



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 07:41 PM EST

PDB ID : 4WPO  
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with elongation factor G in the pre-translocational state  
Authors : Lin, J.; Gagnon, M.G.; Steitz, T.A.  
Deposited on : 2014-10-20  
Resolution : 2.80 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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

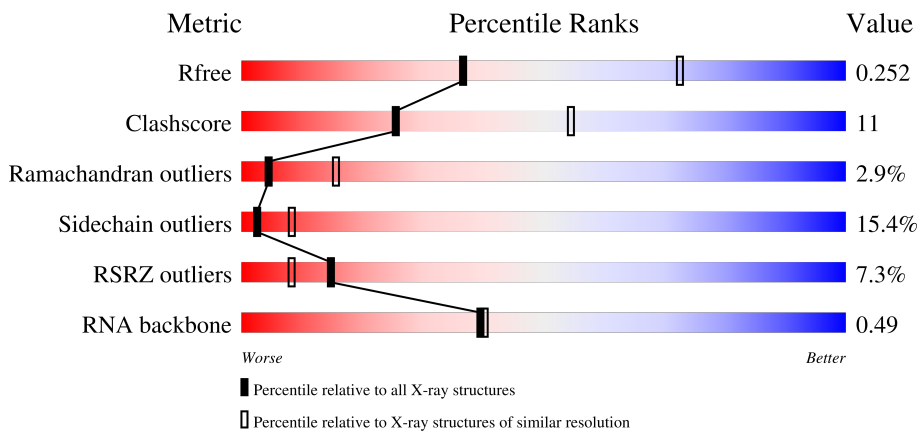
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	2915	
1	CA	2915	
2	AB	121	
2	CB	121	

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Mol	Chain	Length	Quality of chain
3	AC	228	50% 21% 29% 10% 40%
3	CC	228	55% 21% 29% 10% 40%
4	AD	276	% 71% 21% 7%
4	CD	276	66% 27% 6%
5	AE	206	66% 26% 7% .
5	CE	206	67% 23% 8% .
6	AF	210	65% 27% . .
6	CF	210	62% 28% 7% .
7	AG	182	2% 58% 34% 7% ..
7	CG	182	4% 57% 34% 9% .
8	AH	180	% 70% 23% . .
8	CH	180	7% 57% 33% 7% .
9	AK	173	16% 51% 21% . 25%
9	CK	173	41% 53% 18% . 25%
10	AL	147	34% 24% 19% . 55%
10	CL	147	36% 26% 16% . . 55%
11	AN	140	63% 32% 5%
11	CN	140	% 68% 27% 5%
12	AO	122	65% 29% 6% .
12	CO	122	66% 29% 6%
13	AP	150	67% 27% 6% .
13	CP	150	3% 65% 27% 7% ..
14	AQ	141	65% 28% 6% .
14	CQ	141	66% 28% 6%
15	AR	118	64% 29% 7%

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Mol	Chain	Length	Quality of chain
15	CR	118	60% 34% 6%
16	AS	112	70% 22% 6% .
16	CS	112	4% 45% 44% 10% .
17	AT	146	57% 28% 5% 10%
17	CT	146	59% 25% 5% 10%
18	AU	118	69% 24% 6% .
18	CU	118	66% 26% 6% .
19	AV	101	72% 22% 5% .
19	CV	101	62% 32% 5% .
20	AW	113	76% 18% 5% .
20	CW	113	69% 27% . .
21	AX	96	69% 27% . . .
21	CX	96	4% 67% 28% . .
22	AY	110	64% 29% 5% .
22	CY	110	6% 53% 36% 7% . .
23	AZ	206	5% 50% 24% 8% 17%
23	CZ	206	10% 49% 32% . 16%
24	A0	85	2% 74% 21% . .
24	C0	85	7% 69% 27% . .
25	A1	98	2% 66% 31% . .
25	C1	98	67% 23% 8% .
26	A2	72	3% 69% 25% . .
26	C2	72	61% 31% 6% .
27	A3	60	2% 77% 20% . .
27	C3	60	8% 67% 22% 10% .

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Mol	Chain	Length	Quality of chain
28	A4	71	13% 44% 46% . . .
28	C4	71	15% 49% 39% 8% .
29	A5	60	73% 22% . . .
29	C5	60	2% 77% 17% 5% .
30	A6	54	63% 22% 13% .
30	C6	54	2% 57% 37% . .
31	A7	49	4% 61% 35% . .
31	C7	49	2% 65% 29% . .
32	A8	65	54% 37% 8% .
32	C8	65	66% 26% 6% .
33	A9	37	68% 27% 5%
33	C9	37	3% 57% 41% .
34	BA	1521	3% 49% 39% 9% . .
34	DA	1521	3% 48% 39% 11% . .
35	BB	256	7% 41% 35% 13% . 10%
35	DB	256	12% 38% 43% 9% 10%
36	BC	239	4% 55% 25% 6% 14%
36	DC	239	10% 47% 32% 7% 14%
37	BD	209	% 61% 31% 8%
37	DD	209	% 60% 33% 6%
38	BE	162	49% 40% . 9%
38	DE	162	2% 47% 38% 6% . 9%
39	BF	101	59% 35% 5%
39	DF	101	69% 24% 5%
40	BG	156	8% 72% 21% 5%




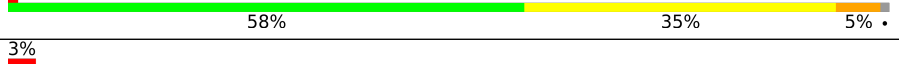


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Mol	Chain	Length	Quality of chain
40	DG	156	11% 69% 28% ..
41	BH	138	% 60% 34% ..
41	DH	138	4% 55% 34% 9% ..
42	BI	128	7% 54% 41% 5% .
42	DI	128	22% 59% 34% 7% .
43	BJ	105	13% 52% 33% 7% 8%
43	DJ	105	24% 45% 42% 5% 9%
44	BK	129	53% 30% .. 12%
44	DK	129	% 61% 24% . 12%
45	BL	132	78% 13% . 8%
45	DL	132	2% 63% 27% . 8%
46	BM	126	7% 61% 29% 6% ..
46	DM	126	13% 49% 40% 8% .
47	BN	61	8% 52% 34% 11% .
47	DN	61	33% 46% 39% 13% .
48	BO	89	2% 61% 35% ..
48	DO	89	65% 31% ..
49	BP	88	% 48% 42% . 7%
49	DP	88	2% 57% 33% . 7%
50	BQ	105	61% 25% 9% 6%
50	DQ	105	60% 28% 7% 6%
51	BR	88	5% 42% 28% 7% 23%
51	DR	88	5% 48% 24% 6% 23%
52	BS	93	16% 43% 44% . 10%
52	DS	93	42% 57% 31% . 11%

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Mol	Chain	Length	Quality of chain
53	BT	106	
53	DT	106	
54	BU	27	
54	DU	27	
55	BV	24	
55	DV	24	
56	BW	76	
56	DW	76	
57	BX	77	
57	DX	77	
58	BY	76	
58	DY	76	
59	BZ	758	
59	DZ	758	

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	PSU	DW	55	-	-	-	X
56	4SU	DW	8	-	-	-	X
58	PSU	DY	55	-	-	-	X
60	MG	A0	104	-	-	-	X
60	MG	AA	3015	-	-	-	X
60	MG	AA	3051	-	-	-	X
60	MG	AA	3059	-	-	-	X
60	MG	AA	3088	-	-	-	X
60	MG	AA	3093	-	-	-	X
60	MG	AA	3108	-	-	-	X
60	MG	AA	3110	-	-	-	X
60	MG	AA	3136	-	-	-	X
60	MG	AA	3152	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	AA	3159	-	-	-	X
60	MG	AA	3161	-	-	-	X
60	MG	AA	3183	-	-	-	X
60	MG	AA	3192	-	-	-	X
60	MG	AA	3203	-	-	-	X
60	MG	AA	3210	-	-	-	X
60	MG	AA	3225	-	-	-	X
60	MG	AA	3234	-	-	-	X
60	MG	AA	3246	-	-	-	X
60	MG	AA	3249	-	-	-	X
60	MG	AA	3263	-	-	-	X
60	MG	AA	3490	-	-	-	X
60	MG	AA	3599	-	-	-	X
60	MG	AA	3640	-	-	-	X
60	MG	AA	3692	-	-	-	X
60	MG	AA	3702	-	-	-	X
60	MG	AA	3713	-	-	-	X
60	MG	AA	3739	-	-	-	X
60	MG	AA	3770	-	-	-	X
60	MG	AA	3805	-	-	-	X
60	MG	AA	3828	-	-	-	X
60	MG	AF	304	-	-	-	X
60	MG	BA	1621	-	-	-	X
60	MG	BA	1646	-	-	-	X
60	MG	BA	1657	-	-	-	X
60	MG	BA	1800	-	-	-	X
60	MG	BA	1804	-	-	-	X
60	MG	BK	3101	-	-	-	X
60	MG	BW	101	-	-	-	X
60	MG	CA	3015	-	-	-	X
60	MG	CA	3016	-	-	-	X
60	MG	CA	3031	-	-	-	X
60	MG	CA	3032	-	-	-	X
60	MG	CA	3042	-	-	-	X
60	MG	CA	3057	-	-	-	X
60	MG	CA	3063	-	-	-	X
60	MG	CA	3067	-	-	-	X
60	MG	CA	3070	-	-	-	X
60	MG	CA	3073	-	-	-	X
60	MG	CA	3079	-	-	-	X
60	MG	CA	3080	-	-	-	X
60	MG	CA	3085	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	CA	3087	-	-	-	X
60	MG	CA	3089	-	-	-	X
60	MG	CA	3090	-	-	-	X
60	MG	CA	3092	-	-	-	X
60	MG	CA	3098	-	-	-	X
60	MG	CA	3113	-	-	-	X
60	MG	CA	3139	-	-	-	X
60	MG	CA	3155	-	-	-	X
60	MG	CA	3177	-	-	-	X
60	MG	CA	3183	-	-	-	X
60	MG	CA	3194	-	-	-	X
60	MG	CA	3199	-	-	-	X
60	MG	CA	3206	-	-	-	X
60	MG	CA	3222	-	-	-	X
60	MG	CA	3467	-	-	-	X
60	MG	CA	3491	-	-	-	X
60	MG	CA	3543	-	-	-	X
60	MG	CA	3575	-	-	-	X
60	MG	CA	3590	-	-	-	X
60	MG	CA	3597	-	-	-	X
60	MG	CA	3653	-	-	-	X
60	MG	CF	306	-	-	-	X
60	MG	CQ	201	-	-	-	X
60	MG	DA	1608	-	-	-	X
60	MG	DA	1615	-	-	-	X
60	MG	DA	1671	-	-	-	X
60	MG	DA	1715	-	-	-	X
60	MG	DA	1739	-	-	-	X
60	MG	DA	1764	-	-	-	X
60	MG	DW	3001	-	-	-	X
60	MG	DX	3001	-	-	-	X

## 2 Entry composition [i](#)

There are 65 unique types of molecules in this entry. The entry contains 313372 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	AA	2872	Total	C	N	O	P	0	0	0
			61861	27532	11574	19884	2871			
1	CA	2868	Total	C	N	O	P	0	0	0
			61771	27492	11554	19858	2867			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	AB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			
2	CB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 3 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	AC	137	Total	C	N	O	S	0	0	0
			1063	669	201	192	1			
3	CC	137	Total	C	N	O	S	0	0	0
			1063	669	201	192	1			

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	AD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
4	CD	275	Total	C	N	O	S	0	0	0
			2142	1352	426	361	3			

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
5	CE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 6 is a protein called 50S ribosomal protein L4.

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

- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	181	Total	C	N	O	S	0	0	0
			1425	914	256	251	4			
7	CG	181	Total	C	N	O	S	0	0	0
			1424	911	258	251	4			

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
8	CH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AK	130	Total	C	N	O	0	0	0
			641	381	130	130			
9	CK	130	Total	C	N	O	0	0	0
			641	381	130	130			

- Molecule 10 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AL	66	Total	C	N	O	S	0	0	0
			498	310	93	92	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CL	66	Total	C	N	O	S	0	0	0
			498	310	93	92	3			

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			
11	CN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
12	CO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AP	149	Total	C	N	O	S	0	0	0
			1139	709	231	196	3			
13	CP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 14 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
14	CQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
15	CR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
16	AS	110	877	553	175	149	0	0	0
16	CS	110	870	549	173	148	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	AT	131	1091	680	225	185	1	0	0	0
17	CT	131	1083	675	224	183	1	0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
18	AU	116	959	608	201	149	1	0	0	0
18	CU	116	959	608	201	149	1	0	0	0

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	AV	101	771	495	140	135	1	0	0	0
19	CV	101	771	495	140	135	1	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	AW	112	886	557	174	153	2	0	0	0
20	CW	112	886	557	174	153	2	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
21	CX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AY	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			
22	CY	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AZ	171	Total	C	N	O	S	0	0	0
			1349	862	243	242	2			
23	CZ	174	Total	C	N	O	S	0	0	0
			1360	870	243	245	2			

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	A0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
24	C0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	A1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			
25	C1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	A2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	C2	70	588	365	118	103	2	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	A3	59	469	298	90	81		0	0	0
27	C3	59	464	296	90	78		0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	A4	69	558	352	102	99	5	0	0	0
28	C4	69	532	339	97	91	5	0	0	0

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	A5	59	455	285	89	76	5	0	0	0
29	C5	59	455	285	89	76	5	0	0	0

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	A6	53	453	281	91	77	4	0	0	0
30	C6	53	449	279	91	75	4	0	0	0

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	A7	48	418	257	104	55	2	0	0	0
31	C7	48	418	257	104	55	2	0	0	0

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	A8	64	Total 517	C 331	N 102	O 82	S 2	0	0	0
32	C8	64	Total 517	C 331	N 102	O 82	S 2	0	0	0

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	A9	37	Total 307	C 188	N 68	O 47	S 4	0	0	0
33	C9	37	Total 307	C 188	N 68	O 47	S 4	0	0	0

- Molecule 34 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
34	BA	1497	Total 32185	C 14324	N 5968	O 10396	P 1497	0	0	0
34	DA	1503	Total 32312	C 14381	N 5990	O 10438	P 1503	0	0	0

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
35	BB	231	Total 1846	C 1179	N 331	O 331	S 5	0	0	0
35	DB	231	Total 1825	C 1167	N 326	O 327	S 5	0	0	0

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
36	BC	206	Total 1552	C 976	N 302	O 273	S 1	0	0	0
36	DC	206	Total 1544	C 970	N 300	O 273	S 1	0	0	0

- Molecule 37 is a protein called 30S ribosomal protein S4.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
37	BD	208	Total 1659	C 1040	N 326	O 286	S 7	0	0	0
37	DD	208	Total 1678	C 1052	N 333	O 286	S 7	0	0	0

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
38	BE	148	Total 1129	C 714	N 213	O 198	S 4	0	0	0
38	DE	148	Total 1133	C 716	N 214	O 199	S 4	0	0	0

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
39	BF	100	Total 812	C 514	N 146	O 149	S 3	0	0	0
39	DF	100	Total 820	C 518	N 147	O 152	S 3	0	0	0

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
40	BG	155	Total 1231	C 766	N 243	O 216	S 6	0	0	0
40	DG	155	Total 1235	C 769	N 244	O 216	S 6	0	0	0

- Molecule 41 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
41	BH	137	Total 1088	C 689	N 206	O 191	S 2	0	0	0
41	DH	137	Total 1088	C 689	N 206	O 191	S 2	0	0	0

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
42	BI	127	Total 986	C 626	N 193	O 167	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
42	DI	127	978	619	190	169	0	0	0

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
43	BJ	97	709	440	138	131	0	0	0
43	DJ	96	714	445	138	131	0	0	0

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	BK	114	833	519	156	155	3	0	0	0
44	DK	114	833	519	156	155	3	0	0	0

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	BL	122	930	585	185	159	1	0	0	0
45	DL	122	930	585	185	159	1	0	0	0

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	BM	123	966	598	200	166	2	0	0	0
46	DM	122	950	586	197	165	2	0	0	0

- Molecule 47 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	BN	60	492	312	104	72	4	0	0	0
47	DN	60	492	312	104	72	4	0	0	0

- Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BO	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			
48	DO	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BP	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
49	DP	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
50	DQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	BR	68	Total	C	N	O	0	0	0
			555	355	108	92			
51	DR	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BS	84	Total	C	N	O	S	0	0	0
			661	423	122	114	2			
52	DS	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BT	96	Total	C	N	O	S	0	0	0
			728	446	156	124	2			
53	DT	96	Total	C	N	O	S	0	0	0
			731	449	156	124	2			

- Molecule 54 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	BU	23	Total	C	N	O	0	0	0
			199	122	48	29			
54	DU	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 55 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BV	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
55	DV	12	Total	C	N	O	P	0	0	0
			252	115	46	80	11			

- Molecule 56 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
56	BW	74	Total	C	N	O	P	S	0	0	0
			1599	722	287	515	73	2			
56	DW	72	Total	C	N	O	P	S	0	0	0
			1552	697	280	502	72	1			

- Molecule 57 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
57	BX	76	Total	C	N	O	P	S	0	0	0
			1635	731	296	530	76	2			
57	DX	76	Total	C	N	O	P	S	0	0	0
			1635	731	296	530	76	2			

- Molecule 58 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
58	BY	74	Total	C	N	O	P	S	0	0	0
			1581	707	285	515	73	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S		
58	DY	73	1561	698	283	507	72	1	0	0

- Molecule 59 is a protein called 50S ribosomal protein L9, Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
59	BZ	728	5663	3599	973	1072	19	0	0	
59	DZ	730	5682	3611	978	1074	19	0	0	

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AA	834	Total	Mg	0	0
			834	834		
60	AB	23	Total	Mg	0	0
			23	23		
60	AD	10	Total	Mg	0	0
			10	10		
60	AE	5	Total	Mg	0	0
			5	5		
60	AF	5	Total	Mg	0	0
			5	5		
60	AG	2	Total	Mg	0	0
			2	2		
60	AH	1	Total	Mg	0	0
			1	1		
60	AN	3	Total	Mg	0	0
			3	3		
60	AO	1	Total	Mg	0	0
			1	1		
60	AP	2	Total	Mg	0	0
			2	2		
60	AQ	3	Total	Mg	0	0
			3	3		
60	AR	1	Total	Mg	0	0
			1	1		
60	AU	4	Total	Mg	0	0
			4	4		
60	AV	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AW	4	Total 4	Mg 4	0	0
60	AX	2	Total 2	Mg 2	0	0
60	AY	1	Total 1	Mg 1	0	0
60	AZ	1	Total 1	Mg 1	0	0
60	A0	5	Total 5	Mg 5	0	0
60	A1	2	Total 2	Mg 2	0	0
60	A2	1	Total 1	Mg 1	0	0
60	A4	1	Total 1	Mg 1	0	0
60	A5	1	Total 1	Mg 1	0	0
60	A6	1	Total 1	Mg 1	0	0
60	A7	1	Total 1	Mg 1	0	0
60	A8	2	Total 2	Mg 2	0	0
60	A9	1	Total 1	Mg 1	0	0
60	BA	213	Total 213	Mg 213	0	0
60	BB	1	Total 1	Mg 1	0	0
60	BD	1	Total 1	Mg 1	0	0
60	BE	1	Total 1	Mg 1	0	0
60	BF	1	Total 1	Mg 1	0	0
60	BK	1	Total 1	Mg 1	0	0
60	BL	2	Total 2	Mg 2	0	0
60	BM	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	BN	2	Total Mg 2 2	0	0
60	BT	1	Total Mg 1 1	0	0
60	BV	1	Total Mg 1 1	0	0
60	BW	2	Total Mg 2 2	0	0
60	BX	15	Total Mg 15 15	0	0
60	BY	2	Total Mg 2 2	0	0
60	BZ	1	Total Mg 1 1	0	0
60	CA	664	Total Mg 664 664	0	0
60	CB	13	Total Mg 13 13	0	0
60	CD	4	Total Mg 4 4	0	0
60	CE	6	Total Mg 6 6	0	0
60	CF	6	Total Mg 6 6	0	0
60	CG	1	Total Mg 1 1	0	0
60	CN	1	Total Mg 1 1	0	0
60	CO	2	Total Mg 2 2	0	0
60	CP	1	Total Mg 1 1	0	0
60	CQ	4	Total Mg 4 4	0	0
60	CR	2	Total Mg 2 2	0	0
60	CU	1	Total Mg 1 1	0	0
60	CV	2	Total Mg 2 2	0	0
60	CY	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	C0	2	Total Mg 2 2	0	0
60	C3	1	Total Mg 1 1	0	0
60	C5	1	Total Mg 1 1	0	0
60	C7	1	Total Mg 1 1	0	0
60	C8	1	Total Mg 1 1	0	0
60	DA	168	Total Mg 168 168	0	0
60	DD	1	Total Mg 1 1	0	0
60	DE	2	Total Mg 2 2	0	0
60	DF	1	Total Mg 1 1	0	0
60	DJ	1	Total Mg 1 1	0	0
60	DK	2	Total Mg 2 2	0	0
60	DT	1	Total Mg 1 1	0	0
60	DW	1	Total Mg 1 1	0	0
60	DX	1	Total Mg 1 1	0	0
60	DZ	1	Total Mg 1 1	0	0

- Molecule 61 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	AA	1	Total K 1 1	0	0

- Molecule 62 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	AY	1	Total Zn 1 1	0	0

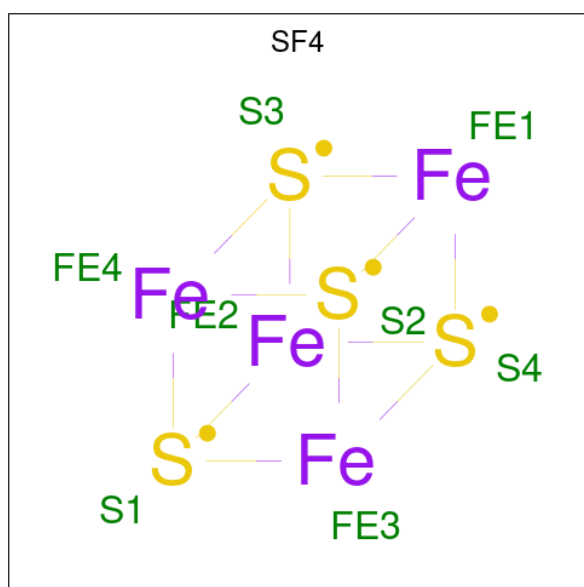
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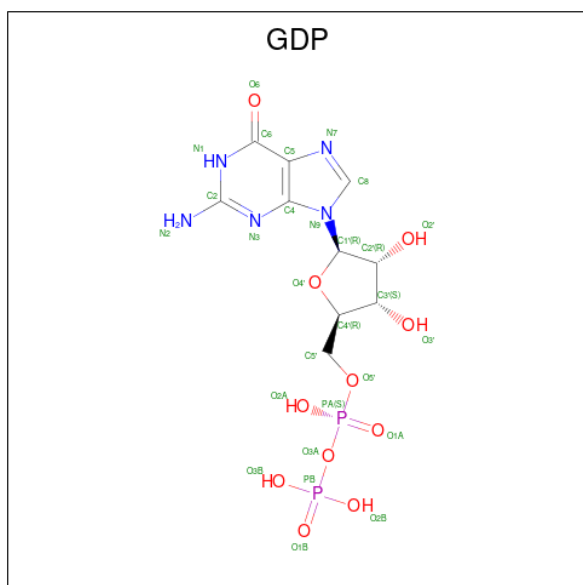
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	A4	1	Total Zn 1 1	0	0
62	A5	1	Total Zn 1 1	0	0
62	A6	1	Total Zn 1 1	0	0
62	A9	1	Total Zn 1 1	0	0
62	BN	1	Total Zn 1 1	0	0
62	CY	1	Total Zn 1 1	0	0
62	C4	1	Total Zn 1 1	0	0
62	C5	1	Total Zn 1 1	0	0
62	C6	1	Total Zn 1 1	0	0
62	C9	1	Total Zn 1 1	0	0
62	DN	1	Total Zn 1 1	0	0

- Molecule 63 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	BD	1	Total	Fe	S	0	0
			8	4	4		
63	DD	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 64 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
64	BZ	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
64	DZ	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 65 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
65	AA	1408	Total	O	0	0
			1408	1408		
65	AB	36	Total	O	0	0
			36	36		
65	AD	15	Total	O	0	0
			15	15		
65	AE	19	Total	O	0	0
			19	19		
65	AF	7	Total	O	0	0
			7	7		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
65	AG	3	Total 3	O 3	0	0
65	AH	1	Total 1	O 1	0	0
65	AN	2	Total 2	O 2	0	0
65	AO	1	Total 1	O 1	0	0
65	AP	15	Total 15	O 15	0	0
65	AQ	4	Total 4	O 4	0	0
65	AR	2	Total 2	O 2	0	0
65	AS	1	Total 1	O 1	0	0
65	AT	2	Total 2	O 2	0	0
65	AU	5	Total 5	O 5	0	0
65	AV	2	Total 2	O 2	0	0
65	AW	2	Total 2	O 2	0	0
65	AX	3	Total 3	O 3	0	0
65	AZ	1	Total 1	O 1	0	0
65	A0	6	Total 6	O 6	0	0
65	A1	1	Total 1	O 1	0	0
65	A3	1	Total 1	O 1	0	0
65	A5	3	Total 3	O 3	0	0
65	A6	2	Total 2	O 2	0	0
65	A7	4	Total 4	O 4	0	0
65	A8	10	Total 10	O 10	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
65	BA	212	Total 212	O 212	0	0
65	BD	2	Total 2	O 2	0	0
65	BE	2	Total 2	O 2	0	0
65	BL	1	Total 1	O 1	0	0
65	BM	1	Total 1	O 1	0	0
65	BV	2	Total 2	O 2	0	0
65	BW	3	Total 3	O 3	0	0
65	BX	8	Total 8	O 8	0	0
65	BY	1	Total 1	O 1	0	0
65	BZ	2	Total 2	O 2	0	0
65	CA	985	Total 985	O 985	0	0
65	CB	9	Total 9	O 9	0	0
65	CD	14	Total 14	O 14	0	0
65	CE	13	Total 13	O 13	0	0
65	CF	7	Total 7	O 7	0	0
65	CN	2	Total 2	O 2	0	0
65	CP	10	Total 10	O 10	0	0
65	CQ	1	Total 1	O 1	0	0
65	CR	1	Total 1	O 1	0	0
65	CT	3	Total 3	O 3	0	0
65	CU	2	Total 2	O 2	0	0

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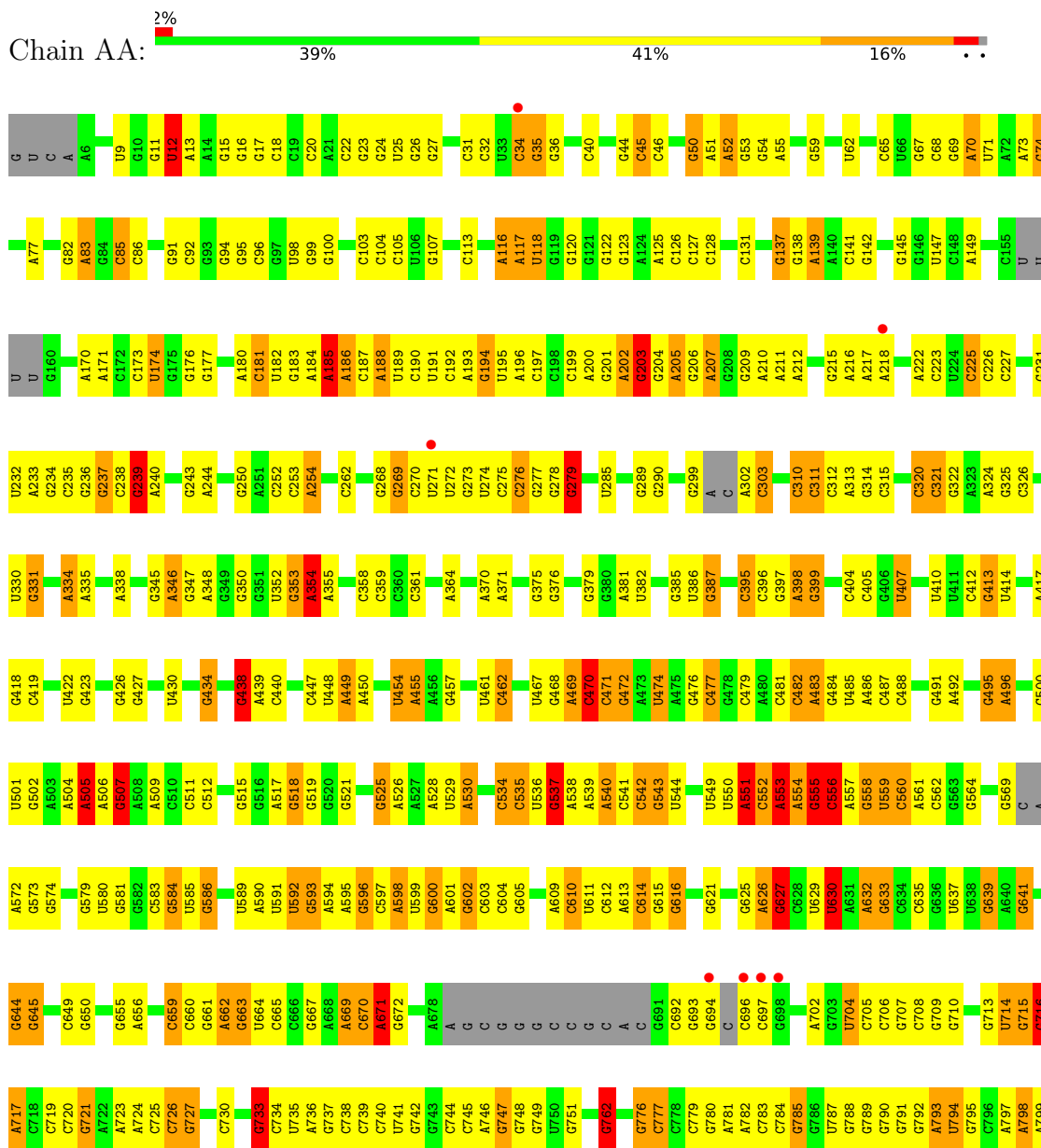
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
65	CV	1	Total 1	O 1	0	0
65	CY	1	Total 1	O 1	0	0
65	C0	6	Total 6	O 6	0	0
65	C1	2	Total 2	O 2	0	0
65	C3	2	Total 2	O 2	0	0
65	C6	1	Total 1	O 1	0	0
65	C7	1	Total 1	O 1	0	0
65	C8	3	Total 3	O 3	0	0
65	DA	155	Total 155	O 155	0	0
65	DE	4	Total 4	O 4	0	0
65	DJ	1	Total 1	O 1	0	0
65	DK	2	Total 2	O 2	0	0
65	DL	1	Total 1	O 1	0	0
65	DW	2	Total 2	O 2	0	0
65	DX	1	Total 1	O 1	0	0

### 3 Residue-property plots [i](#)

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

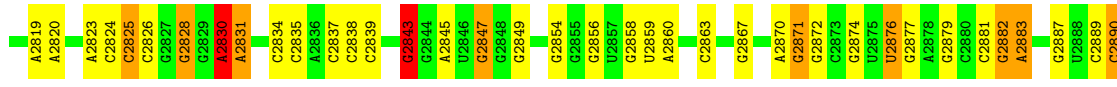
- Molecule 1: 23S Ribosomal RNA



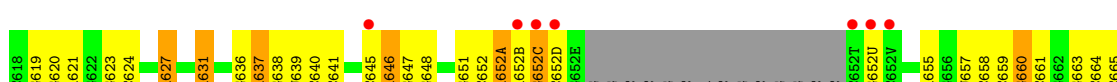
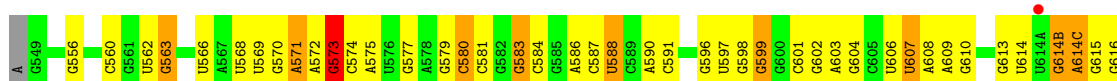
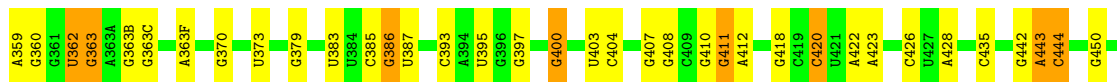
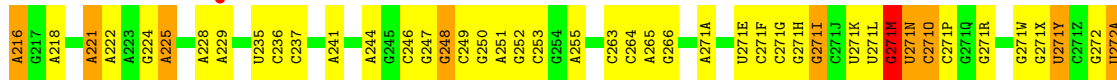
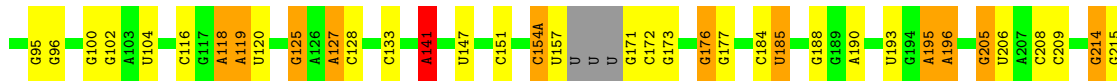
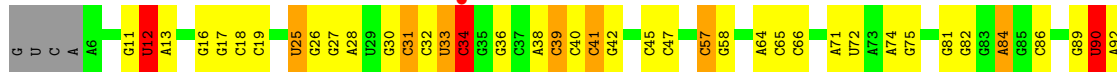
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C864	G865	A866	G867	U868	G870	A871	C872	U873	U874	U875	A876	G877	G878	U879	U880	C881	A882	G883	C884	U885	U886	C887	A888	C891	G892	C893	U894	G895	A896	C897	U898	G899	U905	G906	U907	A908	G909	U988	U989	C912	A913	G916	U917	U918	U924	A925	G926	G927	C1000	G1001	U1002	U1003	A1004	C1005	A934
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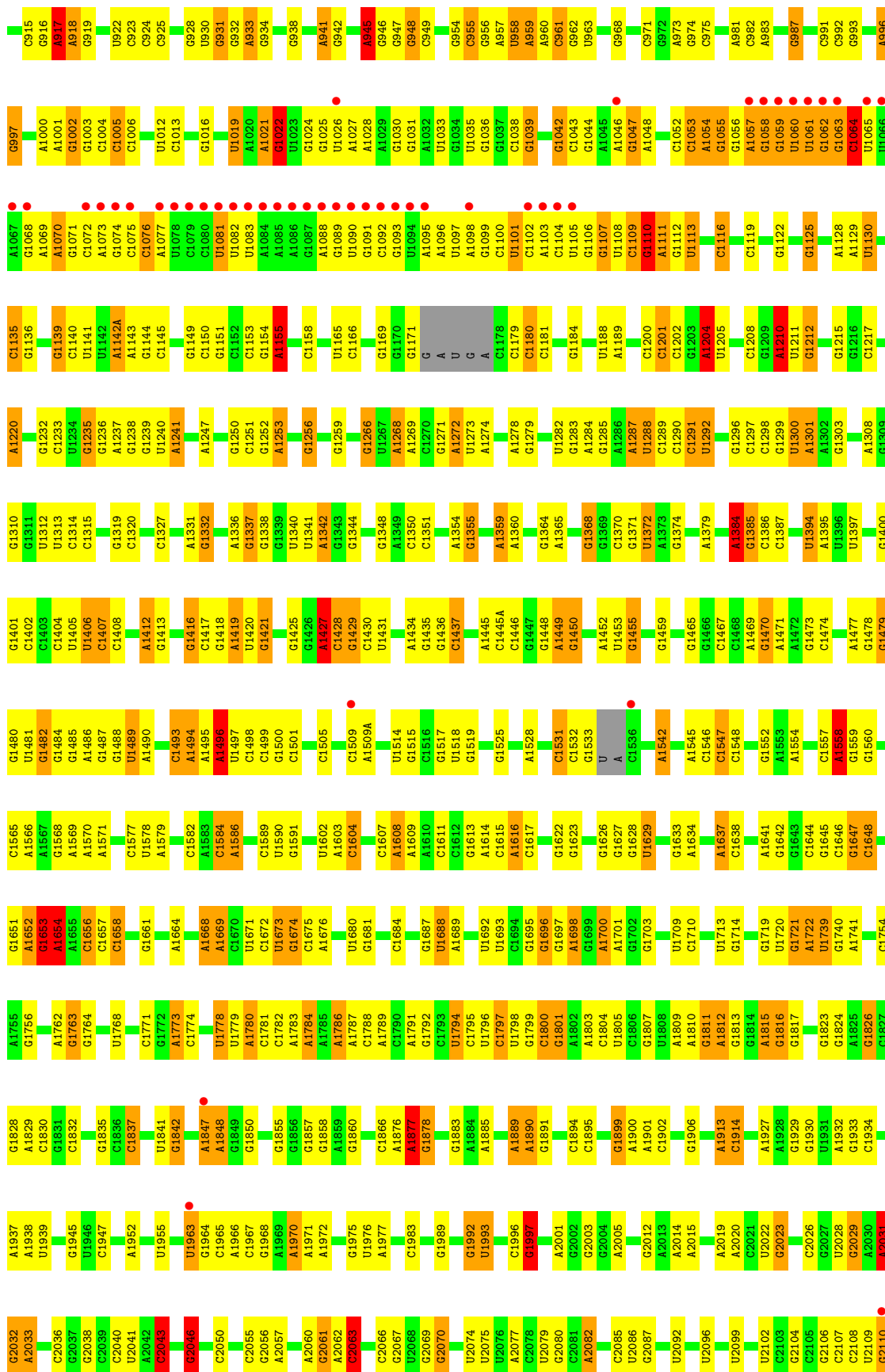
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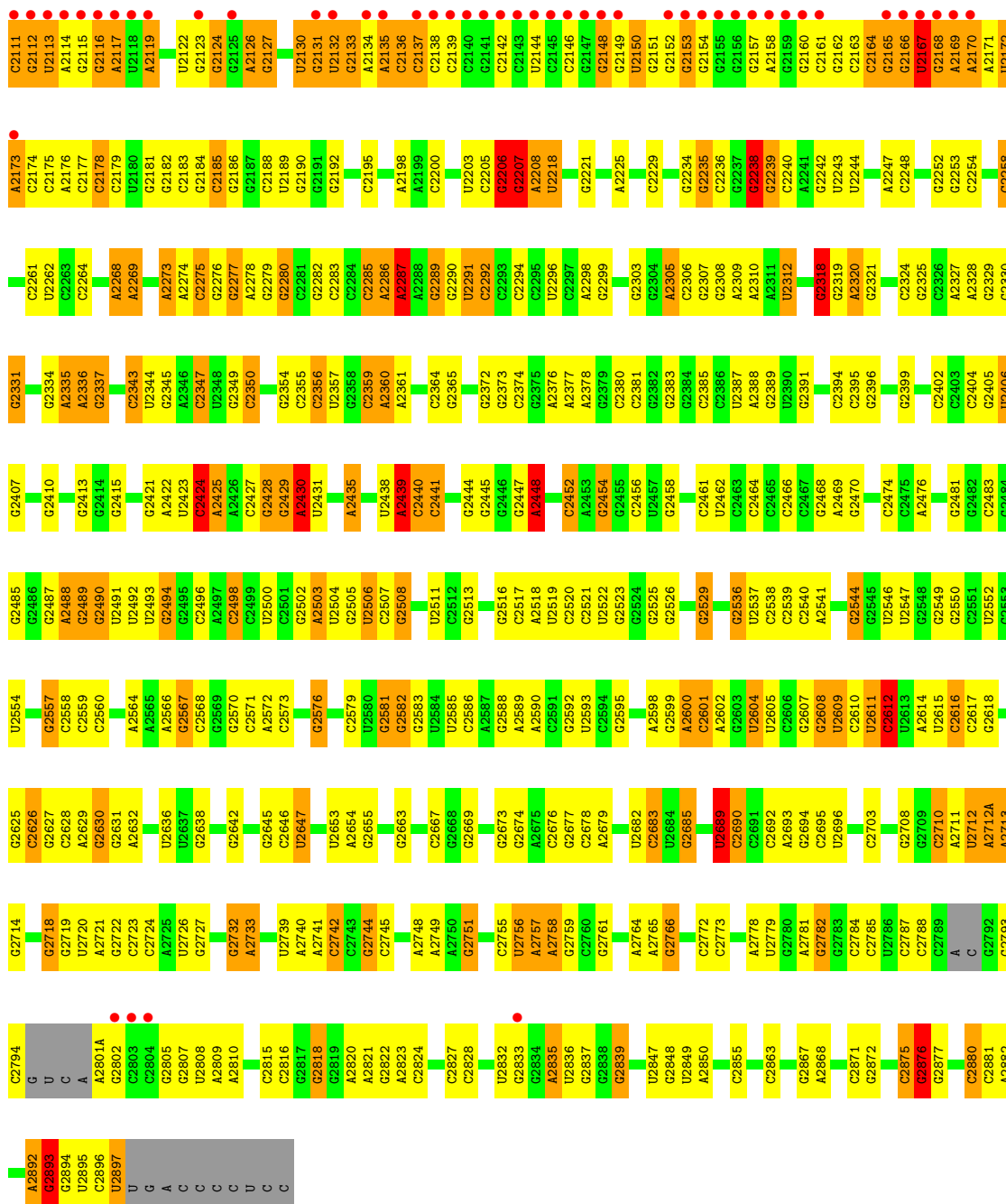




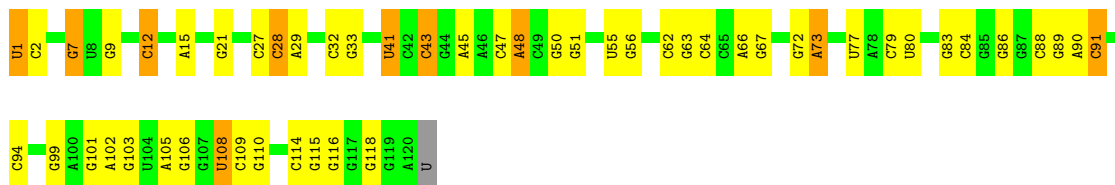
• Molecule 1: 23S Ribosomal RNA



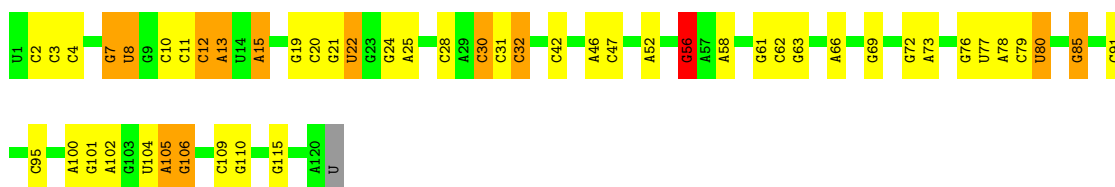




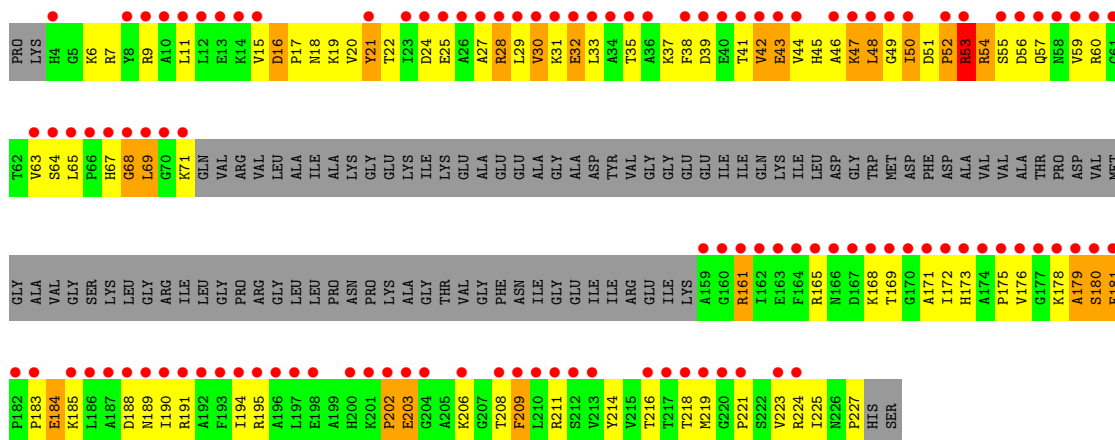
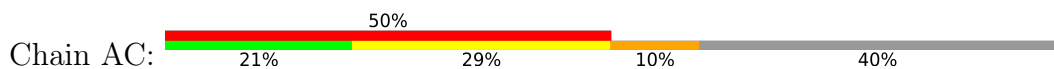
• Molecule 2: 5S Ribosomal RNA



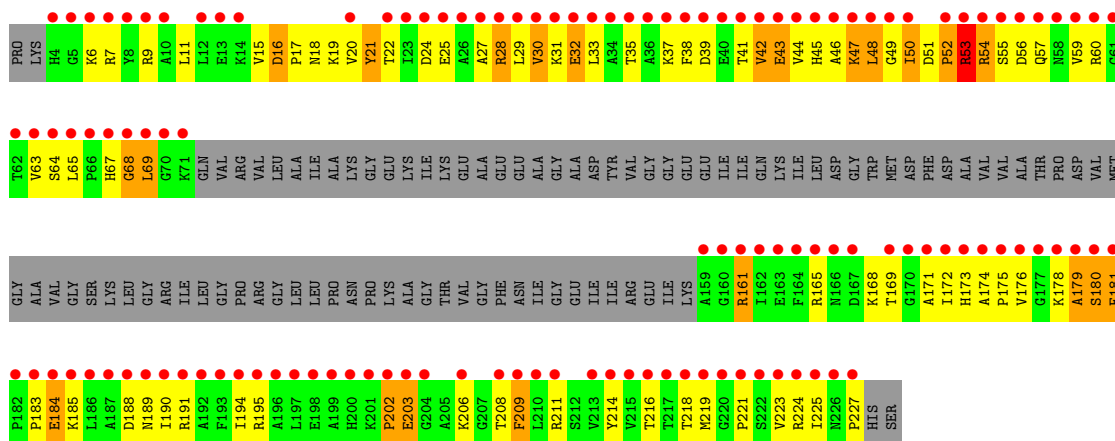
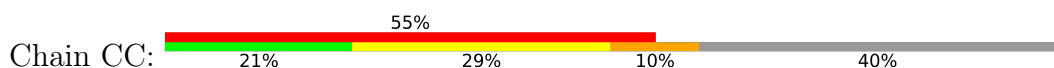
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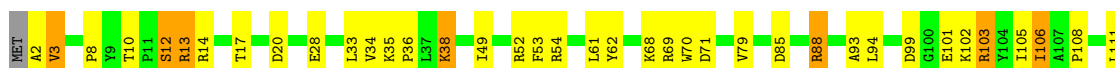
● Molecule 3: 50S ribosomal protein L1

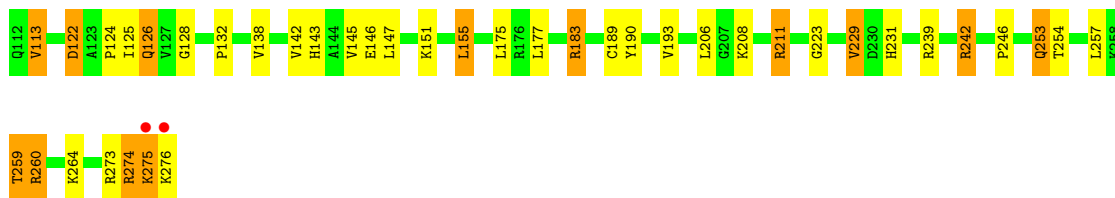


● Molecule 3: 50S ribosomal protein L1



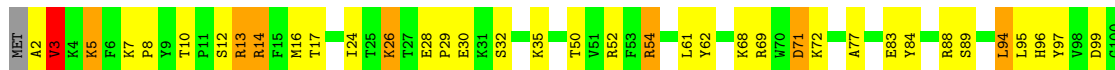
● Molecule 4: 50S ribosomal protein L2





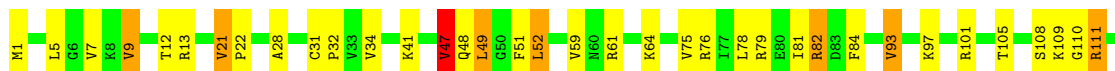
- Molecule 4: 50S ribosomal protein L2

Chain CD: 66% 27% 6%



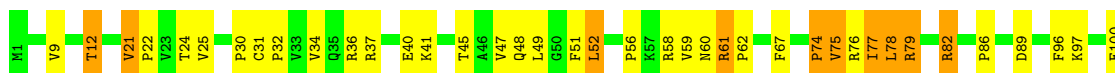
- Molecule 5: 50S ribosomal protein L3

Chain AE: 66% 26% 7%



- Molecule 5: 50S ribosomal protein L3

Chain CE: 67% 23% 8%



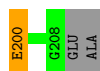
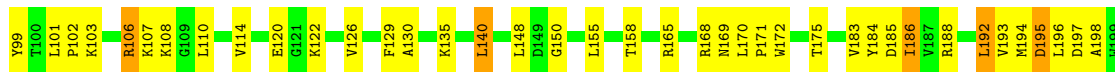
- Molecule 6: 50S ribosomal protein L4

Chain AF: 65% 27% 8%

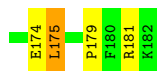




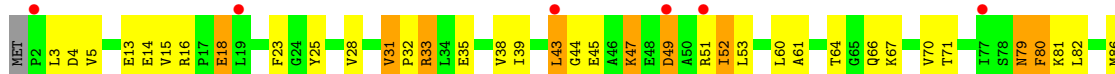
• Molecule 6: 50S ribosomal protein L4



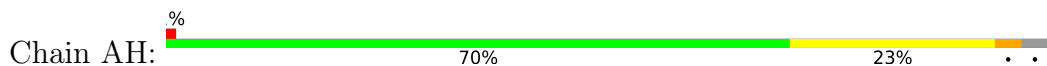
• Molecule 7: 50S ribosomal protein L5

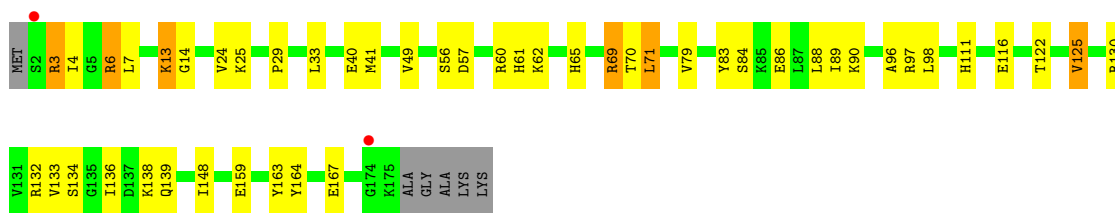


• Molecule 7: 50S ribosomal protein L5

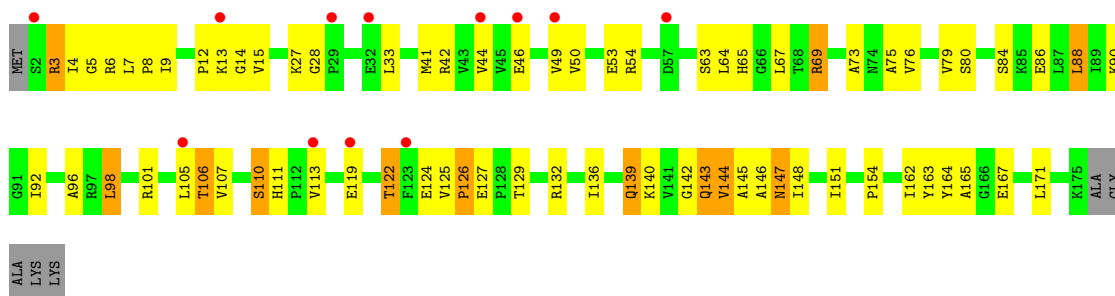


• Molecule 8: 50S ribosomal protein L6

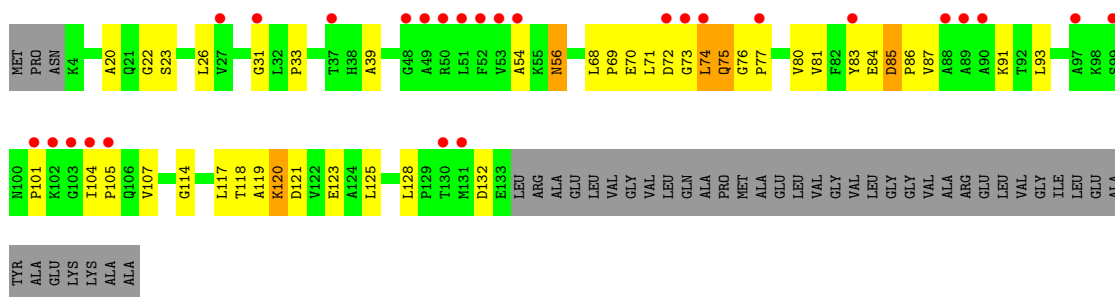




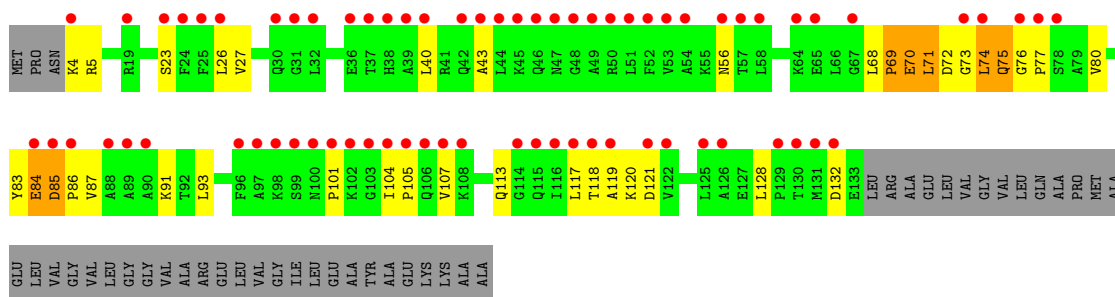
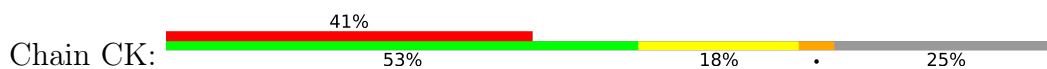
• Molecule 8: 50S ribosomal protein L6



• Molecule 9: 50S ribosomal protein L10

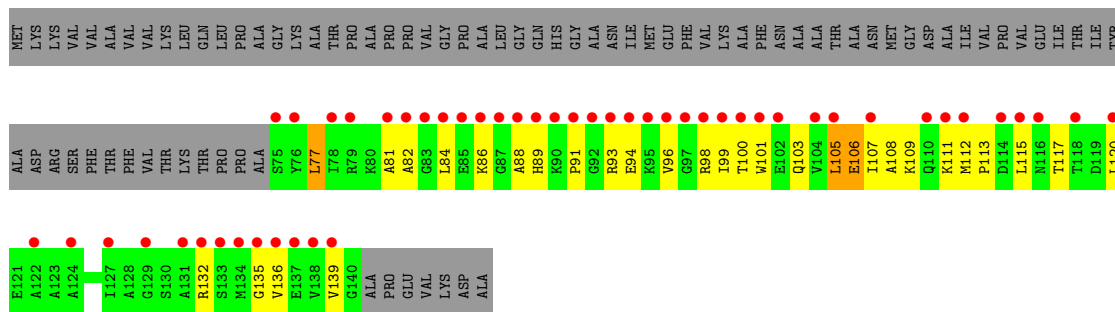


• Molecule 9: 50S ribosomal protein L10

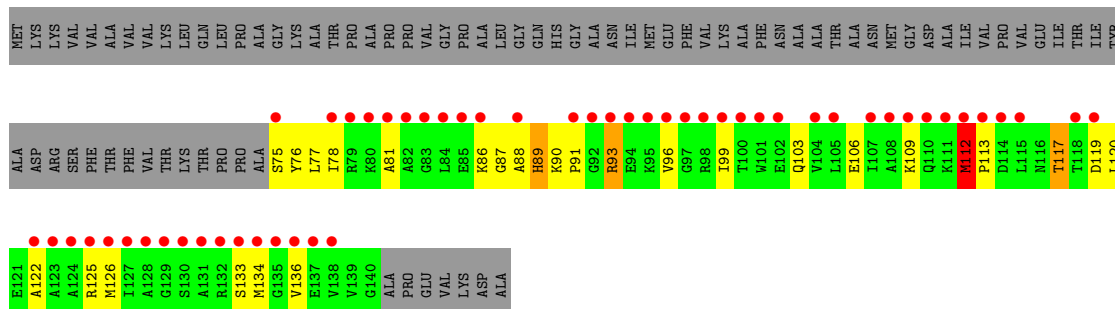


• Molecule 10: 50S ribosomal protein L11

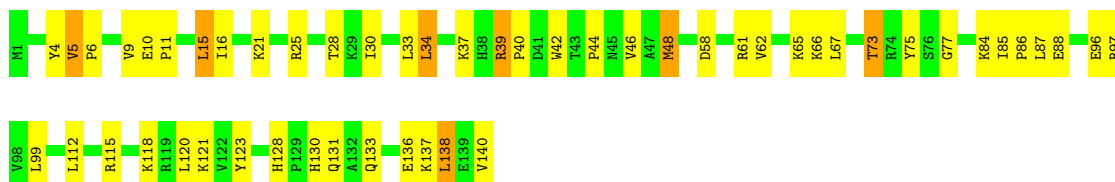




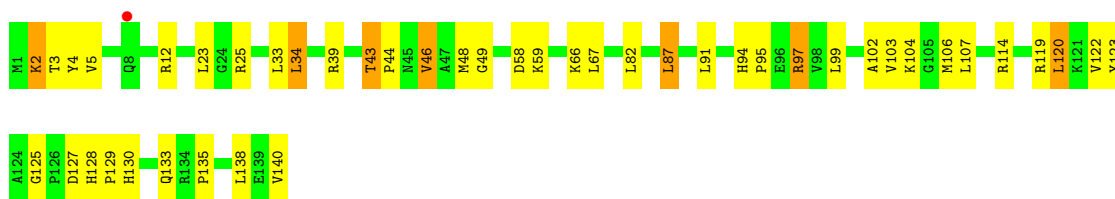
• Molecule 10: 50S ribosomal protein L11



• Molecule 11: 50S ribosomal protein L13



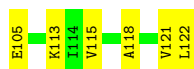
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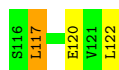
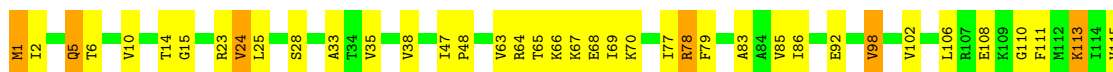
• Molecule 12: 50S ribosomal protein L14



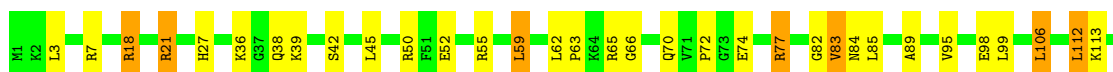




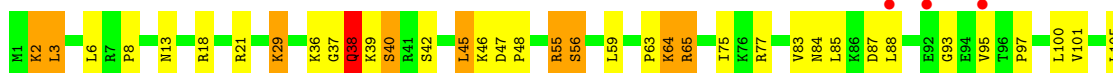
- Molecule 12: 50S ribosomal protein L14



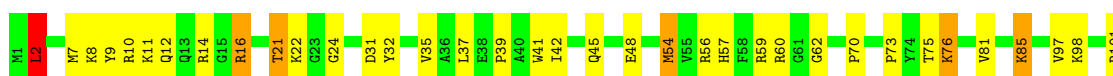
- Molecule 13: 50S ribosomal protein L15



- Molecule 13: 50S ribosomal protein L15

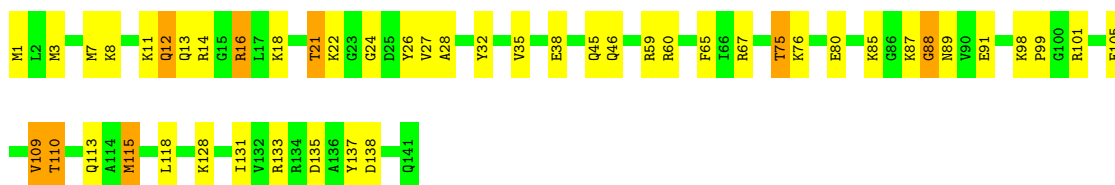


- Molecule 14: 50S ribosomal protein L16

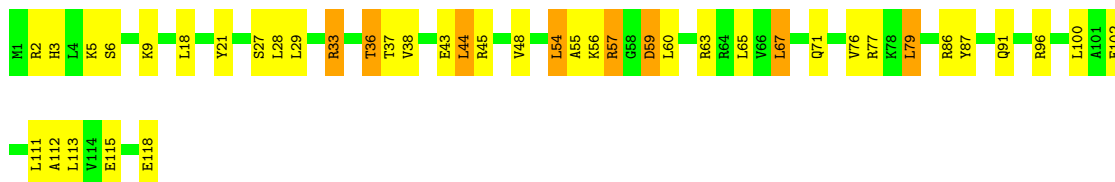


- Molecule 14: 50S ribosomal protein L16

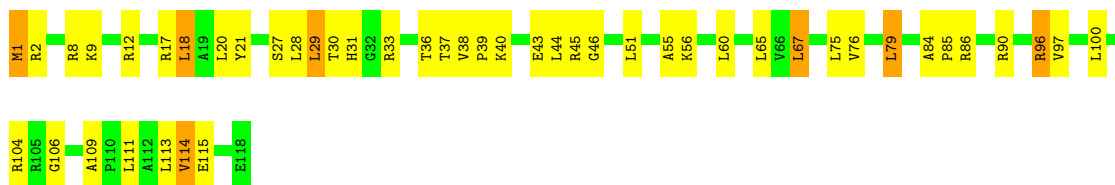




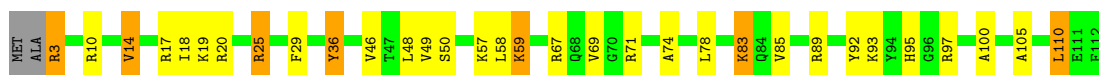
- Molecule 15: 50S ribosomal protein L17



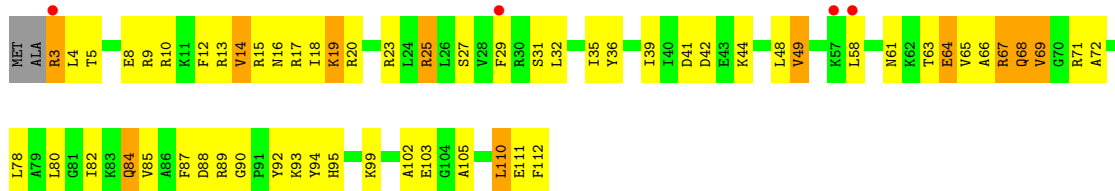
- Molecule 15: 50S ribosomal protein L17



- Molecule 16: 50S ribosomal protein L18

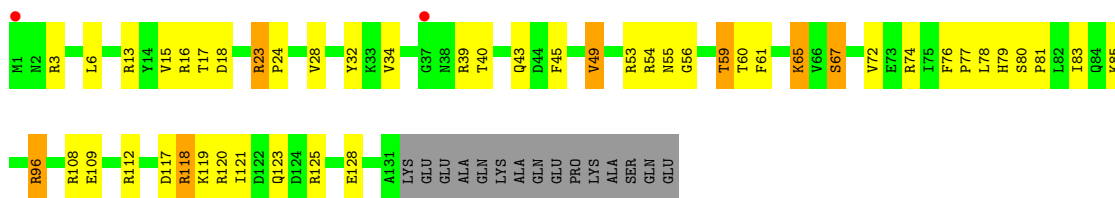


- Molecule 16: 50S ribosomal protein L18

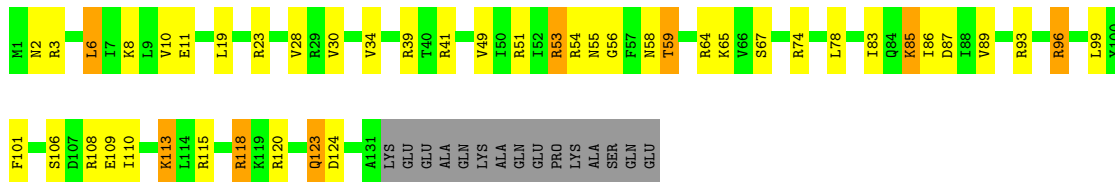


- Molecule 17: 50S ribosomal protein L19

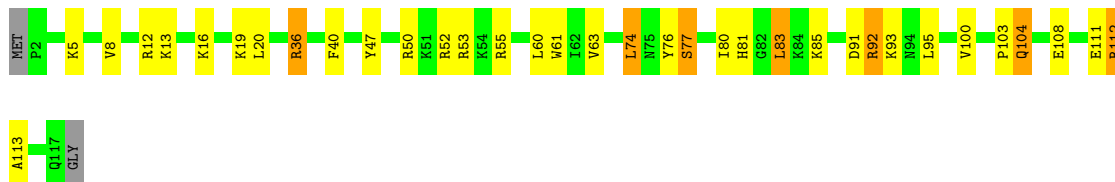




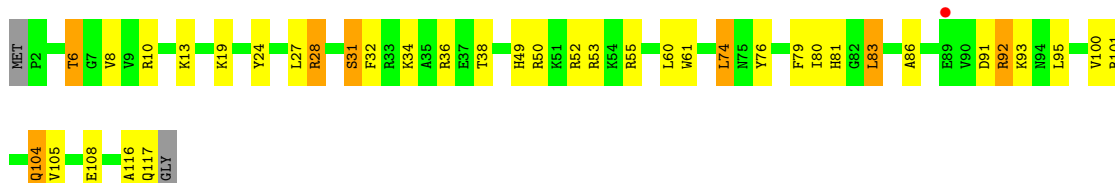
• Molecule 17: 50S ribosomal protein L19



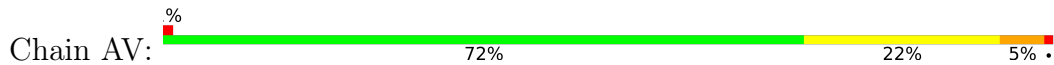
• Molecule 18: 50S ribosomal protein L20



• Molecule 18: 50S ribosomal protein L20



• Molecule 19: 50S ribosomal protein L21



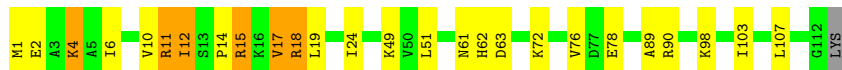
• Molecule 19: 50S ribosomal protein L21





- Molecule 20: 50S ribosomal protein L22

Chain AW: 76% 18% 5%



- Molecule 20: 50S ribosomal protein L22

Chain CW: 69% 27% 4%



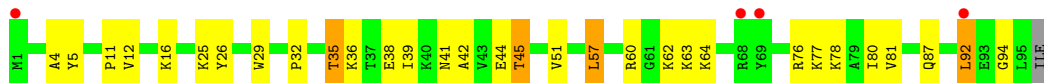
- Molecule 21: 50S ribosomal protein L23

Chain AX: 69% 27% 4%



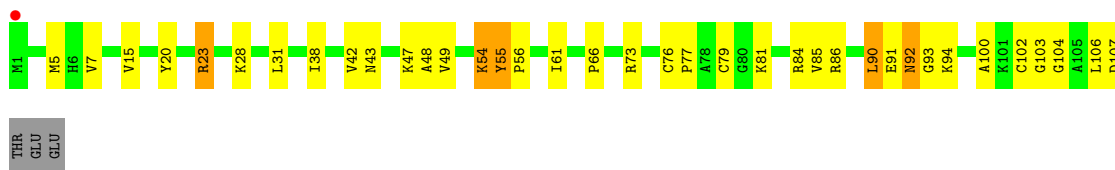
- Molecule 21: 50S ribosomal protein L23

Chain CX: 67% 28% 4%



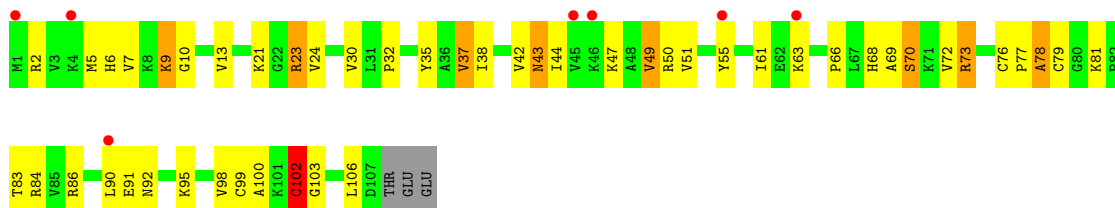
- Molecule 22: 50S ribosomal protein L24

Chain AY: 64% 29% 5%



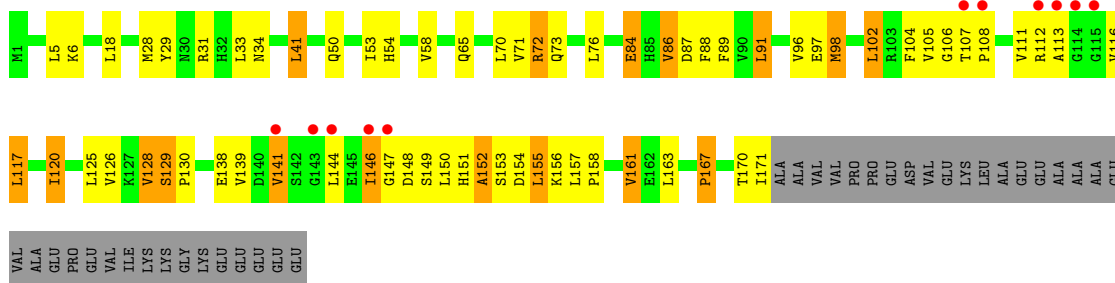
- Molecule 22: 50S ribosomal protein L24

Chain CY: 



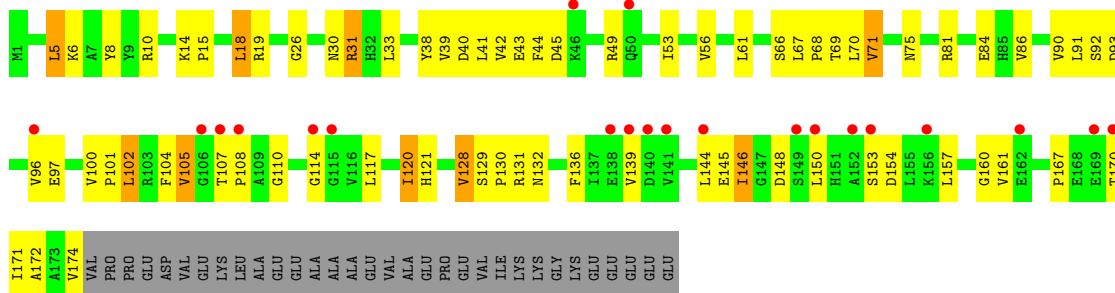
• Molecule 23: 50S ribosomal protein L25

Chain AZ: 




• Molecule 23: 50S ribosomal protein L25

Chain CZ: 



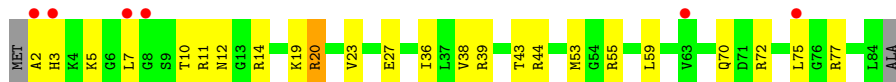
• Molecule 24: 50S ribosomal protein L27

Chain A0: 

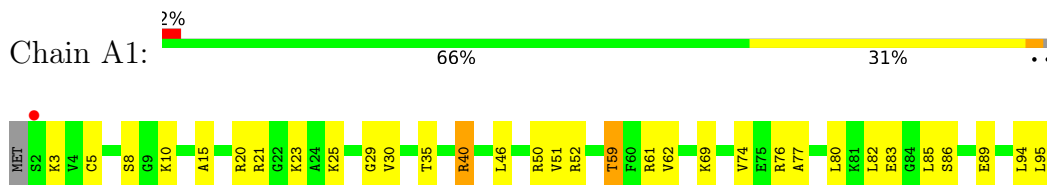


• Molecule 24: 50S ribosomal protein L27

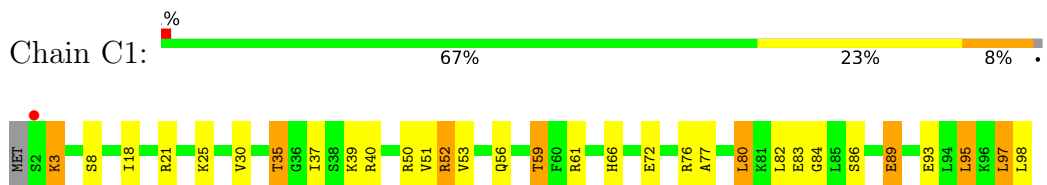
Chain C0: 



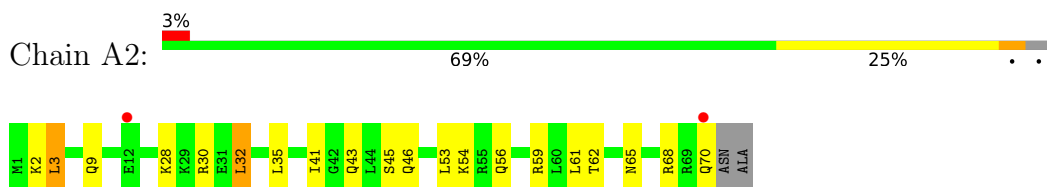
- Molecule 25: 50S ribosomal protein L28



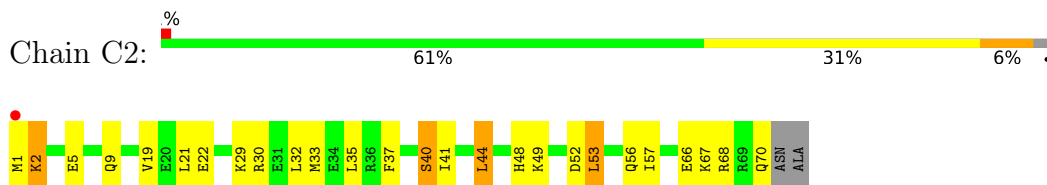
- Molecule 25: 50S ribosomal protein L28



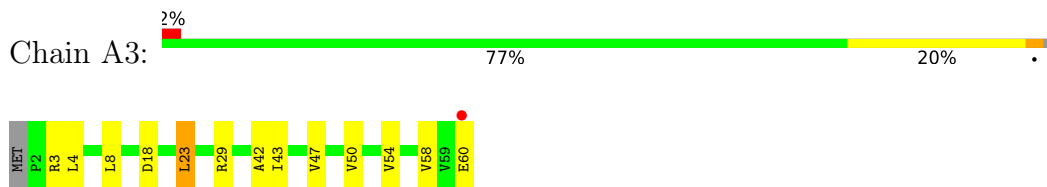
- Molecule 26: 50S ribosomal protein L29



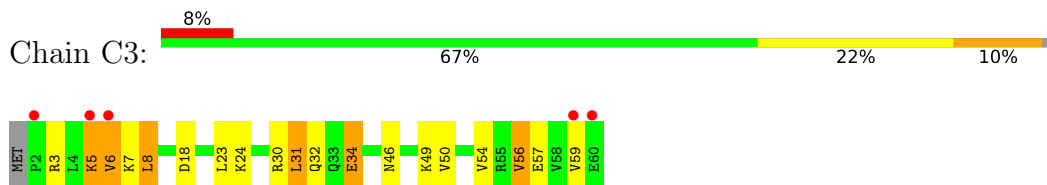
- Molecule 26: 50S ribosomal protein L29



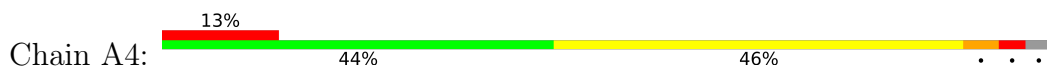
- Molecule 27: 50S ribosomal protein L30



- Molecule 27: 50S ribosomal protein L30



- Molecule 28: 50S ribosomal protein L31





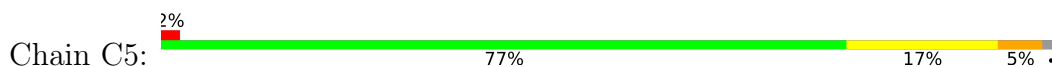
- Molecule 28: 50S ribosomal protein L31



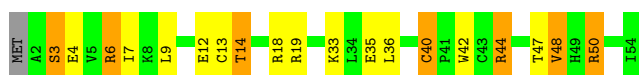
- Molecule 29: 50S ribosomal protein L32



- Molecule 29: 50S ribosomal protein L32



- Molecule 30: 50S ribosomal protein L33



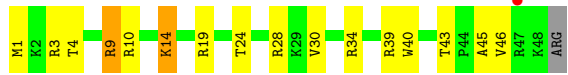
- Molecule 30: 50S ribosomal protein L33



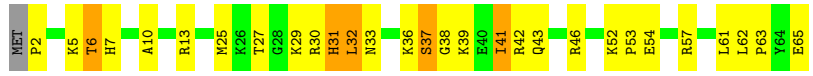
- Molecule 31: 50S ribosomal protein L34



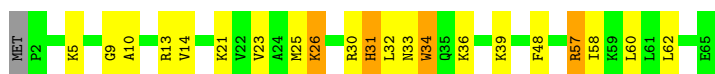
- Molecule 31: 50S ribosomal protein L34



• Molecule 32: 50S ribosomal protein L35



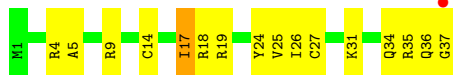
• Molecule 32: 50S ribosomal protein L35



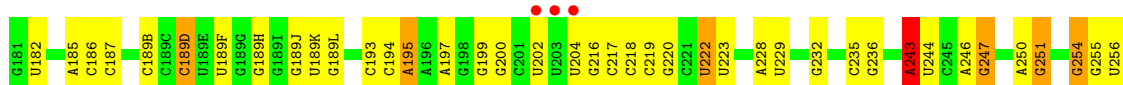
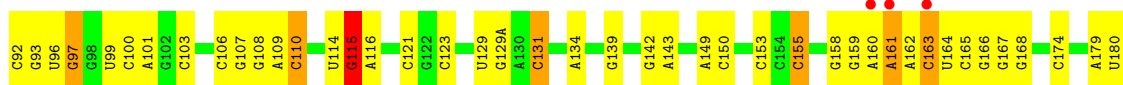
• Molecule 33: 50S ribosomal protein L36



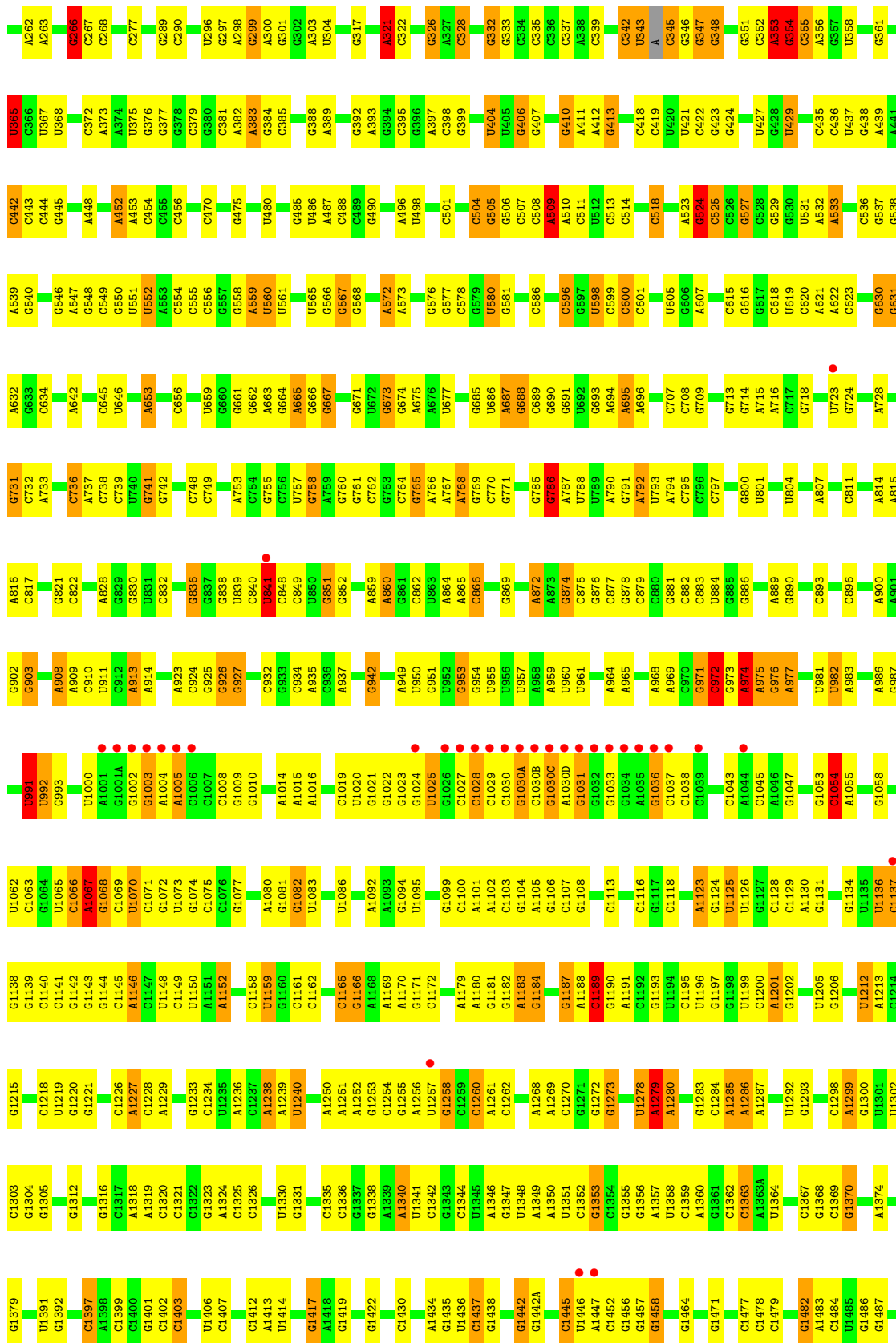
• Molecule 33: 50S ribosomal protein L36

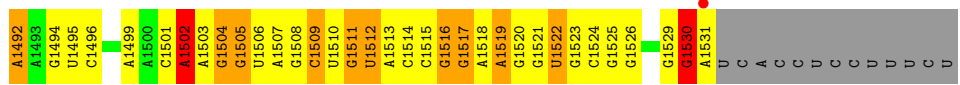


• Molecule 34: 16S Ribosomal RNA

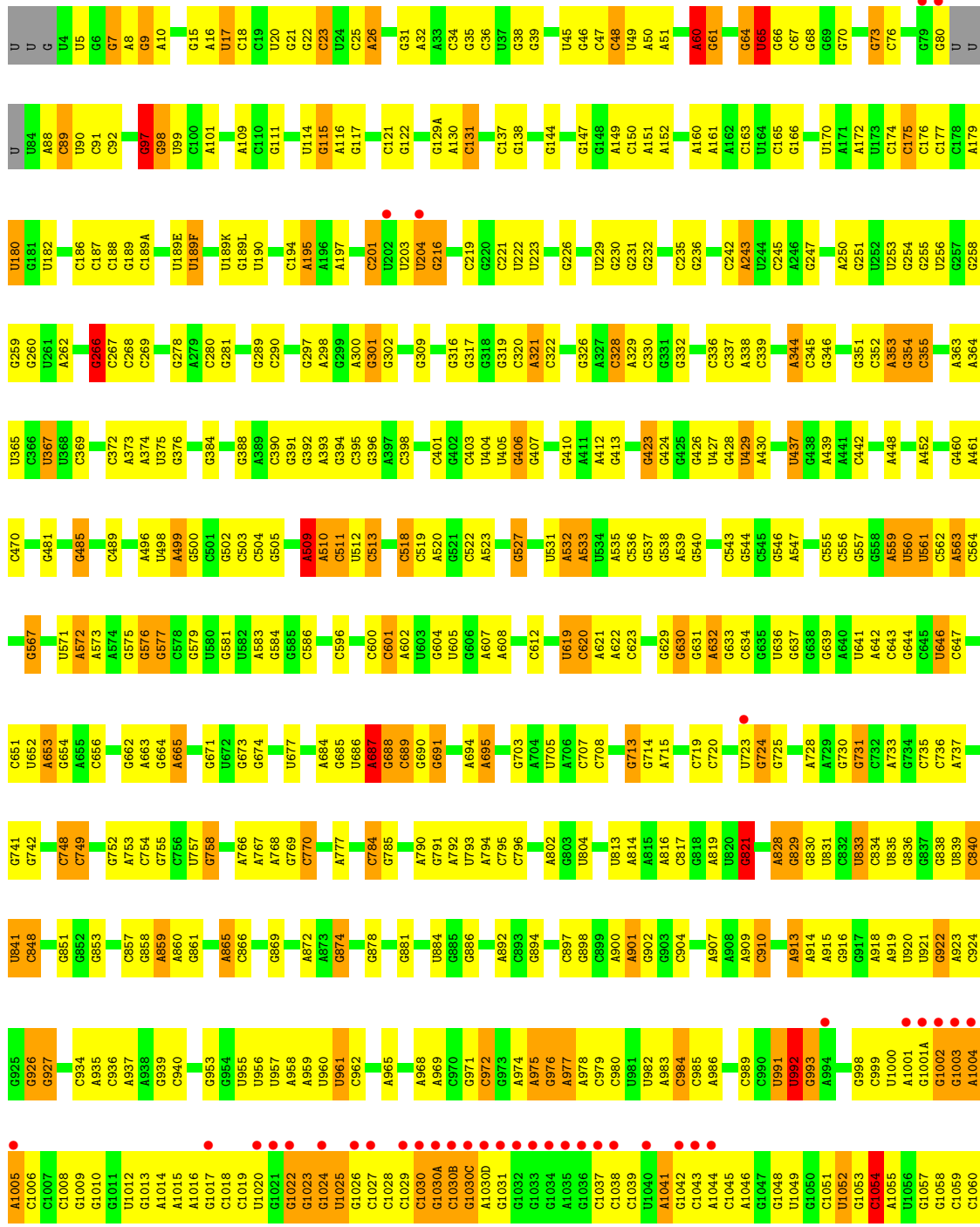


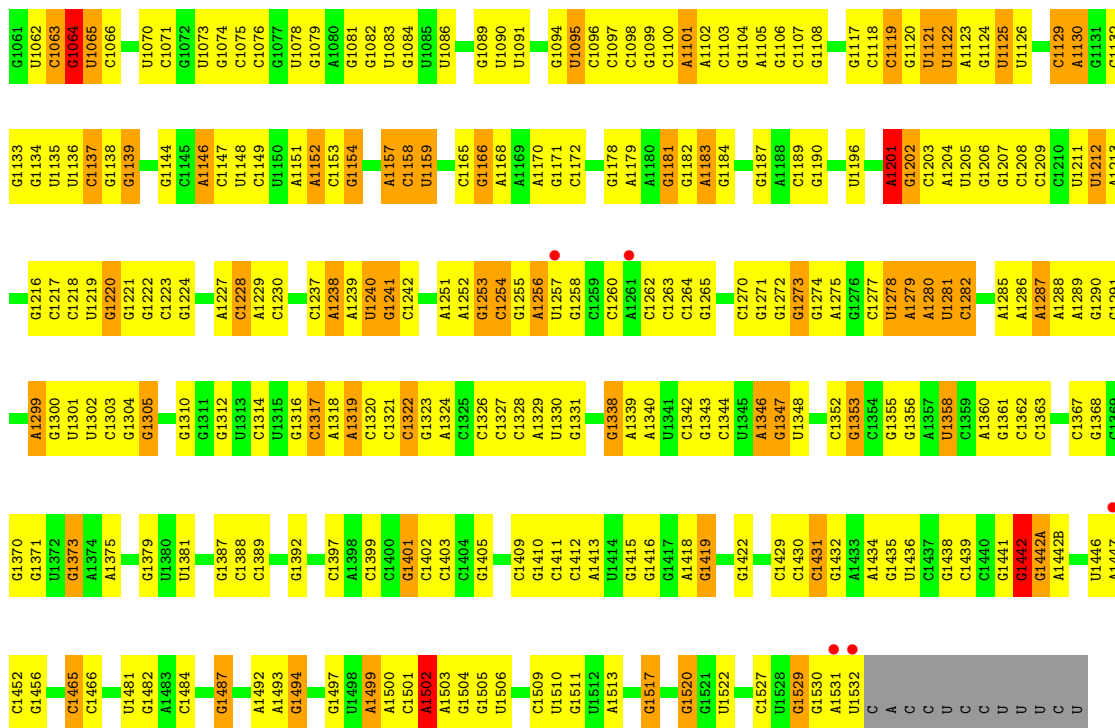






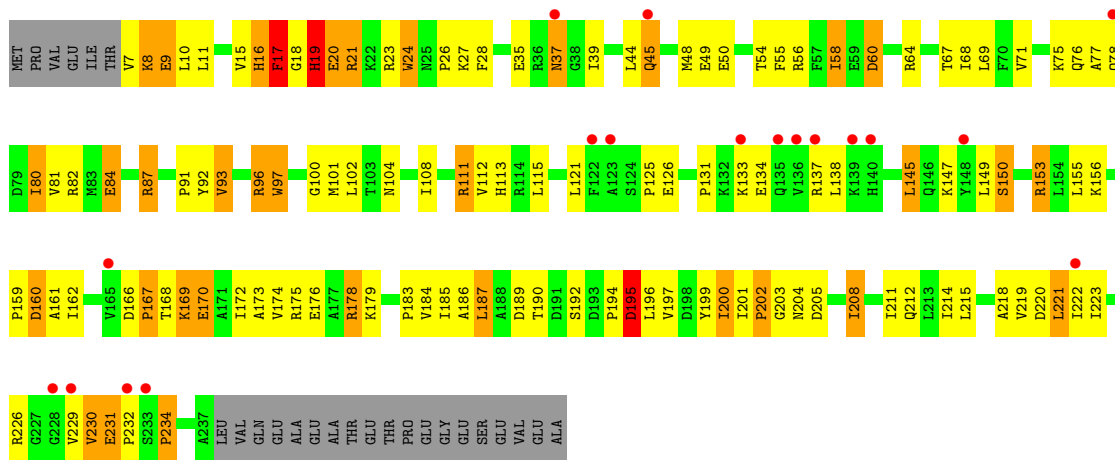
• Molecule 34: 16S Ribosomal RNA





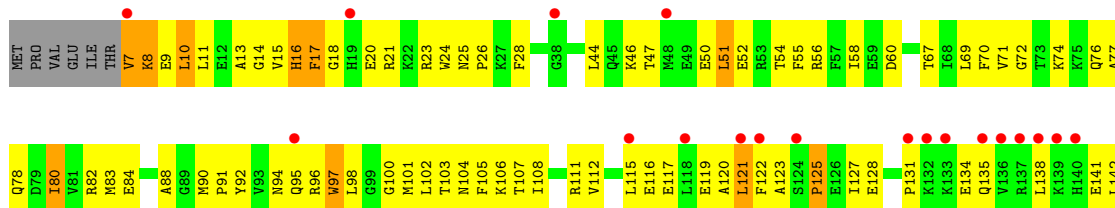
• Molecule 35: 30S ribosomal protein S2

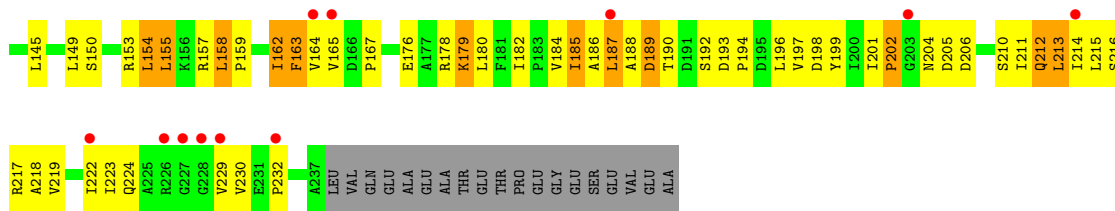
Chain BB: 7% 41% 35% 13% 10%



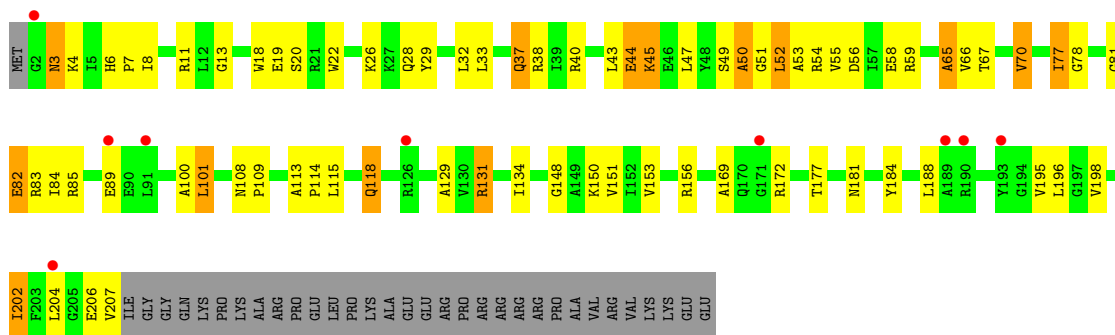
• Molecule 35: 30S ribosomal protein S2

Chain DB: 12% 38% 43% 9% 10%

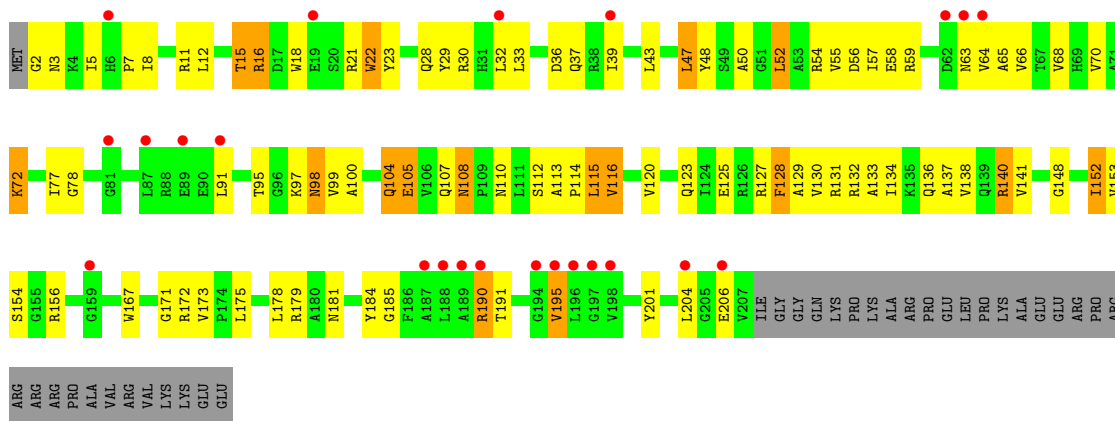




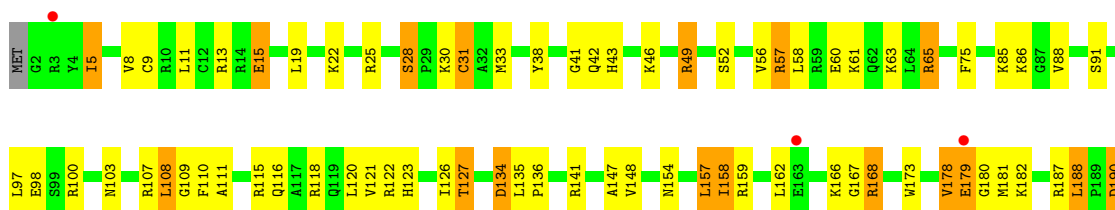
• Molecule 36: 30S ribosomal protein S3



• Molecule 36: 30S ribosomal protein S3

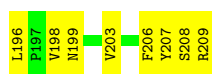


• Molecule 37: 30S ribosomal protein S4

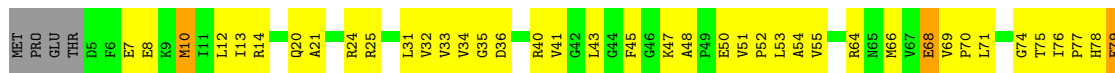




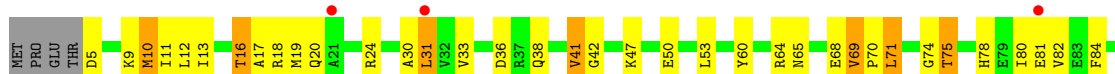
• Molecule 37: 30S ribosomal protein S4



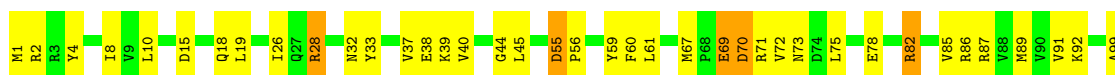
• Molecule 38: 30S ribosomal protein S5



• Molecule 38: 30S ribosomal protein S5



• Molecule 39: 30S ribosomal protein S6




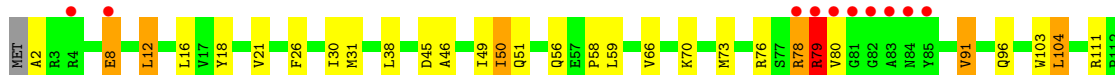
- Molecule 39: 30S ribosomal protein S6

Chain DF:  69% 24% 5% ..



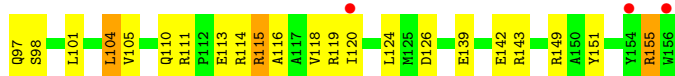
- Molecule 40: 30S ribosomal protein S7

Chain BG:  8% 72% 21% 5% ..



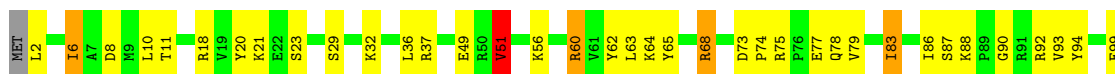
- Molecule 40: 30S ribosomal protein S7

Chain DG:  11% 69% 28% ..



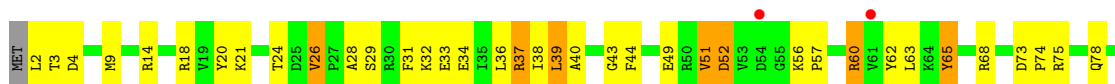
- Molecule 41: 30S ribosomal protein S8

Chain BH:  % 60% 34% ..

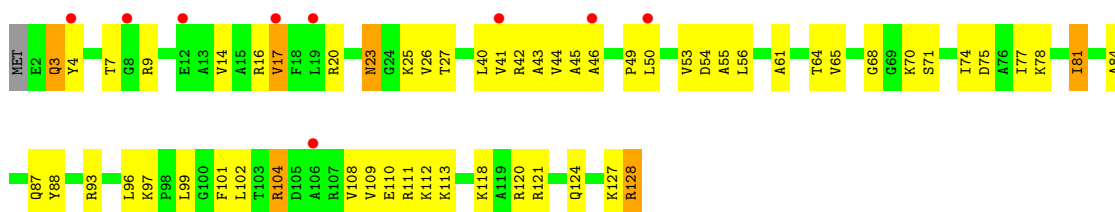


- Molecule 41: 30S ribosomal protein S8

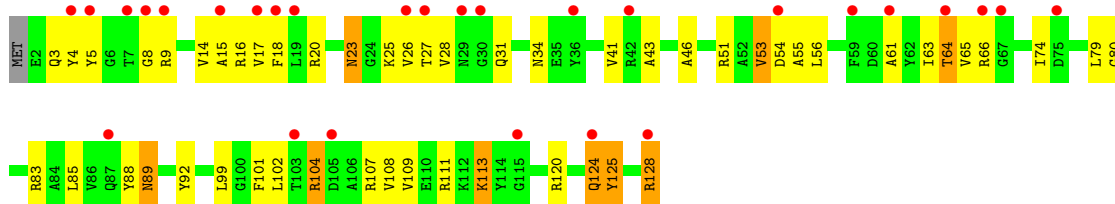
Chain DH:  4% 55% 34% 9% ..



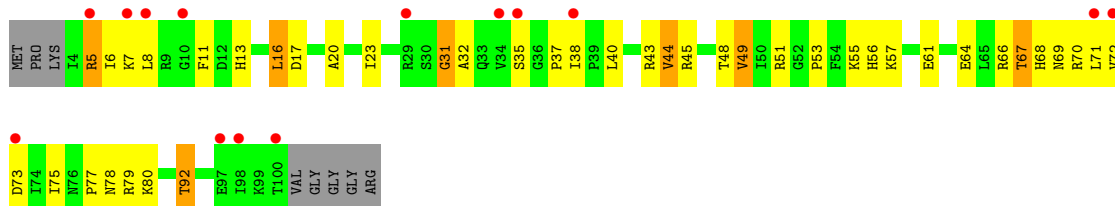
- Molecule 42: 30S ribosomal protein S9



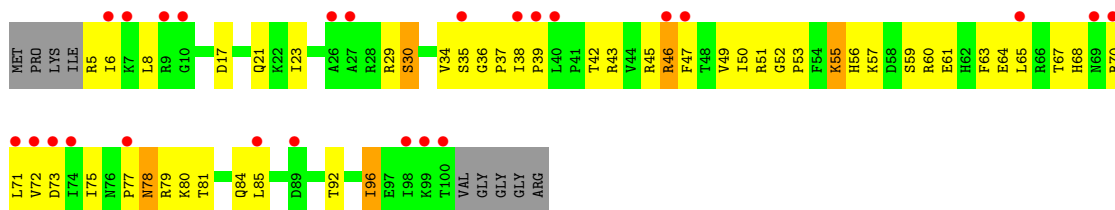
- Molecule 42: 30S ribosomal protein S9



- Molecule 43: 30S ribosomal protein S10

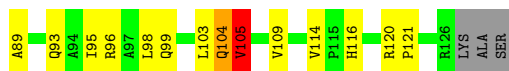


- Molecule 43: 30S ribosomal protein S10



- Molecule 44: 30S ribosomal protein S11

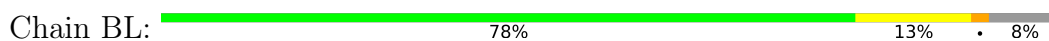




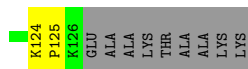
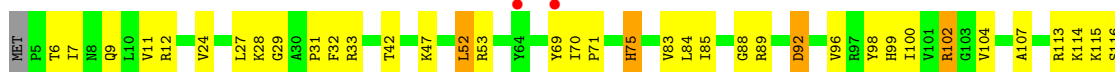
• Molecule 44: 30S ribosomal protein S11



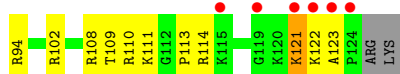
• Molecule 45: 30S ribosomal protein S12



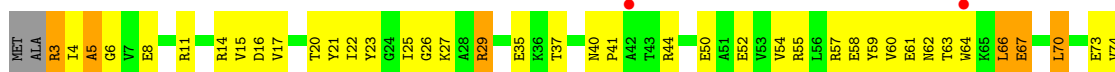
• Molecule 45: 30S ribosomal protein S12



• Molecule 46: 30S ribosomal protein S13



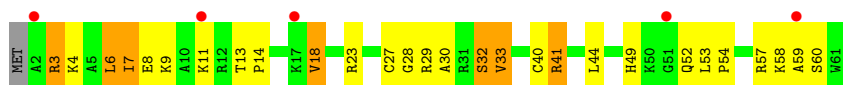
• Molecule 46: 30S ribosomal protein S13



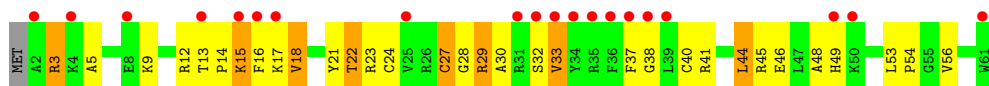




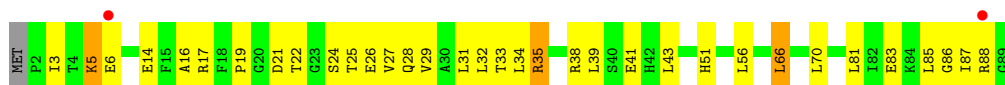
• Molecule 47: 30S ribosomal protein S14 type Z



• Molecule 47: 30S ribosomal protein S14 type Z



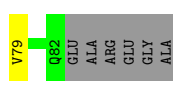
• Molecule 48: 30S ribosomal protein S15



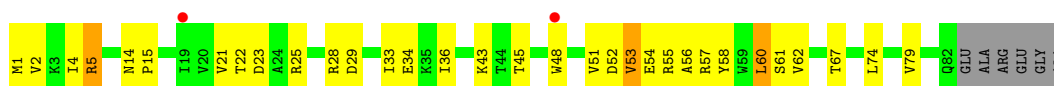
• Molecule 48: 30S ribosomal protein S15



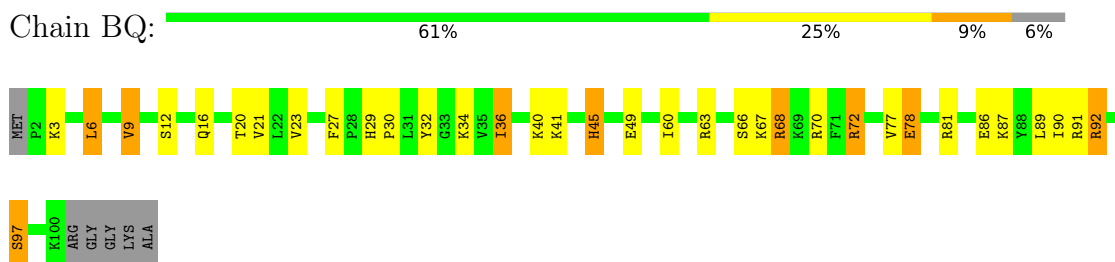
• Molecule 49: 30S ribosomal protein S16



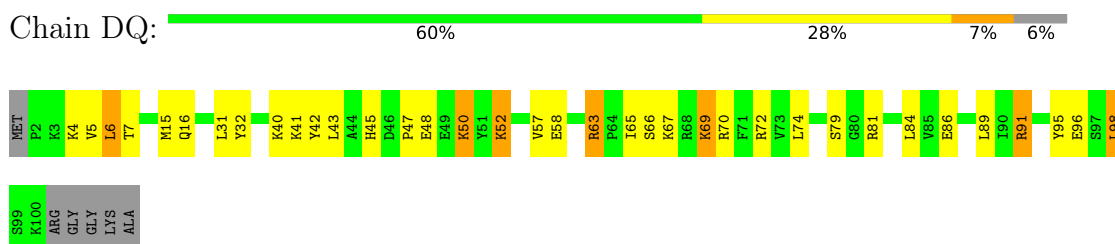
• Molecule 49: 30S ribosomal protein S16



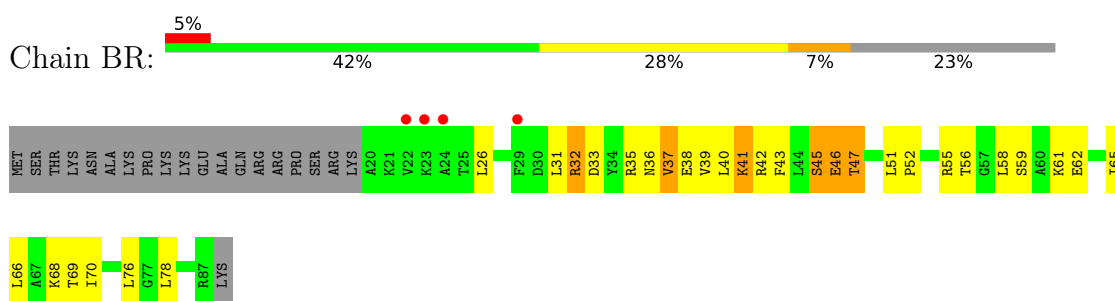
• Molecule 50: 30S ribosomal protein S17



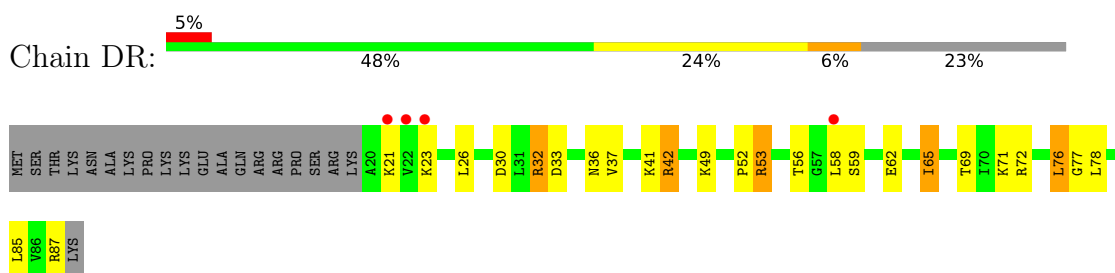
• Molecule 50: 30S ribosomal protein S17



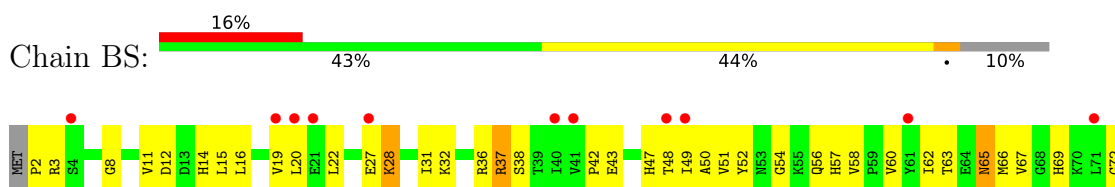
• Molecule 51: 30S ribosomal protein S18

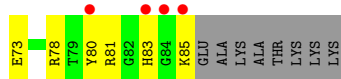


• Molecule 51: 30S ribosomal protein S18

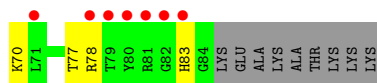
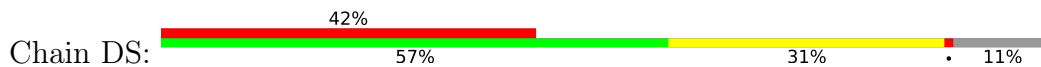


• Molecule 52: 30S ribosomal protein S19

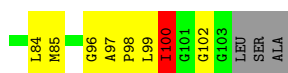




- Molecule 52: 30S ribosomal protein S19



- Molecule 53: 30S ribosomal protein S20



- Molecule 53: 30S ribosomal protein S20



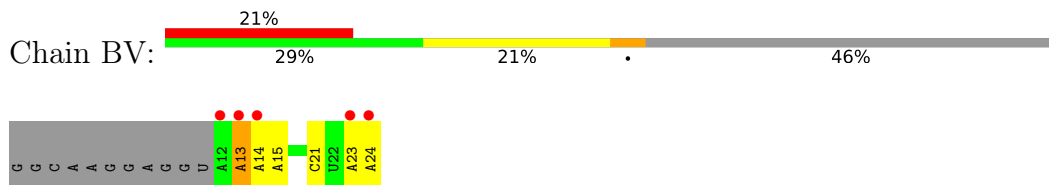
- Molecule 54: 30S ribosomal protein Thx



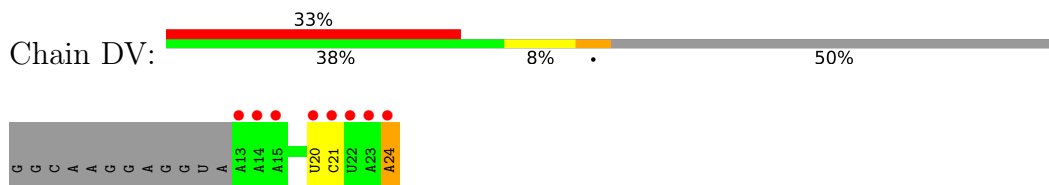
- Molecule 54: 30S ribosomal protein Thx



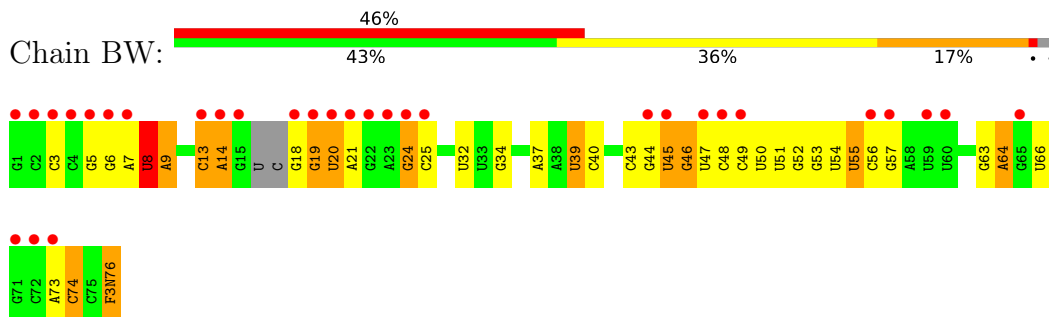
• Molecule 55: mRNA



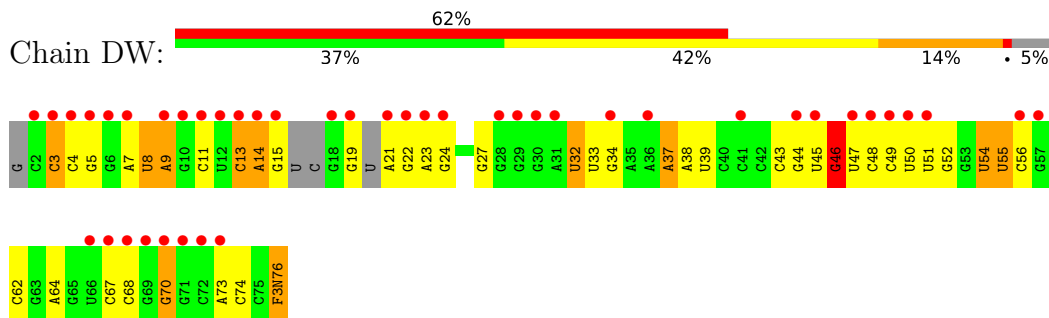
• Molecule 55: mRNA



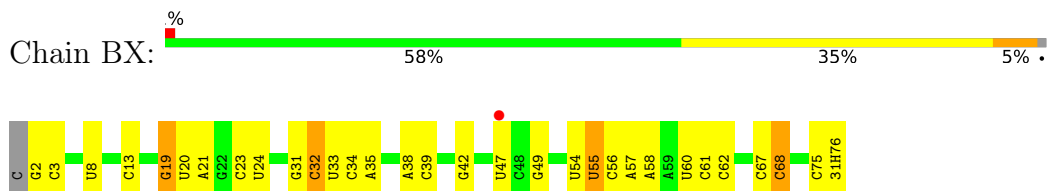
• Molecule 56: A-site tRNA



• Molecule 56: A-site tRNA

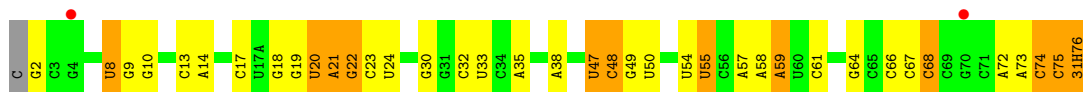


• Molecule 57: P-site tRNA

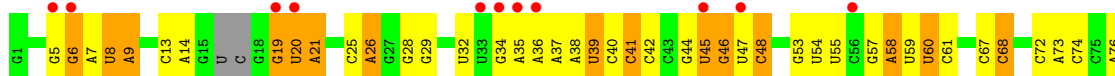


• Molecule 57: P-site tRNA

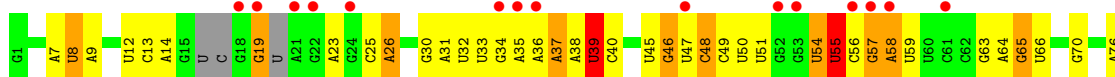




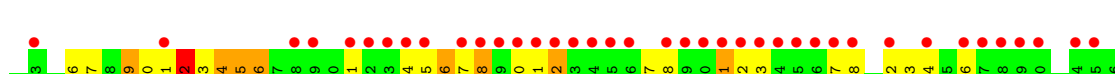
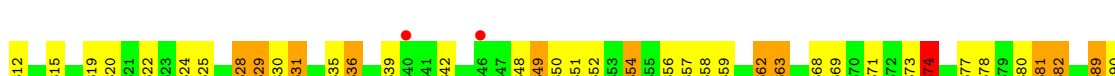
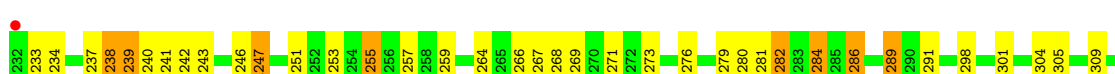
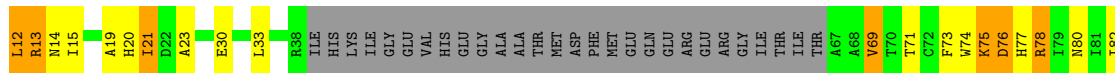
• Molecule 58: E-site tRNA

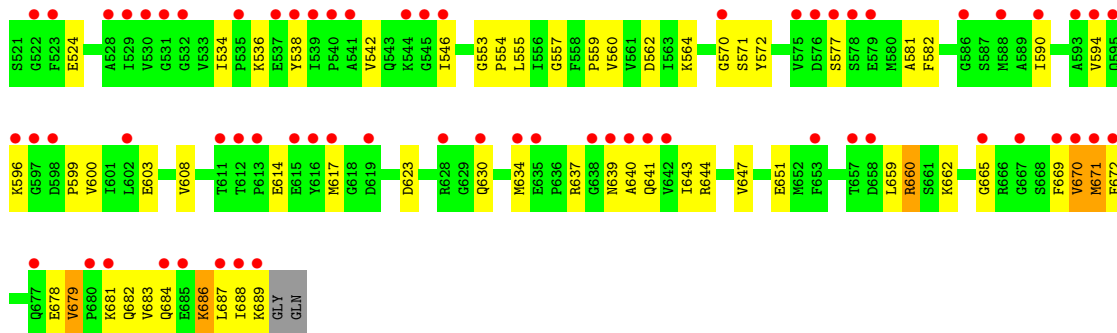


• Molecule 58: E-site tRNA

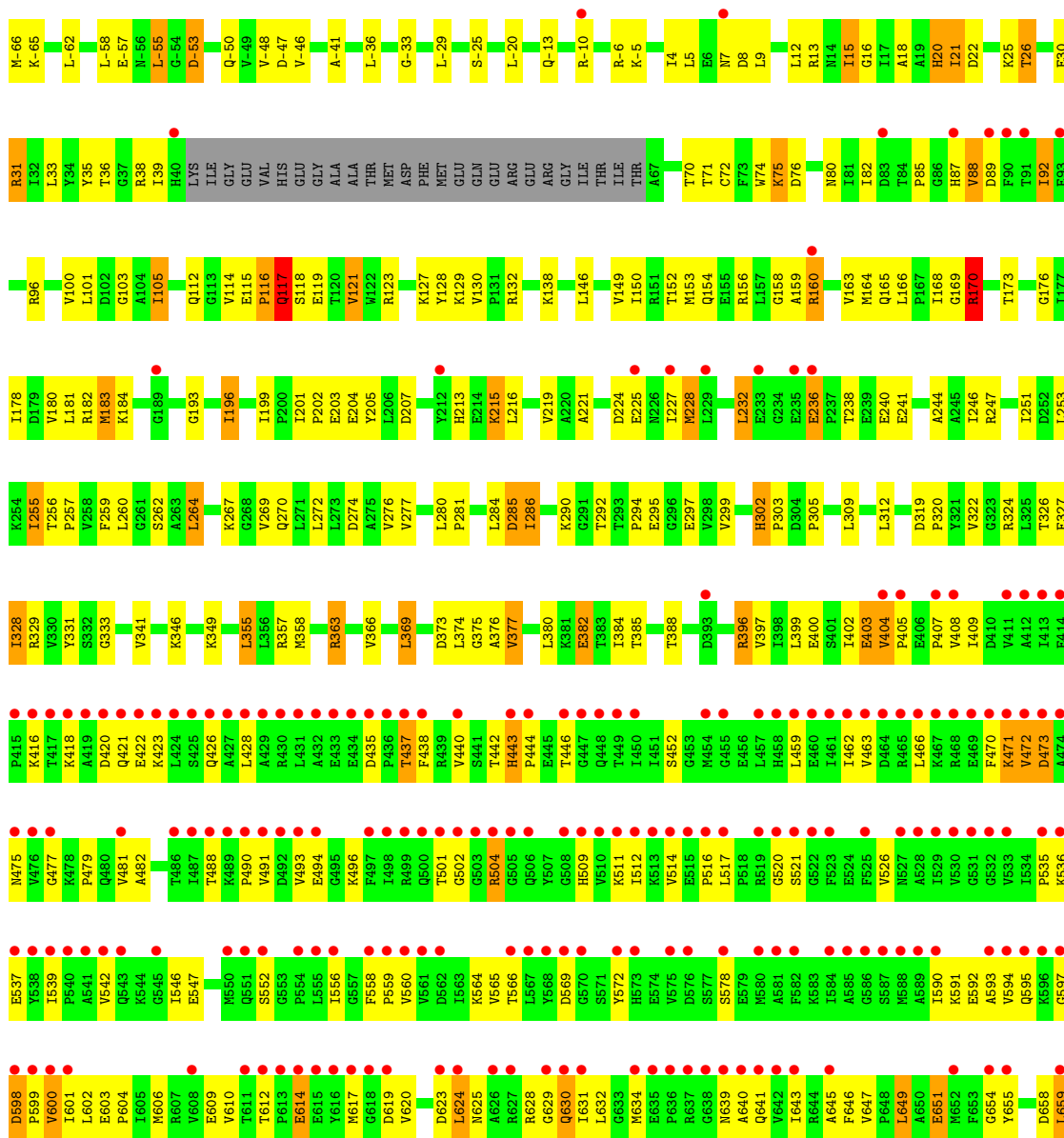


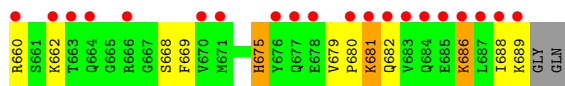
• Molecule 59: 50S ribosomal protein L9, Elongation factor G





• Molecule 59: 50S ribosomal protein L9, Elongation factor G





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.89Å 449.03Å 622.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.63 – 2.80 49.63 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.63-2.80) 99.0 (49.63-2.80)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 2.81Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, $R_{free}$	0.202 , 0.252 0.203 , 0.252	Depositor DCC
$R_{free}$ test set	71166 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.8	Xtrriage
Anisotropy	0.148	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 67.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	313372	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 31H, K, 4SU, PSU, SF4, ZN, 5MU, MG, F3N, MIA, 7MG, 5MC, GDP

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	1.20	165/69281 (0.2%)	1.78	2173/108144 (2.0%)
1	CA	0.89	30/69179 (0.0%)	1.46	878/107984 (0.8%)
2	AB	0.97	0/2878	1.65	57/4490 (1.3%)
2	CB	0.63	0/2878	1.24	15/4490 (0.3%)
3	AC	0.34	0/1083	0.65	0/1460
3	CC	0.34	0/1083	0.65	0/1460
4	AD	0.80	2/2186 (0.1%)	0.91	2/2944 (0.1%)
4	CD	0.65	0/2192	0.81	2/2951 (0.1%)
5	AE	0.81	0/1592	0.89	1/2149 (0.0%)
5	CE	0.63	0/1592	0.80	0/2149
6	AF	0.75	0/1619	0.91	2/2193 (0.1%)
6	CF	0.57	0/1615	0.74	0/2188
7	AG	0.51	0/1450	0.70	0/1959
7	CG	0.39	0/1449	0.59	0/1958
8	AH	0.67	0/1356	0.79	0/1834
8	CH	0.41	0/1356	0.62	0/1834
9	AK	0.33	0/640	0.63	0/889
9	CK	0.26	0/640	0.58	0/889
10	AL	0.31	0/503	0.53	0/673
10	CL	0.34	0/503	0.54	0/673
11	AN	0.81	0/1144	0.90	1/1543 (0.1%)
11	CN	0.57	0/1144	0.71	0/1543
12	AO	0.76	0/943	0.84	1/1269 (0.1%)
12	CO	0.68	0/943	0.75	0/1269
13	AP	0.70	0/1156	0.87	2/1537 (0.1%)
13	CP	0.51	0/1152	0.80	0/1533
14	AQ	0.77	0/1143	0.86	1/1527 (0.1%)
14	CQ	0.58	0/1143	0.69	0/1527
15	AR	0.73	0/982	0.87	0/1312
15	CR	0.58	0/982	0.77	0/1312
16	AS	0.58	0/887	0.76	1/1180 (0.1%)
16	CS	0.46	0/880	0.71	0/1172

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AT	0.74	0/1105	0.88	0/1477
17	CT	0.58	0/1097	0.74	0/1468
18	AU	0.89	1/977 (0.1%)	0.92	1/1301 (0.1%)
18	CU	0.62	0/977	0.71	2/1301 (0.2%)
19	AV	0.80	0/782	0.90	1/1049 (0.1%)
19	CV	0.52	0/782	0.74	0/1049
20	AW	0.91	0/897	0.93	3/1205 (0.2%)
20	CW	0.70	0/897	0.81	0/1205
21	AX	0.82	1/764 (0.1%)	0.80	1/1025 (0.1%)
21	CX	0.62	0/764	0.75	1/1025 (0.1%)
22	AY	0.74	0/819	0.85	0/1095
22	CY	0.54	0/819	0.69	0/1095
23	AZ	0.52	0/1379	0.70	1/1873 (0.1%)
23	CZ	0.39	0/1390	0.58	0/1890
24	A0	0.67	0/662	0.88	1/881 (0.1%)
24	C0	0.56	0/662	0.68	0/881
25	A1	0.70	0/762	0.81	0/1014
25	C1	0.61	0/762	0.77	0/1014
26	A2	0.78	0/590	0.78	0/781
26	C2	0.53	0/590	0.63	0/781
27	A3	0.82	0/474	0.91	0/635
27	C3	0.49	0/469	0.69	0/630
28	A4	0.43	0/571	0.70	0/768
28	C4	0.35	0/545	0.60	0/737
29	A5	0.89	1/469 (0.2%)	1.00	2/635 (0.3%)
29	C5	0.66	0/469	0.82	0/635
30	A6	0.86	1/460 (0.2%)	0.79	0/613
30	C6	0.62	0/456	0.74	0/608
31	A7	0.84	0/426	0.99	2/561 (0.4%)
31	C7	0.70	0/426	0.78	0/561
32	A8	0.82	0/525	0.90	0/691
32	C8	0.61	0/525	0.78	0/691
33	A9	0.80	0/310	0.94	0/407
33	C9	0.60	0/310	0.73	0/407
34	BA	0.70	4/36027 (0.0%)	1.28	246/56227 (0.4%)
34	DA	0.64	1/36170 (0.0%)	1.21	131/56452 (0.2%)
35	BB	0.40	0/1881	0.67	1/2542 (0.0%)
35	DB	0.36	0/1860	0.61	0/2518
36	BC	0.38	0/1576	0.59	0/2130
36	DC	0.35	0/1568	0.57	0/2122
37	BD	0.48	0/1689	0.67	0/2267
37	DD	0.48	0/1708	0.70	1/2289 (0.0%)
38	BE	0.51	0/1145	0.69	1/1543 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DE	0.44	0/1149	0.67	0/1548
39	BF	0.52	0/825	0.70	0/1118
39	DF	0.52	0/833	0.69	1/1128 (0.1%)
40	BG	0.43	0/1250	0.58	0/1679
40	DG	0.37	0/1254	0.56	0/1683
41	BH	0.48	0/1108	0.68	0/1494
41	DH	0.42	0/1108	0.64	0/1494
42	BI	0.42	0/1005	0.62	0/1350
42	DI	0.36	0/997	0.58	0/1343
43	BJ	0.38	0/722	0.58	0/982
43	DJ	0.34	0/727	0.59	0/988
44	BK	0.49	0/848	0.66	0/1149
44	DK	0.50	0/848	0.66	0/1149
45	BL	0.56	0/946	0.70	0/1274
45	DL	0.52	0/946	0.68	0/1274
46	BM	0.41	0/977	0.64	0/1310
46	DM	0.35	0/961	0.56	0/1291
47	BN	0.44	0/501	0.70	0/664
47	DN	0.37	0/501	0.59	1/664 (0.2%)
48	BO	0.50	0/739	0.71	0/985
48	DO	0.46	0/739	0.63	0/985
49	BP	0.53	0/697	0.69	0/939
49	DP	0.52	0/693	0.66	0/935
50	BQ	0.53	0/836	0.69	1/1117 (0.1%)
50	DQ	0.50	0/836	0.68	0/1117
51	BR	0.51	0/560	0.74	0/746
51	DR	0.52	0/560	0.66	0/746
52	BS	0.36	0/676	0.58	0/911
52	DS	0.32	0/661	0.64	0/893
53	BT	0.45	0/730	0.71	0/965
53	DT	0.46	0/733	0.69	0/969
54	BU	0.40	0/203	0.62	0/266
54	DU	0.35	0/203	0.62	0/266
55	BV	0.65	0/310	1.02	1/480 (0.2%)
55	DV	0.54	0/282	0.91	0/437
56	BW	0.43	0/1577	0.96	1/2454 (0.0%)
56	DW	0.36	0/1531	0.94	0/2379
57	BX	0.71	1/1700 (0.1%)	1.22	2/2650 (0.1%)
57	DX	0.63	1/1700 (0.1%)	1.12	4/2650 (0.2%)
58	BY	0.43	0/1602	0.98	1/2493 (0.0%)
58	DY	0.36	0/1579	0.86	0/2455
59	BZ	0.44	0/5763	0.68	2/7804 (0.0%)
59	DZ	0.41	0/5784	0.63	0/7835

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.82	208/333310 (0.1%)	1.32	3545/497173 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	1
28	A4	0	1
35	BB	0	1
53	BT	0	1
53	DT	0	1
59	DZ	0	1
All	All	0	6

All (208) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1188	A	N9-C4	-13.96	1.29	1.37
1	AA	354	A	N9-C4	-13.07	1.30	1.37
1	CA	528	A	N9-C4	-11.34	1.31	1.37
57	DX	74	C	O3'-P	-11.14	1.47	1.61
1	AA	2299	A	N9-C4	-10.50	1.31	1.37
1	AA	1249	A	N9-C4	-10.39	1.31	1.37
1	AA	990	A	N9-C4	-10.29	1.31	1.37
1	AA	1745	A	N9-C4	-9.99	1.31	1.37
1	AA	990	A	N3-C4	-9.67	1.29	1.34
1	AA	1067	A	N9-C4	-9.60	1.32	1.37
1	AA	990	A	C5-C6	-9.56	1.32	1.41
1	AA	978	A	N9-C4	-9.49	1.32	1.37
1	CA	945	A	N9-C4	-9.28	1.32	1.37
1	CA	1142(A)	A	N9-C4	-9.24	1.32	1.37
1	AA	254	A	N7-C5	-8.38	1.34	1.39
4	AD	28	GLU	CG-CD	8.35	1.64	1.51
1	AA	555	G	C2-N3	-8.30	1.26	1.32
1	AA	808	A	N7-C5	-8.10	1.34	1.39
1	AA	553	A	N9-C8	8.04	1.44	1.37
1	AA	254	A	C5-C6	-7.96	1.33	1.41
1	CA	1652	A	N9-C4	-7.86	1.33	1.37
4	AD	28	GLU	CB-CG	7.72	1.66	1.52
1	AA	1249	A	N3-C4	-7.68	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	1021	A	N9-C4	-7.62	1.33	1.37
1	AA	990	A	N7-C5	-7.55	1.34	1.39
1	AA	555	G	C6-N1	-7.52	1.34	1.39
1	AA	2490	A	N9-C4	-7.47	1.33	1.37
1	CA	945	A	C5-C6	-7.45	1.34	1.41
1	AA	1605	A	N9-C4	-7.38	1.33	1.37
1	AA	553	A	N9-C4	-7.30	1.33	1.37
1	AA	1188	A	N3-C4	-7.29	1.30	1.34
1	AA	1745	A	N3-C4	-7.15	1.30	1.34
1	AA	1157	A	N9-C4	-7.11	1.33	1.37
1	AA	830	A	N7-C5	-7.05	1.35	1.39
1	CA	1698	A	N3-C4	-6.99	1.30	1.34
18	AU	111	GLU	CG-CD	6.93	1.62	1.51
1	AA	808	A	N3-C4	-6.90	1.30	1.34
1	AA	1745	A	C5-C6	-6.88	1.34	1.41
1	AA	2527	C	N1-C6	-6.86	1.33	1.37
1	CA	2287	A	N9-C4	-6.76	1.33	1.37
1	AA	2405	A	N9-C4	-6.76	1.33	1.37
1	AA	139	A	N9-C4	-6.64	1.33	1.37
1	AA	978	A	N3-C4	-6.57	1.30	1.34
34	BA	900	A	N9-C4	-6.56	1.33	1.37
1	AA	851	A	N9-C4	-6.54	1.33	1.37
1	CA	1698	A	N9-C4	-6.51	1.33	1.37
1	AA	2553	A	N7-C5	-6.51	1.35	1.39
1	AA	2072	C	N1-C6	-6.50	1.33	1.37
1	CA	1204	A	N9-C4	-6.46	1.33	1.37
1	AA	1820	A	N7-C5	-6.41	1.35	1.39
1	AA	1829	U	C2-N3	-6.38	1.33	1.37
1	AA	16	G	C6-N1	-6.33	1.35	1.39
1	CA	185	U	C2-N3	-6.29	1.33	1.37
1	AA	2553	A	C5-C6	-6.24	1.35	1.41
1	AA	555	G	N9-C8	6.23	1.42	1.37
1	AA	2715	C	N1-C6	-6.23	1.33	1.37
1	AA	254	A	N9-C4	-6.22	1.34	1.37
1	AA	127	C	N1-C6	-6.21	1.33	1.37
1	AA	354	A	C5-C6	-6.20	1.35	1.41
21	AX	15	GLU	CG-CD	6.19	1.61	1.51
1	AA	354	A	N9-C8	6.18	1.42	1.37
1	AA	1249	A	N9-C8	6.17	1.42	1.37
1	AA	644	G	C6-N1	-6.16	1.35	1.39
1	AA	448	U	C2-N3	-6.15	1.33	1.37
1	CA	1142(A)	A	N3-C4	-6.15	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	330	A	N9-C4	-6.11	1.34	1.37
1	AA	2298	A	N3-C4	-6.10	1.31	1.34
1	AA	1188	A	C5-C6	-6.09	1.35	1.41
1	AA	553	A	N3-C4	-6.06	1.31	1.34
1	AA	592	U	N1-C2	-6.06	1.33	1.38
1	AA	2530	A	N7-C5	-6.00	1.35	1.39
1	AA	2515	A	N9-C4	5.99	1.41	1.37
1	AA	1741	C	N1-C6	-5.96	1.33	1.37
1	AA	591	U	C4-O4	-5.93	1.19	1.23
1	CA	1784	A	N9-C4	-5.91	1.34	1.37
1	CA	784	A	C6-N1	-5.89	1.31	1.35
1	AA	2659	U	C2-N3	-5.89	1.33	1.37
1	CA	792	G	C5-C4	-5.87	1.34	1.38
1	AA	538	A	N3-C4	-5.84	1.31	1.34
1	AA	2466	G	N1-C2	-5.82	1.33	1.37
1	AA	2298	A	N7-C5	-5.81	1.35	1.39
1	AA	1048	G	N1-C2	-5.78	1.33	1.37
1	CA	826	U	C2-N3	-5.77	1.33	1.37
1	AA	978	A	C5-C6	-5.77	1.35	1.41
1	AA	591	U	N3-C4	-5.75	1.33	1.38
1	AA	254	A	N3-C4	-5.74	1.31	1.34
1	AA	593	G	N7-C5	-5.73	1.35	1.39
1	AA	2298	A	C5-C4	5.68	1.42	1.38
1	AA	897	C	N3-C4	-5.67	1.29	1.33
1	AA	600	G	N7-C5	-5.66	1.35	1.39
1	AA	322	G	N7-C5	-5.66	1.35	1.39
1	AA	2299	A	C5-C6	-5.65	1.35	1.41
1	CA	1184	G	N7-C5	-5.63	1.35	1.39
1	AA	719	C	C4-N4	-5.63	1.28	1.33
1	AA	2024	G	C8-N7	-5.63	1.27	1.30
1	AA	2104	A	N9-C4	-5.61	1.34	1.37
1	CA	2593	U	C4-O4	-5.60	1.19	1.23
1	AA	2883	A	N3-C4	-5.60	1.31	1.34
1	AA	831	A	C5-C4	-5.58	1.34	1.38
1	AA	2054	G	C6-N1	-5.58	1.35	1.39
1	AA	553	A	C5-C4	5.55	1.42	1.38
1	AA	553	A	C5-C6	-5.53	1.36	1.41
1	AA	2854	G	N9-C4	-5.52	1.33	1.38
1	AA	594	A	N3-C4	5.51	1.38	1.34
1	AA	905	U	C2-N3	-5.50	1.33	1.37
1	AA	2601	A	N3-C4	-5.50	1.31	1.34
1	AA	1292	A	N3-C4	-5.50	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	455	A	N3-C4	-5.50	1.31	1.34
1	AA	2858	G	C6-N1	-5.49	1.35	1.39
1	AA	1234	A	N9-C4	-5.48	1.34	1.37
1	AA	1321	A	N9-C8	-5.48	1.33	1.37
1	AA	2073	A	N3-C4	-5.47	1.31	1.34
1	AA	528	A	N7-C5	-5.47	1.35	1.39
1	AA	808	A	C5-C6	-5.47	1.36	1.41
1	AA	1001	G	C6-N1	5.46	1.43	1.39
1	AA	1380	G	N3-C4	-5.45	1.31	1.35
1	CA	1815	A	N3-C4	-5.45	1.31	1.34
1	AA	993	G	N9-C4	-5.45	1.33	1.38
1	AA	1067	A	N7-C5	-5.43	1.35	1.39
30	A6	40	CYS	CB-SG	-5.43	1.73	1.81
1	AA	830	A	C6-N1	-5.42	1.31	1.35
1	AA	1281	G	N3-C4	-5.42	1.31	1.35
34	BA	1512	U	C2-N3	-5.42	1.33	1.37
1	AA	2701	U	C3'-O3'	5.41	1.49	1.42
1	AA	199	C	N3-C4	-5.41	1.30	1.33
1	AA	990	A	N1-C2	5.41	1.39	1.34
1	AA	2496	G	C5-C4	-5.40	1.34	1.38
1	AA	1605	A	C5-C6	-5.40	1.36	1.41
1	AA	1026	A	N9-C4	-5.38	1.34	1.37
1	AA	1679	A	N3-C4	-5.37	1.31	1.34
1	AA	2602	A	N3-C4	-5.37	1.31	1.34
1	AA	1067	A	N3-C4	-5.36	1.31	1.34
1	AA	2602	A	N9-C4	-5.34	1.34	1.37
1	AA	1001	G	C6-O6	5.33	1.28	1.24
1	AA	894	U	N3-C4	-5.33	1.33	1.38
1	CA	1890	A	N9-C4	-5.33	1.34	1.37
1	AA	2084	A	N9-C4	5.32	1.41	1.37
34	BA	317	G	N7-C5	-5.32	1.36	1.39
1	CA	960	A	N9-C4	-5.32	1.34	1.37
1	AA	1306	G	C6-O6	5.31	1.28	1.24
1	AA	2677	A	N7-C5	-5.31	1.36	1.39
1	AA	2803	A	N9-C4	5.31	1.41	1.37
57	BX	75	C	N1-C6	-5.29	1.33	1.37
1	AA	1067	A	C5-C6	-5.29	1.36	1.41
1	AA	724	A	N7-C5	-5.29	1.36	1.39
1	AA	2611	G	N3-C4	-5.29	1.31	1.35
1	AA	1259	A	N7-C5	-5.28	1.36	1.39
1	AA	2272	C	N1-C6	-5.27	1.33	1.37
1	AA	2876	U	N3-C4	-5.26	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	719	C	N3-C4	-5.26	1.30	1.33
1	AA	2459	G	C6-N1	-5.26	1.35	1.39
1	CA	2033	A	N3-C4	-5.25	1.31	1.34
1	AA	2081	A	N7-C5	-5.25	1.36	1.39
1	AA	2066	C	N1-C6	-5.25	1.34	1.37
1	AA	1679	A	C8-N7	-5.24	1.27	1.31
1	AA	1315	A	N9-C4	-5.24	1.34	1.37
1	AA	2112	G	C5-C4	-5.23	1.34	1.38
1	AA	1274	G	C6-N1	-5.21	1.35	1.39
1	CA	450	G	C6-O6	-5.21	1.19	1.24
1	AA	2294	G	C5-C6	-5.21	1.37	1.42
1	CA	2676	C	N1-C6	-5.20	1.34	1.37
1	CA	2458	G	C6-N1	-5.20	1.35	1.39
1	AA	2466	G	C6-N1	-5.19	1.35	1.39
29	A5	13	LYS	CE-NZ	5.19	1.62	1.49
1	AA	2299	A	N7-C5	-5.17	1.36	1.39
1	AA	741	U	C2-O2	-5.17	1.17	1.22
1	AA	591	U	N1-C2	-5.17	1.33	1.38
1	AA	823	G	C6-N1	-5.17	1.35	1.39
1	AA	2609	G	C5-C4	-5.17	1.34	1.38
1	AA	1518	A	N9-C4	5.16	1.41	1.37
34	DA	250	A	N9-C4	5.15	1.41	1.37
1	CA	1021	A	C5-C6	-5.15	1.36	1.41
1	AA	1605	A	N9-C8	5.14	1.41	1.37
1	AA	2331	G	N9-C4	-5.14	1.33	1.38
1	AA	1323	G	N7-C5	-5.13	1.36	1.39
1	AA	847	A	N3-C4	-5.12	1.31	1.34
1	AA	1068	G	C2-N2	-5.12	1.29	1.34
1	AA	2092	G	C5-C4	-5.12	1.34	1.38
1	AA	2571	C	C2-N3	-5.12	1.31	1.35
1	AA	1786	A	N9-C4	-5.11	1.34	1.37
1	AA	1068	G	N9-C4	-5.10	1.33	1.38
1	AA	586	G	N1-C2	-5.10	1.33	1.37
1	AA	2054	G	C5-C4	-5.09	1.34	1.38
1	AA	1299	A	C5-C4	-5.09	1.35	1.38
1	CA	530	G	N9-C8	5.09	1.41	1.37
1	AA	1068	G	N1-C2	-5.07	1.33	1.37
1	AA	2605	U	C2-N3	-5.07	1.34	1.37
1	AA	808	A	N9-C4	-5.07	1.34	1.37
1	AA	1848	G	C6-N1	-5.07	1.36	1.39
1	AA	990	A	N9-C8	5.06	1.41	1.37
34	BA	903	G	C5-C4	-5.06	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1665	G	C6-N1	-5.06	1.36	1.39
1	AA	2520	G	N9-C8	-5.06	1.34	1.37
1	CA	580	C	N1-C6	-5.05	1.34	1.37
1	CA	2875	C	N1-C6	-5.05	1.34	1.37
1	AA	182	U	C2-N3	-5.05	1.34	1.37
1	AA	2502	G	C6-N1	-5.05	1.36	1.39
1	AA	1709	C	N3-C4	-5.04	1.30	1.33
1	AA	990	A	C5-C4	5.04	1.42	1.38
1	AA	1249	A	N7-C5	-5.04	1.36	1.39
1	AA	2084	A	N3-C4	5.04	1.37	1.34
1	AA	2591	C	N1-C6	-5.03	1.34	1.37
1	AA	492	A	N7-C5	-5.03	1.36	1.39
1	AA	2052	A	C5-C6	-5.02	1.36	1.41
1	AA	2584	A	N3-C4	-5.02	1.31	1.34
1	AA	1324	A	N3-C4	-5.02	1.31	1.34
1	AA	2055	A	C6-N6	-5.01	1.29	1.33
1	AA	669	A	N7-C5	-5.00	1.36	1.39

All (3545) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	990	A	N1-C6-N6	23.54	132.72	118.60
1	AA	354	A	C2-N3-C4	-21.82	99.69	110.60
1	AA	990	A	C6-C5-N7	-21.49	117.25	132.30
1	AA	1188	A	C2-N3-C4	-21.02	100.09	110.60
1	AA	990	A	C5-N7-C8	-19.83	93.98	103.90
1	AA	1067	A	C2-N3-C4	-19.66	100.77	110.60
1	AA	990	A	C2-N3-C4	-18.70	101.25	110.60
1	AA	1745	A	C2-N3-C4	-18.36	101.42	110.60
1	AA	1249	A	C2-N3-C4	-18.05	101.58	110.60
1	AA	2045	G	O5'-P-OP1	-17.97	89.13	110.70
1	AA	990	A	C4-C5-N7	16.94	119.17	110.70
1	AA	1605	A	C2-N3-C4	-16.25	102.47	110.60
1	AA	2299	A	C2-N3-C4	-16.18	102.51	110.60
1	AA	553	A	C5-N7-C8	-15.70	96.05	103.90
1	CA	528	A	C2-N3-C4	-15.31	102.95	110.60
1	AA	990	A	N1-C2-N3	15.24	136.92	129.30
1	CA	1698	A	C2-N3-C4	-15.20	103.00	110.60
1	AA	2298	A	N7-C8-N9	14.95	121.27	113.80
1	AA	354	A	N3-C4-C5	14.76	137.13	126.80
1	AA	990	A	N7-C8-N9	14.24	120.92	113.80
1	AA	1249	A	C5-N7-C8	-14.21	96.79	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	553	A	N7-C8-N9	14.12	120.86	113.80
1	AA	894	U	C5-C4-O4	14.08	134.35	125.90
1	AA	978	A	C5-N7-C8	-13.99	96.91	103.90
1	AA	553	A	C2-N3-C4	-13.88	103.66	110.60
1	AA	254	A	C2-N3-C4	-13.85	103.67	110.60
1	AA	139	A	C5-N7-C8	-13.73	97.04	103.90
1	AA	354	A	N3-C4-N9	-13.65	116.48	127.40
1	CA	945	A	C4-C5-N7	13.51	117.46	110.70
1	AA	1188	A	N3-C4-C5	13.18	136.03	126.80
1	AA	990	A	C4-C5-C6	13.15	123.58	117.00
1	AA	2298	A	C8-N9-C4	-13.14	100.55	105.80
1	CA	2023	G	O5'-P-OP1	-13.14	93.88	105.70
1	AA	553	A	C8-N9-C4	-13.11	100.56	105.80
1	AA	2298	A	C2-N3-C4	-12.90	104.15	110.60
1	CA	945	A	C5-N7-C8	-12.87	97.47	103.90
1	AA	553	A	N1-C6-N6	12.81	126.28	118.60
1	AA	2298	A	N1-C2-N3	12.80	135.70	129.30
1	AA	474	U	O5'-P-OP2	-12.58	94.38	105.70
1	AA	2355	C	O5'-P-OP1	-12.50	94.45	105.70
1	AA	139	A	N7-C8-N9	12.48	120.04	113.80
1	AA	1188	A	N3-C4-N9	-12.37	117.51	127.40
1	AA	990	A	C5-C6-N6	-12.27	113.88	123.70
1	AA	2298	A	C5-N7-C8	-12.26	97.77	103.90
1	AA	1745	A	C5-N7-C8	-12.15	97.83	103.90
1	AA	537	G	O4'-C1'-N9	12.15	117.92	108.20
1	AA	555	G	C5-C6-O6	12.11	135.87	128.60
1	AA	1067	A	C5-N7-C8	-12.10	97.85	103.90
1	AA	726	C	N3-C4-C5	12.06	126.72	121.90
1	CA	963	U	O5'-P-OP1	-12.04	94.86	105.70
1	CA	1021	A	C2-N3-C4	-11.92	104.64	110.60
1	CA	141	A	N7-C8-N9	11.89	119.75	113.80
1	AA	254	A	C6-C5-N7	-11.82	124.02	132.30
1	AA	1237	G	C5-N7-C8	11.76	110.18	104.30
1	CA	945	A	C2-N3-C4	-11.75	104.73	110.60
1	CA	819	A	O5'-P-OP1	-11.73	95.14	105.70
1	AA	978	A	C2-N3-C4	-11.70	104.75	110.60
1	CA	945	A	N1-C6-N6	11.65	125.59	118.60
1	AA	2442	A	O5'-P-OP2	-11.61	95.25	105.70
1	AA	2298	A	C6-C5-N7	-11.59	124.19	132.30
1	AA	555	G	N3-C4-N9	-11.59	119.05	126.00
1	AA	2694	U	O5'-P-OP2	-11.58	95.28	105.70
1	AA	1249	A	N7-C8-N9	11.49	119.54	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1067	A	N3-C4-N9	-11.30	118.36	127.40
1	AA	2834	C	C5-C4-N4	-11.30	112.29	120.20
1	CA	1368	G	O5'-P-OP2	-11.27	95.56	105.70
1	AA	254	A	N1-C6-N6	11.27	125.36	118.60
1	AA	553	A	C4-C5-N7	11.26	116.33	110.70
1	AA	1686	U	O5'-P-OP2	-11.26	95.56	105.70
1	AA	1231	G	C5-C6-N1	11.25	117.13	111.50
1	CA	1142(A)	A	C2-N3-C4	-11.25	104.98	110.60
1	AA	978	A	N7-C8-N9	11.24	119.42	113.80
1	AA	792	G	C5-C6-O6	-11.22	121.86	128.60
1	CA	1698	A	N1-C2-N3	11.22	134.91	129.30
1	AA	1188	A	C5-N7-C8	-11.20	98.30	103.90
1	CA	141	A	C5-N7-C8	-11.17	98.31	103.90
1	CA	961	C	O5'-P-OP2	-11.08	95.73	105.70
1	AA	2834	C	N3-C4-N4	11.05	125.74	118.00
1	CA	528	A	N3-C4-C5	10.98	134.49	126.80
1	AA	235	C	C6-N1-C2	10.96	124.68	120.30
1	AA	1067	A	C5-C6-N1	-10.94	112.23	117.70
1	AA	354	A	C5-N7-C8	-10.92	98.44	103.90
1	CA	2824	C	C6-N1-C2	10.88	124.65	120.30
1	AA	1157	A	O4'-C1'-N9	10.87	116.89	108.20
1	AA	1249	A	C8-N9-C4	-10.86	101.46	105.80
1	AA	1067	A	C8-N9-C4	-10.84	101.47	105.80
1	CA	945	A	N3-C4-C5	10.82	134.37	126.80
1	AA	1021	G	O5'-P-OP2	-10.69	96.08	105.70
1	CA	2576	G	O5'-P-OP1	-10.68	96.09	105.70
1	AA	555	G	N3-C4-C5	10.67	133.93	128.60
1	CA	330	A	C2-N3-C4	-10.66	105.27	110.60
1	AA	1188	A	C5-C6-N1	-10.64	112.38	117.70
1	CA	1614	A	O5'-P-OP1	-10.63	96.13	105.70
1	AA	1067	A	N3-C4-C5	10.63	134.24	126.80
1	AA	2281	A	O5'-P-OP1	-10.62	96.14	105.70
1	AA	1067	A	N7-C8-N9	10.60	119.10	113.80
1	AA	894	U	N3-C4-O4	-10.58	112.00	119.40
1	CA	512	G	O4'-C1'-N9	10.51	116.60	108.20
1	CA	2708	G	C8-N9-C4	10.46	110.58	106.40
1	AA	1874	C	C6-N1-C2	10.43	124.47	120.30
1	AA	2287	C	O5'-P-OP2	-10.42	96.32	105.70
34	BA	365	U	C5-C6-N1	-10.38	117.51	122.70
1	AA	1347	A	O5'-P-OP1	-10.36	96.38	105.70
1	AA	592	U	N1-C2-O2	-10.35	115.56	122.80
1	AA	1154	U	N3-C2-O2	-10.34	114.97	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	2331	G	N3-C4-N9	-10.31	119.82	126.00
1	AA	2641	A	N1-C2-N3	10.30	134.45	129.30
1	AA	345	G	C5-C6-O6	-10.29	122.42	128.60
1	AA	1237	G	N7-C8-N9	-10.28	107.96	113.10
1	AA	1695	C	O5'-P-OP1	-10.27	96.46	105.70
1	AA	542	C	C5-C4-N4	-10.23	113.04	120.20
1	CA	614	U	N3-C2-O2	-10.23	115.04	122.20
1	AA	1249	A	N3-C4-N9	-10.22	119.23	127.40
1	AA	254	A	C5-N7-C8	-10.16	98.82	103.90
1	CA	847	U	C2-N1-C1'	-10.16	105.51	117.70
1	AA	1037	C	C2-N3-C4	-10.13	114.83	119.90
1	AA	555	G	C6-N1-C2	10.12	131.17	125.10
1	CA	1130	U	O5'-P-OP1	-10.11	96.60	105.70
1	AA	2045	G	O5'-P-OP2	10.00	122.70	110.70
1	AA	552	C	N1-C2-N3	9.97	126.18	119.20
1	AA	1605	A	N3-C4-C5	9.97	133.78	126.80
1	AA	1150	C	OP1-P-O3'	-9.97	83.27	105.20
1	AA	978	A	C4-C5-N7	9.95	115.68	110.70
1	AA	1249	A	N3-C4-C5	9.95	133.77	126.80
1	CA	141	A	C8-N9-C4	-9.92	101.83	105.80
1	AA	2427	G	C5-C6-O6	-9.88	122.67	128.60
1	CA	2626	C	C6-N1-C2	9.88	124.25	120.30
1	AA	2298	A	C4-C5-C6	9.86	121.93	117.00
1	AA	2331	G	C8-N9-C4	-9.86	102.46	106.40
1	AA	2776	G	C4-C5-N7	9.85	114.74	110.80
1	AA	1611	C	O5'-P-OP2	-9.75	96.92	105.70
1	AA	205	A	O5'-P-OP1	-9.75	96.93	105.70
2	CB	30	C	C6-N1-C2	-9.74	116.40	120.30
1	AA	481	C	O5'-P-OP2	-9.73	96.94	105.70
1	AA	2386	C	C6-N1-C2	9.73	124.19	120.30
1	AA	2331	G	C5-N7-C8	-9.72	99.44	104.30
1	AA	555	G	C8-N9-C4	-9.71	102.52	106.40
1	AA	798	A	O5'-P-OP2	9.71	122.35	110.70
1	AA	2876	U	C5-C6-N1	-9.68	117.86	122.70
1	AA	2515	A	N1-C6-N6	9.68	124.41	118.60
1	AA	1342	G	N1-C6-O6	-9.66	114.10	119.90
1	AA	2475	C	C6-N1-C2	9.65	124.16	120.30
1	AA	2776	G	N9-C4-C5	-9.63	101.55	105.40
1	AA	1037	C	C5-C6-N1	-9.62	116.19	121.00
1	AA	598	A	O5'-P-OP1	-9.60	97.06	105.70
1	AA	555	G	C5-N7-C8	-9.59	99.51	104.30
1	CA	450	G	N1-C6-O6	-9.58	114.15	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1837	C	O5'-P-OP1	-9.58	97.08	105.70
1	AA	2287	C	O5'-P-OP1	9.55	122.16	110.70
1	AA	596	G	C6-N1-C2	-9.54	119.37	125.10
1	AA	2710	U	O5'-P-OP2	-9.54	97.11	105.70
1	CA	1656	C	N3-C4-C5	9.53	125.71	121.90
1	AA	1856	A	N1-C6-N6	-9.51	112.90	118.60
1	AA	2089	G	C8-N9-C4	-9.51	102.60	106.40
1	CA	856	C	C6-N1-C2	-9.50	116.50	120.30
1	AA	2643	G	O5'-P-OP1	-9.47	97.17	105.70
1	AA	1249	A	N1-C2-N3	9.47	134.03	129.30
1	AA	1745	A	C4-C5-N7	9.45	115.42	110.70
1	AA	1745	A	N3-C4-C5	9.43	133.40	126.80
1	AA	2528	G	N1-C6-O6	-9.43	114.24	119.90
1	AA	2265	G	C8-N9-C4	9.42	110.17	106.40
1	AA	2631	C	C5-C6-N1	-9.41	116.29	121.00
1	AA	894	U	N3-C2-O2	-9.38	115.64	122.20
1	AA	2299	A	N3-C4-C5	9.37	133.36	126.80
1	AA	1318	A	O5'-P-OP2	-9.37	97.27	105.70
1	AA	991	G	O5'-P-OP1	-9.37	97.27	105.70
34	BA	365	U	C5-C4-O4	9.37	131.52	125.90
1	AA	859	C	N3-C4-C5	9.36	125.64	121.90
1	AA	1006	C	O5'-P-OP2	-9.36	97.28	105.70
1	CA	2287	A	C2-N3-C4	-9.36	105.92	110.60
1	AA	1249	A	O4'-C1'-N9	9.35	115.68	108.20
1	AA	792	G	N1-C6-O6	9.31	125.49	119.90
1	CA	1204	A	C2-N3-C4	-9.31	105.94	110.60
1	AA	1001	G	N1-C6-O6	9.30	125.48	119.90
1	CA	1698	A	C5-N7-C8	-9.29	99.25	103.90
1	AA	555	G	C2-N3-C4	-9.29	107.26	111.90
1	AA	2638	C	C5-C6-N1	-9.24	116.38	121.00
1	AA	1067	A	N1-C2-N3	9.22	133.91	129.30
2	AB	80	U	C5-C6-N1	-9.22	118.09	122.70
1	AA	1963	C	N1-C2-O2	-9.19	113.39	118.90
1	AA	186	A	OP1-P-OP2	-9.18	105.83	119.60
1	AA	2754	A	C8-N9-C4	9.18	109.47	105.80
2	AB	91	C	C5-C4-N4	-9.16	113.79	120.20
1	AA	2336	C	C6-N1-C2	9.16	123.96	120.30
1	AA	542	C	C6-N1-C2	9.14	123.96	120.30
1	CA	34	C	N1-C2-O2	9.14	124.39	118.90
1	AA	798	A	O5'-P-OP1	-9.13	97.48	105.70
1	CA	1204	A	N1-C6-N6	9.11	124.07	118.60
1	AA	1723	A	C8-N9-C4	9.11	109.44	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	851	A	C8-N9-C4	9.11	109.44	105.80
1	AA	139	A	C8-N9-C4	-9.09	102.16	105.80
1	AA	1150	C	OP2-P-O3'	-9.08	85.23	105.20
2	AB	91	C	C6-N1-C2	9.06	123.93	120.30
1	AA	2641	A	C6-C5-N7	-9.06	125.96	132.30
1	CA	1653	G	P-O3'-C3'	9.05	130.56	119.70
1	AA	856	G	C5-C6-O6	9.04	134.03	128.60
1	AA	2162	C	C2-N1-C1'	9.04	128.75	118.80
1	CA	141	A	C4-C5-N7	9.04	115.22	110.70
1	AA	2657	G	C4-C5-N7	9.03	114.41	110.80
1	AA	354	A	C5-C6-N1	-9.02	113.19	117.70
1	AA	1605	A	C5-C6-N1	-9.02	113.19	117.70
1	AA	2515	A	C5-C6-N6	-9.01	116.49	123.70
1	AA	2776	G	C5-C6-O6	-9.01	123.19	128.60
1	AA	2049	G	N1-C6-O6	-9.00	114.50	119.90
1	CA	141	A	N1-C6-N6	9.00	124.00	118.60
1	AA	2046	G	C8-N9-C4	9.00	110.00	106.40
1	AA	2571	C	N3-C4-C5	9.00	125.50	121.90
1	CA	963	U	C5-C4-O4	-8.99	120.50	125.90
1	AA	553	A	O4'-C1'-N9	-8.99	101.01	108.20
1	AA	1249	A	C4-C5-N7	8.98	115.19	110.70
1	CA	528	A	N3-C4-N9	-8.96	120.23	127.40
1	AA	2331	G	N7-C8-N9	8.96	117.58	113.10
1	AA	627	G	O5'-P-OP2	-8.96	97.64	105.70
1	AA	1728	G	C4-C5-N7	8.93	114.37	110.80
1	AA	2571	C	N1-C2-O2	8.92	124.25	118.90
1	CA	915	C	C6-N1-C2	-8.90	116.74	120.30
1	AA	254	A	C4-C5-N7	8.89	115.15	110.70
1	AA	1184	G	O5'-P-OP2	-8.88	97.70	105.70
1	CA	450	G	C5-C6-N1	8.88	115.94	111.50
2	AB	91	C	N3-C4-C5	8.88	125.45	121.90
1	CA	1142(A)	A	N3-C4-N9	-8.88	120.30	127.40
1	CA	614	U	C5-C4-O4	8.87	131.22	125.90
1	CA	847	U	N1-C2-O2	-8.87	116.59	122.80
1	AA	470	C	O5'-P-OP1	8.86	121.34	110.70
1	AA	1715	A	O5'-P-OP2	-8.87	97.72	105.70
1	AA	1745	A	N1-C2-N3	8.85	133.73	129.30
1	AA	2331	G	N3-C4-C5	8.85	133.03	128.60
1	AA	552	C	C4-C5-C6	8.85	121.83	117.40
1	AA	2882	G	N1-C6-O6	-8.85	114.59	119.90
1	AA	2041	A	N7-C8-N9	-8.84	109.38	113.80
1	AA	139	A	C4-C5-N7	8.82	115.11	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	86	G	C5-C6-O6	-8.81	123.31	128.60
1	AA	1232	G	N1-C6-O6	-8.80	114.62	119.90
1	AA	1374	G	C5-C6-N1	8.77	115.88	111.50
1	AA	1593	C	C6-N1-C2	-8.76	116.80	120.30
1	CA	330	A	C5-N7-C8	-8.76	99.52	103.90
1	CA	2595	G	O5'-P-OP1	-8.73	97.84	105.70
1	AA	2559	U	N1-C2-N3	8.71	120.13	114.90
1	CA	1698	A	C6-C5-N7	-8.72	126.20	132.30
1	AA	553	A	C6-C5-N7	-8.71	126.20	132.30
1	AA	1718	U	O5'-P-OP2	-8.71	97.86	105.70
1	AA	776	G	O5'-P-OP2	-8.70	97.87	105.70
1	AA	1812	C	C6-N1-C2	8.70	123.78	120.30
1	AA	1188	A	N1-C2-N3	8.69	133.65	129.30
1	AA	2631	C	C6-N1-C2	8.69	123.78	120.30
1	AA	1291	G	N1-C6-O6	-8.69	114.69	119.90
1	AA	553	A	N1-C2-N3	8.68	133.64	129.30
1	AA	1412	A	C8-N9-C4	8.68	109.27	105.80
1	AA	792	G	C8-N9-C4	8.67	109.87	106.40
1	AA	958	C	C6-N1-C2	-8.67	116.83	120.30
1	CA	1673	U	C5-C6-N1	-8.67	118.37	122.70
34	BA	665	A	O5'-P-OP1	-8.66	97.90	105.70
1	CA	1780	A	O5'-P-OP1	-8.66	97.91	105.70
1	AA	555	G	N7-C8-N9	8.65	117.43	113.10
1	AA	1249	A	C5-C6-N1	-8.65	113.37	117.70
1	AA	2525	G	O5'-P-OP2	-8.65	97.92	105.70
1	AA	2743	C	N3-C4-N4	-8.64	111.95	118.00
1	CA	1993	U	O5'-P-OP1	-8.64	97.92	105.70
1	AA	1030	A	O5'-P-OP1	-8.63	97.93	105.70
1	CA	527	C	N3-C4-N4	-8.63	111.96	118.00
34	BA	1495	U	O5'-P-OP2	-8.62	97.94	105.70
1	AA	410	U	C5-C6-N1	-8.62	118.39	122.70
1	AA	990	A	C5-C6-N1	-8.62	113.39	117.70
1	AA	2312	G	C8-N9-C4	-8.60	102.96	106.40
1	AA	2608	U	C5-C6-N1	-8.59	118.40	122.70
1	AA	1745	A	C5-C6-N1	-8.58	113.41	117.70
1	CA	1658	C	C6-N1-C2	-8.57	116.87	120.30
1	AA	990	A	O5'-P-OP1	-8.56	98.00	105.70
1	AA	1237	G	C4-C5-N7	-8.55	107.38	110.80
1	CA	1626	G	N1-C6-O6	-8.55	114.77	119.90
1	CA	1644	C	C6-N1-C2	-8.55	116.88	120.30
1	CA	2850	A	O5'-P-OP2	-8.55	98.01	105.70
1	AA	552	C	C2-N3-C4	-8.54	115.63	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	2298	A	N1-C6-N6	8.53	123.72	118.60
34	BA	365	U	C2-N1-C1'	-8.51	107.49	117.70
1	AA	2585	C	C2-N3-C4	-8.50	115.65	119.90
1	AA	2638	C	C6-N1-C2	8.50	123.70	120.30
1	AA	1050	C	N1-C2-O2	-8.49	113.80	118.90
1	AA	2849	G	C8-N9-C4	8.49	109.80	106.40
1	AA	1860	A	O5'-P-OP2	-8.49	98.06	105.70
1	AA	2876	U	C5-C4-O4	8.49	130.99	125.90
1	AA	2041	A	C8-N9-C4	8.48	109.19	105.80
1	AA	978	A	C8-N9-C4	-8.48	102.41	105.80
1	CA	1787	A	O5'-P-OP1	-8.48	98.07	105.70
1	AA	2641	A	N1-C6-N6	8.48	123.69	118.60
1	AA	831	A	O4'-C1'-N9	8.47	114.98	108.20
1	AA	2609	G	C5-C6-O6	-8.47	123.52	128.60
1	AA	630	U	O5'-P-OP1	-8.45	98.09	105.70
1	AA	543	G	O5'-P-OP2	-8.45	98.10	105.70
1	AA	1346	U	C5-C4-O4	-8.43	120.84	125.90
1	CA	772	C	C6-N1-C2	8.43	123.67	120.30
1	AA	1655	A	C5-C6-N6	-8.43	116.96	123.70
1	AA	1664	A	N1-C6-N6	-8.43	113.55	118.60
1	AA	745	C	O5'-P-OP2	-8.42	98.12	105.70
34	DA	34	C	C6-N1-C2	8.41	123.67	120.30
1	AA	2515	A	N1-C2-N3	-8.41	125.09	129.30
1	AA	359	C	C6-N1-C2	8.40	123.66	120.30
1	AA	2299	A	C5-C6-N1	-8.40	113.50	117.70
34	BA	1417	G	N9-C4-C5	-8.40	102.04	105.40
1	AA	1418	U	N3-C4-O4	8.40	125.28	119.40
34	DA	1484	C	C6-N1-C2	8.38	123.65	120.30
1	CA	1272	A	O5'-P-OP2	-8.36	98.18	105.70
34	BA	1417	G	C5-C6-O6	-8.35	123.59	128.60
1	AA	139	A	C2-N3-C4	-8.35	106.43	110.60
1	AA	595	A	O5'-P-OP1	-8.34	98.19	105.70
1	CA	1673	U	C2-N3-C4	-8.34	122.00	127.00
1	CA	1899	G	C5-C6-O6	-8.33	123.60	128.60
1	AA	45	C	O5'-P-OP2	-8.33	98.20	105.70
1	AA	2033	U	N1-C2-N3	8.32	119.89	114.90
34	BA	1502	A	N1-C2-N3	8.31	133.45	129.30
1	AA	1695	C	O5'-P-OP2	8.30	120.67	110.70
1	CA	2503	A	N1-C2-N3	-8.29	125.15	129.30
1	AA	894	U	C5-C6-N1	-8.29	118.55	122.70
1	AA	1694	G	O4'-C1'-N9	-8.29	101.57	108.20
1	AA	1655	A	C8-N9-C4	8.28	109.11	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	2383	G	C4-C5-N7	8.28	114.11	110.80
1	AA	2609	G	C5-C6-N1	8.28	115.64	111.50
1	AA	195	U	C5-C6-N1	-8.27	118.56	122.70
1	AA	1813	C	N3-C4-C5	8.27	125.21	121.90
1	AA	2657	G	C5-C6-O6	-8.27	123.64	128.60
1	AA	1812	C	N3-C4-N4	8.25	123.78	118.00
1	AA	36	G	O5'-P-OP2	-8.25	98.28	105.70
1	AA	2475	C	N3-C4-C5	8.25	125.20	121.90
1	AA	123	G	C5-C6-N1	8.25	115.62	111.50
1	AA	1605	A	N3-C4-N9	-8.24	120.80	127.40
1	AA	978	A	O4'-C1'-N9	8.24	114.79	108.20
1	AA	2054	G	N7-C8-N9	-8.23	108.99	113.10
34	BA	266	G	C5-N7-C8	-8.22	100.19	104.30
1	AA	2466	G	N1-C2-N2	-8.22	108.80	116.20
1	AA	1462	G	O5'-P-OP2	-8.21	98.31	105.70
1	AA	1750	G	O5'-P-OP2	-8.20	98.32	105.70
1	AA	345	G	C4-C5-N7	8.20	114.08	110.80
1	AA	881	C	N1-C2-O2	-8.19	113.98	118.90
1	CA	510	C	O5'-P-OP2	-8.19	98.33	105.70
34	BA	525	C	C6-N1-C2	-8.19	117.03	120.30
1	AA	990	A	C8-N9-C4	-8.18	102.53	105.80
1	AA	2054	G	C5-N7-C8	8.17	108.39	104.30
1	CA	949	C	N1-C2-O2	-8.17	114.00	118.90
1	AA	2101	U	N1-C2-N3	8.16	119.80	114.90
1	AA	2502	G	N9-C4-C5	-8.16	102.13	105.40
2	AB	41	U	C5-C6-N1	-8.16	118.62	122.70
1	AA	2066	C	C2-N3-C4	-8.16	115.82	119.90
1	AA	1011	G	C5-C6-O6	8.16	133.50	128.60
1	AA	1397	C	OP1-P-O3'	8.15	123.14	105.20
1	AA	893	C	C5-C6-N1	-8.15	116.93	121.00
34	DA	245	C	C6-N1-C2	8.14	123.56	120.30
2	AB	101	G	C8-N9-C4	8.14	109.66	106.40
1	AA	194	G	C8-N9-C4	8.14	109.66	106.40
1	AA	2740	G	O5'-P-OP2	-8.13	98.38	105.70
1	AA	1208	G	C4-C5-N7	-8.13	107.55	110.80
1	AA	1848	G	C5-C6-O6	8.13	133.48	128.60
1	CA	1500	G	N1-C6-O6	8.12	124.77	119.90
1	AA	861	C	C2-N3-C4	-8.11	115.84	119.90
1	AA	1605	A	C5-N7-C8	-8.11	99.84	103.90
34	BA	266	G	C4-C5-N7	8.11	114.04	110.80
1	AA	254	A	N7-C8-N9	8.10	117.85	113.80
1	AA	1861	C	N1-C2-O2	-8.10	114.04	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1824	C	O5'-P-OP1	-8.09	98.42	105.70
1	CA	2824	C	C5-C6-N1	-8.09	116.95	121.00
1	CA	2612	C	O5'-P-OP2	-8.09	98.42	105.70
1	AA	1312	G	C5-C6-N1	8.08	115.54	111.50
1	AA	370	A	O5'-P-OP2	-8.08	98.43	105.70
1	AA	496	A	O5'-P-OP1	-8.07	98.43	105.70
1	AA	1745	A	N7-C8-N9	8.07	117.84	113.80
1	CA	330	A	C4-C5-N7	8.07	114.74	110.70
2	AB	86	G	C5-C6-N1	8.07	115.54	111.50
1	AA	978	A	C6-C5-N7	-8.06	126.66	132.30
1	AA	1655	A	N9-C4-C5	-8.06	102.58	105.80
1	AA	2632	C	N3-C4-C5	8.05	125.12	121.90
1	AA	2258	G	C8-N9-C4	8.05	109.62	106.40
34	BA	328	C	O5'-P-OP1	-8.05	98.46	105.70
2	AB	102	A	O5'-P-OP2	8.05	120.36	110.70
1	AA	345	G	N1-C6-O6	8.05	124.73	119.90
1	CA	1807	G	C8-N9-C4	8.04	109.62	106.40
1	AA	2299	A	C5-N7-C8	-8.04	99.88	103.90
1	AA	1744	G	C5-C6-O6	-8.04	123.78	128.60
1	AA	616	G	O5'-P-OP2	-8.03	98.47	105.70
1	AA	55	A	C2-N3-C4	-8.03	106.59	110.60
1	AA	596	G	C5-C6-N1	8.03	115.51	111.50
1	AA	2603	C	C6-N1-C2	8.03	123.51	120.30
1	AA	1728	G	C5-N7-C8	-8.02	100.29	104.30
1	AA	978	A	N3-C4-C5	8.02	132.41	126.80
34	BA	1502	A	N7-C8-N9	8.02	117.81	113.80
1	AA	1356	G	O5'-P-OP1	-8.01	98.49	105.70
1	CA	945	A	N9-C4-C5	-8.01	102.60	105.80
1	CA	1021	A	C5-N7-C8	-8.01	99.89	103.90
1	AA	22	C	N3-C4-N4	-8.00	112.40	118.00
1	CA	568	U	C5-C4-O4	-8.00	121.10	125.90
1	AA	2697	G	C5-C6-N1	8.00	115.50	111.50
1	AA	1234	A	N1-C6-N6	7.98	123.39	118.60
1	AA	2697	G	C6-N1-C2	-7.98	120.31	125.10
1	CA	1966	A	C8-N9-C4	7.98	108.99	105.80
34	BA	514	C	N1-C2-O2	-7.97	114.12	118.90
1	AA	2299	A	N1-C6-N6	7.96	123.38	118.60
1	CA	1812	A	OP1-P-OP2	7.96	131.54	119.60
1	AA	2835	C	C2-N3-C4	-7.96	115.92	119.90
1	AA	2607	G	C5-C6-O6	7.95	133.37	128.60
1	AA	1745	A	C6-C5-N7	-7.95	126.74	132.30
1	CA	330	A	N1-C6-N6	7.94	123.36	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1444	C	N3-C4-C5	7.93	125.07	121.90
1	AA	1342	G	C5-C6-O6	7.92	133.35	128.60
1	CA	1500	G	C5-C6-O6	-7.92	123.84	128.60
1	AA	477	C	C5-C6-N1	-7.91	117.04	121.00
1	CA	2374	C	C6-N1-C2	7.91	123.47	120.30
1	AA	2631	C	C2-N3-C4	-7.91	115.94	119.90
1	AA	2049	G	C4-C5-N7	-7.90	107.64	110.80
1	AA	1181	G	C8-N9-C4	7.90	109.56	106.40
34	BA	550	G	O5'-P-OP1	-7.90	98.59	105.70
1	AA	2251	G	C5-C6-O6	-7.90	123.86	128.60
1	CA	494	G	C5-C6-N1	-7.89	107.55	111.50
1	CA	807	U	C5-C4-O4	-7.89	121.16	125.90
1	CA	2589	A	N1-C2-N3	7.89	133.25	129.30
1	CA	2253	G	N1-C6-O6	7.89	124.63	119.90
1	AA	2515	A	C2-N3-C4	7.88	114.54	110.60
1	CA	141	A	C6-C5-N7	-7.88	126.78	132.30
1	CA	1661	G	C8-N9-C4	7.88	109.55	106.40
1	AA	2290	A	OP1-P-OP2	-7.88	107.78	119.60
2	AB	7	G	C5-C6-O6	-7.88	123.87	128.60
1	CA	494	G	C2-N3-C4	-7.88	107.96	111.90
1	AA	1539	C	N3-C2-O2	-7.87	116.39	121.90
1	AA	1009	C	N3-C2-O2	-7.87	116.39	121.90
1	AA	2052	A	N1-C6-N6	7.87	123.32	118.60
1	CA	2827	C	C6-N1-C2	7.86	123.44	120.30
1	AA	1812	C	C5-C4-N4	-7.86	114.70	120.20
1	AA	472	G	C2-N3-C4	7.85	115.82	111.90
1	AA	2386	C	C5-C6-N1	-7.85	117.08	121.00
1	CA	1698	A	N7-C8-N9	7.83	117.72	113.80
1	AA	2019	G	O5'-P-OP2	-7.83	98.65	105.70
1	AA	1232	G	C4-C5-C6	-7.82	114.11	118.80
1	CA	1688	U	O5'-P-OP2	-7.81	98.67	105.70
1	CA	847	U	C6-N1-C1'	7.80	132.13	121.20
2	AB	90	A	C8-N9-C4	7.79	108.92	105.80
1	AA	2788	A	N1-C6-N6	-7.79	113.93	118.60
34	BA	1417	G	C5-C6-N1	7.79	115.39	111.50
1	AA	194	G	N1-C6-O6	7.79	124.57	119.90
34	BA	786	G	C5-C6-O6	7.79	133.27	128.60
1	AA	779	C	N1-C2-O2	-7.79	114.23	118.90
1	CA	806	C	N3-C4-C5	7.78	125.01	121.90
34	BA	1520	G	C5-C6-O6	-7.77	123.94	128.60
1	AA	1240	G	C2-N3-C4	7.77	115.79	111.90
1	AA	2838	C	C6-N1-C2	7.77	123.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	851	A	C2-N3-C4	-7.77	106.72	110.60
1	AA	1743	G	O5'-P-OP2	-7.77	98.71	105.70
1	AA	1625	U	O5'-P-OP2	-7.76	98.71	105.70
1	AA	2802	C	C2-N1-C1'	-7.76	110.26	118.80
34	DA	689	C	C6-N1-C2	-7.75	117.20	120.30
1	CA	915	C	N3-C2-O2	-7.75	116.48	121.90
1	AA	742	G	N1-C6-O6	-7.74	115.26	119.90
1	AA	2727	G	O5'-P-OP2	-7.73	98.74	105.70
1	CA	955	C	N3-C4-C5	-7.73	118.81	121.90
1	AA	1667	U	C6-N1-C2	7.71	125.63	121.00
1	AA	2858	G	O4'-C1'-N9	7.71	114.37	108.20
1	AA	1418	U	C5-C4-O4	-7.70	121.28	125.90
1	CA	2503	A	C2-N3-C4	7.70	114.45	110.60
1	AA	2632	C	C2-N3-C4	-7.70	116.05	119.90
1	AA	1053	C	N3-C4-C5	7.69	124.98	121.90
1	CA	1698	A	C5-C6-N1	-7.69	113.86	117.70
34	BA	1524	C	N1-C2-O2	-7.69	114.29	118.90
1	CA	12	U	C2-N1-C1'	7.69	126.93	117.70
1	CA	2441	C	O5'-P-OP1	-7.69	98.78	105.70
1	AA	176	G	C6-C5-N7	-7.68	125.79	130.40
56	BW	74	C	N1-C2-O2	7.68	123.51	118.90
1	AA	188	A	O5'-P-OP2	-7.68	98.79	105.70
1	AA	2342	G	C5-C6-O6	-7.68	123.99	128.60
1	AA	856	G	N1-C6-O6	-7.67	115.30	119.90
1	CA	2286	A	C2-N3-C4	-7.67	106.76	110.60
1	AA	724	A	N1-C2-N3	7.67	133.13	129.30
34	BA	1499	A	N1-C6-N6	7.67	123.20	118.60
1	AA	866	A	O5'-P-OP2	-7.66	98.80	105.70
1	AA	1299	A	C8-N9-C4	7.66	108.86	105.80
1	AA	1741	C	C2-N3-C4	-7.66	116.07	119.90
1	AA	254	A	C4-C5-C6	7.66	120.83	117.00
1	AA	894	U	N1-C2-N3	7.66	119.49	114.90
1	CA	530	G	C4-C5-N7	7.65	113.86	110.80
1	AA	2734	A	C8-N9-C4	7.65	108.86	105.80
1	AA	2162	C	N1-C2-O2	7.64	123.49	118.90
1	AA	1033	G	C4-C5-N7	-7.64	107.74	110.80
58	BY	74	C	C6-N1-C2	7.64	123.36	120.30
1	AA	2510	C	O5'-P-OP1	7.63	119.86	110.70
1	AA	893	C	C6-N1-C2	7.63	123.35	120.30
1	AA	906	G	C8-N9-C4	7.62	109.45	106.40
1	AA	2641	A	O4'-C1'-N9	7.62	114.29	108.20
1	AA	1645	C	C2-N3-C4	-7.61	116.09	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	176	G	C5-C6-O6	-7.60	124.04	128.60
1	AA	595	A	C8-N9-C4	-7.60	102.76	105.80
1	AA	285	U	O4'-C1'-N1	7.59	114.28	108.20
1	AA	1816	A	C8-N9-C4	-7.59	102.76	105.80
1	AA	2451	A	O5'-P-OP2	-7.59	98.87	105.70
1	AA	1721	G	C4-C5-N7	7.59	113.84	110.80
1	AA	2034	G	C4-C5-N7	7.59	113.83	110.80
34	BA	1113	C	C6-N1-C2	-7.57	117.27	120.30
1	CA	1210	A	P-O3'-C3'	7.57	128.78	119.70
1	AA	254	A	N1-C2-N3	7.56	133.08	129.30
1	CA	2689	U	P-O3'-C3'	7.56	128.78	119.70
1	AA	1231	G	C5-C6-O6	-7.56	124.06	128.60
1	AA	1243	U	C2-N3-C4	-7.56	122.46	127.00
1	AA	2533	C	C6-N1-C2	7.56	123.32	120.30
34	BA	764	C	N1-C2-O2	7.56	123.43	118.90
1	AA	542	C	N3-C4-C5	7.55	124.92	121.90
1	AA	872	C	C5-C6-N1	-7.55	117.22	121.00
1	AA	2535	G	C5-C6-O6	-7.55	124.07	128.60
1	AA	2238	C	C5-C6-N1	-7.55	117.22	121.00
1	AA	2509	A	N1-C6-N6	-7.54	114.07	118.60
34	BA	1417	G	C4-C5-N7	7.54	113.82	110.80
1	AA	2392	C	C2-N3-C4	-7.53	116.14	119.90
1	CA	265	A	C5-N7-C8	-7.52	100.14	103.90
1	CA	1692	U	N1-C2-O2	-7.52	117.54	122.80
1	AA	2559	U	C2-N3-C4	-7.51	122.49	127.00
1	CA	1826	G	C4-C5-N7	-7.51	107.80	110.80
1	CA	2289	G	O5'-P-OP2	-7.50	98.94	105.70
1	AA	122	G	O5'-P-OP2	-7.50	98.95	105.70
1	AA	1986	G	O5'-P-OP1	-7.50	98.95	105.70
34	BA	841	U	C5-C6-N1	7.50	126.45	122.70
1	AA	1683	C	C5-C6-N1	-7.50	117.25	121.00
1	AA	553	A	N3-C4-C5	7.50	132.05	126.80
1	AA	1151	U	OP1-P-OP2	7.50	130.84	119.60
1	AA	2001	C	N1-C2-O2	-7.49	114.40	118.90
1	AA	139	A	O4'-C1'-N9	7.48	114.18	108.20
1	AA	1719	C	N1-C2-O2	-7.47	114.42	118.90
1	AA	1374	G	C6-N1-C2	-7.45	120.63	125.10
1	AA	1255	A	P-O3'-C3'	7.45	128.64	119.70
1	AA	1843	A	N1-C6-N6	-7.45	114.13	118.60
1	AA	2049	G	N3-C4-C5	-7.45	124.87	128.60
1	AA	2561	G	C4-C5-N7	7.45	113.78	110.80
1	AA	2597	U	N3-C2-O2	-7.45	116.98	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	2636	G	C6-N1-C2	-7.45	120.63	125.10
1	CA	1142(A)	A	N3-C4-C5	7.45	132.01	126.80
1	AA	2250	G	OP1-P-OP2	7.45	130.77	119.60
1	AA	2294	G	O5'-P-OP1	-7.44	99.00	105.70
1	AA	2581	G	N1-C6-O6	-7.44	115.44	119.90
1	AA	1031	C	C6-N1-C2	-7.43	117.33	120.30
1	AA	859	C	C2-N3-C4	-7.43	116.18	119.90
34	BA	1501	C	N1-C2-O2	-7.43	114.44	118.90
1	CA	2585	U	N3-C4-O4	-7.43	114.20	119.40
1	AA	1788	U	C6-N1-C2	7.43	125.45	121.00
1	AA	1745	A	O4'-C1'-N9	7.42	114.14	108.20
1	AA	2039	U	N3-C2-O2	-7.42	117.00	122.20
1	CA	588	U	O5'-P-OP2	-7.42	99.02	105.70
1	CA	1901	A	C2-N3-C4	7.42	114.31	110.60
1	AA	637	U	N3-C2-O2	-7.41	117.01	122.20
1	AA	1299	A	C5-C6-N1	7.41	121.41	117.70
1	AA	370	A	C8-N9-C4	7.41	108.76	105.80
1	AA	1920	U	N3-C4-O4	-7.41	114.22	119.40
1	AA	50	G	N3-C4-C5	-7.40	124.90	128.60
1	AA	790	G	C5-C6-O6	7.40	133.04	128.60
1	AA	1291	G	C5-C6-O6	7.40	133.04	128.60
1	CA	752	A	P-O3'-C3'	7.40	128.57	119.70
1	AA	1961	U	C4-C5-C6	-7.39	115.27	119.70
1	AA	197	C	C4-C5-C6	7.39	121.09	117.40
1	AA	1660	A	O5'-P-OP1	-7.39	99.05	105.70
1	CA	34	C	C2-N1-C1'	7.38	126.92	118.80
1	AA	2466	G	N1-C6-O6	-7.38	115.47	119.90
1	AA	1264	G	C2-N3-C4	-7.38	108.21	111.90
1	AA	2451	A	C5-N7-C8	-7.38	100.21	103.90
1	AA	1605	A	N1-C6-N6	7.38	123.03	118.60
1	CA	2238	G	OP1-P-OP2	7.37	130.66	119.60
1	AA	872	C	C6-N1-C2	7.37	123.25	120.30
1	AA	69	G	N1-C6-O6	-7.37	115.48	119.90
1	AA	2377	G	C5-C6-N1	7.37	115.19	111.50
1	AA	98	U	C5-C4-O4	7.37	130.32	125.90
1	AA	990	A	O4'-C1'-N9	7.36	114.08	108.20
1	AA	1344	C	N3-C4-C5	7.35	124.84	121.90
1	AA	1745	A	N3-C4-N9	-7.35	121.52	127.40
1	AA	1243	U	N1-C2-N3	7.35	119.31	114.90
1	AA	2657	G	C5-N7-C8	-7.35	100.63	104.30
1	AA	1721	G	C5-C6-O6	-7.34	124.19	128.60
1	CA	1673	U	C2-N1-C1'	-7.34	108.89	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	961	C	C6-N1-C2	-7.34	117.36	120.30
1	AA	207	A	C2-N3-C4	-7.33	106.93	110.60
1	AA	978	A	C5-C6-N1	-7.33	114.03	117.70
1	CA	265	A	N7-C8-N9	7.33	117.47	113.80
1	AA	2571	C	N3-C2-O2	-7.33	116.77	121.90
34	BA	1502	A	C2-N3-C4	-7.32	106.94	110.60
34	BA	736	C	N3-C4-C5	7.32	124.83	121.90
1	AA	2831	A	C2-N3-C4	-7.32	106.94	110.60
1	AA	254	A	C5-C6-N1	-7.31	114.04	117.70
1	CA	2229	C	C6-N1-C2	7.31	123.22	120.30
1	AA	1766	G	C4-C5-N7	7.31	113.72	110.80
34	BA	365	U	N1-C2-N3	7.30	119.28	114.90
1	AA	723	A	C8-N9-C4	7.29	108.72	105.80
1	CA	2085	C	N1-C2-O2	-7.29	114.52	118.90
1	AA	2743	C	N3-C4-C5	7.29	124.82	121.90
1	AA	1874	C	N3-C4-C5	7.29	124.82	121.90
1	AA	2620	G	C5-C6-N1	7.29	115.14	111.50
2	AB	7	G	C4-C5-N7	7.29	113.71	110.80
1	CA	195	A	P-O3'-C3'	7.29	128.44	119.70
1	AA	1920	U	N1-C2-O2	7.28	127.90	122.80
1	AA	1298	G	OP2-P-O3'	7.28	121.22	105.20
1	AA	199	C	N3-C4-N4	-7.28	112.91	118.00
1	AA	645	G	C8-N9-C4	7.28	109.31	106.40
1	AA	1426	G	C8-N9-C4	7.28	109.31	106.40
34	BA	1502	A	O5'-P-OP2	-7.27	99.15	105.70
1	AA	1155	C	C5-C6-N1	7.27	124.63	121.00
1	CA	1202	C	C6-N1-C2	7.27	123.21	120.30
1	AA	906	G	N3-C4-C5	7.26	132.23	128.60
1	AA	2531	U	C5-C6-N1	-7.26	119.07	122.70
1	AA	2751	A	C8-N9-C4	7.26	108.70	105.80
1	CA	2207	G	N1-C6-O6	7.25	124.25	119.90
1	AA	874	U	C6-N1-C2	7.25	125.35	121.00
1	AA	1009	C	C6-N1-C2	-7.25	117.40	120.30
1	AA	194	G	N9-C4-C5	-7.24	102.50	105.40
1	AA	354	A	C4-C5-N7	7.24	114.32	110.70
1	CA	2504	U	O5'-P-OP1	-7.24	99.19	105.70
1	AA	893	C	C2-N3-C4	-7.23	116.28	119.90
1	CA	1200	C	C5-C6-N1	-7.23	117.38	121.00
1	AA	2641	A	N9-C1'-C2'	7.23	123.39	114.00
1	CA	1212	G	N3-C4-N9	7.23	130.34	126.00
1	AA	2464	C	N3-C4-C5	7.22	124.79	121.90
1	AA	2641	A	C4-N9-C1'	7.22	139.30	126.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1204	A	C5-N7-C8	-7.22	100.29	103.90
1	AA	2732	G	C5-C6-O6	-7.22	124.27	128.60
1	CA	1947	C	C6-N1-C2	7.22	123.19	120.30
31	A7	39	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	AA	1204	C	C5-C6-N1	-7.21	117.39	121.00
1	AA	2468	C	C6-N1-C2	7.21	123.19	120.30
1	AA	404	C	C6-N1-C2	7.21	123.18	120.30
34	BA	1195	C	C6-N1-C2	-7.21	117.42	120.30
1	AA	714	U	C5-C6-N1	-7.21	119.10	122.70
34	BA	266	G	N7-C8-N9	7.21	116.70	113.10
1	CA	1626	G	N9-C4-C5	7.20	108.28	105.40
1	CA	2685	G	N1-C6-O6	-7.20	115.58	119.90
1	AA	1154	U	N1-C2-O2	7.20	127.84	122.80
1	AA	128	C	O5'-P-OP1	-7.20	99.22	105.70
1	AA	2506	G	C5-C6-O6	7.20	132.92	128.60
1	CA	1204	A	C4-C5-N7	7.20	114.30	110.70
1	AA	907	U	O5'-P-OP2	-7.19	99.22	105.70
1	AA	69	G	N3-C2-N2	7.19	124.94	119.90
1	AA	1691	C	N3-C2-O2	-7.19	116.87	121.90
1	AA	2451	A	N7-C8-N9	7.19	117.39	113.80
1	AA	254	A	O4'-C1'-N9	7.19	113.95	108.20
1	AA	1001	G	N3-C2-N2	-7.19	114.87	119.90
1	AA	1827	U	OP1-P-OP2	7.18	130.37	119.60
1	CA	2708	G	N7-C8-N9	-7.18	109.51	113.10
1	AA	1821	C	P-O3'-C3'	7.18	128.31	119.70
1	CA	847	U	C5-C6-N1	-7.18	119.11	122.70
1	AA	1723	A	N7-C8-N9	-7.17	110.21	113.80
1	AA	1827	U	C6-N1-C2	7.17	125.30	121.00
1	CA	945	A	C6-C5-N7	-7.17	127.28	132.30
2	AB	79	C	C6-N1-C2	-7.16	117.44	120.30
1	AA	197	C	C5-C6-N1	-7.16	117.42	121.00
1	AA	2331	G	C2-N3-C4	-7.16	108.32	111.90
1	AA	637	U	C5-C4-O4	7.15	130.19	125.90
1	AA	123	G	C6-N1-C2	-7.15	120.81	125.10
1	AA	215	G	O4'-C1'-N9	7.15	113.92	108.20
1	AA	2641	A	C4-C5-C6	7.14	120.57	117.00
34	BA	365	U	C4-C5-C6	7.14	123.99	119.70
1	AA	1717	C	N3-C4-C5	-7.12	119.05	121.90
1	AA	2014	G	C5-C6-N1	7.12	115.06	111.50
1	CA	2523	G	C6-C5-N7	-7.12	126.13	130.40
1	AA	1038	C	C5-C4-N4	-7.12	115.22	120.20
1	CA	1604	C	N3-C4-C5	7.12	124.75	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	933	A	N7-C8-N9	7.11	117.36	113.80
1	CA	527	C	C5-C4-N4	7.11	125.18	120.20
1	AA	1645	C	N1-C2-O2	-7.11	114.64	118.90
1	CA	784	A	N1-C6-N6	-7.11	114.33	118.60
1	AA	1543	U	C5-C4-O4	7.10	130.16	125.90
1	CA	1899	G	N1-C6-O6	7.10	124.16	119.90
34	DA	821	G	O5'-P-OP1	-7.10	99.31	105.70
1	AA	12	U	C2-N1-C1'	7.10	126.22	117.70
1	AA	471	C	C4-C5-C6	7.09	120.95	117.40
1	AA	1249	A	C6-C5-N7	-7.09	127.34	132.30
1	CA	1781	C	N3-C4-N4	-7.09	113.04	118.00
1	AA	1812	C	N3-C2-O2	7.09	126.86	121.90
1	AA	2049	G	C5-C6-O6	7.09	132.85	128.60
1	AA	216	A	N1-C2-N3	7.08	132.84	129.30
1	AA	1605	A	C4-C5-N7	7.08	114.24	110.70
1	CA	1658	C	N3-C4-C5	-7.08	119.07	121.90
1	CA	474	G	O5'-P-OP2	-7.08	99.33	105.70
1	CA	393	C	N1-C2-O2	-7.08	114.65	118.90
1	AA	2849	G	N3-C2-N2	7.07	124.85	119.90
1	AA	354	A	C6-N1-C2	7.07	122.84	118.60
1	AA	990	A	C4-N9-C1'	7.07	139.02	126.30
1	CA	528	A	C5-N7-C8	-7.07	100.37	103.90
34	BA	365	U	C6-N1-C1'	7.06	131.08	121.20
1	AA	954	C	N1-C2-O2	-7.05	114.67	118.90
1	CA	1204	A	O4'-C1'-N9	7.05	113.84	108.20
1	CA	2552	U	N3-C4-O4	-7.05	114.47	119.40
1	AA	2072	C	N3-C4-C5	-7.04	119.08	121.90
1	CA	2824	C	C2-N3-C4	-7.04	116.38	119.90
1	AA	2838	C	N3-C4-C5	7.03	124.71	121.90
1	CA	2683	C	N3-C4-C5	-7.03	119.09	121.90
1	AA	2631	C	C4-C5-C6	7.02	120.91	117.40
1	CA	1783	A	OP1-P-OP2	-7.02	109.07	119.60
1	AA	720	C	N1-C2-O2	7.02	123.11	118.90
1	AA	1422	C	N3-C4-C5	7.02	124.71	121.90
1	AA	2597	U	N1-C2-O2	7.01	127.71	122.80
1	AA	2608	U	C2-N3-C4	-7.01	122.79	127.00
1	AA	1861	C	N3-C2-O2	7.01	126.81	121.90
1	AA	980	C	C5-C6-N1	-7.01	117.50	121.00
1	AA	853	C	N3-C4-C5	7.01	124.70	121.90
1	AA	2331	G	O4'-C1'-N9	7.01	113.81	108.20
1	AA	2111	U	C5-C6-N1	-7.00	119.20	122.70
1	AA	1456	G	C5-C6-O6	-7.00	124.40	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	DA	898	G	C5-C6-O6	-7.00	124.40	128.60
1	AA	851	A	N1-C6-N6	7.00	122.80	118.60
1	AA	993	G	O5'-P-OP1	-7.00	99.40	105.70
1	AA	2162	C	C6-N1-C2	-7.00	117.50	120.30
1	AA	792	G	N9-C4-C5	-6.99	102.60	105.40
1	CA	1142(A)	A	C5-N7-C8	-6.99	100.40	103.90
34	BA	866	C	N1-C2-O2	-6.99	114.71	118.90
1	AA	2641	A	N7-C8-N9	6.98	117.29	113.80
1	AA	785	G	C5-N7-C8	-6.98	100.81	104.30
1	AA	2515	A	N9-C4-C5	-6.98	103.01	105.80
1	AA	534	C	C6-N1-C2	6.98	123.09	120.30
34	BA	913	A	P-O3'-C3'	6.98	128.08	119.70
1	AA	139	A	C6-C5-N7	-6.98	127.42	132.30
1	AA	1011	G	C2-N3-C4	-6.98	108.41	111.90
1	AA	2502	G	C8-N9-C4	6.98	109.19	106.40
1	AA	2722	C	O5'-P-OP1	-6.98	99.42	105.70
1	AA	995	G	C5-N7-C8	-6.98	100.81	104.30
1	AA	1745	A	N1-C6-N6	6.98	122.79	118.60
1	AA	2684	G	OP2-P-O3'	6.98	120.55	105.20
1	AA	1179	U	C5-C6-N1	-6.97	119.21	122.70
1	AA	354	A	N1-C2-N3	6.97	132.79	129.30
1	AA	978	A	N1-C6-N6	6.97	122.78	118.60
1	AA	2632	C	C5-C6-N1	-6.97	117.52	121.00
1	AA	194	G	C2-N3-C4	-6.97	108.42	111.90
1	AA	1788	U	C5-C6-N1	-6.97	119.22	122.70
1	AA	2441	G	O5'-P-OP1	6.97	119.06	110.70
2	AB	101	G	N7-C8-N9	-6.97	109.62	113.10
1	AA	1237	G	C8-N9-C4	6.96	109.19	106.40
1	AA	2060	G	C5-C6-O6	6.96	132.78	128.60
1	AA	176	G	N3-C4-N9	6.96	130.18	126.00
1	AA	1244	U	C5-C6-N1	-6.96	119.22	122.70
1	CA	1664	A	C8-N9-C4	-6.96	103.02	105.80
1	AA	2605	U	N3-C4-O4	-6.95	114.53	119.40
1	AA	980	C	C2-N3-C4	-6.95	116.42	119.90
1	AA	2298	A	C5-C6-N1	-6.95	114.22	117.70
1	AA	2405	A	C2-N3-C4	-6.95	107.12	110.60
1	CA	1296	G	N1-C6-O6	-6.95	115.73	119.90
34	DA	754	C	C2-N1-C1'	6.95	126.44	118.80
1	AA	2528	G	C5-C6-O6	6.95	132.77	128.60
1	AA	553	A	N3-C4-N9	-6.95	121.84	127.40
1	AA	724	A	C4-C5-C6	6.95	120.47	117.00
1	AA	1023	G	O5'-P-OP2	-6.94	99.45	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	798	A	N1-C6-N6	6.94	122.77	118.60
1	AA	616	G	C4-C5-N7	-6.94	108.03	110.80
1	AA	2040	G	C5-C6-N1	6.94	114.97	111.50
1	CA	794	G	N3-C2-N2	6.94	124.75	119.90
1	AA	912	C	N1-C2-O2	-6.93	114.74	118.90
1	AA	790	G	N1-C6-O6	-6.93	115.74	119.90
34	BA	1442	G	N7-C8-N9	6.93	116.56	113.10
1	CA	933	A	C5-N7-C8	-6.93	100.44	103.90
1	CA	1947	C	N3-C4-C5	6.93	124.67	121.90
1	AA	1254	G	C5-C6-N1	6.93	114.96	111.50
1	AA	1067	A	C4-C5-N7	6.92	114.16	110.70
21	CX	57	LEU	CA-CB-CG	6.92	131.23	115.30
1	AA	2299	A	C4-C5-N7	6.92	114.16	110.70
1	AA	477	C	C6-N1-C2	6.92	123.07	120.30
1	AA	555	G	C5-C6-N1	-6.92	108.04	111.50
1	AA	1966	U	N3-C4-O4	-6.91	114.56	119.40
1	AA	1755	C	C6-N1-C2	6.91	123.06	120.30
1	AA	1665	G	N3-C2-N2	6.91	124.73	119.90
1	AA	500	G	C8-N9-C4	-6.90	103.64	106.40
1	AA	1965	U	C5-C6-N1	-6.90	119.25	122.70
1	AA	470	C	C5-C6-N1	-6.90	117.55	121.00
1	AA	511	C	O5'-P-OP2	6.90	118.98	110.70
1	CA	2286	A	C6-C5-N7	-6.89	127.47	132.30
1	AA	1848	G	N3-C2-N2	6.89	124.72	119.90
1	AA	2264	G	N9-C4-C5	6.89	108.15	105.40
1	AA	2329	C	C6-N1-C2	-6.89	117.55	120.30
1	AA	2889	C	N3-C2-O2	-6.88	117.08	121.90
1	AA	649	C	C2-N3-C4	-6.88	116.46	119.90
1	AA	2077	C	C6-N1-C2	6.88	123.05	120.30
34	BA	345	C	C6-N1-C2	-6.88	117.55	120.30
34	DA	1154	G	C4-N9-C1'	6.87	135.43	126.50
1	AA	2448	G	N1-C6-O6	-6.87	115.78	119.90
1	AA	2460	A	N9-C4-C5	6.87	108.55	105.80
1	AA	1026	A	N9-C4-C5	-6.87	103.05	105.80
1	AA	2423	A	C8-N9-C4	6.86	108.54	105.80
1	CA	2536	G	N1-C6-O6	6.86	124.01	119.90
2	CB	30	C	N3-C4-C5	-6.86	119.16	121.90
1	AA	2571	C	N3-C4-N4	-6.85	113.20	118.00
1	AA	2613	C	OP2-P-O3'	6.85	120.28	105.20
34	BA	247	G	N3-C4-C5	-6.85	125.17	128.60
1	AA	1543	U	N3-C4-O4	-6.85	114.60	119.40
1	CA	334	C	C6-N1-C2	6.85	123.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1828	G	O5'-P-OP1	-6.85	99.54	105.70
1	AA	720	C	N3-C2-O2	-6.85	117.11	121.90
1	AA	1374	G	N3-C4-N9	6.85	130.11	126.00
1	AA	2046	G	N7-C8-N9	-6.85	109.68	113.10
1	AA	2667	G	O4'-C1'-N9	6.85	113.68	108.20
1	CA	1021	A	N3-C4-C5	6.85	131.59	126.80
1	AA	407	U	C5-C6-N1	-6.84	119.28	122.70
34	BA	910	C	C6-N1-C2	6.84	123.04	120.30
1	AA	405	C	N1-C2-O2	-6.84	114.80	118.90
34	BA	1401	G	N3-C2-N2	-6.84	115.11	119.90
1	AA	1273	G	C4-C5-N7	-6.84	108.06	110.80
1	AA	1667	U	C5-C6-N1	-6.84	119.28	122.70
1	CA	614	U	N3-C4-O4	-6.84	114.61	119.40
34	DA	770	C	O5'-P-OP2	-6.83	99.55	105.70
1	CA	39	C	C6-N1-C2	6.83	123.03	120.30
1	CA	1425	G	C6-C5-N7	-6.83	126.30	130.40
34	BA	1502	A	C5-N7-C8	-6.83	100.48	103.90
1	AA	345	G	N9-C4-C5	-6.83	102.67	105.40
1	AA	1190	G	N1-C6-O6	-6.83	115.80	119.90
1	AA	2454	C	C5-C6-N1	-6.83	117.59	121.00
1	AA	2512	U	C5-C4-O4	-6.83	121.80	125.90
1	AA	2745	G	N9-C4-C5	6.83	108.13	105.40
1	AA	240	A	C8-N9-C4	6.83	108.53	105.80
1	AA	1643	A	C8-N9-C4	6.83	108.53	105.80
1	AA	2600	G	C8-N9-C4	6.82	109.13	106.40
21	AX	57	LEU	CA-CB-CG	6.82	130.99	115.30
1	AA	1369	U	N3-C4-C5	6.82	118.69	114.60
34	BA	1520	G	O5'-P-OP2	-6.82	99.56	105.70
34	DA	245	C	C5-C6-N1	-6.82	117.59	121.00
1	AA	1184	G	O5'-P-OP1	6.82	118.88	110.70
1	AA	2801	C	N1-C2-O2	-6.82	114.81	118.90
1	CA	1811	G	N1-C6-O6	-6.82	115.81	119.90
1	AA	1001	G	C5-C6-N1	-6.81	108.09	111.50
1	AA	2492	C	N3-C4-C5	-6.81	119.17	121.90
1	CA	751	A	C8-N9-C4	6.81	108.53	105.80
1	CA	1669	A	C4-C5-C6	6.81	120.41	117.00
1	CA	933	A	O4'-C1'-N9	6.81	113.65	108.20
34	DA	567	G	O5'-P-OP1	-6.81	99.57	105.70
1	AA	616	G	C5-C6-O6	6.81	132.68	128.60
1	CA	1437	C	C6-N1-C2	-6.81	117.58	120.30
1	AA	993	G	C8-N9-C4	6.80	109.12	106.40
1	AA	1812	C	N1-C2-N3	-6.80	114.44	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1199	C	N1-C2-O2	-6.80	114.82	118.90
1	AA	1474	C	O5'-P-OP1	-6.80	99.58	105.70
1	AA	1992	A	N1-C6-N6	6.80	122.68	118.60
1	AA	860	U	N3-C4-O4	-6.80	114.64	119.40
1	CA	1976	U	N1-C2-N3	6.80	118.98	114.90
1	AA	500	G	N7-C8-N9	6.80	116.50	113.10
1	AA	706	C	C5-C6-N1	-6.79	117.60	121.00
1	CA	705	A	N1-C6-N6	6.79	122.68	118.60
1	CA	1654	A	O5'-P-OP2	6.79	118.85	110.70
1	AA	1316	C	C6-N1-C2	6.79	123.02	120.30
34	BA	219	C	C6-N1-C2	-6.79	117.58	120.30
1	CA	1763	G	C8-N9-C4	6.79	109.12	106.40
1	CA	941	A	C2-N3-C4	-6.79	107.20	110.60
1	AA	2636	G	C5-C6-O6	-6.78	124.53	128.60
1	AA	873	U	C5-C6-N1	-6.78	119.31	122.70
1	AA	1845	G	N1-C6-O6	6.78	123.97	119.90
1	CA	2818	G	C8-N9-C4	6.78	109.11	106.40
37	DD	188	LEU	CA-CB-CG	6.78	130.89	115.30
1	AA	1210	G	C5-C6-O6	6.78	132.66	128.60
1	AA	1232	G	N3-C2-N2	6.78	124.64	119.90
1	AA	2441	G	O5'-P-OP2	-6.77	99.60	105.70
1	CA	2609	U	O5'-P-OP2	-6.77	99.60	105.70
34	DA	1502	A	C6-C5-N7	-6.77	127.56	132.30
1	AA	585	U	N3-C4-C5	6.77	118.66	114.60
1	AA	1014	U	N3-C4-C5	6.77	118.66	114.60
1	AA	1346	U	N3-C4-O4	6.77	124.14	119.40
1	CA	460	A	N1-C2-N3	6.77	132.68	129.30
1	AA	1829	U	N3-C4-C5	6.76	118.66	114.60
2	AB	50	G	O5'-P-OP2	-6.76	99.61	105.70
1	AA	726	C	N3-C4-N4	-6.76	113.27	118.00
1	AA	1232	G	C5-C6-N1	6.76	114.88	111.50
1	AA	1766	G	C5-N7-C8	-6.76	100.92	104.30
1	AA	2220	A	OP1-P-O3'	6.76	120.08	105.20
1	AA	69	G	N1-C2-N2	-6.76	110.12	116.20
1	AA	2354	C	N1-C2-O2	-6.76	114.84	118.90
1	AA	859	C	C5-C6-N1	-6.75	117.62	121.00
1	AA	1757	C	C6-N1-C2	6.75	123.00	120.30
1	AA	1261	G	C5-C6-O6	-6.75	124.55	128.60
1	AA	1968	U	N1-C2-N3	6.75	118.95	114.90
34	BA	1442	G	C5-N7-C8	-6.75	100.93	104.30
34	DA	64	G	N1-C6-O6	6.74	123.95	119.90
1	AA	555	G	C4-C5-N7	6.74	113.50	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	2028	C	C2-N3-C4	-6.74	116.53	119.90
1	AA	2298	A	C4-N9-C1'	6.74	138.43	126.30
1	AA	191	U	C6-N1-C2	6.74	125.04	121.00
1	AA	2703	C	C6-N1-C2	6.74	122.99	120.30
1	CA	1652	A	C8-N9-C4	6.74	108.49	105.80
1	CA	672	C	C6-N1-C2	6.73	122.99	120.30
1	CA	2490	G	C4-C5-N7	6.73	113.49	110.80
1	AA	254	A	C8-N9-C4	-6.73	103.11	105.80
1	CA	2626	C	N3-C2-O2	6.73	126.61	121.90
1	AA	978	A	N3-C4-N9	-6.73	122.02	127.40
34	BA	1201	A	P-O3'-C3'	6.72	127.77	119.70
1	AA	1728	G	C6-C5-N7	-6.72	126.37	130.40
34	BA	1030(B)	C	C2-N1-C1'	6.71	126.19	118.80
1	AA	2458	G	C8-N9-C4	-6.71	103.72	106.40
1	AA	2500	A	C8-N9-C4	6.71	108.48	105.80
1	AA	2760	G	C5-C6-O6	-6.71	124.57	128.60
1	CA	1287	A	C8-N9-C4	-6.71	103.11	105.80
1	AA	122	G	N1-C6-O6	6.71	123.93	119.90
1	AA	1411	A	C8-N9-C4	6.71	108.48	105.80
1	CA	82	G	C8-N9-C4	6.71	109.08	106.40
34	BA	1407	C	C4-C5-C6	-6.70	114.05	117.40
34	BA	792	A	C8-N9-C4	6.70	108.48	105.80
1	CA	1021	A	N3-C4-N9	-6.70	122.04	127.40
1	CA	1278	A	C2-N3-C4	-6.70	107.25	110.60
1	AA	2641	A	C5-N7-C8	-6.70	100.55	103.90
1	AA	999	G	C5-C6-O6	6.70	132.62	128.60
1	AA	735	U	C5-C6-N1	-6.70	119.35	122.70
1	AA	2393	C	C2-N3-C4	-6.70	116.55	119.90
1	AA	2471	A	C2-N3-C4	6.70	113.95	110.60
1	CA	205	G	OP1-P-OP2	6.70	129.64	119.60
1	CA	2253	G	C5-C6-O6	-6.70	124.58	128.60
1	AA	187	C	O5'-P-OP2	-6.69	99.68	105.70
1	AA	1255	A	OP2-P-O3'	6.69	119.91	105.20
1	CA	962	G	C2-N3-C4	-6.69	108.56	111.90
1	CA	2347	C	N1-C2-O2	6.69	122.91	118.90
1	AA	792	G	N7-C8-N9	-6.68	109.76	113.10
1	AA	999	G	N1-C6-O6	-6.68	115.89	119.90
1	AA	2265	G	N9-C4-C5	-6.68	102.73	105.40
1	AA	2610	A	OP2-P-O3'	6.68	119.91	105.20
34	BA	365	U	N3-C4-O4	-6.68	114.72	119.40
11	AN	65	LYS	CD-CE-NZ	6.68	127.06	111.70
34	DA	509	A	C8-N9-C4	-6.68	103.13	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1698	A	C4-C5-N7	6.68	114.04	110.70
1	AA	2096	U	N3-C4-O4	6.68	124.07	119.40
1	CA	460	A	N1-C6-N6	6.68	122.61	118.60
1	CA	1253	A	N1-C6-N6	-6.68	114.59	118.60
1	AA	82	G	C8-N9-C4	6.67	109.07	106.40
1	CA	2546	U	C4-C5-C6	6.67	123.70	119.70
1	AA	1474	C	C4-C5-C6	6.67	120.74	117.40
34	BA	900	A	O5'-P-OP2	6.67	118.71	110.70
1	CA	2424	C	C6-N1-C2	6.67	122.97	120.30
1	AA	1605	A	N1-C2-N3	6.67	132.63	129.30
1	AA	2553	A	C6-C5-N7	-6.67	127.63	132.30
1	CA	2221	G	N9-C4-C5	6.67	108.07	105.40
1	AA	1831	C	C2-N3-C4	-6.67	116.57	119.90
1	CA	669	G	OP1-P-OP2	-6.67	109.60	119.60
1	AA	2876	U	N3-C4-O4	-6.66	114.74	119.40
1	AA	2895	C	N3-C4-N4	6.66	122.66	118.00
1	AA	2490	A	C8-N9-C4	6.66	108.47	105.80
1	AA	992	G	N3-C2-N2	6.66	124.56	119.90
1	AA	1440	U	C5-C6-N1	6.66	126.03	122.70
1	AA	2054	G	OP1-P-OP2	6.66	129.59	119.60
1	CA	1337	G	C8-N9-C4	6.66	109.06	106.40
1	CA	2893	G	N3-C4-N9	6.66	130.00	126.00
1	AA	2496	G	C2-N3-C4	6.66	115.23	111.90
34	BA	345	C	C5-C6-N1	6.66	124.33	121.00
1	CA	195	A	OP2-P-O3'	6.65	119.83	105.20
1	AA	1605	A	O4'-C1'-N9	6.65	113.52	108.20
1	AA	2515	A	N3-C4-N9	6.65	132.72	127.40
1	AA	1976	G	N1-C6-O6	6.64	123.89	119.90
1	AA	604	C	C5-C6-N1	-6.64	117.68	121.00
1	AA	1874	C	C2-N3-C4	-6.64	116.58	119.90
1	CA	1142(A)	A	C5-C6-N1	-6.64	114.38	117.70
1	CA	2618	G	N7-C8-N9	-6.64	109.78	113.10
1	AA	1232	G	O5'-P-OP2	-6.64	99.73	105.70
1	CA	530	G	C5-N7-C8	-6.64	100.98	104.30
1	AA	85	C	C6-N1-C2	6.63	122.95	120.30
1	AA	2039	U	C5-C6-N1	-6.63	119.38	122.70
1	CA	933	A	C8-N9-C4	-6.63	103.15	105.80
1	CA	2394	C	N3-C4-C5	6.63	124.55	121.90
1	CA	2893	G	C2-N3-C4	6.63	115.22	111.90
1	AA	182	U	N1-C2-N3	6.63	118.88	114.90
1	AA	1859	G	C2-N3-C4	-6.63	108.59	111.90
1	CA	1558	A	P-O3'-C3'	6.63	127.65	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1771	C	C2-N3-C4	-6.62	116.59	119.90
1	CA	705	A	C5-C6-N6	-6.62	118.40	123.70
1	CA	442	G	O5'-P-OP1	-6.62	99.74	105.70
2	AB	28	C	O5'-P-OP2	-6.62	99.74	105.70
34	DA	1502	A	C4-C5-N7	6.62	114.01	110.70
1	AA	552	C	C5-C6-N1	-6.62	117.69	121.00
2	CB	104	U	O5'-P-OP2	-6.61	99.75	105.70
1	AA	834	U	O5'-P-OP1	-6.61	99.75	105.70
1	AA	884	C	C2-N3-C4	-6.61	116.60	119.90
1	AA	345	G	C6-C5-N7	-6.61	126.44	130.40
1	AA	2459	G	C8-N9-C4	6.61	109.04	106.40
1	AA	2660	C	C2-N3-C4	-6.61	116.60	119.90
34	BA	1499	A	C8-N9-C4	6.60	108.44	105.80
34	BA	1522	U	OP1-P-OP2	6.60	129.51	119.60
1	AA	2513	C	C2-N1-C1'	-6.60	111.54	118.80
34	BA	687	A	P-O3'-C3'	6.60	127.62	119.70
1	CA	2207	G	C6-C5-N7	-6.60	126.44	130.40
1	AA	196	A	N1-C6-N6	6.59	122.56	118.60
1	AA	1342	G	N3-C2-N2	6.59	124.52	119.90
1	AA	182	U	C5-C6-N1	-6.59	119.41	122.70
1	AA	2745	G	C8-N9-C4	-6.59	103.76	106.40
57	BX	75	C	C5-C4-N4	-6.59	115.59	120.20
1	CA	2679	A	O5'-P-OP2	-6.59	99.77	105.70
1	AA	185	A	N1-C6-N6	6.59	122.55	118.60
1	AA	1059	C	N3-C4-C5	6.58	124.53	121.90
1	CA	2464	C	C2-N3-C4	-6.58	116.61	119.90
34	DA	1502	A	N1-C6-N6	6.58	122.55	118.60
1	CA	2247	A	C8-N9-C4	6.58	108.43	105.80
1	AA	199	C	C5-C6-N1	-6.58	117.71	121.00
1	AA	399	G	O4'-C1'-N9	6.58	113.46	108.20
1	AA	1822	A	OP1-P-OP2	-6.58	109.73	119.60
1	AA	2375	C	N3-C4-N4	-6.58	113.40	118.00
1	AA	2690	C	N1-C2-O2	-6.58	114.95	118.90
1	AA	2649	U	N1-C2-N3	6.57	118.84	114.90
1	CA	2026	C	N1-C2-O2	-6.57	114.95	118.90
34	DA	1501	C	N1-C2-O2	-6.57	114.96	118.90
1	AA	2761	A	C8-N9-C4	6.57	108.43	105.80
1	AA	1311	A	O5'-P-OP2	-6.57	99.79	105.70
34	BA	504	C	O5'-P-OP1	-6.57	99.79	105.70
1	AA	139	A	N1-C6-N6	6.57	122.54	118.60
1	AA	1438	A	C5-C6-N6	-6.57	118.45	123.70
1	AA	1701	A	C5-C6-N1	-6.57	114.42	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1291	G	C6-C5-N7	6.56	134.34	130.40
1	AA	629	U	OP2-P-O3'	6.56	119.64	105.20
1	AA	1281	G	C2-N3-C4	-6.56	108.62	111.90
1	CA	672	C	C5-C6-N1	-6.56	117.72	121.00
1	CA	2447	G	C8-N9-C4	6.56	109.02	106.40
57	BX	75	C	N3-C4-N4	6.55	122.59	118.00
1	CA	1692	U	C5-C6-N1	-6.55	119.42	122.70
1	AA	549	U	N3-C4-C5	6.55	118.53	114.60
1	AA	476	G	N1-C6-O6	-6.55	115.97	119.90
2	AB	86	G	N3-C4-N9	6.55	129.93	126.00
1	CA	1799	G	O5'-P-OP2	-6.55	99.80	105.70
1	AA	539	A	OP2-P-O3'	6.55	119.61	105.20
1	AA	1458	A	O5'-P-OP2	6.55	118.56	110.70
34	DA	481	G	N3-C4-C5	-6.55	125.33	128.60
1	AA	530	A	C8-N9-C4	-6.55	103.18	105.80
1	AA	2418	U	O5'-P-OP2	6.55	118.56	110.70
1	AA	1985	U	C2-N1-C1'	6.55	125.56	117.70
1	AA	992	G	O5'-P-OP1	-6.54	99.81	105.70
1	AA	1029	A	C5-C6-N6	6.54	128.94	123.70
1	AA	2383	G	N9-C4-C5	-6.54	102.78	105.40
1	AA	1175	A	OP1-P-OP2	6.54	129.41	119.60
1	AA	23	G	C4-C5-N7	-6.54	108.19	110.80
1	CA	1698	A	O4'-C1'-N9	6.54	113.43	108.20
1	CA	2500	U	C5-C6-N1	-6.54	119.43	122.70
1	AA	1522	G	O5'-P-OP1	-6.54	99.82	105.70
1	CA	782	A	N1-C6-N6	6.54	122.52	118.60
1	CA	2221	G	N1-C6-O6	-6.54	115.98	119.90
34	DA	1154	G	C8-N9-C1'	-6.53	118.51	127.00
1	AA	1805	C	N3-C4-C5	6.53	124.51	121.90
1	AA	2641	A	C6-N1-C2	-6.53	114.68	118.60
1	CA	1004	C	N1-C2-O2	-6.53	114.98	118.90
1	CA	2286	A	C5-N7-C8	-6.53	100.64	103.90
1	CA	2875	C	C6-N1-C2	6.53	122.91	120.30
1	AA	2882	G	C5-C6-O6	6.53	132.52	128.60
1	AA	1233	U	C5-C4-O4	6.53	129.82	125.90
1	AA	1986	G	C8-N9-C4	6.53	109.01	106.40
1	CA	955	C	C6-N1-C2	-6.53	117.69	120.30
1	CA	1479	G	O5'-P-OP2	-6.53	99.83	105.70
1	CA	2394	C	C6-N1-C2	6.53	122.91	120.30
1	CA	1968	G	N3-C2-N2	-6.52	115.33	119.90
1	AA	2464	C	C4-C5-C6	-6.52	114.14	117.40
1	CA	1675	C	N3-C4-C5	-6.52	119.29	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	206	U	O5'-P-OP2	-6.52	99.83	105.70
1	AA	641	G	O5'-P-OP2	-6.52	99.83	105.70
1	AA	1316	C	C5-C6-N1	-6.52	117.74	121.00
1	AA	2471	A	C5-C6-N1	6.52	120.96	117.70
1	AA	2652	G	N9-C4-C5	6.51	108.00	105.40
1	AA	749	G	O5'-P-OP2	-6.51	99.84	105.70
1	AA	2605	U	N3-C4-C5	6.51	118.50	114.60
1	AA	2830	A	N1-C6-N6	6.51	122.50	118.60
1	CA	476	G	O5'-P-OP2	-6.50	99.85	105.70
1	AA	2383	G	C8-N9-C4	6.50	109.00	106.40
1	AA	2466	G	N3-C2-N2	6.50	124.45	119.90
1	CA	2286	A	C5-C6-N1	-6.50	114.45	117.70
1	AA	855	G	O5'-P-OP2	-6.50	99.85	105.70
1	AA	1462	G	O4'-C1'-N9	6.50	113.40	108.20
1	AA	1647	G	C8-N9-C4	6.50	109.00	106.40
1	AA	2497	G	N3-C2-N2	6.50	124.45	119.90
1	AA	1231	G	O5'-P-OP2	-6.49	99.86	105.70
1	AA	1911	A	N1-C6-N6	-6.49	114.70	118.60
1	AA	2083	G	C5-C6-O6	-6.49	124.70	128.60
1	AA	2701	U	N1-C2-N3	6.49	118.80	114.90
1	CA	1779	U	O4'-C1'-N1	6.49	113.39	108.20
1	AA	1815	A	O5'-P-OP2	-6.49	99.86	105.70
2	AB	48	A	C2-N3-C4	-6.49	107.36	110.60
1	AA	1247	C	N1-C2-O2	-6.49	115.01	118.90
1	CA	1558	A	C2-N3-C4	-6.48	107.36	110.60
34	DA	713	G	O5'-P-OP1	-6.48	99.87	105.70
1	AA	191	U	N3-C4-C5	6.48	118.49	114.60
1	AA	708	C	C2-N3-C4	-6.48	116.66	119.90
59	BZ	374	LEU	CA-CB-CG	6.48	130.20	115.30
1	AA	1920	U	N3-C4-C5	6.48	118.49	114.60
1	CA	2430	A	O4'-C1'-N9	6.48	113.38	108.20
2	AB	83	G	C5-C6-O6	6.47	132.48	128.60
34	BA	804	U	N3-C4-O4	-6.47	114.87	119.40
1	CA	2570	G	N9-C4-C5	6.47	107.99	105.40
1	AA	2238	C	C6-N1-C2	6.47	122.89	120.30
34	BA	243	A	O5'-P-OP1	-6.47	99.88	105.70
1	AA	279	G	C5-C6-N1	-6.47	108.27	111.50
1	AA	1992	A	C5-C6-N6	-6.46	118.53	123.70
34	BA	1499	A	N9-C4-C5	-6.46	103.22	105.80
1	AA	1423	G	N1-C6-O6	-6.46	116.02	119.90
1	CA	1215	G	C5-C6-N1	6.46	114.73	111.50
1	AA	1597	C	N1-C2-O2	-6.46	115.03	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1848	G	N1-C2-N2	-6.46	110.39	116.20
1	AA	604	C	C2-N3-C4	-6.46	116.67	119.90
1	CA	1673	U	N3-C4-O4	-6.46	114.88	119.40
1	CA	2337	G	N1-C6-O6	6.46	123.77	119.90
1	AA	177	G	N1-C2-N2	-6.46	110.39	116.20
1	CA	90	U	N3-C2-O2	-6.45	117.68	122.20
1	CA	963	U	O5'-P-OP2	6.45	118.44	110.70
1	AA	35	G	O5'-P-OP1	-6.45	99.89	105.70
1	AA	820	U	N1-C2-N3	6.45	118.77	114.90
34	BA	509	A	C8-N9-C4	-6.45	103.22	105.80
1	AA	1844	G	C8-N9-C4	6.45	108.98	106.40
1	AA	2587	C	N3-C4-C5	6.45	124.48	121.90
1	CA	1656	C	N3-C4-N4	-6.45	113.49	118.00
1	AA	1190	G	C5-C6-N1	6.44	114.72	111.50
1	AA	1814	A	O5'-P-OP2	-6.44	99.90	105.70
1	CA	1781	C	C2-N1-C1'	-6.44	111.71	118.80
1	AA	891	C	C6-N1-C2	6.44	122.88	120.30
34	BA	1517	G	N3-C4-N9	-6.44	122.14	126.00
1	AA	797	A	OP2-P-O3'	6.44	119.36	105.20
1	CA	1824	G	N3-C4-N9	-6.44	122.14	126.00
1	AA	2501	G	N3-C4-N9	6.44	129.86	126.00
1	AA	2889	C	N1-C2-O2	6.44	122.76	118.90
34	DA	1405	G	N3-C4-C5	-6.44	125.38	128.60
1	CA	2682	U	O5'-P-OP2	-6.43	99.91	105.70
1	AA	1980	C	N1-C2-O2	-6.43	115.04	118.90
1	AA	2619	G	N1-C6-O6	-6.43	116.04	119.90
1	CA	1698	A	N1-C6-N6	6.43	122.46	118.60
1	AA	855	G	C5-C6-N1	6.43	114.72	111.50
1	AA	2498	G	C5-C6-N1	6.43	114.72	111.50
1	CA	2046	G	C2-N3-C4	-6.43	108.69	111.90
1	CA	2782	G	N1-C6-O6	6.43	123.76	119.90
1	AA	477	C	C2-N3-C4	-6.42	116.69	119.90
1	AA	1546	G	N1-C6-O6	6.42	123.75	119.90
1	CA	312	G	O5'-P-OP1	-6.42	99.92	105.70
1	AA	2041	A	C5-N7-C8	6.42	107.11	103.90
1	AA	127	C	C2-N3-C4	-6.42	116.69	119.90
1	AA	1090	G	N1-C6-O6	-6.42	116.05	119.90
1	AA	2083	G	C6-N1-C2	-6.42	121.25	125.10
1	AA	2503	U	C5-C4-O4	-6.42	122.05	125.90
1	CA	1692	U	C5-C4-O4	-6.42	122.05	125.90
1	AA	2496	G	C5-C6-N1	6.42	114.71	111.50
2	AB	33	G	C8-N9-C4	6.41	108.97	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	2286	A	N1-C6-N6	6.41	122.45	118.60
1	AA	45	C	O5'-P-OP1	6.41	118.39	110.70
1	AA	1264	G	N1-C6-O6	6.41	123.75	119.90
1	AA	1479	U	C5-C6-N1	-6.41	119.49	122.70
34	DA	1502	A	C5-N7-C8	-6.41	100.69	103.90
1	AA	2266	C	N1-C2-O2	-6.41	115.06	118.90
1	AA	2291	G	N1-C6-O6	6.41	123.74	119.90
1	AA	2587	C	C6-N1-C2	6.41	122.86	120.30
1	AA	2590	G	N9-C4-C5	-6.41	102.84	105.40
1	CA	1425	G	N9-C4-C5	-6.41	102.84	105.40
1	AA	1836	U	OP1-P-OP2	-6.40	110.00	119.60
1	AA	726	C	C2-N3-C4	-6.40	116.70	119.90
1	AA	2443	U	C2-N3-C4	-6.40	123.16	127.00
1	AA	2331	G	C4-C5-N7	6.40	113.36	110.80
1	AA	2876	U	N1-C2-N3	6.40	118.74	114.90
1	CA	2252	G	C8-N9-C4	6.40	108.96	106.40
1	AA	704	U	C5-C6-N1	-6.40	119.50	122.70
1	AA	1278	G	O5'-P-OP2	6.40	118.38	110.70
1	AA	808	A	C5-C6-N1	-6.39	114.50	117.70
1	AA	2520	G	N9-C4-C5	6.39	107.96	105.40
1	AA	2036	A	C8-N9-C4	6.39	108.36	105.80
1	CA	272(F)	C	C6-N1-C2	6.39	122.86	120.30
1	CA	1337	G	N7-C8-N9	-6.39	109.90	113.10
1	AA	2383	G	C5-C6-N1	6.39	114.70	111.50
1	AA	2594	G	O5'-P-OP2	-6.39	99.95	105.70
1	CA	2626	C	C5-C4-N4	-6.39	115.73	120.20
1	AA	2294	G	C4-C5-N7	6.39	113.36	110.80
1	CA	807	U	N3-C4-O4	6.38	123.87	119.40
1	AA	2273	C	C4-C5-C6	6.38	120.59	117.40
1	AA	1022	C	C6-N1-C2	-6.38	117.75	120.30
1	AA	1318	A	O4'-C1'-N9	6.38	113.31	108.20
1	AA	2340	A	C8-N9-C4	6.38	108.35	105.80
1	AA	2590	G	C8-N9-C4	6.38	108.95	106.40
1	AA	2743	C	C5-C6-N1	-6.38	117.81	121.00
1	CA	848	G	N3-C4-C5	-6.38	125.41	128.60
1	CA	1384	A	C2-N3-C4	6.38	113.79	110.60
1	CA	1668	A	O5'-P-OP1	-6.38	99.96	105.70
1	AA	92	C	C6-N1-C2	-6.38	117.75	120.30
1	AA	2515	A	O5'-P-OP1	-6.38	99.96	105.70
1	AA	744	C	O5'-P-OP2	-6.38	99.96	105.70
1	AA	1290	G	N1-C2-N2	-6.37	110.46	116.20
1	AA	1518	A	C8-N9-C4	-6.37	103.25	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	2535	G	C4-C5-N7	6.37	113.35	110.80
1	CA	961	C	C6-N1-C2	6.37	122.85	120.30
1	AA	858	U	O5'-P-OP2	-6.37	99.97	105.70
1	AA	85	C	N3-C4-C5	6.37	124.45	121.90
1	AA	851	A	N9-C4-C5	-6.37	103.25	105.80
1	AA	2298	A	C4-C5-N7	6.37	113.88	110.70
1	CA	917	A	O5'-P-OP1	6.37	118.34	110.70
1	AA	581	G	N1-C6-O6	-6.37	116.08	119.90
1	AA	2480	G	C8-N9-C4	6.37	108.95	106.40
1	AA	2540	U	O5'-P-OP1	-6.37	99.97	105.70
1	AA	25	U	C5-C4-O4	-6.36	122.08	125.90
1	AA	650	G	C8-N9-C4	-6.36	103.85	106.40
1	AA	1422	C	C2-N3-C4	-6.36	116.72	119.90
1	AA	2872	G	N1-C6-O6	-6.36	116.08	119.90
1	AA	2625	U	N3-C2-O2	-6.36	117.75	122.20
31	A7	39	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	AA	1402	G	C5-C6-O6	-6.36	124.78	128.60
12	AO	8	LEU	CA-CB-CG	6.36	129.93	115.30
1	AA	176	G	N1-C6-O6	6.36	123.72	119.90
1	AA	1703	C	C6-N1-C2	6.35	122.84	120.30
1	AA	555	G	N1-C6-O6	-6.35	116.09	119.90
1	AA	846	G	N1-C2-N2	-6.35	110.49	116.20
1	AA	2014	G	P-O3'-C3'	6.35	127.32	119.70
1	AA	2299	A	N3-C4-N9	-6.34	122.32	127.40
1	AA	2724	U	C6-N1-C2	6.34	124.81	121.00
1	AA	637	U	N3-C4-O4	-6.34	114.96	119.40
1	AA	1026	A	N1-C6-N6	6.34	122.41	118.60
1	AA	2520	G	C4-C5-N7	-6.34	108.26	110.80
1	AA	585	U	O5'-P-OP1	-6.34	100.00	105.70
1	AA	1976	G	C5-C6-O6	-6.34	124.80	128.60
1	AA	2251	G	N1-C6-O6	6.34	123.70	119.90
34	BA	1067	A	O4'-C1'-N9	-6.34	103.13	108.20
1	AA	240	A	N1-C6-N6	-6.34	114.80	118.60
1	AA	235	C	C5-C6-N1	-6.33	117.83	121.00
34	BA	546	G	C8-N9-C4	-6.33	103.87	106.40
1	CA	141	A	C5-C6-N6	-6.33	118.63	123.70
1	CA	2012	G	C8-N9-C4	-6.33	103.87	106.40
1	AA	1347	A	OP1-P-OP2	6.33	129.09	119.60
1	CA	917	A	O5'-P-OP2	-6.33	100.00	105.70
1	CA	2589	A	C6-N1-C2	-6.33	114.80	118.60
1	AA	2418	U	O4'-C1'-N1	-6.33	103.14	108.20
1	CA	2818	G	N3-C2-N2	6.33	124.33	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	2585	C	C4-C5-C6	6.33	120.56	117.40
1	AA	2601	A	N9-C4-C5	6.32	108.33	105.80
1	CA	330	A	C6-C5-N7	-6.32	127.87	132.30
1	CA	1824	G	C5-C6-O6	6.32	132.39	128.60
1	AA	2825	C	N3-C2-O2	-6.32	117.48	121.90
1	CA	1696	G	C2-N3-C4	6.32	115.06	111.90
1	CA	2582	G	O5'-P-OP2	-6.32	100.01	105.70
1	AA	2502	G	C5-C6-N1	6.32	114.66	111.50
1	AA	1304	C	C6-N1-C2	6.32	122.83	120.30
1	AA	1354	A	C5-C6-N6	6.32	128.75	123.70
1	AA	1561	C	C6-N1-C2	6.32	122.83	120.30
1	AA	2372	A	O5'-P-OP2	-6.32	100.01	105.70
1	CA	205	G	O5'-P-OP2	-6.32	100.01	105.70
1	CA	1626	G	C2-N3-C4	6.32	115.06	111.90
1	CA	2740	A	C8-N9-C4	6.32	108.33	105.80
1	AA	2301	G	N1-C2-N3	-6.32	120.11	123.90
1	AA	629	U	O5'-P-OP2	-6.31	100.02	105.70
1	AA	2791	A	N1-C2-N3	6.31	132.46	129.30
1	AA	2835	C	C5-C6-N1	-6.31	117.84	121.00
1	AA	27	G	O5'-P-OP2	-6.31	100.02	105.70
1	AA	1021	G	OP1-P-OP2	6.31	129.07	119.60
1	CA	2036	C	C6-N1-C2	6.31	122.82	120.30
1	AA	1000	C	O5'-P-OP2	-6.31	100.02	105.70
1	AA	2346	G	N3-C4-N9	6.31	129.78	126.00
1	CA	1565	C	C6-N1-C2	6.31	122.82	120.30
1	CA	2286	A	N7-C8-N9	6.31	116.95	113.80
1	CA	1789	A	C5-C6-N6	6.31	128.75	123.70
34	BA	1442	G	C6-C5-N7	-6.30	126.62	130.40
34	DA	499	A	C8-N9-C4	6.30	108.32	105.80
1	AA	470	C	C2-N3-C4	-6.30	116.75	119.90
1	AA	906	G	O4'-C1'-N9	-6.30	103.16	108.20
1	AA	540	A	N1-C6-N6	-6.30	114.82	118.60
1	AA	1359	U	C2-N1-C1'	6.30	125.26	117.70
1	AA	2621	U	OP2-P-O3'	6.30	119.06	105.20
1	AA	977	G	C4-C5-N7	-6.30	108.28	110.80
1	AA	1709	C	N3-C4-C5	6.30	124.42	121.90
1	AA	2443	U	N3-C4-C5	6.30	118.38	114.60
1	AA	2606	C	N3-C2-O2	-6.30	117.49	121.90
1	AA	2092	G	C6-N1-C2	-6.29	121.32	125.10
34	BA	1530	G	N3-C4-C5	6.29	131.75	128.60
1	AA	1809	U	N3-C2-O2	6.29	126.60	122.20
1	AA	2067	C	C4-C5-C6	6.29	120.55	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	84	C	N1-C2-O2	6.29	122.67	118.90
1	AA	2514	G	O5'-P-OP1	-6.29	100.04	105.70
1	CA	528	A	C5-C6-N1	-6.29	114.56	117.70
1	AA	993	G	C5-C6-O6	-6.29	124.83	128.60
1	AA	50	G	N3-C4-N9	6.28	129.77	126.00
1	AA	1657	C	N1-C2-N3	6.28	123.60	119.20
1	AA	2276	C	C5-C6-N1	-6.28	117.86	121.00
1	AA	2220	A	O4'-C1'-N9	6.28	113.22	108.20
1	AA	2276	C	C6-N1-C2	6.28	122.81	120.30
6	AF	74	ARG	NE-CZ-NH1	6.28	123.44	120.30
34	BA	1417	G	N3-C4-N9	6.28	129.77	126.00
1	AA	2291	G	C5-C6-O6	-6.28	124.83	128.60
1	AA	1281	G	C6-C5-N7	-6.28	126.64	130.40
1	CA	2287	A	N3-C4-C5	6.28	131.19	126.80
1	AA	2049	G	N9-C4-C5	6.27	107.91	105.40
1	CA	851	U	C5-C6-N1	-6.27	119.56	122.70
1	CA	1394	U	O5'-P-OP2	6.27	118.23	110.70
1	AA	595	A	N9-C4-C5	6.27	108.31	105.80
1	CA	562	U	O5'-P-OP1	-6.27	100.06	105.70
1	AA	1665	G	N1-C6-O6	-6.27	116.14	119.90
1	CA	2605	U	N3-C4-O4	-6.27	115.01	119.40
1	CA	768	G	C5-C6-O6	6.27	132.36	128.60
1	AA	525	G	C8-N9-C4	6.26	108.91	106.40
1	AA	747	G	N9-C4-C5	6.26	107.91	105.40
1	CA	1313	U	C2-N1-C1'	6.26	125.22	117.70
1	AA	616	G	N9-C4-C5	6.26	107.91	105.40
1	AA	1290	G	C5-C6-O6	6.26	132.36	128.60
1	AA	1329	G	N3-C4-N9	6.26	129.76	126.00
1	AA	85	C	C2-N3-C4	-6.26	116.77	119.90
1	AA	2341	G	N3-C2-N2	6.25	124.28	119.90
1	AA	2451	A	N1-C6-N6	6.25	122.35	118.60
1	AA	2791	A	C2-N3-C4	-6.25	107.47	110.60
1	AA	1290	G	N1-C6-O6	-6.25	116.15	119.90
34	BA	896	C	C6-N1-C2	6.25	122.80	120.30
1	CA	16	G	C8-N9-C4	6.25	108.90	106.40
1	CA	1899	G	N3-C2-N2	-6.25	115.52	119.90
1	AA	1069	U	O5'-P-OP2	-6.25	100.08	105.70
1	AA	1097	G	C5-C6-O6	-6.25	124.85	128.60
1	AA	1388	A	C6-N1-C2	-6.25	114.85	118.60
34	BA	297	G	N9-C4-C5	-6.25	102.90	105.40
1	CA	2387	U	C5-C6-N1	-6.25	119.58	122.70
1	AA	2383	G	C5-C6-O6	-6.25	124.85	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	820	U	C2-N3-C4	-6.24	123.25	127.00
1	AA	2052	A	C5-C6-N6	-6.24	118.70	123.70
1	CA	1425	G	C4-C5-N7	6.24	113.30	110.80
1	AA	1612	C	O5'-P-OP2	-6.24	100.08	105.70
1	AA	2579	G	N1-C6-O6	-6.24	116.16	119.90
1	CA	665	C	C6-N1-C2	6.24	122.80	120.30
1	CA	847	U	C5-C4-O4	6.24	129.64	125.90
1	AA	1342	G	N1-C2-N2	-6.24	110.59	116.20
1	AA	1069	U	N1-C2-N3	6.24	118.64	114.90
1	AA	1829	U	C2-N3-C4	-6.24	123.26	127.00
1	AA	2882	G	N9-C4-C5	6.24	107.89	105.40
1	CA	728	G	O5'-P-OP2	-6.23	100.09	105.70
1	CA	2586	C	C6-N1-C2	-6.23	117.81	120.30
1	AA	422	U	O4'-C1'-N1	6.23	113.19	108.20
1	AA	727	G	O5'-P-OP1	-6.23	100.09	105.70
2	AB	115	G	OP1-P-OP2	6.23	128.95	119.60
1	AA	2387	G	N7-C8-N9	-6.23	109.99	113.10
1	AA	2798	C	C6-N1-C2	-6.23	117.81	120.30
1	AA	2553	A	C4-C5-N7	6.22	113.81	110.70
1	AA	884	C	C5-C6-N1	-6.22	117.89	121.00
34	BA	1505	G	N3-C4-C5	6.22	131.71	128.60
1	CA	834	C	N1-C2-O2	-6.22	115.17	118.90
1	CA	1351	C	C6-N1-C2	6.22	122.79	120.30
1	AA	2384	G	C5-C6-O6	-6.21	124.87	128.60
1	CA	1774	C	N3-C2-O2	-6.21	117.55	121.90
1	CA	1781	C	C5-C4-N4	6.21	124.55	120.20
34	DA	992	U	P-O3'-C3'	6.21	127.15	119.70
1	AA	2669	A	O5'-P-OP2	-6.21	100.11	105.70
1	AA	2162	C	N3-C2-O2	-6.20	117.56	121.90
1	CA	482	A	N1-C2-N3	6.20	132.40	129.30
1	AA	1076	G	N3-C2-N2	6.20	124.24	119.90
34	BA	442	C	C6-N1-C2	-6.20	117.82	120.30
1	AA	1721	G	N3-C4-N9	6.20	129.72	126.00
1	AA	2576	A	N9-C4-C5	6.20	108.28	105.80
1	AA	1312	G	C6-N1-C2	-6.19	121.38	125.10
1	AA	1253	C	C2-N3-C4	-6.19	116.80	119.90
4	AD	229	VAL	CB-CA-C	-6.19	99.63	111.40
1	CA	1623	G	C5-C6-N1	-6.19	108.40	111.50
1	CA	2407	G	N3-C4-C5	-6.19	125.50	128.60
1	AA	2466	G	C5-C6-O6	6.19	132.31	128.60
1	CA	1789	A	N1-C6-N6	-6.19	114.89	118.60
1	CA	2407	G	N3-C4-N9	6.19	129.71	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	50	G	C6-N1-C2	-6.19	121.39	125.10
1	AA	830	A	C4-C5-C6	6.19	120.09	117.00
1	CA	2415	G	C5-C6-N1	6.19	114.59	111.50
1	AA	2898	C	C2-N3-C4	-6.18	116.81	119.90
34	BA	244	U	N1-C2-O2	6.18	127.12	122.80
1	AA	1188	A	N1-C6-N6	6.18	122.31	118.60
1	AA	1001	G	N1-C2-N2	6.17	121.76	116.20
2	AB	86	G	N9-C4-C5	-6.17	102.93	105.40
34	BA	771	G	N9-C4-C5	6.17	107.87	105.40
1	CA	2276	G	C2-N3-C4	6.17	114.99	111.90
1	AA	2527	C	C2-N3-C4	-6.17	116.81	119.90
1	AA	1029	A	N1-C6-N6	-6.17	114.90	118.60
1	AA	2397	C	N1-C2-O2	-6.17	115.20	118.90
1	AA	2787	C	C6-N1-C2	-6.17	117.83	120.30
34	DA	901	A	O5'-P-OP1	-6.17	100.14	105.70
1	AA	2523	U	C5-C6-N1	-6.17	119.61	122.70
1	CA	1201	C	N1-C2-O2	-6.17	115.20	118.90
1	CA	2238	G	O5'-P-OP1	-6.17	100.15	105.70
34	DA	1529	G	C4-N9-C1'	6.17	134.52	126.50
1	AA	883	G	C2-N3-C4	6.17	114.98	111.90
1	AA	1324	A	C2-N3-C4	-6.17	107.52	110.60
34	DA	754	C	N1-C2-O2	6.17	122.60	118.90
1	AA	1821	C	OP1-P-O3'	6.16	118.76	105.20
1	CA	2588	G	N3-C4-N9	-6.16	122.30	126.00
1	AA	543	G	O5'-P-OP1	6.16	118.09	110.70
1	CA	1837	C	O5'-P-OP2	6.16	118.09	110.70
1	AA	593	G	C5-C6-N1	6.16	114.58	111.50
1	AA	1026	A	C4-C5-N7	6.16	113.78	110.70
1	AA	2101	U	N1-C2-O2	-6.16	118.49	122.80
1	AA	197	C	N1-C2-O2	-6.16	115.20	118.90
1	AA	352	U	N1-C2-N3	6.16	118.60	114.90
1	AA	55	A	N1-C2-N3	6.16	132.38	129.30
1	AA	2594	G	N3-C2-N2	6.16	124.21	119.90
1	AA	851	A	N3-C4-C5	6.16	131.11	126.80
1	AA	2583	C	C5-C6-N1	-6.16	117.92	121.00
1	CA	668	G	O5'-P-OP1	-6.16	100.16	105.70
1	AA	1312	G	C5-C6-O6	-6.15	124.91	128.60
1	AA	2090	U	C5-C6-N1	-6.15	119.62	122.70
1	AA	1688	A	C8-N9-C4	-6.15	103.34	105.80
34	BA	841	U	C2-N1-C1'	6.15	125.08	117.70
1	AA	1187	U	C5-C4-O4	-6.15	122.21	125.90
1	AA	2049	G	C2-N3-C4	6.15	114.97	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	2856	G	O5'-P-OP1	-6.15	100.17	105.70
1	CA	1963	U	C2-N1-C1'	6.15	125.08	117.70
1	AA	147	U	N3-C4-C5	6.15	118.29	114.60
1	AA	962	G	O5'-P-OP1	-6.15	100.17	105.70
1	CA	1841	U	OP1-P-OP2	6.14	128.81	119.60
1	AA	1053	C	C2-N3-C4	-6.14	116.83	119.90
1	AA	2426	G	N1-C6-O6	6.14	123.58	119.90
1	AA	856	G	N3-C2-N2	6.14	124.20	119.90
1	AA	1207	C	C2-N3-C4	-6.14	116.83	119.90
1	AA	2754	A	N7-C8-N9	-6.14	110.73	113.80
1	CA	2818	G	N9-C4-C5	-6.14	102.95	105.40
1	AA	40	C	N1-C2-O2	-6.13	115.22	118.90
1	AA	1741	C	C5-C6-N1	-6.13	117.93	121.00
1	AA	1655	A	N1-C6-N6	6.13	122.28	118.60
1	CA	2280	G	N1-C6-O6	-6.13	116.22	119.90
34	DA	1405	G	N3-C2-N2	6.13	124.19	119.90
1	AA	592	U	N3-C2-O2	6.13	126.49	122.20
1	AA	1022	C	OP2-P-O3'	6.13	118.68	105.20
34	BA	1482	G	N3-C4-N9	6.13	129.68	126.00
1	AA	185	A	C6-C5-N7	-6.13	128.01	132.30
1	AA	1246	C	N3-C4-C5	6.13	124.35	121.90
1	AA	1966	U	C5-C4-O4	6.13	129.58	125.90
1	AA	2073	A	N9-C4-C5	6.13	108.25	105.80
1	AA	2531	U	C2-N3-C4	-6.13	123.32	127.00
34	BA	971	G	O4'-C1'-N9	6.13	113.10	108.20
1	AA	1657	C	N3-C2-O2	-6.12	117.61	121.90
1	AA	2074	G	C6-C5-N7	6.12	134.07	130.40
1	AA	1655	A	C5-C6-N1	6.12	120.76	117.70
34	BA	1505	G	C2-N3-C4	-6.12	108.84	111.90
1	CA	1385	G	N3-C4-C5	6.12	131.66	128.60
1	CA	2549	G	C5-C6-O6	-6.12	124.93	128.60
34	BA	1054	C	O5'-P-OP2	-6.12	100.19	105.70
1	CA	1850	G	N1-C6-O6	6.12	123.57	119.90
34	BA	1530	G	N3-C4-N9	-6.12	122.33	126.00
2	AB	94	C	C5-C4-N4	6.12	124.48	120.20
1	CA	265	A	N1-C6-N6	6.12	122.27	118.60
1	CA	2029	G	N1-C6-O6	6.12	123.57	119.90
1	AA	290	G	C8-N9-C4	6.11	108.85	106.40
1	CA	1385	G	C4-N9-C1'	-6.11	118.55	126.50
1	CA	420	C	N1-C2-O2	6.11	122.57	118.90
1	AA	1344	C	N3-C2-O2	6.11	126.18	121.90
1	AA	1921	G	C5-C6-O6	-6.11	124.93	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	2701	U	P-O3'-C3'	6.11	127.03	119.70
2	AB	41	U	C2-N3-C4	-6.11	123.33	127.00
1	CA	1637	A	N1-C6-N6	-6.11	114.93	118.60
1	AA	2622	C	N1-C2-O2	6.11	122.56	118.90
1	AA	1054	C	N1-C2-O2	-6.11	115.23	118.90
1	AA	1423	G	N1-C2-N2	-6.11	110.70	116.20
1	CA	774	A	O5'-P-OP2	-6.11	100.20	105.70
1	CA	1945	G	C4-N9-C1'	6.11	134.44	126.50
2	CB	22	U	C5-C6-N1	6.11	125.75	122.70
1	AA	977	G	O5'-P-OP2	-6.11	100.20	105.70
1	AA	2611	G	OP2-P-O3'	6.11	118.63	105.20
1	AA	1179	U	N1-C2-O2	-6.10	118.53	122.80
1	AA	1571	G	O5'-P-OP1	-6.10	100.21	105.70
1	AA	2527	C	N1-C2-O2	-6.10	115.24	118.90
1	AA	2633	A	C4-C5-C6	-6.10	113.95	117.00
1	CA	2488	A	C8-N9-C4	6.10	108.24	105.80
1	AA	748	G	OP2-P-O3'	6.10	118.62	105.20
34	DA	1183	A	P-O3'-C3'	6.10	127.02	119.70
1	AA	602	G	C2-N3-C4	6.10	114.95	111.90
1	AA	916	G	O5'-P-OP1	-6.10	100.21	105.70
1	AA	1420	G	OP1-P-OP2	-6.10	110.45	119.60
1	AA	1782	C	N3-C2-O2	6.10	126.17	121.90
2	CB	72	G	C8-N9-C4	6.10	108.84	106.40
1	AA	2503	U	C2-N3-C4	-6.10	123.34	127.00
1	CA	1697	G	C8-N9-C4	6.10	108.84	106.40
1	AA	2298	A	N9-C1'-C2'	6.09	121.92	114.00
1	AA	2459	G	N1-C6-O6	-6.09	116.24	119.90
1	AA	2732	G	N1-C6-O6	6.09	123.56	119.90
1	AA	1665	G	N1-C2-N2	-6.09	110.72	116.20
1	AA	177	G	N3-C2-N2	6.09	124.16	119.90
1	AA	202	A	OP2-P-O3'	6.09	118.60	105.20
1	AA	714	U	C2-N3-C4	-6.09	123.35	127.00
1	AA	723	A	C6-N1-C2	6.09	122.25	118.60
1	AA	1448	C	C5-C6-N1	6.09	124.04	121.00
13	AP	18	ARG	NE-CZ-NH1	6.09	123.34	120.30
34	DA	1513	A	OP1-P-OP2	6.09	128.74	119.60
1	AA	1393	G	C5-C6-N1	6.09	114.54	111.50
1	CA	768	G	C4-C5-N7	-6.09	108.36	110.80
34	DA	754	C	C6-N1-C2	-6.09	117.86	120.30
1	CA	2287	A	N1-C6-N6	6.09	122.25	118.60
1	CA	2444	G	N1-C2-N3	6.09	127.55	123.90
1	CA	2576	G	C8-N9-C4	6.09	108.83	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	1515	C	C5-C4-N4	-6.08	115.94	120.20
1	AA	2263	G	N1-C6-O6	-6.08	116.25	119.90
1	CA	1412	A	C8-N9-C4	-6.08	103.37	105.80
1	CA	1602	U	C6-N1-C2	6.08	124.65	121.00
1	CA	1110	G	N3-C2-N2	-6.08	115.64	119.90
1	AA	1033	G	N3-C2-N2	-6.08	115.65	119.90
1	AA	1254	G	C6-N1-C2	-6.08	121.45	125.10
1	CA	2337	G	C5-C6-O6	-6.08	124.95	128.60
1	CA	2490	G	C5-C6-O6	-6.08	124.95	128.60
1	AA	2632	C	C6-N1-C2	6.07	122.73	120.30
1	AA	1044	C	N1-C2-O2	-6.07	115.26	118.90
34	DA	1431	C	C6-N1-C2	-6.07	117.87	120.30
1	AA	604	C	N1-C2-O2	-6.07	115.26	118.90
1	CA	773	U	C5-C6-N1	-6.07	119.66	122.70
1	CA	784	A	O4'-C1'-N9	6.07	113.06	108.20
1	CA	962	G	C5-C6-N1	-6.07	108.47	111.50
1	CA	1692	U	C2-N3-C4	-6.07	123.36	127.00
1	CA	2822	G	C4-C5-N7	6.07	113.23	110.80
1	AA	2559	U	C5-C6-N1	-6.07	119.67	122.70
34	BA	741	G	C8-N9-C4	-6.07	103.97	106.40
1	CA	185	U	N1-C2-O2	6.07	127.05	122.80
1	AA	379	G	N1-C6-O6	6.06	123.54	119.90
1	AA	2561	G	C5-C6-O6	-6.06	124.96	128.60
1	CA	2689	U	N3-C2-O2	-6.06	117.95	122.20
1	AA	46	C	C6-N1-C2	6.06	122.72	120.30
1	AA	1983	C	C6-N1-C2	6.06	122.72	120.30
1	AA	2882	G	C4-C5-N7	-6.06	108.38	110.80
1	CA	2092	U	N3-C2-O2	6.06	126.44	122.20
1	AA	730	C	N3-C4-N4	-6.06	113.76	118.00
1	CA	827	U	C6-N1-C2	6.06	124.64	121.00
1	AA	1617	A	N1-C6-N6	6.06	122.23	118.60
1	AA	1704	C	C2-N3-C4	-6.06	116.87	119.90
1	AA	2005	C	N1-C2-O2	-6.06	115.27	118.90
1	CA	2057	A	O5'-P-OP1	6.06	117.97	110.70
1	CA	1142(A)	A	C8-N9-C4	-6.06	103.38	105.80
1	AA	1612	C	C6-N1-C2	6.05	122.72	120.30
1	AA	2537	G	C5-C6-N1	6.05	114.53	111.50
1	CA	794	G	O5'-P-OP2	-6.05	100.25	105.70
1	CA	2253	G	C2-N3-C4	-6.05	108.87	111.90
1	AA	1172	A	C8-N9-C4	-6.05	103.38	105.80
1	CA	1291	C	N3-C4-C5	6.05	124.32	121.90
1	AA	2063	U	N3-C4-O4	6.05	123.64	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	2115	G	N3-C2-N2	-6.05	115.66	119.90
34	BA	345	C	C2-N3-C4	6.05	122.92	119.90
1	AA	831	A	OP1-P-O3'	6.05	118.51	105.20
1	AA	735	U	C4-C5-C6	6.05	123.33	119.70
34	BA	297	G	C5-C6-O6	-6.05	124.97	128.60
1	CA	1966	A	N7-C8-N9	-6.05	110.78	113.80
1	AA	817	G	C8-N9-C4	6.05	108.82	106.40
1	AA	1068	G	N3-C2-N2	-6.05	115.67	119.90
1	AA	1453	C	N1-C2-O2	-6.05	115.27	118.90
1	AA	1874	C	C5-C6-N1	-6.05	117.98	121.00
34	BA	1030(B)	C	N1-C2-O2	6.05	122.53	118.90
1	CA	2206	G	C8-N9-C4	6.05	108.82	106.40
1	AA	621	G	N9-C4-C5	6.04	107.82	105.40
1	AA	1037	C	C4-C5-C6	6.04	120.42	117.40
34	DA	1158	C	C2-N1-C1'	6.04	125.44	118.80
1	AA	346	A	C8-N9-C4	6.04	108.22	105.80
1	AA	2565	G	C2-N3-C4	6.04	114.92	111.90
47	DN	44	LEU	CA-CB-CG	6.04	129.19	115.30
1	CA	915	C	N1-C2-O2	6.04	122.52	118.90
1	AA	2340	A	C2-N3-C4	-6.04	107.58	110.60
1	AA	2510	C	C5-C4-N4	6.03	124.42	120.20
34	BA	1189	C	N1-C2-O2	6.03	122.52	118.90
1	CA	1661	G	N9-C4-C5	-6.03	102.99	105.40
1	AA	1204	C	C6-N1-C2	6.03	122.71	120.30
1	AA	1721	G	C6-C5-N7	-6.03	126.78	130.40
34	BA	529	G	N1-C6-O6	6.03	123.52	119.90
34	BA	1482	G	N3-C2-N2	6.03	124.12	119.90
1	AA	1314	A	C5-C6-N1	-6.03	114.69	117.70
34	BA	1067	A	P-O3'-C3'	6.02	126.93	119.70
34	BA	1519	A	C8-N9-C4	-6.02	103.39	105.80
1	AA	893	C	N3-C4-C5	6.02	124.31	121.90
1	AA	991	G	OP1-P-O3'	6.02	118.45	105.20
2	AB	114	C	C6-N1-C2	6.02	122.71	120.30
1	AA	279	G	N7-C8-N9	6.02	116.11	113.10
1	AA	2843	G	C8-N9-C4	-6.02	103.99	106.40
1	CA	1842	G	C5-C6-O6	-6.02	124.99	128.60
1	CA	2001	A	C5-C6-N1	6.02	120.71	117.70
1	AA	990	A	N9-C4-C5	-6.02	103.39	105.80
1	AA	2484	G	N3-C4-C5	-6.02	125.59	128.60
34	DA	23	C	O5'-P-OP2	6.02	117.92	110.70
1	AA	2399	U	C4-C5-C6	6.01	123.31	119.70
1	CA	1826	G	C5-N7-C8	6.01	107.31	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	869	U	C5-C6-N1	6.01	125.71	122.70
1	AA	15	G	C5-C6-N1	-6.01	108.49	111.50
1	CA	1427	A	P-O3'-C3'	6.01	126.91	119.70
1	AA	906	G	C4-N9-C1'	-6.01	118.69	126.50
1	AA	2018	C	N3-C4-C5	6.01	124.30	121.90
1	AA	806	G	C5-C6-O6	-6.01	125.00	128.60
1	AA	1694	G	C6-C5-N7	6.01	134.00	130.40
1	AA	2299	A	C6-C5-N7	-6.01	128.09	132.30
1	AA	2759	U	O5'-P-OP2	-6.01	100.29	105.70
1	CA	1975	G	C8-N9-C4	6.01	108.80	106.40
1	CA	2544	G	C5-C6-O6	-6.01	125.00	128.60
34	DA	355	C	C6-N1-C2	-6.01	117.90	120.30
1	AA	552	C	N1-C2-O2	-6.00	115.30	118.90
34	DA	754	C	N3-C2-O2	-6.00	117.70	121.90
1	AA	1924	C	C4-C5-C6	6.00	120.40	117.40
2	AB	27	C	O5'-P-OP2	-6.00	100.30	105.70
1	AA	470	C	OP1-P-OP2	-6.00	110.60	119.60
34	DA	784	C	N1-C2-O2	-6.00	115.30	118.90
1	AA	1324	A	N1-C2-N3	6.00	132.30	129.30
1	AA	2599	A	O5'-P-OP1	-6.00	100.30	105.70
1	CA	2032	G	C8-N9-C4	6.00	108.80	106.40
1	AA	113	C	C6-N1-C2	6.00	122.70	120.30
34	BA	442	C	C5-C6-N1	6.00	124.00	121.00
1	CA	330	A	N3-C4-C5	6.00	131.00	126.80
1	AA	1188	A	C4-C5-N7	5.99	113.70	110.70
1	AA	1755	C	N3-C4-C5	5.99	124.30	121.90
1	AA	223	C	N3-C2-O2	-5.99	117.71	121.90
1	CA	614	U	N1-C2-N3	5.99	118.50	114.90
1	AA	540	A	N9-C4-C5	5.99	108.20	105.80
1	CA	84	A	O4'-C1'-N9	5.99	112.99	108.20
34	BA	1501	C	C4-C5-C6	5.99	120.39	117.40
1	CA	1673	U	N3-C4-C5	5.99	118.19	114.60
1	AA	2676	G	N1-C6-O6	5.99	123.49	119.90
1	AA	2519	C	C5-C4-N4	5.99	124.39	120.20
2	AB	7	G	N1-C6-O6	5.99	123.49	119.90
1	CA	1332	G	O5'-P-OP2	-5.99	100.31	105.70
1	AA	1069	U	C2-N3-C4	-5.98	123.41	127.00
1	AA	1316	C	C2-N3-C4	-5.98	116.91	119.90
1	CA	2407	G	C4-N9-C1'	5.98	134.28	126.50
1	AA	1236	G	C8-N9-C4	5.98	108.79	106.40
1	AA	1405	A	N1-C2-N3	-5.98	126.31	129.30
34	BA	836	G	N1-C6-O6	5.98	123.49	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1832	G	O5'-P-OP1	-5.98	100.32	105.70
34	BA	760	G	N1-C6-O6	5.98	123.49	119.90
1	CA	2503	A	C5-C6-N6	-5.98	118.92	123.70
1	AA	2453	C	C2-N3-C4	-5.98	116.91	119.90
1	AA	723	A	C5-C6-N1	-5.98	114.71	117.70
1	AA	2556	G	N3-C2-N2	-5.98	115.72	119.90
34	BA	290	C	C6-N1-C2	5.98	122.69	120.30
1	AA	2613	C	C4-C5-C6	5.98	120.39	117.40
55	BV	21	C	C6-N1-C2	-5.97	117.91	120.30
1	AA	635	C	C6-N1-C2	5.97	122.69	120.30
1	AA	1233	U	N3-C4-O4	-5.97	115.22	119.40
1	AA	1296	G	N1-C6-O6	-5.97	116.32	119.90
34	BA	1036	G	C4-N9-C1'	5.97	134.26	126.50
1	CA	1064	C	C2-N1-C1'	5.97	125.37	118.80
1	CA	2373	G	N3-C2-N2	-5.97	115.72	119.90
34	BA	1442	G	C4-C5-N7	5.97	113.19	110.80
1	AA	1805	C	C2-N3-C4	-5.97	116.92	119.90
1	CA	556	G	N1-C6-O6	5.97	123.48	119.90
1	AA	785	G	C4-C5-N7	5.97	113.19	110.80
1	AA	44	G	N1-C6-O6	-5.97	116.32	119.90
1	AA	846	G	N3-C2-N2	5.97	124.08	119.90
1	AA	2576	A	N1-C6-N6	-5.97	115.02	118.60
1	AA	2895	C	C6-N1-C2	-5.97	117.91	120.30
1	AA	438	G	N1-C2-N3	5.96	127.48	123.90
1	AA	1914	C	N1-C2-O2	-5.96	115.32	118.90
1	AA	2889	C	O5'-P-OP2	-5.96	100.33	105.70
1	CA	1021	A	N7-C8-N9	5.96	116.78	113.80
1	AA	206	G	N3-C2-N2	-5.96	115.73	119.90
1	AA	481	C	N3-C4-C5	5.96	124.28	121.90
1	AA	521	G	C5-C6-O6	5.96	132.18	128.60
1	CA	945	A	O4'-C1'-N9	5.96	112.97	108.20
1	AA	1539	C	N1-C2-O2	5.96	122.47	118.90
1	AA	747	G	C4-C5-N7	-5.96	108.42	110.80
1	AA	194	G	C6-C5-N7	-5.95	126.83	130.40
1	AA	1845	G	C4-C5-N7	5.95	113.18	110.80
1	AA	2327	G	C8-N9-C4	5.95	108.78	106.40
1	AA	1244	U	C2-N3-C4	-5.95	123.43	127.00
1	AA	1369	U	C6-N1-C2	5.95	124.57	121.00
1	CA	420	C	N3-C2-O2	-5.95	117.73	121.90
34	BA	1502	A	C8-N9-C4	-5.95	103.42	105.80
1	CA	1656	C	C4-C5-C6	-5.95	114.42	117.40
1	AA	995	G	OP1-P-OP2	-5.95	110.68	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1067	A	O5'-P-OP1	-5.95	100.35	105.70
1	CA	176	G	C8-N9-C4	5.95	108.78	106.40
1	AA	2557	G	OP2-P-O3'	5.95	118.28	105.20
1	AA	751	G	O4'-C1'-N9	5.95	112.96	108.20
1	AA	958	C	C5-C6-N1	5.95	123.97	121.00
1	AA	1252	C	N3-C2-O2	-5.95	117.74	121.90
34	BA	297	G	C4-C5-N7	5.95	113.18	110.80
1	CA	2718	G	N1-C6-O6	5.95	123.47	119.90
1	CA	2855	C	C6-N1-C2	-5.95	117.92	120.30
1	AA	1332	A	C8-N9-C4	-5.94	103.42	105.80
1	CA	265	A	C6-C5-N7	-5.94	128.14	132.30
34	DA	437	U	O5'-P-OP1	-5.94	100.35	105.70
1	AA	1866	G	O5'-P-OP2	-5.94	100.35	105.70
1	AA	354	A	N7-C8-N9	5.94	116.77	113.80
1	AA	1696	G	N1-C6-O6	-5.94	116.34	119.90
1	AA	2355	C	OP1-P-OP2	5.94	128.51	119.60
34	BA	764	C	N3-C2-O2	-5.94	117.74	121.90
34	DA	897	C	C6-N1-C2	5.94	122.67	120.30
1	AA	615	G	OP2-P-O3'	5.94	118.26	105.20
1	AA	779	C	N3-C2-O2	5.94	126.06	121.90
34	BA	771	G	C8-N9-C4	-5.93	104.03	106.40
1	AA	2595	G	N3-C2-N2	-5.93	115.75	119.90
1	AA	2700	U	N3-C4-O4	5.93	123.55	119.40
1	CA	1407	C	N1-C2-O2	-5.93	115.34	118.90
1	AA	600	G	O5'-P-OP2	-5.93	100.37	105.70
1	AA	1659	G	C8-N9-C4	-5.93	104.03	106.40
1	AA	2162	C	C5-C6-N1	5.93	123.96	121.00
34	DA	1527	C	N3-C4-C5	5.93	124.27	121.90
1	CA	271(Y)	U	N3-C2-O2	-5.92	118.05	122.20
1	CA	25	U	N1-C2-O2	-5.92	118.65	122.80
34	DA	1154	G	C6-C5-N7	-5.92	126.85	130.40
1	AA	1245	C	O5'-P-OP2	-5.92	100.37	105.70
1	AA	2641	A	C5-C6-N6	-5.92	118.96	123.70
1	CA	1372	U	N3-C4-O4	5.92	123.55	119.40
1	CA	2324	C	C6-N1-C2	5.92	122.67	120.30
1	CA	34	C	N3-C2-O2	-5.92	117.76	121.90
1	AA	350	G	N9-C4-C5	5.92	107.77	105.40
1	AA	535	C	N3-C2-O2	-5.92	117.76	121.90
1	CA	2552	U	N3-C4-C5	5.92	118.15	114.60
1	AA	103	C	OP2-P-O3'	5.92	118.22	105.20
1	AA	741	U	C2-N3-C4	-5.92	123.45	127.00
34	DA	579	G	N1-C6-O6	5.92	123.45	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	127	C	N1-C2-O2	-5.91	115.35	118.90
1	AA	553	A	C5-C6-N6	-5.91	118.97	123.70
1	AA	2162	C	C6-N1-C1'	-5.91	113.71	120.80
1	AA	553	A	C5-C6-N1	-5.91	114.75	117.70
1	CA	2080	G	C5-N7-C8	5.91	107.25	104.30
1	CA	400	G	N1-C6-O6	5.91	123.44	119.90
1	CA	2335	A	O4'-C1'-N9	5.91	112.93	108.20
1	CA	2576	G	O5'-P-OP2	5.91	117.79	110.70
1	AA	518	G	C5-N7-C8	5.91	107.25	104.30
1	AA	846	G	N3-C4-N9	5.91	129.54	126.00
1	AA	977	G	O5'-P-OP1	5.91	117.79	110.70
1	CA	2487	G	N9-C4-C5	-5.91	103.04	105.40
1	AA	2258	G	N7-C8-N9	-5.90	110.15	113.10
1	AA	2616	U	OP1-P-O3'	5.90	118.19	105.20
24	A0	12	ASN	C-N-CA	-5.90	109.90	122.30
1	AA	1038	C	C2-N3-C4	-5.90	116.95	119.90
1	AA	2835	C	C6-N1-C2	5.90	122.66	120.30
1	AA	279	G	C6-C5-N7	-5.90	126.86	130.40
1	AA	1924	C	N3-C4-C5	-5.90	119.54	121.90
1	AA	1961	U	N3-C4-C5	5.90	118.14	114.60
1	AA	193	A	C2-N3-C4	5.90	113.55	110.60
1	AA	996	C	N3-C4-N4	-5.90	113.87	118.00
1	AA	1175	A	O5'-P-OP2	-5.89	100.39	105.70
1	AA	1387	U	N3-C2-O2	5.89	126.33	122.20
34	BA	1341	U	N3-C2-O2	-5.89	118.07	122.20
1	CA	1204	A	N9-C4-C5	-5.89	103.44	105.80
1	CA	1626	G	C8-N9-C4	-5.89	104.04	106.40
1	CA	2235	G	N1-C6-O6	5.89	123.44	119.90
1	AA	2078	G	N1-C6-O6	-5.89	116.36	119.90
1	AA	126	C	O5'-P-OP1	-5.89	100.40	105.70
1	AA	1981	G	OP2-P-O3'	5.89	118.16	105.20
1	AA	338	A	C5-N7-C8	-5.89	100.95	103.90
1	AA	1184	G	N9-C4-C5	5.89	107.76	105.40
1	AA	2033	U	C5-C4-O4	5.89	129.43	125.90
1	CA	1850	G	C5-C6-O6	-5.89	125.07	128.60
1	AA	988	U	O5'-P-OP2	-5.89	100.40	105.70
1	AA	31	C	O5'-P-OP1	-5.89	100.40	105.70
1	AA	502	G	C8-N9-C4	5.89	108.75	106.40
1	AA	1067	A	C6-C5-N7	-5.89	128.18	132.30
1	AA	2063	U	N1-C2-O2	-5.89	118.68	122.80
1	AA	2264	G	C5-C6-O6	5.89	132.13	128.60
1	CA	12	U	N1-C2-O2	5.89	126.92	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	DA	1158	C	C6-N1-C2	-5.89	117.94	120.30
1	AA	2189	U	C2-N1-C1'	5.88	124.76	117.70
1	CA	265	A	C2-N3-C4	-5.88	107.66	110.60
1	CA	2421	G	C8-N9-C4	5.88	108.75	106.40
1	CA	2689	U	C6-N1-C2	-5.88	117.47	121.00
1	AA	1336	C	OP2-P-O3'	5.88	118.14	105.20
1	AA	1703	C	N3-C4-C5	5.88	124.25	121.90
1	AA	2399	U	C5-C6-N1	-5.88	119.76	122.70
34	DA	219	C	C6-N1-C2	-5.88	117.95	120.30
34	DA	354	G	C6-C5-N7	-5.88	126.87	130.40
1	AA	708	C	C5-C6-N1	-5.88	118.06	121.00
29	A5	16	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	CA	1429	G	C2-N3-C4	5.88	114.84	111.90
34	BA	659	U	O5'-P-OP2	-5.87	100.41	105.70
1	AA	2641	A	C8-N9-C1'	-5.87	117.13	127.70
1	AA	2849	G	N9-C4-C5	-5.87	103.05	105.40
34	DA	1079	G	O5'-P-OP1	-5.87	100.42	105.70
1	AA	2553	A	N1-C6-N6	5.87	122.12	118.60
34	BA	53	A	C8-N9-C4	-5.87	103.45	105.80
34	DA	1064	G	P-O3'-C3'	5.87	126.74	119.70
1	AA	887	C	C2-N3-C4	-5.87	116.97	119.90
1	AA	1188	A	N7-C8-N9	5.87	116.73	113.80
1	AA	2381	A	N1-C6-N6	-5.87	115.08	118.60
34	BA	326	G	C6-C5-N7	-5.87	126.88	130.40
1	AA	639	G	C4-C5-N7	-5.87	108.45	110.80
1	AA	2521	G	N9-C4-C5	-5.87	103.05	105.40
1	AA	2529	C	C4-C5-C6	-5.87	114.47	117.40
1	AA	2571	C	C4-C5-C6	-5.87	114.47	117.40
1	CA	2617	C	C6-N1-C2	5.87	122.65	120.30
1	AA	352	U	OP1-P-O3'	5.86	118.10	105.20
1	AA	1006	C	C2-N1-C1'	-5.86	112.35	118.80
1	CA	1122	G	C5-C6-O6	-5.86	125.08	128.60
1	AA	1657	C	C2-N3-C4	-5.86	116.97	119.90
2	AB	114	C	N3-C4-C5	5.86	124.24	121.90
34	BA	410	G	C8-N9-C4	-5.86	104.06	106.40
1	CA	2360	A	N7-C8-N9	-5.86	110.87	113.80
34	BA	1523	G	OP1-P-OP2	5.86	128.39	119.60
1	AA	2039	U	O5'-P-OP1	-5.86	100.43	105.70
1	AA	2641	A	C8-N9-C4	-5.86	103.46	105.80
1	CA	2085	C	N3-C4-C5	5.86	124.24	121.90
34	BA	1082	G	C5-C6-O6	-5.85	125.09	128.60
1	AA	22	C	N1-C2-O2	5.85	122.41	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	592	U	N3-C4-O4	5.85	123.50	119.40
1	AA	671	A	C8-N9-C4	-5.85	103.46	105.80
1	AA	710	G	N3-C2-N2	-5.85	115.80	119.90
1	AA	870	G	N1-C6-O6	-5.85	116.39	119.90
1	AA	1000	C	N1-C2-O2	-5.85	115.39	118.90
1	AA	1157	A	C2-N3-C4	-5.85	107.67	110.60
2	CB	91	C	C6-N1-C2	5.85	122.64	120.30
1	AA	870	G	N9-C4-C5	5.85	107.74	105.40
1	AA	833	C	N3-C4-N4	-5.85	113.91	118.00
1	AA	1845	G	C5-C6-O6	-5.85	125.09	128.60
1	CA	756	C	N1-C2-O2	-5.85	115.39	118.90
1	CA	2875	C	C5-C6-N1	-5.85	118.08	121.00
34	DA	1158	C	N1-C2-O2	5.85	122.41	118.90
1	AA	1231	G	C6-N1-C2	-5.85	121.59	125.10
34	BA	758	G	O5'-P-OP1	5.85	117.72	110.70
1	AA	1463	C	OP1-P-OP2	-5.85	110.83	119.60
1	AA	1870	G	N1-C6-O6	-5.85	116.39	119.90
1	CA	151	C	C6-N1-C2	5.85	122.64	120.30
1	CA	1696	G	O5'-P-OP2	-5.85	100.44	105.70
1	AA	1423	G	N3-C2-N2	5.84	123.99	119.90
1	AA	1593	C	O5'-P-OP1	-5.84	100.44	105.70
1	AA	2052	A	C8-N9-C4	5.84	108.14	105.80
34	BA	1524	C	N1-C2-N3	5.84	123.29	119.20
1	CA	1204	A	N3-C4-C5	5.84	130.89	126.80
1	CA	2029	G	C5-C6-O6	-5.84	125.09	128.60
1	AA	645	G	N9-C4-C5	-5.84	103.06	105.40
1	AA	849	A	N1-C6-N6	-5.84	115.09	118.60
1	CA	2206	G	C4-N9-C1'	-5.84	118.90	126.50
1	AA	491	G	N7-C8-N9	5.84	116.02	113.10
1	AA	138	G	OP1-P-OP2	-5.84	110.84	119.60
1	AA	1961	U	N1-C2-N3	-5.84	111.40	114.90
1	AA	2043	C	C5-C6-N1	-5.84	118.08	121.00
1	AA	2605	U	C2-N3-C4	-5.84	123.50	127.00
1	CA	961	C	N3-C4-C5	5.84	124.23	121.90
1	CA	596	G	N1-C6-O6	-5.84	116.40	119.90
1	CA	2023	G	C5-C6-O6	-5.83	125.10	128.60
1	CA	2546	U	C5-C6-N1	-5.83	119.78	122.70
1	AA	52	A	N1-C2-N3	5.83	132.22	129.30
1	AA	1403	U	N3-C2-O2	-5.83	118.12	122.20
1	AA	2521	G	C4-C5-N7	5.83	113.13	110.80
1	AA	2574	U	N3-C2-O2	-5.83	118.12	122.20
1	AA	1009	C	N1-C2-O2	5.83	122.40	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	2364	A	C8-N9-C4	5.83	108.13	105.80
1	AA	331	G	N3-C4-C5	-5.83	125.69	128.60
1	AA	1401	G	N1-C6-O6	-5.83	116.41	119.90
1	AA	2542	A	C2-N3-C4	-5.83	107.69	110.60
1	AA	2802	C	O4'-C1'-N1	5.83	112.86	108.20
1	CA	2867	G	O4'-C1'-N9	5.83	112.86	108.20
1	AA	1728	G	N1-C6-O6	5.82	123.39	119.90
1	CA	674	G	N1-C6-O6	5.82	123.39	119.90
1	AA	808	A	C2-N3-C4	-5.82	107.69	110.60
1	AA	831	A	C5-N7-C8	5.82	106.81	103.90
34	DA	687	A	P-O3'-C3'	5.82	126.69	119.70
1	AA	234	G	C2-N3-C4	-5.82	108.99	111.90
1	AA	817	G	N3-C2-N2	5.82	123.97	119.90
1	AA	2501	G	N3-C4-C5	-5.82	125.69	128.60
1	AA	1185	C	N1-C2-O2	-5.82	115.41	118.90
1	AA	1637	G	N1-C6-O6	-5.82	116.41	119.90
34	BA	852	G	O5'-P-OP2	-5.82	100.46	105.70
1	CA	577	G	N9-C4-C5	-5.82	103.07	105.40
1	CA	2513	G	C5-C6-O6	-5.82	125.11	128.60
1	CA	1885	A	C8-N9-C4	5.82	108.13	105.80
1	CA	2447	G	O5'-P-OP2	-5.82	100.47	105.70
1	AA	1513	G	OP2-P-O3'	5.81	117.99	105.20
34	BA	972	C	C6-N1-C2	-5.81	117.97	120.30
1	CA	1299	G	C8-N9-C4	-5.81	104.07	106.40
1	AA	892	G	O4'-C1'-N9	5.81	112.85	108.20
1	AA	1020	C	O5'-P-OP1	-5.81	100.47	105.70
1	CA	1992	G	N1-C6-O6	-5.81	116.41	119.90
1	AA	1059	C	C6-N1-C2	5.81	122.62	120.30
1	AA	1646	C	C4-C5-C6	5.81	120.31	117.40
1	AA	2565	G	C5-C6-N1	5.81	114.41	111.50
1	AA	2603	C	N3-C4-C5	5.81	124.22	121.90
1	CA	2618	G	C8-N9-C4	5.81	108.72	106.40
1	AA	2265	G	N7-C8-N9	-5.81	110.20	113.10
1	AA	2303	U	C5-C6-N1	-5.81	119.80	122.70
1	CA	2724	C	N3-C4-C5	5.81	124.22	121.90
1	AA	85	C	C5-C6-N1	-5.81	118.10	121.00
1	CA	2070	G	N1-C2-N3	5.80	127.38	123.90
1	AA	1302	G	N9-C4-C5	-5.80	103.08	105.40
1	AA	2022	G	OP1-P-OP2	5.80	128.30	119.60
1	AA	107	G	N1-C6-O6	-5.80	116.42	119.90
13	AP	18	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	CA	2273	A	O5'-P-OP2	-5.80	100.48	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	976	G	C6-N1-C2	-5.80	121.62	125.10
1	AA	1018	A	OP1-P-OP2	-5.80	110.90	119.60
1	AA	2093	A	C2-N3-C4	-5.80	107.70	110.60
1	AA	2824	C	N1-C2-O2	-5.80	115.42	118.90
1	CA	1235	G	N1-C6-O6	5.80	123.38	119.90
1	AA	123	G	C5-C6-O6	-5.80	125.12	128.60
1	AA	853	C	C4-C5-C6	-5.80	114.50	117.40
1	AA	2565	G	N3-C4-N9	5.80	129.48	126.00
34	BA	600	C	O5'-P-OP2	-5.80	100.48	105.70
1	AA	560	C	C5-C6-N1	-5.79	118.10	121.00
34	DA	884	U	N1-C2-O2	-5.79	118.75	122.80
1	AA	1029	A	O5'-P-OP2	-5.79	100.49	105.70
1	AA	1410	G	C5-C6-O6	-5.79	125.12	128.60
1	AA	1920	U	N3-C2-O2	-5.79	118.15	122.20
1	AA	1965	U	C2-N3-C4	-5.79	123.53	127.00
1	CA	1279	G	C2-N3-C4	-5.79	109.00	111.90
1	CA	1698	A	C8-N9-C4	-5.79	103.48	105.80
1	AA	426	G	C8-N9-C4	5.79	108.72	106.40
1	AA	2561	G	N1-C6-O6	5.79	123.37	119.90
1	AA	2002	G	C8-N9-C4	-5.79	104.08	106.40
1	AA	894	U	C6-N1-C1'	5.79	129.30	121.20
1	AA	918	U	C5-C4-O4	-5.78	122.43	125.90
1	AA	1030	A	N1-C6-N6	-5.78	115.13	118.60
1	AA	1069	U	C5-C6-N1	-5.78	119.81	122.70
1	AA	2243	C	C4-C5-C6	5.78	120.29	117.40
1	AA	2738	A	C2-N3-C4	-5.78	107.71	110.60
1	CA	2372	G	C8-N9-C4	-5.78	104.09	106.40
1	AA	2871	G	C5-C6-O6	-5.78	125.13	128.60
34	BA	335	C	N1-C2-O2	5.78	122.37	118.90
1	CA	1855	G	C8-N9-C4	5.78	108.71	106.40
1	AA	235	C	N3-C4-C5	5.78	124.21	121.90
1	AA	716	G	OP1-P-OP2	-5.78	110.93	119.60
1	AA	2553	A	C5-N7-C8	-5.78	101.01	103.90
1	CA	2490	G	N9-C4-C5	-5.78	103.09	105.40
1	CA	2847	U	C5-C4-O4	-5.78	122.43	125.90
1	AA	960	C	C5-C6-N1	-5.78	118.11	121.00
1	AA	2378	A	N1-C6-N6	5.78	122.06	118.60
1	CA	686	G	O4'-C1'-N9	5.78	112.82	108.20
34	BA	266	G	C6-C5-N7	-5.77	126.94	130.40
1	AA	542	C	N3-C4-N4	5.77	122.04	118.00
1	CA	1496	A	C8-N9-C4	-5.77	103.49	105.80
1	AA	2082	A	C2-N3-C4	-5.77	107.72	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	AW	17	VAL	CB-CA-C	-5.77	100.44	111.40
1	AA	491	G	C8-N9-C4	-5.77	104.09	106.40
1	AA	1691	C	N1-C2-O2	5.77	122.36	118.90
1	AA	2264	G	C4-C5-N7	-5.77	108.49	110.80
34	BA	321	A	O5'-P-OP2	-5.77	100.51	105.70
1	CA	670	A	O4'-C1'-N9	-5.77	103.58	108.20
34	DA	910	C	C6-N1-C2	5.77	122.61	120.30
1	AA	1623	U	N3-C2-O2	-5.77	118.16	122.20
1	AA	2481	A	OP2-P-O3'	5.77	117.89	105.20
1	AA	2607	G	N1-C6-O6	-5.77	116.44	119.90
1	AA	1312	G	C2-N3-C4	5.77	114.78	111.90
1	AA	1814	A	N9-C4-C5	5.77	108.11	105.80
1	AA	852	G	N1-C6-O6	-5.76	116.44	119.90
1	AA	980	C	C6-N1-C2	5.76	122.61	120.30
1	AA	1240	G	N1-C2-N2	5.76	121.39	116.20
1	CA	704	G	O4'-C1'-N9	5.76	112.81	108.20
1	CA	799	G	C5-C6-O6	-5.76	125.14	128.60
1	CA	2361	A	C2-N3-C4	-5.76	107.72	110.60
1	CA	1977	A	C5-C6-N6	5.76	128.31	123.70
1	AA	361	C	C6-N1-C2	5.76	122.60	120.30
1	AA	801	C	C2-N3-C4	-5.76	117.02	119.90
1	AA	2029	C	C6-N1-C2	-5.76	118.00	120.30
1	AA	2066	C	N1-C2-N3	5.76	123.23	119.20
34	BA	266	G	P-O3'-C3'	5.76	126.61	119.70
2	AB	1	U	N1-C2-O2	5.76	126.83	122.80
1	CA	1021	A	C8-N9-C4	-5.76	103.50	105.80
1	CA	2742	C	C6-N1-C2	5.76	122.60	120.30
1	AA	556	C	C2-N3-C4	-5.76	117.02	119.90
1	AA	1431	G	O4'-C1'-N9	5.76	112.80	108.20
1	AA	2346	G	C6-C5-N7	-5.76	126.95	130.40
1	AA	2387	G	C8-N9-C4	5.76	108.70	106.40
34	BA	615	C	C6-N1-C2	-5.75	118.00	120.30
1	AA	2585	C	C5-C6-N1	-5.75	118.12	121.00
34	BA	769	G	O5'-P-OP1	5.75	117.60	110.70
34	BA	1442	G	C2-N3-C4	-5.75	109.02	111.90
1	CA	2028	U	N3-C2-O2	-5.75	118.17	122.20
34	DA	1054	C	O4'-C1'-N1	5.75	112.80	108.20
1	AA	1751	G	N1-C6-O6	-5.75	116.45	119.90
1	AA	2609	G	C4-C5-N7	5.75	113.10	110.80
1	CA	528	A	N1-C2-N3	5.75	132.17	129.30
1	CA	2824	C	C5-C4-N4	-5.75	116.18	120.20
57	DX	20	U	C2-N1-C1'	5.75	124.60	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	960	C	C6-N1-C2	5.75	122.60	120.30
1	CA	829	A	N1-C6-N6	5.75	122.05	118.60
1	CA	1672	C	C6-N1-C2	-5.75	118.00	120.30
1	AA	1983	C	C5-C6-N1	-5.75	118.13	121.00
1	CA	1781	C	C6-N1-C1'	5.74	127.69	120.80
1	AA	894	U	C2-N1-C1'	-5.74	110.81	117.70
1	AA	2460	A	C8-N9-C4	-5.74	103.50	105.80
1	CA	2003	G	O5'-P-OP1	-5.74	100.53	105.70
1	AA	2528	G	C4-C5-N7	-5.74	108.50	110.80
1	AA	784	C	C6-N1-C2	5.74	122.59	120.30
1	AA	1313	U	N3-C4-O4	-5.74	115.38	119.40
1	AA	2219	U	C4-C5-C6	5.74	123.14	119.70
1	AA	2655	G	N9-C4-C5	-5.74	103.11	105.40
34	BA	1397	C	C5-C4-N4	5.74	124.22	120.20
1	AA	560	C	N1-C2-N3	5.74	123.22	119.20
1	AA	457	G	C5-C6-O6	-5.74	125.16	128.60
1	AA	1370	G	N1-C2-N3	5.74	127.34	123.90
1	AA	2264	G	N3-C4-N9	-5.74	122.56	126.00
1	AA	2345	A	P-O3'-C3'	5.74	126.58	119.70
1	AA	2643	G	OP1-P-OP2	5.73	128.20	119.60
1	AA	2849	G	N7-C8-N9	-5.73	110.23	113.10
2	AB	63	G	O5'-P-OP2	-5.73	100.54	105.70
1	AA	59	G	C5-C6-O6	-5.73	125.16	128.60
1	AA	430	U	N3-C2-O2	-5.73	118.19	122.20
1	AA	725	C	N1-C2-O2	-5.73	115.46	118.90
1	AA	2696	U	C5-C6-N1	-5.73	119.83	122.70
34	BA	890	G	N3-C2-N2	5.73	123.91	119.90
1	CA	383	U	O4'-C1'-N1	5.73	112.79	108.20
1	AA	240	A	N1-C2-N3	-5.73	126.43	129.30
1	AA	827	G	N3-C2-N2	-5.73	115.89	119.90
1	AA	2472	U	O5'-P-OP1	-5.73	100.54	105.70
1	CA	563	G	C4-C5-N7	5.73	113.09	110.80
1	CA	1797	C	N3-C4-C5	5.73	124.19	121.90
1	CA	2377	A	C2-N3-C4	-5.73	107.73	110.60
1	CA	2647	U	C5-C6-N1	-5.73	119.83	122.70
1	AA	131	C	N1-C2-O2	5.73	122.34	118.90
1	AA	395	C	N1-C2-O2	-5.73	115.46	118.90
1	CA	2407	G	C8-N9-C1'	-5.73	119.55	127.00
34	DA	266	G	C5-N7-C8	-5.73	101.44	104.30
1	AA	1849	U	N3-C4-C5	5.73	118.04	114.60
1	AA	715	G	C4-C5-N7	5.73	113.09	110.80
1	AA	1208	G	C5-N7-C8	5.73	107.16	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1042	A	N1-C6-N6	-5.72	115.17	118.60
1	CA	2050	C	N3-C4-C5	5.72	124.19	121.90
1	AA	125	A	C8-N9-C4	5.72	108.09	105.80
1	AA	621	G	C8-N9-C4	-5.72	104.11	106.40
1	AA	1097	G	C4-C5-N7	5.72	113.09	110.80
1	AA	1721	G	N9-C4-C5	-5.72	103.11	105.40
1	CA	2242	G	C8-N9-C4	5.72	108.69	106.40
1	CA	147	U	C5-C6-N1	-5.72	119.84	122.70
1	AA	1321	A	C5-N7-C8	5.72	106.76	103.90
1	AA	2776	G	C8-N9-C4	5.72	108.69	106.40
4	AD	111	LEU	CA-CB-CG	5.72	128.45	115.30
1	AA	2461	U	N3-C4-O4	5.72	123.40	119.40
1	AA	1296	G	N7-C8-N9	-5.72	110.24	113.10
1	AA	1415	G	C5-C6-O6	-5.72	125.17	128.60
1	AA	1484	U	N3-C4-O4	5.71	123.40	119.40
1	AA	583	C	C5-C6-N1	-5.71	118.14	121.00
1	AA	891	C	N3-C4-C5	5.71	124.18	121.90
1	AA	2581	G	C5-C6-N1	5.71	114.35	111.50
1	AA	2604	G	OP2-P-O3'	5.71	117.76	105.20
1	CA	2523	G	N3-C4-N9	5.71	129.43	126.00
1	CA	2772	C	C6-N1-C2	-5.71	118.02	120.30
34	BA	554	C	N1-C2-O2	-5.71	115.48	118.90
1	CA	1355	G	N3-C4-C5	-5.71	125.75	128.60
1	AA	2745	G	N3-C2-N2	-5.70	115.91	119.90
34	DA	266	G	P-O3'-C3'	5.70	126.55	119.70
1	AA	782	A	C5-C6-N1	-5.70	114.85	117.70
1	AA	1179	U	C2-N3-C4	-5.70	123.58	127.00
1	CA	1977	A	C4-C5-N7	-5.70	107.85	110.70
1	CA	2541	A	N1-C2-N3	5.70	132.15	129.30
1	AA	123	G	C2-N3-C4	5.70	114.75	111.90
1	CA	474	G	N3-C4-C5	-5.70	125.75	128.60
1	CA	1212	G	N3-C4-C5	-5.70	125.75	128.60
1	AA	107	G	C5-C6-N1	5.70	114.35	111.50
1	AA	200	A	N1-C2-N3	5.70	132.15	129.30
1	CA	410	G	N1-C6-O6	-5.70	116.48	119.90
2	CB	10	C	C6-N1-C2	-5.70	118.02	120.30
1	AA	1487	G	N1-C2-N2	5.70	121.33	116.20
1	AA	184	A	P-O3'-C3'	5.70	126.53	119.70
1	AA	471	C	C6-N1-C2	-5.70	118.02	120.30
1	AA	491	G	C4-C5-N7	5.70	113.08	110.80
1	AA	2783	G	C8-N9-C4	5.70	108.68	106.40
1	CA	2019	A	C5-N7-C8	5.70	106.75	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1204	A	C5-C6-N1	-5.69	114.85	117.70
1	CA	1313	U	O4'-C1'-N1	5.69	112.76	108.20
2	CB	115	G	C8-N9-C4	5.69	108.68	106.40
1	AA	419	C	O5'-P-OP1	-5.69	100.58	105.70
1	AA	1438	A	C5-C6-N1	5.69	120.55	117.70
1	AA	139	A	N1-C2-N3	5.69	132.15	129.30
1	AA	1817	A	C8-N9-C4	5.69	108.08	105.80
1	AA	2448	G	OP1-P-O3'	5.69	117.72	105.20
1	CA	2848	G	O4'-C1'-N9	5.69	112.75	108.20
1	AA	2052	A	C4-C5-N7	5.69	113.54	110.70
1	CA	1788	C	N3-C4-C5	-5.69	119.62	121.90
1	CA	2718	G	C5-C6-O6	-5.69	125.19	128.60
1	AA	541	C	N3-C4-C5	5.69	124.17	121.90
1	AA	847	A	N1-C2-N3	5.69	132.14	129.30
1	AA	2096	U	N1-C2-O2	-5.69	118.82	122.80
1	AA	2117	C	O5'-P-OP2	-5.69	100.58	105.70
1	AA	2544	G	C5-C6-O6	-5.69	125.19	128.60
1	CA	1613	G	C5-C6-O6	-5.69	125.19	128.60
1	CA	2077	A	N1-C6-N6	5.69	122.01	118.60
34	DA	1500	A	N1-C6-N6	5.69	122.01	118.60
1	AA	2052	A	N9-C4-C5	-5.69	103.53	105.80
1	AA	1427	G	C5-C6-O6	-5.68	125.19	128.60
1	AA	2552	C	N3-C4-C5	5.68	124.17	121.90
34	BA	1464	G	N1-C6-O6	5.68	123.31	119.90
1	CA	2425	A	C5-C6-N1	5.68	120.54	117.70
34	DA	886	G	N9-C4-C5	-5.68	103.13	105.40
1	AA	518	G	N7-C8-N9	-5.68	110.26	113.10
1	AA	715	G	OP2-P-O3'	5.68	117.70	105.20
1	AA	2364	A	O5'-P-OP1	-5.68	100.59	105.70
1	AA	2511	C	N1-C2-O2	-5.68	115.49	118.90
1	CA	981	A	C8-N9-C4	5.68	108.07	105.80
1	CA	1842	G	N9-C4-C5	-5.68	103.13	105.40
1	AA	833	C	N3-C4-C5	5.68	124.17	121.90
1	AA	2372	A	O5'-P-OP1	5.68	117.51	110.70
1	AA	2561	G	C5-N7-C8	-5.68	101.46	104.30
1	AA	2659	U	C6-N1-C2	5.68	124.41	121.00
1	AA	2707	C	C6-N1-C2	5.68	122.57	120.30
1	AA	2837	C	N1-C2-O2	-5.68	115.49	118.90
1	CA	529	A	C5-N7-C8	-5.68	101.06	103.90
1	CA	1204	A	C6-C5-N7	-5.68	128.33	132.30
1	AA	2773	C	O5'-P-OP1	-5.67	100.59	105.70
1	CA	560	C	C5-C6-N1	-5.67	118.16	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1292	U	N1-C2-O2	-5.67	118.83	122.80
1	CA	2517	C	N3-C4-C5	5.67	124.17	121.90
1	CA	2373	G	N1-C6-O6	5.67	123.30	119.90
1	AA	200	A	C4-C5-C6	5.67	119.84	117.00
1	AA	2528	G	C6-C5-N7	5.67	133.80	130.40
1	AA	2625	U	C5-C4-O4	5.67	129.30	125.90
1	AA	2887	G	N1-C6-O6	-5.67	116.50	119.90
1	CA	188	G	N3-C2-N2	5.67	123.87	119.90
34	DA	532	A	OP1-P-O3'	5.67	117.68	105.20
1	AA	830	A	C8-N9-C4	-5.67	103.53	105.80
1	AA	1438	A	N9-C4-C5	-5.67	103.53	105.80
34	BA	44	G	N3-C2-N2	-5.67	115.93	119.90
1	CA	668	G	C2-N3-C4	-5.67	109.07	111.90
1	CA	2593	U	N3-C4-C5	5.67	118.00	114.60
1	AA	1695	C	C2-N1-C1'	-5.67	112.57	118.80
1	AA	2370	G	C2-N3-C4	-5.67	109.07	111.90
1	AA	2397	C	C2-N3-C4	-5.67	117.07	119.90
1	AA	2802	C	C5-C6-N1	-5.67	118.17	121.00
34	BA	1505	G	C5-C6-N1	-5.67	108.67	111.50
1	AA	526	A	N1-C2-N3	5.66	132.13	129.30
1	AA	954	C	C2-N3-C4	-5.66	117.07	119.90
1	AA	2696	U	C2-N3-C4	-5.66	123.60	127.00
1	CA	918	A	O5'-P-OP1	-5.66	100.60	105.70
1	AA	713	G	OP2-P-O3'	5.66	117.66	105.20
1	AA	20	C	N3-C4-N4	-5.66	114.04	118.00
34	BA	1442	G	N1-C6-O6	5.66	123.30	119.90
1	CA	426	C	N3-C2-O2	-5.66	117.94	121.90
1	CA	1385	G	O4'-C1'-N9	5.66	112.73	108.20
1	AA	957	A	N1-C6-N6	-5.66	115.20	118.60
1	AA	2498	G	N3-C4-N9	5.66	129.40	126.00
1	AA	1037	C	N3-C4-C5	5.65	124.16	121.90
1	AA	1849	U	C2-N3-C4	-5.65	123.61	127.00
34	BA	110	C	N1-C2-O2	5.65	122.29	118.90
1	AA	2089	G	N9-C4-C5	5.65	107.66	105.40
1	AA	2823	A	N1-C6-N6	-5.65	115.21	118.60
34	BA	1442	G	C8-N9-C4	-5.65	104.14	106.40
34	BA	1502	A	C6-C5-N7	-5.65	128.34	132.30
1	CA	1499	C	N3-C4-C5	5.65	124.16	121.90
1	AA	1070	G	C6-C5-N7	-5.65	127.01	130.40
1	AA	1810	U	C5-C4-O4	-5.65	122.51	125.90
1	CA	1901	A	O5'-P-OP1	-5.65	100.62	105.70
1	AA	1488	G	C8-N9-C4	-5.65	104.14	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	2797	C	N3-C2-O2	-5.65	117.95	121.90
34	BA	277	C	C2-N3-C4	-5.64	117.08	119.90
34	BA	567	G	O5'-P-OP1	-5.64	100.62	105.70
1	CA	1681	G	C5-N7-C8	-5.64	101.48	104.30
1	AA	870	G	C5-C6-O6	5.64	131.99	128.60
1	AA	1805	C	N3-C2-O2	-5.64	117.95	121.90
1	AA	2520	G	N3-C4-C5	-5.64	125.78	128.60
1	AA	2602	A	OP1-P-OP2	-5.64	111.14	119.60
1	AA	2292	G	OP2-P-O3'	5.64	117.61	105.20
1	AA	1712	A	C8-N9-C4	-5.64	103.54	105.80
1	AA	2538	G	C5-C6-O6	5.64	131.98	128.60
1	AA	2632	C	C2-N1-C1'	-5.64	112.60	118.80
1	AA	371	A	N1-C2-N3	5.64	132.12	129.30
1	AA	1015	C	C5-C6-N1	5.64	123.82	121.00
1	AA	1252	C	C4-C5-C6	5.64	120.22	117.40
1	AA	2693	C	C6-N1-C2	-5.64	118.05	120.30
1	CA	2605	U	N3-C4-C5	5.64	117.98	114.60
1	AA	2346	G	C8-N9-C1'	-5.63	119.67	127.00
34	DA	1405	G	N3-C4-N9	5.63	129.38	126.00
1	CA	778	G	C4-C5-N7	5.63	113.05	110.80
1	CA	2085	C	C5-C4-N4	-5.63	116.26	120.20
1	AA	491	G	C5-N7-C8	-5.63	101.48	104.30
1	AA	663	G	N1-C6-O6	-5.63	116.52	119.90
34	BA	123	C	C6-N1-C2	5.63	122.55	120.30
1	CA	2318	G	O4'-C1'-N9	5.63	112.71	108.20
1	CA	2387	U	C2-N1-C1'	-5.63	110.94	117.70
1	AA	1813	C	O5'-P-OP2	5.63	117.45	110.70
34	BA	115	G	P-O3'-C3'	5.63	126.45	119.70
1	CA	1616	A	C2-N3-C4	-5.63	107.78	110.60
1	AA	2650	G	N3-C4-N9	5.63	129.38	126.00
1	CA	2503	A	N1-C6-N6	5.63	121.98	118.60
34	DA	795	C	C2-N3-C4	-5.63	117.09	119.90
1	AA	783	C	C6-N1-C2	5.62	122.55	120.30
1	AA	2898	C	N3-C4-N4	-5.62	114.06	118.00
34	DA	894	G	C5-C6-O6	-5.62	125.22	128.60
1	AA	1023	G	C8-N9-C4	-5.62	104.15	106.40
1	AA	1742	G	C4-C5-N7	5.62	113.05	110.80
1	AA	2544	G	N1-C6-O6	5.62	123.27	119.90
1	AA	877	G	N1-C6-O6	-5.62	116.53	119.90
1	AA	2503	U	N3-C4-C5	5.62	117.97	114.60
1	CA	1501	C	C5-C6-N1	5.62	123.81	121.00
1	AA	2504	U	N3-C2-O2	-5.62	118.27	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1029	A	O5'-P-OP1	5.62	117.44	110.70
1	AA	1243	U	C5-C6-N1	-5.62	119.89	122.70
1	AA	2520	G	N1-C6-O6	-5.62	116.53	119.90
1	AA	2607	G	N3-C4-N9	-5.62	122.63	126.00
1	CA	34	C	C5-C6-N1	5.62	123.81	121.00
34	BA	1526	G	C5-C6-N1	5.61	114.31	111.50
1	CA	2456	C	C6-N1-C2	5.61	122.55	120.30
1	AA	1463	C	N3-C4-N4	5.61	121.93	118.00
1	AA	777	C	N1-C2-N3	5.61	123.13	119.20
1	AA	707	G	N1-C6-O6	5.61	123.26	119.90
1	AA	874	U	C5-C6-N1	-5.61	119.90	122.70
1	AA	1020	C	N3-C4-C5	5.61	124.14	121.90
1	AA	2074	G	N9-C4-C5	5.61	107.64	105.40
1	AA	2898	C	C5-C6-N1	-5.61	118.20	121.00
34	DA	97	G	O4'-C1'-N9	5.61	112.69	108.20
1	AA	252	C	C6-N1-C2	5.61	122.54	120.30
1	CA	845	G	O4'-C1'-N9	5.61	112.69	108.20
34	DA	320	C	C6-N1-C2	5.61	122.54	120.30
1	CA	1552	G	O5'-P-OP2	-5.60	100.66	105.70
1	AA	2450	U	C2-N3-C4	-5.60	123.64	127.00
1	AA	1412	A	N9-C4-C5	-5.60	103.56	105.80
1	AA	1712	A	N9-C4-C5	5.60	108.04	105.80
1	AA	2331	G	N9-C1'-C2'	5.60	121.28	114.00
34	BA	1113	C	C5-C6-N1	5.60	123.80	121.00
1	AA	438	G	C8-N9-C4	-5.60	104.16	106.40
1	AA	2400	A	OP1-P-OP2	-5.60	111.20	119.60
34	BA	254	G	O5'-P-OP1	-5.60	100.66	105.70
1	CA	1945	G	C8-N9-C1'	-5.60	119.72	127.00
1	CA	2674	G	C8-N9-C4	5.60	108.64	106.40
1	AA	2064	A	O5'-P-OP1	5.60	117.42	110.70
2	AB	72	G	C2-N3-C4	-5.60	109.10	111.90
1	CA	532	A	O4'-C1'-N9	5.60	112.68	108.20
1	CA	945	A	N7-C8-N9	5.60	116.60	113.80
34	DA	1502	A	O5'-P-OP2	-5.60	100.66	105.70
1	AA	352	U	N3-C2-O2	-5.60	118.28	122.20
1	AA	370	A	N9-C4-C5	-5.60	103.56	105.80
1	AA	353	G	C5-C6-O6	-5.59	125.24	128.60
1	AA	2529	C	O4'-C1'-N1	5.59	112.68	108.20
1	CA	1139	G	O5'-P-OP2	-5.59	100.67	105.70
1	CA	1695	G	O5'-P-OP2	-5.59	100.67	105.70
1	CA	2618	G	N1-C6-O6	-5.59	116.54	119.90
1	CA	2031	A	C4-C5-C6	5.59	119.80	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	DA	65	U	P-O3'-C3'	5.59	126.41	119.70
2	CB	10	C	N3-C2-O2	-5.59	117.99	121.90
1	AA	141	C	OP2-P-O3'	5.59	117.49	105.20
1	AA	2331	G	N3-C2-N2	-5.59	115.99	119.90
1	AA	2674	A	C8-N9-C4	-5.59	103.56	105.80
34	BA	1509	C	N1-C2-O2	-5.59	115.55	118.90
1	AA	736	A	N7-C8-N9	-5.59	111.01	113.80
1	AA	2502	G	N3-C2-N2	5.59	123.81	119.90
34	BA	1464	G	C5-C6-O6	-5.59	125.25	128.60
1	CA	1977	A	N1-C6-N6	-5.59	115.25	118.60
34	DA	290	C	N3-C4-C5	5.58	124.13	121.90
1	AA	12	U	O4'-C1'-N1	-5.58	103.73	108.20
1	CA	2645	G	N1-C6-O6	5.58	123.25	119.90
1	CA	265	A	C4-C5-N7	5.58	113.49	110.70
1	CA	2523	G	C4-C5-C6	5.58	122.15	118.80
34	DA	1499	A	C8-N9-C4	5.58	108.03	105.80
1	AA	1232	G	C8-N9-C4	5.58	108.63	106.40
1	AA	2529	C	C2-N3-C4	5.58	122.69	119.90
1	AA	2599	A	OP1-P-O3'	5.58	117.47	105.20
1	CA	1899	G	C4-C5-N7	5.58	113.03	110.80
1	CA	2876	G	C8-N9-C4	5.58	108.63	106.40
1	AA	724	A	C4-C5-N7	-5.58	107.91	110.70
1	AA	808	A	N1-C6-N6	5.58	121.95	118.60
1	AA	2022	G	C2-N3-C4	5.58	114.69	111.90
1	CA	2253	G	C8-N9-C4	5.58	108.63	106.40
1	AA	847	A	N9-C4-C5	5.57	108.03	105.80
1	AA	2770	A	N1-C2-N3	-5.57	126.51	129.30
20	AW	18	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	AA	859	C	C6-N1-C2	5.57	122.53	120.30
1	AA	2657	G	N9-C4-C5	-5.57	103.17	105.40
1	CA	1629	U	C5-C6-N1	5.57	125.49	122.70
1	AA	943	C	C2-N1-C1'	5.57	124.92	118.80
1	CA	963	U	C6-N1-C2	5.57	124.34	121.00
1	AA	507	G	O5'-P-OP2	-5.57	100.69	105.70
1	AA	639	G	N1-C6-O6	-5.57	116.56	119.90
1	AA	2431	U	C6-N1-C2	5.57	124.34	121.00
34	BA	770	C	OP1-P-OP2	-5.57	111.25	119.60
34	BA	1344	C	O5'-P-OP2	-5.57	100.69	105.70
1	AA	137	G	N3-C4-N9	5.56	129.34	126.00
1	AA	721	G	N3-C2-N2	5.56	123.79	119.90
1	AA	742	G	C4-C5-N7	-5.56	108.58	110.80
1	AA	1002	A	O5'-P-OP2	-5.56	100.69	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1183	G	O5'-P-OP1	-5.56	100.69	105.70
1	AA	1187	U	N3-C4-O4	5.56	123.29	119.40
1	AA	1273	G	C5-N7-C8	5.56	107.08	104.30
1	CA	798	G	C5-C6-O6	5.56	131.94	128.60
1	CA	2431	U	C5-C6-N1	-5.56	119.92	122.70
1	AA	706	C	C6-N1-C2	5.56	122.52	120.30
1	CA	2576	G	N7-C8-N9	-5.56	110.32	113.10
1	AA	1312	G	N3-C4-N9	5.56	129.34	126.00
1	AA	1432	C	N1-C2-O2	-5.56	115.56	118.90
1	AA	2708	U	C5-C6-N1	-5.56	119.92	122.70
1	CA	12	U	N3-C2-O2	-5.56	118.31	122.20
1	CA	2571	C	C2-N3-C4	-5.56	117.12	119.90
1	AA	1029	A	C4-C5-N7	-5.56	107.92	110.70
1	AA	1274	G	C5-C6-O6	5.56	131.94	128.60
1	AA	2727	G	O5'-P-OP1	5.56	117.37	110.70
1	CA	1653	G	N1-C2-N3	5.56	127.23	123.90
1	AA	801	C	C5-C6-N1	-5.56	118.22	121.00
1	AA	2570	C	N3-C4-C5	5.56	124.12	121.90
1	CA	743	G	N1-C2-N2	-5.56	111.20	116.20
1	CA	2822	G	C6-C5-N7	-5.56	127.07	130.40
1	CA	2824	C	N1-C2-O2	-5.56	115.57	118.90
1	AA	2831	A	N1-C2-N3	5.55	132.08	129.30
1	CA	1634	A	C6-N1-C2	-5.55	115.27	118.60
1	AA	174	U	N1-C2-N3	5.55	118.23	114.90
1	AA	663	G	C5-C6-O6	5.55	131.93	128.60
1	AA	1474	C	N1-C2-O2	-5.55	115.57	118.90
1	AA	1751	G	C5-C6-O6	5.55	131.93	128.60
34	BA	243	A	OP1-P-OP2	5.55	127.93	119.60
34	BA	884	U	N3-C2-O2	5.55	126.09	122.20
1	CA	673	C	O5'-P-OP2	-5.55	100.70	105.70
1	AA	2346	G	OP2-P-O3'	5.55	117.41	105.20
1	AA	2620	G	C6-N1-C2	-5.55	121.77	125.10
1	AA	2663	C	C6-N1-C2	5.55	122.52	120.30
34	BA	792	A	O4'-C1'-N9	5.55	112.64	108.20
1	CA	665	C	N3-C4-C5	5.55	124.12	121.90
1	CA	1997	G	C5'-C4'-O4'	5.55	115.76	109.10
1	AA	2583	C	C6-N1-C2	5.55	122.52	120.30
1	CA	1288	U	N3-C2-O2	-5.55	118.32	122.20
1	CA	2082	A	C8-N9-C4	-5.55	103.58	105.80
1	AA	320	C	C6-N1-C2	5.54	122.52	120.30
1	AA	31	C	C2-N1-C1'	-5.54	112.70	118.80
1	AA	1240	G	C5-C6-O6	-5.54	125.27	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	2422	G	O5'-P-OP1	-5.54	100.71	105.70
1	CA	827	U	C2-N3-C4	-5.54	123.67	127.00
1	AA	1683	C	C4-C5-C6	5.54	120.17	117.40
1	CA	2273	A	C8-N9-C4	5.54	108.02	105.80
1	AA	709	G	OP1-P-OP2	-5.54	111.29	119.60
1	AA	2876	U	C4-C5-C6	5.54	123.02	119.70
1	CA	1768	U	C5-C4-O4	5.54	129.22	125.90
1	CA	2570	G	C4-C5-N7	-5.54	108.58	110.80
1	AA	644	G	C5-C6-N1	5.54	114.27	111.50
1	AA	1438	A	C8-N9-C4	5.54	108.02	105.80
1	AA	18	C	C4-C5-C6	5.54	120.17	117.40
1	CA	973	A	N1-C6-N6	-5.54	115.28	118.60
1	AA	209	G	C8-N9-C4	5.53	108.61	106.40
1	AA	1014	U	N3-C4-O4	-5.53	115.53	119.40
1	AA	2802	C	N1-C2-O2	-5.53	115.58	118.90
1	AA	2051	G	N3-C2-N2	-5.53	116.03	119.90
1	AA	471	C	OP1-P-OP2	-5.53	111.31	119.60
1	AA	784	C	N3-C2-O2	5.53	125.77	121.90
1	AA	800	C	C6-N1-C2	5.53	122.51	120.30
1	AA	605	G	C2-N3-C4	-5.53	109.14	111.90
1	AA	799	A	N1-C6-N6	5.53	121.92	118.60
1	AA	2641	A	C4-C5-N7	5.53	113.46	110.70
1	AA	2712	C	C6-N1-C2	5.53	122.51	120.30
1	CA	2550	G	N1-C2-N3	5.53	127.22	123.90
1	CA	2855	C	C5-C6-N1	5.53	123.76	121.00
1	AA	1290	G	N3-C2-N2	5.53	123.77	119.90
1	AA	1385	G	C8-N9-C4	5.53	108.61	106.40
1	AA	1925	G	O5'-P-OP1	-5.53	100.73	105.70
1	AA	2775	G	N1-C6-O6	-5.53	116.58	119.90
1	CA	1047	G	N3-C4-N9	5.53	129.31	126.00
1	CA	2287	A	C5-C6-N1	-5.53	114.94	117.70
1	CA	2608	G	O5'-P-OP2	-5.53	100.73	105.70
4	CD	229	VAL	CB-CA-C	-5.53	100.90	111.40
1	AA	1964	C	C4-C5-C6	-5.52	114.64	117.40
1	AA	23	G	N9-C4-C5	5.52	107.61	105.40
1	AA	2273	C	N1-C2-N3	5.52	123.07	119.20
1	AA	2745	G	N1-C2-N3	5.52	127.21	123.90
34	BA	353	A	OP2-P-O3'	5.52	117.35	105.20
1	CA	315	G	O5'-P-OP2	-5.52	100.73	105.70
1	CA	1698	A	C4-C5-C6	5.52	119.76	117.00
1	CA	2618	G	C5-N7-C8	5.52	107.06	104.30
1	AA	279	G	C8-N9-C4	-5.52	104.19	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	593	G	C8-N9-C4	-5.52	104.19	106.40
34	BA	1530	G	C4-N9-C1'	-5.52	119.32	126.50
1	CA	2050	C	C2-N3-C4	-5.52	117.14	119.90
1	CA	2598	A	C2-N3-C4	-5.52	107.84	110.60
34	DA	1484	C	C5-C4-N4	-5.52	116.34	120.20
1	AA	31	C	C6-N1-C1'	5.52	127.42	120.80
1	AA	2096	U	N3-C4-C5	-5.52	111.29	114.60
1	CA	33	U	N3-C2-O2	-5.52	118.34	122.20
1	CA	2067	G	C8-N9-C4	-5.52	104.19	106.40
34	DA	1522	U	OP2-P-O3'	5.52	117.34	105.20
1	AA	2050	U	N3-C4-O4	-5.52	115.54	119.40
1	AA	2641	A	C2-N3-C4	-5.52	107.84	110.60
1	AA	2359	C	N3-C2-O2	-5.51	118.04	121.90
34	BA	893	C	N3-C4-N4	5.51	121.86	118.00
1	CA	2604	U	N1-C2-O2	5.51	126.66	122.80
1	AA	16	G	N1-C6-O6	-5.51	116.59	119.90
34	BA	1407	C	N3-C2-O2	5.51	125.76	121.90
1	CA	599	G	N3-C4-N9	5.51	129.31	126.00
1	AA	2221	A	C8-N9-C4	-5.51	103.59	105.80
1	CA	1021	A	C4-C5-N7	5.51	113.46	110.70
1	AA	488	C	N1-C2-O2	-5.51	115.59	118.90
1	AA	530	A	N7-C8-N9	5.51	116.56	113.80
1	AA	981	C	N1-C2-O2	-5.51	115.59	118.90
1	AA	1834	A	OP2-P-O3'	5.51	117.32	105.20
1	AA	2676	G	N3-C4-N9	5.51	129.31	126.00
34	DA	576	G	N9-C4-C5	-5.51	103.20	105.40
34	DA	705	U	O5'-P-OP2	-5.51	100.74	105.70
1	AA	26	G	N3-C4-C5	-5.51	125.85	128.60
1	AA	236	G	N1-C6-O6	5.51	123.20	119.90
1	AA	449	A	OP1-P-OP2	-5.51	111.34	119.60
1	AA	1314	A	C2-N3-C4	-5.51	107.85	110.60
1	AA	1719	C	N3-C2-O2	5.51	125.75	121.90
1	AA	2584	A	OP1-P-O3'	5.51	117.32	105.20
34	BA	322	C	C6-N1-C2	5.51	122.50	120.30
1	CA	2557	G	N1-C2-N2	-5.50	111.25	116.20
1	AA	2398	C	C5-C4-N4	5.50	124.05	120.20
34	DA	489	C	C6-N1-C2	-5.50	118.10	120.30
1	AA	2556	G	C5-C6-O6	-5.50	125.30	128.60
34	BA	321	A	N1-C6-N6	5.50	121.90	118.60
1	CA	2559	C	C6-N1-C2	5.50	122.50	120.30
1	CA	2560	C	C5-C4-N4	-5.50	116.35	120.20
1	AA	398	A	N1-C6-N6	5.50	121.90	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1371	G	C2-N3-C4	5.50	114.65	111.90
1	AA	2456	G	C5-C6-O6	-5.50	125.30	128.60
1	AA	22	C	N3-C2-O2	-5.50	118.05	121.90
1	AA	549	U	C2-N3-C4	-5.50	123.70	127.00
1	AA	781	A	N1-C6-N6	5.50	121.90	118.60
1	AA	1359	U	N3-C2-O2	-5.50	118.35	122.20
1	AA	1674	G	O5'-P-OP1	-5.50	100.75	105.70
1	CA	2454	G	C5-C6-O6	5.50	131.90	128.60
1	AA	714	U	N1-C2-O2	-5.50	118.95	122.80
1	AA	721	G	C6-N1-C2	5.50	128.40	125.10
1	AA	2113	U	N1-C2-N3	5.50	118.20	114.90
1	AA	2233	G	C5-C6-O6	5.50	131.90	128.60
1	AA	2312	G	N9-C4-C5	5.50	107.60	105.40
1	AA	2566	U	O5'-P-OP1	-5.50	100.75	105.70
1	AA	17	G	C6-N1-C2	-5.49	121.80	125.10
1	AA	118	U	OP1-P-OP2	-5.49	111.36	119.60
1	AA	1427	G	C4-C5-N7	5.49	113.00	110.80
1	AA	2373	A	N1-C6-N6	5.49	121.90	118.60
2	AB	101	G	O5'-P-OP2	5.49	117.29	110.70
1	CA	704	G	N3-C4-N9	5.49	129.30	126.00
1	AA	585	U	C4-C5-C6	-5.49	116.41	119.70
34	BA	244	U	N3-C2-O2	-5.49	118.36	122.20
1	CA	692	C	N3-C4-N4	-5.49	114.16	118.00
1	AA	1296	G	N3-C2-N2	5.49	123.74	119.90
1	AA	2529	C	O5'-P-OP1	5.49	117.29	110.70
2	AB	83	G	N1-C6-O6	-5.49	116.61	119.90
1	CA	945	A	N3-C4-N9	-5.49	123.01	127.40
1	AA	83	A	O4'-C1'-N9	5.49	112.59	108.20
1	AA	455	A	C5'-C4'-C3'	-5.49	107.22	116.00
1	AA	1157	A	C5-N7-C8	-5.49	101.16	103.90
1	AA	1597	C	C5-C4-N4	-5.49	116.36	120.20
1	AA	2446	A	N1-C6-N6	-5.49	115.31	118.60
1	AA	2798	C	C4-C5-C6	5.48	120.14	117.40
34	BA	1520	G	N1-C6-O6	5.48	123.19	119.90
1	AA	410	U	O4'-C1'-N1	5.48	112.58	108.20
1	CA	2539	C	C5-C6-N1	-5.48	118.26	121.00
34	DA	1416	G	C8-N9-C4	5.48	108.59	106.40
1	AA	551	A	C5-C6-N6	5.48	128.08	123.70
1	AA	2252	C	O5'-P-OP2	-5.48	100.77	105.70
34	BA	1414	U	C6-N1-C2	5.48	124.29	121.00
1	CA	1965	C	N1-C2-O2	-5.48	115.61	118.90
1	AA	614	C	N3-C4-C5	5.47	124.09	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1028	C	C5-C6-N1	5.47	123.74	121.00
1	AA	2757	G	C8-N9-C4	5.47	108.59	106.40
34	BA	953	G	O5'-P-OP2	-5.47	100.77	105.70
1	CA	746	A	O4'-C1'-N9	5.47	112.58	108.20
1	AA	2775	G	O5'-P-OP2	-5.47	100.78	105.70
1	AA	2271	G	N1-C2-N2	-5.47	111.28	116.20
34	BA	771	G	N3-C2-N2	-5.47	116.07	119.90
1	CA	933	A	C4-C5-N7	5.47	113.44	110.70
1	CA	2287	A	C5-N7-C8	-5.47	101.17	103.90
1	CA	2221	G	C5-C6-O6	5.47	131.88	128.60
1	AA	1180	C	N1-C2-O2	-5.47	115.62	118.90
1	AA	1984	C	C4-C5-C6	-5.47	114.67	117.40
1	CA	1142(A)	A	N7-C8-N9	5.47	116.53	113.80
1	AA	2451	A	C8-N9-C4	-5.46	103.61	105.80
34	BA	1074	G	N1-C6-O6	5.46	123.18	119.90
1	CA	1125	G	C8-N9-C4	5.46	108.59	106.40
1	CA	1661	G	N7-C8-N9	-5.46	110.37	113.10
1	CA	806	C	C4-C5-C6	-5.46	114.67	117.40
1	CA	2424	C	N1-C2-O2	-5.46	115.62	118.90
1	AA	784	C	N1-C2-O2	-5.46	115.62	118.90
1	AA	1617	A	C5-C6-N6	-5.46	119.33	123.70
1	AA	2024	G	C8-N9-C4	5.46	108.58	106.40
1	AA	2375	C	N3-C2-O2	-5.46	118.08	121.90
34	BA	785	G	N1-C6-O6	5.46	123.18	119.90
1	CA	34	C	C6-N1-C2	-5.46	118.11	120.30
1	CA	2254	C	OP2-P-O3'	5.46	117.21	105.20
34	DA	1442	G	P-O3'-C3'	5.46	126.25	119.70
1	AA	888	A	N1-C6-N6	5.46	121.88	118.60
1	AA	2250	G	OP2-P-O3'	5.46	117.21	105.20
34	BA	886	G	N3-C2-N2	-5.46	116.08	119.90
1	CA	1022	G	N3-C4-N9	-5.46	122.72	126.00
1	CA	57	C	N1-C2-O2	-5.46	115.63	118.90
1	AA	412	C	C6-N1-C2	-5.46	118.12	120.30
1	AA	1264	G	C6-C5-N7	-5.46	127.13	130.40
1	CA	1812	A	O5'-P-OP1	-5.46	100.79	105.70
1	AA	841	G	C8-N9-C4	5.45	108.58	106.40
1	AA	872	C	C2-N3-C4	-5.45	117.17	119.90
1	CA	1022	G	N9-C4-C5	5.45	107.58	105.40
1	CA	2610	C	O5'-P-OP1	-5.45	100.79	105.70
1	AA	2751	A	N7-C8-N9	-5.45	111.07	113.80
2	AB	79	C	N3-C4-C5	-5.45	119.72	121.90
1	AA	2636	G	N3-C2-N2	-5.45	116.08	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	99	G	C4-C5-N7	5.45	112.98	110.80
1	CA	1807	G	N9-C4-C5	-5.45	103.22	105.40
34	DA	1405	G	N1-C2-N2	-5.45	111.29	116.20
1	AA	818	G	N1-C6-O6	-5.45	116.63	119.90
1	AA	2776	G	N1-C6-O6	5.45	123.17	119.90
1	CA	2766	G	C4-C5-N7	5.45	112.98	110.80
1	CA	1259	G	N1-C2-N2	-5.45	111.30	116.20
1	AA	843	C	C4-C5-C6	5.45	120.12	117.40
1	CA	2540	C	N3-C4-C5	5.45	124.08	121.90
34	DA	510	A	N1-C6-N6	-5.45	115.33	118.60
34	DA	1502	A	N7-C8-N9	5.45	116.52	113.80
1	CA	1282	U	C5-C4-O4	5.44	129.17	125.90
1	CA	2690	C	N1-C2-O2	-5.44	115.63	118.90
1	AA	555	G	OP2-P-O3'	5.44	117.17	105.20
1	AA	1253	C	C4-C5-C6	5.44	120.12	117.40
1	AA	2259	A	N1-C2-N3	5.44	132.02	129.30
1	CA	1425	G	N3-C4-N9	5.44	129.26	126.00
34	DA	897	C	C5-C6-N1	-5.44	118.28	121.00
1	AA	725	C	N3-C2-O2	5.44	125.71	121.90
1	AA	2251	G	OP1-P-OP2	-5.44	111.44	119.60
1	AA	2890	C	N3-C2-O2	-5.44	118.09	121.90
34	BA	881	G	O5'-P-OP1	5.44	117.23	110.70
1	AA	542	C	OP2-P-O3'	5.44	117.17	105.20
1	AA	2077	C	C2-N1-C1'	-5.44	112.82	118.80
1	CA	2579	C	C6-N1-C2	-5.44	118.12	120.30
1	AA	2622	C	O5'-P-OP2	-5.44	100.81	105.70
1	CA	1692	U	N3-C2-O2	5.44	126.01	122.20
1	CA	2023	G	C6-C5-N7	-5.44	127.14	130.40
1	AA	1360	C	C2-N3-C4	-5.43	117.18	119.90
1	CA	945	A	C5-C6-N6	-5.43	119.35	123.70
1	CA	1407	C	N3-C2-O2	5.43	125.70	121.90
1	CA	2424	C	C5-C6-N1	-5.43	118.28	121.00
1	AA	1014	U	OP2-P-O3'	5.43	117.15	105.20
1	AA	1426	G	N7-C8-N9	-5.43	110.38	113.10
1	AA	1835	C	OP1-P-OP2	-5.43	111.45	119.60
1	AA	2443	U	C5-C6-N1	-5.43	119.98	122.70
1	AA	2538	G	C2-N3-C4	-5.43	109.18	111.90
1	CA	583	G	N3-C2-N2	-5.43	116.10	119.90
1	CA	2832	U	C6-N1-C2	5.43	124.26	121.00
1	AA	2475	C	C5-C6-N1	-5.43	118.28	121.00
1	CA	1208	C	OP2-P-O3'	5.43	117.15	105.20
1	CA	2690	C	C2-N1-C1'	-5.43	112.83	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	2233	G	C4-C5-N7	-5.43	108.63	110.80
1	AA	2497	G	C8-N9-C4	5.43	108.57	106.40
1	CA	786	C	N3-C4-C5	5.43	124.07	121.90
1	AA	839	G	O5'-P-OP1	-5.43	100.82	105.70
1	AA	1796	C	N3-C4-C5	5.43	124.07	121.90
34	BA	1193	G	O5'-P-OP1	-5.43	100.82	105.70
1	CA	599	G	N3-C4-C5	-5.43	125.89	128.60
1	AA	1735	U	N3-C4-O4	-5.42	115.60	119.40
1	AA	2367	C	O5'-P-OP1	-5.42	100.82	105.70
1	AA	2370	G	N1-C2-N2	-5.42	111.32	116.20
34	DA	1158	C	N3-C2-O2	-5.42	118.10	121.90
1	AA	1955	G	C4-N9-C1'	5.42	133.55	126.50
1	AA	2619	G	C6-N1-C2	-5.42	121.85	125.10
1	CA	2772	C	N3-C4-C5	-5.42	119.73	121.90
1	AA	2113	U	C4-C5-C6	5.42	122.95	119.70
1	AA	2434	A	O4'-C1'-N9	5.42	112.54	108.20
1	CA	2740	A	N7-C8-N9	-5.42	111.09	113.80
1	CA	2755	C	C5-C6-N1	5.42	123.71	121.00
1	CA	2832	U	C5-C6-N1	-5.42	119.99	122.70
1	AA	2095	C	OP2-P-O3'	5.42	117.12	105.20
1	AA	2502	G	N3-C4-N9	5.42	129.25	126.00
1	AA	2715	C	C4-C5-C6	5.42	120.11	117.40
1	CA	2601	C	C6-N1-C2	-5.42	118.13	120.30
1	CA	2710	C	C6-N1-C2	5.42	122.47	120.30
1	AA	182	U	C4-C5-C6	5.42	122.95	119.70
1	AA	887	C	C5-C6-N1	-5.42	118.29	121.00
1	AA	1048	G	O5'-P-OP2	-5.42	100.83	105.70
1	AA	2229	A	O4'-C1'-N9	5.42	112.53	108.20
34	BA	1515	C	N3-C4-C5	5.42	124.07	121.90
39	DF	87	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	AA	552	C	C6-N1-C2	-5.42	118.13	120.30
1	CA	1801	G	O4'-C1'-N9	5.42	112.53	108.20
1	AA	145	G	O5'-P-OP2	-5.41	100.83	105.70
1	AA	1006	C	C6-N1-C1'	5.41	127.30	120.80
1	AA	1234	A	C5-C6-N6	-5.41	119.37	123.70
1	AA	1264	G	N9-C4-C5	-5.41	103.23	105.40
34	BA	1496	C	C6-N1-C2	5.41	122.47	120.30
1	AA	417	A	N1-C6-N6	5.41	121.85	118.60
1	CA	945	A	C6-N1-C2	5.41	121.85	118.60
1	AA	1807	G	O5'-P-OP2	-5.41	100.83	105.70
1	CA	673	C	N1-C2-O2	-5.41	115.65	118.90
1	AA	992	G	N1-C2-N2	-5.41	111.33	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1374	G	C5-C6-O6	-5.41	125.36	128.60
1	AA	1440	U	N1-C2-O2	5.41	126.59	122.80
1	AA	2708	U	C2-N3-C4	-5.41	123.75	127.00
1	AA	1385	G	C5-C6-N1	5.41	114.20	111.50
1	CA	1489	U	C5-C4-O4	5.41	129.14	125.90
1	CA	1696	G	N1-C6-O6	-5.41	116.66	119.90
34	DA	266	G	C2-N3-C4	-5.41	109.20	111.90
1	AA	1265	A	N1-C6-N6	5.41	121.84	118.60
1	AA	1378	G	C6-C5-N7	-5.41	127.16	130.40
1	AA	2029	C	C4-C5-C6	5.41	120.10	117.40
1	AA	2072	C	C4-C5-C6	5.41	120.10	117.40
1	AA	2427	G	N1-C6-O6	5.41	123.14	119.90
1	CA	2511	U	N3-C4-O4	-5.41	115.62	119.40
34	DA	1484	C	N3-C2-O2	5.41	125.68	121.90
1	AA	554	A	C5-N7-C8	-5.40	101.20	103.90
1	AA	887	C	C4-C5-C6	5.40	120.10	117.40
1	AA	1204	C	C2-N3-C4	-5.40	117.20	119.90
1	AA	2497	G	N1-C6-O6	-5.40	116.66	119.90
1	AA	2565	G	N3-C4-C5	-5.40	125.90	128.60
1	AA	2637	G	C6-C5-N7	5.40	133.64	130.40
34	DA	1484	C	N3-C4-C5	5.40	124.06	121.90
1	AA	1030	A	N7-C8-N9	-5.40	111.10	113.80
1	AA	2479	C	OP2-P-O3'	5.40	117.08	105.20
1	AA	2882	G	C6-C5-N7	5.40	133.64	130.40
1	CA	2285	C	O5'-P-OP2	-5.40	100.84	105.70
1	AA	2788	A	C5-C6-N6	5.40	128.02	123.70
34	BA	1403	C	N3-C4-N4	-5.40	114.22	118.00
1	AA	1026	A	C5-N7-C8	-5.40	101.20	103.90
1	AA	1067	A	N1-C6-N6	5.40	121.84	118.60
1	AA	2083	G	C5-C6-N1	5.40	114.20	111.50
1	CA	786	C	O5'-P-OP1	-5.40	100.84	105.70
1	CA	1653	G	N1-C6-O6	-5.40	116.66	119.90
1	CA	1899	G	C5-N7-C8	-5.40	101.60	104.30
1	AA	1050	C	N3-C2-O2	5.39	125.68	121.90
1	AA	2118	U	OP2-P-O3'	5.39	117.07	105.20
1	AA	800	C	C5-C6-N1	-5.39	118.30	121.00
1	AA	1598	C	C4-C5-C6	5.39	120.10	117.40
1	AA	1457	C	N3-C2-O2	-5.39	118.13	121.90
1	CA	2221	G	C8-N9-C4	-5.39	104.24	106.40
1	AA	596	G	C8-N9-C4	-5.39	104.25	106.40
1	CA	577	G	C5-C6-O6	-5.39	125.37	128.60
1	AA	231	G	OP1-P-OP2	-5.39	111.52	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	558	G	C4-C5-C6	-5.39	115.57	118.80
1	AA	585	U	N3-C2-O2	-5.39	118.43	122.20
1	AA	894	U	C4-C5-C6	5.39	122.93	119.70
1	AA	2285	A	C8-N9-C4	5.39	107.95	105.80
1	AA	2477	C	C6-N1-C2	5.39	122.45	120.30
1	AA	2487	C	C6-N1-C2	-5.39	118.14	120.30
34	DA	913	A	P-O3'-C3'	5.39	126.16	119.70
1	AA	1613	A	N1-C2-N3	-5.38	126.61	129.30
1	AA	1846	A	N1-C2-N3	5.38	131.99	129.30
1	AA	2494	G	N1-C6-O6	5.38	123.13	119.90
34	BA	43	C	C6-N1-C2	5.38	122.45	120.30
34	BA	317	G	C8-N9-C4	-5.38	104.25	106.40
1	CA	2536	G	C5-C6-O6	-5.38	125.37	128.60
1	AA	2344	U	C5-C6-N1	-5.38	120.01	122.70
1	AA	2461	U	C5-C4-O4	-5.38	122.67	125.90
1	AA	2620	G	C5-C6-O6	-5.38	125.37	128.60
2	AB	62	C	N1-C2-O2	-5.38	115.67	118.90
1	CA	2519	U	N1-C2-O2	-5.38	119.03	122.80
1	AA	601	A	C5-C6-N6	5.38	128.00	123.70
1	AA	2287	C	C5'-C4'-O4'	-5.38	102.64	109.10
34	BA	1520	G	C4-C5-N7	5.38	112.95	110.80
1	CA	1626	G	C4-C5-N7	-5.38	108.65	110.80
1	CA	2452	C	OP2-P-O3'	5.38	117.04	105.20
1	CA	2439	A	C5'-C4'-O4'	-5.38	102.64	109.10
1	AA	808	A	C4-C5-C6	5.38	119.69	117.00
1	AA	1306	G	OP2-P-O3'	5.38	117.03	105.20
1	AA	2093	A	O5'-P-OP2	-5.38	100.86	105.70
1	AA	2475	C	N3-C4-N4	-5.38	114.23	118.00
34	BA	801	U	C5-C6-N1	-5.38	120.01	122.70
1	CA	847	U	N1-C2-N3	5.38	118.13	114.90
1	CA	1992	G	P-O3'-C3'	5.38	126.15	119.70
1	CA	2360	A	C8-N9-C4	5.38	107.95	105.80
1	AA	1232	G	N1-C2-N3	-5.38	120.67	123.90
16	AS	25	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	CA	271(M)	G	OP1-P-O3'	5.38	117.03	105.20
1	CA	1794	U	N1-C2-N3	5.38	118.12	114.90
1	CA	2708	G	N9-C4-C5	-5.38	103.25	105.40
1	AA	1804	A	O5'-P-OP1	5.38	117.15	110.70
1	AA	777	C	C2-N3-C4	-5.37	117.21	119.90
1	AA	1020	C	OP1-P-O3'	5.37	117.02	105.20
1	CA	515	A	C2-N3-C4	5.37	113.29	110.60
34	DA	354	G	C4-N9-C1'	5.37	133.49	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1169	C	N3-C4-C5	5.37	124.05	121.90
1	AA	2502	G	C4-C5-N7	5.37	112.95	110.80
2	AB	84	C	C2-N1-C1'	5.37	124.71	118.80
1	CA	2032	G	N1-C6-O6	-5.37	116.68	119.90
34	DA	1529	G	C8-N9-C1'	-5.37	120.02	127.00
1	AA	730	C	N3-C2-O2	-5.37	118.14	121.90
1	AA	1921	G	N3-C4-N9	5.37	129.22	126.00
1	AA	2021	C	N1-C2-O2	-5.37	115.68	118.90
34	BA	1401	G	C5-C6-N1	-5.37	108.81	111.50
1	AA	1329	G	N9-C4-C5	-5.37	103.25	105.40
1	AA	2264	G	C5-C6-N1	-5.37	108.82	111.50
1	AA	2427	G	C5-C6-N1	5.37	114.18	111.50
1	AA	2427	G	N3-C2-N2	-5.37	116.14	119.90
1	AA	2639	G	N3-C2-N2	5.37	123.66	119.90
1	AA	2713	C	C4-C5-C6	5.37	120.08	117.40
1	CA	321	G	O4'-C1'-N9	5.37	112.50	108.20
1	CA	1989	G	O5'-P-OP1	-5.37	100.87	105.70
1	AA	2797	C	N1-C2-O2	5.37	122.12	118.90
1	AA	2883	A	C5-N7-C8	-5.37	101.22	103.90
1	CA	1425	G	C5-C6-O6	-5.37	125.38	128.60
1	AA	899	G	C5-C6-O6	5.37	131.82	128.60
1	AA	2588	G	N1-C2-N2	5.37	121.03	116.20
1	CA	1266	G	C5-C6-O6	-5.37	125.38	128.60
1	AA	780	G	C5-N7-C8	5.36	106.98	104.30
1	AA	2001	C	C6-N1-C2	-5.36	118.16	120.30
1	CA	782	A	C5-C6-N6	-5.36	119.41	123.70
34	DA	329	A	N1-C6-N6	5.36	121.82	118.60
34	DA	915	A	O5'-P-OP2	-5.36	100.87	105.70
1	AA	1985	U	OP1-P-O3'	5.36	117.00	105.20
1	AA	2050	U	N1-C2-O2	5.36	126.55	122.80
2	AB	102	A	N1-C6-N6	5.36	121.82	118.60
1	AA	1329	G	C8-N9-C4	5.36	108.54	106.40
1	AA	1802	C	C2-N3-C4	-5.36	117.22	119.90
1	AA	2513	C	C6-N1-C2	5.36	122.44	120.30
34	BA	527	G	C8-N9-C4	-5.36	104.25	106.40
34	BA	889	A	O5'-P-OP2	-5.36	100.88	105.70
1	AA	2245	U	N1-C2-N3	5.36	118.12	114.90
1	AA	2433	G	N1-C6-O6	5.36	123.11	119.90
1	CA	2893	G	N3-C4-C5	-5.36	125.92	128.60
1	AA	912	C	N3-C4-C5	-5.36	119.76	121.90
1	AA	2399	U	N1-C2-O2	-5.36	119.05	122.80
1	CA	2581	G	O5'-P-OP2	-5.36	100.88	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1055	A	C2-N3-C4	5.36	113.28	110.60
1	AA	2043	C	N3-C4-C5	5.36	124.04	121.90
1	AA	2069	U	C5-C4-O4	-5.36	122.69	125.90
1	AA	2513	C	C5-C6-N1	-5.36	118.32	121.00
1	AA	2802	C	C6-N1-C1'	5.36	127.23	120.80
1	AA	2825	C	N1-C2-O2	5.36	122.11	118.90
34	BA	404	U	N3-C2-O2	-5.36	118.45	122.20
34	BA	852	G	C8-N9-C4	5.36	108.54	106.40
1	AA	800	C	N3-C4-C5	5.35	124.04	121.90
1	AA	880	U	O5'-P-OP1	-5.35	100.88	105.70
1	AA	2427	G	N1-C2-N2	5.35	121.02	116.20
1	AA	468	G	C5-C6-O6	-5.35	125.39	128.60
1	AA	869	U	C6-N1-C2	-5.35	117.79	121.00
1	AA	1324	A	N9-C4-C5	5.35	107.94	105.80
34	BA	317	G	C6-C5-N7	-5.35	127.19	130.40
1	CA	31	C	C2-N3-C4	-5.35	117.22	119.90
1	CA	176	G	N9-C4-C5	-5.35	103.26	105.40
1	CA	2897	U	C2-N1-C1'	5.35	124.12	117.70
1	AA	181	C	N1-C2-O2	-5.35	115.69	118.90
1	AA	788	G	O5'-P-OP1	-5.35	100.89	105.70
1	AA	845	G	N7-C8-N9	-5.35	110.43	113.10
2	AB	7	G	C5-N7-C8	-5.35	101.63	104.30
34	BA	1406	U	C5-C6-N1	-5.35	120.03	122.70
1	CA	2835	A	OP1-P-O3'	5.35	116.97	105.20
1	AA	2498	G	N3-C4-C5	-5.35	125.93	128.60
2	AB	109	C	O4'-C1'-N1	5.35	112.48	108.20
1	CA	2448	A	N1-C6-N6	5.35	121.81	118.60
1	CA	2645	G	C6-C5-N7	-5.35	127.19	130.40
1	AA	203	G	OP2-P-O3'	5.34	116.96	105.20
34	BA	1407	C	C6-N1-C2	5.34	122.44	120.30
34	DA	830	G	N1-C6-O6	5.34	123.11	119.90
1	AA	77	A	C2-N3-C4	-5.34	107.93	110.60
1	AA	2277	U	N1-C2-O2	-5.34	119.06	122.80
1	CA	1416	G	O4'-C1'-N9	5.34	112.47	108.20
1	AA	1487	G	N3-C2-N2	-5.34	116.16	119.90
1	AA	2043	C	C2-N3-C4	-5.34	117.23	119.90
1	AA	2393	C	C5-C6-N1	-5.34	118.33	121.00
1	AA	2657	G	N1-C6-O6	5.34	123.11	119.90
1	CA	185	U	N3-C4-O4	-5.34	115.66	119.40
1	CA	418	G	C8-N9-C4	5.34	108.54	106.40
1	CA	1842	G	C8-N9-C4	5.34	108.54	106.40
34	DA	866	C	N3-C2-O2	-5.34	118.16	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	737	G	N7-C8-N9	-5.34	110.43	113.10
1	AA	1725	G	C6-C5-N7	-5.34	127.20	130.40
1	AA	2271	G	N3-C2-N2	5.34	123.64	119.90
34	BA	299	G	N1-C6-O6	5.34	123.10	119.90
1	AA	502	G	N7-C8-N9	-5.34	110.43	113.10
1	AA	1457	C	N1-C2-O2	5.34	122.10	118.90
1	AA	1842	G	C4-C5-N7	-5.34	108.67	110.80
1	CA	2877	G	N1-C6-O6	5.34	123.10	119.90
34	DA	367	U	N3-C4-O4	5.34	123.14	119.40
34	BA	1484	C	C6-N1-C2	5.33	122.43	120.30
1	AA	413	G	N3-C4-C5	-5.33	125.93	128.60
1	AA	2586	G	C5-C6-N1	5.33	114.17	111.50
1	AA	1434	G	C5-N7-C8	5.33	106.97	104.30
1	AA	2542	A	C5-C6-N1	-5.33	115.03	117.70
34	BA	438	G	C8-N9-C4	-5.33	104.27	106.40
1	CA	2867	G	N3-C4-C5	5.33	131.27	128.60
1	AA	40	C	C2-N3-C4	-5.33	117.23	119.90
1	AA	2756	C	O5'-P-OP1	-5.33	100.90	105.70
38	BE	53	LEU	CA-CB-CG	5.33	127.56	115.30
1	CA	435	C	N1-C2-O2	5.33	122.10	118.90
1	CA	659	C	C5-C6-N1	-5.33	118.33	121.00
1	AA	55	A	O5'-P-OP1	-5.33	100.90	105.70
1	AA	990	A	C6-N1-C2	-5.33	115.40	118.60
1	AA	2039	U	C4-C5-C6	5.33	122.90	119.70
1	AA	2533	C	C5-C6-N1	-5.33	118.34	121.00
1	CA	1809	A	C5-C6-N6	-5.33	119.44	123.70
1	CA	2448	A	O5'-P-OP1	-5.33	100.91	105.70
57	DX	17	C	C2-N1-C1'	5.33	124.66	118.80
1	AA	205	A	C8-N9-C4	5.33	107.93	105.80
1	AA	1011	G	C5-C6-N1	-5.33	108.84	111.50
1	AA	2617	U	O5'-P-OP2	-5.33	100.91	105.70
1	CA	2292	C	N3-C4-C5	5.33	124.03	121.90
1	CA	2595	G	O5'-P-OP2	5.33	117.09	110.70
1	AA	471	C	N1-C2-N3	5.32	122.93	119.20
1	AA	1728	G	C5-C6-O6	-5.32	125.41	128.60
34	BA	529	G	C5-C6-O6	-5.32	125.41	128.60
35	BB	9	GLU	N-CA-C	5.32	125.37	111.00
1	CA	1937	A	O4'-C1'-N9	5.32	112.46	108.20
1	CA	769	G	C8-N9-C4	5.32	108.53	106.40
1	CA	1406	U	N3-C4-O4	-5.32	115.67	119.40
1	AA	888	A	C2-N3-C4	-5.32	107.94	110.60
1	AA	1218	G	O4'-C1'-N9	5.32	112.46	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1593	C	N3-C4-C5	-5.32	119.77	121.90
1	AA	2312	G	N7-C8-N9	5.32	115.76	113.10
1	AA	2477	C	N3-C4-N4	-5.32	114.28	118.00
2	AB	73	A	OP1-P-OP2	5.32	127.58	119.60
1	CA	2043	C	N1-C2-O2	5.32	122.09	118.90
1	CA	2402	C	N1-C2-O2	-5.32	115.71	118.90
1	AA	550	U	O5'-P-OP2	-5.32	100.91	105.70
1	AA	1518	A	N7-C8-N9	5.32	116.46	113.80
1	AA	2735	G	C2-N3-C4	5.32	114.56	111.90
34	BA	1417	G	C8-N9-C4	5.32	108.53	106.40
1	AA	1745	A	N9-C1'-C2'	5.32	120.91	114.00
1	AA	2454	C	C4-C5-C6	5.32	120.06	117.40
2	AB	15	A	N9-C4-C5	-5.32	103.67	105.80
1	CA	1400	G	C8-N9-C4	-5.32	104.27	106.40
1	AA	315	C	C6-N1-C2	5.32	122.43	120.30
1	AA	1299	A	N7-C8-N9	-5.32	111.14	113.80
1	CA	2513	G	N1-C6-O6	5.32	123.09	119.90
1	CA	2080	G	N7-C8-N9	-5.31	110.44	113.10
1	AA	98	U	N3-C4-O4	-5.31	115.68	119.40
1	AA	555	G	C8-N9-C1'	5.31	133.91	127.00
1	AA	2015	U	O5'-P-OP1	-5.31	100.92	105.70
34	BA	811	C	C6-N1-C2	5.31	122.42	120.30
1	CA	1675	C	C6-N1-C2	-5.31	118.17	120.30
34	DA	17	U	N1-C2-O2	5.31	126.52	122.80
34	DA	1154	G	C4-C5-N7	5.31	112.92	110.80
1	AA	644	G	N1-C2-N2	-5.31	111.42	116.20
1	AA	1384	G	N1-C2-N3	5.31	127.09	123.90
1	AA	184	A	C5-N7-C8	-5.31	101.25	103.90
1	AA	395	C	N1-C2-N3	5.31	122.92	119.20
1	CA	1047	G	N3-C4-C5	-5.31	125.95	128.60
1	CA	2496	C	N3-C4-N4	-5.31	114.28	118.00
1	AA	584	G	C5-C6-N1	5.31	114.15	111.50
1	AA	893	C	O4'-C1'-N1	5.31	112.45	108.20
1	AA	1273	G	N7-C8-N9	-5.31	110.45	113.10
1	AA	2024	G	N9-C4-C5	-5.31	103.28	105.40
1	CA	185	U	N3-C2-O2	-5.31	118.48	122.20
1	CA	408	G	O5'-P-OP2	-5.31	100.92	105.70
1	AA	1248	G	C5-C6-N1	5.31	114.15	111.50
34	BA	830	G	OP1-P-OP2	-5.31	111.64	119.60
1	AA	334	A	C8-N9-C4	5.30	107.92	105.80
1	AA	511	C	O5'-P-OP1	-5.30	100.93	105.70
1	AA	1344	C	N1-C2-O2	-5.30	115.72	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1474	C	C5-C6-N1	-5.30	118.35	121.00
1	AA	2583	C	N3-C4-C5	5.30	124.02	121.90
34	BA	1406	U	O5'-P-OP2	-5.30	100.92	105.70
1	CA	2337	G	C6-C5-N7	-5.30	127.22	130.40
1	AA	354	A	C4-C5-C6	-5.30	114.35	117.00
34	BA	733	A	OP1-P-OP2	5.30	127.56	119.60
1	AA	358	C	N1-C2-O2	-5.30	115.72	118.90
1	AA	1370	G	OP1-P-O3'	5.30	116.86	105.20
1	AA	2598	C	N3-C4-C5	5.30	124.02	121.90
34	BA	1286	A	C8-N9-C4	-5.30	103.68	105.80
1	CA	852	G	C5-C6-O6	5.30	131.78	128.60
1	CA	2067	G	N3-C4-C5	-5.30	125.95	128.60
1	AA	505	A	O4'-C1'-N9	5.30	112.44	108.20
1	CA	1238	G	O5'-P-OP2	-5.30	100.93	105.70
1	CA	1697	G	N9-C4-C5	-5.30	103.28	105.40
1	AA	2587	C	C6-N1-C1'	-5.30	114.44	120.80
1	AA	236	G	C5-C6-O6	-5.30	125.42	128.60
1	AA	1385	G	N3-C4-N9	5.30	129.18	126.00
1	AA	1872	U	OP1-P-O3'	5.30	116.85	105.20
1	AA	793	A	O5'-P-OP2	5.29	117.05	110.70
1	AA	817	G	N9-C4-C5	-5.29	103.28	105.40
1	CA	2200	C	O5'-P-OP2	-5.29	100.94	105.70
1	AA	238	C	C6-N1-C2	5.29	122.42	120.30
1	AA	472	G	N1-C2-N3	-5.29	120.72	123.90
1	AA	1169	C	C2-N3-C4	-5.29	117.25	119.90
1	AA	1757	C	N1-C2-O2	-5.29	115.73	118.90
1	AA	2831	A	N1-C6-N6	5.29	121.78	118.60
1	CA	659	C	C6-N1-C2	5.29	122.42	120.30
1	AA	1281	G	N1-C2-N3	5.29	127.07	123.90
1	AA	74	G	N1-C6-O6	5.29	123.07	119.90
1	AA	227	C	C5-C4-N4	-5.29	116.50	120.20
1	AA	1714	G	N1-C6-O6	-5.29	116.73	119.90
1	AA	1844	G	N9-C4-C5	-5.29	103.28	105.40
1	AA	2729	U	N1-C2-O2	-5.29	119.10	122.80
1	AA	2849	G	N1-C2-N2	-5.29	111.44	116.20
1	CA	840	C	N1-C2-O2	-5.29	115.73	118.90
1	CA	1697	G	C5-C6-O6	-5.29	125.43	128.60
1	AA	1617	A	C4-C5-N7	5.29	113.34	110.70
1	CA	1850	G	C6-C5-N7	-5.29	127.23	130.40
1	AA	1154	U	OP1-P-O3'	5.29	116.83	105.20
1	AA	1236	G	O5'-P-OP1	-5.29	100.94	105.70
1	CA	513	A	C2-N3-C4	-5.29	107.96	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	671	C	C5-C6-N1	5.29	123.64	121.00
1	CA	840	C	N3-C4-N4	5.29	121.70	118.00
1	CA	945	A	C5-C6-N1	-5.29	115.06	117.70
1	CA	1647	G	O4'-C1'-N9	-5.29	103.97	108.20
1	CA	1809	A	N1-C6-N6	5.29	121.77	118.60
1	AA	976	G	N3-C2-N2	-5.28	116.20	119.90
1	AA	1643	A	N7-C8-N9	-5.28	111.16	113.80
1	AA	1952	G	C5-N7-C8	5.28	106.94	104.30
1	AA	2608	U	C6-N1-C2	5.28	124.17	121.00
34	BA	860	A	C8-N9-C4	-5.28	103.69	105.80
1	AA	1243	U	N1-C2-O2	-5.28	119.10	122.80
1	AA	2060	G	N1-C6-O6	-5.28	116.73	119.90
1	CA	692	C	C5-C4-N4	5.28	123.90	120.20
34	DA	204	U	C2-N1-C1'	5.28	124.04	117.70
1	AA	418	G	C6-C5-N7	-5.28	127.23	130.40
1	CA	942	G	C8-N9-C4	5.28	108.51	106.40
1	AA	564	G	C2-N3-C4	5.28	114.54	111.90
1	AA	2045	G	N1-C6-O6	5.28	123.07	119.90
34	BA	332	G	N1-C6-O6	5.28	123.07	119.90
1	CA	816	C	OP1-P-O3'	5.28	116.81	105.20
1	AA	2598	C	C5-C4-N4	-5.28	116.51	120.20
1	AA	2871	G	N1-C6-O6	5.28	123.07	119.90
1	CA	2521	C	N1-C2-O2	-5.28	115.73	118.90
1	AA	206	G	N1-C6-O6	5.28	123.06	119.90
1	AA	1019	G	N3-C2-N2	-5.28	116.21	119.90
1	AA	1080	G	OP1-P-OP2	5.28	127.51	119.60
1	AA	1710	C	C4-C5-C6	5.28	120.04	117.40
1	AA	853	C	N3-C4-N4	-5.27	114.31	118.00
34	BA	991	U	P-O3'-C3'	5.27	126.03	119.70
1	CA	2359	C	C5-C4-N4	5.27	123.89	120.20
1	AA	126	C	OP1-P-OP2	5.27	127.51	119.60
1	AA	1535	U	O5'-P-OP1	-5.27	100.95	105.70
1	CA	2592	G	C8-N9-C4	-5.27	104.29	106.40
1	AA	418	G	N1-C6-O6	5.27	123.06	119.90
1	CA	1832	C	N3-C2-O2	5.27	125.59	121.90
1	AA	559	U	C6-N1-C2	5.27	124.16	121.00
1	AA	2019	G	N1-C2-N2	-5.27	111.46	116.20
1	AA	2085	C	O5'-P-OP1	-5.27	100.96	105.70
1	AA	2459	G	N3-C2-N2	5.27	123.59	119.90
34	BA	533	A	O5'-P-OP1	-5.27	100.96	105.70
1	AA	2335	G	C6-C5-N7	-5.27	127.24	130.40
1	AA	2707	C	N1-C2-O2	5.27	122.06	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	1458	G	C8-N9-C4	5.27	108.51	106.40
34	DA	60	A	P-O3'-C3'	5.27	126.02	119.70
1	AA	969	C	N1-C2-O2	-5.27	115.74	118.90
34	BA	518	C	N3-C2-O2	-5.27	118.21	121.90
1	CA	2413	G	N1-C6-O6	5.27	123.06	119.90
1	AA	841	G	OP1-P-OP2	-5.26	111.70	119.60
1	AA	969	C	N3-C2-O2	5.26	125.58	121.90
1	AA	1024	G	C5-C6-O6	5.26	131.76	128.60
1	AA	1925	G	N7-C8-N9	5.26	115.73	113.10
34	BA	1508	G	C4-C5-N7	-5.26	108.69	110.80
1	CA	2239	G	C8-N9-C4	5.26	108.50	106.40
34	DA	1465	C	N3-C2-O2	-5.26	118.22	121.90
1	AA	591	U	N3-C4-O4	-5.26	115.72	119.40
1	AA	723	A	N7-C8-N9	-5.26	111.17	113.80
1	AA	2081	A	O4'-C1'-N9	5.26	112.41	108.20
1	AA	2773	C	N3-C4-C5	5.26	124.00	121.90
1	AA	2303	U	C5-C4-O4	5.26	129.06	125.90
34	BA	1340	A	C8-N9-C4	5.26	107.90	105.80
34	DA	619	U	N3-C2-O2	-5.26	118.52	122.20
1	AA	1404	G	C5-C6-O6	5.26	131.76	128.60
1	AA	1674	G	OP1-P-O3'	5.26	116.77	105.20
1	AA	1688	A	C5-N7-C8	-5.26	101.27	103.90
1	AA	2788	A	C6-C5-N7	5.26	135.98	132.30
1	AA	2902	G	C4-C5-N7	5.26	112.90	110.80
34	BA	389	A	N1-C6-N6	5.26	121.76	118.60
1	CA	1505	C	C6-N1-C2	-5.26	118.20	120.30
34	DA	533	A	C8-N9-C4	-5.26	103.70	105.80
1	AA	735	U	N1-C2-N3	5.26	118.06	114.90
1	AA	1231	G	OP1-P-O3'	5.26	116.76	105.20
1	AA	1744	G	N1-C6-O6	5.26	123.05	119.90
1	CA	1217	C	C6-N1-C2	-5.26	118.20	120.30
1	CA	1421	G	N1-C6-O6	5.26	123.05	119.90
1	CA	1531	C	C2-N1-C1'	5.26	124.58	118.80
1	CA	1774	C	C6-N1-C2	-5.26	118.20	120.30
1	AA	2734	A	N7-C8-N9	-5.25	111.17	113.80
1	CA	2406	U	O4'-C1'-N1	-5.25	104.00	108.20
1	CA	2516	G	C2-N3-C4	-5.25	109.27	111.90
1	AA	193	A	C5-C6-N1	5.25	120.33	117.70
34	BA	1279	A	N7-C8-N9	5.25	116.43	113.80
1	CA	1813	G	C8-N9-C4	5.25	108.50	106.40
1	CA	2195	C	OP1-P-O3'	5.25	116.76	105.20
1	AA	2539	C	C6-N1-C2	5.25	122.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	664	C	N3-C4-C5	5.25	124.00	121.90
1	CA	744	G	N1-C6-O6	5.25	123.05	119.90
1	CA	1877	A	N1-C6-N6	5.25	121.75	118.60
1	CA	2003	G	C5-C6-O6	5.25	131.75	128.60
1	CA	2399	G	N1-C6-O6	-5.25	116.75	119.90
34	DA	831	U	C6-N1-C2	-5.25	117.85	121.00
1	AA	615	G	O5'-P-OP2	-5.25	100.98	105.70
1	AA	1312	G	N3-C4-C5	-5.25	125.98	128.60
1	AA	1921	G	C4-C5-N7	5.25	112.90	110.80
34	BA	841	U	C6-N1-C2	-5.25	117.85	121.00
34	DA	38	G	C8-N9-C4	5.25	108.50	106.40
1	AA	596	G	N3-C4-C5	-5.25	125.98	128.60
1	AA	848	G	C2-N3-C4	-5.25	109.28	111.90
34	BA	1437	C	N3-C2-O2	-5.25	118.23	121.90
1	CA	987	G	O5'-P-OP2	5.25	117.00	110.70
1	AA	193	A	N1-C6-N6	-5.24	115.45	118.60
1	AA	1026	A	C5-C6-N6	-5.24	119.51	123.70
1	AA	1098	C	C6-N1-C2	-5.24	118.20	120.30
1	AA	358	C	C4-C5-C6	5.24	120.02	117.40
1	AA	961	C	N3-C4-C5	-5.24	119.80	121.90
1	AA	1954	A	O5'-P-OP1	-5.24	100.98	105.70
34	BA	155	C	N1-C2-O2	5.24	122.05	118.90
1	AA	1728	G	N7-C8-N9	5.24	115.72	113.10
1	AA	1753	U	N1-C2-O2	5.24	126.47	122.80
34	BA	572	A	C8-N9-C4	5.24	107.90	105.80
1	CA	1348	G	N1-C6-O6	5.24	123.04	119.90
1	CA	1355	G	N1-C6-O6	-5.24	116.76	119.90
34	DA	813	U	OP1-P-OP2	-5.24	111.74	119.60
1	AA	1785	C	C4-C5-C6	5.24	120.02	117.40
1	CA	2521	C	C6-N1-C2	5.24	122.39	120.30
1	AA	2346	G	C4-N9-C1'	5.24	133.31	126.50
1	AA	2398	C	C2-N1-C1'	-5.24	113.04	118.80
34	BA	1524	C	C6-N1-C2	-5.24	118.21	120.30
1	AA	32	C	O5'-P-OP2	-5.23	100.99	105.70
1	AA	2403	G	O5'-P-OP2	-5.23	100.99	105.70
1	CA	614	U	N1-C2-O2	5.23	126.46	122.80
1	CA	2593	U	N3-C4-O4	-5.23	115.74	119.40
1	CA	2828	C	N1-C2-O2	5.23	122.04	118.90
1	AA	1839	U	N3-C2-O2	5.23	125.86	122.20
1	AA	2370	G	N3-C2-N2	5.23	123.56	119.90
1	AA	2839	C	C6-N1-C2	5.23	122.39	120.30
1	AA	1678	A	C5-C6-N1	-5.23	115.08	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1688	A	N7-C8-N9	5.23	116.42	113.80
1	AA	1171	G	C5-C6-O6	-5.23	125.46	128.60
34	BA	596	C	C6-N1-C2	5.23	122.39	120.30
1	AA	581	G	N3-C2-N2	5.23	123.56	119.90
1	AA	740	C	N3-C4-N4	-5.23	114.34	118.00
1	AA	1807	G	C8-N9-C4	5.23	108.49	106.40
1	AA	2303	U	C4-C5-C6	5.23	122.84	119.70
1	AA	2480	G	N1-C6-O6	5.23	123.04	119.90
1	AA	2590	G	N3-C2-N2	5.23	123.56	119.90
1	AA	2799	U	N3-C4-C5	5.23	117.74	114.60
1	AA	2858	G	N1-C6-O6	-5.23	116.76	119.90
1	AA	321	C	C4-C5-C6	5.23	120.01	117.40
1	AA	1184	G	C8-N9-C4	-5.23	104.31	106.40
1	AA	2863	C	C5-C6-N1	-5.23	118.39	121.00
34	BA	869	G	N1-C6-O6	5.23	123.04	119.90
1	AA	500	G	N1-C2-N3	5.22	127.03	123.90
1	AA	1440	U	OP1-P-OP2	-5.22	111.76	119.60
1	AA	2441	G	OP1-P-OP2	-5.22	111.76	119.60
18	CU	74	LEU	CA-CB-CG	5.22	127.32	115.30
34	BA	795	C	N1-C2-O2	-5.22	115.77	118.90
1	CA	2066	C	O5'-P-OP1	-5.22	101.00	105.70
1	AA	199	C	C2-N1-C1'	-5.22	113.06	118.80
1	AA	1849	U	N1-C2-O2	-5.22	119.14	122.80
1	AA	2637	G	N1-C6-O6	-5.22	116.77	119.90
1	AA	512	C	OP1-P-O3'	5.22	116.68	105.20
1	AA	615	G	N1-C6-O6	-5.22	116.77	119.90
1	AA	2572	C	C4-C5-C6	5.22	120.01	117.40
1	AA	2879	G	C5-C6-N1	-5.22	108.89	111.50
34	BA	787	A	OP2-P-O3'	5.22	116.68	105.20
1	CA	154(A)	C	N1-C2-O2	5.22	122.03	118.90
1	AA	250	G	C5-C6-O6	-5.22	125.47	128.60
1	AA	1835	C	C6-N1-C2	-5.22	118.21	120.30
2	AB	90	A	N7-C8-N9	-5.22	111.19	113.80
34	DA	175	C	C6-N1-C2	-5.22	118.21	120.30
1	AA	974	G	C6-C5-N7	-5.22	127.27	130.40
1	AA	1659	G	N1-C6-O6	-5.22	116.77	119.90
1	AA	2576	A	C5-C6-N6	5.22	127.87	123.70
1	AA	2783	G	C5-C6-O6	-5.22	125.47	128.60
1	CA	241	A	O5'-P-OP2	-5.22	101.00	105.70
1	AA	410	U	C4-C5-C6	5.21	122.83	119.70
1	CA	1284	A	N9-C4-C5	-5.21	103.71	105.80
34	DA	577	G	OP2-P-O3'	5.21	116.67	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1301	U	C4-C5-C6	-5.21	116.57	119.70
1	CA	2570	G	C5-C6-O6	5.21	131.73	128.60
1	AA	558	G	C5-C6-N1	5.21	114.11	111.50
1	AA	2014	G	C2'-C3'-O3'	5.21	122.04	113.70
1	AA	2033	U	C6-N1-C2	-5.21	117.87	121.00
1	AA	2504	U	OP2-P-O3'	5.21	116.67	105.20
1	CA	2085	C	C2-N3-C4	-5.21	117.29	119.90
2	CB	30	C	C2-N1-C1'	5.21	124.53	118.80
1	AA	2858	G	N3-C2-N2	5.21	123.55	119.90
1	CA	2822	G	N9-C4-C5	-5.21	103.32	105.40
1	AA	990	A	C8-N9-C1'	-5.21	118.32	127.70
1	AA	1704	C	OP2-P-O3'	5.21	116.66	105.20
1	AA	2006	G	OP2-P-O3'	5.21	116.66	105.20
1	AA	2320	G	C5-N7-C8	-5.21	101.70	104.30
1	AA	2676	G	C5-C6-O6	-5.21	125.47	128.60
1	CA	1350	C	N1-C2-O2	-5.21	115.78	118.90
1	CA	1355	G	C2-N3-C4	5.21	114.50	111.90
1	AA	1024	G	C8-N9-C4	5.21	108.48	106.40
1	AA	1200	G	OP1-P-OP2	-5.21	111.79	119.60
1	AA	2101	U	C4-C5-C6	5.21	122.82	119.70
1	CA	411	G	O4'-C1'-N9	-5.21	104.03	108.20
1	AA	22	C	C5-C4-N4	5.21	123.84	120.20
34	BA	552	U	C5-C6-N1	-5.21	120.10	122.70
2	CB	56	G	N3-C4-C5	-5.21	126.00	128.60
1	AA	65	C	N3-C4-N4	-5.20	114.36	118.00
1	AA	995	G	N7-C8-N9	5.20	115.70	113.10
1	AA	2633	A	O5'-P-OP1	-5.20	101.02	105.70
1	CA	426	C	N1-C2-O2	5.20	122.02	118.90
1	CA	1964	G	O4'-C1'-N9	-5.20	104.04	108.20
34	BA	822	C	C6-N1-C2	5.20	122.38	120.30
1	CA	948	G	N9-C4-C5	5.20	107.48	105.40
1	CA	961	C	OP1-P-OP2	5.20	127.40	119.60
1	AA	472	G	C5-C6-O6	-5.20	125.48	128.60
1	AA	1646	C	C5-C6-N1	-5.20	118.40	121.00
1	AA	1967	G	N1-C2-N3	5.20	127.02	123.90
1	AA	2389	A	N1-C6-N6	5.20	121.72	118.60
1	AA	2632	C	N3-C4-N4	-5.20	114.36	118.00
1	AA	2826	C	N3-C4-N4	-5.20	114.36	118.00
1	CA	1374	G	N1-C6-O6	5.20	123.02	119.90
1	CA	1885	A	N7-C8-N9	-5.20	111.20	113.80
34	BA	768	A	N1-C2-N3	5.20	131.90	129.30
34	BA	1511	G	C8-N9-C4	5.20	108.48	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	474	G	C6-N1-C2	-5.20	121.98	125.10
1	AA	187	C	N3-C4-C5	5.20	123.98	121.90
1	AA	1697	G	OP1-P-OP2	-5.20	111.81	119.60
1	AA	2303	U	N1-C2-N3	5.20	118.02	114.90
1	CA	2599	G	C6-C5-N7	5.20	133.52	130.40
1	AA	31	C	N3-C4-N4	-5.20	114.36	118.00
1	AA	479	C	C5-C6-N1	-5.20	118.40	121.00
34	BA	1471	G	N1-C6-O6	-5.20	116.78	119.90
1	CA	2431	U	N3-C4-C5	5.20	117.72	114.60
34	DA	1481	U	C5-C4-O4	5.20	129.02	125.90
1	AA	2561	G	C6-C5-N7	-5.19	127.28	130.40
1	AA	2294	G	N9-C4-C5	-5.19	103.32	105.40
1	AA	2619	G	N1-C2-N3	5.19	127.02	123.90
1	AA	2877	G	O4'-C1'-N9	5.19	112.36	108.20
1	CA	1611	C	N1-C2-O2	5.19	122.02	118.90
1	CA	1721	G	C5-C6-O6	-5.19	125.48	128.60
1	CA	2356	C	C6-N1-C2	5.19	122.38	120.30
1	AA	898	U	C5-C6-N1	-5.19	120.10	122.70
34	BA	791	G	O5'-P-OP2	5.19	116.93	110.70
1	CA	795	C	C4-C5-C6	5.19	120.00	117.40
2	CB	15	A	C8-N9-C4	5.19	107.88	105.80
1	AA	1332	A	O5'-P-OP2	-5.19	101.03	105.70
1	AA	2221	A	O5'-P-OP2	5.19	116.93	110.70
1	CA	1778	U	C5-C6-N1	-5.19	120.11	122.70
1	AA	884	C	C4-C5-C6	5.19	119.99	117.40
1	AA	999	G	N1-C2-N2	-5.19	111.53	116.20
1	AA	1097	G	N1-C6-O6	5.19	123.01	119.90
1	AA	1254	G	C5-C6-O6	-5.19	125.49	128.60
1	AA	1343	C	N3-C4-N4	-5.19	114.37	118.00
1	AA	2374	G	N7-C8-N9	-5.19	110.51	113.10
1	CA	826	U	N3-C4-O4	-5.19	115.77	119.40
1	CA	1155	A	OP1-P-O3'	5.19	116.61	105.20
1	CA	1372	U	C5-C4-O4	-5.19	122.79	125.90
1	AA	479	C	C6-N1-C2	5.18	122.37	120.30
1	AA	551	A	C4-C5-N7	-5.18	108.11	110.70
1	AA	2017	U	N3-C2-O2	-5.18	118.57	122.20
1	AA	2281	A	N1-C6-N6	5.18	121.71	118.60
1	AA	2726	A	C8-N9-C4	5.18	107.87	105.80
1	AA	2761	A	N7-C8-N9	-5.18	111.21	113.80
34	BA	1482	G	C8-N9-C1'	-5.18	120.26	127.00
1	AA	438	G	N3-C2-N2	-5.18	116.27	119.90
1	AA	2260	C	O5'-P-OP2	-5.18	101.04	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1210	A	OP2-P-O3'	5.18	116.60	105.20
1	CA	1976	U	C2-N3-C4	-5.18	123.89	127.00
1	AA	74	G	N3-C4-C5	5.18	131.19	128.60
1	AA	1078	A	C8-N9-C4	5.18	107.87	105.80
1	AA	1472	G	C5-C6-N1	5.18	114.09	111.50
1	AA	1983	C	C4-C5-C6	5.18	119.99	117.40
1	CA	2508	G	N1-C6-O6	-5.18	116.79	119.90
1	AA	1242	G	C8-N9-C4	5.18	108.47	106.40
1	AA	2056	U	N1-C2-N3	5.18	118.01	114.90
1	CA	556	G	C5-C6-O6	-5.18	125.49	128.60
1	CA	1251	C	OP1-P-OP2	5.18	127.37	119.60
1	CA	2046	G	C8-N9-C4	5.18	108.47	106.40
1	CA	2647	U	C6-N1-C2	5.18	124.11	121.00
1	AA	1811	A	OP1-P-O3'	5.18	116.59	105.20
1	CA	1374	G	C6-C5-N7	-5.18	127.29	130.40
34	DA	691	G	N1-C6-O6	5.18	123.01	119.90
1	AA	1247	C	C5-C4-N4	-5.18	116.58	120.20
34	BA	266	G	C8-N9-C4	-5.18	104.33	106.40
1	CA	17	G	OP1-P-OP2	-5.18	111.83	119.60
1	CA	501	A	O5'-P-OP2	-5.18	101.04	105.70
1	CA	934	G	C6-C5-N7	-5.18	127.29	130.40
1	CA	2526	G	N1-C6-O6	5.18	123.01	119.90
34	DA	557	G	O5'-P-OP2	-5.18	101.04	105.70
1	AA	1299	A	C5-C6-N6	-5.17	119.56	123.70
34	BA	760	G	C5-C6-O6	-5.17	125.50	128.60
1	CA	823	G	C5-C6-N1	5.17	114.09	111.50
14	AQ	2	LEU	CA-CB-CG	5.17	127.20	115.30
34	BA	1227	A	C2-N3-C4	-5.17	108.01	110.60
1	CA	791	C	N3-C4-N4	-5.17	114.38	118.00
1	AA	74	G	C4-C5-N7	5.17	112.87	110.80
1	AA	816	G	N1-C6-O6	-5.17	116.80	119.90
1	AA	1024	G	N1-C6-O6	-5.17	116.80	119.90
1	AA	1361	C	C6-N1-C2	-5.17	118.23	120.30
1	AA	1612	C	N1-C2-O2	-5.17	115.80	118.90
1	AA	2051	G	N9-C4-C5	5.17	107.47	105.40
1	AA	2400	A	O4'-C1'-N9	5.17	112.34	108.20
18	AU	20	LEU	CB-CG-CD1	-5.17	102.21	111.00
19	AV	35	LEU	CA-CB-CG	5.17	127.19	115.30
1	CA	1989	G	C4-C5-N7	5.17	112.87	110.80
1	AA	884	C	OP1-P-OP2	-5.17	111.84	119.60
1	AA	454	U	OP1-P-O3'	5.17	116.57	105.20
1	AA	859	C	N3-C4-N4	-5.17	114.38	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1387	U	N1-C2-O2	-5.17	119.18	122.80
2	AB	15	A	C8-N9-C4	5.17	107.87	105.80
1	CA	987	G	C4-N9-C1'	-5.17	119.78	126.50
1	AA	1155	C	C6-N1-C2	-5.17	118.23	120.30
1	AA	1401	G	C5-C6-O6	5.17	131.70	128.60
1	AA	2075	G	O5'-P-OP2	-5.17	101.05	105.70
1	AA	2550	C	C6-N1-C2	5.17	122.37	120.30
1	CA	185	U	C5-C6-N1	-5.17	120.12	122.70
1	AA	455	A	C5-C6-N1	-5.17	115.12	117.70
1	AA	1281	G	N1-C6-O6	5.16	123.00	119.90
1	AA	1623	U	OP2-P-O3'	5.16	116.56	105.20
2	AB	62	C	OP1-P-OP2	5.16	127.35	119.60
1	CA	666	G	N1-C2-N2	-5.16	111.55	116.20
1	CA	2863	C	N3-C4-C5	5.16	123.97	121.90
1	AA	777	C	N3-C2-O2	-5.16	118.29	121.90
34	DA	866	C	N1-C2-O2	5.16	122.00	118.90
1	AA	200	A	C2-N3-C4	-5.16	108.02	110.60
1	AA	971	C	C2-N3-C4	-5.16	117.32	119.90
1	AA	2114	U	N1-C2-O2	5.16	126.41	122.80
1	AA	2117	C	OP2-P-O3'	5.16	116.55	105.20
1	CA	2063	C	OP2-P-O3'	5.16	116.55	105.20
34	DA	1527	C	C6-N1-C2	5.16	122.36	120.30
1	AA	310	C	C6-N1-C2	5.16	122.36	120.30
1	AA	2016	C	N3-C4-C5	-5.16	119.84	121.90
1	AA	2035	A	N9-C4-C5	-5.16	103.74	105.80
1	CA	1647	G	C6-C5-N7	5.16	133.50	130.40
1	CA	2032	G	N7-C8-N9	-5.16	110.52	113.10
2	CB	80	U	C5-C4-O4	5.16	129.00	125.90
2	AB	55	U	N1-C2-O2	-5.16	119.19	122.80
1	CA	2292	C	C6-N1-C2	5.16	122.36	120.30
1	CA	2720	U	N3-C2-O2	-5.16	118.59	122.20
34	BA	1477	C	C6-N1-C2	-5.16	118.24	120.30
1	CA	827	U	N3-C4-C5	5.16	117.69	114.60
1	CA	2766	G	C4-N9-C1'	5.16	133.20	126.50
1	AA	1405	A	C6-N1-C2	5.15	121.69	118.60
34	BA	872	A	O4'-C1'-N9	5.15	112.32	108.20
1	CA	2642	G	OP2-P-O3'	5.15	116.54	105.20
1	AA	45	C	O4'-C1'-N1	5.15	112.32	108.20
1	AA	818	G	C4-C5-N7	-5.15	108.74	110.80
1	AA	1757	C	N3-C2-O2	5.15	125.51	121.90
2	AB	48	A	N1-C6-N6	5.15	121.69	118.60
1	CA	715	G	O5'-P-OP2	-5.15	101.06	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	997	G	O5'-P-OP1	-5.15	101.06	105.70
1	CA	1019	U	C5-C4-O4	5.15	128.99	125.90
1	AA	239	G	C8-N9-C4	-5.15	104.34	106.40
1	AA	1434	G	N3-C4-C5	-5.15	126.03	128.60
1	AA	1515	C	N1-C2-O2	-5.15	115.81	118.90
34	BA	786	G	N1-C6-O6	-5.15	116.81	119.90
1	CA	225	A	O5'-P-OP2	-5.15	101.06	105.70
4	CD	52	ARG	NE-CZ-NH1	-5.15	117.72	120.30
34	DA	1487	G	C8-N9-C4	-5.15	104.34	106.40
1	AA	1232	G	C6-C5-N7	5.15	133.49	130.40
34	BA	753	A	OP1-P-O3'	5.15	116.53	105.20
1	AA	816	G	N3-C2-N2	5.15	123.50	119.90
1	AA	2115	G	C5-C6-O6	-5.15	125.51	128.60
1	AA	2274	U	N1-C2-N3	5.15	117.99	114.90
34	DA	1079	G	C8-N9-C4	-5.15	104.34	106.40
34	BA	1482	G	N9-C4-C5	-5.15	103.34	105.40
1	CA	410	G	C5-C6-O6	5.15	131.69	128.60
1	CA	2655	G	C8-N9-C4	5.15	108.46	106.40
1	AA	724	A	N9-C4-C5	5.14	107.86	105.80
1	AA	621	G	N3-C4-C5	-5.14	126.03	128.60
1	AA	1917	C	OP2-P-O3'	5.14	116.51	105.20
1	AA	2364	A	N9-C4-C5	-5.14	103.74	105.80
1	CA	127	A	O5'-P-OP2	-5.14	101.07	105.70
2	AB	12	C	O5'-P-OP1	-5.14	101.07	105.70
1	AA	2511	C	N3-C2-O2	5.14	125.50	121.90
1	AA	2547	G	C8-N9-C4	-5.14	104.34	106.40
1	AA	2801	C	N3-C4-C5	5.14	123.96	121.90
1	AA	2897	U	N3-C4-C5	5.14	117.68	114.60
1	CA	2608	G	C5-C6-O6	5.14	131.68	128.60
34	DA	1154	G	O4'-C1'-N9	5.14	112.31	108.20
1	AA	1963	C	N3-C2-O2	5.14	125.50	121.90
1	AA	2231	G	N1-C6-O6	5.14	122.98	119.90
1	AA	2243	C	C5-C6-N1	-5.14	118.43	121.00
1	CA	2286	A	C8-N9-C4	-5.14	103.75	105.80
1	AA	2510	C	C6-N1-C2	-5.14	118.25	120.30
34	BA	821	G	N1-C6-O6	-5.14	116.82	119.90
1	CA	850	C	O5'-P-OP1	-5.14	101.08	105.70
1	CA	2454	G	N1-C6-O6	-5.14	116.82	119.90
34	DA	1119	C	C6-N1-C2	-5.14	118.25	120.30
34	DA	1201	A	P-O3'-C3'	5.14	125.86	119.70
1	AA	1236	G	N7-C8-N9	-5.13	110.53	113.10
1	AA	1344	C	C6-N1-C2	5.13	122.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	2048	C	OP2-P-O3'	5.13	116.50	105.20
34	DA	1004	A	O4'-C1'-N9	5.13	112.31	108.20
59	BZ	378	VAL	CB-CA-C	-5.13	101.65	111.40
1	CA	668	G	OP2-P-O3'	5.13	116.49	105.20
34	DA	865	A	C2-N3-C4	-5.13	108.03	110.60
1	AA	131	C	O5'-P-OP2	-5.13	101.08	105.70
1	AA	2011	G	N3-C2-N2	5.13	123.49	119.90
1	AA	2456	G	O5'-P-OP1	-5.13	101.08	105.70
34	BA	800	G	O5'-P-OP2	-5.13	101.08	105.70
1	CA	934	G	N1-C6-O6	5.13	122.98	119.90
1	CA	1331	A	N1-C2-N3	5.13	131.87	129.30
1	AA	137	G	N3-C4-C5	-5.13	126.04	128.60
34	BA	974	A	N1-C6-N6	5.13	121.68	118.60
1	AA	1154	U	C5-C4-O4	5.12	128.97	125.90
34	BA	1036	G	C8-N9-C1'	-5.12	120.34	127.00
1	CA	1684	C	N1-C2-O2	-5.12	115.83	118.90
1	AA	199	C	C6-N1-C2	5.12	122.35	120.30
1	AA	1742	G	C5-C6-O6	-5.12	125.53	128.60
34	DA	354	G	C8-N9-C1'	-5.12	120.34	127.00
1	AA	24	G	O5'-P-OP1	-5.12	101.09	105.70
1	AA	1843	A	C4-C5-N7	-5.12	108.14	110.70
1	AA	2217	C	OP1-P-O3'	5.12	116.47	105.20
1	AA	2560	G	O5'-P-OP1	-5.12	101.09	105.70
1	CA	540	C	N1-C2-O2	5.12	121.97	118.90
1	CA	668	G	N3-C4-C5	5.12	131.16	128.60
1	CA	708	C	N1-C2-O2	5.12	121.97	118.90
1	CA	2616	C	N1-C2-O2	5.12	121.97	118.90
1	AA	826	U	C5-C4-O4	-5.12	122.83	125.90
1	AA	1772	C	C6-N1-C2	-5.12	118.25	120.30
2	AB	118	G	C8-N9-C4	5.12	108.45	106.40
34	DA	1501	C	C4-C5-C6	5.12	119.96	117.40
1	AA	354	A	C8-N9-C1'	5.12	136.91	127.70
1	AA	1033	G	N9-C4-C5	5.12	107.45	105.40
1	AA	2056	U	C4-C5-C6	5.12	122.77	119.70
34	BA	354	G	O5'-P-OP2	-5.12	101.09	105.70
1	CA	2525	G	O5'-P-OP2	-5.12	101.09	105.70
1	CA	28	A	N1-C6-N6	-5.12	115.53	118.60
1	CA	1647	G	O5'-P-OP1	-5.12	101.09	105.70
1	AA	1303	C	C4-C5-C6	5.12	119.96	117.40
1	AA	1380	G	N9-C4-C5	5.12	107.45	105.40
1	AA	2257	U	C6-N1-C2	5.12	124.07	121.00
1	AA	2535	G	C6-C5-N7	-5.12	127.33	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	2896	G	N3-C2-N2	-5.12	116.32	119.90
34	BA	518	C	N1-C2-O2	5.12	121.97	118.90
1	CA	387	U	OP1-P-O3'	5.12	116.45	105.20
1	CA	1579	A	N1-C6-N6	5.12	121.67	118.60
1	AA	54	G	N1-C6-O6	-5.11	116.83	119.90
1	AA	192	C	N3-C4-C5	5.11	123.95	121.90
1	AA	434	G	N3-C4-C5	-5.11	126.04	128.60
1	AA	2847	G	C4-C5-C6	5.11	121.87	118.80
2	CB	85	G	N9-C4-C5	-5.11	103.36	105.40
1	CA	298	G	N9-C4-C5	-5.11	103.36	105.40
57	DX	74	C	OP2-P-O3'	-5.11	93.95	105.20
1	AA	738	C	C2-N3-C4	-5.11	117.34	119.90
1	AA	837	C	N3-C4-C5	5.11	123.94	121.90
1	AA	2251	G	N7-C8-N9	-5.11	110.55	113.10
1	CA	866	A	OP1-P-O3'	5.11	116.44	105.20
1	CA	2598	A	N1-C6-N6	5.11	121.67	118.60
1	AA	2467	G	N1-C2-N2	-5.11	111.60	116.20
34	BA	1483	A	O5'-P-OP1	-5.11	101.10	105.70
1	CA	385	C	N1-C2-O2	5.11	121.97	118.90
1	AA	474	U	C5-C4-O4	5.11	128.97	125.90
1	CA	827	U	C5-C6-N1	-5.11	120.15	122.70
1	CA	1681	G	C4-C5-N7	5.11	112.84	110.80
1	AA	581	G	O5'-P-OP2	-5.11	101.11	105.70
1	AA	1655	A	N1-C2-N3	-5.11	126.75	129.30
1	AA	1829	U	C5-C6-N1	-5.11	120.15	122.70
1	AA	1062	G	C8-N9-C4	-5.10	104.36	106.40
1	CA	571	A	OP1-P-OP2	-5.10	111.94	119.60
1	CA	1799	G	C4-C5-N7	-5.10	108.76	110.80
1	CA	2242	G	N7-C8-N9	-5.10	110.55	113.10
1	AA	471	C	N1-C2-O2	-5.10	115.84	118.90
1	AA	1961	U	O5'-P-OP1	-5.10	101.11	105.70
2	AB	108	U	C6-N1-C2	5.10	124.06	121.00
34	BA	7	G	N3-C4-C5	5.10	131.15	128.60
1	CA	2258	C	N3-C4-C5	5.10	123.94	121.90
1	CA	2708	G	N3-C4-C5	5.10	131.15	128.60
1	AA	479	C	C5-C4-N4	5.10	123.77	120.20
1	AA	2530	A	N1-C6-N6	5.10	121.66	118.60
1	AA	584	G	C2-N3-C4	5.10	114.45	111.90
1	CA	453	C	C6-N1-C2	5.10	122.34	120.30
1	CA	2242	G	C5-N7-C8	5.10	106.85	104.30
1	CA	2435	A	N7-C8-N9	5.10	116.35	113.80
1	CA	2732	G	N1-C6-O6	-5.10	116.84	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	704	U	C6-N1-C2	5.10	124.06	121.00
1	AA	1025	G	C5-C6-N1	5.10	114.05	111.50
1	AA	1385	G	C5-C6-O6	-5.10	125.54	128.60
1	AA	1551	C	C6-N1-C2	-5.10	118.26	120.30
1	AA	1647	G	N7-C8-N9	-5.10	110.55	113.10
1	AA	2340	A	N7-C8-N9	-5.10	111.25	113.80
1	AA	2743	C	C6-N1-C2	5.10	122.34	120.30
1	CA	516	C	C6-N1-C2	5.10	122.34	120.30
1	CA	1779	U	C5-C4-O4	-5.10	122.84	125.90
1	AA	2256	U	N3-C4-O4	-5.10	115.83	119.40
1	AA	876	A	C4-C5-N7	5.09	113.25	110.70
34	BA	890	G	N1-C6-O6	-5.09	116.84	119.90
1	CA	1788	C	C4-C5-C6	5.09	119.95	117.40
1	AA	866	A	OP2-P-O3'	5.09	116.41	105.20
6	AF	38	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	CA	482	A	C4-C5-C6	5.09	119.55	117.00
1	CA	1681	G	C2-N3-C4	-5.09	109.35	111.90
1	AA	632	A	C8-N9-C4	5.09	107.84	105.80
1	AA	814	U	C2-N3-C4	-5.09	123.94	127.00
1	AA	1068	G	N3-C4-N9	-5.09	122.94	126.00
1	AA	1412	A	N7-C8-N9	-5.09	111.25	113.80
1	AA	1815	A	C5-C6-N1	-5.09	115.15	117.70
1	AA	2238	C	C2-N3-C4	-5.09	117.35	119.90
34	BA	345	C	N3-C4-C5	-5.09	119.86	121.90
34	BA	524	G	C5-C6-O6	-5.09	125.55	128.60
34	BA	807	A	N1-C6-N6	-5.09	115.55	118.60
34	DA	1373	G	N3-C4-C5	-5.09	126.05	128.60
34	DA	1482	G	C8-N9-C1'	-5.09	120.38	127.00
1	AA	645	G	N3-C2-N2	5.09	123.46	119.90
1	AA	762	G	C6-C5-N7	-5.09	127.35	130.40
1	AA	2553	A	C5-C6-N6	-5.09	119.63	123.70
1	AA	358	C	C5-C6-N1	-5.09	118.46	121.00
1	CA	2057	A	O5'-P-OP2	-5.09	101.12	105.70
1	AA	742	G	C5-C6-O6	5.09	131.65	128.60
1	AA	1449	C	O5'-P-OP1	-5.09	101.12	105.70
1	AA	2467	G	N1-C6-O6	-5.09	116.85	119.90
1	AA	2686	G	C8-N9-C4	-5.09	104.36	106.40
1	CA	40	C	C5-C6-N1	-5.09	118.46	121.00
1	AA	913	A	C2-N3-C4	-5.08	108.06	110.60
1	CA	798	G	N1-C6-O6	-5.08	116.85	119.90
1	AA	414	U	N3-C2-O2	5.08	125.76	122.20
1	AA	2335	G	C4-C5-N7	5.08	112.83	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	2515	A	C6-C5-N7	-5.08	128.74	132.30
1	AA	2723	A	N9-C4-C5	-5.08	103.77	105.80
1	CA	2331	G	C2-N3-C4	-5.08	109.36	111.90
1	AA	781	A	C5-C6-N6	-5.08	119.63	123.70
1	AA	2484	G	C6-N1-C2	-5.08	122.05	125.10
1	AA	2773	C	N1-C2-O2	-5.08	115.85	118.90
20	AW	18	ARG	NE-CZ-NH2	-5.08	117.76	120.30
34	BA	580	U	C5-C6-N1	-5.08	120.16	122.70
1	CA	1181	C	C6-N1-C2	5.08	122.33	120.30
1	AA	1617	A	N9-C4-C5	-5.08	103.77	105.80
1	AA	1544	C	OP1-P-O3'	5.08	116.37	105.20
1	AA	25	U	C2-N3-C4	-5.08	123.95	127.00
1	AA	1365	G	OP2-P-O3'	5.08	116.37	105.20
1	AA	1441	A	C8-N9-C4	5.08	107.83	105.80
1	AA	1809	U	N1-C2-N3	-5.08	111.85	114.90
1	AA	2701	U	C6-N1-C2	-5.08	117.95	121.00
1	CA	1687	G	N3-C2-N2	5.08	123.45	119.90
1	AA	32	C	C5-C6-N1	-5.08	118.46	121.00
1	AA	240	A	C6-C5-N7	5.08	135.85	132.30
1	AA	1026	A	C8-N9-C4	5.08	107.83	105.80
1	AA	2759	U	C5-C6-N1	-5.08	120.16	122.70
2	AB	103	G	N1-C6-O6	5.08	122.95	119.90
34	DA	7	G	C8-N9-C1'	5.08	133.60	127.00
34	DA	907	A	OP2-P-O3'	5.08	116.37	105.20
1	AA	2019	G	N1-C6-O6	-5.07	116.86	119.90
1	AA	2233	G	N1-C6-O6	-5.07	116.86	119.90
1	AA	2441	G	N1-C2-N3	5.07	126.94	123.90
1	AA	2801	C	C2-N3-C4	-5.07	117.36	119.90
34	BA	423	G	N3-C4-N9	5.07	129.04	126.00
34	DA	532	A	P-O3'-C3'	5.07	125.79	119.70
1	AA	630	U	N3-C2-O2	5.07	125.75	122.20
1	AA	2059	G	N7-C8-N9	-5.07	110.56	113.10
1	AA	225	C	N3-C4-C5	5.07	123.93	121.90
1	AA	2638	C	C2-N3-C4	-5.07	117.36	119.90
1	CA	1644	C	N3-C4-C5	-5.07	119.87	121.90
1	AA	1275	G	N1-C6-O6	5.07	122.94	119.90
1	AA	2272	C	C4-C5-C6	5.07	119.93	117.40
34	BA	1030(B)	C	N3-C2-O2	-5.07	118.35	121.90
1	AA	199	C	C5-C4-N4	5.07	123.75	120.20
1	AA	536	U	N1-C2-O2	-5.07	119.25	122.80
2	AB	64	C	C5-C6-N1	-5.07	118.47	121.00
5	AE	47	VAL	CB-CA-C	-5.07	101.77	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1054	C	C6-N1-C2	5.07	122.33	120.30
1	AA	2276	C	C2-N3-C4	-5.07	117.37	119.90
1	AA	2576	A	C8-N9-C4	-5.07	103.77	105.80
34	BA	605	U	C5-C4-O4	5.07	128.94	125.90
34	BA	1458	G	C5-C6-O6	-5.07	125.56	128.60
34	DA	904	C	C5-C4-N4	-5.07	116.65	120.20
1	AA	1376	C	C5-C6-N1	-5.06	118.47	121.00
1	CA	1687	G	OP2-P-O3'	5.06	116.34	105.20
1	CA	2712	U	N3-C4-C5	5.06	117.64	114.60
34	BA	578	C	C2-N3-C4	-5.06	117.37	119.90
1	AA	1240	G	C5-C6-N1	5.06	114.03	111.50
1	AA	1720	U	O4'-C1'-N1	5.06	112.25	108.20
1	AA	2344	U	N3-C4-O4	-5.06	115.86	119.40
34	BA	598	U	N3-C4-O4	5.06	122.94	119.40
1	AA	17	G	N1-C6-O6	-5.06	116.86	119.90
1	AA	1585	G	N1-C6-O6	5.06	122.94	119.90
1	AA	2611	G	N1-C6-O6	-5.06	116.86	119.90
34	BA	546	G	N9-C4-C5	5.06	107.42	105.40
1	CA	116	C	O5'-P-OP2	-5.06	101.15	105.70
34	DA	758	G	C5-C6-O6	5.06	131.63	128.60
1	AA	174	U	OP2-P-O3'	5.06	116.33	105.20
1	AA	733	G	O4'-C1'-N9	5.06	112.25	108.20
1	AA	2403	G	O4'-C1'-N9	5.06	112.25	108.20
1	AA	2437	A	N1-C6-N6	5.06	121.63	118.60
29	A5	20	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	CA	1680	U	N1-C2-O2	-5.06	119.26	122.80
1	CA	2167	U	C2-N1-C1'	5.06	123.77	117.70
1	AA	1258	A	C6-N1-C2	-5.06	115.57	118.60
1	AA	2775	G	C5-C6-O6	5.06	131.63	128.60
1	CA	1129	A	OP1-P-OP2	5.06	127.18	119.60
1	AA	1545	C	C5-C6-N1	-5.05	118.47	121.00
1	CA	660	G	C5-C6-O6	5.05	131.63	128.60
1	CA	1256	G	N1-C6-O6	5.05	122.93	119.90
1	CA	2439	A	N1-C6-N6	5.05	121.63	118.60
1	CA	2523	G	C4-N9-C1'	5.05	133.07	126.50
1	CA	2625	G	C8-N9-C4	5.05	108.42	106.40
34	DA	1502	A	C5-C6-N6	-5.05	119.66	123.70
1	AA	730	C	N3-C4-C5	5.05	123.92	121.90
1	AA	2016	C	C4-C5-C6	5.05	119.93	117.40
1	AA	2701	U	N3-C2-O2	-5.05	118.66	122.20
1	CA	2277	G	N9-C4-C5	5.05	107.42	105.40
1	AA	2375	C	C5-C4-N4	5.05	123.74	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	BQ	9	VAL	CB-CA-C	-5.05	101.80	111.40
34	DA	1517	G	O5'-P-OP2	-5.05	101.15	105.70
1	AA	2682	A	N1-C6-N6	-5.05	115.57	118.60
1	CA	1531	C	C5-C6-N1	5.05	123.53	121.00
1	CA	1784	A	C8-N9-C4	5.05	107.82	105.80
1	AA	655	G	O5'-P-OP2	-5.05	101.16	105.70
1	AA	893	C	C2-N1-C1'	-5.05	113.25	118.80
1	AA	2828	G	OP1-P-OP2	5.05	127.17	119.60
34	BA	770	C	N3-C2-O2	-5.05	118.37	121.90
1	CA	794	G	N1-C2-N2	-5.05	111.66	116.20
1	AA	632	A	N7-C8-N9	-5.05	111.28	113.80
1	AA	875	U	N1-C2-O2	-5.05	119.27	122.80
1	AA	2074	G	C4-C5-N7	-5.05	108.78	110.80
34	BA	337	C	N1-C2-O2	5.05	121.93	118.90
1	CA	2496	C	C5-C4-N4	5.05	123.73	120.20
1	AA	592	U	N1-C2-N3	5.04	117.93	114.90
34	BA	852	G	N7-C8-N9	-5.04	110.58	113.10
1	AA	739	C	OP1-P-OP2	-5.04	112.03	119.60
1	AA	1653	C	N3-C4-C5	-5.04	119.88	121.90
1	AA	2578	A	O4'-C1'-N9	5.04	112.23	108.20
1	AA	2883	A	C8-N9-C4	-5.04	103.78	105.80
34	BA	769	G	OP2-P-O3'	5.04	116.30	105.20
1	AA	201	G	N7-C8-N9	-5.04	110.58	113.10
1	AA	1848	G	N1-C6-O6	-5.04	116.88	119.90
1	CA	125	G	O4'-C1'-N9	-5.04	104.17	108.20
1	CA	528	A	C4-C5-N7	5.04	113.22	110.70
1	CA	2286	A	C4-C5-N7	5.04	113.22	110.70
34	DA	784	C	N3-C2-O2	5.04	125.43	121.90
1	AA	1418	U	C2-N1-C1'	5.04	123.75	117.70
1	AA	2243	C	C2-N3-C4	-5.04	117.38	119.90
1	CA	2415	G	C5-C6-O6	-5.04	125.58	128.60
1	AA	953	U	OP2-P-O3'	5.04	116.28	105.20
1	AA	1256	U	OP1-P-OP2	-5.04	112.04	119.60
1	AA	1824	C	N3-C4-C5	5.04	123.92	121.90
1	CA	141	A	O4'-C1'-N9	5.04	112.23	108.20
1	CA	2413	G	N3-C2-N2	-5.04	116.37	119.90
34	DA	319	G	N1-C6-O6	-5.04	116.88	119.90
34	DA	646	U	N3-C2-O2	-5.04	118.67	122.20
34	DA	1063	C	C5-C6-N1	5.04	123.52	121.00
1	CA	856	C	C3'-C2'-C1'	-5.04	97.47	101.50
1	AA	17	G	C5-C6-N1	5.04	114.02	111.50
1	AA	199	C	C2-N3-C4	-5.04	117.38	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	777	C	C5-C6-N1	-5.04	118.48	121.00
1	AA	1398	U	OP1-P-OP2	-5.04	112.05	119.60
1	AA	555	G	C4-C5-C6	-5.03	115.78	118.80
1	AA	2057	G	O4'-C1'-N9	5.03	112.23	108.20
34	BA	1430	C	N3-C4-N4	-5.03	114.48	118.00
1	CA	1797	C	C2-N3-C4	-5.03	117.38	119.90
1	AA	448	U	N3-C4-O4	-5.03	115.88	119.40
1	AA	2416	C	C2-N1-C1'	-5.03	113.27	118.80
2	AB	80	U	C6-N1-C2	5.03	124.02	121.00
1	CA	663	G	C4-C5-N7	-5.03	108.79	110.80
1	CA	1425	G	C8-N9-C1'	-5.03	120.46	127.00
1	CA	2043	C	N3-C2-O2	-5.03	118.38	121.90
1	AA	596	G	C2-N3-C4	5.03	114.42	111.90
1	AA	610	C	C5-C6-N1	5.03	123.52	121.00
1	AA	1589	A	C8-N9-C4	-5.03	103.79	105.80
1	AA	2026	G	N1-C6-O6	5.03	122.92	119.90
1	CA	47	C	C5-C6-N1	-5.03	118.48	121.00
1	CA	753	C	O5'-P-OP2	5.03	116.74	110.70
1	CA	1901	A	C5-C6-N1	5.03	120.22	117.70
1	CA	2570	G	O5'-P-OP1	-5.03	101.17	105.70
1	AA	2229	A	N1-C6-N6	5.03	121.62	118.60
1	AA	723	A	N1-C6-N6	5.03	121.62	118.60
1	AA	1924	C	OP2-P-O3'	5.03	116.26	105.20
1	AA	2384	G	C4-C5-N7	5.03	112.81	110.80
1	AA	2902	G	C5-N7-C8	-5.03	101.79	104.30
1	CA	1397	U	O4'-C1'-N1	5.03	112.22	108.20
1	CA	2040	C	C5-C6-N1	-5.03	118.49	121.00
1	CA	2489	G	OP2-P-O3'	5.03	116.26	105.20
1	CA	2538	C	C6-N1-C2	5.03	122.31	120.30
1	AA	126	C	N1-C2-O2	-5.03	115.89	118.90
1	AA	874	U	O5'-P-OP2	-5.03	101.18	105.70
1	AA	1256	U	C5-C6-N1	-5.03	120.19	122.70
1	AA	1713	G	O4'-C1'-N9	5.03	112.22	108.20
34	BA	1445	C	C6-N1-C2	-5.03	118.29	120.30
34	DA	322	C	C6-N1-C2	5.03	122.31	120.30
1	AA	1665	G	N3-C4-N9	5.02	129.01	126.00
1	CA	460	A	C4-C5-C6	5.02	119.51	117.00
34	DA	31	G	N3-C4-C5	5.02	131.11	128.60
1	AA	279	G	C4-C5-C6	5.02	121.81	118.80
1	AA	549	U	OP2-P-O3'	5.02	116.25	105.20
1	AA	777	C	C4-C5-C6	5.02	119.91	117.40
1	AA	1645	C	C5-C6-N1	-5.02	118.49	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1814	A	C8-N9-C4	-5.02	103.79	105.80
1	AA	1925	G	O5'-P-OP2	-5.02	101.18	105.70
1	AA	2277	U	N3-C2-O2	5.02	125.72	122.20
1	CA	671	C	C6-N1-C2	-5.02	118.29	120.30
1	CA	1284	A	C5-C6-N6	-5.02	119.68	123.70
1	AA	831	A	N7-C8-N9	-5.02	111.29	113.80
34	BA	1457	G	C4-C5-N7	-5.02	108.79	110.80
1	CA	2003	G	N1-C6-O6	-5.02	116.89	119.90
18	CU	28	ARG	NE-CZ-NH1	-5.02	117.79	120.30
1	AA	183	G	OP2-P-O3'	5.02	116.24	105.20
1	AA	462	C	C6-N1-C2	5.02	122.31	120.30
1	AA	1181	G	C5-C6-N1	5.02	114.01	111.50
1	AA	1930	C	C4-C5-C6	5.02	119.91	117.40
23	AZ	86	VAL	CB-CA-C	-5.02	101.86	111.40
1	CA	2291	U	C5-C4-O4	5.02	128.91	125.90
1	CA	2589	A	C2-N3-C4	-5.02	108.09	110.60
1	AA	495	G	C8-N9-C4	5.02	108.41	106.40
1	AA	854	U	N1-C2-N3	5.02	117.91	114.90
1	AA	1178	A	OP1-P-OP2	5.02	127.13	119.60
1	AA	1941	A	N9-C4-C5	-5.02	103.79	105.80
2	AB	43	C	C6-N1-C2	-5.02	118.29	120.30
34	BA	821	G	C2-N3-C4	5.02	114.41	111.90
1	CA	573	G	C2-N3-C4	5.02	114.41	111.90
1	CA	1387	C	C6-N1-C2	-5.02	118.29	120.30
1	CA	1470	G	N3-C4-C5	5.02	131.11	128.60
57	DX	20	U	N1-C2-O2	5.02	126.31	122.80
1	CA	246	C	C6-N1-C2	5.02	122.31	120.30
1	CA	1180	C	C6-N1-C2	5.02	122.31	120.30
1	CA	1786	A	OP1-P-O3'	5.02	116.23	105.20
1	AA	470	C	C6-N1-C2	5.01	122.31	120.30
1	AA	661	G	N3-C2-N2	-5.01	116.39	119.90
1	AA	1479	U	C6-N1-C2	5.01	124.01	121.00
1	AA	1567	G	C8-N9-C4	-5.01	104.39	106.40
1	AA	2567	U	OP1-P-OP2	-5.01	112.08	119.60
34	BA	599	C	N1-C2-O2	5.01	121.91	118.90
1	CA	778	G	C5-C6-O6	-5.01	125.59	128.60
1	CA	2438	U	O5'-P-OP2	-5.01	101.19	105.70
1	AA	31	C	N1-C2-O2	-5.01	115.89	118.90
1	AA	1495	G	C8-N9-C4	5.01	108.41	106.40
1	AA	2044	U	C4-C5-C6	5.01	122.71	119.70
1	AA	820	U	C5-C6-N1	-5.01	120.19	122.70
1	AA	854	U	N3-C2-O2	-5.01	118.69	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1369	U	N1-C2-N3	-5.01	111.89	114.90
1	AA	2723	A	N1-C6-N6	5.01	121.61	118.60
1	AA	2724	U	N1-C2-O2	5.01	126.31	122.80
1	CA	133	C	N3-C4-C5	5.01	123.91	121.90
1	CA	992	C	N3-C4-C5	5.01	123.91	121.90
1	CA	1268	A	OP1-P-O3'	5.01	116.22	105.20
1	AA	1812	C	C6-N1-C1'	-5.01	114.79	120.80
1	AA	1962	U	N1-C2-N3	5.01	117.91	114.90
1	CA	709	U	O5'-P-OP1	5.01	116.71	110.70
1	CA	2614	A	N1-C6-N6	-5.01	115.59	118.60
1	AA	176	G	C4-C5-N7	5.01	112.80	110.80
1	AA	1612	C	C5-C4-N4	-5.01	116.69	120.20
1	AA	2877	G	N3-C4-N9	-5.01	123.00	126.00
1	CA	379	G	OP2-P-O3'	5.01	116.22	105.20
1	AA	738	C	C5-C6-N1	-5.01	118.50	121.00
1	AA	1485	A	C8-N9-C4	5.01	107.80	105.80
1	AA	2696	U	C4-C5-C6	5.01	122.70	119.70
2	AB	114	C	C5-C6-N1	-5.01	118.50	121.00
34	BA	862	C	OP2-P-O3'	5.01	116.22	105.20
1	CA	2547	U	N3-C4-O4	5.01	122.91	119.40
1	AA	704	U	N3-C4-O4	-5.00	115.90	119.40
1	AA	1020	C	N3-C4-N4	-5.00	114.50	118.00
1	AA	2627	U	N3-C2-O2	-5.00	118.70	122.20
1	AA	2798	C	N3-C4-C5	-5.00	119.90	121.90
1	CA	2876	G	N9-C4-C5	-5.00	103.40	105.40
1	AA	331	G	N1-C6-O6	-5.00	116.90	119.90
1	AA	1359	U	O4'-C1'-N1	5.00	112.20	108.20
1	AA	1437	U	N1-C2-O2	5.00	126.30	122.80
1	AA	2451	A	C5'-C4'-O4'	-5.00	103.09	109.10
1	AA	2625	U	N3-C4-O4	-5.00	115.90	119.40
2	AB	106	G	C4-C5-N7	5.00	112.80	110.80
1	CA	1899	G	N1-C2-N2	5.00	120.70	116.20
34	DA	804	U	C5-C4-O4	5.00	128.90	125.90
1	AA	1214	G	N1-C2-N2	-5.00	111.70	116.20
1	AA	2530	A	C4-C5-C6	5.00	119.50	117.00
1	CA	2517	C	C5-C4-N4	-5.00	116.70	120.20
1	CA	2600	A	N1-C2-N3	5.00	131.80	129.30
2	CB	105	A	C8-N9-C4	5.00	107.80	105.80

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	A4	59	PHE	Peptide
1	AA	537	G	Sidechain
35	BB	8	LYS	Peptide
53	BT	9	ASN	Peptide
53	DT	9	ASN	Peptide
59	DZ	159	ALA	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	61861	0	31186	660	2
1	CA	61771	0	31146	786	0
2	AB	2573	0	1306	15	0
2	CB	2573	0	1306	26	0
3	AC	1063	0	1091	140	5
3	CC	1063	0	1089	150	10
4	AD	2136	0	2218	55	0
4	CD	2142	0	2229	67	0
5	AE	1559	0	1618	48	0
5	CE	1559	0	1618	42	0
6	AF	1584	0	1625	39	0
6	CF	1580	0	1619	50	0
7	AG	1425	0	1443	47	0
7	CG	1424	0	1434	42	0
8	AH	1330	0	1407	24	0
8	CH	1330	0	1407	42	0
9	AK	641	0	309	11	0
9	CK	641	0	309	13	0
10	AL	498	0	521	17	0
10	CL	498	0	521	21	0
11	AN	1117	0	1184	26	0
11	CN	1117	0	1184	21	0
12	AO	933	0	996	29	0
12	CO	933	0	996	22	0
13	AP	1139	0	1223	34	0
13	CP	1135	0	1212	47	0
14	AQ	1122	0	1179	36	0
14	CQ	1122	0	1179	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	AR	968	0	1033	19	0
15	CR	968	0	1033	27	0
16	AS	877	0	938	20	0
16	CS	870	0	923	35	0
17	AT	1091	0	1151	31	0
17	CT	1083	0	1136	28	0
18	AU	959	0	1019	25	0
18	CU	959	0	1019	30	0
19	AV	771	0	830	13	0
19	CV	771	0	830	19	0
20	AW	886	0	940	15	0
20	CW	886	0	940	18	0
21	AX	750	0	814	20	0
21	CX	750	0	814	19	0
22	AY	806	0	881	29	0
22	CY	806	0	882	37	0
23	AZ	1349	0	1355	38	0
23	CZ	1360	0	1363	41	0
24	A0	653	0	674	20	0
24	C0	653	0	674	20	0
25	A1	755	0	826	20	0
25	C1	755	0	826	20	0
26	A2	588	0	643	9	0
26	C2	588	0	643	14	0
27	A3	469	0	518	6	0
27	C3	464	0	514	8	0
28	A4	558	0	545	22	0
28	C4	532	0	506	20	0
29	A5	455	0	465	7	0
29	C5	455	0	465	11	0
30	A6	453	0	473	13	0
30	C6	449	0	469	13	0
31	A7	418	0	467	11	0
31	C7	418	0	467	9	0
32	A8	517	0	582	23	0
32	C8	517	0	582	19	0
33	A9	307	0	335	8	0
33	C9	307	0	335	11	0
34	BA	32185	0	16245	438	0
34	DA	32312	0	16308	510	1
35	BB	1846	0	1867	80	0
35	DB	1825	0	1828	101	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	BC	1552	0	1546	52	0
36	DC	1544	0	1524	65	0
37	BD	1659	0	1676	58	0
37	DD	1678	0	1718	53	0
38	BE	1129	0	1185	42	0
38	DE	1133	0	1191	41	0
39	BF	812	0	804	18	0
39	DF	820	0	814	23	0
40	BG	1231	0	1238	21	0
40	DG	1235	0	1249	31	0
41	BH	1088	0	1126	39	0
41	DH	1088	0	1126	37	0
42	BI	986	0	995	39	0
42	DI	978	0	966	42	0
43	BJ	709	0	650	34	0
43	DJ	714	0	672	33	0
44	BK	833	0	836	23	0
44	DK	833	0	836	16	0
45	BL	930	0	980	10	0
45	DL	930	0	980	30	0
46	BM	966	0	1024	33	0
46	DM	950	0	988	39	0
47	BN	492	0	529	22	0
47	DN	492	0	531	33	0
48	BO	728	0	760	17	0
48	DO	728	0	760	14	0
49	BP	681	0	697	27	0
49	DP	677	0	686	20	0
50	BQ	823	0	891	24	0
50	DQ	823	0	891	23	0
51	BR	555	0	618	16	0
51	DR	555	0	618	20	0
52	BS	661	0	675	39	0
52	DS	646	0	644	25	0
53	BT	728	0	798	29	0
53	DT	731	0	807	22	0
54	BU	199	0	208	7	0
54	DU	199	0	208	5	0
55	BV	277	0	140	3	0
55	DV	252	0	130	3	0
56	BW	1599	0	830	26	0
56	DW	1552	0	794	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	BX	1635	0	838	15	0
57	DX	1635	0	839	25	0
58	BY	1581	0	805	21	0
58	DY	1561	0	796	18	0
59	BZ	5663	0	5746	246	10
59	DZ	5682	0	5766	192	6
60	A0	5	0	0	0	0
60	A1	2	0	0	0	0
60	A2	1	0	0	0	0
60	A4	1	0	0	0	0
60	A5	1	0	0	0	0
60	A6	1	0	0	0	0
60	A7	1	0	0	0	0
60	A8	2	0	0	0	0
60	A9	1	0	0	0	0
60	AA	834	0	0	0	0
60	AB	23	0	0	0	0
60	AD	10	0	0	0	0
60	AE	5	0	0	0	0
60	AF	5	0	0	0	0
60	AG	2	0	0	0	0
60	AH	1	0	0	0	0
60	AN	3	0	0	0	0
60	AO	1	0	0	0	0
60	AP	2	0	0	0	0
60	AQ	3	0	0	0	0
60	AR	1	0	0	0	0
60	AU	4	0	0	0	0
60	AV	1	0	0	0	0
60	AW	4	0	0	0	0
60	AX	2	0	0	0	0
60	AY	1	0	0	0	0
60	AZ	1	0	0	0	0
60	BA	213	0	0	0	0
60	BB	1	0	0	0	0
60	BD	1	0	0	0	0
60	BE	1	0	0	0	0
60	BF	1	0	0	0	0
60	BK	1	0	0	0	0
60	BL	2	0	0	0	0
60	BM	1	0	0	0	0
60	BN	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	BT	1	0	0	0	0
60	BV	1	0	0	0	0
60	BW	2	0	0	0	0
60	BX	15	0	0	0	0
60	BY	2	0	0	0	0
60	BZ	1	0	0	0	0
60	C0	2	0	0	0	0
60	C3	1	0	0	0	0
60	C5	1	0	0	0	0
60	C7	1	0	0	0	0
60	C8	1	0	0	0	0
60	CA	664	0	0	0	0
60	CB	13	0	0	0	0
60	CD	4	0	0	0	0
60	CE	6	0	0	0	0
60	CF	6	0	0	0	0
60	CG	1	0	0	0	0
60	CN	1	0	0	0	0
60	CO	2	0	0	0	0
60	CP	1	0	0	0	0
60	CQ	4	0	0	0	0
60	CR	2	0	0	0	0
60	CU	1	0	0	0	0
60	CV	2	0	0	0	0
60	CY	1	0	0	0	0
60	DA	168	0	0	0	0
60	DD	1	0	0	0	0
60	DE	2	0	0	0	0
60	DF	1	0	0	0	0
60	DJ	1	0	0	0	0
60	DK	2	0	0	0	0
60	DT	1	0	0	0	0
60	DW	1	0	0	0	0
60	DX	1	0	0	0	0
60	DZ	1	0	0	0	0
61	AA	1	0	0	0	0
62	A4	1	0	0	0	0
62	A5	1	0	0	0	0
62	A6	1	0	0	0	0
62	A9	1	0	0	0	0
62	AY	1	0	0	0	0
62	BN	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	C4	1	0	0	0	0
62	C5	1	0	0	0	0
62	C6	1	0	0	0	0
62	C9	1	0	0	0	0
62	CY	1	0	0	0	0
62	DN	1	0	0	0	0
63	BD	8	0	0	1	0
63	DD	8	0	0	1	0
64	BZ	28	0	12	6	0
64	DZ	28	0	12	7	0
65	A0	6	0	0	0	0
65	A1	1	0	0	0	0
65	A3	1	0	0	0	0
65	A5	3	0	0	0	0
65	A6	2	0	0	0	0
65	A7	4	0	0	1	0
65	A8	10	0	0	1	0
65	AA	1408	0	0	48	0
65	AB	36	0	0	1	0
65	AD	15	0	0	1	0
65	AE	19	0	0	1	0
65	AF	7	0	0	0	0
65	AG	3	0	0	0	0
65	AH	1	0	0	0	0
65	AN	2	0	0	0	0
65	AO	1	0	0	0	0
65	AP	15	0	0	2	0
65	AQ	4	0	0	2	0
65	AR	2	0	0	2	0
65	AS	1	0	0	0	0
65	AT	2	0	0	0	0
65	AU	5	0	0	0	0
65	AV	2	0	0	0	0
65	AW	2	0	0	0	0
65	AX	3	0	0	0	0
65	AZ	1	0	0	0	0
65	BA	212	0	0	13	0
65	BD	2	0	0	0	0
65	BE	2	0	0	0	0
65	BL	1	0	0	0	0
65	BM	1	0	0	0	0
65	BV	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
65	BW	3	0	0	0	0
65	BX	8	0	0	0	0
65	BY	1	0	0	0	0
65	BZ	2	0	0	0	0
65	C0	6	0	0	1	0
65	C1	2	0	0	0	0
65	C3	2	0	0	0	0
65	C6	1	0	0	1	0
65	C7	1	0	0	0	0
65	C8	3	0	0	0	0
65	CA	985	0	0	52	0
65	CB	9	0	0	1	0
65	CD	14	0	0	0	0
65	CE	13	0	0	1	0
65	CF	7	0	0	0	0
65	CN	2	0	0	0	0
65	CP	10	0	0	1	0
65	CQ	1	0	0	0	0
65	CR	1	0	0	0	0
65	CT	3	0	0	0	0
65	CU	2	0	0	0	0
65	CV	1	0	0	0	0
65	CY	1	0	0	0	0
65	DA	155	0	0	6	0
65	DE	4	0	0	0	0
65	DJ	1	0	0	0	0
65	DK	2	0	0	0	0
65	DL	1	0	0	0	0
65	DW	2	0	0	0	0
65	DX	1	0	0	0	0
All	All	313372	0	210866	5329	17

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 11.

All (5329) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1860:G:H5'	3:CC:206:LYS:CD	1.27	1.64
1:CA:1860:G:H5''	3:CC:206:LYS:CG	1.28	1.64
1:AA:1891:G:C5'	3:AC:206:LYS:HD2	1.35	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1860:G:C5'	3:CC:206:LYS:HD2	1.25	1.53
1:CA:1860:G:C5'	3:CC:206:LYS:CG	1.84	1.50
1:CA:1860:G:C5'	3:CC:206:LYS:CD	1.76	1.45
1:CA:1053:C:H42	1:CA:1107:G:N2	1.04	1.41
1:CA:1053:C:N4	1:CA:1107:G:H22	1.16	1.38
1:CA:1860:G:C4'	3:CC:206:LYS:HD2	1.53	1.35
1:CA:1860:G:H4'	3:CC:206:LYS:CD	1.59	1.32
1:AA:1891:G:C5'	3:AC:206:LYS:CD	2.09	1.31
1:AA:1891:G:C4'	3:AC:206:LYS:HD2	1.58	1.31
1:AA:1891:G:H4'	3:AC:206:LYS:CD	1.60	1.29
1:CA:1860:G:C4'	3:CC:206:LYS:CD	2.06	1.29
1:AA:1891:G:H5''	3:AC:206:LYS:CG	1.68	1.22
1:AA:1891:G:H5'	3:AC:206:LYS:HD2	1.20	1.09
1:CA:1798:U:H5'	4:CD:259:THR:HG22	1.34	1.09
1:AA:1891:G:H5''	3:AC:206:LYS:HG2	1.36	1.06
1:AA:1891:G:O3'	3:AC:206:LYS:HG3	1.54	1.05
1:AA:2198:A:HO2'	3:AC:45:HIS:CD2	1.74	1.04
1:CA:1860:G:C4'	3:CC:206:LYS:HG3	1.87	1.02
1:CA:2132:U:N3	3:CC:6:LYS:HE3	1.74	1.02
1:CA:1860:G:C4'	3:CC:206:LYS:CG	2.32	1.02
1:AA:1249:A:H2	1:AA:1287:A:H62	1.06	1.02
1:CA:1860:G:H5'	3:CC:206:LYS:CE	1.90	1.01
1:CA:1053:C:N4	1:CA:1107:G:N2	1.87	1.00
1:AA:9:U:H3	1:AA:2641:A:H2	1.08	0.99
21:AX:31:HIS:HD2	21:AX:33:LYS:H	1.07	0.99
59:BZ:99:ARG:HB3	59:BZ:99:ARG:HH11	1.26	0.99
1:AA:1829:U:H5'	4:AD:259:THR:HG22	1.43	0.98
1:CA:1860:G:H4'	3:CC:206:LYS:HD3	1.42	0.98
1:AA:2198:A:O2'	3:AC:45:HIS:CD2	2.17	0.98
1:CA:1860:G:H5''	3:CC:206:LYS:HG3	1.38	0.98
1:AA:1891:G:H5''	3:AC:206:LYS:CD	1.86	0.96
1:AA:1405:A:H61	1:AA:1418:U:H3	1.10	0.96
59:BZ:13:ARG:HH12	59:BZ:247:ARG:HH22	1.11	0.96
21:CX:35:THR:HG22	21:CX:38:GLU:H	1.30	0.95
1:AA:535:C:OP1	65:AA:4769:HOH:O	1.83	0.95
1:CA:1204:A:H2	1:CA:1241:A:H62	1.14	0.95
1:AA:1891:G:C4'	3:AC:206:LYS:CD	2.26	0.95
59:DZ:119:GLU:OE1	59:DZ:156:ARG:NH1	2.00	0.94
34:BA:160:A:N6	34:BA:345:C:OP2	2.01	0.94
35:BB:16:HIS:HB2	35:BB:204:ASN:HB3	1.49	0.94
13:AP:39:LYS:NZ	65:AP:307:HOH:O	2.00	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1736:A:H62	1:AA:1745:A:H2	1.13	0.94
1:AA:1891:G:C5'	3:AC:206:LYS:CG	2.42	0.93
1:CA:1689:A:H62	1:CA:1698:A:H2	1.04	0.93
1:AA:1090:G:O2'	1:AA:1157:A:N6	2.01	0.93
34:DA:1086:U:H3	34:DA:1099:G:H22	1.16	0.92
1:CA:397:G:N7	65:CA:4556:HOH:O	2.03	0.92
1:CA:1860:G:H5''	3:CC:206:LYS:HG2	0.94	0.92
34:BA:1158:C:H5	34:BA:1181:G:H1	1.19	0.90
1:CA:1021:A:H62	1:CA:1141:U:H3	1.15	0.90
1:AA:1065:U:HO2'	1:AA:1067:A:H2	1.18	0.90
1:AA:2511:C:OP1	65:AA:5078:HOH:O	1.87	0.89
22:CY:102:CYS:SG	22:CY:103:GLY:N	2.42	0.89
20:AW:12:ILE:HD13	20:AW:17:VAL:HG22	1.55	0.89
59:BZ:78:ARG:HH11	59:BZ:78:ARG:HG3	1.38	0.89
23:AZ:29:TYR:HB3	23:AZ:34:ASN:HD22	1.37	0.89
34:BA:975:A:H4'	34:BA:976:G:H5''	1.56	0.88
34:BA:964:A:OP1	65:BA:2060:HOH:O	1.88	0.88
3:CC:31:LYS:NZ	3:CC:181:PHE:O	2.06	0.88
17:CT:55:ASN:H	17:CT:59:THR:HG22	1.36	0.87
34:BA:937:A:OP2	65:BA:2015:HOH:O	1.92	0.87
3:AC:31:LYS:NZ	3:AC:181:PHE:O	2.06	0.87
6:CF:185:ASP:HA	6:CF:188:ARG:HD3	1.57	0.87
35:DB:185:ILE:HG22	35:DB:199:TYR:HB2	1.55	0.86
3:AC:52:PRO:HG2	3:AC:53:ARG:HD3	1.57	0.86
1:CA:2714:G:OP2	65:CA:3993:HOH:O	1.91	0.86
34:DA:975:A:H4'	34:DA:976:G:H5''	1.58	0.86
34:DA:376:G:H5''	49:DP:5:ARG:HD3	1.58	0.86
3:CC:52:PRO:HG2	3:CC:53:ARG:HD3	1.57	0.86
24:C0:10:THR:HG22	24:C0:12:ASN:H	1.40	0.85
1:AA:1716:A:OP2	65:AA:5038:HOH:O	1.94	0.85
1:AA:2201:C:O4'	3:AC:169:THR:HG22	1.76	0.85
22:AY:54:LYS:HA	22:AY:56:PRO:HD3	1.58	0.85
44:BK:79:SER:HA	44:BK:104:GLN:HB2	1.59	0.85
13:CP:100:LEU:HD12	13:CP:112:LEU:HD11	1.57	0.84
18:AU:108:GLU:OE2	18:AU:112:ARG:NH1	2.10	0.84
59:BZ:169:GLY:HA3	59:BZ:174:PHE:HA	1.59	0.84
34:BA:1502:A:H2	34:BA:1505:G:H1	1.24	0.84
43:BJ:35:SER:HB3	43:BJ:73:ASP:HB2	1.58	0.84
1:AA:1356:G:OP2	31:A7:9:ARG:NH1	2.10	0.84
1:AA:1891:G:H4'	3:AC:206:LYS:HD3	1.56	0.84
59:BZ:405:PRO:HD2	59:BZ:406:GLU:HG2	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:DA:1166:G:N2	34:DA:1170:A:OP2	2.09	0.83
34:BA:538:G:H5''	45:BL:114:LYS:HB2	1.60	0.83
34:BA:664:G:H22	34:BA:741:G:H1	1.24	0.83
1:CA:1603:A:OP1	65:CA:4478:HOH:O	1.95	0.83
12:AO:2:ILE:HD12	12:AO:6:THR:HG21	1.59	0.83
1:CA:2178:C:O2'	3:CC:169:THR:HB	1.76	0.83
34:DA:656:C:O2'	48:DO:28:GLN:NE2	2.12	0.83
1:AA:1094:A:OP2	1:AA:1155:C:N4	2.12	0.82
1:AA:2297:C:OP2	30:A6:6:ARG:NH1	2.12	0.82
14:AQ:111:GLU:OE1	14:AQ:133:ARG:NH2	2.13	0.82
34:DA:922:G:H4'	38:DE:20:GLN:HA	1.59	0.82
13:CP:39:LYS:HB2	13:CP:45:LEU:HG	1.61	0.82
3:AC:54:ARG:NH2	3:AC:56:ASP:HB3	1.95	0.82
1:CA:1860:G:H4'	3:CC:206:LYS:CG	2.03	0.82
1:CA:2206:G:H3'	1:CA:2207:G:C8	2.15	0.82
8:CH:98:LEU:HD22	8:CH:125:VAL:HG23	1.61	0.82
1:AA:1100:A:H62	1:AA:1151:U:H3	1.29	0.81
1:AA:2128:G:H1	1:AA:2205:C:H42	1.27	0.81
43:DJ:49:VAL:HG23	47:DN:41:ARG:HB2	1.61	0.81
5:AE:179:GLU:HB3	5:AE:181:LEU:HD22	1.60	0.81
34:BA:1129:C:H5''	42:BI:16:ARG:HH12	1.46	0.81
34:DA:653:A:OP1	41:DH:56:LYS:NZ	2.13	0.81
38:DE:122:GLU:O	38:DE:126:ARG:NH1	2.14	0.81
59:BZ:97:SER:O	59:BZ:99:ARG:N	2.12	0.81
45:DL:24:VAL:HG11	45:DL:27:LEU:HD22	1.62	0.81
35:BB:69:LEU:HB3	35:BB:162:ILE:HG22	1.60	0.81
3:CC:54:ARG:NH2	3:CC:56:ASP:HB3	1.95	0.81
53:DT:10:LEU:HB3	53:DT:12:ALA:H	1.45	0.81
1:AA:927:G:N2	1:AA:944:C:N3	2.29	0.80
24:A0:11:ARG:O	24:A0:14:ARG:NH2	2.14	0.80
1:CA:1019:U:H3	1:CA:1142(A):A:H62	1.27	0.80
58:DY:19:G:N2	58:DY:56:C:N3	2.29	0.80
35:BB:111:ARG:HG2	35:BB:111:ARG:HH11	1.46	0.80
1:AA:2299:A:H62	1:AA:2356:U:H3	1.27	0.80
59:BZ:357:ARG:NH1	59:BZ:373:ASP:OD1	2.15	0.79
40:BG:111:ARG:NH1	40:BG:113:GLU:OE2	2.15	0.79
34:DA:664:G:H22	34:DA:741:G:H1	1.25	0.79
1:AA:1219:A:H1'	1:AA:1220:U:H5''	1.62	0.79
7:CG:80:PHE:O	7:CG:82:LEU:N	2.15	0.79
34:BA:376:G:H5''	49:BP:5:ARG:HG2	1.64	0.79
36:BC:37:GLN:NE2	47:BN:52:GLN:OE1	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:2132:U:C4	3:CC:6:LYS:HE3	2.18	0.79
34:BA:656:C:O2'	48:BO:28:GLN:NE2	2.15	0.79
38:DE:74:GLY:HA3	38:DE:116:THR:HG22	1.64	0.79
41:DH:51:VAL:HG11	41:DH:60:ARG:HH11	1.46	0.79
1:CA:529:A:N6	1:CA:2041:U:O2	2.15	0.79
24:C0:11:ARG:O	24:C0:14:ARG:NH2	2.16	0.79
59:BZ:380:LEU:HD21	59:BZ:389:LEU:HD21	1.64	0.79
17:AT:55:ASN:H	17:AT:59:THR:HG22	1.45	0.79
1:AA:1891:G:C4'	3:AC:206:LYS:CG	2.61	0.79
59:BZ:363:ARG:HG2	59:BZ:363:ARG:HH11	1.46	0.79
1:CA:1860:G:C3'	3:CC:206:LYS:HG3	2.12	0.79
1:CA:2287:A:H62	1:CA:2344:U:H3	1.30	0.79
34:DA:115:G:OP1	65:DA:1871:HOH:O	2.01	0.79
34:DA:1320:C:N3	52:DS:36:ARG:NH2	2.31	0.78
59:BZ:480:GLN:O	59:BZ:482:ALA:N	2.17	0.78
1:CA:1860:G:C5'	3:CC:206:LYS:HG2	1.77	0.78
28:C4:36:CYS:SG	28:C4:37:SER:N	2.55	0.78
4:AD:69:ARG:NH2	4:AD:128:GLY:O	2.16	0.78
22:AY:92:ASN:H	22:AY:92:ASN:HD22	1.29	0.78
58:DY:7:A:H61	58:DY:66:U:H3	1.30	0.78
35:BB:115:LEU:HD13	35:BB:145:LEU:HB3	1.65	0.78
1:CA:880:G:H22	1:CA:898:C:H1'	1.46	0.78
1:CA:2296:U:OP2	16:CS:9:ARG:NH2	2.17	0.78
59:BZ:169:GLY:O	59:BZ:173:THR:OG1	2.02	0.78
1:CA:1817:G:OP1	4:CD:88:ARG:NH2	2.16	0.78
36:BC:58:GLU:HB3	43:BJ:92:THR:HG21	1.65	0.78
1:CA:631:A:OP1	13:CP:65:ARG:NH1	2.16	0.78
24:C0:5:LYS:NZ	57:DX:2:G:OP1	2.17	0.78
42:BI:17:VAL:HG21	42:BI:81:ILE:HG22	1.65	0.77
4:CD:148:GLU:HB2	4:CD:151:LYS:HD2	1.66	0.77
14:AQ:21:THR:HG21	14:AQ:101:ARG:HD3	1.64	0.77
1:CA:528:A:O2'	1:CA:529:A:H5''	1.83	0.77
1:AA:1100:A:N6	1:AA:1151:U:H3	1.81	0.77
35:BB:150:SER:O	35:BB:153:ARG:NH1	2.17	0.77
34:DA:344:A:H5''	34:DA:345:C:H5	1.48	0.77
36:DC:70:VAL:HG22	36:DC:72:LYS:H	1.49	0.77
3:AC:20:VAL:O	3:AC:21:TYR:HB2	1.83	0.77
21:AX:31:HIS:CD2	21:AX:33:LYS:H	1.98	0.77
22:AY:92:ASN:HB2	22:AY:94:LYS:H	1.48	0.77
34:DA:48:C:OP2	65:DA:1871:HOH:O	2.03	0.77
39:DF:87:ARG:HH11	39:DF:87:ARG:HG3	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AV:98:GLU:OE2	19:AV:100:ARG:NH1	2.17	0.77
23:AZ:117:LEU:HD11	23:AZ:144:LEU:HD22	1.66	0.77
56:BW:5:G:H2'	56:BW:6:G:H8	1.50	0.77
59:BZ:329:ARG:HH11	59:BZ:331:TYR:HE1	1.33	0.77
3:AC:27:ALA:O	3:AC:30:VAL:HG22	1.85	0.77
15:AR:33:ARG:NH1	15:AR:115:GLU:OE2	2.16	0.77
36:DC:179:ARG:NH1	36:DC:206:GLU:OE1	2.17	0.77
1:AA:1007:G:OP1	65:AA:4764:HOH:O	2.03	0.76
53:BT:10:LEU:HB3	53:BT:12:ALA:H	1.50	0.76
1:CA:1155:A:H5''	18:CU:55:ARG:HH11	1.50	0.76
3:CC:20:VAL:O	3:CC:21:TYR:HB2	1.83	0.76
1:AA:992:G:OP2	65:AA:4762:HOH:O	2.03	0.76
3:AC:24:ASP:O	3:AC:28:ARG:HG3	1.85	0.76
59:BZ:78:ARG:HH11	59:BZ:78:ARG:CG	1.96	0.76
1:CA:1031:G:H21	33:C9:36:GLN:HE22	1.31	0.76
15:AR:67:LEU:HD13	15:AR:76:VAL:HG21	1.67	0.76
3:CC:24:ASP:O	3:CC:28:ARG:HG3	1.85	0.76
1:AA:1829:U:OP2	4:AD:274:ARG:NH2	2.19	0.76
59:BZ:148:LEU:O	59:BZ:152:THR:OG1	2.04	0.76
34:DA:1224:G:O2'	34:DA:1322:C:OP1	2.04	0.76
59:DZ:247:ARG:NH1	59:DZ:251:ILE:HD11	2.00	0.76
1:AA:1740:U:O2'	4:AD:14:ARG:NH2	2.18	0.76
1:CA:1310:G:OP2	31:C7:9:ARG:NH1	2.19	0.76
1:AA:1016:C:OP2	65:AA:5195:HOH:O	2.03	0.76
1:AA:2658:C:OP2	1:AA:2745:G:O2'	2.02	0.76
56:BW:50:U:H3	56:BW:64:A:H61	1.33	0.76
1:CA:827:U:OP1	65:CA:4250:HOH:O	2.02	0.76
1:CA:1039:G:O6	1:CA:1116:C:N4	2.19	0.76
34:DA:1103:C:OP1	35:DB:96:ARG:NH2	2.18	0.76
1:CA:271(R):G:H5''	25:C1:97:LEU:HD21	1.66	0.76
3:CC:27:ALA:O	3:CC:30:VAL:HG22	1.85	0.76
56:DW:76:F3N:H5'	56:DW:76:F3N:H8	1.66	0.76
59:DZ:165:GLN:HE21	59:DZ:260:LEU:H	1.33	0.76
1:CA:878:A:N6	1:CA:899:A:O2'	2.18	0.76
1:AA:1891:G:C3'	3:AC:206:LYS:HG3	2.16	0.76
6:AF:195:ASP:HB3	6:AF:198:ALA:H	1.50	0.75
1:CA:731:C:OP2	65:CA:4229:HOH:O	2.02	0.75
1:AA:894:U:OP2	65:AA:4336:HOH:O	2.02	0.75
56:BW:19:G:H1	56:BW:56:C:H42	1.33	0.75
1:CA:301:G:OP2	22:CY:84:ARG:NH2	2.18	0.75
59:BZ:373:ASP:OD2	59:BZ:374:LEU:N	2.18	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:614(B):G:H2'	6:CF:44:ARG:HH11	1.51	0.75
4:CD:96:HIS:HD2	4:CD:102:LYS:HG2	1.52	0.75
1:AA:139:A:H8	1:AA:1454:C:HO2'	1.34	0.75
1:AA:2227:G:H5'	1:AA:2228:G:N7	2.02	0.75
59:DZ:129:LYS:HD3	59:DZ:521:SER:HB2	1.67	0.75
1:AA:927:G:H2'	1:AA:928:G:H8	1.52	0.75
34:DA:677:U:H3	34:DA:713:G:H22	1.35	0.75
34:DA:838:G:H1	34:DA:848:C:H42	1.34	0.75
15:AR:3:HIS:NE2	65:AR:5101:HOH:O	2.20	0.75
4:CD:125:ILE:HB	39:DF:81:ILE:HD11	1.68	0.75
20:CW:34:ASN:OD1	20:CW:37:ARG:NH2	2.18	0.75
1:CA:1024:G:OP2	65:CA:4575:HOH:O	2.03	0.75
1:CA:2138:C:H42	1:CA:2153:G:H1	1.35	0.75
34:BA:504:C:OP1	65:BA:2083:HOH:O	2.04	0.74
34:DA:1255:G:OP1	43:DJ:45:ARG:NH2	2.19	0.74
1:CA:370:G:N7	65:CA:3748:HOH:O	2.20	0.74
15:CR:55:ALA:HB2	15:CR:79:LEU:HD13	1.69	0.74
1:AA:1151:U:H2'	1:AA:1152:G:C8	2.22	0.74
1:AA:2122:G:H1	1:AA:2211:U:H3	1.33	0.74
37:BD:49:ARG:HE	37:BD:49:ARG:H	1.35	0.74
59:DZ:116:PRO:O	59:DZ:118:SER:N	2.21	0.74
1:CA:2099:U:H3	1:CA:2190:G:H1	1.35	0.74
34:DA:619:U:N3	37:DD:134:ASP:OD1	2.21	0.74
59:DZ:-66:MET:N	59:DZ:-46:VAL:O	2.19	0.74
59:DZ:203:GLU:N	59:DZ:203:GLU:OE2	2.20	0.74
3:CC:48:LEU:HB3	3:CC:50:ILE:HD12	1.70	0.74
46:DM:58:GLU:O	46:DM:62:ASN:ND2	2.20	0.74
1:AA:427:G:N7	65:AA:4917:HOH:O	2.19	0.74
34:DA:992:U:H3	34:DA:1044:A:H62	1.36	0.74
34:DA:953:G:H5'	34:DA:965:A:H61	1.51	0.74
1:CA:1860:G:O3'	3:CC:206:LYS:HG3	1.88	0.74
44:DK:92:GLU:OE2	51:DR:87:ARG:NH1	2.21	0.74
34:BA:165:C:H2'	34:BA:166:G:C8	2.23	0.74
1:AA:1405:A:N6	1:AA:1418:U:H3	1.84	0.73
43:DJ:29:ARG:HB2	43:DJ:84:GLN:HE22	1.53	0.73
1:CA:2646:C:OP2	1:CA:2732:G:O2'	2.06	0.73
59:DZ:21:ILE:HD11	59:DZ:117:GLN:HE22	1.51	0.73
34:BA:560:U:OP2	65:BA:1956:HOH:O	2.07	0.73
1:CA:1842:G:O2'	4:CD:253:GLN:NE2	2.21	0.73
13:CP:38:GLN:O	13:CP:40:SER:N	2.22	0.73
1:AA:2825:C:H5'	29:A5:29:THR:HG21	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:517:C:OP1	29:C5:16:ARG:NH2	2.22	0.73
35:BB:16:HIS:O	35:BB:18:GLY:N	2.21	0.73
59:DZ:363:ARG:HG2	59:DZ:363:ARG:HH11	1.53	0.73
34:BA:1305:G:N2	34:BA:1331:G:H1'	2.02	0.73
59:BZ:13:ARG:HH12	59:BZ:247:ARG:NH2	1.84	0.73
1:CA:2176:A:O2'	3:CC:45:HIS:CD2	2.41	0.73
1:AA:1873:G:O2'	4:AD:253:GLN:NE2	2.22	0.73
5:AE:127:ASP:OD2	65:AE:406:HOH:O	2.07	0.73
20:AW:4:LYS:HE2	20:AW:6:ILE:HD11	1.70	0.73
34:DA:1075:C:OP1	35:DB:179:LYS:NZ	2.22	0.73
37:BD:178:VAL:O	37:BD:180:GLY:N	2.21	0.73
1:CA:2177:C:O2	3:CC:173:HIS:CE1	2.42	0.73
23:CZ:45:ASP:OD2	23:CZ:49:ARG:NH1	2.22	0.73
1:AA:1055:A:OP2	11:AN:37:LYS:NZ	2.22	0.73
35:BB:7:VAL:HG11	35:BB:221:LEU:HD23	1.70	0.73
34:DA:137:C:H42	34:DA:226:G:H1	1.37	0.73
34:DA:1030(A):G:N2	34:DA:1030(D):A:OP2	2.20	0.73
41:DH:29:SER:HB3	41:DH:32:LYS:HG3	1.70	0.73
1:AA:2324:U:H5'	7:AG:88:ILE:HD11	1.71	0.73
1:AA:2859:U:O4	17:AT:23:ARG:NH2	2.21	0.73
12:AO:97:ARG:NH1	34:BA:339:C:OP2	2.20	0.73
7:CG:38:VAL:HG22	7:CG:93:THR:HG23	1.71	0.73
15:CR:33:ARG:NH2	29:C5:57:VAL:O	2.22	0.73
1:AA:929:G:N2	1:AA:941:U:O2	2.22	0.72
6:AF:185:ASP:HA	6:AF:188:ARG:HD3	1.71	0.72
34:BA:166:G:H2'	34:BA:167:G:H8	1.53	0.72
34:BA:505:G:N7	65:BA:2082:HOH:O	2.22	0.72
34:BA:558:G:OP1	65:BA:1960:HOH:O	2.07	0.72
28:C4:61:ARG:HG3	52:DS:42:PRO:HG3	1.71	0.72
38:DE:100:VAL:O	38:DE:107:ARG:NH2	2.22	0.72
1:AA:1001:G:OP2	14:AQ:14:ARG:NH2	2.22	0.72
34:BA:1030(C):G:N7	34:BA:1031:G:N2	2.37	0.72
49:BP:53:VAL:HG13	49:BP:79:VAL:HG22	1.70	0.72
56:DW:11:C:H42	56:DW:24:G:H1	1.36	0.72
1:AA:1065:U:H3	1:AA:1188:A:H62	1.35	0.72
1:CA:2357:U:OP1	24:C0:20:ARG:NH1	2.22	0.72
42:DI:16:ARG:HB2	42:DI:64:THR:HG23	1.70	0.72
36:BC:40:ARG:NH2	36:BC:55:VAL:O	2.22	0.72
35:DB:178:ARG:HH22	41:DH:68:ARG:HH22	1.35	0.72
1:AA:831:A:OP2	65:AA:4557:HOH:O	2.08	0.72
1:CA:323:G:HO2'	1:CA:1205:U:H3	0.75	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:991:C:OP2	65:CA:4148:HOH:O	2.08	0.72
1:CA:2046:G:H5'	29:C5:19:ARG:HA	1.70	0.72
34:BA:167:G:H2'	34:BA:168:G:H8	1.55	0.72
42:BI:128:ARG:NH2	57:BX:33:U:OP2	2.21	0.72
59:BZ:102:ASP:OD2	59:BZ:329:ARG:NH2	2.22	0.72
1:AA:1657:C:OP1	65:AA:5025:HOH:O	2.07	0.72
34:BA:1054:C:OP2	65:BA:1976:HOH:O	2.07	0.72
38:DE:88:LYS:HB3	38:DE:123:LEU:HB2	1.71	0.72
34:DA:1065:U:OP2	34:DA:1190:G:N2	2.22	0.72
35:DB:69:LEU:HB3	35:DB:162:ILE:HG22	1.70	0.72
1:AA:467:U:O2	6:AF:46:ARG:NH2	2.23	0.72
20:AW:2:GLU:OE2	20:AW:72:LYS:HE2	1.90	0.72
50:DQ:66:SER:O	50:DQ:70:ARG:NH1	2.23	0.72
59:BZ:13:ARG:NH1	59:BZ:247:ARG:HH22	1.86	0.72
59:BZ:363:ARG:HG2	59:BZ:363:ARG:NH1	2.01	0.72
1:CA:2445:G:OP1	6:CF:74:ARG:NH2	2.23	0.72
12:CO:63:VAL:HG12	12:CO:106:LEU:HD11	1.72	0.72
34:DA:1239:A:H4'	34:DA:1240:U:H5'	1.70	0.72
1:AA:1189:A:OP1	11:AN:25:ARG:NH2	2.23	0.71
42:BI:40:LEU:O	42:BI:42:ARG:N	2.23	0.71
1:AA:1151:U:H2'	1:AA:1152:G:H8	1.51	0.71
3:AC:48:LEU:HB3	3:AC:50:ILE:HD12	1.70	0.71
17:AT:60:THR:HG22	17:AT:77:PRO:HA	1.70	0.71
1:CA:1622:G:OP2	65:CA:3921:HOH:O	2.08	0.71
48:DO:5:LYS:H	48:DO:5:LYS:HD3	1.55	0.71
1:AA:2337:G:OP2	65:AA:5135:HOH:O	2.06	0.71
1:CA:641:C:O2'	1:CA:2350:C:OP1	2.04	0.71
1:CA:1754:C:OP1	17:CT:96:ARG:NH1	2.22	0.71
6:CF:53:THR:HG22	6:CF:56:GLU:HG3	1.71	0.71
37:DD:187:ARG:NH2	37:DD:193:ASP:OD2	2.23	0.71
59:DZ:82:ILE:HD12	59:DZ:101:LEU:HB3	1.72	0.71
59:DZ:466:LEU:HG	59:DZ:472:VAL:HG21	1.71	0.71
14:AQ:14:ARG:HG2	14:AQ:41:TRP:HH2	1.55	0.71
45:DL:32:PHE:HB3	45:DL:84:LEU:HD11	1.72	0.71
1:AA:1891:G:C4'	3:AC:206:LYS:HG3	2.20	0.71
1:CA:775:G:N3	65:CA:4199:HOH:O	2.23	0.71
1:AA:2291:G:N7	24:A0:14:ARG:NH1	2.37	0.71
34:BA:1226:C:O2'	46:BM:111:LYS:NZ	2.23	0.71
1:CA:740:U:OP2	65:CA:4169:HOH:O	2.07	0.71
1:CA:2124:G:H4'	3:CC:175:PRO:HG3	1.72	0.71
34:BA:255:G:H1'	50:BQ:16:GLN:HE21	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:BZ:396:ARG:HG3	59:BZ:396:ARG:HH21	1.56	0.71
1:CA:971:C:OP2	65:CA:4574:HOH:O	2.07	0.71
8:CH:107:VAL:HG11	8:CH:162:ILE:HD11	1.70	0.71
34:DA:1238:A:OP2	65:DA:1861:HOH:O	2.07	0.71
3:AC:51:ASP:HB3	3:AC:57:GLN:OE1	1.91	0.71
41:BH:10:LEU:HD22	41:BH:83:ILE:HD11	1.72	0.71
3:CC:51:ASP:HB3	3:CC:57:GLN:OE1	1.91	0.71
59:DZ:225:GLU:HA	59:DZ:228:MET:HB3	1.72	0.71
48:DO:39:LEU:HD13	48:DO:56:LEU:HB2	1.73	0.71
59:DZ:466:LEU:HA	59:DZ:470:PHE:HD2	1.56	0.71
19:AV:40:LEU:HB2	19:AV:46:VAL:HG13	1.72	0.71
1:CA:2823:A:OP1	5:CE:159:HIS:NE2	2.21	0.71
1:AA:1391:C:OP2	65:AA:3960:HOH:O	2.08	0.70
3:AC:55:SER:O	3:AC:57:GLN:N	2.22	0.70
34:BA:427:U:OP1	37:BD:13:ARG:NH2	2.23	0.70
59:BZ:87:HIS:O	59:BZ:89:ASP:N	2.24	0.70
1:CA:2022:U:OP1	65:CA:4131:HOH:O	2.07	0.70
47:DN:21:TYR:OH	47:DN:23:ARG:NH2	2.24	0.70
59:DZ:169:GLY:H	59:DZ:170:ARG:HH12	1.39	0.70
36:BC:150:LYS:HG3	36:BC:169:ALA:HB2	1.73	0.70
52:BS:32:LYS:HA	52:BS:50:ALA:HB3	1.72	0.70
59:BZ:114:VAL:CG1	59:BZ:156:ARG:HH12	2.05	0.70
38:BE:43:LEU:HD21	38:BE:132:ALA:HB1	1.73	0.70
38:BE:100:VAL:O	38:BE:107:ARG:NH2	2.24	0.70
1:AA:1891:G:H4'	3:AC:206:LYS:CG	2.21	0.70
34:BA:953:G:H5'	34:BA:965:A:H61	1.56	0.70
3:CC:55:SER:O	3:CC:57:GLN:N	2.22	0.70
31:A7:24:THR:HG22	31:A7:27:GLY:H	1.56	0.70
7:CG:101:ILE:HG22	7:CG:105:LYS:HE2	1.73	0.70
1:AA:325:G:OP2	22:AY:84:ARG:NH2	2.24	0.70
36:BC:181:ASN:HD22	36:BC:204:LEU:HB2	1.57	0.70
1:CA:1026:U:OP1	65:CA:4575:HOH:O	2.09	0.70
1:CA:1860:G:H5'	3:CC:206:LYS:HD2	0.85	0.70
10:CL:99:ILE:HG23	10:CL:103:GLN:HB2	1.74	0.70
38:DE:75:THR:OG1	38:DE:117:ASP:O	2.07	0.70
59:BZ:329:ARG:NH1	59:BZ:331:TYR:HE1	1.89	0.70
59:BZ:546:ILE:HG23	59:BZ:590:ILE:HG13	1.73	0.70
15:CR:67:LEU:HD13	15:CR:76:VAL:HG21	1.73	0.70
17:CT:54:ARG:HA	17:CT:59:THR:HB	1.72	0.70
1:AA:2442:A:OP1	65:AA:4780:HOH:O	2.08	0.70
1:CA:1108:U:C5	1:CA:1109:C:C5	2.79	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:BK:19:ALA:HB3	44:BK:82:VAL:HG22	1.73	0.70
41:DH:119:LEU:HD13	41:DH:123:GLU:HG2	1.74	0.70
1:AA:2299:A:H2	1:AA:2358:A:H62	1.40	0.70
1:AA:2459:G:OP2	65:AA:4485:HOH:O	2.08	0.70
42:BI:23:ASN:HD22	42:BI:25:LYS:HG2	1.57	0.70
59:BZ:165:GLN:HE21	59:BZ:259:PHE:HB3	1.56	0.70
38:DE:80:ILE:HD13	41:DH:104:ARG:HH21	1.56	0.69
46:DM:37:THR:O	46:DM:55:ARG:NH1	2.24	0.69
37:BD:15:GLU:HG3	37:BD:63:LYS:HD3	1.74	0.69
39:BF:28:ARG:O	39:BF:32:ASN:ND2	2.24	0.69
3:CC:25:GLU:HA	3:CC:28:ARG:HD2	1.74	0.69
7:CG:64:THR:HB	7:CG:94:LEU:HD21	1.74	0.69
3:AC:57:GLN:HG3	3:AC:57:GLN:O	1.93	0.69
1:CA:1528:A:OP2	65:CA:3946:HOH:O	2.09	0.69
1:CA:1762:A:N1	65:CA:4246:HOH:O	2.25	0.69
7:CG:64:THR:HG21	7:CG:92:VAL:HG11	1.74	0.69
34:DA:254:G:OP1	50:DQ:66:SER:OG	2.10	0.69
10:CL:106:GLU:HA	10:CL:109:LYS:HD3	1.74	0.69
32:C8:10:ALA:HB3	32:C8:62:LEU:HD21	1.73	0.69
1:AA:2801:C:OP1	5:AE:61:ARG:NH2	2.25	0.69
3:AC:183:PRO:HG2	3:AC:184:GLU:OE2	1.92	0.69
34:BA:1086:U:H3	34:BA:1099:G:H22	1.38	0.69
1:CA:1419:A:OP2	65:CA:4417:HOH:O	2.09	0.69
35:DB:120:ALA:O	35:DB:122:PHE:N	2.25	0.69
1:AA:1221:G:H1'	1:AA:1222:A:H5'	1.75	0.69
1:AA:1324:A:OP1	15:AR:36:THR:HG23	1.91	0.69
29:A5:16:ARG:HG3	29:A5:17:ASP:N	2.08	0.69
34:BA:1191:A:H5''	36:BC:4:LYS:HZ2	1.58	0.69
42:BI:3:GLN:OE1	42:BI:20:ARG:NH2	2.21	0.69
59:BZ:227:ILE:HG23	59:BZ:237:PRO:HG2	1.74	0.69
3:CC:15:VAL:O	3:CC:16:ASP:HB3	1.92	0.69
17:CT:65:LYS:HE2	17:CT:67:SER:HB2	1.75	0.69
43:DJ:30:SER:O	43:DJ:81:THR:OG1	2.10	0.69
1:AA:483:A:H5''	65:AA:5243:HOH:O	1.93	0.69
3:AC:15:VAL:O	3:AC:16:ASP:HB3	1.92	0.69
9:AK:73:GLY:O	9:AK:75:GLN:N	2.24	0.69
1:AA:671:A:H2'	1:AA:672:G:O4'	1.93	0.69
22:AY:102:CYS:SG	22:AY:103:GLY:N	2.66	0.69
34:BA:356:A:N3	34:BA:368:U:O2'	2.24	0.69
1:CA:526:A:OP1	65:CA:4143:HOH:O	2.10	0.69
3:CC:46:ALA:HB3	3:CC:172:ILE:CG2	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CC:46:ALA:HB3	3:CC:172:ILE:HG22	1.75	0.69
34:DA:353:A:H8	34:DA:353:A:H5'	1.57	0.69
1:AA:553:A:C8	1:AA:553:A:H3'	2.28	0.68
3:AC:46:ALA:HB3	3:AC:172:ILE:HG22	1.75	0.68
3:CC:183:PRO:HG2	3:CC:184:GLU:OE2	1.93	0.68
4:CD:276:LYS:H	4:CD:276:LYS:HD3	1.58	0.68
34:DA:1060:C:C5	36:DC:2:GLY:HA3	2.28	0.68
59:DZ:26:THR:OG1	64:DZ:702:GDP:O1B	2.10	0.68
1:AA:2146:G:H1	1:AA:2196:C:H42	1.41	0.68
46:BM:17:VAL:O	46:BM:20:THR:OG1	2.09	0.68
1:CA:1061:U:H4'	1:CA:1070:A:H1'	1.75	0.68
44:DK:99:GLN:HG2	44:DK:105:VAL:HG21	1.74	0.68
1:AA:2200:C:O2'	3:AC:169:THR:HB	1.93	0.68
3:AC:25:GLU:HA	3:AC:28:ARG:HD2	1.75	0.68
17:AT:54:ARG:HA	17:AT:59:THR:HB	1.76	0.68
59:BZ:87:HIS:HB3	59:BZ:90:PHE:HB3	1.75	0.68
37:DD:150:GLU:HA	37:DD:153:ARG:HE	1.59	0.68
1:AA:932:C:H3'	1:AA:933:C:H5''	1.75	0.68
34:BA:1255:G:O2'	34:BA:1258:G:O2'	2.10	0.68
3:CC:30:VAL:HG23	3:CC:31:LYS:H	1.58	0.68
34:DA:117:G:OP2	65:DA:1839:HOH:O	2.11	0.68
34:DA:1060:C:H5	36:DC:2:GLY:HA3	1.58	0.68
46:DM:14:ARG:HG3	46:DM:44:ARG:HH11	1.58	0.68
56:DW:27:G:H1	56:DW:43:C:H42	1.40	0.68
2:CB:76:G:N7	65:CB:3103:HOH:O	2.25	0.68
28:C4:44:THR:O	28:C4:46:GLN:N	2.26	0.68
34:DA:983:A:N1	34:DA:1222:G:N2	2.41	0.68
1:AA:2007:G:OP2	65:AA:4909:HOH:O	2.11	0.68
34:DA:976:G:H5'	34:DA:1358:U:O2'	1.94	0.68
1:AA:1431:G:O2'	1:AA:1442:U:O2	2.10	0.68
22:AY:102:CYS:SG	22:AY:104:GLY:N	2.63	0.68
41:BH:114:THR:OG1	41:BH:117:GLY:O	2.11	0.68
5:CE:97:LYS:N	5:CE:100:GLU:OE1	2.24	0.68
16:CS:5:THR:N	16:CS:8:GLU:OE1	2.26	0.68
34:DA:1004:A:H62	34:DA:1037:C:H2'	1.59	0.68
34:DA:1255:G:P	43:DJ:45:ARG:HH22	2.16	0.68
1:AA:2586:G:OP1	65:AA:4113:HOH:O	2.11	0.68
3:AC:30:VAL:HG23	3:AC:31:LYS:H	1.58	0.68
35:BB:60:ASP:OD1	35:BB:64:ARG:NH2	2.26	0.68
58:BY:60:U:H5''	58:BY:61:C:H5	1.56	0.68
1:CA:299:A:H5''	22:CY:86:ARG:HH21	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:307:G:H21	1:CA:330:A:H62	1.42	0.68
1:CA:1604:C:OP2	65:CA:4479:HOH:O	2.11	0.68
5:CE:12:THR:HG21	17:CT:11:GLU:OE2	1.92	0.68
56:BW:5:G:H2'	56:BW:6:G:C8	2.30	0.68
3:CC:30:VAL:HG23	3:CC:31:LYS:N	2.09	0.68
1:AA:1114:G:N2	1:AA:1141:A:O3'	2.27	0.67
3:AC:30:VAL:HG23	3:AC:31:LYS:N	2.09	0.67
59:BZ:114:VAL:HG23	59:BZ:152:THR:HB	1.75	0.67
42:DI:99:LEU:HB3	42:DI:101:PHE:CE1	2.29	0.67
47:DN:23:ARG:HH11	47:DN:30:ALA:HB2	1.58	0.67
1:AA:2457:G:OP1	6:AF:74:ARG:NH2	2.27	0.67
3:AC:46:ALA:HB3	3:AC:172:ILE:CG2	2.23	0.67
4:AD:206:LEU:HD22	4:AD:211:ARG:HG2	1.75	0.67
26:A2:9:GLN:HE22	26:A2:56:GLN:HB3	1.58	0.67
1:CA:813:U:H2'	1:CA:814:C:C6	2.30	0.67
1:CA:882:G:H2'	1:CA:883:G:H8	1.59	0.67
1:CA:2611:U:C4	29:C5:3:LYS:HG2	2.30	0.67
12:CO:64:ARG:HG2	12:CO:79:PHE:CG	2.29	0.67
23:CZ:150:LEU:H	23:CZ:172:ALA:HB3	1.59	0.67
37:BD:178:VAL:HG12	37:BD:179:GLU:H	1.58	0.67
42:BI:43:ALA:O	42:BI:45:ALA:N	2.28	0.67
3:CC:176:VAL:HG11	3:CC:190:ILE:HD13	1.76	0.67
34:DA:1502:A:H2	34:DA:1505:G:H1	1.38	0.67
46:DM:25:ILE:HG23	46:DM:29:ARG:HB3	1.75	0.67
1:AA:399:G:OP2	25:A1:69:LYS:NZ	2.24	0.67
1:AA:626:A:H4'	1:AA:627:G:H5'	1.76	0.67
1:AA:2227:G:H3'	1:AA:2228:G:C8	2.30	0.67
38:BE:110:LEU:HD13	38:BE:118:ILE:HD13	1.77	0.67
6:CF:101:LEU:O	6:CF:106:ARG:NH1	2.26	0.67
8:CH:9:ILE:HB	8:CH:50:VAL:HB	1.74	0.67
34:DA:1305:G:N2	34:DA:1331:G:H1'	2.09	0.67
38:DE:102:ALA:HB1	38:DE:106:PRO:HG2	1.75	0.67
48:DO:41:GLU:HA	48:DO:44:LYS:HD2	1.75	0.67
9:AK:26:LEU:HA	9:AK:84:GLU:HA	1.74	0.67
34:BA:353:A:H5'	34:BA:353:A:H8	1.60	0.67
37:BD:111:ALA:HB2	37:BD:120:LEU:HD12	1.75	0.67
1:CA:1430:C:H2'	1:CA:1431:U:C6	2.30	0.67
1:CA:1547:C:H2'	1:CA:1548:C:H6	1.60	0.67
1:CA:2070:G:OP2	65:CA:4420:HOH:O	2.12	0.67
34:DA:1316:G:OP1	47:DN:17:LYS:NZ	2.25	0.67
51:DR:56:THR:HB	51:DR:58:LEU:HD23	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:BC:50:ALA:HB1	36:BC:70:VAL:HG21	1.74	0.67
1:CA:1057:A:O2'	1:CA:1058:G:OP1	2.09	0.67
36:DC:52:LEU:HD23	36:DC:55:VAL:HG23	1.75	0.67
1:AA:2772:G:N7	65:AA:4053:HOH:O	2.27	0.67
1:CA:2114:A:N1	1:CA:2171:A:N6	2.40	0.67
3:CC:57:GLN:O	3:CC:57:GLN:HG3	1.93	0.67
28:C4:16:CYS:SG	28:C4:17:GLY:N	2.67	0.67
34:DA:920:U:H2'	34:DA:921:U:C6	2.29	0.67
43:DJ:17:ASP:OD1	43:DJ:70:ARG:NH1	2.26	0.67
1:AA:2396:G:OP2	24:A0:55:ARG:NH1	2.26	0.67
2:AB:7:G:OP2	65:AB:3127:HOH:O	2.11	0.67
44:BK:18:ARG:NH1	44:BK:20:TYR:OH	2.27	0.67
1:CA:2104:G:H1	1:CA:2185:C:H42	1.42	0.67
42:BI:128:ARG:NH1	57:BX:35:A:OP2	2.27	0.67
1:CA:1022:G:N7	11:CN:66:LYS:HE2	2.10	0.67
3:CC:42:VAL:HG13	3:CC:43:GLU:N	2.10	0.67
34:DA:560:U:O2'	34:DA:561:U:OP2	2.13	0.67
59:DZ:494:GLU:HG2	59:DZ:511:LYS:HG2	1.75	0.67
37:BD:187:ARG:NH1	37:BD:190:ASP:OD1	2.28	0.67
44:BK:34:ASP:HB3	44:BK:40:ILE:HD11	1.75	0.67
45:BL:53:ARG:HG3	45:BL:93:LEU:HD21	1.76	0.67
59:BZ:20:HIS:ND1	59:BZ:115:GLU:HB3	2.09	0.67
1:CA:2177:C:O2	3:CC:173:HIS:HE1	1.78	0.67
1:CA:2286:A:H4'	1:CA:2287:A:O4'	1.95	0.67
1:AA:925:A:H61	1:AA:945:A:H1'	1.59	0.66
3:AC:42:VAL:HG13	3:AC:43:GLU:N	2.10	0.66
9:AK:70:GLU:O	9:AK:72:ASP:N	2.28	0.66
1:CA:1970:A:OP1	65:CA:3914:HOH:O	2.12	0.66
3:AC:31:LYS:NZ	3:AC:180:SER:O	2.28	0.66
40:BG:111:ARG:NH2	40:BG:126:ASP:OD2	2.28	0.66
59:DZ:329:ARG:HD3	59:DZ:331:TYR:CZ	2.31	0.66
1:AA:237:G:OP1	65:AA:4920:HOH:O	2.13	0.66
1:AA:1154:U:HO2'	1:AA:1155:C:H6	1.43	0.66
34:BA:1303:C:OP1	65:BA:2008:HOH:O	2.14	0.66
37:BD:107:ARG:HH22	37:BD:194:LEU:HD11	1.59	0.66
9:CK:73:GLY:O	9:CK:75:GLN:N	2.21	0.66
1:AA:1249:A:H2	1:AA:1287:A:N6	1.88	0.66
1:CA:2590:A:OP2	4:CD:238:GLY:HA2	1.94	0.66
4:CD:8:PRO:HB3	4:CD:14:ARG:HB2	1.76	0.66
10:AL:106:GLU:HA	10:AL:109:LYS:HD3	1.77	0.66
34:BA:1069:C:OP2	65:BA:1906:HOH:O	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:BW:51:U:H2'	56:BW:52:G:H8	1.60	0.66
35:DB:52:GLU:O	35:DB:56:ARG:HG2	1.96	0.66
57:DX:73:A:H5''	57:DX:74:C:H5'	1.76	0.66
22:AY:15:VAL:HG21	22:AY:42:VAL:HG11	1.78	0.66
34:BA:1221:G:OP1	34:BA:1320:C:N4	2.23	0.66
1:CA:2136:C:O2'	1:CA:2137:C:O5'	2.13	0.66
3:CC:63:VAL:O	3:CC:161:ARG:HA	1.96	0.66
42:DI:28:VAL:HG22	42:DI:63:ILE:HB	1.76	0.66
43:DJ:38:ILE:HD11	43:DJ:71:LEU:HD23	1.78	0.66
59:DZ:181:LEU:HD12	59:DZ:216:LEU:HD21	1.78	0.66
1:AA:1711:A:OP1	65:AA:5092:HOH:O	2.13	0.66
34:DA:1054:C:C4	56:DW:34:G:H1'	2.29	0.66
37:BD:22:LYS:HB2	63:BD:501:SF4:S4	2.36	0.66
36:DC:59:ARG:HG3	36:DC:64:VAL:HG13	1.77	0.66
3:AC:176:VAL:HG11	3:AC:190:ILE:HD13	1.76	0.66
34:BA:166:G:H2'	34:BA:167:G:C8	2.30	0.66
34:BA:1348:U:H4'	42:BI:120:ARG:HD2	1.77	0.66
1:CA:833:U:O2	13:CP:55:ARG:NH2	2.29	0.66
1:CA:855:G:O2'	24:C0:27:GLU:OE2	2.14	0.66
1:CA:1341:U:OP2	1:CA:1394:U:O2'	2.11	0.66
3:CC:65:LEU:HB3	3:CC:189:ASN:ND2	2.11	0.66
35:DB:201:ILE:HG21	35:DB:214:ILE:HG21	1.78	0.66
34:BA:193:C:H2'	34:BA:194:C:H6	1.61	0.66
34:DA:1239:A:H62	34:DA:1299:A:H62	1.41	0.66
1:AA:1079:U:OP1	33:A9:9:ARG:NH2	2.29	0.65
3:AC:65:LEU:HB3	3:AC:189:ASN:ND2	2.11	0.65
20:AW:18:ARG:NH1	20:AW:76:VAL:O	2.29	0.65
59:DZ:264:LEU:HB2	64:DZ:702:GDP:C6	2.31	0.65
1:CA:1332:G:OP1	65:CA:4126:HOH:O	2.14	0.65
1:CA:1671:U:HO2'	1:CA:1673:U:H5	1.44	0.65
17:CT:56:GLY:O	17:CT:59:THR:HG23	1.96	0.65
18:CU:76:TYR:OH	18:CU:92:ARG:NH1	2.28	0.65
1:CA:300:A:P	22:CY:86:ARG:HH22	2.19	0.65
1:CA:1604:C:OP2	65:CA:4478:HOH:O	2.15	0.65
34:DA:222:U:H2'	34:DA:223:U:C6	2.30	0.65
3:AC:41:THR:O	3:AC:42:VAL:HB	1.94	0.65
3:AC:63:VAL:O	3:AC:161:ARG:HA	1.95	0.65
7:AG:179:PRO:HB2	28:A4:42:PHE:HE1	1.61	0.65
1:CA:1315:C:OP2	65:CA:4126:HOH:O	2.15	0.65
28:C4:40:HIS:HB3	28:C4:43:TYR:HB2	1.78	0.65
34:DA:266:G:H5''	34:DA:268:C:H41	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:137:GLU:HG2	7:AG:152:LEU:HD13	1.78	0.65
17:AT:16:ARG:NH2	17:AT:83:ILE:O	2.29	0.65
3:CC:206:LYS:NZ	3:CC:206:LYS:HB3	2.12	0.65
42:DI:43:ALA:HA	42:DI:74:ILE:HD13	1.77	0.65
13:AP:50:ARG:HD3	32:A8:7:HIS:CD2	2.32	0.65
34:BA:200:G:H1	34:BA:217:C:H42	1.43	0.65
34:BA:1304:G:OP2	65:BA:2008:HOH:O	2.15	0.65
35:BB:195:ASP:O	41:BH:68:ARG:NH2	2.30	0.65
59:BZ:191:ASP:O	59:BZ:266:ASN:ND2	2.22	0.65
1:CA:2327:A:H2'	1:CA:2328:A:C8	2.31	0.65
3:CC:41:THR:O	3:CC:42:VAL:HB	1.94	0.65
35:DB:91:PRO:HG3	35:DB:155:LEU:HD23	1.79	0.65
35:DB:162:ILE:HD11	35:DB:184:VAL:HG22	1.78	0.65
34:BA:642:A:N3	41:BH:113:SER:OG	2.30	0.65
1:CA:1495:A:H2'	1:CA:1496:A:C8	2.32	0.65
1:AA:1087:C:H42	1:AA:1160:G:H1	1.45	0.65
1:AA:2138:G:N2	1:AA:2184:G:OP1	2.26	0.65
20:AW:14:PRO:HG2	20:AW:78:GLU:HG2	1.77	0.65
42:BI:42:ARG:NH1	42:BI:71:SER:OG	2.29	0.65
59:BZ:160:ARG:HD2	59:BZ:160:ARG:H	1.61	0.65
34:DA:1000:U:H3	34:DA:1041:A:H61	1.44	0.65
35:DB:100:GLY:O	35:DB:104:ASN:N	2.25	0.65
37:DD:127:THR:HB	37:DD:132:ARG:HA	1.79	0.65
1:AA:2199:C:O2	3:AC:173:HIS:CE1	2.50	0.65
19:CV:21:ARG:HG2	19:CV:91:TYR:CD2	2.31	0.65
34:DA:403:C:OP1	37:DD:137:SER:OG	2.14	0.65
47:DN:22:THR:HB	47:DN:33:VAL:HB	1.79	0.65
1:AA:2776:G:OP2	65:AA:4635:HOH:O	2.13	0.65
23:AZ:53:ILE:HG22	23:AZ:71:VAL:HG12	1.79	0.65
34:BA:1369:C:H2'	34:BA:1370:G:C8	2.31	0.65
1:CA:816:C:OP2	65:CA:4596:HOH:O	2.13	0.65
59:DZ:610:VAL:HG13	59:DZ:659:LEU:HD11	1.78	0.65
1:AA:1891:G:H5'	3:AC:206:LYS:CD	2.00	0.64
20:CW:65:LEU:HD12	20:CW:68:ARG:HE	1.62	0.64
1:AA:1093:G:HO2'	1:AA:1156:G:H1	1.44	0.64
3:AC:206:LYS:HB3	3:AC:206:LYS:NZ	2.12	0.64
34:DA:1129:C:H2'	34:DA:1139:G:N7	2.11	0.64
37:DD:61:LYS:NZ	37:DD:207:TYR:OH	2.31	0.64
56:DW:3:C:O2	56:DW:70:G:N2	2.17	0.64
1:AA:1219:A:H4'	1:AA:1220:U:OP1	1.97	0.64
7:AG:41:GLN:NE2	7:AG:154:GLY:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:BH:73:ASP:OD2	41:BH:75:ARG:NH1	2.31	0.64
30:A6:44:ARG:HB3	30:A6:44:ARG:NH1	2.12	0.64
57:BX:61:C:H2'	57:BX:62:C:H6	1.62	0.64
1:CA:848:G:H2'	1:CA:849:A:C8	2.33	0.64
30:C6:13:CYS:SG	30:C6:47:THR:HG21	2.37	0.64
41:DH:86:ILE:HG21	41:DH:133:LEU:HD13	1.78	0.64
3:AC:69:LEU:O	3:AC:178:LYS:HG3	1.98	0.64
34:BA:1318:A:H1'	52:BS:37:ARG:HH21	1.61	0.64
1:CA:1082:U:H4'	10:CL:117:THR:HB	1.78	0.64
23:CZ:117:LEU:HD12	23:CZ:174:VAL:HG22	1.80	0.64
1:AA:2460:A:OP1	65:AA:5078:HOH:O	2.14	0.64
1:AA:2601:A:OP1	65:AA:4557:HOH:O	2.14	0.64
3:AC:68:GLY:N	3:AC:189:ASN:HD21	1.96	0.64
1:CA:1800:C:OP2	4:CD:183:ARG:NH2	2.29	0.64
34:DA:396:G:OP1	59:DZ:349:LYS:NZ	2.31	0.64
42:DI:8:GLY:N	42:DI:15:ALA:O	2.27	0.64
1:AA:630:U:OP1	6:AF:102:PRO:HA	1.98	0.64
36:BC:52:LEU:HD23	36:BC:53:ALA:H	1.63	0.64
1:CA:1250:G:N7	13:CP:18:ARG:NH2	2.45	0.64
10:CL:81:ALA:HB1	10:CL:99:ILE:HD11	1.79	0.64
12:CO:35:VAL:HG23	12:CO:65:THR:HG23	1.78	0.64
34:DA:189(F):U:O2	50:DQ:63:ARG:NH2	2.30	0.64
37:DD:18:LYS:NZ	37:DD:31:CYS:SG	2.71	0.64
1:AA:9:U:N3	1:AA:2641:A:H2	1.89	0.64
1:AA:239:G:OP2	32:A8:13:ARG:NH2	2.31	0.64
22:AY:92:ASN:HB2	22:AY:94:LYS:N	2.12	0.64
23:AZ:157:LEU:HD21	23:AZ:163:LEU:HD13	1.79	0.64
36:BC:114:PRO:O	36:BC:118:GLN:NE2	2.31	0.64
1:CA:528:A:C2	1:CA:2043:C:H4'	2.33	0.64
19:CV:62:LEU:HD23	19:CV:93:GLU:HG2	1.80	0.64
35:DB:204:ASN:OD1	35:DB:205:ASP:N	2.31	0.64
59:DZ:170:ARG:N	59:DZ:170:ARG:HH11	1.96	0.64
7:AG:41:GLN:HB3	7:AG:43:LEU:HD22	1.79	0.64
34:BA:1158:C:H5	34:BA:1181:G:N1	1.95	0.64
34:BA:1182:G:H4'	34:BA:1183:A:H5'	1.80	0.64
45:BL:7:ILE:HA	45:BL:10:LEU:HD12	1.80	0.64
46:BM:59:TYR:O	46:BM:63:THR:OG1	2.15	0.64
1:CA:2424:C:O2	1:CA:2429:G:O2'	2.14	0.64
3:CC:69:LEU:O	3:CC:178:LYS:HG3	1.97	0.64
28:C4:24:THR:OG1	28:C4:25:TYR:N	2.27	0.64
35:BB:54:THR:HG21	35:BB:201:ILE:HD11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:BY:8:4SU:H4'	58:BY:48:C:H4'	1.80	0.64
1:AA:791:G:OP1	65:AA:4626:HOH:O	2.15	0.63
4:AD:122:ASP:OD1	4:AD:122:ASP:N	2.24	0.63
7:AG:48:GLU:HA	7:AG:51:ARG:HE	1.62	0.63
1:CA:2243:U:H2'	1:CA:2244:U:C6	2.33	0.63
15:CR:21:TYR:OH	15:CR:43:GLU:HG2	1.98	0.63
3:AC:29:LEU:O	3:AC:32:GLU:N	2.32	0.63
8:AH:90:LYS:HD3	8:AH:159:GLU:HG2	1.79	0.63
13:AP:125:VAL:HG21	13:AP:138:LEU:HD21	1.80	0.63
34:BA:600:C:H2'	34:BA:601:C:C6	2.33	0.63
59:BZ:82:ILE:HD12	59:BZ:101:LEU:HD23	1.80	0.63
3:CC:31:LYS:NZ	3:CC:180:SER:O	2.28	0.63
11:CN:123:TYR:OH	11:CN:130:HIS:NE2	2.31	0.63
34:DA:986:A:O2'	52:DS:55:LYS:O	2.16	0.63
50:DQ:81:ARG:HB3	50:DQ:84:LEU:HD12	1.80	0.63
59:DZ:363:ARG:HH11	59:DZ:363:ARG:CG	2.09	0.63
3:AC:44:VAL:CG2	3:AC:176:VAL:HG21	2.28	0.63
30:A6:13:CYS:SG	30:A6:47:THR:HG21	2.39	0.63
12:CO:25:LEU:HD12	12:CO:38:VAL:HG12	1.80	0.63
35:DB:213:LEU:HD22	35:DB:214:ILE:HD13	1.80	0.63
59:DZ:-53:ASP:H	59:DZ:-50:GLN:NE2	1.97	0.63
59:DZ:117:GLN:O	59:DZ:121:VAL:N	2.30	0.63
3:AC:7:ARG:O	3:AC:11:LEU:HD23	1.99	0.63
14:AQ:10:ARG:HG2	14:AQ:11:LYS:HG3	1.80	0.63
52:BS:63:THR:OG1	52:BS:65:ASN:ND2	2.32	0.63
3:CC:7:ARG:O	3:CC:11:LEU:HD23	1.99	0.63
44:DK:98:LEU:O	44:DK:101:SER:OG	2.06	0.63
11:AN:46:VAL:HG23	11:AN:48:MET:HG2	1.80	0.63
59:BZ:73:PHE:CE2	59:BZ:78:ARG:NH1	2.67	0.63
49:DP:5:ARG:HB3	49:DP:67:THR:HG23	1.80	0.63
58:DY:12:U:H3	58:DY:23:A:H61	1.45	0.63
34:BA:421:U:OP2	34:BA:422:C:N4	2.30	0.63
59:BZ:184:LYS:HD2	59:BZ:198:GLU:OE2	1.98	0.63
34:DA:1130:A:O2'	42:DI:3:GLN:OE1	2.17	0.63
42:DI:99:LEU:HB3	42:DI:101:PHE:HE1	1.62	0.63
1:CA:1143:A:OP1	11:CN:25:ARG:NH2	2.31	0.63
1:CA:1860:G:C5'	3:CC:206:LYS:HG3	1.88	0.63
3:CC:68:GLY:N	3:CC:189:ASN:HD21	1.96	0.63
20:CW:18:ARG:NH1	20:CW:76:VAL:O	2.31	0.63
34:DA:986:A:H1'	52:DS:55:LYS:HA	1.81	0.63
34:DA:1118:C:OP1	42:DI:104:ARG:NH1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:DP:52:ASP:O	49:DP:54:GLU:N	2.32	0.63
1:AA:1218:G:O2'	1:AA:1219:A:O4'	2.16	0.63
3:AC:6:LYS:HG3	3:AC:7:ARG:N	2.14	0.63
4:AD:71:ASP:OD2	4:AD:103:ARG:NH2	2.32	0.63
1:CA:96:G:H4'	26:C2:48:HIS:CD2	2.33	0.63
17:CT:39:ARG:NH2	34:DA:345:C:OP2	2.32	0.63
1:AA:990:A:OP2	65:AA:4345:HOH:O	2.16	0.63
34:BA:992:U:O2	34:BA:1043:C:N4	2.32	0.63
34:BA:1525:G:OP1	44:BK:120:ARG:NH2	2.32	0.63
53:BT:9:ASN:HB3	53:BT:10:LEU:HD12	1.80	0.63
59:BZ:78:ARG:HG3	59:BZ:78:ARG:NH1	2.07	0.63
59:BZ:127:LYS:HG3	59:BZ:520:GLY:HA3	1.81	0.63
3:CC:6:LYS:HG3	3:CC:7:ARG:N	2.14	0.63
3:CC:44:VAL:CG2	3:CC:176:VAL:HG21	2.28	0.63
37:DD:103:ASN:OD1	37:DD:114:ARG:NE	2.28	0.63
39:DF:23:LYS:HG2	39:DF:61:LEU:HD21	1.81	0.63
43:DJ:5:ARG:N	43:DJ:73:ASP:OD1	2.32	0.63
1:AA:2045:G:H5'	1:AA:2629:C:H4'	1.79	0.62
1:AA:2152:U:H4'	1:AA:2155:G:H4'	1.81	0.62
34:BA:972:C:O2'	43:BJ:55:LYS:O	2.16	0.62
38:BE:68:GLU:HG2	38:BE:70:PRO:HD3	1.81	0.62
59:BZ:238:THR:HG23	59:BZ:241:GLU:HB2	1.80	0.62
1:CA:2176:A:H2'	1:CA:2177:C:C6	2.34	0.62
3:CC:29:LEU:O	3:CC:32:GLU:N	2.31	0.62
15:CR:56:LYS:NZ	15:CR:90:ARG:O	2.32	0.62
42:DI:128:ARG:NH2	57:DX:33:U:OP2	2.32	0.62
57:DX:9:G:O2'	57:DX:10:G:N7	2.24	0.62
1:AA:1199:C:OP1	18:AU:92:ARG:NH1	2.32	0.62
50:BQ:45:HIS:HB3	50:BQ:72:ARG:HB3	1.82	0.62
6:CF:185:ASP:OD1	6:CF:188:ARG:NH1	2.31	0.62
1:AA:1480:A:H61	1:AA:1605:A:H62	1.47	0.62
3:AC:68:GLY:H	3:AC:189:ASN:HD21	1.47	0.62
35:BB:17:PHE:HB2	35:BB:44:LEU:HD21	1.81	0.62
35:BB:155:LEU:HD21	35:BB:159:PRO:HD3	1.82	0.62
1:CA:2785:C:OP1	5:CE:41:LYS:NZ	2.32	0.62
1:AA:1501:U:OP1	15:AR:77:ARG:NH1	2.32	0.62
21:AX:57:LEU:HD21	21:AX:78:LYS:HE2	1.80	0.62
34:BA:598:U:H4'	41:BH:94:TYR:CD2	2.34	0.62
36:BC:19:GLU:HB3	36:BC:40:ARG:HH22	1.65	0.62
1:CA:731:C:OP1	65:CA:4291:HOH:O	2.16	0.62
1:CA:2206:G:H3'	1:CA:2207:G:N7	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:2839:G:H5'	15:CR:46:GLY:HA2	1.81	0.62
6:CF:155:LEU:HD23	6:CF:186:ILE:HG13	1.81	0.62
1:AA:611:U:H2'	1:AA:612:C:C6	2.35	0.62
1:CA:1798:U:OP2	4:CD:274:ARG:NH2	2.32	0.62
34:DA:406:G:H5'	37:DD:5:ILE:HD11	1.82	0.62
34:DA:1133:G:H2'	34:DA:1134:G:H8	1.63	0.62
34:DA:1228:C:OP1	46:DM:115:LYS:N	2.30	0.62
36:DC:58:GLU:HB3	43:DJ:92:THR:HG21	1.82	0.62
36:DC:65:ALA:HA	36:DC:100:ALA:HB3	1.81	0.62
34:BA:153:C:H42	34:BA:168:G:H1	1.48	0.62
48:BO:17:ARG:HG3	48:BO:17:ARG:HH11	1.64	0.62
1:CA:2788:C:O2'	1:CA:2809:A:N3	2.30	0.62
34:DA:958:A:N6	52:DS:77:THR:O	2.32	0.62
1:AA:927:G:H2'	1:AA:928:G:C8	2.34	0.62
56:BW:63:G:H2'	56:BW:64:A:O4'	2.00	0.62
26:C2:1:MET:N	26:C2:52:ASP:OD1	2.23	0.62
34:DA:1318:A:H1'	52:DS:37:ARG:HD3	1.80	0.62
35:DB:16:HIS:CG	35:DB:17:PHE:H	2.17	0.62
1:AA:798:A:H5'	20:AW:90:ARG:HA	1.82	0.62
1:AA:957:A:H2'	14:AQ:9:TYR:OH	2.00	0.62
1:AA:1154:U:O2'	1:AA:1155:C:H6	1.82	0.62
13:AP:59:LEU:HD11	32:A8:10:ALA:HB2	1.81	0.62
3:CC:53:ARG:HD3	3:CC:53:ARG:H	1.65	0.62
30:C6:6:ARG:NH1	30:C6:26:ASN:HB2	2.14	0.62
34:DA:1073:U:H2'	34:DA:1074:G:H8	1.65	0.62
34:BA:255:G:H1'	50:BQ:16:GLN:NE2	2.15	0.62
42:BI:99:LEU:HB3	42:BI:101:PHE:HE1	1.64	0.62
6:CF:101:LEU:HD12	6:CF:102:PRO:HD2	1.82	0.62
34:DA:523:A:H61	45:DL:92:ASP:HB2	1.64	0.62
1:AA:202:A:H2'	1:AA:203:G:O4'	2.00	0.62
1:AA:2209:G:O2'	1:AA:2210:C:OP1	2.18	0.62
3:AC:53:ARG:HD3	3:AC:53:ARG:H	1.65	0.62
34:BA:1062:U:H2'	34:BA:1063:C:C6	2.35	0.62
1:CA:993:G:OP1	18:CU:50:ARG:NH2	2.32	0.62
3:CC:11:LEU:HD12	3:CC:33:LEU:HA	1.82	0.62
1:AA:1405:A:N1	1:AA:1418:U:O4	2.33	0.61
1:AA:1529:G:O6	1:AA:1553:A:N6	2.33	0.61
6:AF:28:ILE:O	6:AF:30:PRO:HD3	1.99	0.61
19:AV:49:THR:HG22	19:AV:49:THR:O	2.00	0.61
34:BA:877:C:H5''	41:BH:88:LYS:HD3	1.82	0.61
59:BZ:319:ASP:OD1	59:BZ:363:ARG:NH2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:2328:A:H2'	1:CA:2329:G:C8	2.35	0.61
1:CA:2805:G:H2'	1:CA:2807:G:C8	2.35	0.61
34:DA:460:G:O6	34:DA:470:C:H5''	2.00	0.61
34:DA:991:U:H4'	34:DA:992:U:OP1	1.99	0.61
19:AV:76:LYS:HB2	19:AV:81:TYR:HB3	1.82	0.61
1:CA:2355:C:H1'	24:C0:39:ARG:HH21	1.63	0.61
19:CV:98:GLU:OE1	19:CV:100:ARG:NH1	2.33	0.61
35:DB:13:ALA:N	35:DB:14:GLY:HA3	2.15	0.61
7:AG:110:ALA:HB1	7:AG:140:ILE:HG23	1.82	0.61
34:BA:1123:A:H61	34:BA:1149:C:H42	1.49	0.61
59:BZ:328:ILE:O	59:BZ:374:LEU:HB2	2.00	0.61
1:CA:1109:C:H2'	1:CA:1110:G:C8	2.35	0.61
34:DA:1010:G:N2	34:DA:1020:U:O2	2.34	0.61
14:AQ:12:GLN:HG2	14:AQ:73:PRO:HD2	1.83	0.61
49:BP:75:ARG:O	49:BP:78:GLY:N	2.27	0.61
1:CA:2238:G:N7	65:CA:4455:HOH:O	2.31	0.61
14:CQ:85:LYS:HG2	24:C0:7:LEU:HB3	1.82	0.61
34:DA:1002:G:C4	34:DA:1003:G:H8	2.18	0.61
34:DA:1302:U:OP2	46:DM:21:TYR:OH	2.10	0.61
34:BA:266:G:H5''	34:BA:268:C:H41	1.65	0.61
1:CA:1876:A:H2'	1:CA:1877:A:C8	2.35	0.61
5:CE:59:VAL:HG21	5:CE:74:PRO:HB3	1.82	0.61
1:AA:1834:A:H4'	4:AD:259:THR:HG23	1.83	0.61
4:AD:71:ASP:HB3	4:AD:103:ARG:HH22	1.66	0.61
28:A4:10:VAL:HG21	28:A4:29:PRO:HG3	1.81	0.61
1:CA:1081:U:OP1	10:CL:125:ARG:NH1	2.33	0.61
4:CD:142:VAL:HG13	4:CD:191:ALA:HB1	1.81	0.61
14:CQ:138:ASP:OD2	23:CZ:81:ARG:NH1	2.34	0.61
59:DZ:659:LEU:HD12	59:DZ:669:PHE:HD1	1.66	0.61
7:AG:161:THR:HG22	7:AG:163:ALA:H	1.65	0.61
28:A4:44:THR:O	28:A4:46:GLN:N	2.34	0.61
36:BC:134:ILE:HG23	36:BC:151:VAL:HB	1.83	0.61
1:CA:1019:U:HO2'	1:CA:1021:A:H2	1.48	0.61
34:DA:1022:G:H2'	34:DA:1023:G:H8	1.64	0.61
34:DA:1062:U:H2'	34:DA:1063:C:C6	2.35	0.61
42:DI:8:GLY:HA2	42:DI:79:LEU:HD23	1.83	0.61
58:DY:51:U:H3	58:DY:63:G:H1	1.46	0.61
1:AA:354:A:H2	1:AA:1255:A:HO2'	1.49	0.61
1:AA:625:G:O2'	1:AA:702:A:N6	2.34	0.61
1:AA:1604:C:OP2	1:AA:1605:A:O2'	2.19	0.61
23:AZ:72:ARG:NH2	23:AZ:97:GLU:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A6:44:ARG:HB3	30:A6:44:ARG:HH11	1.66	0.61
59:BZ:509:HIS:HB3	59:BZ:571:SER:H	1.66	0.61
1:CA:300:A:OP2	22:CY:86:ARG:NH2	2.34	0.61
34:DA:959:A:HO2'	34:DA:984:C:HO2'	1.43	0.61
34:DA:1312:G:H5'	52:DS:5:LEU:HD11	1.81	0.61
1:AA:542:C:OP1	29:A5:16:ARG:NH2	2.30	0.61
5:AE:117:MET:SD	5:AE:136:ARG:HB3	2.41	0.61
36:DC:125:GLU:HG3	36:DC:190:ARG:O	2.01	0.61
42:DI:3:GLN:HG2	42:DI:20:ARG:HE	1.64	0.61
1:AA:2348:A:H61	24:A0:43:THR:CG2	2.14	0.61
7:AG:41:GLN:HE22	7:AG:153:ARG:HB3	1.66	0.61
34:BA:1255:G:OP1	43:BJ:45:ARG:NH2	2.33	0.61
35:BB:100:GLY:O	35:BB:104:ASN:N	2.27	0.61
43:BJ:40:LEU:HB2	43:BJ:69:ASN:HB2	1.83	0.61
56:BW:9:A:N3	56:BW:45:U:H2'	2.16	0.61
1:CA:1816:G:O6	4:CD:35:LYS:NZ	2.23	0.61
1:CA:2169:A:H2'	1:CA:2170:A:C8	2.36	0.61
42:DI:51:ARG:HG2	42:DI:56:LEU:HD21	1.83	0.61
1:AA:2348:A:H61	24:A0:43:THR:HG21	1.65	0.60
13:CP:138:LEU:HD23	13:CP:145:PRO:HG3	1.82	0.60
35:DB:103:THR:HA	35:DB:180:LEU:HD11	1.83	0.60
58:DY:33:U:H2'	58:DY:35:A:OP2	2.01	0.60
59:DZ:491:VAL:HG21	59:DZ:597:GLY:HA3	1.83	0.60
21:AX:35:THR:HG22	21:AX:38:GLU:HB2	1.83	0.60
34:BA:742:G:OP2	48:BO:35:ARG:NH2	2.32	0.60
56:BW:51:U:H2'	56:BW:52:G:C8	2.35	0.60
1:CA:289:A:H2'	1:CA:290:G:O4'	2.01	0.60
6:CF:34:TRP:CZ2	13:CP:8:PRO:HG3	2.35	0.60
34:DA:427:U:OP1	37:DD:13:ARG:NH2	2.34	0.60
34:DA:630:G:H2'	34:DA:631:G:H8	1.65	0.60
34:DA:924:C:O2'	34:DA:1502:A:N6	2.35	0.60
49:DP:51:VAL:HG12	49:DP:53:VAL:H	1.66	0.60
1:AA:1093:G:N2	1:AA:1156:G:O2'	2.33	0.60
1:AA:2130:C:H2'	1:AA:2131:U:H6	1.66	0.60
1:AA:2303:U:H2'	1:AA:2304:C:C6	2.36	0.60
1:AA:2331:G:H22	16:AS:3:ARG:NE	1.99	0.60
1:CA:636:G:O2'	1:CA:638:G:O2'	2.19	0.60
1:CA:1493:C:N4	1:CA:2206:G:O2'	2.34	0.60
1:CA:2875:C:OP1	17:CT:3:ARG:NH2	2.35	0.60
30:C6:8:LYS:HD3	32:C8:34:TRP:CD2	2.36	0.60
34:DA:1055:A:N3	36:DC:156:ARG:NH1	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:232:U:OP1	32:A8:6:THR:OG1	2.16	0.60
11:AN:42:TRP:CH2	11:AN:44:PRO:HB3	2.36	0.60
34:BA:524:G:H2'	34:BA:525:C:C6	2.36	0.60
35:BB:200:ILE:HB	35:BB:202:PRO:HD3	1.82	0.60
36:BC:19:GLU:HB3	36:BC:40:ARG:NH2	2.16	0.60
58:BY:67:C:H2'	58:BY:68:C:C6	2.36	0.60
59:BZ:-64:VAL:HG12	59:BZ:-29:LEU:HA	1.82	0.60
7:CG:15:VAL:HA	7:CG:175:LEU:HD23	1.83	0.60
34:DA:986:A:N3	52:DS:52:TYR:OH	2.33	0.60
36:DC:8:ILE:HD13	36:DC:184:TYR:HB3	1.82	0.60
1:AA:2044:U:O2'	1:AA:2629:C:H5'	2.02	0.60
3:AC:194:ILE:HD11	3:AC:227:PRO:CB	2.32	0.60
59:BZ:20:HIS:HA	59:BZ:117:GLN:HB2	1.81	0.60
1:CA:271(M):G:H4'	1:CA:271(N):U:OP1	2.01	0.60
1:CA:400:G:N7	65:CA:4345:HOH:O	2.32	0.60
28:C4:59:PHE:HA	28:C4:61:ARG:N	2.17	0.60
1:AA:553:A:H3'	1:AA:553:A:H8	1.66	0.60
1:AA:2262:G:OP1	14:AQ:85:LYS:HE3	2.01	0.60
1:AA:2585:C:H3'	65:AA:4113:HOH:O	2.00	0.60
3:AC:214:TYR:CE2	3:AC:224:ARG:HG2	2.36	0.60
5:AE:105:THR:OG1	5:AE:199:ARG:NH2	2.35	0.60
4:CD:146:GLU:HB2	4:CD:189:CYS:HB3	1.84	0.60
8:CH:101:ARG:HH22	8:CH:122:THR:HG23	1.67	0.60
34:DA:630:G:H2'	34:DA:631:G:C8	2.37	0.60
42:DI:23:ASN:HD22	42:DI:23:ASN:H	1.49	0.60
59:DZ:363:ARG:HG2	59:DZ:363:ARG:NH1	2.11	0.60
1:AA:1766:G:H3'	1:AA:1767:A:H5''	1.81	0.60
1:AA:2697:G:H5'	12:AO:68:GLU:OE1	2.02	0.60
13:AP:39:LYS:HD2	13:AP:45:LEU:HD11	1.82	0.60
41:BH:112:LEU:HA	41:BH:134:ILE:HG12	1.81	0.60
59:BZ:12:LEU:HD12	59:BZ:78:ARG:HD2	1.83	0.60
59:BZ:99:ARG:HH11	59:BZ:99:ARG:CB	2.09	0.60
20:CW:88:ARG:NH1	20:CW:94:ASP:OD2	2.34	0.60
34:DA:390:C:O3'	49:DP:28:ARG:NH2	2.34	0.60
34:DA:982:U:O2	34:DA:1222:G:N1	2.31	0.60
34:DA:1189:C:OP1	43:DJ:51:ARG:NH2	2.34	0.60
41:DH:49:GLU:OE2	41:DH:62:TYR:OH	2.15	0.60
51:DR:58:LEU:HD12	51:DR:62:GLU:HB3	1.84	0.60
1:AA:2504:U:H2'	1:AA:2505:U:C6	2.37	0.60
35:BB:187:LEU:HA	35:BB:201:ILE:HB	1.82	0.60
57:BX:61:C:H2'	57:BX:62:C:C6	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1021:A:C8	1:CA:1021:A:H3'	2.37	0.60
3:CC:68:GLY:H	3:CC:189:ASN:HD21	1.47	0.60
3:CC:214:TYR:CE2	3:CC:224:ARG:HG2	2.36	0.60
5:CE:56:PRO:HG3	5:CE:74:PRO:HG2	1.84	0.60
14:CQ:26:TYR:CE1	14:CQ:28:ALA:HB2	2.37	0.60
25:C1:72:GLU:OE1	25:C1:76:ARG:NH2	2.35	0.60
35:DB:74:LYS:HD2	35:DB:165:VAL:HG11	1.84	0.60
59:DZ:13:ARG:NE	59:DZ:280:LEU:O	2.30	0.60
1:AA:1312:G:O5'	20:AW:15:ARG:NH2	2.35	0.60
1:AA:2075:G:OP1	5:AE:144:ARG:HG2	2.02	0.60
3:AC:11:LEU:HD12	3:AC:33:LEU:HA	1.82	0.60
16:AS:14:VAL:O	16:AS:18:ILE:HG12	2.01	0.60
18:AU:76:TYR:CE1	18:AU:80:ILE:HG13	2.36	0.60
34:BA:1251:A:H2'	34:BA:1252:A:C8	2.37	0.60
34:DA:975:A:N6	43:DJ:60:ARG:HH12	2.00	0.60
38:DE:81:GLU:HG2	38:DE:90:VAL:HG13	1.82	0.60
41:DH:37:ARG:HH21	41:DH:38:ILE:HD11	1.66	0.60
45:DL:83:VAL:HG23	45:DL:107:ALA:HB2	1.82	0.60
36:BC:43:LEU:HD22	36:BC:47:LEU:HD11	1.83	0.60
59:BZ:276:VAL:HG13	59:BZ:280:LEU:HD12	1.82	0.60
4:CD:17:THR:O	4:CD:211:ARG:NH2	2.34	0.60
42:DI:53:VAL:O	42:DI:55:ALA:N	2.34	0.60
7:AG:3:LEU:HD12	7:AG:5:VAL:HG12	1.84	0.59
34:BA:1305:G:H22	34:BA:1331:G:H1'	1.65	0.59
36:BC:6:HIS:HD2	36:BC:8:ILE:H	1.50	0.59
1:CA:793:A:O2'	65:CA:4198:HOH:O	2.14	0.59
1:CA:1153:C:OP1	18:CU:92:ARG:NH1	2.35	0.59
4:CD:131:LEU:HB2	4:CD:136:ILE:HD11	1.83	0.59
34:DA:1003:G:N2	34:DA:1025:U:O4	2.35	0.59
55:DV:20:U:H2'	55:DV:21:C:H6	1.67	0.59
59:DZ:35:TYR:HE2	59:DZ:269:VAL:HB	1.66	0.59
59:DZ:438:PHE:HE2	59:DZ:440:VAL:HG23	1.65	0.59
1:AA:2008:A:OP1	65:AA:4321:HOH:O	2.16	0.59
28:A4:26:SER:OG	28:A4:27:THR:N	2.35	0.59
47:BN:4:LYS:HA	47:BN:7:ILE:HG23	1.83	0.59
1:CA:854:G:O6	65:CA:4561:HOH:O	2.13	0.59
1:CA:918:A:N3	2:CB:80:U:O2'	2.32	0.59
4:CD:96:HIS:CD2	4:CD:102:LYS:HG2	2.34	0.59
13:CP:85:LEU:HA	13:CP:88:LEU:HD12	1.84	0.59
23:CZ:19:ARG:NH1	23:CZ:84:GLU:O	2.35	0.59
34:DA:664:G:N2	34:DA:741:G:H1	1.99	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:DA:878:G:H5'	41:DH:89:PRO:HG2	1.82	0.59
34:DA:1118:C:H2'	34:DA:1119:C:H6	1.66	0.59
1:AA:2201:C:O4'	3:AC:169:THR:CG2	2.48	0.59
10:AL:77:LEU:HD21	10:AL:111:LYS:HD2	1.84	0.59
14:AQ:56:ARG:NH1	56:BW:52:G:H4'	2.17	0.59
34:BA:193:C:H2'	34:BA:194:C:C6	2.36	0.59
34:BA:555:C:H2'	34:BA:556:C:C6	2.37	0.59
36:BC:53:ALA:HB2	36:BC:115:LEU:HD13	1.84	0.59
59:BZ:179:ASP:N	59:BZ:184:LYS:O	2.29	0.59
1:CA:2273:A:O2'	1:CA:2274:A:H5'	2.02	0.59
1:CA:2781:A:H5''	1:CA:2782:G:H5'	1.84	0.59
5:CE:78:LEU:O	5:CE:79:ARG:HG2	2.01	0.59
7:CG:113:ARG:NH1	7:CG:139:LEU:O	2.34	0.59
34:DA:920:U:H2'	34:DA:921:U:H6	1.67	0.59
34:DA:1073:U:H2'	34:DA:1074:G:C8	2.37	0.59
39:DF:2:ARG:NE	39:DF:69:GLU:HG2	2.17	0.59
1:AA:2255:U:H2'	1:AA:2256:U:C6	2.37	0.59
8:AH:164:TYR:HB2	8:AH:167:GLU:HB2	1.83	0.59
10:AL:77:LEU:HD12	10:AL:107:ILE:HG23	1.85	0.59
12:AO:35:VAL:HG21	12:AO:69:ILE:HD13	1.84	0.59
34:BA:1240:U:OP2	40:BG:116:ALA:N	2.27	0.59
1:CA:908:C:OP2	14:CQ:22:LYS:NZ	2.35	0.59
1:CA:1053:C:C4	1:CA:1107:G:N2	2.68	0.59
1:CA:1589:C:H2'	1:CA:1590:U:C6	2.37	0.59
1:CA:2132:U:C2	3:CC:6:LYS:HE3	2.37	0.59
1:CA:2485:G:H5''	14:CQ:46:GLN:HE21	1.67	0.59
3:CC:194:ILE:HD11	3:CC:227:PRO:CB	2.32	0.59
14:CQ:110:THR:HG23	14:CQ:113:GLN:HB2	1.83	0.59
23:CZ:108:PRO:HG2	23:CZ:117:LEU:HD13	1.85	0.59
34:DA:1030:C:H42	34:DA:1031:G:H1	1.50	0.59
34:DA:1123:A:H4'	43:DJ:37:PRO:HD2	1.85	0.59
35:DB:189:ASP:OD1	35:DB:189:ASP:N	2.27	0.59
49:DP:43:LYS:HG2	49:DP:48:TRP:CG	2.38	0.59
59:DZ:407:PRO:HB3	59:DZ:452:SER:HB3	1.85	0.59
1:AA:1338:U:H2'	1:AA:1339:C:C6	2.37	0.59
8:AH:88:LEU:HD13	8:AH:130:ARG:HG2	1.84	0.59
42:BI:3:GLN:HG3	42:BI:20:ARG:HE	1.67	0.59
1:CA:1108:U:H6	1:CA:1108:U:O5'	1.85	0.59
1:CA:2166:G:H3'	1:CA:2167:U:H5''	1.84	0.59
44:DK:22:HIS:HB3	44:DK:29:ILE:HB	1.85	0.59
1:AA:331:G:H21	1:AA:354:A:H62	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:2013:U:H2'	1:AA:2014:G:H5''	1.84	0.59
34:BA:736:C:H2'	34:BA:737:A:C8	2.37	0.59
35:BB:178:ARG:NH2	41:BH:74:PRO:HB3	2.18	0.59
37:BD:60:GLU:OE1	37:BD:198:VAL:HA	2.01	0.59
16:AS:3:ARG:C	16:AS:3:ARG:HD3	2.22	0.59
34:BA:103:C:P	53:BT:17:ARG:HH21	2.25	0.59
1:CA:2148:G:H2'	1:CA:2149:G:C8	2.37	0.59
1:CA:2165:G:H22	1:CA:2172:U:H5	1.51	0.59
1:CA:2320:A:H2'	1:CA:2320:A:N3	2.17	0.59
3:CC:41:THR:HG22	3:CC:42:VAL:N	2.17	0.59
35:DB:16:HIS:O	35:DB:18:GLY:N	2.36	0.59
37:DD:13:ARG:NH1	37:DD:38:TYR:O	2.36	0.59
49:DP:43:LYS:HG2	49:DP:48:TRP:CD2	2.37	0.59
34:BA:1326:C:OP1	54:BU:12:LYS:NZ	2.23	0.59
35:BB:201:ILE:HG21	35:BB:214:ILE:HG21	1.83	0.59
36:BC:13:GLY:HA3	47:BN:57:ARG:HH21	1.66	0.59
59:BZ:20:HIS:ND1	59:BZ:117:GLN:HG2	2.18	0.59
1:CA:1792:G:O2'	1:CA:1830:C:OP1	2.20	0.59
1:CA:2139:C:H42	1:CA:2152:G:H1	1.51	0.59
27:C3:8:LEU:HD13	27:C3:31:LEU:HD23	1.84	0.59
41:DH:73:ASP:OD1	41:DH:75:ARG:NH1	2.36	0.59
42:DI:14:VAL:HG23	42:DI:66:ARG:HB3	1.83	0.59
52:DS:63:THR:OG1	52:DS:64:GLU:N	2.35	0.59
1:AA:1159:U:H2'	1:AA:1160:G:C8	2.38	0.59
41:BH:51:VAL:HG21	41:BH:60:ARG:HH11	1.67	0.59
1:CA:309:G:N3	1:CA:329:G:O2'	2.35	0.59
53:DT:9:ASN:O	53:DT:10:LEU:HB2	2.02	0.59
59:DZ:346:LYS:HZ1	59:DZ:384:ILE:HG23	1.68	0.59
1:AA:1775:C:H5'	1:AA:1776:G:OP2	2.03	0.59
36:BC:3:ASN:OD1	36:BC:3:ASN:N	2.36	0.59
42:BI:110:GLU:OE2	42:BI:113:LYS:NZ	2.35	0.59
59:BZ:146:LEU:HD12	59:BZ:167:PRO:HD3	1.85	0.59
1:CA:1108:U:C5	1:CA:1109:C:C4	2.91	0.59
18:CU:86:ALA:HB2	18:CU:116:ALA:HB2	1.84	0.59
34:DA:1330:U:H4'	46:DM:23:TYR:CE1	2.37	0.59
1:AA:278:G:H2'	1:AA:279:G:H5''	1.85	0.58
1:AA:1154:U:H1'	1:AA:1155:C:OP1	2.03	0.58
3:AC:214:TYR:CZ	3:AC:224:ARG:HG2	2.37	0.58
4:AD:52:ARG:NH2	65:AD:412:HOH:O	2.29	0.58
43:BJ:38:ILE:HD11	43:BJ:71:LEU:HD23	1.84	0.58
1:CA:90:U:H1'	1:CA:92:A:C8	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:2183:C:H2'	1:CA:2184:G:H8	1.68	0.58
12:CO:120:GLU:OE1	17:CT:67:SER:OG	2.21	0.58
16:CS:10:ARG:O	16:CS:14:VAL:HG13	2.03	0.58
34:DA:839:U:H5''	34:DA:840:C:H5	1.68	0.58
34:DA:1202:G:O4'	47:DN:29:ARG:NH1	2.34	0.58
59:DZ:74:TRP:O	59:DZ:76:ASP:N	2.36	0.58
1:AA:1688:A:H2'	1:AA:1689:G:O4'	2.03	0.58
3:AC:41:THR:HG22	3:AC:42:VAL:N	2.17	0.58
25:A1:3:LYS:HB2	25:A1:61:ARG:NH1	2.18	0.58
34:BA:1125:U:H4'	43:BJ:5:ARG:NH2	2.18	0.58
50:BQ:66:SER:O	50:BQ:70:ARG:NH1	2.36	0.58
56:BW:7:A:H61	56:BW:66:U:H3	1.49	0.58
59:BZ:138:LYS:HG2	64:BZ:702:GDP:C6	2.38	0.58
1:CA:307:G:N1	1:CA:310:A:OP2	2.32	0.58
3:CC:214:TYR:CZ	3:CC:224:ARG:HG2	2.37	0.58
14:CQ:16:ARG:HG2	14:CQ:16:ARG:HH11	1.68	0.58
28:C4:34:GLU:HG2	46:DM:3:ARG:HB3	1.84	0.58
35:DB:71:VAL:HG22	35:DB:164:VAL:HA	1.84	0.58
39:DF:35:ALA:HA	39:DF:67:MET:HB3	1.84	0.58
58:DY:50:U:H3	58:DY:64:A:H61	1.51	0.58
1:AA:1232:G:H5''	19:AV:81:TYR:CE1	2.37	0.58
14:AQ:2:LEU:HD22	65:AQ:3104:HOH:O	2.02	0.58
34:BA:653:A:OP1	41:BH:56:LYS:NZ	2.36	0.58
46:BM:11:ARG:HB2	46:BM:46:LYS:HB3	1.84	0.58
59:BZ:289:ILE:HD11	59:BZ:331:TYR:HB3	1.85	0.58
1:CA:208:C:H2'	1:CA:209:C:C6	2.39	0.58
1:CA:657:U:H2'	1:CA:658:C:C6	2.38	0.58
8:CH:64:LEU:HD23	8:CH:67:LEU:HD23	1.86	0.58
34:DA:1022:G:H2'	34:DA:1023:G:C8	2.38	0.58
37:DD:173:TRP:HB2	37:DD:187:ARG:O	2.02	0.58
39:DF:8:ILE:HD11	39:DF:79:LEU:HD13	1.85	0.58
47:DN:9:LYS:HG3	47:DN:12:ARG:HD3	1.85	0.58
9:AK:74:LEU:O	9:AK:76:GLY:N	2.35	0.58
12:AO:2:ILE:HG13	12:AO:8:LEU:HD11	1.86	0.58
34:BA:1325:C:H2'	34:BA:1326:C:H6	1.69	0.58
51:BR:56:THR:HB	51:BR:58:LEU:HD23	1.85	0.58
1:CA:244:A:C2	1:CA:255:A:C4	2.92	0.58
1:CA:774:A:HO2'	1:CA:775:G:H8	1.50	0.58
1:CA:1427:A:H4'	1:CA:1428:C:O5'	2.02	0.58
48:DO:29:VAL:HG11	48:DO:81:LEU:HD21	1.85	0.58
11:AN:128:HIS:O	11:AN:131:GLN:NE2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BA:347:G:H2'	34:BA:348:G:O4'	2.03	0.58
34:BA:974:A:OP2	47:BN:29:ARG:NH2	2.36	0.58
46:BM:84:ILE:HG13	46:BM:86:CYS:H	1.67	0.58
59:BZ:247:ARG:O	59:BZ:251:ILE:HG13	2.04	0.58
34:DA:1052:U:H5''	34:DA:1053:G:OP2	2.03	0.58
42:DI:9:ARG:HG2	42:DI:14:VAL:HG12	1.84	0.58
42:DI:80:GLY:HA2	42:DI:83:ARG:HB2	1.84	0.58
1:AA:1898:A:H2'	1:AA:1899:A:C8	2.37	0.58
39:BF:44:GLY:O	39:BF:60:PHE:N	2.30	0.58
47:BN:23:ARG:NH1	47:BN:30:ALA:HB2	2.19	0.58
59:BZ:217:VAL:HA	59:BZ:220:ALA:HB3	1.86	0.58
6:CF:126:VAL:HG21	6:CF:129:PHE:CZ	2.39	0.58
34:DA:998:G:N2	34:DA:1043:C:N3	2.47	0.58
34:DA:1220:G:N2	52:DS:54:GLY:O	2.36	0.58
59:DZ:4:ILE:HG22	59:DZ:5:LEU:HD23	1.86	0.58
34:BA:149:A:H2'	34:BA:150:C:C6	2.39	0.58
59:BZ:-36:LEU:HD21	59:BZ:-29:LEU:HD22	1.84	0.58
59:DZ:357:ARG:HD2	59:DZ:366:VAL:HG11	1.85	0.58
59:DZ:404:VAL:H	59:DZ:405:PRO:HD3	1.69	0.58
1:AA:551:A:H5''	1:AA:552:C:OP1	2.03	0.58
34:BA:142:G:H2'	34:BA:143:A:H8	1.68	0.58
38:BE:71:LEU:HD21	38:BE:115:VAL:HG22	1.85	0.58
59:BZ:-58:LEU:HD21	59:BZ:-32:LEU:HD22	1.85	0.58
1:CA:1430:C:H2'	1:CA:1431:U:H6	1.69	0.58
4:CD:26:LYS:NZ	4:CD:30:GLU:HG2	2.19	0.58
24:C0:2:ALA:N	65:C0:202:HOH:O	2.37	0.58
34:DA:64:G:H4'	34:DA:65:U:H3'	1.86	0.58
34:DA:834:C:H2'	34:DA:835:U:C6	2.39	0.58
34:DA:978:A:O2'	34:DA:1322:C:N3	2.33	0.58
34:DA:1001:A:H2'	34:DA:1001(A):G:H8	1.68	0.58
47:DN:27:CYS:SG	47:DN:29:ARG:HB2	2.44	0.58
1:AA:173:C:H2'	1:AA:174:U:C6	2.39	0.58
30:A6:14:THR:HB	30:A6:48:VAL:O	2.04	0.58
34:BA:232:G:H1'	34:BA:262:A:N1	2.19	0.58
1:CA:2349:G:OP1	65:CA:3743:HOH:O	2.17	0.58
1:CA:2815:C:H5'	29:C5:29:THR:HG21	1.85	0.58
34:DA:673:G:H2'	34:DA:674:G:C8	2.38	0.58
1:AA:181:C:OP1	65:AA:3944:HOH:O	2.17	0.58
1:AA:1101:G:O2'	1:AA:1131:A:N1	2.30	0.58
1:AA:1123:A:O2'	10:AL:132:ARG:O	2.21	0.58
21:AX:11:PRO:HB3	21:AX:92:LEU:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:BQ:97:SER:O	50:BQ:97:SER:OG	2.21	0.58
1:CA:2788:C:OP1	5:CE:61:ARG:NH2	2.37	0.58
17:CT:23:ARG:HG3	17:CT:120:ARG:NH1	2.19	0.58
25:C1:18:ILE:HG12	25:C1:37:ILE:HG23	1.86	0.58
1:AA:1891:G:H4'	3:AC:206:LYS:HD2	1.25	0.57
1:AA:2227:G:O2'	1:AA:2228:G:OP1	2.22	0.57
1:AA:2787:C:H2'	1:AA:2788:A:O4'	2.03	0.57
11:AN:42:TRP:CE3	18:AU:63:VAL:HG11	2.39	0.57
34:BA:410:G:OP1	37:BD:30:LYS:NZ	2.24	0.57
59:BZ:13:ARG:NH1	59:BZ:280:LEU:O	2.37	0.57
59:BZ:246:ILE:HG23	59:BZ:255:ILE:HD11	1.85	0.57
1:CA:796:C:H2'	1:CA:797:C:C6	2.39	0.57
34:DA:344:A:H5''	34:DA:345:C:C5	2.35	0.57
34:DA:1321:C:H4'	46:DM:87:TYR:CE2	2.39	0.57
40:DG:72:ARG:N	40:DG:142:GLU:OE2	2.36	0.57
59:DZ:-62:LEU:HD11	59:DZ:-48:VAL:HG22	1.86	0.57
1:AA:1296:G:N7	13:AP:18:ARG:NH2	2.52	0.57
1:AA:2141:A:O2'	1:AA:2142:G:H5'	2.04	0.57
1:AA:2585:C:OP1	65:AA:4112:HOH:O	2.17	0.57
34:BA:1323:G:H2'	34:BA:1324:A:C8	2.39	0.57
49:BP:56:ALA:O	49:BP:60:LEU:HB2	2.04	0.57
51:BR:32:ARG:HA	51:BR:69:THR:HG21	1.86	0.57
1:CA:1364:G:OP2	25:C1:3:LYS:HG3	2.04	0.57
16:CS:41:ASP:OD2	16:CS:44:LYS:HE2	2.04	0.57
34:DA:1126:U:H4'	34:DA:1281:U:H1'	1.85	0.57
35:DB:77:ALA:HA	35:DB:80:ILE:HG22	1.84	0.57
1:AA:610:C:OP2	13:AP:21:ARG:NH2	2.36	0.57
1:AA:1077:G:H21	33:A9:36:GLN:HE22	1.52	0.57
1:AA:2417:G:P	13:AP:77:ARG:HH22	2.26	0.57
28:A4:61:ARG:HH21	52:BS:42:PRO:HD2	1.69	0.57
42:BI:99:LEU:HB3	42:BI:101:PHE:CE1	2.38	0.57
59:BZ:225:GLU:HA	59:BZ:228:MET:HB3	1.86	0.57
1:CA:2179:C:O4'	3:CC:169:THR:HG22	2.03	0.57
1:CA:2749:A:H1'	8:CH:63:SER:HB3	1.86	0.57
8:CH:143:GLN:O	8:CH:146:ALA:N	2.38	0.57
35:DB:80:ILE:HD11	35:DB:212:GLN:HA	1.87	0.57
37:DD:61:LYS:HB2	37:DD:203:VAL:HG22	1.85	0.57
46:DM:16:ASP:OD1	46:DM:16:ASP:N	2.38	0.57
47:DN:48:ALA:HB2	47:DN:53:LEU:HD12	1.86	0.57
59:DZ:114:VAL:HG21	59:DZ:156:ARG:HB2	1.86	0.57
1:AA:1201:A:OP1	18:AU:55:ARG:HD3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:43:LEU:HD11	7:AG:153:ARG:HG2	1.87	0.57
34:BA:131:C:O2'	34:BA:262:A:N3	2.34	0.57
35:BB:185:ILE:HG23	35:BB:199:TYR:HB2	1.85	0.57
42:BI:70:LYS:O	42:BI:74:ILE:HG13	2.04	0.57
1:CA:1021:A:H3'	1:CA:1021:A:H8	1.70	0.57
1:CA:1062:G:O2'	10:CL:133:SER:O	2.17	0.57
1:CA:1648:C:OP1	65:CA:4161:HOH:O	2.17	0.57
9:CK:69:PRO:O	9:CK:71:LEU:N	2.35	0.57
28:C4:62:ARG:O	28:C4:64:GLY:N	2.37	0.57
34:DA:736:C:H2'	34:DA:737:A:C8	2.39	0.57
35:DB:74:LYS:O	35:DB:78:GLN:HB2	2.04	0.57
1:AA:1112:U:N3	1:AA:1114:G:OP2	2.37	0.57
1:AA:2735:G:H2'	1:AA:2736:C:C6	2.39	0.57
25:A1:77:ALA:HB2	25:A1:94:LEU:HD21	1.85	0.57
49:BP:17:TYR:CE2	49:BP:41:PRO:HG3	2.40	0.57
59:BZ:-53:ASP:H	59:BZ:-50:GLN:NE2	2.02	0.57
59:BZ:162:VAL:HG21	59:BZ:255:ILE:HD12	1.85	0.57
1:CA:1338:G:N7	21:CX:62:LYS:NZ	2.49	0.57
1:CA:1568:G:N7	65:CA:4604:HOH:O	2.32	0.57
34:DA:1171:G:H2'	34:DA:1172:C:C6	2.40	0.57
35:DB:16:HIS:HB2	35:DB:204:ASN:HB3	1.86	0.57
56:DW:51:U:H2'	56:DW:52:G:C8	2.40	0.57
59:DZ:294:PRO:HG3	59:DZ:396:ARG:HB2	1.85	0.57
1:AA:561:A:H2'	1:AA:562:C:C6	2.40	0.57
1:AA:2158:C:H42	1:AA:2177:G:H1	1.53	0.57
37:BD:162:LEU:HD13	37:BD:181:MET:HG2	1.87	0.57
59:BZ:-53:ASP:H	59:BZ:-50:GLN:HE21	1.53	0.57
1:CA:955:C:OP1	14:CQ:87:LYS:NZ	2.34	0.57
1:CA:2744:G:N2	8:CH:143:GLN:OE1	2.37	0.57
12:CO:24:VAL:HB	12:CO:33:ALA:HB2	1.87	0.57
34:DA:834:C:H2'	34:DA:835:U:H6	1.69	0.57
34:DA:962:C:O2'	65:DA:1841:HOH:O	2.15	0.57
59:DZ:619:ASP:HB3	59:DZ:662:LYS:HD2	1.86	0.57
1:AA:1067:A:H8	1:AA:1068:G:H5''	1.70	0.57
5:AE:111:ARG:HG3	5:AE:160:TYR:CD2	2.40	0.57
34:BA:167:G:H2'	34:BA:168:G:C8	2.37	0.57
34:BA:395:C:O3'	59:BZ:349:LYS:NZ	2.37	0.57
35:BB:77:ALA:HB2	35:BB:211:ILE:HD13	1.87	0.57
35:BB:111:ARG:HG2	35:BB:111:ARG:NH1	2.17	0.57
37:BD:154:ASN:HA	37:BD:159:ARG:HH21	1.69	0.57
40:BG:18:TYR:CE2	40:BG:59:LEU:HB2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:BJ:8:LEU:HD12	43:BJ:20:ALA:HB2	1.87	0.57
46:BM:3:ARG:HD2	46:BM:9:ILE:HG12	1.86	0.57
1:CA:882:G:N2	1:CA:894:C:O2	2.34	0.57
6:CF:195:ASP:HB3	6:CF:198:ALA:H	1.70	0.57
26:C2:35:LEU:HD22	26:C2:44:LEU:HD11	1.84	0.57
34:DA:646:U:H2'	34:DA:647:C:C6	2.40	0.57
34:DA:1256:A:H61	34:DA:1278:U:H1'	1.70	0.57
59:DZ:16:GLY:HA3	59:DZ:101:LEU:HD22	1.85	0.57
34:BA:1239:A:H4'	34:BA:1240:U:H5''	1.85	0.57
36:BC:40:ARG:O	36:BC:44:GLU:HB2	2.05	0.57
38:BE:152:ARG:HA	41:BH:64:LYS:NZ	2.19	0.57
59:BZ:74:TRP:CD1	59:BZ:273:LEU:HB3	2.39	0.57
1:CA:1108:U:C6	1:CA:1109:C:C5	2.92	0.57
1:CA:1693:U:O2'	4:CD:14:ARG:NH2	2.37	0.57
15:CR:104:ARG:HD2	15:CR:109:ALA:HB3	1.85	0.57
34:DA:188:C:H2'	34:DA:189:G:H8	1.69	0.57
34:DA:316:G:OP2	34:DA:351:G:O2'	2.22	0.57
34:DA:503:C:OP2	45:DL:116:SER:HB3	2.04	0.57
34:DA:1001:A:H2'	34:DA:1001(A):G:C8	2.40	0.57
35:DB:7:VAL:HG12	35:DB:8:LYS:HG2	1.86	0.57
48:DO:56:LEU:O	48:DO:60:VAL:HG23	2.05	0.57
1:AA:469:A:H1'	1:AA:1246:C:O4'	2.04	0.57
5:AE:101:ARG:NH1	5:AE:169:ASN:O	2.34	0.57
33:A9:2:LYS:HE2	33:A9:31:LYS:O	2.04	0.57
35:BB:37:ASN:N	35:BB:37:ASN:OD1	2.38	0.57
1:CA:1899:G:H2'	1:CA:1899:G:N3	2.20	0.57
8:CH:3:ARG:CZ	8:CH:4:ILE:H	2.17	0.57
19:CV:3:ALA:HB3	19:CV:14:VAL:HG23	1.86	0.57
21:CX:41:ASN:O	21:CX:45:THR:HG23	2.05	0.57
30:C6:10:LEU:HD23	30:C6:22:ALA:HB2	1.86	0.57
34:DA:1135:U:H2'	34:DA:1137:C:C2	2.40	0.57
38:DE:139:LEU:C	38:DE:141:GLN:H	2.08	0.57
1:AA:185:A:H62	13:AP:38:GLN:HE22	1.51	0.57
6:AF:184:TYR:O	6:AF:188:ARG:HG3	2.05	0.57
7:AG:38:VAL:HG22	7:AG:93:THR:HG23	1.87	0.57
34:BA:673:G:H2'	34:BA:674:G:C8	2.40	0.57
34:BA:731:G:H5'	34:BA:766:A:H4'	1.87	0.57
1:CA:214:G:O2'	1:CA:216:A:O2'	2.19	0.57
6:CF:184:TYR:CE1	13:CP:3:LEU:HD21	2.39	0.57
34:DA:881:G:OP2	45:DL:12:ARG:NH2	2.38	0.57
34:DA:1353:G:OP1	54:DU:10:ARG:NH1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:DB:184:VAL:HG12	35:DB:197:VAL:HG13	1.87	0.57
46:DM:78:ILE:HD12	46:DM:92:HIS:CE1	2.40	0.57
1:AA:990:A:H2	65:AA:4753:HOH:O	1.87	0.56
1:AA:1827:U:H2'	1:AA:1828:C:C6	2.40	0.56
14:AQ:110:THR:HG23	14:AQ:113:GLN:OE1	2.05	0.56
35:BB:97:TRP:CH2	35:BB:101:MET:HB2	2.40	0.56
59:BZ:75:LYS:H	59:BZ:75:LYS:HZ3	1.51	0.56
59:BZ:247:ARG:HE	59:BZ:251:ILE:HD11	1.70	0.56
8:CH:7:LEU:HD23	8:CH:69:ARG:HH12	1.70	0.56
9:CK:26:LEU:HA	9:CK:84:GLU:HA	1.86	0.56
23:CZ:145:GLU:H	23:CZ:148:ASP:HB2	1.70	0.56
34:DA:1106:G:H5''	36:DC:172:ARG:HG2	1.87	0.56
59:DZ:138:LYS:HG2	64:DZ:702:GDP:C5	2.40	0.56
59:DZ:224:ASP:HB3	59:DZ:227:ILE:HG12	1.87	0.56
1:AA:843:C:H2'	1:AA:844:C:C6	2.40	0.56
1:AA:1067:A:C8	1:AA:1067:A:H3'	2.40	0.56
4:AD:2:ALA:O	4:AD:3:VAL:HB	2.05	0.56
7:AG:61:ALA:O	28:A4:7:PRO:HG2	2.05	0.56
35:BB:55:PHE:HA	35:BB:58:ILE:HG13	1.87	0.56
1:CA:1688:U:O2	1:CA:1700:A:H5'	2.06	0.56
1:CA:1721:G:N1	1:CA:1739:U:OP2	2.38	0.56
13:CP:64:LYS:HA	32:C8:13:ARG:HB3	1.87	0.56
34:DA:527:G:O2'	34:DA:535:A:N1	2.37	0.56
35:DB:16:HIS:CD2	35:DB:204:ASN:HB3	2.40	0.56
46:DM:22:ILE:HG23	46:DM:67:GLU:HG2	1.86	0.56
1:AA:1785:C:OP1	17:AT:96:ARG:NH1	2.35	0.56
3:AC:6:LYS:HG3	3:AC:7:ARG:H	1.69	0.56
37:BD:168:ARG:HB2	37:BD:168:ARG:HH11	1.69	0.56
46:BM:11:ARG:HA	46:BM:45:VAL:HB	1.86	0.56
49:BP:39:TYR:CD2	49:BP:73:LEU:HD11	2.40	0.56
59:BZ:20:HIS:CE1	59:BZ:117:GLN:HG2	2.40	0.56
59:BZ:129:LYS:HA	59:BZ:253:LEU:HD21	1.88	0.56
59:BZ:403:GLU:HG2	59:BZ:404:VAL:HG22	1.86	0.56
1:CA:535:C:O3'	18:CU:53:ARG:NH1	2.38	0.56
1:CA:566:U:H5''	13:CP:29:LYS:HE3	1.86	0.56
1:CA:957:A:H5'	14:CQ:76:LYS:HD2	1.87	0.56
1:CA:1149:G:H2'	1:CA:1150:C:C6	2.41	0.56
1:CA:1794:U:H2'	1:CA:1795:C:H6	1.71	0.56
1:CA:2132:U:C2	3:CC:6:LYS:CD	2.88	0.56
5:CE:111:ARG:HG3	5:CE:160:TYR:CD2	2.40	0.56
6:CF:34:TRP:CE2	13:CP:8:PRO:HG3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:C5:16:ARG:HG2	29:C5:16:ARG:HH11	1.70	0.56
38:DE:9:LYS:HB2	38:DE:112:LEU:HD11	1.87	0.56
59:DZ:150:ILE:O	59:DZ:154:GLN:HG2	2.05	0.56
1:AA:2121:U:H3	1:AA:2212:G:H1	1.54	0.56
34:BA:179:A:H2'	34:BA:180:U:C6	2.41	0.56
34:DA:1147:C:HO2'	42:DI:5:TYR:HH	1.52	0.56
39:DF:7:ASN:HD22	39:DF:7:ASN:N	2.04	0.56
55:DV:20:U:H2'	55:DV:21:C:C6	2.40	0.56
59:DZ:138:LYS:HG2	64:DZ:702:GDP:C6	2.41	0.56
1:AA:1068:G:N2	1:AA:1188:A:C2	2.74	0.56
14:AQ:104:PHE:HE2	14:AQ:125:LEU:HD11	1.70	0.56
22:AY:55:TYR:N	22:AY:55:TYR:CD1	2.74	0.56
34:BA:179:A:H2'	34:BA:180:U:H6	1.70	0.56
37:BD:25:ARG:HA	37:BD:28:SER:HB3	1.88	0.56
43:BJ:37:PRO:HA	43:BJ:72:VAL:HG12	1.86	0.56
59:BZ:125:ALA:HB1	59:BZ:132:ARG:NH1	2.20	0.56
59:BZ:555:LEU:HD11	59:BZ:599:PRO:HG2	1.87	0.56
7:CG:145:THR:HG23	7:CG:147:ASP:H	1.71	0.56
21:CX:26:TYR:O	21:CX:81:VAL:HG22	2.06	0.56
22:CY:90:LEU:HB3	22:CY:92:ASN:HB3	1.87	0.56
34:DA:1348:U:H4'	42:DI:120:ARG:HD3	1.85	0.56
34:DA:1441:G:H5''	34:DA:1442:G:H5'	1.88	0.56
59:DZ:369:LEU:HD21	59:DZ:375:GLY:HA3	1.88	0.56
17:AT:56:GLY:O	17:AT:59:THR:HG23	2.05	0.56
34:BA:1103:C:OP1	35:BB:96:ARG:NH2	2.38	0.56
1:CA:1359:A:N6	1:CA:1372:U:H3	2.04	0.56
1:CA:1518:U:H2'	1:CA:1519:G:O4'	2.06	0.56
25:C1:3:LYS:HB2	25:C1:61:ARG:NH1	2.21	0.56
30:C6:23:THR:OG1	30:C6:24:GLU:N	2.34	0.56
34:DA:748:C:H4'	34:DA:749:C:O5'	2.05	0.56
1:AA:1218:G:O2'	1:AA:1219:A:O5'	2.24	0.56
59:BZ:495:GLY:N	59:BZ:510:VAL:O	2.38	0.56
3:CC:49:GLY:N	3:CC:209:PHE:O	2.39	0.56
16:CS:84:GLN:H	16:CS:111:GLU:HB2	1.71	0.56
19:CV:72:VAL:HG13	19:CV:85:LYS:HB3	1.86	0.56
23:CZ:5:LEU:HD22	23:CZ:6:LYS:H	1.71	0.56
34:DA:1016:A:O2'	34:DA:1217:C:O2'	2.21	0.56
36:DC:57:ILE:HG13	36:DC:66:VAL:HG22	1.88	0.56
1:AA:552:C:C5	1:AA:2792:U:H2'	2.41	0.56
1:AA:1123:A:H4'	10:AL:91:PRO:HB2	1.87	0.56
1:AA:1154:U:O2'	1:AA:1155:C:H5''	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A5:35:GLU:HG3	29:A5:51:TYR:CD2	2.41	0.56
34:BA:159:G:N2	34:BA:161:A:O5'	2.39	0.56
1:CA:1412:A:H2'	1:CA:1413:G:C8	2.40	0.56
1:CA:1782:C:H1'	1:CA:2609:U:H5''	1.86	0.56
1:CA:1803:A:O2'	4:CD:259:THR:HG21	2.06	0.56
3:CC:42:VAL:O	3:CC:216:THR:O	2.24	0.56
4:CD:121:PRO:HB3	4:CD:135:PHE:CE2	2.41	0.56
5:CE:111:ARG:HA	15:CR:1:MET:HE3	1.88	0.56
45:DL:71:PRO:O	45:DL:102:ARG:HD3	2.05	0.56
46:DM:40:ASN:HD22	46:DM:41:PRO:HD2	1.71	0.56
59:DZ:630:GLN:HG2	59:DZ:646:PHE:HB2	1.86	0.56
1:AA:482:C:H4'	65:AA:5243:HOH:O	2.04	0.56
1:AA:1825:U:H2'	1:AA:1826:C:C6	2.41	0.56
18:AU:81:HIS:CE1	18:AU:85:LYS:HD2	2.41	0.56
51:BR:56:THR:HB	51:BR:58:LEU:CD2	2.36	0.56
1:CA:1668:A:OP1	12:CO:5:GLN:HG2	2.04	0.56
1:CA:2074:U:H2'	1:CA:2075:U:C6	2.41	0.56
10:CL:89:HIS:O	10:CL:91:PRO:HD3	2.06	0.56
10:CL:134:MET:HG3	10:CL:136:VAL:HG12	1.87	0.56
13:CP:63:PRO:HG2	32:C8:25:MET:HB2	1.86	0.56
18:CU:28:ARG:NH1	18:CU:38:THR:OG1	2.38	0.56
36:DC:12:LEU:HD23	36:DC:16:ARG:HB3	1.86	0.56
44:DK:79:SER:HB2	44:DK:106:LYS:HE3	1.87	0.56
59:DZ:614:GLU:HA	59:DZ:617:MET:HG3	1.86	0.56
1:AA:670:C:H5''	1:AA:671:A:OP2	2.06	0.56
3:AC:49:GLY:N	3:AC:209:PHE:O	2.39	0.56
7:AG:77:ILE:HG22	7:AG:80:PHE:H	1.71	0.56
15:AR:57:ARG:HB3	15:AR:59:ASP:OD1	2.06	0.56
35:BB:21:ARG:HB3	35:BB:39:ILE:HG12	1.88	0.56
35:BB:201:ILE:O	35:BB:203:GLY:N	2.39	0.56
48:BO:16:ALA:HB1	48:BO:21:ASP:HB3	1.87	0.56
59:BZ:-38:TYR:HD2	59:BZ:-37:LEU:HD23	1.71	0.56
1:CA:897:C:H1'	56:DW:56:C:H41	1.71	0.56
30:C6:6:ARG:NH2	65:C6:4001:HOH:O	2.30	0.56
34:DA:1118:C:H2'	34:DA:1119:C:C6	2.41	0.56
34:DA:1326:C:H2'	34:DA:1327:C:C6	2.41	0.56
1:AA:555:G:N3	1:AA:555:G:O4'	2.34	0.55
1:AA:1116:A:H5'	1:AA:1118:C:OP2	2.06	0.55
25:A1:51:VAL:HG11	25:A1:74:VAL:HG21	1.87	0.55
34:BA:1356:G:H2'	34:BA:1357:A:C8	2.40	0.55
44:BK:99:GLN:HG2	44:BK:105:VAL:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:922:U:H2'	1:CA:923:C:C6	2.40	0.55
1:CA:1794:U:H2'	1:CA:1795:C:C6	2.41	0.55
3:CC:6:LYS:HG3	3:CC:7:ARG:H	1.69	0.55
16:CS:39:ILE:HB	16:CS:49:VAL:HG12	1.88	0.55
34:DA:1095:U:OP1	34:DA:1108:G:N2	2.29	0.55
48:DO:54:ARG:O	48:DO:58:MET:HG3	2.06	0.55
1:AA:1423:G:H2'	65:AA:5230:HOH:O	2.06	0.55
6:AF:120:GLU:HB2	6:AF:122:LYS:HG3	1.88	0.55
6:AF:132:VAL:HG22	6:AF:163:VAL:HG22	1.88	0.55
10:AL:105:LEU:HD23	10:AL:120:LEU:HD22	1.87	0.55
34:BA:262:A:H2'	34:BA:263:A:C8	2.41	0.55
34:BA:662:G:H2'	34:BA:663:A:C8	2.41	0.55
41:BH:116:LYS:HD3	41:BH:127:LEU:HD23	1.88	0.55
6:CF:197:ASP:OD1	6:CF:198:ALA:N	2.39	0.55
18:CU:91:ASP:O	18:CU:95:LEU:HD13	2.05	0.55
24:C0:53:MET:HG3	24:C0:59:LEU:HD23	1.87	0.55
1:AA:1539:C:H5''	1:AA:1539:C:O2	2.06	0.55
17:AT:16:ARG:NH1	17:AT:18:ASP:OD1	2.39	0.55
17:AT:39:ARG:NH2	34:BA:345:C:OP1	2.39	0.55
34:BA:537:G:H5''	45:BL:113:ARG:NH1	2.21	0.55
36:BC:113:ALA:HB2	36:BC:202:ILE:HG13	1.89	0.55
59:BZ:126:GLU:OE2	59:BZ:132:ARG:NH2	2.40	0.55
1:CA:492:A:H2'	1:CA:493:G:O4'	2.06	0.55
1:CA:639:U:H2'	1:CA:640:C:C6	2.40	0.55
1:CA:1689:A:N6	1:CA:1698:A:H2	1.88	0.55
8:CH:46:GLU:HB2	8:CH:49:VAL:HG12	1.88	0.55
10:CL:75:SER:OG	10:CL:134:MET:SD	2.65	0.55
34:DA:742:G:OP2	48:DO:35:ARG:NH2	2.39	0.55
35:DB:16:HIS:CD2	35:DB:17:PHE:H	2.24	0.55
35:DB:91:PRO:HD3	35:DB:154:LEU:HD12	1.88	0.55
44:DK:15:ALA:HB1	44:DK:78:GLN:HG3	1.87	0.55
1:AA:2874:G:OP1	17:AT:119:LYS:HE3	2.06	0.55
35:BB:69:LEU:HD13	35:BB:91:PRO:HB2	1.88	0.55
44:BK:84:VAL:HG21	44:BK:95:ILE:HD11	1.87	0.55
46:BM:3:ARG:HG2	46:BM:8:GLU:HA	1.87	0.55
50:BQ:6:LEU:HG	50:BQ:23:VAL:HG11	1.87	0.55
1:CA:1709:U:H2'	1:CA:1710:C:C6	2.41	0.55
1:CA:2653:U:O2'	8:CH:110:SER:HB3	2.07	0.55
17:CT:2:ASN:O	17:CT:6:LEU:HD22	2.06	0.55
22:CY:23:ARG:HG2	22:CY:42:VAL:HG22	1.88	0.55
28:C4:16:CYS:HA	28:C4:33:VAL:HB	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:DL:24:VAL:CG1	45:DL:27:LEU:HD22	2.33	0.55
50:DQ:66:SER:OG	50:DQ:67:LYS:N	2.38	0.55
54:DU:9:ARG:O	54:DU:13:ILE:HG13	2.07	0.55
1:AA:2504:U:H2'	1:AA:2505:U:H6	1.71	0.55
23:AZ:111:VAL:HG23	23:AZ:117:LEU:HD13	1.88	0.55
24:A0:43:THR:O	24:A0:43:THR:HG23	2.07	0.55
36:BC:153:VAL:HG22	36:BC:198:VAL:HG22	1.88	0.55
41:BH:73:ASP:OD1	41:BH:75:ARG:HD3	2.06	0.55
1:CA:954:G:H5''	14:CQ:13:GLN:HB3	1.88	0.55
34:DA:957:U:H2'	34:DA:959:A:OP2	2.07	0.55
34:DA:1273:G:H3'	34:DA:1274:G:H8	1.71	0.55
35:DB:55:PHE:CD1	35:DB:58:ILE:HD12	2.42	0.55
1:AA:943:C:O4'	56:BW:56:C:H5	1.89	0.55
1:AA:2146:G:C5'	3:AC:175:PRO:HG3	2.35	0.55
3:AC:42:VAL:O	3:AC:216:THR:O	2.24	0.55
3:AC:52:PRO:HB2	3:AC:168:LYS:O	2.07	0.55
5:AE:7:VAL:HG12	5:AE:51:PHE:HE2	1.72	0.55
11:AN:58:ASP:OD1	11:AN:58:ASP:N	2.33	0.55
35:BB:82:ARG:HG3	35:BB:92:TYR:CZ	2.41	0.55
37:BD:43:HIS:O	37:BD:46:LYS:HB2	2.07	0.55
38:BE:75:THR:OG1	38:BE:76:ILE:N	2.40	0.55
59:BZ:114:VAL:HB	59:BZ:156:ARG:HH12	1.71	0.55
1:CA:1412:A:H2'	1:CA:1413:G:H8	1.72	0.55
1:CA:2572:A:C8	5:CE:144:ARG:HD2	2.42	0.55
3:CC:52:PRO:HB2	3:CC:168:LYS:O	2.07	0.55
6:CF:53:THR:HG23	6:CF:55:GLY:H	1.70	0.55
34:DA:1003:G:H2'	34:DA:1004:A:O4'	2.06	0.55
59:DZ:22:ASP:HA	64:DZ:702:GDP:H5'	1.89	0.55
1:AA:1825:U:H2'	1:AA:1826:C:H6	1.71	0.55
12:AO:35:VAL:HG11	12:AO:103:ALA:HB3	1.89	0.55
38:BE:40:ARG:NH2	38:BE:68:GLU:HA	2.22	0.55
46:BM:122:LYS:HD3	46:BM:123:ALA:H	1.72	0.55
49:BP:43:LYS:HA	49:BP:48:TRP:HB3	1.89	0.55
1:CA:1155:A:OP1	18:CU:55:ARG:HD2	2.05	0.55
1:CA:1359:A:H61	1:CA:1372:U:H3	1.54	0.55
16:CS:48:LEU:HD23	16:CS:82:ILE:HD11	1.89	0.55
34:DA:255:G:H2'	34:DA:256:U:C6	2.41	0.55
34:DA:1218:C:H2'	34:DA:1219:U:C6	2.41	0.55
36:DC:129:ALA:HB3	36:DC:132:ARG:HB3	1.89	0.55
40:DG:115:ARG:HG2	40:DG:118:VAL:HG23	1.87	0.55
1:AA:2346:G:H4'	1:AA:2347:A:OP2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:2699:U:H2'	1:AA:2700:U:O4'	2.07	0.55
36:BC:82:GLU:HA	36:BC:85:ARG:HH21	1.71	0.55
37:BD:8:VAL:HG23	37:BD:11:LEU:HD22	1.88	0.55
58:BY:6:G:O6	58:BY:7:A:N6	2.40	0.55
1:CA:2345:G:N3	1:CA:2381:C:H2'	2.21	0.55
5:CE:120:TRP:CE3	5:CE:155:LYS:HD3	2.41	0.55
35:DB:189:ASP:O	35:DB:192:SER:OG	2.24	0.55
42:DI:28:VAL:HA	42:DI:63:ILE:O	2.07	0.55
53:DT:54:LYS:HA	53:DT:57:ARG:NH2	2.22	0.55
59:DZ:303:PRO:O	59:DZ:305:PRO:HD3	2.07	0.55
1:AA:2221:A:H5''	1:AA:2222:C:OP2	2.07	0.55
36:BC:148:GLY:HA3	36:BC:172:ARG:O	2.07	0.55
38:BE:12:LEU:HD11	38:BE:14:ARG:HD3	1.89	0.55
59:BZ:99:ARG:HG3	59:BZ:128:TYR:HE1	1.71	0.55
59:BZ:608:VAL:HG22	59:BZ:671:MET:HG3	1.89	0.55
1:CA:1336:A:OP2	21:CX:64:LYS:HE3	2.07	0.55
1:CA:2292:C:OP1	16:CS:17:ARG:NH2	2.29	0.55
7:CG:15:VAL:HG21	7:CG:176:LEU:HD23	1.88	0.55
15:CR:38:VAL:HB	15:CR:39:PRO:HD3	1.89	0.55
34:DA:1000:U:H2'	34:DA:1001:A:C8	2.42	0.55
1:AA:354:A:H2	1:AA:1255:A:H2'	1.72	0.55
1:AA:1473:A:H4'	1:AA:1474:C:O5'	2.07	0.55
1:AA:2442:A:H2'	1:AA:2442:A:N3	2.22	0.55
18:AU:76:TYR:CZ	18:AU:80:ILE:HG13	2.41	0.55
34:BA:942:G:H21	42:BI:124:GLN:NE2	2.04	0.55
35:BB:134:GLU:O	35:BB:138:LEU:HG	2.07	0.55
39:BF:19:LEU:HD11	39:BF:59:TYR:CE2	2.42	0.55
40:BG:16:LEU:HD22	40:BG:16:LEU:H	1.71	0.55
46:BM:11:ARG:HG3	46:BM:12:ASN:ND2	2.22	0.55
48:BO:24:SER:OG	48:BO:25:THR:N	2.40	0.55
59:BZ:-38:TYR:O	59:BZ:-35:PRO:HD2	2.07	0.55
59:BZ:363:ARG:HH11	59:BZ:363:ARG:CG	2.17	0.55
34:DA:235:C:H2'	34:DA:236:G:H8	1.72	0.55
34:DA:707:C:H4'	44:DK:20:TYR:CD2	2.42	0.55
34:DA:1239:A:H62	34:DA:1299:A:N6	2.05	0.55
57:DX:75:C:H5''	57:DX:76:31H:OP1	2.07	0.55
1:AA:543:G:H2'	1:AA:544:U:C6	2.42	0.54
1:AA:1109:G:H1	1:AA:1121:C:H42	1.55	0.54
3:AC:54:ARG:CZ	3:AC:56:ASP:HB3	2.38	0.54
5:AE:116:VAL:HG13	5:AE:122:PHE:HB2	1.89	0.54
18:AU:83:LEU:HD13	18:AU:113:ALA:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:A4:61:ARG:HG3	28:A4:62:ARG:N	2.21	0.54
32:A8:42:ARG:HD2	65:A8:6306:HOH:O	2.06	0.54
34:BA:406:G:H5'	37:BD:5:ILE:HD11	1.87	0.54
59:BZ:639:ASN:HA	59:BZ:640:ALA:O	2.07	0.54
1:CA:271(H):G:HO2'	1:CA:271(I):G:H8	1.53	0.54
1:CA:800:A:H8	1:CA:800:A:OP1	1.90	0.54
3:CC:194:ILE:HD11	3:CC:227:PRO:HB3	1.89	0.54
8:CH:3:ARG:NH2	8:CH:4:ILE:H	2.05	0.54
34:DA:174:C:H2'	34:DA:175:C:H6	1.72	0.54
34:DA:1240:U:OP2	40:DG:116:ALA:N	2.39	0.54
42:DI:128:ARG:NH1	57:DX:35:A:OP2	2.40	0.54
50:DQ:4:LYS:HE2	50:DQ:6:LEU:HD11	1.88	0.54
1:AA:1261:G:P	18:AU:12:ARG:HH21	2.29	0.54
7:AG:77:ILE:HD12	7:AG:82:LEU:HD12	1.88	0.54
9:AK:118:THR:N	9:AK:121:ASP:O	2.38	0.54
13:AP:95:VAL:HG22	13:AP:125:VAL:HG12	1.88	0.54
34:BA:189(K):U:H2'	34:BA:189(L):G:C8	2.42	0.54
34:BA:1123:A:O2'	43:BJ:37:PRO:O	2.22	0.54
51:BR:40:LEU:O	51:BR:42:ARG:N	2.40	0.54
1:CA:1106:G:C6	1:CA:1107:G:C5	2.95	0.54
22:CY:30:VAL:HG22	22:CY:37:VAL:HG12	1.89	0.54
34:DA:1316:G:H22	34:DA:1319:A:H5''	1.72	0.54
35:DB:210:SER:OG	35:DB:211:ILE:HG13	2.07	0.54
38:DE:84:PHE:HB3	38:DE:134:ALA:HB2	1.89	0.54
1:AA:469:A:C5	6:AF:45:ARG:HD2	2.43	0.54
1:AA:776:G:C6	4:AD:208:LYS:HB2	2.43	0.54
1:AA:2764:G:H4'	8:AH:4:ILE:HD11	1.88	0.54
34:BA:1435:G:H2'	34:BA:1436:U:C6	2.42	0.54
39:BF:10:LEU:HB2	39:BF:59:TYR:HB3	1.90	0.54
49:BP:3:LYS:N	49:BP:22:THR:O	2.41	0.54
59:BZ:348:ARG:HG2	59:BZ:348:ARG:HH11	1.72	0.54
23:CZ:92:SER:O	23:CZ:130:PRO:HG2	2.07	0.54
34:DA:985:C:H2'	34:DA:986:A:C8	2.43	0.54
34:DA:1053:G:O5'	34:DA:1054:C:H5'	2.07	0.54
34:DA:1104:G:H4'	35:DB:111:ARG:NH1	2.22	0.54
59:DZ:496:LYS:HE2	59:DZ:509:HIS:CE1	2.42	0.54
1:AA:2653:G:H5''	1:AA:2653:G:H8	1.71	0.54
3:AC:52:PRO:HG2	3:AC:53:ARG:H	1.73	0.54
7:AG:109:VAL:C	7:AG:112:PRO:HD2	2.28	0.54
11:AN:121:LYS:HB3	11:AN:123:TYR:HE2	1.72	0.54
28:A4:33:VAL:HG12	28:A4:35:VAL:H	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BA:555:C:H2'	34:BA:556:C:H6	1.73	0.54
37:BD:41:GLY:O	37:BD:43:HIS:N	2.41	0.54
44:BK:48:ILE:O	44:BK:48:ILE:HG12	2.05	0.54
50:BQ:41:LYS:NZ	50:BQ:92:ARG:HH21	2.05	0.54
1:CA:1149:G:H2'	1:CA:1150:C:H6	1.71	0.54
16:CS:15:ARG:HB3	16:CS:19:LYS:NZ	2.22	0.54
32:C8:9:GLY:O	32:C8:13:ARG:HG2	2.08	0.54
34:DA:1316:G:H4'	47:DN:18:VAL:HG13	1.90	0.54
59:DZ:116:PRO:HA	59:DZ:119:GLU:HG3	1.89	0.54
1:AA:559:U:H2'	1:AA:560:C:C6	2.43	0.54
3:AC:194:ILE:HD11	3:AC:227:PRO:HB3	1.89	0.54
16:AS:10:ARG:O	16:AS:14:VAL:HG13	2.07	0.54
34:BA:1505:G:O2'	55:BV:13:A:O2'	2.26	0.54
43:BJ:11:PHE:HE1	43:BJ:67:THR:HG22	1.73	0.54
1:CA:2882:A:OP1	15:CR:96:ARG:NE	2.30	0.54
4:CD:121:PRO:HB3	4:CD:135:PHE:CD2	2.42	0.54
7:CG:145:THR:HG22	7:CG:148:MET:HG2	1.89	0.54
12:CO:64:ARG:HB2	12:CO:83:ALA:HB3	1.90	0.54
27:C3:46:ASN:O	27:C3:50:VAL:HG22	2.08	0.54
34:DA:1133:G:H2'	34:DA:1134:G:C8	2.42	0.54
34:DA:1387:G:H2'	34:DA:1388:C:C6	2.42	0.54
45:DL:83:VAL:HG21	45:DL:100:ILE:HD13	1.90	0.54
59:DZ:603:GLU:OE2	59:DZ:628:ARG:NH2	2.28	0.54
1:AA:2576:A:C2	1:AA:2659:U:H4'	2.43	0.54
34:BA:1191:A:H5''	36:BC:4:LYS:NZ	2.22	0.54
35:BB:16:HIS:CG	35:BB:17:PHE:N	2.76	0.54
46:BM:9:ILE:HB	46:BM:18:ALA:HB1	1.88	0.54
3:CC:44:VAL:HG23	3:CC:176:VAL:HG21	1.89	0.54
14:CQ:21:THR:HG21	14:CQ:101:ARG:HD3	1.90	0.54
34:DA:858:G:O6	34:DA:869:G:H3'	2.07	0.54
38:DE:12:LEU:HD12	38:DE:128:PRO:HB2	1.90	0.54
49:DP:28:ARG:HG3	49:DP:29:ASP:OD1	2.07	0.54
52:DS:12:ASP:OD1	52:DS:37:ARG:NH1	2.40	0.54
1:AA:714:U:O2	32:A8:2:PRO:HD2	2.07	0.54
34:BA:1239:A:H62	34:BA:1299:A:N6	2.06	0.54
59:BZ:227:ILE:HD13	59:BZ:242:LEU:HD23	1.89	0.54
4:CD:206:LEU:HD22	4:CD:211:ARG:HG2	1.88	0.54
16:CS:31:SER:OG	16:CS:32:LEU:N	2.41	0.54
34:DA:353:A:H5'	34:DA:353:A:C8	2.42	0.54
59:DZ:404:VAL:H	59:DZ:405:PRO:CD	2.21	0.54
1:AA:486:A:H2'	1:AA:487:C:O4'	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AY:92:ASN:N	22:AY:93:GLY:HA2	2.23	0.54
34:BA:134:A:H61	49:BP:25:ARG:NH1	2.06	0.54
34:BA:957:U:O2'	34:BA:959:A:N7	2.30	0.54
41:BH:120:THR:H	41:BH:123:GLU:HB3	1.72	0.54
50:BQ:77:VAL:HG12	50:BQ:78:GLU:HB2	1.89	0.54
59:BZ:-25:SER:O	59:BZ:-22:LYS:HB2	2.07	0.54
59:BZ:239:GLU:O	59:BZ:243:VAL:HG23	2.07	0.54
1:CA:584:C:OP2	18:CU:6:THR:OG1	2.23	0.54
1:CA:774:A:H2'	1:CA:774:A:N3	2.22	0.54
3:CC:6:LYS:HA	3:CC:9:ARG:HH11	1.72	0.54
17:CT:108:ARG:NH2	34:DA:1465:C:OP2	2.41	0.54
34:DA:255:G:H2'	34:DA:256:U:H6	1.73	0.54
34:DA:1321:C:H4'	46:DM:87:TYR:HE2	1.72	0.54
46:DM:25:ILE:HG13	46:DM:29:ARG:HG2	1.90	0.54
59:DZ:264:LEU:HB2	64:DZ:702:GDP:C5	2.42	0.54
59:DZ:346:LYS:NZ	59:DZ:384:ILE:HG23	2.22	0.54
1:AA:715:G:H5'	1:AA:716:G:OP2	2.07	0.54
1:AA:2023:A:H2'	1:AA:2024:G:C8	2.43	0.54
34:BA:49:U:O4	34:BA:365:U:H5	1.90	0.54
39:BF:86:ARG:O	39:BF:87:ARG:HG2	2.07	0.54
1:CA:1063:G:H2'	1:CA:1064:C:H6	1.72	0.54
1:CA:2132:U:C2	3:CC:6:LYS:HD2	2.42	0.54
10:CL:112:MET:H	10:CL:113:PRO:HD2	1.73	0.54
14:CQ:76:LYS:HB3	14:CQ:91:GLU:HG3	1.89	0.54
23:CZ:132:ASN:HD21	23:CZ:160:GLY:H	1.54	0.54
47:DN:23:ARG:NH1	47:DN:30:ALA:HB2	2.22	0.54
59:DZ:38:ARG:HH12	59:DZ:270:GLN:NE2	2.05	0.54
59:DZ:276:VAL:HG13	59:DZ:280:LEU:HD12	1.90	0.54
1:AA:664:U:H2'	1:AA:665:C:C6	2.43	0.54
1:AA:1452:U:H2'	1:AA:1453:C:C6	2.42	0.54
1:AA:1846:A:H8	1:AA:1846:A:OP1	1.91	0.54
1:AA:2349:G:OP1	65:AA:4051:HOH:O	2.18	0.54
34:BA:1238:A:OP2	65:BA:2031:HOH:O	2.19	0.54
59:BZ:85:PRO:HD2	59:BZ:94:VAL:HG13	1.89	0.54
59:BZ:114:VAL:CB	59:BZ:156:ARG:HH12	2.21	0.54
1:CA:956:G:OP2	14:CQ:14:ARG:NH2	2.35	0.54
1:CA:1165:U:H2'	1:CA:1166:C:C6	2.43	0.54
41:DH:39:LEU:HD12	41:DH:44:PHE:HB2	1.90	0.54
51:DR:53:ARG:HD2	51:DR:59:SER:O	2.07	0.54
59:DZ:5:LEU:HD13	59:DZ:305:PRO:HG2	1.90	0.54
1:AA:354:A:HO2'	1:AA:355:A:H8	1.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:553:A:H2'	1:AA:554:A:H5'	1.90	0.53
1:AA:1102:G:H5''	1:AA:1103:A:O4'	2.08	0.53
1:AA:2658:C:H2'	1:AA:2659:U:O4'	2.08	0.53
3:AC:30:VAL:HG23	3:AC:31:LYS:HG2	1.89	0.53
34:BA:159:G:H2'	34:BA:161:A:OP2	2.07	0.53
41:BH:121:ASP:OD2	41:BH:121:ASP:N	2.37	0.53
1:CA:1495:A:OP2	65:CA:3810:HOH:O	2.19	0.53
3:CC:48:LEU:CB	3:CC:50:ILE:HD12	2.38	0.53
7:CG:13:GLU:O	7:CG:15:VAL:N	2.40	0.53
30:C6:9:LEU:HA	30:C6:54:ILE:HB	1.89	0.53
59:DZ:96:ARG:NH1	59:DZ:96:ARG:HB2	2.23	0.53
59:DZ:129:LYS:HZ1	59:DZ:517:LEU:HG	1.74	0.53
8:AH:3:ARG:HG2	8:AH:6:ARG:HD2	1.90	0.53
22:AY:92:ASN:H	22:AY:92:ASN:ND2	2.02	0.53
34:BA:1014:A:H4'	52:BS:14:HIS:NE2	2.24	0.53
34:BA:1349:A:OP2	42:BI:118:LYS:HE3	2.08	0.53
34:BA:1355:G:H2'	34:BA:1356:G:C8	2.43	0.53
43:BJ:49:VAL:CG2	47:BN:41:ARG:HB2	2.38	0.53
52:BS:11:VAL:HG11	52:BS:16:LEU:HB2	1.90	0.53
59:BZ:165:GLN:NE2	59:BZ:259:PHE:HB3	2.22	0.53
1:CA:127:A:H5''	1:CA:128:C:C6	2.44	0.53
1:CA:856:C:H2'	1:CA:857:C:C6	2.43	0.53
1:CA:880:G:N2	1:CA:898:C:H1'	2.20	0.53
1:CA:910:A:H62	14:CQ:12:GLN:HA	1.72	0.53
22:CY:49:VAL:HG11	22:CY:55:TYR:CD2	2.44	0.53
34:DA:688:G:H2'	34:DA:689:C:H6	1.73	0.53
34:DA:1402:C:H2'	34:DA:1403:C:O4'	2.08	0.53
46:DM:5:ALA:HB3	46:DM:22:ILE:HD12	1.90	0.53
59:DZ:639:ASN:N	59:DZ:640:ALA:HB3	2.23	0.53
1:AA:2289:G:P	24:A0:10:THR:HG21	2.49	0.53
5:AE:143:ASN:HD22	5:AE:147:PRO:HD3	1.73	0.53
6:AF:24:LEU:HB3	6:AF:115:ALA:HB2	1.90	0.53
42:BI:43:ALA:C	42:BI:45:ALA:H	2.12	0.53
52:BS:3:ARG:NH1	52:BS:8:GLY:O	2.42	0.53
59:BZ:181:LEU:HD12	59:BZ:216:LEU:HD21	1.90	0.53
1:CA:184:C:H2'	1:CA:185:U:C6	2.43	0.53
1:CA:247:G:H4'	1:CA:386:G:C5	2.43	0.53
1:CA:997:G:OP1	18:CU:92:ARG:HG2	2.09	0.53
1:CA:2207:G:H3'	1:CA:2208:A:H5''	1.90	0.53
1:CA:2305:A:H5''	7:CG:134:GLY:HA3	1.90	0.53
3:CC:30:VAL:HG23	3:CC:31:LYS:HG2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:DG:111:ARG:NH2	40:DG:126:ASP:OD2	2.41	0.53
42:DI:8:GLY:O	42:DI:15:ALA:N	2.27	0.53
46:DM:20:THR:HA	46:DM:25:ILE:HG22	1.89	0.53
59:DZ:165:GLN:HE21	59:DZ:260:LEU:N	2.04	0.53
3:AC:6:LYS:HA	3:AC:9:ARG:HH11	1.72	0.53
3:AC:171:ALA:HB1	3:AC:173:HIS:CE1	2.44	0.53
12:AO:104:ARG:HH12	17:AT:43:GLN:HE22	1.57	0.53
24:A0:27:GLU:HG3	24:A0:68:GLU:HA	1.89	0.53
34:BA:354:G:H2'	34:BA:355:C:H5'	1.90	0.53
34:BA:1030(D):A:N6	34:BA:1031:G:H21	2.07	0.53
34:BA:1367:C:H4'	43:BJ:48:THR:HG21	1.89	0.53
59:BZ:138:LYS:HE2	64:BZ:702:GDP:C4	2.44	0.53
1:CA:2277:G:H5''	14:CQ:87:LYS:HB3	1.90	0.53
4:CD:129:ASN:O	4:CD:193:VAL:HG13	2.08	0.53
14:CQ:26:TYR:CD1	14:CQ:28:ALA:HB2	2.44	0.53
21:CX:29:TRP:CZ3	21:CX:78:LYS:HB3	2.44	0.53
36:DC:63:ASN:HB2	36:DC:98:ASN:HB2	1.91	0.53
57:DX:50:U:H3	57:DX:64:G:H1	1.56	0.53
1:AA:704:U:H2'	1:AA:705:C:C6	2.44	0.53
1:AA:2053:A:C6	1:AA:2510:C:H1'	2.43	0.53
1:AA:2296:C:OP1	30:A6:3:SER:OG	2.15	0.53
34:BA:381:C:H2'	34:BA:382:A:O4'	2.09	0.53
34:BA:404:U:H5'	37:BD:122:ARG:HD3	1.89	0.53
34:BA:507:C:OP2	34:BA:508:C:O2'	2.20	0.53
41:BH:87:SER:HA	41:BH:93:VAL:HG23	1.90	0.53
53:BT:26:ASN:ND2	53:BT:71:THR:OG1	2.41	0.53
59:BZ:213:HIS:O	59:BZ:217:VAL:HG23	2.09	0.53
1:CA:2166:G:H3'	1:CA:2167:U:C5'	2.38	0.53
35:DB:119:GLU:OE2	35:DB:153:ARG:NH1	2.32	0.53
36:DC:137:ALA:HA	36:DC:140:ARG:HH11	1.72	0.53
42:DI:26:VAL:HG13	42:DI:61:ALA:HB3	1.88	0.53
1:AA:2389:A:H2'	1:AA:2390:A:C8	2.43	0.53
1:AA:2798:C:OP1	5:AE:41:LYS:NZ	2.35	0.53
65:AA:5297:HOH:O	25:A1:20:ARG:HD3	2.07	0.53
3:AC:64:SER:HA	3:AC:161:ARG:H	1.74	0.53
4:AD:68:LYS:HD2	4:AD:70:TRP:CZ2	2.44	0.53
34:BA:1024:G:H2'	34:BA:1025:U:H5''	1.90	0.53
51:BR:37:VAL:O	51:BR:41:LYS:HG2	2.09	0.53
52:BS:22:LEU:HB3	52:BS:27:GLU:HG3	1.91	0.53
52:BS:27:GLU:HB3	52:BS:28:LYS:HB3	1.91	0.53
3:CC:42:VAL:HG13	3:CC:43:GLU:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:CE:47:VAL:HG11	5:CE:86:PRO:HD2	1.89	0.53
7:CG:49:ASP:OD1	7:CG:49:ASP:N	2.41	0.53
8:CH:154:PRO:HB3	8:CH:163:TYR:CE2	2.44	0.53
34:DA:1286:A:C8	34:DA:1287:A:H4'	2.44	0.53
35:DB:28:PHE:CD1	35:DB:190:THR:HG22	2.44	0.53
59:DZ:284:LEU:HD22	59:DZ:284:LEU:H	1.74	0.53
1:AA:1381:U:H2'	1:AA:1382:A:O4'	2.09	0.53
1:AA:2287:C:C2	14:AQ:85:LYS:HE2	2.44	0.53
35:BB:97:TRP:CZ2	35:BB:102:LEU:HD13	2.43	0.53
42:BI:9:ARG:HD3	42:BI:14:VAL:HG22	1.91	0.53
1:CA:668:G:H5'	1:CA:669:G:OP2	2.09	0.53
1:CA:1359:A:C2	1:CA:1372:U:O4	2.61	0.53
3:CC:54:ARG:CZ	3:CC:56:ASP:HB3	2.37	0.53
16:CS:14:VAL:O	16:CS:18:ILE:HG12	2.08	0.53
16:CS:67:ARG:HH11	16:CS:67:ARG:HB2	1.73	0.53
34:DA:45:U:H2'	34:DA:46:G:C8	2.44	0.53
34:DA:857:C:H2'	34:DA:858:G:O4'	2.09	0.53
35:DB:164:VAL:HB	35:DB:186:ALA:HB2	1.90	0.53
1:AA:1157:A:H8	1:AA:1158:G:H1'	1.73	0.53
1:AA:2146:G:H5'	3:AC:175:PRO:HG3	1.90	0.53
3:AC:44:VAL:HG23	3:AC:176:VAL:HG21	1.89	0.53
6:AF:162:LEU:HA	6:AF:165:ARG:HD3	1.91	0.53
10:AL:88:ALA:HB3	10:AL:135:GLY:HA3	1.90	0.53
32:A8:61:LEU:O	32:A8:63:PRO:HD3	2.09	0.53
34:BA:250:A:H4'	34:BA:251:G:O5'	2.08	0.53
34:BA:677:U:H3	34:BA:713:G:H22	1.55	0.53
34:BA:790:A:OP1	57:BX:38:A:O2'	2.25	0.53
49:BP:17:TYR:HE2	49:BP:41:PRO:HG3	1.72	0.53
59:BZ:138:LYS:HG2	64:BZ:702:GDP:C5	2.43	0.53
1:CA:489:G:N7	20:CW:49:LYS:NZ	2.57	0.53
1:CA:637:A:H8	13:CP:117:GLU:HG3	1.73	0.53
1:CA:1065:U:O2	1:CA:1074:G:N2	2.42	0.53
6:CF:192:LEU:HD13	6:CF:194:MET:HE2	1.89	0.53
34:DA:1388:C:H2'	34:DA:1389:C:C6	2.44	0.53
35:DB:72:GLY:O	35:DB:94:ASN:HA	2.09	0.53
59:DZ:435:ASP:OD2	59:DZ:437:THR:OG1	2.26	0.53
1:AA:602:G:H2'	1:AA:603:C:C6	2.44	0.53
3:AC:42:VAL:HG13	3:AC:43:GLU:H	1.73	0.53
44:BK:44:SER:OG	44:BK:47:VAL:HG23	2.09	0.53
56:BW:43:C:H2'	56:BW:44:G:C8	2.44	0.53
1:CA:958:U:OP2	14:CQ:14:ARG:NH1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CC:65:LEU:HD22	3:CC:189:ASN:HB3	1.91	0.53
4:CD:130:ALA:C	4:CD:131:LEU:HD12	2.29	0.53
7:CG:79:ASN:OD1	7:CG:79:ASN:N	2.40	0.53
34:DA:972:C:O2'	43:DJ:55:LYS:O	2.27	0.53
36:DC:152:ILE:HB	36:DC:167:TRP:HB3	1.90	0.53
43:DJ:78:ASN:O	43:DJ:80:LYS:N	2.41	0.53
59:DZ:168:ILE:HG12	59:DZ:205:TYR:CE2	2.44	0.53
1:AA:2204:G:H2'	1:AA:2205:C:C6	2.44	0.53
3:AC:65:LEU:HD22	3:AC:189:ASN:HB3	1.91	0.53
6:AF:123:LEU:HD13	6:AF:192:LEU:HD13	1.90	0.53
34:BA:67:C:H2'	34:BA:68:G:C8	2.44	0.53
34:BA:452:A:H62	34:BA:480:U:H3	1.56	0.53
35:BB:175:ARG:O	35:BB:179:LYS:N	2.36	0.53
37:BD:57:ARG:HE	37:BD:202:LEU:HD22	1.74	0.53
59:BZ:264:LEU:HB2	64:BZ:702:GDP:C5	2.43	0.53
1:CA:673:C:H5''	6:CF:81:PRO:HD2	1.91	0.53
6:CF:165:ARG:HG2	6:CF:168:ARG:HH21	1.74	0.53
22:CY:77:PRO:HD3	22:CY:106:LEU:HD23	1.90	0.53
34:DA:1218:C:P	47:DN:9:LYS:HZ3	2.31	0.53
28:A4:63:TYR:CD1	28:A4:63:TYR:N	2.77	0.52
34:BA:1458:G:H5''	53:BT:31:SER:HB2	1.91	0.52
35:BB:231:GLU:HB3	35:BB:232:PRO:HD3	1.90	0.52
42:BI:50:LEU:HB2	42:BI:81:ILE:HD11	1.89	0.52
53:BT:9:ASN:O	53:BT:10:LEU:HB2	2.08	0.52
59:BZ:682:GLN:O	59:BZ:686:LYS:HB3	2.09	0.52
1:CA:1144:G:H2'	1:CA:1145:C:C6	2.44	0.52
1:CA:2287:A:N6	1:CA:2344:U:H3	2.02	0.52
1:CA:2291:U:H2'	1:CA:2292:C:C6	2.44	0.52
3:CC:52:PRO:HG2	3:CC:53:ARG:H	1.73	0.52
5:CE:116:VAL:HG13	5:CE:122:PHE:HB2	1.90	0.52
6:CF:24:LEU:HD21	6:CF:114:VAL:HG12	1.90	0.52
34:DA:201:C:H42	34:DA:216:G:H1	1.57	0.52
40:DG:54:THR:O	40:DG:56:GLN:N	2.41	0.52
53:DT:57:ARG:HH12	53:DT:100:ILE:HD12	1.74	0.52
34:BA:976:G:N2	34:BA:1363:C:OP2	2.36	0.52
3:CC:51:ASP:OD2	3:CC:54:ARG:HB2	2.09	0.52
3:CC:171:ALA:HB1	3:CC:173:HIS:CE1	2.43	0.52
34:DA:1062:U:H2'	34:DA:1063:C:C5	2.45	0.52
34:DA:1435:G:H2'	34:DA:1436:U:C6	2.44	0.52
45:DL:28:LYS:N	45:DL:29:GLY:HA2	2.24	0.52
58:DY:55:PSU:HN1	58:DY:57:G:H5'	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1157:A:O2'	1:AA:1158:G:H4'	2.10	0.52
1:AA:2638:C:H2'	1:AA:2639:G:O4'	2.08	0.52
23:AZ:151:HIS:O	23:AZ:153:SER:N	2.35	0.52
34:BA:8:A:N6	37:BD:205:GLU:O	2.43	0.52
34:BA:1125:U:H4'	43:BJ:5:ARG:HH22	1.74	0.52
1:CA:1057:A:HO2'	1:CA:1058:G:P	2.32	0.52
1:CA:1068:G:H21	1:CA:1096:A:H5'	1.74	0.52
1:CA:1721:G:H8	1:CA:1741:A:H62	1.55	0.52
2:CB:46:A:H2'	2:CB:47:C:C6	2.44	0.52
24:C0:70:GLN:NE2	24:C0:72:ARG:HD2	2.24	0.52
33:C9:17:ILE:HG22	33:C9:24:TYR:HB2	1.92	0.52
34:DA:620:C:H2'	34:DA:621:A:O4'	2.10	0.52
46:DM:3:ARG:NH1	46:DM:3:ARG:O	2.42	0.52
1:AA:470:C:H4'	6:AF:49:ALA:HB2	1.91	0.52
1:AA:1525:G:O2'	1:AA:1605:A:C2	2.62	0.52
1:AA:1921:G:H2'	1:AA:1921:G:N3	2.25	0.52
3:AC:48:LEU:CB	3:AC:50:ILE:HD12	2.38	0.52
25:A1:15:ALA:HB3	25:A1:40:ARG:HD3	1.91	0.52
36:BC:11:ARG:NH2	36:BC:177:THR:O	2.41	0.52
43:BJ:17:ASP:OD1	43:BJ:70:ARG:NH1	2.43	0.52
59:BZ:428:LEU:O	59:BZ:432:ALA:N	2.42	0.52
1:CA:335:C:H4'	22:CY:73:ARG:CZ	2.40	0.52
1:CA:1237:A:OP1	65:CA:4443:HOH:O	2.19	0.52
1:CA:1453:U:O2'	1:CA:1455:G:N7	2.40	0.52
1:CA:1815:A:OP2	4:CD:54:ARG:NH2	2.40	0.52
14:CQ:32:TYR:CE1	14:CQ:133:ARG:HD3	2.45	0.52
34:DA:1218:C:OP2	47:DN:9:LYS:NZ	2.39	0.52
1:AA:939:C:H2'	1:AA:940:C:C6	2.44	0.52
1:AA:1648:U:O4	65:AA:4154:HOH:O	2.10	0.52
3:AC:51:ASP:OD2	3:AC:54:ARG:HB2	2.09	0.52
4:AD:101:GLU:OE1	4:AD:103:ARG:HD3	2.10	0.52
34:BA:1165:C:H2'	34:BA:1166:G:O4'	2.08	0.52
36:BC:77:ILE:O	36:BC:84:ILE:N	2.34	0.52
40:BG:113:GLU:HG2	40:BG:119:ARG:HG2	1.92	0.52
59:BZ:405:PRO:HB2	59:BZ:406:GLU:HA	1.92	0.52
1:CA:607:U:OP1	6:CF:102:PRO:HA	2.10	0.52
1:CA:811:U:H2'	13:CP:21:ARG:HA	1.91	0.52
1:CA:2695:C:H2'	1:CA:2696:U:H6	1.75	0.52
3:CC:67:HIS:CG	3:CC:185:LYS:HD2	2.45	0.52
9:CK:74:LEU:O	9:CK:76:GLY:N	2.40	0.52
19:CV:40:LEU:HB2	19:CV:46:VAL:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:CX:11:PRO:HB3	21:CX:92:LEU:HD11	1.91	0.52
34:DA:921:U:O2	38:DE:19:MET:HB2	2.09	0.52
35:DB:97:TRP:CZ3	35:DB:101:MET:HB2	2.45	0.52
1:AA:11:G:H2'	1:AA:12:U:H5''	1.91	0.52
1:AA:2343:G:H4'	24:A0:43:THR:H	1.74	0.52
3:AC:29:LEU:O	3:AC:30:VAL:C	2.48	0.52
4:AD:17:THR:O	4:AD:211:ARG:NH2	2.40	0.52
34:BA:186:C:H2'	34:BA:187:C:C6	2.45	0.52
35:BB:197:VAL:HG12	35:BB:200:ILE:HD13	1.90	0.52
36:BC:58:GLU:H	36:BC:65:ALA:HB3	1.75	0.52
49:BP:18:ARG:O	49:BP:20:VAL:HB	2.09	0.52
59:BZ:156:ARG:NH1	59:BZ:156:ARG:HB3	2.25	0.52
1:CA:491:G:H2'	1:CA:492:A:C8	2.44	0.52
2:CB:105:A:H2'	2:CB:106:G:O4'	2.08	0.52
6:CF:21:ALA:HB3	6:CF:22:ALA:HA	1.92	0.52
9:CK:40:LEU:HA	9:CK:43:ALA:HB3	1.91	0.52
16:CS:27:SER:HA	16:CS:88:ASP:HB3	1.92	0.52
34:DA:1012:U:H2'	34:DA:1013:G:C8	2.44	0.52
34:DA:1317:C:OP1	47:DN:17:LYS:HG2	2.09	0.52
37:DD:189:PRO:HB2	37:DD:194:LEU:HD11	1.92	0.52
38:DE:139:LEU:O	38:DE:141:GLN:N	2.42	0.52
38:DE:152:ARG:HG3	41:DH:43:GLY:O	2.09	0.52
59:DZ:165:GLN:NE2	59:DZ:260:LEU:H	2.04	0.52
59:DZ:592:GLU:HA	59:DZ:595:GLN:HB3	1.92	0.52
34:BA:1399:C:C2	34:BA:1502:A:N6	2.77	0.52
36:BC:22:TRP:CE2	47:BN:54:PRO:HG3	2.45	0.52
49:BP:3:LYS:O	49:BP:21:VAL:HA	2.09	0.52
1:CA:1059:G:H3'	1:CA:1060:U:C6	2.45	0.52
34:DA:859:A:H2'	34:DA:860:A:O4'	2.09	0.52
35:DB:178:ARG:NH1	35:DB:196:LEU:O	2.42	0.52
36:DC:7:PRO:HG3	36:DC:201:TYR:HE2	1.75	0.52
45:DL:69:TYR:HB2	45:DL:96:VAL:HG11	1.91	0.52
46:DM:84:ILE:O	46:DM:86:CYS:N	2.40	0.52
49:DP:23:ASP:OD1	49:DP:25:ARG:HD3	2.10	0.52
1:AA:1221:G:H1'	1:AA:1222:A:C5'	2.39	0.52
1:AA:1834:A:O2'	4:AD:259:THR:HG21	2.09	0.52
1:AA:2734:A:H5''	65:AA:4044:HOH:O	2.10	0.52
34:BA:418:C:H1'	34:BA:540:G:O2'	2.09	0.52
34:BA:600:C:H2'	34:BA:601:C:H6	1.73	0.52
40:BG:46:ALA:O	40:BG:50:ILE:HG23	2.10	0.52
1:CA:1028:A:N6	1:CA:1125:G:H2'	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CB:20:C:H42	2:CB:63:G:H1	1.57	0.52
3:CC:64:SER:HA	3:CC:161:ARG:H	1.74	0.52
7:CG:43:LEU:HD12	7:CG:45:GLU:HG3	1.92	0.52
8:CH:12:PRO:O	8:CH:15:VAL:HG12	2.09	0.52
14:CQ:16:ARG:HG2	14:CQ:16:ARG:NH1	2.24	0.52
17:CT:19:LEU:HD13	17:CT:86:ILE:HD12	1.90	0.52
20:CW:59:VAL:HG12	20:CW:60:ASN:HD22	1.75	0.52
31:C7:30:VAL:O	31:C7:34:ARG:HG3	2.10	0.52
34:DA:539:A:H2'	34:DA:540:G:H8	1.75	0.52
34:DA:1008:C:H2'	34:DA:1009:G:O4'	2.10	0.52
44:DK:48:ILE:O	44:DK:50:TYR:N	2.43	0.52
1:AA:2331:G:N2	16:AS:3:ARG:HA	2.25	0.52
1:AA:2643:G:O2'	1:AA:2820:A:N1	2.32	0.52
34:BA:1068:G:H8	34:BA:1068:G:OP2	1.92	0.52
34:BA:1106:G:C6	34:BA:1107:C:C4	2.98	0.52
35:BB:77:ALA:O	35:BB:81:VAL:HG22	2.10	0.52
37:BD:190:ASP:OD1	37:BD:190:ASP:N	2.42	0.52
1:CA:330:A:HO2'	1:CA:331:A:H8	1.56	0.52
1:CA:1815:A:H8	1:CA:1815:A:OP1	1.92	0.52
1:CA:1932:A:H2'	1:CA:1933:G:O4'	2.10	0.52
1:CA:2871:C:N4	65:CA:4204:HOH:O	2.42	0.52
6:CF:184:TYR:CE2	6:CF:188:ARG:HD2	2.45	0.52
18:CU:81:HIS:HB3	18:CU:117:GLN:HE22	1.73	0.52
25:C1:8:SER:HB3	25:C1:66:HIS:CD2	2.45	0.52
34:DA:278:G:OP2	50:DQ:41:LYS:NZ	2.43	0.52
36:DC:18:TRP:CD1	47:DN:54:PRO:HA	2.45	0.52
38:DE:11:ILE:HG21	38:DE:105:VAL:HG22	1.92	0.52
6:AF:129:PHE:HB3	6:AF:132:VAL:HG13	1.92	0.52
30:A6:40:CYS:SG	30:A6:42:TRP:HB2	2.50	0.52
34:BA:368:U:N3	59:BZ:354:ARG:NH1	2.58	0.52
39:BF:60:PHE:CE2	51:BR:78:LEU:HD21	2.45	0.52
1:CA:1110:G:H2'	1:CA:1110:G:N3	2.25	0.52
1:CA:2275:C:H5'	1:CA:2275:C:H6	1.74	0.52
7:CG:23:PHE:HB2	7:CG:25:TYR:CZ	2.44	0.52
8:CH:96:ALA:HB2	8:CH:105:LEU:HD23	1.92	0.52
14:CQ:85:LYS:HB2	24:C0:7:LEU:HD12	1.91	0.52
34:DA:539:A:H2'	34:DA:540:G:C8	2.45	0.52
34:DA:1352:C:H2'	34:DA:1353:G:C8	2.45	0.52
38:DE:110:LEU:HD13	38:DE:118:ILE:HG21	1.92	0.52
1:AA:1882:U:H2'	1:AA:1883:C:O4'	2.10	0.51
3:AC:67:HIS:CG	3:AC:185:LYS:HD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BA:1047:G:HO2'	34:BA:1215:G:HO2'	1.58	0.51
41:BH:87:SER:HB2	41:BH:93:VAL:H	1.75	0.51
59:BZ:2:LYS:O	59:BZ:6:GLU:N	2.42	0.51
59:BZ:78:ARG:HH21	59:BZ:357:ARG:CZ	2.23	0.51
59:BZ:494:GLU:HG2	59:BZ:511:LYS:HG2	1.91	0.51
1:CA:65:C:H2'	1:CA:66:C:C6	2.45	0.51
1:CA:1101:U:H2'	1:CA:1102:C:C6	2.45	0.51
7:CG:44:GLY:O	7:CG:47:LYS:HB2	2.10	0.51
34:DA:130:A:O2'	34:DA:131:C:O5'	2.23	0.51
34:DA:1316:G:N2	34:DA:1319:A:H5''	2.25	0.51
35:DB:122:PHE:HA	35:DB:127:ILE:HD12	1.92	0.51
57:DX:75:C:H5''	57:DX:76:31H:P	2.49	0.51
59:DZ:238:THR:O	59:DZ:241:GLU:HG2	2.10	0.51
1:AA:1091:A:H4'	1:AA:1092:A:H5'	1.93	0.51
1:AA:2304:C:P	16:AS:17:ARG:HH12	2.33	0.51
4:AD:3:VAL:HG13	4:AD:17:THR:HB	1.92	0.51
30:A6:18:ARG:HD2	30:A6:42:TRP:CD1	2.45	0.51
34:BA:10:A:OP2	38:BE:126:ARG:HD2	2.09	0.51
34:BA:767:A:H2'	34:BA:768:A:O4'	2.11	0.51
50:BQ:12:SER:HB3	50:BQ:20:THR:HB	1.91	0.51
50:BQ:67:LYS:O	50:BQ:68:ARG:HG2	2.10	0.51
59:BZ:114:VAL:HG11	59:BZ:156:ARG:HH12	1.75	0.51
59:BZ:247:ARG:HG3	59:BZ:247:ARG:HH11	1.75	0.51
1:CA:1359:A:N1	1:CA:1372:U:C4	2.78	0.51
3:CC:218:THR:HG22	3:CC:219:MET:SD	2.50	0.51
1:AA:2564:U:C2	1:AA:2566:U:H5'	2.45	0.51
2:AB:77:U:H4'	23:AZ:84:GLU:OE2	2.10	0.51
5:AE:59:VAL:HG12	5:AE:64:LYS:HG3	1.91	0.51
26:A2:32:LEU:HD11	26:A2:54:LYS:HG3	1.93	0.51
34:BA:882:C:O2'	34:BA:883:C:H5'	2.11	0.51
34:BA:1305:G:H5''	54:BU:4:GLY:HA3	1.93	0.51
3:CC:65:LEU:HB3	3:CC:189:ASN:HD22	1.75	0.51
4:CD:71:ASP:HB3	4:CD:103:ARG:HH22	1.75	0.51
20:CW:41:LYS:HE3	29:C5:25:LEU:HD21	1.91	0.51
34:DA:437:U:O2'	37:DD:123:HIS:HD2	1.94	0.51
34:DA:1004:A:H8	34:DA:1005:A:H4'	1.75	0.51
1:AA:1072:U:H4'	1:AA:1073:A:OP1	2.09	0.51
1:AA:2123:G:H1	1:AA:2210:C:H42	1.58	0.51
1:AA:2149:G:H21	1:AA:2195:A:H1'	1.76	0.51
32:A8:61:LEU:C	32:A8:63:PRO:HD3	2.30	0.51
34:BA:976:G:OP1	47:BN:32:SER:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BA:1353:G:OP1	54:BU:10:ARG:NH1	2.43	0.51
39:BF:1:MET:HA	39:BF:67:MET:O	2.10	0.51
43:BJ:8:LEU:HB2	43:BJ:70:ARG:HB2	1.92	0.51
1:CA:208:C:H2'	1:CA:209:C:H6	1.74	0.51
1:CA:1796:U:H2'	1:CA:1797:C:C6	2.45	0.51
1:CA:2312:U:H5'	7:CG:88:ILE:HD11	1.92	0.51
15:CR:37:THR:OG1	15:CR:40:LYS:HG3	2.09	0.51
21:CX:12:VAL:HG22	21:CX:29:TRP:CE2	2.45	0.51
34:DA:392:G:H2'	34:DA:393:A:H8	1.76	0.51
34:DA:1305:G:H22	34:DA:1331:G:H1'	1.74	0.51
35:DB:9:GLU:O	35:DB:11:LEU:N	2.44	0.51
36:DC:125:GLU:N	36:DC:125:GLU:OE2	2.43	0.51
36:DC:140:ARG:HH12	36:DC:141:VAL:HG23	1.76	0.51
40:DG:151:TYR:OH	44:DK:54:ARG:HD2	2.11	0.51
53:DT:39:LYS:O	53:DT:42:GLN:N	2.42	0.51
1:AA:509:A:O4'	22:AY:48:ALA:HB1	2.10	0.51
2:AB:105:A:OP1	23:AZ:72:ARG:NH1	2.44	0.51
3:AC:65:LEU:HB3	3:AC:189:ASN:HD22	1.74	0.51
3:AC:218:THR:HG22	3:AC:219:MET:SD	2.50	0.51
13:AP:89:ALA:HA	13:AP:121:LYS:HE2	1.92	0.51
17:AT:119:LYS:O	17:AT:123:GLN:HG3	2.10	0.51
34:BA:45:U:H2'	34:BA:46:G:C8	2.46	0.51
34:BA:103:C:OP2	53:BT:17:ARG:NH2	2.43	0.51
34:BA:1379:G:O6	40:BG:2:ALA:HB3	2.10	0.51
1:CA:323:G:C8	6:CF:171:PRO:HG3	2.46	0.51
1:CA:2784:C:H1'	5:CE:37:ARG:HH12	1.75	0.51
4:CD:69:ARG:NH2	4:CD:128:GLY:O	2.43	0.51
4:CD:77:ALA:HB2	4:CD:97:TYR:CD2	2.44	0.51
34:DA:1152:A:H2'	34:DA:1153:C:H6	1.76	0.51
34:DA:1178:G:N2	34:DA:1181:G:OP2	2.42	0.51
36:DC:136:GLN:C	36:DC:138:VAL:H	2.13	0.51
38:DE:33:VAL:HG13	38:DE:112:LEU:HD12	1.92	0.51
41:DH:4:ASP:OD2	41:DH:85:ARG:NH1	2.44	0.51
49:DP:28:ARG:NH1	49:DP:29:ASP:OD2	2.43	0.51
57:DX:2:G:N3	57:DX:2:G:H2'	2.25	0.51
59:DZ:264:LEU:HD12	64:DZ:702:GDP:N3	2.25	0.51
1:AA:1476:C:H2'	1:AA:1477:U:C6	2.46	0.51
3:AC:6:LYS:N	3:AC:9:ARG:NH1	2.58	0.51
3:AC:50:ILE:H	3:AC:50:ILE:HD13	1.76	0.51
9:AK:56:ASN:HA	9:AK:83:TYR:HA	1.93	0.51
10:AL:98:ARG:HA	10:AL:136:VAL:HG23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BA:110:C:O2'	49:BP:25:ARG:O	2.26	0.51
38:BE:135:THR:O	38:BE:139:LEU:HG	2.11	0.51
59:BZ:145:ASP:HB3	59:BZ:148:LEU:HD23	1.92	0.51
1:CA:1102:C:H2'	1:CA:1103:A:C8	2.45	0.51
1:CA:1653:G:H3'	15:CR:2:ARG:HD3	1.93	0.51
8:CH:143:GLN:O	8:CH:145:ALA:N	2.43	0.51
11:CN:94:HIS:O	11:CN:97:ARG:HB2	2.11	0.51
22:CY:99:CYS:SG	22:CY:100:ALA:N	2.84	0.51
34:DA:280:C:OP1	50:DQ:91:ARG:NH1	2.43	0.51
34:DA:828:A:H2'	34:DA:829:G:O4'	2.11	0.51
51:DR:32:ARG:HD2	51:DR:65:ILE:HG21	1.92	0.51
1:AA:95:G:OP1	26:A2:46:GLN:NE2	2.39	0.51
3:AC:68:GLY:H	3:AC:189:ASN:ND2	2.09	0.51
4:AD:2:ALA:N	4:AD:20:ASP:OD2	2.44	0.51
4:AD:102:LYS:C	4:AD:103:ARG:HG2	2.30	0.51
59:BZ:78:ARG:HE	59:BZ:357:ARG:NH1	2.08	0.51
59:BZ:485:GLU:HB3	59:BZ:560:VAL:HG22	1.93	0.51
1:CA:221:A:O2'	1:CA:266:G:N7	2.42	0.51
1:CA:236:C:H2'	1:CA:237:C:C6	2.44	0.51
1:CA:863:A:H2'	1:CA:864:G:C8	2.46	0.51
1:CA:2572:A:N7	5:CE:144:ARG:HD2	2.26	0.51
1:CA:2880:C:O3'	15:CR:90:ARG:NH1	2.43	0.51
2:CB:7:G:H4'	16:CS:29:PHE:CD2	2.46	0.51
3:CC:50:ILE:H	3:CC:50:ILE:HD13	1.76	0.51
8:CH:86:GLU:OE2	8:CH:132:ARG:NH2	2.43	0.51
34:DA:1401:G:C2	34:DA:1402:C:H1'	2.46	0.51
1:AA:934:A:O2'	1:AA:935:C:OP2	2.23	0.51
1:AA:1387:U:O2	21:AX:80:ILE:HD12	2.10	0.51
1:AA:1496:A:H5'	1:AA:1497:G:OP2	2.11	0.51
8:AH:89:ILE:CD1	8:AH:96:ALA:HB2	2.41	0.51
34:BA:17:U:H2'	34:BA:18:C:C6	2.46	0.51
36:BC:52:LEU:HD23	36:BC:53:ALA:N	2.25	0.51
39:BF:8:ILE:HD13	39:BF:26:ILE:HD13	1.93	0.51
59:BZ:417:THR:HA	59:BZ:418:LYS:HG2	1.93	0.51
1:CA:706:A:OP1	4:CD:7:LYS:NZ	2.42	0.51
1:CA:1448:G:H4'	1:CA:1542:A:OP1	2.11	0.51
1:CA:2638:G:P	5:CE:82:ARG:NH2	2.84	0.51
1:CA:2815:C:H2'	1:CA:2816:C:H6	1.75	0.51
3:CC:6:LYS:N	3:CC:9:ARG:NH1	2.59	0.51
21:CX:36:LYS:HA	21:CX:39:ILE:HD12	1.93	0.51
37:DD:150:GLU:O	37:DD:153:ARG:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:DL:24:VAL:HG13	45:DL:98:TYR:CE1	2.46	0.51
53:DT:63:ILE:HD13	53:DT:80:ARG:HB3	1.93	0.51
59:DZ:373:ASP:OD2	59:DZ:374:LEU:N	2.44	0.51
59:DZ:539:ILE:O	59:DZ:542:VAL:HG12	2.11	0.51
1:AA:1040:C:OP1	18:AU:53:ARG:NH2	2.44	0.51
11:AN:30:ILE:HG22	11:AN:34:LEU:HD22	1.93	0.51
16:AS:58:LEU:HD22	16:AS:59:LYS:HG3	1.92	0.51
34:BA:523:A:H61	45:BL:92:ASP:HB2	1.75	0.51
34:BA:976:G:H5'	34:BA:1358:U:O2'	2.11	0.51
49:BP:20:VAL:HG21	49:BP:32:TYR:CD2	2.46	0.51
1:CA:1247:A:OP1	6:CF:95:ARG:NH2	2.43	0.51
1:CA:1547:C:H2'	1:CA:1548:C:C6	2.43	0.51
1:CA:1786:A:H1'	1:CA:1938:A:N6	2.25	0.51
1:CA:1877:A:H5'	1:CA:1878:G:OP2	2.11	0.51
1:CA:2836:U:H2'	1:CA:2837:G:C8	2.45	0.51
3:CC:54:ARG:HD2	3:CC:55:SER:H	1.76	0.51
4:CD:10:THR:OG1	4:CD:13:ARG:HB2	2.10	0.51
7:CG:18:GLU:HG2	7:CG:175:LEU:HD21	1.93	0.51
13:CP:39:LYS:HD2	13:CP:45:LEU:HD11	1.93	0.51
34:DA:979:C:H42	47:DN:18:VAL:HB	1.76	0.51
34:DA:1166:G:H5'	34:DA:1168:A:OP2	2.11	0.51
34:DA:1347:G:HO2'	34:DA:1373:G:H1	1.58	0.51
39:DF:87:ARG:HH11	39:DF:87:ARG:CG	2.20	0.51
59:DZ:129:LYS:NZ	59:DZ:517:LEU:HG	2.26	0.51
59:DZ:169:GLY:N	59:DZ:170:ARG:HH12	2.09	0.51
1:AA:553:A:C2'	1:AA:554:A:H5'	2.41	0.51
1:AA:1289:G:O2'	13:AP:7:ARG:NH2	2.43	0.51
1:AA:2434:A:O4'	58:BY:76:A:N6	2.44	0.51
6:AF:53:THR:CG2	6:AF:55:GLY:H	2.24	0.51
15:AR:33:ARG:HD2	15:AR:113:LEU:HD13	1.91	0.51
34:BA:8:A:N6	37:BD:209:ARG:HB2	2.26	0.51
34:BA:134:A:H61	49:BP:25:ARG:HH12	1.58	0.51
34:BA:1278:U:H5'	34:BA:1279:A:O4'	2.11	0.51
37:BD:190:ASP:HB2	37:BD:193:ASP:HB2	1.93	0.51
1:CA:1429:G:H2'	1:CA:1430:C:C6	2.46	0.51
1:CA:1939:U:OP1	1:CA:2604:U:O2'	2.26	0.51
1:CA:2365:G:N7	32:C8:39:LYS:NZ	2.54	0.51
2:CB:31:C:C2'	2:CB:32:C:H5'	2.41	0.51
34:DA:427:U:H3'	34:DA:428:G:H2'	1.93	0.51
34:DA:892:A:O2'	34:DA:1415:G:H4'	2.11	0.51
35:DB:97:TRP:CH2	35:DB:101:MET:HB2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:DH:28:ALA:HB3	41:DH:57:PRO:HB2	1.93	0.51
43:DJ:8:LEU:HD23	43:DJ:96:ILE:HG23	1.93	0.51
59:DZ:18:ALA:HB1	59:DZ:121:VAL:HG21	1.93	0.51
59:DZ:610:VAL:HG22	59:DZ:669:PHE:HB3	1.92	0.51
1:AA:553:A:H2	1:AA:2065:C:H5'	1.75	0.50
1:AA:1686:U:O2'	1:AA:1687:C:H5'	2.11	0.50
3:AC:42:VAL:CG1	3:AC:43:GLU:N	2.73	0.50
18:AU:61:TRP:CH2	18:AU:93:LYS:HB2	2.46	0.50
34:BA:114:U:O2'	34:BA:115:G:H5'	2.10	0.50
35:BB:160:ASP:N	35:BB:160:ASP:OD1	2.44	0.50
46:BM:60:VAL:HG13	46:BM:64:TRP:HZ3	1.76	0.50
59:BZ:177:ILE:HD12	59:BZ:188:TYR:CE2	2.46	0.50
1:CA:1778:U:H2'	1:CA:1784:A:N6	2.26	0.50
3:CC:42:VAL:CG1	3:CC:43:GLU:N	2.73	0.50
16:CS:66:ALA:O	16:CS:69:VAL:HG13	2.11	0.50
34:DA:1279:A:H5''	34:DA:1280:A:OP1	2.11	0.50
35:DB:84:GLU:HB3	35:DB:219:VAL:HG21	1.93	0.50
35:DB:96:ARG:O	35:DB:98:LEU:HD22	2.11	0.50
35:DB:229:VAL:HG12	35:DB:230:VAL:H	1.76	0.50
36:DC:28:GLN:O	36:DC:32:LEU:HD23	2.11	0.50
37:DD:117:ALA:O	37:DD:121:VAL:HG23	2.10	0.50
59:DZ:491:VAL:HG12	59:DZ:493:VAL:HG13	1.93	0.50
1:AA:484:G:O2'	1:AA:495:G:O6	2.24	0.50
1:AA:1553:A:O2'	1:AA:1554:A:O4'	2.29	0.50
10:AL:108:ALA:O	10:AL:112:MET:HB3	2.11	0.50
11:AN:121:LYS:HB3	11:AN:123:TYR:CE2	2.47	0.50
23:AZ:70:LEU:HG	23:AZ:91:LEU:HD21	1.92	0.50
40:BG:66:VAL:HG12	40:BG:70:LYS:HE3	1.93	0.50
59:BZ:76:ASP:OD2	59:BZ:76:ASP:N	2.42	0.50
1:CA:176:G:O2'	1:CA:177:G:H5'	2.11	0.50
1:CA:297:C:OP1	22:CY:95:LYS:NZ	2.43	0.50
1:CA:1204:A:H2	1:CA:1241:A:N6	1.97	0.50
1:CA:2061:G:OP2	65:CA:4063:HOH:O	2.19	0.50
7:CG:98:ARG:HA	7:CG:101:ILE:HD12	1.93	0.50
14:CQ:109:VAL:HG22	14:CQ:113:GLN:OE1	2.11	0.50
34:DA:23:C:OP2	34:DA:561:U:N3	2.34	0.50
34:DA:559:A:OP1	38:DE:126:ARG:NH2	2.44	0.50
34:DA:1118:C:H1'	34:DA:1179:A:C4	2.46	0.50
59:DZ:302:HIS:CD2	59:DZ:303:PRO:HD2	2.45	0.50
1:AA:139:A:H8	1:AA:1454:C:O2'	1.91	0.50
1:AA:515:G:N7	20:AW:49:LYS:NZ	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:943:C:H4'	56:BW:55:PSU:O3'	2.11	0.50
3:AC:54:ARG:HD2	3:AC:55:SER:H	1.76	0.50
3:AC:57:GLN:HB2	3:AC:202:PRO:HG2	1.93	0.50
23:AZ:111:VAL:HG12	23:AZ:112:ARG:H	1.77	0.50
59:BZ:329:ARG:HD2	59:BZ:331:TYR:CE1	2.47	0.50
1:CA:34:C:O2	1:CA:34:C:H2'	2.10	0.50
1:CA:86:C:OP1	22:CY:32:PRO:HG2	2.11	0.50
1:CA:1044:G:H21	1:CA:1111:A:H2	1.59	0.50
1:CA:1052:C:N4	1:CA:1053:C:H41	2.09	0.50
1:CA:1288:U:O4	15:CR:106:GLY:HA3	2.12	0.50
1:CA:2567:G:H2'	1:CA:2568:C:C6	2.47	0.50
1:CA:2805:G:H2'	1:CA:2807:G:H8	1.74	0.50
3:CC:44:VAL:HG21	3:CC:176:VAL:HG21	1.92	0.50
5:CE:9:VAL:HG13	5:CE:25:VAL:O	2.11	0.50
34:DA:665:A:H1'	34:DA:733:A:O4'	2.11	0.50
34:DA:1346:A:H5''	42:DI:120:ARG:HH12	1.76	0.50
35:DB:178:ARG:HH22	41:DH:68:ARG:NH2	2.05	0.50
40:DG:111:ARG:NH1	40:DG:113:GLU:OE1	2.44	0.50
42:DI:88:TYR:CD2	42:DI:89:ASN:HB2	2.46	0.50
50:DQ:65:ILE:HB	50:DQ:69:LYS:HB3	1.93	0.50
59:DZ:629:GLY:HA3	59:DZ:647:VAL:HG12	1.93	0.50
1:AA:1211:U:H2'	1:AA:1212:C:C6	2.46	0.50
1:AA:1410:G:P	25:A1:3:LYS:HG3	2.51	0.50
1:AA:2860:A:OP2	1:AA:2876:U:H5	1.93	0.50
5:AE:5:LEU:HD12	5:AE:51:PHE:HB2	1.92	0.50
28:A4:59:PHE:HB3	52:BS:67:VAL:HG11	1.94	0.50
32:A8:62:LEU:HB3	32:A8:65:GLU:HG2	1.93	0.50
34:BA:200:G:H1	34:BA:217:C:N4	2.10	0.50
34:BA:353:A:H5'	34:BA:353:A:C8	2.42	0.50
34:BA:955:U:O2'	52:BS:83:HIS:HD2	1.94	0.50
34:BA:1179:A:H2'	34:BA:1180:A:O4'	2.12	0.50
1:CA:11:G:H2'	1:CA:12:U:H5''	1.93	0.50
1:CA:1371:G:H2'	1:CA:1372:U:H5	1.77	0.50
1:CA:1482:G:H2'	1:CA:1484:G:H8	1.76	0.50
1:CA:1798:U:H5'	4:CD:259:THR:CG2	2.24	0.50
1:CA:2031:A:C6	1:CA:2498:C:H1'	2.47	0.50
3:CC:29:LEU:O	3:CC:30:VAL:C	2.48	0.50
3:CC:68:GLY:H	3:CC:189:ASN:ND2	2.08	0.50
19:CV:24:LYS:HA	19:CV:92:THR:OG1	2.11	0.50
21:CX:25:LYS:HA	21:CX:81:VAL:O	2.12	0.50
25:C1:89:GLU:O	25:C1:93:GLU:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:DA:1070:U:H2'	34:DA:1071:C:H6	1.75	0.50
34:DA:1412:C:H2'	34:DA:1413:A:C8	2.47	0.50
36:DC:113:ALA:O	36:DC:116:VAL:N	2.44	0.50
48:DO:15:PHE:CZ	48:DO:85:LEU:HD21	2.47	0.50
58:DY:55:PSU:N3	58:DY:58:A:N7	2.49	0.50
59:DZ:154:GLN:O	59:DZ:158:GLY:HA2	2.12	0.50
1:AA:721:G:H1'	6:AF:74:ARG:HD3	1.92	0.50
1:AA:2843:G:H8	1:AA:2843:G:OP1	1.95	0.50
12:AO:48:PRO:HB3	34:BA:1422:G:H5'	1.94	0.50
34:BA:1511:G:H2'	34:BA:1512:U:O4'	2.10	0.50
35:BB:153:ARG:NH1	35:BB:153:ARG:HB3	2.26	0.50
38:BE:51:VAL:O	38:BE:55:VAL:HG23	2.11	0.50
44:BK:41:THR:OG1	44:BK:42:TRP:N	2.43	0.50
48:BO:81:LEU:O	48:BO:85:LEU:HB2	2.11	0.50
59:BZ:21:ILE:HD13	59:BZ:21:ILE:N	2.25	0.50
59:BZ:554:PRO:HG3	59:BZ:594:VAL:HG12	1.93	0.50
59:BZ:623:ASP:CG	59:BZ:662:LYS:HE3	2.31	0.50
1:CA:298:G:H5''	1:CA:299:A:OP1	2.10	0.50
1:CA:733:G:OP2	65:CA:3724:HOH:O	2.20	0.50
1:CA:987:G:O2'	1:CA:1000:A:N3	2.41	0.50
1:CA:2113:U:H3	1:CA:2170:A:H61	1.59	0.50
1:CA:2126:A:N6	1:CA:2172:U:H5'	2.27	0.50
1:CA:2572:A:N7	5:CE:145:LYS:HB2	2.27	0.50
1:CA:2876:G:H4'	17:CT:2:ASN:ND2	2.26	0.50
3:CC:191:ARG:O	3:CC:195:ARG:HG2	2.11	0.50
13:CP:111:ARG:HD3	13:CP:128:HIS:CD2	2.47	0.50
34:DA:728:A:N7	48:DO:54:ARG:HD2	2.26	0.50
34:DA:1095:U:P	34:DA:1108:G:H1	2.35	0.50
34:DA:1509:C:H2'	34:DA:1510:U:O4'	2.12	0.50
50:DQ:48:GLU:OE2	50:DQ:50:LYS:HE3	2.12	0.50
1:AA:2574:U:O2'	12:AO:23:ARG:HD3	2.11	0.50
4:AD:155:LEU:HD23	4:AD:177:LEU:HD22	1.94	0.50
6:AF:64:ILE:HD12	6:AF:65:TRP:CD2	2.47	0.50
34:BA:52:G:H2'	34:BA:53:A:H8	1.75	0.50
34:BA:765:G:H5''	34:BA:766:A:OP1	2.12	0.50
38:BE:20:GLN:HG2	38:BE:25:ARG:HD2	1.93	0.50
1:CA:1098:A:H2'	1:CA:1099:G:O4'	2.11	0.50
1:CA:2150:U:H2'	1:CA:2151:G:C8	2.47	0.50
3:CC:54:ARG:HH22	3:CC:56:ASP:HB3	1.75	0.50
3:CC:57:GLN:HB2	3:CC:202:PRO:HG2	1.93	0.50
23:CZ:96:VAL:N	23:CZ:128:VAL:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1284:G:OP2	65:AA:4926:HOH:O	2.19	0.50
1:AA:1553:A:O2'	1:AA:1554:A:O5'	2.29	0.50
1:AA:1846:A:O3'	65:AA:4736:HOH:O	2.18	0.50
1:AA:2287:C:O2	14:AQ:85:LYS:HG3	2.12	0.50
3:AC:44:VAL:HG21	3:AC:176:VAL:HG21	1.92	0.50
3:AC:191:ARG:O	3:AC:195:ARG:HG2	2.11	0.50
10:AL:99:ILE:O	10:AL:139:VAL:N	2.39	0.50
11:AN:5:VAL:HG23	11:AN:6:PRO:HD2	1.94	0.50
34:BA:109:A:H2'	34:BA:326:G:N2	2.27	0.50
34:BA:1312:G:N7	52:BS:2:PRO:HD2	2.27	0.50
37:BD:134:ASP:O	37:BD:136:PRO:HD3	2.11	0.50
54:BU:3:LYS:HB3	54:BU:14:TRP:CG	2.47	0.50
59:BZ:517:LEU:HD13	59:BZ:564:LYS:HB2	1.94	0.50
1:CA:271(E):U:H2'	1:CA:271(F):C:C6	2.46	0.50
1:CA:2365:G:O6	32:C8:39:LYS:NZ	2.45	0.50
16:CS:12:PHE:O	16:CS:16:ASN:ND2	2.44	0.50
18:CU:79:PHE:CZ	18:CU:83:LEU:HD21	2.46	0.50
34:DA:17:U:H2'	34:DA:18:C:C6	2.47	0.50
34:DA:1152:A:H2'	34:DA:1153:C:C6	2.47	0.50
35:DB:102:LEU:HB3	35:DB:180:LEU:HD12	1.93	0.50
35:DB:142:LEU:HA	35:DB:145:LEU:HB2	1.94	0.50
36:DC:97:LYS:O	36:DC:99:VAL:N	2.45	0.50
53:DT:64:ASP:OD2	53:DT:81:LYS:NZ	2.38	0.50
59:DZ:127:LYS:HG3	59:DZ:520:GLY:HA3	1.93	0.50
1:AA:553:A:C8	1:AA:553:A:C3'	2.94	0.50
1:AA:2152:U:H1'	1:AA:2180:A:N1	2.27	0.50
3:AC:183:PRO:C	3:AC:185:LYS:H	2.16	0.50
7:AG:114:ILE:HA	7:AG:140:ILE:HD11	1.93	0.50
25:A1:80:LEU:HB3	25:A1:82:LEU:HG	1.93	0.50
34:BA:1255:G:C2	34:BA:1283:G:C2	3.00	0.50
34:BA:1260:C:OP1	34:BA:1284:C:O2'	2.24	0.50
34:BA:1436:U:OP1	53:BT:23:ARG:NH2	2.44	0.50
34:BA:1509:C:H2'	34:BA:1510:U:O4'	2.12	0.50
59:BZ:-62:LEU:HD11	59:BZ:-48:VAL:HG22	1.93	0.50
59:BZ:216:LEU:HD11	59:BZ:246:ILE:HD11	1.93	0.50
59:BZ:438:PHE:HB3	59:BZ:458:HIS:HE1	1.77	0.50
1:CA:627:A:C6	1:CA:637:A:C8	3.00	0.50
1:CA:1070:A:H2'	1:CA:1097:U:OP1	2.11	0.50
1:CA:2131:G:N7	1:CA:2133:G:N2	2.59	0.50
1:CA:2506:U:O2	56:DW:76:F3N:HD2	2.11	0.50
3:CC:183:PRO:C	3:CC:185:LYS:H	2.16	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:CK:85:ASP:O	9:CK:87:VAL:N	2.45	0.50
23:CZ:69:THR:HG22	23:CZ:90:VAL:HA	1.94	0.50
34:DA:20:U:H2'	34:DA:21:G:O4'	2.12	0.50
34:DA:1203:C:H2'	34:DA:1204:A:C8	2.47	0.50
35:DB:16:HIS:CG	35:DB:17:PHE:N	2.80	0.50
38:DE:69:VAL:HG22	38:DE:71:LEU:HD13	1.94	0.50
48:DO:71:GLN:HB2	48:DO:78:TYR:CD2	2.47	0.50
51:DR:32:ARG:HA	51:DR:69:THR:HG21	1.93	0.50
1:AA:70:A:N7	21:AX:31:HIS:HE1	2.09	0.50
4:AD:79:VAL:HG12	4:AD:113:VAL:HA	1.94	0.50
10:AL:106:GLU:O	10:AL:109:LYS:HB2	2.12	0.50
34:BA:406:G:C2	34:BA:407:G:C8	3.00	0.50
34:BA:714:G:H2'	34:BA:715:A:C8	2.47	0.50
34:BA:1010:G:N2	34:BA:1020:U:H1'	2.26	0.50
34:BA:1456:G:O3'	53:BT:39:LYS:NZ	2.41	0.50
55:BV:14:A:C6	58:BY:34:G:C6	3.00	0.50
1:CA:30:G:H2'	1:CA:31:C:C6	2.46	0.50
1:CA:1237:A:OP1	65:CA:4442:HOH:O	2.19	0.50
1:CA:1300:U:H4'	1:CA:1301:A:C5'	2.42	0.50
1:CA:2298:A:H2'	1:CA:2299:G:O4'	2.12	0.50
1:CA:2364:C:OP1	24:C0:55:ARG:HD3	2.11	0.50
5:CE:77:ILE:HD11	5:CE:79:ARG:NH1	2.27	0.50
29:C5:16:ARG:HD2	29:C5:20:ARG:NH1	2.27	0.50
34:DA:572:A:OP1	65:DA:1836:HOH:O	2.18	0.50
34:DA:1355:G:H2'	34:DA:1356:G:C8	2.46	0.50
35:DB:112:VAL:O	35:DB:116:GLU:HB3	2.12	0.50
53:DT:43:LEU:O	53:DT:47:GLY:N	2.45	0.50
1:AA:1387:U:O4'	21:AX:57:LEU:HD12	2.12	0.49
1:AA:2518:U:C2	1:AA:2597:U:O4	2.65	0.49
2:AB:1:U:O2	2:AB:1:U:H2'	2.11	0.49
14:AQ:14:ARG:HG2	14:AQ:41:TRP:CH2	2.41	0.49
19:AV:14:VAL:HB	19:AV:96:ILE:HG13	1.93	0.49
34:BA:560:U:H5'	34:BA:566:G:N2	2.26	0.49
34:BA:645:C:H2'	34:BA:646:U:C6	2.46	0.49
1:CA:2787:C:HO2'	1:CA:2810:A:HO2'	1.60	0.49
12:CO:23:ARG:HG3	12:CO:24:VAL:N	2.27	0.49
18:CU:49:HIS:HA	18:CU:52:ARG:HB3	1.94	0.49
34:DA:583:A:H2'	34:DA:584:G:O4'	2.12	0.49
35:DB:54:THR:O	35:DB:58:ILE:HG13	2.12	0.49
36:DC:15:THR:HG21	36:DC:181:ASN:HA	1.94	0.49
59:DZ:388:THR:HG21	59:DZ:397:VAL:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:DZ:526:VAL:HG23	59:DZ:566:THR:HA	1.94	0.49
1:AA:346:A:H5'	1:AA:364:A:H1'	1.93	0.49
1:AA:1249:A:N1	1:AA:1287:A:N7	2.59	0.49
14:AQ:24:GLY:O	14:AQ:102:VAL:HG23	2.12	0.49
22:AY:54:LYS:H	22:AY:56:PRO:HG3	1.77	0.49
34:BA:129:U:H5'	50:BQ:3:LYS:NZ	2.27	0.49
34:BA:1228:C:P	46:BM:108:ARG:HH22	2.35	0.49
59:BZ:396:ARG:HH21	59:BZ:396:ARG:CG	2.23	0.49
1:CA:1026:U:H4'	1:CA:1027:A:OP1	2.11	0.49
1:CA:1637:A:H4'	1:CA:2711:A:O2'	2.11	0.49
1:CA:2600:A:H2'	1:CA:2601:C:C6	2.48	0.49
1:CA:2815:C:H2'	1:CA:2816:C:C6	2.47	0.49
4:CD:148:GLU:CB	4:CD:151:LYS:HD2	2.40	0.49
8:CH:75:ALA:O	8:CH:79:VAL:HG22	2.12	0.49
35:DB:150:SER:O	35:DB:153:ARG:HG2	2.12	0.49
43:DJ:47:PHE:HB2	43:DJ:63:PHE:HB2	1.93	0.49
56:DW:21:A:N6	56:DW:46:7MG:N3	2.60	0.49
59:DZ:36:THR:HB	59:DZ:72:CYS:HB2	1.93	0.49
1:AA:225:C:H2'	1:AA:226:C:C6	2.47	0.49
3:AC:191:ARG:O	3:AC:194:ILE:HG22	2.12	0.49
13:AP:62:LEU:O	32:A8:13:ARG:HD3	2.11	0.49
17:AT:65:LYS:HE2	17:AT:67:SER:HB2	1.94	0.49
34:BA:539:A:H2'	34:BA:540:G:C8	2.47	0.49
35:BB:218:ALA:O	35:BB:222:ILE:HG13	2.13	0.49
38:BE:7:GLU:N	38:BE:35:GLY:O	2.45	0.49
53:BT:13:LEU:O	53:BT:17:ARG:HG3	2.12	0.49
1:CA:1188:U:H4'	19:CV:79:VAL:HG22	1.94	0.49
1:CA:1418:G:N7	65:CA:4067:HOH:O	2.35	0.49
1:CA:2116:G:H5'	1:CA:2117:A:OP2	2.11	0.49
12:CO:48:PRO:HB3	34:DA:1422:G:H5'	1.95	0.49
17:CT:83:ILE:HD13	17:CT:86:ILE:HD11	1.94	0.49
34:DA:1084:G:H5'	34:DA:1102:A:OP2	2.12	0.49
36:DC:131:ARG:NH1	38:DE:50:GLU:HG3	2.27	0.49
43:DJ:38:ILE:CG1	43:DJ:71:LEU:HB3	2.42	0.49
53:DT:40:ALA:HB2	53:DT:55:ILE:HG22	1.93	0.49
59:DZ:119:GLU:HB3	59:DZ:123:ARG:HH21	1.77	0.49
1:AA:841:G:H2'	1:AA:842:C:C6	2.47	0.49
1:AA:1074:A:N6	1:AA:1171:G:H2'	2.27	0.49
1:AA:1095:C:H2'	1:AA:1096:A:H5'	1.95	0.49
13:AP:27:HIS:HB2	65:AP:315:HOH:O	2.11	0.49
32:A8:37:SER:OG	32:A8:38:GLY:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BA:674:G:H2'	34:BA:675:A:H8	1.76	0.49
34:BA:688:G:H2'	34:BA:689:C:H6	1.77	0.49
34:BA:1171:G:H2'	34:BA:1172:C:C6	2.47	0.49
59:BZ:328:ILE:HD12	59:BZ:377:VAL:HG12	1.93	0.49
1:CA:1480:G:C6	1:CA:1481:U:N3	2.80	0.49
4:CD:96:HIS:NE2	4:CD:102:LYS:HE2	2.27	0.49
23:CZ:110:GLY:HA3	23:CZ:145:GLU:HA	1.93	0.49
34:DA:254:G:P	50:DQ:66:SER:HG	2.34	0.49
34:DA:1299:A:N3	34:DA:1299:A:H2'	2.27	0.49
35:DB:77:ALA:HB2	35:DB:211:ILE:HD13	1.95	0.49
36:DC:47:LEU:HG	36:DC:68:VAL:HG11	1.93	0.49
37:DD:13:ARG:HD3	37:DD:32:ALA:HB1	1.95	0.49
42:DI:46:ALA:HB2	42:DI:74:ILE:HG23	1.94	0.49
43:DJ:30:SER:O	43:DJ:30:SER:OG	2.29	0.49
45:DL:88:GLY:O	45:DL:99:HIS:HD2	1.96	0.49
59:DZ:160:ARG:NH1	59:DZ:256:THR:OG1	2.37	0.49
1:AA:1466:U:O2'	1:AA:1467:G:OP1	2.28	0.49
1:AA:1712:A:N3	12:AO:1:MET:HE2	2.28	0.49
4:AD:12:SER:HB3	4:AD:208:LYS:HB3	1.95	0.49
11:AN:96:GLU:H	11:AN:96:GLU:CD	2.16	0.49
22:AY:79:CYS:SG	22:AY:81:LYS:HG3	2.52	0.49
35:BB:178:ARG:HH22	41:BH:68:ARG:NH1	2.11	0.49
53:BT:40:ALA:HB2	53:BT:55:ILE:HG22	1.95	0.49
58:BY:34:G:H8	58:BY:34:G:O5'	1.96	0.49
59:BZ:75:LYS:O	59:BZ:77:HIS:HD2	1.95	0.49
1:CA:18:C:H2'	1:CA:19:C:C6	2.48	0.49
1:CA:1782:C:H1'	1:CA:2609:U:C5'	2.43	0.49
1:CA:2758:A:C2	1:CA:2759:G:H1'	2.46	0.49
3:CC:191:ARG:O	3:CC:194:ILE:HG22	2.12	0.49
13:CP:38:GLN:O	13:CP:39:LYS:HB3	2.12	0.49
34:DA:259:G:H2'	34:DA:260:G:O4'	2.13	0.49
34:DA:1107:C:C4	34:DA:1108:G:C8	3.00	0.49
35:DB:46:LYS:O	35:DB:50:GLU:HB2	2.13	0.49
37:DD:59:ARG:O	37:DD:63:LYS:HD3	2.12	0.49
50:DQ:45:HIS:CD2	50:DQ:47:PRO:HD3	2.47	0.49
59:DZ:511:LYS:HB2	59:DZ:569:ASP:HB3	1.94	0.49
1:AA:826:U:OP1	4:AD:49:ILE:HD12	2.13	0.49
1:AA:1834:A:H4'	4:AD:259:THR:CG2	2.41	0.49
1:AA:2200:C:O2'	3:AC:169:THR:CB	2.59	0.49
13:AP:52:GLU:HG2	32:A8:57:ARG:HH22	1.77	0.49
43:BJ:11:PHE:CE1	43:BJ:67:THR:HG22	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:BO:33:THR:HG21	48:BO:85:LEU:HD22	1.93	0.49
51:BR:26:LEU:HD21	51:BR:39:VAL:HG13	1.94	0.49
1:CA:300:A:P	22:CY:86:ARG:NH2	2.84	0.49
1:CA:819:A:C4	1:CA:1189:A:C2	3.00	0.49
1:CA:2171:A:H1'	1:CA:2172:U:C6	2.47	0.49
1:CA:2773:C:H5''	5:CE:164:ARG:HG2	1.93	0.49
1:CA:2849:U:H4'	1:CA:2868:A:C2	2.47	0.49
34:DA:1148:U:H2'	34:DA:1149:C:O4'	2.13	0.49
35:DB:178:ARG:HH21	41:DH:74:PRO:HB3	1.78	0.49
39:DF:87:ARG:HG3	39:DF:87:ARG:NH1	2.18	0.49
42:DI:3:GLN:CG	42:DI:20:ARG:HE	2.26	0.49
46:DM:70:LEU:O	46:DM:74:VAL:HG23	2.12	0.49
1:AA:1220:U:O3'	1:AA:1221:G:H4'	2.13	0.49
1:AA:2830:A:C8	5:AE:109:LYS:HE2	2.47	0.49
13:AP:84:ASN:HB3	13:AP:117:GLU:O	2.13	0.49
17:AT:15:VAL:HG13	17:AT:79:HIS:CE1	2.48	0.49
17:AT:77:PRO:HB2	17:AT:80:SER:HB2	1.94	0.49
23:AZ:73:GLN:HB3	23:AZ:87:ASP:HB2	1.95	0.49
34:BA:21:G:H2'	34:BA:22:G:C8	2.47	0.49
34:BA:92:C:H2'	34:BA:93:G:C8	2.48	0.49
34:BA:693:G:H2'	34:BA:694:A:C8	2.48	0.49
34:BA:903:G:OP1	65:BA:1925:HOH:O	2.19	0.49
34:BA:1342:C:O2'	42:BI:124:GLN:HG3	2.12	0.49
44:BK:73:MET:HG2	44:BK:103:LEU:HD21	1.94	0.49
46:BM:3:ARG:HG3	46:BM:4:ILE:H	1.77	0.49
59:BZ:140:ASP:HA	59:BZ:172:ASP:H	1.78	0.49
1:CA:1130:U:O2	5:CE:149:ARG:NH2	2.40	0.49
1:CA:1498:C:O4'	1:CA:1577:C:H4'	2.13	0.49
1:CA:2396:G:OP1	25:C1:25:LYS:NZ	2.29	0.49
9:CK:27:VAL:HA	9:CK:113:GLN:HA	1.95	0.49
34:DA:9:G:OP1	38:DE:122:GLU:HG3	2.13	0.49
34:DA:91:C:H2'	34:DA:92:C:C6	2.48	0.49
34:DA:977:A:O2'	34:DA:979:C:OP2	2.22	0.49
34:DA:1073:U:O2	35:DB:104:ASN:ND2	2.39	0.49
59:DZ:244:ALA:HA	59:DZ:247:ARG:HB3	1.94	0.49
59:DZ:302:HIS:HD2	59:DZ:303:PRO:HD2	1.77	0.49
1:AA:2096:U:H2'	1:AA:2097:U:C6	2.47	0.49
1:AA:2181:G:H2'	1:AA:2182:G:C8	2.48	0.49
1:AA:2660:C:H2'	1:AA:2661:U:C6	2.48	0.49
18:AU:36:ARG:HD2	18:AU:40:PHE:CZ	2.48	0.49
22:AY:86:ARG:HH11	22:AY:100:ALA:HA	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BA:707:C:H2'	34:BA:708:C:C6	2.48	0.49
34:BA:757:U:H2'	34:BA:758:G:O4'	2.13	0.49
34:BA:1128:C:H4'	34:BA:1148:U:O2	2.13	0.49
53:BT:76:ALA:O	53:BT:80:ARG:HG2	2.13	0.49
1:CA:1169:G:H1	1:CA:1180:C:H42	1.61	0.49
1:CA:2405:G:OP1	13:CP:77:ARG:NH2	2.44	0.49
4:CD:24:ILE:HD13	4:CD:84:TYR:HB2	1.95	0.49
15:CR:30:THR:HG22	15:CR:31:HIS:CD2	2.48	0.49
15:CR:33:ARG:HG3	15:CR:115:GLU:HB3	1.95	0.49
18:CU:34:LYS:HE2	18:CU:34:LYS:HA	1.94	0.49
20:CW:19:LEU:HB3	29:C5:25:LEU:HD11	1.95	0.49
23:CZ:93:ASP:HA	23:CZ:131:ARG:NH2	2.28	0.49
34:DA:767:A:H2'	34:DA:768:A:O4'	2.12	0.49
34:DA:983:A:H3'	34:DA:983:A:N3	2.28	0.49
36:DC:120:VAL:HA	36:DC:123:GLN:HE21	1.78	0.49
51:DR:52:PRO:O	51:DR:56:THR:HG23	2.12	0.49
59:DZ:634:MET:HE3	59:DZ:643:ILE:HG12	1.94	0.49
1:AA:239:G:P	32:A8:13:ARG:HH22	2.35	0.49
1:AA:346:A:H3'	6:AF:169:ASN:HD21	1.77	0.49
1:AA:868:A:H2'	1:AA:991:G:H5''	1.94	0.49
1:AA:1067:A:H8	1:AA:1067:A:H3'	1.76	0.49
1:AA:1468:G:H1'	1:AA:1542:A:N1	2.27	0.49
1:AA:1594:C:H2'	1:AA:1595:C:C6	2.47	0.49
1:AA:2250:G:N3	1:AA:2250:G:H2'	2.26	0.49
1:AA:2285:A:H2'	1:AA:2286:A:C8	2.48	0.49
34:BA:222:U:H2'	34:BA:223:U:C6	2.48	0.49
34:BA:443:C:H2'	34:BA:444:C:C6	2.48	0.49
34:BA:559:A:OP1	38:BE:126:ARG:NH2	2.45	0.49
34:BA:814:A:N7	34:BA:816:A:C4	2.81	0.49
35:BB:20:GLU:HA	35:BB:21:ARG:NH2	2.27	0.49
37:BD:107:ARG:HH12	37:BD:194:LEU:HD21	1.77	0.49
44:BK:48:ILE:O	44:BK:50:TYR:N	2.45	0.49
59:BZ:78:ARG:HH21	59:BZ:357:ARG:NH2	2.10	0.49
59:BZ:147:TRP:O	59:BZ:151:ARG:HB2	2.13	0.49
1:CA:81:G:HO2'	1:CA:295:G:HO2'	1.57	0.49
1:CA:500:G:N2	1:CA:502:A:H3'	2.28	0.49
1:CA:608:A:H2'	1:CA:609:A:C8	2.48	0.49
1:CA:613:G:N2	1:CA:614(C):A:O2'	2.46	0.49
1:CA:1031:G:H21	33:C9:36:GLN:NE2	2.06	0.49
2:CB:61:G:C6	2:CB:62:C:C4	3.01	0.49
34:DA:8:A:N6	37:DD:209:ARG:HB2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:DA:522:C:OP2	45:DL:69:TYR:OH	2.22	0.49
34:DA:790:A:H2'	34:DA:791:G:C8	2.48	0.49
34:DA:909:A:H2'	34:DA:910:C:O4'	2.13	0.49
34:DA:1121:U:C2'	34:DA:1122:U:H5'	2.43	0.49
35:DB:96:ARG:HD2	35:DB:98:LEU:HD13	1.94	0.49
36:DC:32:LEU:HD12	36:DC:59:ARG:NH1	2.27	0.49
40:DG:26:PHE:O	40:DG:30:ILE:HG13	2.13	0.49
45:DL:102:ARG:HE	45:DL:102:ARG:HB3	1.49	0.49
1:AA:656:A:OP1	13:AP:65:ARG:NH1	2.44	0.49
1:AA:794:U:O2	1:AA:2036:A:H1'	2.12	0.49
1:AA:801:C:H2'	1:AA:802:C:C6	2.48	0.49
1:AA:1846:A:P	4:AD:54:ARG:HH22	2.36	0.49
3:AC:42:VAL:HA	3:AC:216:THR:O	2.13	0.49
4:AD:71:ASP:CB	4:AD:103:ARG:HH22	2.26	0.49
41:BH:29:SER:OG	41:BH:32:LYS:HG3	2.13	0.49
59:BZ:519:ARG:HH22	59:BZ:678:GLU:H	1.59	0.49
1:CA:647:G:O5'	1:CA:647:G:H8	1.96	0.49
3:CC:184:GLU:O	3:CC:188:ASP:OD2	2.31	0.49
4:CD:273:ARG:HG2	4:CD:274:ARG:N	2.28	0.49
13:CP:59:LEU:O	32:C8:13:ARG:HD2	2.13	0.49
13:CP:101:VAL:HA	13:CP:106:LEU:O	2.13	0.49
14:CQ:18:LYS:O	14:CQ:98:LYS:NZ	2.35	0.49
17:CT:6:LEU:O	17:CT:10:VAL:HG23	2.12	0.49
34:DA:707:C:H2'	34:DA:708:C:H6	1.78	0.49
34:DA:1101:A:H4'	34:DA:1102:A:O5'	2.12	0.49
34:DA:1251:A:H2'	34:DA:1252:A:C8	2.47	0.49
43:DJ:63:PHE:HE2	47:DN:45:ARG:HA	1.78	0.49
51:DR:33:ASP:OD2	51:DR:36:ASN:HB2	2.13	0.49
59:DZ:169:GLY:H	59:DZ:170:ARG:NH1	2.09	0.49
1:AA:898:U:O2'	27:A3:42:ALA:O	2.29	0.48
1:AA:1890:A:N6	1:AA:1905:G:O2'	2.45	0.48
1:AA:2021:C:H4'	1:AA:2736:C:O2	2.13	0.48
7:AG:126:ASP:HB3	7:AG:130:ASN:H	1.78	0.48
18:AU:61:TRP:CZ2	18:AU:93:LYS:HB2	2.48	0.48
34:BA:429:U:H3'	37:BD:9:CYS:SG	2.53	0.48
34:BA:674:G:H2'	34:BA:675:A:C8	2.48	0.48
37:BD:88:VAL:HG12	37:BD:91:SER:H	1.78	0.48
38:BE:36:ASP:OD2	38:BE:40:ARG:HB2	2.13	0.48
1:CA:272:G:H4'	1:CA:272(A):U:H5''	1.95	0.48
1:CA:1434:A:H61	1:CA:1558:A:N6	2.10	0.48
1:CA:1628:G:H2'	1:CA:1629:U:C6	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CB:12:C:O5'	2:CB:12:C:H6	1.96	0.48
34:DA:687:A:N3	34:DA:688:G:H1'	2.28	0.48
35:DB:103:THR:HG23	35:DB:176:GLU:OE1	2.13	0.48
37:DD:98:GLU:OE1	37:DD:103:ASN:ND2	2.46	0.48
47:DN:27:CYS:SG	47:DN:28:GLY:N	2.86	0.48
52:DS:11:VAL:O	52:DS:13:ASP:N	2.46	0.48
1:AA:311:C:H2'	1:AA:312:C:C6	2.48	0.48
1:AA:537:G:N7	65:AA:4769:HOH:O	2.34	0.48
1:AA:556:C:OP1	1:AA:584:G:N1	2.45	0.48
1:AA:1117:G:H1'	1:AA:1135:G:C8	2.48	0.48
1:AA:1425:A:H4'	1:AA:1426:G:OP2	2.12	0.48
1:AA:1492:C:H2'	1:AA:1493:C:H6	1.78	0.48
5:AE:120:TRP:CD2	5:AE:155:LYS:HG2	2.48	0.48
6:AF:53:THR:HG22	6:AF:56:GLU:HG3	1.95	0.48
10:AL:112:MET:HG2	10:AL:113:PRO:HD3	1.94	0.48
13:AP:83:VAL:HG13	13:AP:112:LEU:HD21	1.94	0.48
14:AQ:56:ARG:HH12	56:BW:52:G:H4'	1.78	0.48
15:AR:86:ARG:NH2	15:AR:87:TYR:OH	2.44	0.48
34:BA:1014:A:H4'	52:BS:14:HIS:CE1	2.48	0.48
35:BB:229:VAL:HG12	35:BB:230:VAL:H	1.77	0.48
58:BY:28:G:H2'	58:BY:29:G:H8	1.78	0.48
59:BZ:-29:LEU:H	59:BZ:-29:LEU:CD2	2.26	0.48
1:CA:1091:G:H2'	1:CA:1092:C:C6	2.49	0.48
4:CD:2:ALA:O	4:CD:3:VAL:HB	2.13	0.48
34:DA:1001(A):G:O6	34:DA:1039:C:N4	2.37	0.48
34:DA:1051:C:H2'	34:DA:1052:U:H6	1.78	0.48
35:DB:219:VAL:O	35:DB:222:ILE:HG12	2.13	0.48
36:DC:39:ILE:O	36:DC:43:LEU:HG	2.13	0.48
40:DG:93:PRO:HA	40:DG:96:GLN:HE21	1.78	0.48
1:AA:1068:G:N7	11:AN:66:LYS:HE2	2.28	0.48
1:AA:1098:C:H2'	1:AA:1099:C:C6	2.48	0.48
1:AA:1117:G:H21	1:AA:1135:G:HO2'	1.61	0.48
1:AA:2331:G:C2	16:AS:3:ARG:HA	2.47	0.48
4:AD:35:LYS:HB2	4:AD:36:PRO:HD2	1.95	0.48
4:AD:124:PRO:O	4:AD:126:GLN:N	2.46	0.48
27:A3:23:LEU:HD13	27:A3:50:VAL:HG11	1.95	0.48
34:BA:91:C:H5'	34:BA:92:C:OP2	2.14	0.48
34:BA:1239:A:C4	34:BA:1298:C:N4	2.81	0.48
35:BB:27:LYS:O	35:BB:194:PRO:HG2	2.12	0.48
37:BD:98:GLU:OE1	37:BD:107:ARG:NH1	2.46	0.48
42:BI:93:ARG:NH1	42:BI:93:ARG:HB2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:BS:51:VAL:O	52:BS:58:VAL:N	2.44	0.48
1:CA:2132:U:C4	3:CC:6:LYS:CE	2.94	0.48
1:CA:2356:C:H2'	1:CA:2357:U:O4'	2.14	0.48
1:CA:2364:C:H2'	1:CA:2365:G:O4'	2.13	0.48
1:CA:2522:U:O2'	1:CA:2647:U:OP1	2.24	0.48
11:CN:128:HIS:CE1	11:CN:135:PRO:HG2	2.48	0.48
20:CW:60:ASN:HD22	20:CW:60:ASN:N	2.11	0.48
32:C8:33:ASN:HA	32:C8:36:LYS:HD3	1.95	0.48
34:DA:363:A:C5	45:DL:31:PRO:HD2	2.47	0.48
34:DA:428:G:OP2	37:DD:10:ARG:NH1	2.47	0.48
34:DA:1355:G:H2'	34:DA:1356:G:H8	1.78	0.48
35:DB:111:ARG:HG2	35:DB:111:ARG:HH11	1.78	0.48
48:DO:24:SER:O	48:DO:28:GLN:HG3	2.12	0.48
59:DZ:103:GLY:H	59:DZ:130:VAL:HG23	1.77	0.48
1:AA:504:A:N1	1:AA:525:G:H4'	2.27	0.48
1:AA:662:A:H4'	1:AA:663:G:O5'	2.14	0.48
1:AA:2584:A:N7	5:AE:144:ARG:HD2	2.27	0.48
1:AA:2686:G:H5'	12:AO:26:LYS:HE2	1.95	0.48
2:AB:48:A:H4'	16:AS:95:HIS:HD2	1.79	0.48
6:AF:8:GLN:HE22	6:AF:21:ALA:HB2	1.78	0.48
14:AQ:54:MET:HG3	14:AQ:117:ALA:HB1	1.96	0.48
15:AR:38:VAL:HG22	15:AR:112:ALA:HB2	1.95	0.48
25:A1:5:CYS:SG	25:A1:62:VAL:HG23	2.53	0.48
25:A1:8:SER:OG	25:A1:10:LYS:HG3	2.13	0.48
34:BA:109:A:H4'	34:BA:110:C:OP2	2.13	0.48
34:BA:1325:C:H2'	34:BA:1326:C:C6	2.48	0.48
35:BB:178:ARG:HH22	41:BH:68:ARG:HH12	1.60	0.48
37:BD:98:GLU:OE1	37:BD:103:ASN:ND2	2.35	0.48
37:BD:187:ARG:HG2	37:BD:188:LEU:N	2.29	0.48
40:BG:50:ILE:HD11	40:BG:58:PRO:HA	1.95	0.48
40:BG:152:ALA:O	40:BG:155:ARG:HB3	2.13	0.48
44:BK:62:GLN:HB2	44:BK:93:GLN:HG3	1.95	0.48
59:BZ:150:ILE:O	59:BZ:154:GLN:HG3	2.13	0.48
1:CA:848:G:N9	1:CA:933:A:H8	2.11	0.48
1:CA:2163:C:C5	1:CA:2164:C:H1'	2.49	0.48
6:CF:51:THR:O	6:CF:93:LYS:HE2	2.13	0.48
12:CO:2:ILE:HD12	12:CO:6:THR:HG21	1.95	0.48
14:CQ:75:THR:HA	14:CQ:89:ASN:O	2.12	0.48
34:DA:769:G:O2'	34:DA:770:C:H5'	2.13	0.48
34:DA:1208:C:H2'	34:DA:1209:C:H6	1.79	0.48
35:DB:16:HIS:HD2	35:DB:204:ASN:HB3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:DZ:606:MET:O	59:DZ:646:PHE:HA	2.14	0.48
1:AA:746:A:H2'	1:AA:747:G:O4'	2.13	0.48
1:AA:908:A:C2	1:AA:963:A:C4	3.01	0.48
1:AA:945:A:O2'	1:AA:946:A:H8	1.96	0.48
1:AA:2372:A:H2'	1:AA:2373:A:O4'	2.14	0.48
4:AD:10:THR:OG1	4:AD:13:ARG:HB2	2.13	0.48
24:A0:32:ARG:H	24:A0:35:ASN:ND2	2.11	0.48
34:BA:153:C:N4	34:BA:168:G:H1	2.11	0.48
35:BB:189:ASP:OD1	35:BB:189:ASP:N	2.33	0.48
38:BE:84:PHE:HB3	38:BE:134:ALA:HB2	1.95	0.48
56:BW:9:A:H1'	56:BW:45:U:O2'	2.14	0.48
59:BZ:2:LYS:HA	59:BZ:5:LEU:HD12	1.95	0.48
59:BZ:221:ALA:HB2	59:BZ:227:ILE:HG22	1.95	0.48
59:BZ:336:THR:O	59:BZ:339:SER:OG	2.24	0.48
1:CA:848:G:C4	1:CA:933:A:H8	2.32	0.48
1:CA:1274:A:N3	1:CA:1297:C:H1'	2.28	0.48
1:CA:2235:G:H2'	1:CA:2236:C:C6	2.48	0.48
1:CA:2695:C:H2'	1:CA:2696:U:C6	2.49	0.48
2:CB:3:C:H2'	2:CB:4:C:H6	1.78	0.48
6:CF:120:GLU:HB2	6:CF:122:LYS:HG2	1.95	0.48
14:CQ:38:GLU:HA	14:CQ:99:PRO:HG3	1.96	0.48
34:DA:690:G:H2'	34:DA:691:G:C8	2.49	0.48
34:DA:1347:G:H5''	42:DI:107:ARG:HB3	1.94	0.48
35:DB:210:SER:OG	35:DB:211:ILE:N	2.46	0.48
45:DL:24:VAL:HG12	45:DL:27:LEU:HB2	1.95	0.48
52:DS:27:GLU:HB3	52:DS:28:LYS:HD3	1.96	0.48
59:DZ:149:VAL:O	59:DZ:153:MET:HB2	2.12	0.48
1:AA:518:G:O6	65:AA:4472:HOH:O	2.18	0.48
1:AA:878:G:O2'	13:AP:38:GLN:NE2	2.47	0.48
4:AD:273:ARG:HG2	4:AD:274:ARG:H	1.79	0.48
5:AE:174:ASP:OD1	5:AE:175:VAL:N	2.47	0.48
6:AF:118:ALA:HB2	6:AF:123:LEU:HD23	1.95	0.48
14:AQ:31:ASP:HB2	14:AQ:32:TYR:CD2	2.49	0.48
25:A1:50:ARG:HG2	25:A1:59:THR:HB	1.95	0.48
34:BA:736:C:H2'	34:BA:737:A:H8	1.78	0.48
34:BA:1053:G:N7	34:BA:1200:C:H5''	2.28	0.48
34:BA:1233:G:H2'	34:BA:1234:C:C6	2.49	0.48
35:BB:101:MET:HA	35:BB:108:ILE:HD12	1.94	0.48
46:BM:86:CYS:HB2	52:BS:73:GLU:HB3	1.96	0.48
57:BX:19:G:H5''	57:BX:60:U:O4	2.12	0.48
1:CA:65:C:H2'	1:CA:66:C:H6	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1025:G:C4	1:CA:1135:C:H1'	2.48	0.48
1:CA:1860:G:H5'	3:CC:206:LYS:HE2	1.87	0.48
1:CA:2107:C:H42	1:CA:2182:G:H1	1.61	0.48
1:CA:2163:C:H5	1:CA:2164:C:H1'	1.78	0.48
1:CA:2359:C:H2'	1:CA:2360:A:O4'	2.13	0.48
4:CD:94:LEU:HD22	4:CD:95:LEU:H	1.79	0.48
9:CK:118:THR:N	9:CK:121:ASP:O	2.47	0.48
28:C4:62:ARG:H	28:C4:62:ARG:NE	2.11	0.48
34:DA:448:A:P	34:DA:485:G:H22	2.36	0.48
34:DA:586:C:O2'	34:DA:878:G:H4'	2.12	0.48
53:DT:54:LYS:HA	53:DT:57:ARG:CZ	2.44	0.48
59:DZ:169:GLY:N	59:DZ:170:ARG:NH1	2.61	0.48
1:AA:908:A:H2'	1:AA:909:G:O4'	2.14	0.48
7:AG:48:GLU:HA	7:AG:51:ARG:NE	2.27	0.48
23:AZ:41:LEU:O	23:AZ:41:LEU:HD22	2.13	0.48
23:AZ:152:ALA:O	23:AZ:155:LEU:HB2	2.14	0.48
34:BA:1144:G:N2	34:BA:1146:A:H62	2.12	0.48
34:BA:1205:U:O2'	36:BC:195:VAL:HG23	2.14	0.48
41:BH:114:THR:HG22	41:BH:130:GLY:O	2.13	0.48
44:BK:20:TYR:HB2	44:BK:31:THR:HG23	1.94	0.48
1:CA:697:C:H2'	1:CA:698:C:C6	2.48	0.48
1:CA:919:G:N2	1:CA:2269:A:OP2	2.47	0.48
1:CA:1005:C:H2'	1:CA:1006:C:C6	2.49	0.48
1:CA:2507:C:H2'	1:CA:2508:G:O4'	2.14	0.48
6:CF:192:LEU:HD22	6:CF:194:MET:HG3	1.96	0.48
15:CR:97:VAL:HG22	15:CR:114:VAL:HG13	1.96	0.48
34:DA:1238:A:N3	34:DA:1241:G:O2'	2.42	0.48
34:DA:1318:A:H5''	52:DS:3:ARG:NH2	2.29	0.48
34:DA:1499:A:H1'	34:DA:1520:G:H5'	1.95	0.48
35:DB:121:LEU:H	35:DB:125:PRO:HG2	1.78	0.48
37:DD:8:VAL:HG23	37:DD:11:LEU:HD22	1.96	0.48
41:DH:20:TYR:HD2	41:DH:65:TYR:CD2	2.32	0.48
43:DJ:5:ARG:N	43:DJ:73:ASP:HA	2.29	0.48
59:DZ:556:ILE:HD13	59:DZ:558:PHE:HD2	1.78	0.48
1:AA:311:C:H2'	1:AA:312:C:H6	1.78	0.48
1:AA:313:A:H61	1:AA:375:G:H1'	1.79	0.48
1:AA:597:C:N3	5:AE:145:LYS:NZ	2.53	0.48
1:AA:997:G:OP1	14:AQ:16:ARG:NH2	2.47	0.48
1:AA:1071:G:C4	1:AA:1180:C:H1'	2.49	0.48
1:AA:1210:G:H2'	1:AA:1211:U:C6	2.49	0.48
1:AA:1769:G:H2'	1:AA:1770:A:H8	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:2181:G:H2'	1:AA:2182:G:H8	1.78	0.48
11:AN:112:LEU:HD12	11:AN:112:LEU:O	2.14	0.48
34:BA:437:U:O2'	37:BD:123:HIS:HD2	1.97	0.48
34:BA:1299:A:N3	34:BA:1299:A:H5''	2.29	0.48
36:BC:8:ILE:HD13	36:BC:184:TYR:HB3	1.94	0.48
39:BF:82:ARG:HB3	39:BF:85:VAL:HG23	1.96	0.48
43:BJ:44:VAL:HG13	43:BJ:66:ARG:HG2	1.95	0.48
1:CA:38:A:H2'	1:CA:39:C:C6	2.49	0.48
1:CA:1142(A):A:C4	1:CA:1144:G:C8	3.02	0.48
1:CA:1384:A:N3	1:CA:1405:U:H1'	2.29	0.48
8:CH:164:TYR:HB2	8:CH:167:GLU:HB2	1.96	0.48
38:DE:16:THR:OG1	38:DE:17:ALA:N	2.45	0.48
40:DG:94:ARG:O	40:DG:97:GLN:HB3	2.14	0.48
59:DZ:514:VAL:HA	59:DZ:564:LYS:O	2.13	0.48
1:AA:116:A:C8	1:AA:117:A:C8	3.02	0.48
1:AA:2567:U:H5''	1:AA:2568:C:OP2	2.14	0.48
21:AX:31:HIS:CD2	21:AX:32:PRO:HD2	2.48	0.48
34:BA:49:U:C2	34:BA:361:G:N2	2.82	0.48
34:BA:1189:C:H5''	34:BA:1190:G:OP2	2.14	0.48
34:BA:1279:A:H5''	34:BA:1280:A:OP1	2.14	0.48
37:BD:31:CYS:SG	37:BD:33:MET:N	2.87	0.48
52:BS:15:LEU:O	52:BS:19:VAL:HG23	2.14	0.48
58:BY:58:A:C2	58:BY:60:U:H2'	2.48	0.48
59:BZ:21:ILE:HD11	59:BZ:117:GLN:NE2	2.29	0.48
59:BZ:132:ARG:N	59:BZ:132:ARG:HD3	2.28	0.48
12:CO:102:VAL:HB	12:CO:106:LEU:HD12	1.94	0.48
34:DA:70:G:H1	34:DA:99:U:H3	1.60	0.48
38:DE:92:LYS:HB3	38:DE:119:LEU:HB2	1.96	0.48
50:DQ:95:TYR:HA	50:DQ:98:LEU:HD12	1.96	0.48
57:DX:49:G:N2	57:DX:66:C:C2	2.82	0.48
1:AA:1566:U:H2'	1:AA:1567:G:O4'	2.14	0.48
1:AA:2339:A:H2'	1:AA:2340:A:C8	2.48	0.48
4:AD:108:PRO:HB3	4:AD:143:HIS:CE1	2.49	0.48
14:AQ:57:HIS:CE1	14:AQ:116:GLU:HG2	2.49	0.48
23:AZ:29:TYR:HB3	23:AZ:34:ASN:ND2	2.17	0.48
28:A4:61:ARG:HH21	52:BS:42:PRO:CD	2.26	0.48
34:BA:1226:C:H4'	52:BS:80:TYR:CZ	2.49	0.48
58:BY:9:A:H1'	58:BY:45:U:H2'	1.96	0.48
1:CA:660:G:O3'	6:CF:38:ARG:NH2	2.47	0.48
1:CA:1220:A:OP2	18:CU:19:LYS:NZ	2.47	0.48
1:CA:1830:C:OP2	65:CA:4300:HOH:O	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CD:134:ARG:NH1	4:CD:188:GLU:OE2	2.47	0.48
15:CR:17:ARG:O	15:CR:20:LEU:HB3	2.14	0.48
18:CU:32:PHE:HZ	18:CU:36:ARG:HH21	1.61	0.48
30:C6:25:LYS:HE3	30:C6:30:THR:O	2.13	0.48
34:DA:300:A:H2'	34:DA:301:G:O4'	2.14	0.48
34:DA:392:G:H2'	34:DA:393:A:C8	2.49	0.48
34:DA:689:C:P	44:DK:46:GLY:HA3	2.54	0.48
35:DB:76:GLN:NE2	35:DB:206:ASP:O	2.47	0.48
38:DE:10:MET:HB3	38:DE:13:ILE:HD11	1.96	0.48
50:DQ:5:VAL:O	50:DQ:6:LEU:HD13	2.14	0.48
59:DZ:170:ARG:HD3	59:DZ:170:ARG:HA	1.62	0.48
59:DZ:328:ILE:HD12	59:DZ:377:VAL:HG12	1.96	0.48
4:AD:146:GLU:HB2	4:AD:189:CYS:HB3	1.96	0.47
5:AE:141:ILE:HD12	5:AE:150:VAL:HG21	1.96	0.47
19:AV:5:VAL:HG21	19:AV:35:LEU:HD23	1.96	0.47
21:AX:88:LYS:NZ	21:AX:90:GLU:OE1	2.47	0.47
34:BA:411:A:C8	34:BA:413:G:C8	3.01	0.47
35:BB:20:GLU:HB3	35:BB:190:THR:OG1	2.14	0.47
38:BE:10:MET:HA	38:BE:32:VAL:HG22	1.95	0.47
53:BT:21:LYS:O	53:BT:25:ARG:HG3	2.15	0.47
1:CA:218:A:C2	1:CA:235:U:H4'	2.49	0.47
1:CA:1514:U:H2'	1:CA:1515:G:C8	2.49	0.47
1:CA:2395:C:O2'	25:C1:30:VAL:HG22	2.14	0.47
1:CA:2712(A):A:H5''	1:CA:2713:A:OP2	2.13	0.47
7:CG:18:GLU:HG3	7:CG:18:GLU:O	2.12	0.47
8:CH:54:ARG:HD3	8:CH:65:HIS:ND1	2.29	0.47
22:CY:13:VAL:HB	22:CY:72:VAL:HG13	1.95	0.47
24:C0:23:VAL:HG22	24:C0:38:VAL:HG22	1.96	0.47
34:DA:563:A:H2'	34:DA:567:G:C8	2.49	0.47
34:DA:993:G:O6	34:DA:1045:C:N4	2.41	0.47
34:DA:1273:G:H3'	34:DA:1274:G:C8	2.48	0.47
34:DA:1342:C:H4'	42:DI:125:TYR:HB3	1.95	0.47
34:DA:1375:A:O2'	40:DG:29:LYS:NZ	2.47	0.47
39:DF:30:LEU:HD23	39:DF:75:LEU:HD21	1.96	0.47
1:AA:354:A:H2	1:AA:1255:A:C2'	2.26	0.47
1:AA:2317:A:H5''	7:AG:134:GLY:HA3	1.96	0.47
6:AF:161:GLU:HG2	6:AF:164:ARG:NH2	2.29	0.47
34:BA:708:C:H2'	34:BA:709:G:H8	1.79	0.47
34:BA:814:A:H2'	34:BA:816:A:H5''	1.96	0.47
35:BB:170:GLU:O	35:BB:174:VAL:HG23	2.14	0.47
49:BP:22:THR:HA	49:BP:33:ILE:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:BZ:146:LEU:HD12	59:BZ:167:PRO:CD	2.44	0.47
59:BZ:168:ILE:HD11	59:BZ:178:ILE:HG13	1.96	0.47
59:BZ:348:ARG:HG2	59:BZ:348:ARG:NH1	2.29	0.47
59:BZ:416:LYS:HB2	59:BZ:474:ALA:HA	1.96	0.47
1:CA:930:U:H4'	1:CA:931:G:O5'	2.14	0.47
1:CA:1641:A:H2'	1:CA:1642:G:O4'	2.14	0.47
1:CA:2611:U:OP2	1:CA:2611:U:H3'	2.14	0.47
1:CA:2693:A:H2'	1:CA:2694:G:H8	1.78	0.47
22:CY:37:VAL:HG21	22:CY:72:VAL:HG21	1.95	0.47
34:DA:149:A:H2'	34:DA:150:C:C6	2.49	0.47
34:DA:714:G:H2'	34:DA:715:A:C8	2.49	0.47
34:DA:920:U:C2	34:DA:921:U:C5	3.02	0.47
34:DA:927:G:OP2	34:DA:927:G:H4'	2.12	0.47
34:DA:1239:A:N6	34:DA:1299:A:H62	2.11	0.47
35:DB:82:ARG:HG3	35:DB:92:TYR:OH	2.14	0.47
35:DB:141:GLU:HG2	35:DB:145:LEU:HD12	1.97	0.47
51:DR:26:LEU:HD21	51:DR:42:ARG:HE	1.79	0.47
1:AA:142:G:H1'	21:AX:37:THR:HG21	1.96	0.47
1:AA:1358:U:H4'	1:AA:1359:U:O5'	2.14	0.47
1:AA:2074:G:H4'	5:AE:143:ASN:O	2.14	0.47
8:AH:89:ILE:HD12	8:AH:96:ALA:HB2	1.95	0.47
12:AO:87:ILE:HD12	12:AO:91:LEU:HA	1.96	0.47
34:BA:164:U:H2'	34:BA:165:C:C6	2.49	0.47
34:BA:927:G:H4'	34:BA:927:G:OP2	2.13	0.47
34:BA:1020:U:H2'	34:BA:1021:G:C8	2.49	0.47
34:BA:1229:A:OP2	46:BM:114:ARG:HD3	2.14	0.47
36:BC:22:TRP:CH2	36:BC:32:LEU:HB2	2.49	0.47
36:BC:52:LEU:HD23	36:BC:54:ARG:H	1.79	0.47
52:BS:52:TYR:HA	52:BS:56:GLN:O	2.14	0.47
59:BZ:534:ILE:HD11	59:BZ:570:GLY:HA3	1.96	0.47
1:CA:185:U:H4'	1:CA:218:A:H4'	1.95	0.47
1:CA:500:G:N1	1:CA:503:A:OP2	2.47	0.47
34:DA:429:U:H3'	37:DD:9:CYS:SG	2.54	0.47
34:DA:636:U:H2'	34:DA:637:G:C8	2.49	0.47
34:DA:1041:A:C6	34:DA:1042:G:C6	3.02	0.47
34:DA:1301:U:O2'	34:DA:1302:U:H5'	2.14	0.47
34:DA:1338:G:C6	34:DA:1339:A:C6	3.02	0.47
37:DD:68:TYR:CE1	37:DD:97:LEU:HB3	2.49	0.47
1:AA:225:C:H2'	1:AA:226:C:H6	1.78	0.47
1:AA:354:A:O2'	1:AA:355:A:H8	1.96	0.47
1:AA:826:U:P	4:AD:49:ILE:HD12	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:955:A:H2'	1:AA:958:C:C5	2.49	0.47
7:AG:79:ASN:OD1	7:AG:79:ASN:N	2.48	0.47
16:AS:83:LYS:HE2	16:AS:83:LYS:HB2	1.60	0.47
34:BA:354:G:C2'	34:BA:355:C:H5'	2.44	0.47
34:BA:436:C:H2'	34:BA:437:U:C6	2.49	0.47
34:BA:1255:G:N7	43:BJ:43:ARG:NH2	2.62	0.47
35:BB:212:GLN:NE2	35:BB:234:PRO:O	2.47	0.47
59:BZ:217:VAL:HG13	59:BZ:242:LEU:HD21	1.95	0.47
59:BZ:542:VAL:HG23	59:BZ:582:PHE:O	2.14	0.47
1:CA:1266:G:O4'	20:CW:15:ARG:NH2	2.47	0.47
1:CA:2203:U:O4'	4:CD:151:LYS:HE2	2.14	0.47
1:CA:2356:C:O3'	24:C0:20:ARG:HD3	2.14	0.47
1:CA:2391:G:OP2	32:C8:32:LEU:HD23	2.13	0.47
10:CL:103:GLN:HA	10:CL:106:GLU:HG2	1.96	0.47
32:C8:10:ALA:CB	32:C8:62:LEU:HD21	2.43	0.47
34:DA:194:C:H2'	34:DA:195:A:H5''	1.97	0.47
34:DA:374:A:C6	34:DA:375:U:C4	3.02	0.47
34:DA:1342:C:H1'	42:DI:124:GLN:HE21	1.79	0.47
35:DB:134:GLU:O	35:DB:138:LEU:HG	2.15	0.47
1:AA:1105:G:H1	1:AA:1125:C:H42	1.61	0.47
3:AC:30:VAL:CG2	3:AC:31:LYS:H	2.27	0.47
3:AC:184:GLU:O	3:AC:188:ASP:OD2	2.31	0.47
34:BA:586:C:O2'	34:BA:878:G:H4'	2.14	0.47
49:BP:74:LEU:O	49:BP:79:VAL:HG23	2.13	0.47
52:BS:36:ARG:HB3	52:BS:72:GLY:CA	2.44	0.47
52:BS:65:ASN:HD22	52:BS:65:ASN:N	2.12	0.47
58:BY:19:G:H4'	58:BY:20:U:OP2	2.12	0.47
1:CA:757:U:H2'	1:CA:758:C:O4'	2.15	0.47
1:CA:870:A:C2	1:CA:908:C:C2	3.02	0.47
1:CA:1486:A:O2'	1:CA:1487:G:H5'	2.14	0.47
1:CA:1847:A:H3'	1:CA:1848:A:H5'	1.97	0.47
1:CA:2166:G:N7	1:CA:2168:G:N2	2.62	0.47
1:CA:2171:A:N3	1:CA:2172:U:N3	2.62	0.47
1:CA:2440:C:OP2	65:CA:4113:HOH:O	2.20	0.47
3:CC:180:SER:O	3:CC:181:PHE:O	2.33	0.47
14:CQ:24:GLY:HA2	14:CQ:67:ARG:NH2	2.29	0.47
19:CV:29:PRO:HA	19:CV:61:VAL:HG22	1.95	0.47
34:DA:321:A:N7	34:DA:328:C:O2'	2.35	0.47
1:AA:592:U:C4	1:AA:593:G:C6	3.03	0.47
6:AF:150:GLY:HA2	6:AF:172:TRP:CD2	2.49	0.47
12:AO:17:ARG:HD2	12:AO:17:ARG:HA	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AO:35:VAL:HG11	12:AO:103:ALA:CB	2.44	0.47
13:AP:134:ALA:O	13:AP:138:LEU:HB2	2.14	0.47
23:AZ:153:SER:HB3	23:AZ:167:PRO:HB3	1.97	0.47
33:A9:27:CYS:SG	33:A9:28:GLU:N	2.87	0.47
48:BO:29:VAL:HG11	48:BO:81:LEU:HD21	1.97	0.47
59:BZ:286:ILE:HD13	59:BZ:286:ILE:H	1.79	0.47
59:BZ:325:LEU:HD23	59:BZ:325:LEU:HA	1.75	0.47
1:CA:839:U:H2'	1:CA:840:C:C6	2.50	0.47
1:CA:1054:A:N6	1:CA:1055:G:C6	2.82	0.47
1:CA:1319:G:C6	1:CA:1320:C:N4	2.82	0.47
1:CA:1477:A:H2'	1:CA:1478:G:O4'	2.13	0.47
1:CA:2469:A:H2'	1:CA:2470:G:O4'	2.15	0.47
11:CN:102:ALA:O	11:CN:106:MET:HG3	2.15	0.47
16:CS:61:ASN:O	16:CS:65:VAL:HG23	2.14	0.47
23:CZ:105:VAL:N	23:CZ:139:VAL:O	2.48	0.47
34:DA:633:G:H2'	34:DA:634:C:C6	2.50	0.47
34:DA:1264:C:H2'	34:DA:1265:G:C8	2.49	0.47
36:DC:123:GLN:O	36:DC:128:PHE:HB2	2.15	0.47
40:DG:50:ILE:HD11	40:DG:58:PRO:HB3	1.95	0.47
40:DG:75:VAL:HA	40:DG:87:VAL:O	2.15	0.47
1:AA:762:G:C2	48:BO:56:LEU:HD21	2.49	0.47
1:AA:821:A:H2'	1:AA:821:A:N3	2.29	0.47
1:AA:1109:G:N2	1:AA:1122:C:O2	2.48	0.47
1:AA:1525:G:H2'	1:AA:1526:G:H8	1.78	0.47
1:AA:2228:G:H2'	1:AA:2229:A:C2	2.50	0.47
3:AC:180:SER:O	3:AC:181:PHE:O	2.32	0.47
4:AD:206:LEU:HD23	4:AD:206:LEU:HA	1.69	0.47
6:AF:101:LEU:HD12	6:AF:102:PRO:HD2	1.96	0.47
7:AG:21:ARG:O	7:AG:21:ARG:HG2	2.13	0.47
7:AG:63:ILE:HD13	7:AG:141:PHE:CG	2.50	0.47
22:AY:38:ILE:HD11	22:AY:66:PRO:HG3	1.97	0.47
34:BA:1233:G:H2'	34:BA:1234:C:H6	1.80	0.47
34:BA:1316:G:N2	34:BA:1318:A:H3'	2.30	0.47
36:BC:6:HIS:CD2	36:BC:7:PRO:HD2	2.49	0.47
39:BF:15:ASP:OD1	39:BF:18:GLN:N	2.39	0.47
47:BN:3:ARG:HB3	47:BN:3:ARG:HH21	1.79	0.47
49:BP:58:TYR:O	49:BP:61:SER:OG	2.22	0.47
51:BR:51:LEU:HD23	51:BR:52:PRO:HD2	1.96	0.47
59:BZ:20:HIS:CE1	59:BZ:115:GLU:HB3	2.49	0.47
59:BZ:359:HIS:ND1	59:BZ:362:HIS:CE1	2.83	0.47
59:BZ:399:LEU:C	59:BZ:401:SER:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:BZ:399:LEU:O	59:BZ:401:SER:N	2.48	0.47
59:BZ:484:ARG:NH1	59:BZ:559:PRO:HG2	2.30	0.47
1:CA:479:A:N3	1:CA:481:G:H5''	2.29	0.47
1:CA:674:G:H1'	6:CF:74:ARG:HD3	1.96	0.47
1:CA:747:U:O2	1:CA:2014:A:H1'	2.15	0.47
1:CA:750:A:H2'	1:CA:751:A:H5''	1.97	0.47
1:CA:2108:C:H2'	1:CA:2109:U:C6	2.50	0.47
1:CA:2126:A:H61	1:CA:2172:U:H5'	1.80	0.47
2:CB:13:A:N1	2:CB:69:G:O2'	2.40	0.47
2:CB:66:A:H61	2:CB:109:C:H5''	1.79	0.47
3:CC:42:VAL:HA	3:CC:216:THR:O	2.13	0.47
4:CD:72:LYS:HG3	4:CD:103:ARG:NH2	2.30	0.47
7:CG:23:PHE:HB2	7:CG:25:TYR:CE1	2.50	0.47
9:CK:70:GLU:O	9:CK:72:ASP:N	2.48	0.47
14:CQ:11:LYS:NZ	14:CQ:88:GLY:O	2.32	0.47
20:CW:29:LEU:O	20:CW:33:ARG:HG3	2.15	0.47
29:C5:35:GLU:HG2	29:C5:51:TYR:CG	2.49	0.47
34:DA:518:C:H5''	34:DA:519:C:C6	2.49	0.47
34:DA:1030(A):G:H2'	34:DA:1030(B):C:H5''	1.97	0.47
34:DA:1076:C:C2	34:DA:1082:G:N2	2.82	0.47
34:DA:1203:C:H2'	34:DA:1204:A:H8	1.80	0.47
34:DA:1278:U:H5'	34:DA:1279:A:C5'	2.44	0.47
34:DA:1305:G:O2'	34:DA:1331:G:N2	2.47	0.47
36:DC:129:ALA:O	36:DC:133:ALA:N	2.41	0.47
38:DE:101:ILE:HG13	38:DE:119:LEU:HD23	1.96	0.47
41:DH:109:ILE:HB	41:DH:120:THR:HG22	1.97	0.47
42:DI:23:ASN:OD1	42:DI:25:LYS:HE2	2.15	0.47
43:DJ:49:VAL:HG12	43:DJ:61:GLU:O	2.14	0.47
47:DN:32:SER:O	47:DN:40:CYS:HA	2.15	0.47
57:DX:23:C:H2'	57:DX:24:U:C6	2.50	0.47
57:DX:67:C:C2'	57:DX:68:C:H5'	2.44	0.47
59:DZ:15:ILE:HA	59:DZ:103:GLY:O	2.14	0.47
59:DZ:272:LEU:O	59:DZ:276:VAL:HG23	2.14	0.47
59:DZ:490:PRO:HG3	59:DZ:516:PRO:HD2	1.96	0.47
1:AA:440:C:OP2	65:AA:4986:HOH:O	2.21	0.47
1:AA:894:U:H5	1:AA:978:A:H62	1.58	0.47
1:AA:2147:G:OP1	3:AC:71:LYS:HE2	2.15	0.47
1:AA:2623:U:H6	1:AA:2623:U:H5'	1.80	0.47
3:AC:68:GLY:N	3:AC:189:ASN:ND2	2.62	0.47
5:AE:12:THR:HG22	5:AE:13:ARG:H	1.80	0.47
12:AO:23:ARG:HG3	12:AO:24:VAL:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:AU:74:LEU:HD12	18:AU:74:LEU:H	1.79	0.47
34:BA:1070:U:H2'	34:BA:1071:C:H6	1.80	0.47
52:BS:27:GLU:HG2	52:BS:47:HIS:NE2	2.29	0.47
59:BZ:114:VAL:O	59:BZ:115:GLU:HB2	2.15	0.47
59:BZ:405:PRO:CB	59:BZ:406:GLU:HA	2.45	0.47
1:CA:196:A:H2'	1:CA:196:A:N3	2.30	0.47
1:CA:1059:G:H5'	1:CA:1060:U:O5'	2.15	0.47
1:CA:1340:U:OP1	21:CX:16:LYS:NZ	2.43	0.47
1:CA:1478:G:HO2'	1:CA:1558:A:H2	1.60	0.47
1:CA:1891:G:O6	65:CA:4398:HOH:O	2.20	0.47
3:CC:6:LYS:HA	3:CC:9:ARG:NH1	2.30	0.47
5:CE:52:LEU:O	5:CE:76:ARG:N	2.38	0.47
6:CF:150:GLY:HA2	6:CF:172:TRP:CE3	2.49	0.47
20:CW:14:PRO:HG2	20:CW:78:GLU:HG2	1.96	0.47
21:CX:44:GLU:OE2	21:CX:51:VAL:N	2.48	0.47
28:C4:48:ARG:HA	28:C4:48:ARG:HD3	1.76	0.47
34:DA:364:A:H2'	34:DA:365:U:C6	2.50	0.47
34:DA:404:U:H2'	34:DA:405:U:H6	1.80	0.47
34:DA:713:G:H2'	34:DA:714:G:C8	2.50	0.47
34:DA:1121:U:H2'	34:DA:1122:U:H5'	1.97	0.47
45:DL:7:ILE:HD13	45:DL:7:ILE:HA	1.78	0.47
49:DP:60:LEU:HD13	49:DP:60:LEU:HA	1.70	0.47
59:DZ:408:VAL:O	59:DZ:482:ALA:HB3	2.15	0.47
1:AA:2720:G:H1'	15:AR:71:GLN:HE22	1.79	0.47
18:AU:104:GLN:CD	18:AU:104:GLN:H	2.16	0.47
28:A4:36:CYS:SG	28:A4:37:SER:N	2.88	0.47
28:A4:57:GLU:HB2	28:A4:58:ARG:HE	1.80	0.47
34:BA:189(D):C:O2	34:BA:189(H):G:C6	2.68	0.47
34:BA:974:A:P	47:BN:29:ARG:HH21	2.37	0.47
34:BA:1037:C:H2'	34:BA:1038:C:C6	2.50	0.47
36:BC:6:HIS:CD2	36:BC:8:ILE:H	2.32	0.47
38:BE:32:VAL:O	38:BE:43:LEU:HD12	2.15	0.47
39:BF:37:VAL:HG12	39:BF:38:GLU:O	2.15	0.47
1:CA:193:U:OP2	65:CA:4435:HOH:O	2.20	0.47
1:CA:660:G:H5'	6:CF:99:TYR:CE2	2.50	0.47
1:CA:1590:U:H2'	1:CA:1591:G:C8	2.49	0.47
1:CA:2119:A:H2	1:CA:2171:A:H5'	1.79	0.47
1:CA:2427:C:H5''	1:CA:2428:G:OP1	2.14	0.47
3:CC:17:PRO:HG2	3:CC:18:ASN:H	1.79	0.47
3:CC:42:VAL:CG1	3:CC:43:GLU:H	2.28	0.47
7:CG:121:ASN:O	7:CG:124:SER:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:CH:139:GLN:HG3	8:CH:140:LYS:N	2.30	0.47
11:CN:67:LEU:HD13	11:CN:87:LEU:HD13	1.97	0.47
34:DA:1049:U:C5	34:DA:1201:A:H5'	2.50	0.47
34:DA:1126:U:C4'	34:DA:1281:U:H1'	2.44	0.47
35:DB:167:PRO:HD3	35:DB:187:LEU:O	2.15	0.47
36:DC:50:ALA:HB1	36:DC:70:VAL:HG21	1.96	0.47
36:DC:137:ALA:HA	36:DC:140:ARG:NH1	2.30	0.47
53:DT:50:GLU:H	53:DT:99:LEU:HD12	1.79	0.47
59:DZ:182:ARG:O	59:DZ:184:LYS:N	2.48	0.47
59:DZ:262:SER:HB3	59:DZ:267:LYS:HB2	1.96	0.47
1:AA:1095:C:C2'	1:AA:1096:A:H5'	2.45	0.47
3:AC:46:ALA:O	3:AC:47:LYS:HB2	2.15	0.47
4:AD:52:ARG:HB2	4:AD:53:PHE:CD2	2.50	0.47
9:AK:54:ALA:HB1	9:AK:83:TYR:O	2.14	0.47
27:A3:18:ASP:OD1	27:A3:18:ASP:N	2.48	0.47
27:A3:43:ILE:O	27:A3:47:VAL:HG23	2.15	0.47
34:BA:696:A:N1	34:BA:797:C:O2'	2.39	0.47
34:BA:738:C:H2'	34:BA:739:C:C6	2.50	0.47
34:BA:1391:U:H2'	34:BA:1392:G:C8	2.50	0.47
34:BA:1456:G:H1'	53:BT:39:LYS:NZ	2.30	0.47
42:BI:53:VAL:O	42:BI:55:ALA:N	2.48	0.47
46:BM:33:ALA:HB2	46:BM:64:TRP:HH2	1.80	0.47
59:BZ:226:ASN:HB3	59:BZ:241:GLU:OE2	2.15	0.47
1:CA:328:U:H4'	22:CY:68:HIS:CE1	2.50	0.47
1:CA:1713:U:H2'	1:CA:1714:G:H8	1.80	0.47
1:CA:2167:U:OP1	1:CA:2167:U:H4'	2.15	0.47
8:CH:7:LEU:HA	8:CH:8:PRO:HD3	1.80	0.47
13:CP:97:PRO:HD3	13:CP:126:VAL:O	2.15	0.47
20:CW:58:ALA:HB1	20:CW:64:MET:HB2	1.96	0.47
34:DA:828:A:N6	34:DA:858:G:O2'	2.47	0.47
34:DA:936:C:H2'	34:DA:937:A:O4'	2.15	0.47
47:DN:24:CYS:HB3	47:DN:27:CYS:SG	2.55	0.47
49:DP:57:ARG:NH2	49:DP:79:VAL:O	2.48	0.47
3:AC:17:PRO:HG2	3:AC:18:ASN:H	1.79	0.46
3:AC:223:VAL:HG23	3:AC:223:VAL:O	2.15	0.46
4:AD:242:ARG:N	4:AD:242:ARG:HD3	2.29	0.46
22:AY:23:ARG:HG2	22:AY:42:VAL:HG22	1.96	0.46
34:BA:1284:C:H3'	34:BA:1285:A:H8	1.80	0.46
34:BA:1346:A:N1	34:BA:1374:A:H5''	2.30	0.46
49:BP:20:VAL:HG21	49:BP:32:TYR:CG	2.50	0.46
58:BY:72:C:H2'	58:BY:73:A:O4'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:620:G:H5'	1:CA:620:G:N3	2.30	0.46
1:CA:882:G:H2'	1:CA:883:G:C8	2.46	0.46
9:CK:23:SER:HA	9:CK:117:LEU:O	2.15	0.46
19:CV:71:LEU:HD23	19:CV:71:LEU:HA	1.72	0.46
27:C3:6:VAL:HG13	27:C3:56:VAL:HG22	1.97	0.46
34:DA:900:A:H2'	34:DA:901:A:C8	2.50	0.46
34:DA:1289:A:C8	34:DA:1290:G:C8	3.03	0.46
36:DC:114:PRO:HA	36:DC:185:GLY:HA3	1.96	0.46
43:DJ:35:SER:HB3	43:DJ:73:ASP:HB2	1.97	0.46
57:DX:55:PSU:O2'	57:DX:57:A:N7	2.31	0.46
1:AA:1907:A:H2'	1:AA:1908:C:O4'	2.14	0.46
8:AH:40:GLU:OE2	8:AH:60:ARG:NH1	2.47	0.46
11:AN:75:TYR:CE2	11:AN:77:GLY:HA2	2.50	0.46
12:AO:2:ILE:HB	12:AO:33:ALA:HB3	1.97	0.46
20:AW:14:PRO:HG2	20:AW:78:GLU:CG	2.44	0.46
32:A8:39:LYS:O	32:A8:43:GLN:HG3	2.14	0.46
57:BX:55:PSU:O2'	57:BX:57:A:N7	2.37	0.46
59:BZ:233:GLU:HB3	59:BZ:234:GLY:H	1.54	0.46
1:CA:579:G:H2'	1:CA:580:C:C6	2.50	0.46
1:CA:740:U:H2'	1:CA:741:G:C8	2.51	0.46
1:CA:993:G:N2	19:CV:23:GLU:OE2	2.45	0.46
1:CA:2014:A:H2'	1:CA:2015:A:C8	2.50	0.46
1:CA:2336:A:H61	24:C0:43:THR:HG21	1.79	0.46
1:CA:2615:U:H2'	1:CA:2616:C:H6	1.80	0.46
3:CC:176:VAL:O	3:CC:176:VAL:HG12	2.15	0.46
4:CD:175:LEU:HD12	4:CD:185:VAL:HG21	1.97	0.46
8:CH:113:VAL:HG11	8:CH:151:ILE:HD13	1.96	0.46
10:CL:78:ILE:O	10:CL:78:ILE:HG12	2.15	0.46
15:CR:29:LEU:HD12	15:CR:29:LEU:HA	1.83	0.46
19:CV:6:LYS:HB2	19:CV:38:LEU:HD21	1.97	0.46
26:C2:9:GLN:OE1	26:C2:56:GLN:HG2	2.15	0.46
34:DA:543:C:O2'	34:DA:544:G:H5'	2.14	0.46
34:DA:992:U:O2'	34:DA:993:G:OP2	2.27	0.46
34:DA:1159:U:O4'	34:DA:1182:G:N2	2.47	0.46
34:DA:1347:G:N2	34:DA:1373:G:H2'	2.29	0.46
1:AA:397:G:H4'	1:AA:398:A:OP2	2.15	0.46
1:AA:1769:G:H2'	1:AA:1770:A:C8	2.51	0.46
5:AE:9:VAL:HB	17:AT:3:ARG:HG2	1.97	0.46
14:AQ:48:GLU:HB2	65:AQ:3104:HOH:O	2.14	0.46
18:AU:112:ARG:HH11	18:AU:112:ARG:CG	2.28	0.46
41:BH:20:TYR:HD2	41:BH:65:TYR:CE2	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:BJ:16:LEU:HD21	43:BJ:70:ARG:HG2	1.97	0.46
46:BM:84:ILE:HG13	46:BM:86:CYS:N	2.29	0.46
1:CA:32:C:O2'	1:CA:33:U:H5'	2.16	0.46
1:CA:861:A:C2	1:CA:917:A:C4	3.03	0.46
1:CA:1042:G:H1	1:CA:1113:U:H3	1.63	0.46
1:CA:2178:C:O2'	3:CC:169:THR:CB	2.56	0.46
1:CA:2454:G:H1'	65:CA:3889:HOH:O	2.15	0.46
14:CQ:21:THR:CG2	14:CQ:101:ARG:HH11	2.28	0.46
34:DA:147:G:H1	34:DA:175:C:H42	1.64	0.46
34:DA:179:A:H2'	34:DA:180:U:C6	2.50	0.46
34:DA:364:A:H2'	34:DA:365:U:H6	1.80	0.46
34:DA:724:G:C2	34:DA:725:G:C8	3.03	0.46
58:DY:25:C:H2'	58:DY:26:A:H8	1.80	0.46
59:DZ:620:VAL:O	59:DZ:624:LEU:HB2	2.16	0.46
1:AA:934:A:HO2'	1:AA:935:C:P	2.37	0.46
1:AA:1913:G:C6	1:AA:1914:C:C4	3.03	0.46
1:AA:2332:A:H2'	1:AA:2332:A:N3	2.31	0.46
1:AA:2430:A:H2'	1:AA:2431:U:C6	2.50	0.46
65:AA:5273:HOH:O	5:AE:147:PRO:HD2	2.15	0.46
3:AC:6:LYS:HA	3:AC:9:ARG:NH1	2.30	0.46
26:A2:35:LEU:HD23	26:A2:35:LEU:HA	1.63	0.46
34:BA:160:A:H2'	34:BA:160:A:N3	2.31	0.46
34:BA:487:A:H2'	34:BA:488:C:O4'	2.16	0.46
34:BA:923:A:OP1	38:BE:21:ALA:HB2	2.14	0.46
34:BA:1148:U:O3'	42:BI:14:VAL:HG11	2.15	0.46
35:BB:18:GLY:O	35:BB:19:HIS:HB3	2.16	0.46
44:BK:27:ASN:OD1	44:BK:55:LYS:HB3	2.15	0.46
51:BR:33:ASP:OD2	51:BR:36:ASN:HB2	2.16	0.46
59:BZ:19:ALA:HB1	59:BZ:23:ALA:HB3	1.97	0.46
59:BZ:165:GLN:HA	59:BZ:180:VAL:HG13	1.95	0.46
1:CA:580:C:H2'	1:CA:581:C:C6	2.51	0.46
1:CA:1001:A:H2'	1:CA:1002:G:O4'	2.14	0.46
1:CA:2261:C:O2'	1:CA:2262:U:H5'	2.15	0.46
1:CA:2430:A:OP2	65:CA:4250:HOH:O	2.20	0.46
1:CA:2483:C:OP1	56:DW:64:A:H4'	2.16	0.46
1:CA:2493:U:H2'	1:CA:2494:G:O4'	2.15	0.46
1:CA:2683:C:O2	12:CO:70:LYS:NZ	2.42	0.46
1:CA:2685:G:N7	65:CA:3903:HOH:O	2.36	0.46
7:CG:39:ILE:N	7:CG:39:ILE:HD12	2.31	0.46
8:CH:13:LYS:HA	8:CH:14:GLY:HA2	1.70	0.46
8:CH:147:ASN:N	8:CH:147:ASN:OD1	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:CL:76:TYR:CD2	10:CL:77:LEU:HD23	2.50	0.46
12:CO:1:MET:HG2	12:CO:67:LYS:HG2	1.96	0.46
16:CS:88:ASP:C	16:CS:90:GLY:H	2.19	0.46
33:C9:25:VAL:HB	33:C9:34:GLN:HB2	1.97	0.46
34:DA:186:C:H2'	34:DA:187:C:H6	1.80	0.46
34:DA:426:G:OP1	37:DD:36:ARG:HD2	2.16	0.46
34:DA:509:A:C8	34:DA:509:A:H3'	2.50	0.46
35:DB:167:PRO:HG3	35:DB:188:ALA:HB2	1.98	0.46
35:DB:218:ALA:O	35:DB:222:ILE:HG23	2.16	0.46
38:DE:68:GLU:OE1	38:DE:70:PRO:HG3	2.15	0.46
1:AA:449:A:H2'	1:AA:450:A:C8	2.50	0.46
1:AA:1343:C:OP1	1:AA:2722:C:H4'	2.16	0.46
3:AC:42:VAL:CG1	3:AC:43:GLU:H	2.27	0.46
7:AG:72:ARG:NH1	7:AG:87:PRO:HG3	2.31	0.46
7:AG:83:ARG:O	7:AG:86:MET:HB2	2.16	0.46
34:BA:52:G:H2'	34:BA:53:A:C8	2.50	0.46
38:BE:148:VAL:HG21	41:BH:107:LEU:HB3	1.98	0.46
40:BG:26:PHE:CE2	40:BG:30:ILE:HD11	2.50	0.46
46:BM:80:ARG:NH2	52:BS:69:HIS:HE1	2.14	0.46
53:BT:57:ARG:HH12	53:BT:100:ILE:HG13	1.79	0.46
59:BZ:145:ASP:HB3	59:BZ:148:LEU:HB3	1.98	0.46
59:BZ:670:VAL:HB	59:BZ:672:PHE:CZ	2.51	0.46
59:BZ:687:LEU:O	59:BZ:689:LYS:N	2.49	0.46
1:CA:621:A:OP2	13:CP:108:LYS:NZ	2.43	0.46
1:CA:908:C:O2'	1:CA:909:A:H5'	2.16	0.46
1:CA:1075:C:H5'	14:CQ:59:ARG:HH21	1.79	0.46
1:CA:1232:G:C6	1:CA:1233:C:C4	3.03	0.46
1:CA:1300:U:H4'	1:CA:1301:A:H5''	1.96	0.46
5:CE:12:THR:HG22	17:CT:58:ASN:HD21	1.81	0.46
6:CF:184:TYR:HE1	13:CP:3:LEU:HD21	1.80	0.46
14:CQ:135:ASP:HB3	14:CQ:137:TYR:H	1.79	0.46
34:DA:165:C:H2'	34:DA:166:G:C8	2.50	0.46
34:DA:1288:A:N1	34:DA:1371:G:H1'	2.30	0.46
36:DC:5:ILE:HD11	47:DN:49:HIS:HE1	1.79	0.46
43:DJ:65:LEU:HD13	47:DN:56:VAL:HG22	1.97	0.46
51:DR:32:ARG:HD2	51:DR:65:ILE:CG2	2.45	0.46
59:DZ:183:MET:SD	59:DZ:213:HIS:HB2	2.56	0.46
1:AA:2086:C:H2'	1:AA:2087:C:C6	2.50	0.46
1:AA:2274:U:H4'	1:AA:2340:A:C2	2.50	0.46
2:AB:66:A:H61	2:AB:108:U:H2'	1.79	0.46
3:AC:176:VAL:O	3:AC:176:VAL:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:176:ILE:HB	5:AE:181:LEU:HB2	1.97	0.46
7:AG:171:ALA:O	7:AG:175:LEU:HD22	2.14	0.46
17:AT:96:ARG:CZ	17:AT:96:ARG:HB3	2.46	0.46
34:BA:836:G:C6	34:BA:851:G:C6	3.04	0.46
34:BA:954:G:H2'	34:BA:955:U:C6	2.51	0.46
34:BA:1036:G:H3'	34:BA:1037:C:H6	1.81	0.46
37:BD:97:LEU:HD23	37:BD:97:LEU:HA	1.70	0.46
38:BE:83:GLU:HG2	38:BE:88:LYS:HD2	1.98	0.46
56:BW:18:G:O2'	56:BW:57:G:N2	2.44	0.46
57:BX:31:G:N7	57:BX:32:5MC:HM52	2.30	0.46
59:BZ:20:HIS:HA	59:BZ:117:GLN:CB	2.45	0.46
1:CA:125:G:OP1	31:C7:14:LYS:HE2	2.15	0.46
1:CA:996:A:C2	1:CA:997:G:C8	3.03	0.46
1:CA:1063:G:O2'	10:CL:89:HIS:O	2.33	0.46
1:CA:1449:A:H5'	1:CA:1450:G:OP2	2.15	0.46
1:CA:1889:A:H2'	1:CA:1890:A:C8	2.51	0.46
1:CA:2061:G:H5''	1:CA:2503:A:C2	2.51	0.46
13:CP:37:GLY:C	13:CP:38:GLN:O	2.49	0.46
19:CV:43:GLU:N	19:CV:43:GLU:OE2	2.49	0.46
34:DA:622:A:C8	34:DA:623:C:C6	3.04	0.46
59:DZ:409:ILE:HG12	59:DZ:459:LEU:HD12	1.97	0.46
1:AA:1057:G:OP1	18:AU:77:SER:OG	2.33	0.46
1:AA:1451:U:H2'	1:AA:1452:U:C6	2.51	0.46
1:AA:1817:A:H8	65:AA:5175:HOH:O	1.98	0.46
3:AC:20:VAL:O	3:AC:224:ARG:O	2.34	0.46
3:AC:211:ARG:HG2	3:AC:211:ARG:HH11	1.81	0.46
4:AD:145:VAL:HG12	4:AD:146:GLU:O	2.15	0.46
8:AH:69:ARG:HG3	8:AH:70:THR:N	2.28	0.46
15:AR:56:LYS:HE3	15:AR:87:TYR:O	2.16	0.46
26:A2:41:ILE:HG13	26:A2:43:GLN:HG3	1.97	0.46
34:BA:452:A:O2'	34:BA:453:A:OP2	2.28	0.46
34:BA:1318:A:OP1	52:BS:3:ARG:NH2	2.49	0.46
36:BC:181:ASN:ND2	36:BC:204:LEU:HD12	2.30	0.46
37:BD:8:VAL:O	37:BD:11:LEU:HB2	2.15	0.46
40:BG:18:TYR:CD2	40:BG:59:LEU:HD13	2.51	0.46
41:BH:132:GLU:O	41:BH:134:ILE:N	2.48	0.46
59:BZ:9:LEU:HD22	59:BZ:284:LEU:HD13	1.96	0.46
59:BZ:280:LEU:HA	59:BZ:281:PRO:HD3	1.76	0.46
59:BZ:342:TYR:N	59:BZ:390:VAL:O	2.47	0.46
1:CA:491:G:H2'	1:CA:492:A:H8	1.81	0.46
1:CA:1210:A:H5''	1:CA:1212:G:O4'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:2079:U:O3'	25:C1:35:THR:OG1	2.32	0.46
1:CA:2113:U:H3	1:CA:2170:A:N6	2.13	0.46
1:CA:2173:A:H2'	1:CA:2174:C:O4'	2.16	0.46
1:CA:2422:A:H5'	58:DY:76:A:H62	1.80	0.46
7:CG:103:LEU:HD23	7:CG:106:LEU:HD23	1.98	0.46
7:CG:109:VAL:HG21	28:C4:14:ILE:HD13	1.96	0.46
8:CH:90:LYS:HD2	8:CH:163:TYR:CD1	2.51	0.46
12:CO:64:ARG:HG2	12:CO:79:PHE:CD1	2.50	0.46
17:CT:106:SER:O	17:CT:110:ILE:HG13	2.15	0.46
34:DA:109:A:H2'	34:DA:326:G:N2	2.29	0.46
34:DA:921:U:H2'	34:DA:922:G:O4'	2.16	0.46
34:DA:1241:G:H2'	34:DA:1242:C:C6	2.51	0.46
34:DA:1318:A:H5''	52:DS:3:ARG:HH22	1.80	0.46
35:DB:90:MET:SD	35:DB:222:ILE:HD12	2.55	0.46
36:DC:77:ILE:HG13	36:DC:78:GLY:H	1.79	0.46
38:DE:5:ASP:OD1	38:DE:5:ASP:N	2.49	0.46
39:DF:30:LEU:HB3	39:DF:35:ALA:HB3	1.98	0.46
56:DW:44:G:H2'	56:DW:45:U:H5'	1.97	0.46
1:AA:553:A:C2	1:AA:2065:C:H4'	2.49	0.46
1:AA:834:U:H5''	1:AA:835:A:H5'	1.98	0.46
1:AA:1993:A:OP1	65:AA:4251:HOH:O	2.20	0.46
23:AZ:128:VAL:HG23	23:AZ:161:VAL:HA	1.97	0.46
34:BA:1104:G:H2'	34:BA:1105:A:H8	1.81	0.46
34:BA:1260:C:O5'	34:BA:1284:C:H4'	2.16	0.46
59:BZ:87:HIS:O	59:BZ:90:PHE:N	2.45	0.46
1:CA:27:G:C2	1:CA:512:G:N3	2.83	0.46
1:CA:271(O):C:H2'	1:CA:271(P):C:C6	2.51	0.46
1:CA:1584:C:H2'	1:CA:1586:A:H5'	1.97	0.46
1:CA:2395:C:H2'	1:CA:2396:G:O4'	2.15	0.46
3:CC:48:LEU:HD23	3:CC:59:VAL:HG21	1.98	0.46
3:CC:211:ARG:HG2	3:CC:211:ARG:HH11	1.81	0.46
5:CE:176:ILE:HB	5:CE:181:LEU:HB2	1.97	0.46
12:CO:111:PHE:O	12:CO:115:VAL:HG23	2.15	0.46
15:CR:33:ARG:HE	15:CR:113:LEU:HD22	1.80	0.46
22:CY:9:LYS:HA	22:CY:10:GLY:HA2	1.59	0.46
22:CY:44:ILE:HA	22:CY:63:LYS:O	2.16	0.46
34:DA:955:U:H2'	34:DA:956:U:O4'	2.16	0.46
34:DA:1305:G:H5'	54:DU:4:GLY:HA3	1.97	0.46
40:DG:113:GLU:HB2	40:DG:119:ARG:HG2	1.97	0.46
45:DL:85:ILE:HG22	45:DL:100:ILE:HG12	1.97	0.46
1:AA:1550:C:H2'	1:AA:1551:C:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:AR:44:LEU:HD22	15:AR:48:VAL:HG23	1.98	0.46
23:AZ:139:VAL:HG22	23:AZ:155:LEU:HD11	1.96	0.46
34:BA:189(B):C:N3	34:BA:189(J):G:C2	2.84	0.46
34:BA:1161:C:H2'	34:BA:1162:C:C6	2.51	0.46
43:BJ:31:GLY:HA2	43:BJ:32:ALA:HA	1.44	0.46
59:BZ:177:ILE:HD12	59:BZ:188:TYR:HE2	1.80	0.46
59:BZ:617:MET:HG2	59:BZ:643:ILE:HD11	1.96	0.46
1:CA:1902:C:H5'	4:CD:246:PRO:HD3	1.98	0.46
2:CB:76:G:H2'	2:CB:77:U:O4'	2.16	0.46
3:CC:46:ALA:O	3:CC:47:LYS:HB2	2.15	0.46
5:CE:108:SER:HB3	5:CE:165:VAL:HG21	1.97	0.46
34:DA:1095:U:H2'	34:DA:1096:C:O4'	2.16	0.46
34:DA:1216:G:H5''	47:DN:5:ALA:HB2	1.97	0.46
36:DC:54:ARG:HB3	36:DC:54:ARG:NH1	2.30	0.46
48:DO:25:THR:HG21	48:DO:70:LEU:HB2	1.98	0.46
59:DZ:236:GLU:H	59:DZ:236:GLU:HG3	1.40	0.46
1:AA:801:C:H2'	1:AA:802:C:H6	1.81	0.46
1:AA:1067:A:H62	1:AA:1186:U:H3	1.63	0.46
1:AA:2087:C:H2'	1:AA:2088:C:C6	2.51	0.46
1:AA:2365:G:H1'	24:A0:34:GLY:HA3	1.97	0.46
2:AB:7:G:H5'	16:AS:29:PHE:CE2	2.51	0.46
32:A8:29:LYS:HB2	32:A8:33:ASN:HD21	1.81	0.46
34:BA:973:G:H3'	34:BA:974:A:H5''	1.98	0.46
34:BA:1350:A:C6	34:BA:1351:U:N3	2.84	0.46
37:BD:120:LEU:HB3	37:BD:126:ILE:HD11	1.97	0.46
40:BG:104:LEU:HD13	40:BG:104:LEU:HA	1.55	0.46
46:BM:65:LYS:O	46:BM:70:LEU:HG	2.16	0.46
57:BX:23:C:H2'	57:BX:24:U:C6	2.51	0.46
59:BZ:-38:TYR:CD2	59:BZ:-37:LEU:HD23	2.51	0.46
1:CA:1053:C:H2'	1:CA:1054:A:O5'	2.16	0.46
1:CA:1545:A:H2'	1:CA:1546:C:O4'	2.16	0.46
1:CA:1589:C:H2'	1:CA:1590:U:H6	1.78	0.46
1:CA:2630:G:H2'	1:CA:2631:G:C8	2.50	0.46
1:CA:2677:G:H2'	1:CA:2678:C:C6	2.51	0.46
1:CA:2741:A:H2'	1:CA:2742:C:O4'	2.16	0.46
31:C7:24:THR:O	31:C7:28:ARG:HG3	2.16	0.46
34:DA:1014:A:OP1	52:DS:18:LYS:NZ	2.49	0.46
35:DB:96:ARG:O	35:DB:98:LEU:N	2.49	0.46
37:DD:4:TYR:O	37:DD:5:ILE:HG22	2.16	0.46
39:DF:10:LEU:HD12	39:DF:85:VAL:HA	1.98	0.46
59:DZ:-41:ALA:O	59:DZ:-36:LEU:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:DZ:546:ILE:HD13	59:DZ:565:VAL:HG11	1.98	0.46
1:AA:1153:G:H4'	9:AK:81:VAL:HA	1.98	0.45
1:AA:1314:A:H2'	1:AA:1315:A:O4'	2.16	0.45
1:AA:1345:G:H5'	1:AA:1347:A:O4'	2.16	0.45
1:AA:1462:G:O2'	1:AA:1463:C:H5	1.99	0.45
1:AA:1529:G:C6	1:AA:1553:A:C6	3.04	0.45
1:AA:2128:G:H1	1:AA:2205:C:N4	2.05	0.45
2:AB:7:G:H5'	16:AS:29:PHE:CD2	2.51	0.45
8:AH:90:LYS:HD2	8:AH:163:TYR:CD1	2.52	0.45
12:AO:115:VAL:HG13	12:AO:121:VAL:HG21	1.98	0.45
14:AQ:2:LEU:HB2	14:AQ:70:PRO:CG	2.46	0.45
21:AX:13:LEU:HD11	26:A2:41:ILE:HG22	1.97	0.45
34:BA:228:A:H2'	34:BA:229:U:O4'	2.16	0.45
34:BA:236:G:OP1	50:BQ:40:LYS:NZ	2.49	0.45
34:BA:1298:C:H4'	34:BA:1299:A:C4	2.51	0.45
35:BB:21:ARG:H	35:BB:21:ARG:HH21	1.65	0.45
46:BM:94:ARG:NH1	52:BS:80:TYR:HD2	2.14	0.45
52:BS:63:THR:HG23	52:BS:66:MET:HE3	1.98	0.45
1:CA:784:A:H5'	1:CA:785:G:OP1	2.16	0.45
1:CA:1063:G:H2'	1:CA:1064:C:C6	2.50	0.45
3:CC:37:LYS:O	3:CC:38:PHE:HB3	2.17	0.45
4:CD:275:LYS:HA	4:CD:276:LYS:C	2.36	0.45
5:CE:21:VAL:HA	5:CE:22:PRO:HD3	1.72	0.45
16:CS:29:PHE:HD1	16:CS:92:TYR:HH	1.61	0.45
34:DA:242:C:H2'	34:DA:243:A:H5'	1.96	0.45
34:DA:860:A:N6	34:DA:861:G:C2	2.84	0.45
34:DA:1023:G:H3'	34:DA:1024:G:H8	1.81	0.45
34:DA:1254:C:O5'	34:DA:1254:C:H6	1.99	0.45
34:DA:1431:C:H2'	34:DA:1432:G:O4'	2.16	0.45
41:DH:127:LEU:HA	41:DH:127:LEU:HD13	1.73	0.45
45:DL:6:THR:HG23	45:DL:9:GLN:OE1	2.16	0.45
49:DP:74:LEU:HG	49:DP:79:VAL:HG21	1.97	0.45
59:DZ:75:LYS:HA	59:DZ:75:LYS:NZ	2.31	0.45
1:AA:67:G:H2'	1:AA:68:C:O4'	2.16	0.45
1:AA:669:A:H4'	1:AA:670:C:H5	1.81	0.45
1:AA:1097:G:H1	1:AA:1154:U:H5	1.64	0.45
1:AA:1261:G:OP2	18:AU:12:ARG:NH2	2.42	0.45
1:AA:2299:A:N6	1:AA:2356:U:H3	2.05	0.45
1:AA:2451:A:C5'	1:AA:2451:A:C8	3.00	0.45
1:AA:2812:A:H1'	1:AA:2904:U:H1'	1.97	0.45
5:AE:167:VAL:HG23	5:AE:170:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AH:41:MET:CE	8:AH:65:HIS:HA	2.46	0.45
21:AX:43:VAL:HG13	21:AX:47:PHE:HD2	1.81	0.45
28:A4:14:ILE:HB	28:A4:22:ILE:HB	1.97	0.45
36:BC:45:LYS:HE3	36:BC:45:LYS:HB2	1.78	0.45
40:BG:78:ARG:NH1	40:BG:79:ARG:HD2	2.31	0.45
44:BK:120:ARG:HA	44:BK:121:PRO:HD3	1.79	0.45
58:BY:40:C:H2'	58:BY:41:C:H6	1.82	0.45
1:CA:1022:G:C5	1:CA:1140:C:C4	3.04	0.45
1:CA:1406:U:H2'	1:CA:1407:C:C6	2.50	0.45
1:CA:1477:A:C2	1:CA:1515:G:C2	3.05	0.45
1:CA:1803:A:H4'	4:CD:259:THR:HG23	1.99	0.45
1:CA:2123:G:H2'	1:CA:2124:G:C8	2.51	0.45
1:CA:2722:G:H2'	1:CA:2723:C:C6	2.51	0.45
2:CB:21:G:H2'	2:CB:22:U:O4'	2.16	0.45
8:CH:144:VAL:O	8:CH:148:ILE:HG12	2.16	0.45
28:C4:33:VAL:HG12	28:C4:35:VAL:H	1.81	0.45
34:DA:160:A:H2'	34:DA:161:A:O4'	2.16	0.45
34:DA:601:C:H2'	34:DA:602:A:C8	2.51	0.45
34:DA:731:G:H5'	34:DA:766:A:H4'	1.97	0.45
34:DA:980:C:HO2'	47:DN:21:TYR:HE2	1.64	0.45
35:DB:44:LEU:HD22	35:DB:44:LEU:H	1.81	0.45
37:DD:153:ARG:HB2	37:DD:181:MET:SD	2.57	0.45
46:DM:90:LEU:HD22	46:DM:93:ARG:HE	1.81	0.45
53:DT:36:LEU:HD12	53:DT:55:ILE:HG23	1.97	0.45
57:DX:72:A:C6	57:DX:73:A:C6	3.04	0.45
58:DY:30:G:H2'	58:DY:31:A:H8	1.81	0.45
59:DZ:166:LEU:O	59:DZ:178:ILE:N	2.41	0.45
59:DZ:609:GLU:O	59:DZ:669:PHE:HA	2.15	0.45
1:AA:354:A:H2	1:AA:1255:A:O2'	1.99	0.45
1:AA:2199:C:O2	3:AC:173:HIS:HE1	1.99	0.45
1:AA:2500:A:H2'	1:AA:2501:G:O4'	2.16	0.45
4:AD:85:ASP:OD2	4:AD:88:ARG:HD2	2.15	0.45
4:AD:106:ILE:O	4:AD:108:PRO:HD3	2.16	0.45
11:AN:4:TYR:CD2	18:AU:100:VAL:HG11	2.52	0.45
21:AX:61:GLY:HA3	21:AX:73:ARG:O	2.17	0.45
23:AZ:54:HIS:O	23:AZ:98:MET:HE1	2.16	0.45
34:BA:13:U:OP1	65:BA:2020:HOH:O	2.21	0.45
34:BA:255:G:H2'	34:BA:256:U:C6	2.52	0.45
34:BA:1417:G:N2	34:BA:1482:G:H2'	2.32	0.45
37:BD:194:LEU:HD12	37:BD:195:ALA:H	1.81	0.45
44:BK:20:TYR:HB2	44:BK:31:THR:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:BK:59:TYR:CE2	44:BK:63:LEU:HD12	2.51	0.45
49:BP:40:ASP:HA	49:BP:41:PRO:HD2	1.76	0.45
53:BT:42:GLN:HG3	53:BT:43:LEU:HD23	1.99	0.45
57:BX:67:C:C2'	57:BX:68:C:H5'	2.46	0.45
59:BZ:10:LYS:O	59:BZ:282:SER:HB2	2.16	0.45
59:BZ:264:LEU:HD12	64:BZ:702:GDP:N3	2.31	0.45
1:CA:602:G:O2'	1:CA:655:A:N6	2.49	0.45
1:CA:1342:A:O2'	1:CA:1344:G:OP2	2.26	0.45
1:CA:2029:G:H2'	1:CA:2031:A:OP1	2.16	0.45
1:CA:2135:A:H2'	1:CA:2136:C:C6	2.51	0.45
22:CY:83:THR:OG1	22:CY:84:ARG:N	2.50	0.45
23:CZ:45:ASP:O	23:CZ:49:ARG:HG3	2.16	0.45
34:DA:302:G:N3	34:DA:556:C:H4'	2.30	0.45
34:DA:369:C:OP2	34:DA:388:G:N2	2.37	0.45
34:DA:757:U:H2'	34:DA:758:G:O4'	2.15	0.45
34:DA:1024:G:C2'	34:DA:1025:U:H5''	2.45	0.45
34:DA:1104:G:C4	34:DA:1105:A:C8	3.04	0.45
34:DA:1205:U:H4'	36:DC:195:VAL:HG23	1.97	0.45
34:DA:1216:G:H5''	47:DN:5:ALA:CB	2.46	0.45
36:DC:104:GLN:HE21	36:DC:105:GLU:N	2.13	0.45
54:DU:2:GLY:O	54:DU:4:GLY:N	2.49	0.45
59:DZ:560:VAL:HG11	59:DZ:594:VAL:HG11	1.99	0.45
1:AA:611:U:O4	1:AA:717:A:H1'	2.15	0.45
1:AA:2804:C:H2'	1:AA:2805:G:H8	1.82	0.45
7:AG:120:LEU:HD12	7:AG:179:PRO:HD2	1.99	0.45
28:A4:59:PHE:HA	28:A4:61:ARG:HG2	1.98	0.45
34:BA:435:C:H2'	34:BA:436:C:C6	2.51	0.45
34:BA:580:U:H2'	34:BA:581:G:O4'	2.16	0.45
34:BA:695:A:H2'	34:BA:696:A:O4'	2.17	0.45
34:BA:718:G:C8	44:BK:116:HIS:HB3	2.51	0.45
43:BJ:64:GLU:HB3	47:BN:59:ALA:HB2	1.99	0.45
43:BJ:67:THR:O	43:BJ:67:THR:OG1	2.34	0.45
47:BN:23:ARG:HD2	47:BN:28:GLY:O	2.16	0.45
59:BZ:14:ASN:OD1	59:BZ:80:ASN:HB2	2.16	0.45
59:BZ:170:ARG:O	59:BZ:173:THR:OG1	2.33	0.45
1:CA:1364:G:P	25:C1:3:LYS:HG3	2.56	0.45
1:CA:1488:G:C6	1:CA:1489:U:N3	2.85	0.45
1:CA:1773:A:H5''	65:CA:4317:HOH:O	2.15	0.45
1:CA:2135:A:OP1	1:CA:2160:G:H1'	2.16	0.45
1:CA:2881:C:H2'	1:CA:2882:A:O4'	2.16	0.45
4:CD:71:ASP:HB3	4:CD:103:ARG:NH2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:CF:184:TYR:O	6:CF:188:ARG:HG3	2.15	0.45
28:C4:16:CYS:SG	28:C4:36:CYS:HB3	2.57	0.45
34:DA:604:G:H2'	34:DA:605:U:O4'	2.16	0.45
34:DA:641:U:O2	34:DA:642:A:N6	2.25	0.45
49:DP:22:THR:HA	49:DP:33:ILE:HG13	1.99	0.45
59:DZ:74:TRP:HA	59:DZ:74:TRP:CE3	2.49	0.45
59:DZ:215:LYS:O	59:DZ:219:VAL:HG23	2.16	0.45
1:AA:303:C:H42	1:AA:385:G:H1	1.63	0.45
1:AA:386:U:O2'	1:AA:387:G:H5''	2.16	0.45
1:AA:555:G:C5	1:AA:2044:U:H5''	2.51	0.45
1:AA:1336:C:H2'	1:AA:1337:C:C6	2.52	0.45
1:AA:1848:G:H2'	1:AA:1849:U:H5'	1.98	0.45
1:AA:2556:G:H1'	1:AA:2658:C:H4'	1.99	0.45
1:AA:2702:C:OP2	1:AA:2702:C:H6	1.99	0.45
1:AA:2891:C:H2'	1:AA:2892:A:O4'	2.17	0.45
2:AB:32:C:C2	2:AB:51:G:N2	2.85	0.45
3:AC:37:LYS:O	3:AC:38:PHE:HB3	2.17	0.45
3:AC:48:LEU:HD23	3:AC:59:VAL:HG21	1.98	0.45
23:AZ:28:MET:HA	23:AZ:88:PHE:O	2.17	0.45
28:A4:40:HIS:CE1	28:A4:42:PHE:HB3	2.52	0.45
34:BA:1118:C:OP1	42:BI:104:ARG:NH1	2.49	0.45
34:BA:1392:G:H21	34:BA:1502:A:H8	1.63	0.45
35:BB:16:HIS:CD2	35:BB:17:PHE:N	2.85	0.45
35:BB:16:HIS:C	35:BB:18:GLY:H	2.18	0.45
35:BB:208:ILE:H	35:BB:208:ILE:HD12	1.82	0.45
37:BD:65:ARG:HG2	37:BD:75:PHE:CD1	2.52	0.45
37:BD:126:ILE:HG22	37:BD:127:THR:H	1.82	0.45
40:BG:12:LEU:H	40:BG:12:LEU:HD12	1.80	0.45
48:BO:25:THR:HG21	48:BO:70:LEU:HB2	1.96	0.45
59:BZ:660:ARG:HE	59:BZ:665:GLY:HA2	1.82	0.45
1:CA:72:U:OP2	26:C2:29:LYS:NZ	2.44	0.45
1:CA:271(H):G:O2'	1:CA:271(I):G:H8	2.00	0.45
1:CA:1109:C:H2'	1:CA:1110:G:N7	2.31	0.45
1:CA:2275:C:H5'	1:CA:2275:C:C6	2.51	0.45
3:CC:20:VAL:O	3:CC:224:ARG:O	2.34	0.45
8:CH:3:ARG:NH2	8:CH:5:GLY:H	2.14	0.45
11:CN:4:TYR:CD2	18:CU:100:VAL:HG11	2.51	0.45
16:CS:3:ARG:HE	16:CS:4:LEU:N	2.14	0.45
18:CU:27:LEU:HB3	18:CU:31:SER:HB3	1.98	0.45
34:DA:97:G:O2'	34:DA:98:G:H5''	2.16	0.45
52:DS:15:LEU:HD12	52:DS:18:LYS:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:DZ:20:HIS:CE1	59:DZ:117:GLN:HG3	2.52	0.45
1:AA:517:A:H2'	1:AA:518:G:O4'	2.17	0.45
1:AA:2051:G:H2'	1:AA:2053:A:OP1	2.16	0.45
1:AA:2564:U:O2	1:AA:2566:U:H5'	2.17	0.45
1:AA:2792:U:H5'	1:AA:2794:A:O4'	2.16	0.45
13:AP:63:PRO:HG2	32:A8:25:MET:HB2	1.97	0.45
20:AW:10:VAL:HG21	20:AW:103:ILE:HD12	1.98	0.45
22:AY:92:ASN:HD22	22:AY:92:ASN:N	2.07	0.45
25:A1:94:LEU:HD23	25:A1:94:LEU:HA	1.72	0.45
32:A8:54:GLU:OE1	32:A8:54:GLU:HA	2.17	0.45
33:A9:7:VAL:HG12	33:A9:34:GLN:HB3	1.97	0.45
34:BA:262:A:C6	34:BA:263:A:C6	3.04	0.45
34:BA:667:G:H4'	48:BO:51:HIS:ND1	2.32	0.45
34:BA:865:A:H2'	34:BA:866:C:C6	2.52	0.45
37:BD:108:LEU:HB3	37:BD:110:PHE:CE1	2.52	0.45
40:BG:91:VAL:HB	40:BG:96:GLN:HG2	1.99	0.45
42:BI:46:ALA:HB1	42:BI:77:ILE:HG22	1.98	0.45
50:BQ:32:TYR:O	50:BQ:34:LYS:N	2.41	0.45
59:BZ:-9:LEU:HD12	59:BZ:-9:LEU:HA	1.71	0.45
59:BZ:93:GLU:HA	59:BZ:96:ARG:HG3	1.99	0.45
59:BZ:182:ARG:O	59:BZ:184:LYS:N	2.50	0.45
1:CA:1064:C:H3'	1:CA:1065:U:C6	2.51	0.45
1:CA:2318:G:N3	1:CA:2318:G:O2'	2.48	0.45
3:CC:194:ILE:HD11	3:CC:227:PRO:HB2	1.99	0.45
3:CC:203:GLU:CD	3:CC:203:GLU:N	2.70	0.45
3:CC:223:VAL:HG23	3:CC:223:VAL:O	2.15	0.45
16:CS:94:TYR:CE1	16:CS:99:LYS:HG3	2.52	0.45
26:C2:37:PHE:O	26:C2:40:SER:OG	2.31	0.45
29:C5:20:ARG:HG2	29:C5:23:HIS:CE1	2.51	0.45
34:DA:503:C:H2'	34:DA:504:C:H6	1.81	0.45
35:DB:51:LEU:O	35:DB:55:PHE:N	2.25	0.45
36:DC:105:GLU:OE1	36:DC:107:GLN:N	2.50	0.45
37:DD:31:CYS:O	37:DD:35:ARG:HG3	2.17	0.45
37:DD:163:GLU:O	37:DD:166:LYS:HG3	2.16	0.45
39:DF:2:ARG:HE	39:DF:69:GLU:HG2	1.80	0.45
59:DZ:357:ARG:NH1	59:DZ:373:ASP:OD1	2.49	0.45
1:AA:269:G:N7	1:AA:270:C:N4	2.65	0.45
1:AA:471:C:H2'	1:AA:472:G:O4'	2.16	0.45
1:AA:1817:A:H1'	1:AA:1960:A:N6	2.32	0.45
1:AA:2105:G:O5'	1:AA:2105:G:H8	2.00	0.45
1:AA:2343:G:O2'	24:A0:43:THR:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:2575:U:O2	1:AA:2577:A:H8	2.00	0.45
3:AC:7:ARG:HH22	3:AC:219:MET:HB2	1.82	0.45
3:AC:16:ASP:OD2	3:AC:19:LYS:HB2	2.17	0.45
5:AE:110:GLY:O	65:AR:5101:HOH:O	2.21	0.45
34:BA:949:A:H2'	34:BA:950:U:O4'	2.17	0.45
34:BA:1402:C:H2'	34:BA:1403:C:O4'	2.17	0.45
35:BB:172:ILE:H	35:BB:172:ILE:HG13	1.56	0.45
39:BF:33:TYR:HE2	39:BF:78:GLU:HG2	1.81	0.45
57:BX:19:G:C5	57:BX:57:A:C2	3.05	0.45
59:BZ:78:ARG:HE	59:BZ:357:ARG:CZ	2.29	0.45
59:BZ:82:ILE:HD13	59:BZ:100:VAL:HG12	1.98	0.45
1:CA:263:C:H2'	1:CA:264:C:O4'	2.17	0.45
1:CA:1030:G:N2	33:C9:5:ALA:O	2.50	0.45
1:CA:1043:C:H2'	1:CA:1044:G:H8	1.82	0.45
2:CB:106:G:H5'	23:CZ:31:ARG:HG2	1.97	0.45
6:CF:196:LEU:HA	6:CF:196:LEU:HD23	1.54	0.45
8:CH:7:LEU:HD23	8:CH:69:ARG:NH1	2.31	0.45
22:CY:35:TYR:CD2	22:CY:69:ALA:HB3	2.51	0.45
34:DA:429:U:H5'	37:DD:9:CYS:SG	2.56	0.45
34:DA:1097:C:H2'	34:DA:1098:C:H6	1.81	0.45
49:DP:14:ASN:N	49:DP:15:PRO:HD3	2.31	0.45
59:DZ:225:GLU:CD	59:DZ:225:GLU:H	2.18	0.45
59:DZ:535:PRO:O	59:DZ:539:ILE:HG12	2.17	0.45
1:AA:1378:G:OP1	65:AA:4576:HOH:O	2.21	0.45
1:AA:1476:C:H2'	1:AA:1477:U:H6	1.81	0.45
1:AA:1478:C:H2'	1:AA:1479:U:O4'	2.16	0.45
1:AA:1671:C:H2'	1:AA:1672:G:O4'	2.17	0.45
3:AC:54:ARG:HH22	3:AC:56:ASP:HB3	1.76	0.45
59:BZ:-32:LEU:HD23	59:BZ:-32:LEU:HA	1.82	0.45
59:BZ:14:ASN:HD22	59:BZ:329:ARG:HH21	1.64	0.45
59:BZ:87:HIS:CB	59:BZ:90:PHE:HB3	2.46	0.45
59:BZ:304:ASP:HA	59:BZ:305:PRO:HD2	1.81	0.45
1:CA:362:U:O2'	1:CA:363:G:H5'	2.17	0.45
1:CA:533:G:H5'	18:CU:24:TYR:CE1	2.52	0.45
1:CA:2751:G:H4'	8:CH:4:ILE:HD11	1.99	0.45
7:CG:115:ARG:HH11	7:CG:115:ARG:H	1.63	0.45
23:CZ:40:ASP:HB3	23:CZ:43:GLU:HG3	1.98	0.45
34:DA:644:G:H4'	41:DH:92:ARG:NH2	2.31	0.45
34:DA:926:G:C6	34:DA:1505:G:C5	3.05	0.45
36:DC:148:GLY:HA3	36:DC:172:ARG:O	2.16	0.45
1:AA:669:A:H4'	1:AA:670:C:C5	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:203:GLU:CD	3:AC:203:GLU:N	2.70	0.45
5:AE:47:VAL:HG22	5:AE:84:PHE:O	2.17	0.45
8:AH:13:LYS:HA	8:AH:14:GLY:HA2	1.71	0.45
8:AH:71:LEU:HD12	8:AH:71:LEU:HA	1.81	0.45
13:AP:125:VAL:O	13:AP:125:VAL:HG23	2.17	0.45
29:A5:35:GLU:HG3	29:A5:51:TYR:CG	2.52	0.45
51:BR:66:LEU:O	51:BR:70:ILE:HG13	2.17	0.45
53:BT:100:ILE:H	53:BT:100:ILE:HG12	1.43	0.45
59:BZ:98:MET:HG2	59:BZ:101:LEU:HD12	1.98	0.45
1:CA:271(A):A:N7	1:CA:271(W):G:N2	2.60	0.45
1:CA:2727:G:O2'	12:CO:70:LYS:NZ	2.48	0.45
25:C1:77:ALA:HB1	25:C1:82:LEU:HD11	1.99	0.45
34:DA:49:U:O4	34:DA:365:U:H5	2.00	0.45
34:DA:111:G:O6	34:DA:330:C:N4	2.44	0.45
34:DA:176:C:H2'	34:DA:177:C:H6	1.81	0.45
34:DA:297:G:N2	34:DA:300:A:OP2	2.45	0.45
34:DA:600:C:C2	34:DA:639:G:C2	3.05	0.45
34:DA:1058:G:H2'	34:DA:1059:C:C6	2.52	0.45
34:DA:1151:A:O2'	34:DA:1152:A:H8	2.00	0.45
34:DA:1157:A:H5'	34:DA:1158:C:C6	2.52	0.45
42:DI:9:ARG:O	42:DI:104:ARG:HG3	2.17	0.45
59:DZ:181:LEU:O	59:DZ:183:MET:N	2.50	0.45
59:DZ:358:MET:HE1	59:DZ:363:ARG:HH12	1.82	0.45
59:DZ:517:LEU:HD13	59:DZ:564:LYS:HB2	1.99	0.45
1:AA:2228:G:O2'	1:AA:2229:A:OP1	2.31	0.45
2:AB:91:C:OP1	14:AQ:16:ARG:HG3	2.17	0.45
3:AC:179:ALA:O	3:AC:180:SER:O	2.35	0.45
4:AD:93:ALA:HB3	4:AD:105:ILE:HG13	1.99	0.45
10:AL:103:GLN:HA	10:AL:106:GLU:HG2	1.98	0.45
15:AR:54:LEU:HD12	15:AR:54:LEU:HA	1.66	0.45
24:A0:24:LYS:O	24:A0:25:ARG:HD3	2.16	0.45
34:BA:453:A:C6	34:BA:454:C:C4	3.05	0.45
34:BA:620:C:H2'	34:BA:621:A:O4'	2.16	0.45
34:BA:838:G:N2	34:BA:849:C:C2	2.85	0.45
48:BO:14:GLU:O	48:BO:14:GLU:HG3	2.17	0.45
49:BP:74:LEU:HG	49:BP:79:VAL:HG21	1.99	0.45
57:BX:31:G:C8	57:BX:32:5MC:HM52	2.52	0.45
59:BZ:-66:MET:N	59:BZ:-46:VAL:O	2.49	0.45
59:BZ:178:ILE:HA	59:BZ:185:ALA:HB2	1.99	0.45
1:CA:89:G:H3'	1:CA:90:U:H5''	1.98	0.45
1:CA:1059:G:O2'	10:CL:126:MET:O	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1494:A:H2'	1:CA:1495:A:C8	2.52	0.45
1:CA:2298:A:N6	1:CA:2318:G:C8	2.85	0.45
3:CC:30:VAL:CG2	3:CC:31:LYS:H	2.27	0.45
3:CC:179:ALA:O	3:CC:180:SER:O	2.35	0.45
5:CE:31:CYS:HA	5:CE:32:PRO:HD2	1.83	0.45
11:CN:58:ASP:OD1	11:CN:125:GLY:N	2.32	0.45
23:CZ:104:PHE:HA	23:CZ:139:VAL:HB	1.99	0.45
25:C1:3:LYS:HB2	25:C1:61:ARG:HH11	1.79	0.45
34:DA:10:A:OP2	38:DE:126:ARG:HD2	2.17	0.45
34:DA:1254:C:OP1	43:DJ:45:ARG:HA	2.16	0.45
36:DC:130:VAL:O	36:DC:134:ILE:HG12	2.17	0.45
38:DE:144:THR:OG1	38:DE:147:ASP:OD2	2.24	0.45
45:DL:70:ILE:HD13	45:DL:75:HIS:CD2	2.51	0.45
46:DM:59:TYR:CE1	46:DM:63:THR:HG21	2.52	0.45
50:DQ:40:LYS:HD3	50:DQ:42:TYR:CZ	2.52	0.45
56:DW:21:A:N6	56:DW:46:7MG:C4	2.85	0.45
59:DZ:246:ILE:HG23	59:DZ:255:ILE:HD11	1.99	0.45
59:DZ:257:PRO:HB2	59:DZ:259:PHE:HE1	1.82	0.45
59:DZ:462:ILE:O	59:DZ:466:LEU:HB2	2.17	0.45
1:AA:864:C:O2'	1:AA:886:U:H5''	2.17	0.44
1:AA:987:G:O2'	1:AA:988:U:H5'	2.17	0.44
1:AA:1002:A:N1	1:AA:2470:G:H4'	2.32	0.44
1:AA:1108:G:H1	1:AA:1122:C:H42	1.65	0.44
1:AA:2650:G:P	5:AE:82:ARG:NH2	2.90	0.44
5:AE:120:TRP:CE2	5:AE:155:LYS:HG2	2.52	0.44
7:AG:145:THR:H	7:AG:148:MET:HE2	1.81	0.44
11:AN:39:ARG:HA	11:AN:40:PRO:HD3	1.80	0.44
28:A4:15:ILE:HD13	28:A4:21:VAL:HG13	1.99	0.44
34:BA:43:C:H42	34:BA:399:G:H1	1.65	0.44
34:BA:506:G:C5	34:BA:507:C:C4	3.05	0.44
34:BA:551:U:H2'	34:BA:552:U:C6	2.52	0.44
34:BA:1005:A:H1'	34:BA:1036:G:H22	1.82	0.44
34:BA:1014:A:H4'	52:BS:14:HIS:CD2	2.52	0.44
34:BA:1152:A:OP1	43:BJ:68:HIS:ND1	2.49	0.44
35:BB:162:ILE:HD11	35:BB:184:VAL:HG22	1.99	0.44
43:BJ:78:ASN:O	43:BJ:80:LYS:N	2.50	0.44
56:BW:13:C:HO2'	56:BW:14:A:P	2.39	0.44
1:CA:530:G:N3	1:CA:530:G:O4'	2.49	0.44
1:CA:1517:G:C6	1:CA:1518:U:N3	2.85	0.44
1:CA:2305:A:H2'	1:CA:2306:C:O4'	2.17	0.44
2:CB:3:C:H2'	2:CB:4:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CC:7:ARG:HH22	3:CC:219:MET:HB2	1.82	0.44
8:CH:3:ARG:HB3	8:CH:6:ARG:HG2	1.99	0.44
34:DA:15:G:H2'	34:DA:16:A:H8	1.81	0.44
34:DA:423:G:H3'	34:DA:423:G:N3	2.32	0.44
34:DA:838:G:H1	34:DA:848:C:N4	2.09	0.44
34:DA:1270:C:H2'	34:DA:1271:G:C8	2.51	0.44
34:DA:1320:C:OP1	52:DS:70:LYS:HE2	2.18	0.44
35:DB:54:THR:HG21	35:DB:201:ILE:HD11	1.98	0.44
37:DD:12:CYS:HB3	37:DD:17:VAL:O	2.17	0.44
47:DN:22:THR:HB	47:DN:33:VAL:CB	2.47	0.44
53:DT:92:LEU:HD23	53:DT:92:LEU:HA	1.81	0.44
58:DY:35:A:H2'	58:DY:36:A:O4'	2.17	0.44
58:DY:37:MIA:H2'	58:DY:38:A:O4'	2.17	0.44
59:DZ:552:SER:HB3	59:DZ:591:LYS:NZ	2.32	0.44
1:AA:116:A:H3'	1:AA:117:A:C5'	2.48	0.44
1:AA:320:C:H2'	1:AA:321:C:H6	1.81	0.44
1:AA:795:G:C8	20:AW:89:ALA:HB1	2.51	0.44
1:AA:866:A:H8	1:AA:866:A:H5''	1.82	0.44
1:AA:1099:C:H2'	1:AA:1100:A:H5''	1.99	0.44
1:AA:1177:G:H21	11:AN:73:THR:CG2	2.30	0.44
1:AA:1355:G:P	31:A7:9:ARG:HD3	2.58	0.44
1:AA:1809:U:H2'	1:AA:1815:A:N6	2.33	0.44
3:AC:55:SER:C	3:AC:57:GLN:N	2.71	0.44
34:BA:142:G:H2'	34:BA:143:A:C8	2.48	0.44
34:BA:841:U:H6	34:BA:841:U:OP2	2.00	0.44
34:BA:1036:G:H3'	34:BA:1037:C:C6	2.53	0.44
34:BA:1356:G:N2	34:BA:1367:C:O2	2.50	0.44
35:BB:223:ILE:HA	35:BB:226:ARG:HB2	2.00	0.44
42:BI:4:TYR:CE1	42:BI:88:TYR:HA	2.52	0.44
42:BI:26:VAL:HG22	42:BI:61:ALA:HB3	1.97	0.44
42:BI:49:PRO:HG3	42:BI:101:PHE:CD2	2.52	0.44
53:BT:45:GLN:HE21	53:BT:45:GLN:HB3	1.66	0.44
58:BY:48:C:OP1	58:BY:48:C:H2'	2.17	0.44
59:BZ:94:VAL:HA	59:BZ:97:SER:HB2	1.99	0.44
1:CA:118:A:O5'	1:CA:119:A:H5''	2.16	0.44
1:CA:300:A:H3'	22:CY:84:ARG:NH2	2.32	0.44
1:CA:601:C:OP1	6:CF:108:LYS:NZ	2.37	0.44
1:CA:647:G:H2'	1:CA:648:G:O4'	2.17	0.44
1:CA:851:U:H5'	27:C3:49:LYS:HD2	1.98	0.44
1:CA:1336:A:H2'	1:CA:1337:G:C8	2.53	0.44
1:CA:2139:C:N4	1:CA:2152:G:H1	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:2303:G:O2'	7:CG:132:ASN:HB2	2.17	0.44
1:CA:2336:A:H61	24:C0:43:THR:CG2	2.30	0.44
4:CD:124:PRO:O	4:CD:126:GLN:N	2.51	0.44
7:CG:67:LYS:H	28:C4:6:HIS:CE1	2.35	0.44
10:CL:119:ASP:HB3	10:CL:120:LEU:H	1.66	0.44
28:C4:59:PHE:CE1	52:DS:64:GLU:HB2	2.52	0.44
34:DA:1252:A:H2'	34:DA:1253:G:O4'	2.17	0.44
35:DB:16:HIS:HB2	35:DB:204:ASN:ND2	2.32	0.44
36:DC:7:PRO:HG3	36:DC:201:TYR:CE2	2.51	0.44
38:DE:12:LEU:O	38:DE:30:ALA:HA	2.18	0.44
43:DJ:42:THR:CG2	43:DJ:68:HIS:HD2	2.30	0.44
50:DQ:7:THR:HA	50:DQ:57:VAL:O	2.17	0.44
59:DZ:169:GLY:O	59:DZ:173:THR:OG1	2.28	0.44
59:DZ:632:LEU:HG	59:DZ:645:ALA:HA	1.99	0.44
1:AA:310:C:H2'	1:AA:311:C:C6	2.52	0.44
1:AA:395:C:H2'	1:AA:396:C:O4'	2.18	0.44
1:AA:886:U:H1'	1:AA:1236:G:H1'	1.99	0.44
1:AA:990:A:C4	1:AA:2460:A:C2	3.06	0.44
1:AA:2102:G:OP1	25:A1:35:THR:HG21	2.18	0.44
4:AD:246:PRO:O	4:AD:254:THR:HG22	2.17	0.44
13:AP:82:GLY:HA2	13:AP:113:LYS:O	2.17	0.44
34:BA:664:G:N2	34:BA:741:G:H1	2.03	0.44
34:BA:1075:C:H5''	35:BB:179:LYS:HE2	1.98	0.44
34:BA:1218:C:H2'	34:BA:1219:U:C6	2.51	0.44
34:BA:1323:G:H4'	34:BA:1363:C:N3	2.33	0.44
34:BA:1478:C:H2'	34:BA:1479:C:C6	2.52	0.44
38:BE:33:VAL:HG21	38:BE:109:ILE:HA	2.00	0.44
41:BH:86:ILE:HG21	41:BH:133:LEU:HD13	1.99	0.44
50:BQ:9:VAL:O	50:BQ:21:VAL:HA	2.17	0.44
58:BY:60:U:H5''	58:BY:61:C:C5	2.45	0.44
1:CA:661:C:H4'	13:CP:13:ASN:OD1	2.18	0.44
1:CA:1289:C:H2'	1:CA:1290:C:H6	1.80	0.44
1:CA:1434:A:H61	1:CA:1558:A:H62	1.64	0.44
1:CA:2607:G:H2'	1:CA:2608:G:O4'	2.17	0.44
34:DA:1082:G:H2'	34:DA:1083:U:O4'	2.17	0.44
34:DA:1119:C:OP1	42:DI:83:ARG:NH2	2.47	0.44
34:DA:1281:U:H5''	34:DA:1282:C:H5	1.81	0.44
59:DZ:247:ARG:NH2	59:DZ:285:ASP:OD1	2.50	0.44
5:AE:31:CYS:HA	5:AE:32:PRO:HD2	1.76	0.44
6:AF:64:ILE:HD11	6:AF:75:HIS:HB2	2.00	0.44
7:AG:121:ASN:HA	7:AG:122:PRO:HD3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AP:112:LEU:HD13	13:AP:127:ALA:HB2	1.99	0.44
14:AQ:62:GLY:HA2	23:AZ:116:VAL:HG21	2.00	0.44
26:A2:61:LEU:HD23	26:A2:61:LEU:HA	1.62	0.44
34:BA:667:G:OP1	34:BA:732:C:O2'	2.21	0.44
34:BA:1129:C:H5''	42:BI:16:ARG:NH1	2.23	0.44
34:BA:1412:C:H2'	34:BA:1413:A:C8	2.53	0.44
35:BB:80:ILE:O	35:BB:80:ILE:HG13	2.17	0.44
35:BB:166:ASP:HB3	35:BB:169:LYS:HB2	1.99	0.44
38:BE:79:GLU:H	38:BE:79:GLU:HG3	1.61	0.44
41:BH:6:ILE:O	41:BH:10:LEU:HG	2.18	0.44
44:BK:30:VAL:HG21	44:BK:65:ALA:HA	1.98	0.44
59:BZ:418:LYS:HD3	59:BZ:418:LYS:HA	1.77	0.44
1:CA:858:U:O2	1:CA:2268:A:H2'	2.18	0.44
1:CA:1021:A:C8	1:CA:1021:A:C3'	3.00	0.44
1:CA:1434:A:O2'	1:CA:1435:G:H5'	2.17	0.44
1:CA:2466:C:H5'	33:C9:5:ALA:HB3	1.98	0.44
2:CB:8:U:O3'	16:CS:25:ARG:NH2	2.38	0.44
3:CC:16:ASP:OD2	3:CC:19:LYS:HB2	2.17	0.44
3:CC:174:ALA:HA	3:CC:175:PRO:HD3	1.82	0.44
4:CD:29:PRO:HA	4:CD:83:GLU:OE1	2.18	0.44
4:CD:94:LEU:O	4:CD:95:LEU:HD23	2.18	0.44
5:CE:96:PHE:O	5:CE:175:VAL:HG11	2.18	0.44
6:CF:36:VAL:HG11	6:CF:183:VAL:CG1	2.48	0.44
16:CS:25:ARG:NH1	16:CS:42:ASP:OD1	2.50	0.44
34:DA:235:C:H5'	50:DQ:70:ARG:HG2	1.98	0.44
34:DA:1013:G:N2	34:DA:1016:A:OP2	2.44	0.44
34:DA:1286:A:H8	34:DA:1287:A:H4'	1.81	0.44
34:DA:1323:G:H2'	34:DA:1324:A:C8	2.53	0.44
59:DZ:115:GLU:O	59:DZ:118:SER:HB2	2.17	0.44
59:DZ:127:LYS:HE2	59:DZ:128:TYR:HE2	1.81	0.44
1:AA:212:A:O2'	1:AA:447:C:O2	2.28	0.44
1:AA:1495:G:H1'	1:AA:1574:A:N1	2.33	0.44
1:AA:2130:C:H2'	1:AA:2131:U:C6	2.51	0.44
1:AA:2417:G:OP1	13:AP:77:ARG:NH2	2.51	0.44
1:AA:2804:C:H2'	1:AA:2805:G:C8	2.53	0.44
3:AC:24:ASP:C	3:AC:24:ASP:OD1	2.55	0.44
23:AZ:111:VAL:C	23:AZ:113:ALA:H	2.21	0.44
27:A3:4:LEU:HD23	27:A3:4:LEU:HA	1.75	0.44
34:BA:410:G:H5''	34:BA:411:A:OP1	2.18	0.44
34:BA:1445:C:H2'	34:BA:1446:U:O4'	2.17	0.44
35:BB:71:VAL:HA	35:BB:93:VAL:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:359:A:H2'	1:CA:360:G:O4'	2.18	0.44
1:CA:459:U:H5''	31:C7:40:TRP:CD2	2.53	0.44
1:CA:1074:G:H2'	1:CA:1075:C:C6	2.53	0.44
1:CA:1894:C:O2'	1:CA:1895:C:H5'	2.16	0.44
1:CA:2148:G:H2'	1:CA:2149:G:H8	1.81	0.44
1:CA:2638:G:P	5:CE:82:ARG:HH21	2.39	0.44
3:CC:68:GLY:N	3:CC:189:ASN:ND2	2.62	0.44
8:CH:73:ALA:O	8:CH:76:VAL:HB	2.18	0.44
13:CP:123:LEU:HD23	13:CP:123:LEU:HA	1.79	0.44
16:CS:105:ALA:O	16:CS:110:LEU:HB2	2.17	0.44
32:C8:31:HIS:O	32:C8:32:LEU:HB2	2.18	0.44
34:DA:235:C:H2'	34:DA:236:G:C8	2.52	0.44
34:DA:833:U:H2'	34:DA:834:C:H6	1.83	0.44
44:DK:43:SER:OG	44:DK:44:SER:N	2.51	0.44
59:DZ:168:ILE:N	59:DZ:176:GLY:O	2.50	0.44
59:DZ:604:PRO:HG2	59:DZ:649:LEU:HB3	1.98	0.44
1:AA:1941:A:H5''	1:AA:1942:C:OP2	2.17	0.44
3:AC:22:THR:HG23	3:AC:25:GLU:OE1	2.17	0.44
8:AH:29:PRO:HD2	8:AH:79:VAL:O	2.18	0.44
12:AO:69:ILE:O	12:AO:69:ILE:HG13	2.16	0.44
34:BA:358:U:P	59:BZ:381:LYS:HZ2	2.40	0.44
34:BA:418:C:H2'	34:BA:419:C:H6	1.83	0.44
34:BA:685:G:O2'	34:BA:686:U:H5'	2.18	0.44
34:BA:1326:C:H5''	54:BU:12:LYS:HE3	1.99	0.44
34:BA:1530:G:H4'	34:BA:1530:G:OP1	2.17	0.44
35:BB:28:PHE:CD1	35:BB:190:THR:HA	2.52	0.44
41:BH:112:LEU:HD13	41:BH:114:THR:HG23	1.98	0.44
54:BU:5:ASP:O	54:BU:11:GLY:HA3	2.17	0.44
59:BZ:553:GLY:H	59:BZ:557:GLY:HA2	1.82	0.44
1:CA:515:A:H1'	1:CA:581:C:H1'	1.99	0.44
1:CA:646:A:H2'	1:CA:647:G:O4'	2.17	0.44
1:CA:752:A:P	31:C7:3:ARG:HH22	2.41	0.44
1:CA:1847:A:H4'	1:CA:1848:A:OP2	2.17	0.44
1:CA:2238:G:H2'	1:CA:2238:G:N3	2.32	0.44
3:CC:22:THR:HG23	3:CC:25:GLU:OE1	2.17	0.44
3:CC:30:VAL:CG2	3:CC:31:LYS:N	2.78	0.44
10:CL:88:ALA:O	10:CL:90:LYS:N	2.50	0.44
34:DA:1262:C:H2'	34:DA:1263:C:H6	1.83	0.44
34:DA:1272:G:C2	34:DA:1273:G:H1'	2.52	0.44
36:DC:7:PRO:O	36:DC:11:ARG:NH1	2.50	0.44
39:DF:49:ALA:HB2	51:DR:78:LEU:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:DH:97:VAL:HA	41:DH:100:ILE:HG13	1.98	0.44
46:DM:40:ASN:ND2	46:DM:41:PRO:HD2	2.32	0.44
52:DS:36:ARG:HD2	52:DS:52:TYR:O	2.18	0.44
59:DZ:681:LYS:HE2	59:DZ:681:LYS:HB3	1.72	0.44
1:AA:1188:A:C4	1:AA:1190:G:C8	3.06	0.44
1:AA:1889:G:N2	1:AA:1905:G:H2'	2.33	0.44
3:AC:39:ASP:O	3:AC:178:LYS:HE3	2.17	0.44
6:AF:53:THR:HG23	6:AF:55:GLY:H	1.81	0.44
7:AG:34:LEU:HD23	7:AG:34:LEU:HA	1.70	0.44
8:AH:111:HIS:CD2	8:AH:111:HIS:H	2.35	0.44
15:AR:55:ALA:HB2	15:AR:79:LEU:HD13	1.99	0.44
20:AW:18:ARG:HG2	20:AW:76:VAL:HB	2.00	0.44
21:AX:60:ARG:NH1	31:A7:47:ARG:HH21	2.15	0.44
28:A4:53:GLU:HB3	28:A4:54:GLY:HA2	2.00	0.44
34:BA:630:G:H2'	34:BA:631:G:H8	1.82	0.44
34:BA:977:A:O2'	34:BA:981:U:N3	2.47	0.44
34:BA:1159:U:OP1	35:BB:133:LYS:NZ	2.48	0.44
34:BA:1268:A:H2'	34:BA:1269:A:C8	2.52	0.44
35:BB:44:LEU:H	35:BB:44:LEU:HD22	1.82	0.44
39:BF:99:ALA:O	39:BF:100:ASN:HB2	2.16	0.44
59:BZ:-38:TYR:O	59:BZ:-34:ARG:HG2	2.18	0.44
59:BZ:177:ILE:O	59:BZ:185:ALA:HA	2.17	0.44
59:BZ:524:GLU:HB3	59:BZ:564:LYS:HG3	2.00	0.44
1:CA:271(X):G:C2	1:CA:271(Y):U:O4	2.70	0.44
1:CA:1019:U:O2'	1:CA:1021:A:H2	1.99	0.44
1:CA:1076:C:H2'	1:CA:1077:A:C8	2.53	0.44
1:CA:1479:G:O2'	1:CA:1558:A:H5'	2.18	0.44
1:CA:1653:G:C6	15:CR:9:LYS:HG3	2.53	0.44
1:CA:2063:C:H1'	57:DX:76:31H:HCN	2.00	0.44
11:CN:103:VAL:O	11:CN:107:LEU:HG	2.17	0.44
17:CT:85:LYS:NZ	17:CT:87:ASP:OD2	2.46	0.44
21:CX:35:THR:HG22	21:CX:38:GLU:N	2.14	0.44
23:CZ:5:LEU:HD13	23:CZ:6:LYS:O	2.18	0.44
34:DA:839:U:H5''	34:DA:840:C:C5	2.51	0.44
34:DA:1165:C:H2'	34:DA:1166:G:O4'	2.18	0.44
37:DD:67:ILE:HG22	37:DD:68:TYR:CD2	2.52	0.44
53:DT:81:LYS:O	53:DT:85:MET:HG3	2.17	0.44
58:DY:55:PSU:HN1	58:DY:57:G:C5'	2.29	0.44
59:DZ:610:VAL:HG21	59:DZ:655:TYR:OH	2.18	0.44
1:AA:34:C:H5''	1:AA:35:G:OP2	2.18	0.44
1:AA:905:U:O2	1:AA:2280:A:H2'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1576:G:H2'	1:AA:1577:C:O4'	2.18	0.44
1:AA:2034:G:OP1	20:AW:11:ARG:NH2	2.44	0.44
1:AA:2421:G:H2'	1:AA:2422:G:O4'	2.18	0.44
1:AA:2653:G:H5''	1:AA:2653:G:C8	2.52	0.44
1:AA:2710:U:H2'	1:AA:2711:C:C6	2.53	0.44
4:AD:147:LEU:HD13	4:AD:155:LEU:HD11	1.99	0.44
10:AL:93:ARG:NH1	10:AL:94:GLU:HB2	2.33	0.44
18:AU:76:TYR:OH	18:AU:92:ARG:NH1	2.43	0.44
28:A4:59:PHE:HD2	52:BS:42:PRO:HG3	1.83	0.44
34:BA:96:U:O2'	34:BA:97:G:H5'	2.18	0.44
34:BA:200:G:N2	34:BA:218:C:C2	2.85	0.44
34:BA:1077:G:N2	34:BA:1080:A:OP2	2.46	0.44
34:BA:1226:C:H4'	52:BS:80:TYR:OH	2.18	0.44
43:BJ:6:ILE:O	43:BJ:71:LEU:HD12	2.18	0.44
46:BM:84:ILE:N	46:BM:85:GLY:HA2	2.33	0.44
59:BZ:94:VAL:HG12	59:BZ:97:SER:HB2	1.99	0.44
59:BZ:243:VAL:HG13	59:BZ:279:TYR:CE1	2.53	0.44
59:BZ:508:GLY:HA3	59:BZ:581:ALA:O	2.18	0.44
1:CA:251:A:C5	1:CA:252:G:H1'	2.53	0.44
1:CA:569:U:C4	1:CA:570:G:C6	3.06	0.44
1:CA:657:U:H2'	1:CA:658:C:H6	1.83	0.44
1:CA:771:G:OP1	31:C7:10:ARG:NH1	2.50	0.44
1:CA:1359:A:N1	1:CA:1372:U:O4	2.51	0.44
1:CA:1607:C:H4'	1:CA:1608:A:O5'	2.17	0.44
1:CA:2282:G:H4'	1:CA:2389:G:O2'	2.16	0.44
3:CC:39:ASP:O	3:CC:178:LYS:HE3	2.18	0.44
11:CN:39:ARG:HE	11:CN:39:ARG:HB3	1.48	0.44
13:CP:88:LEU:HD11	13:CP:114:ILE:HD12	1.99	0.44
14:CQ:16:ARG:HH11	14:CQ:16:ARG:CG	2.29	0.44
17:CT:53:ARG:O	17:CT:59:THR:HB	2.17	0.44
22:CY:38:ILE:HD13	22:CY:66:PRO:HA	2.00	0.44
23:CZ:53:ILE:HG22	23:CZ:71:VAL:HB	2.00	0.44
27:C3:5:LYS:NZ	27:C3:57:GLU:OE2	2.51	0.44
34:DA:25:C:O2'	34:DA:26:A:H5'	2.17	0.44
34:DA:309:G:H1'	34:DA:608:A:C2	2.52	0.44
34:DA:502:G:C2	34:DA:544:G:C2	3.06	0.44
34:DA:1239:A:H4'	34:DA:1240:U:C5'	2.44	0.44
34:DA:1328:C:OP1	54:DU:21:TYR:OH	2.28	0.44
35:DB:88:ALA:HB2	35:DB:219:VAL:HG13	1.99	0.44
41:DH:33:GLU:O	41:DH:36:LEU:N	2.46	0.44
41:DH:125:ARG:HE	41:DH:125:ARG:HB2	1.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:DI:17:VAL:HG11	42:DI:80:GLY:C	2.38	0.44
47:DN:15:LYS:HE2	47:DN:16:PHE:CZ	2.52	0.44
47:DN:45:ARG:O	47:DN:49:HIS:HD2	2.01	0.44
59:DZ:-53:ASP:H	59:DZ:-50:GLN:HE22	1.66	0.44
59:DZ:129:LYS:O	59:DZ:253:LEU:HD11	2.18	0.44
1:AA:104:C:H2'	1:AA:105:C:H6	1.83	0.44
1:AA:243:G:O6	32:A8:5:LYS:HG2	2.17	0.44
1:AA:324:A:P	22:AY:86:ARG:HH22	2.40	0.44
1:AA:504:A:C6	1:AA:506:A:C6	3.06	0.44
1:AA:553:A:C2	1:AA:2065:C:H5'	2.52	0.44
1:AA:808:A:OP1	65:AA:4735:HOH:O	2.21	0.44
1:AA:1249:A:N6	1:AA:1286:U:H2'	2.32	0.44
1:AA:1575:A:N6	1:AA:1588:G:O2'	2.45	0.44
1:AA:1900:G:H2'	1:AA:1901:C:C6	2.52	0.44
4:AD:132:PRO:HD3	4:AD:190:TYR:CZ	2.53	0.44
9:AK:85:ASP:O	9:AK:87:VAL:N	2.51	0.44
13:AP:135:LEU:HD23	13:AP:135:LEU:HA	1.75	0.44
15:AR:118:GLU:H	15:AR:118:GLU:CD	2.21	0.44
20:AW:61:ASN:HB2	20:AW:62:HIS:CD2	2.52	0.44
34:BA:1324:A:H2'	34:BA:1325:C:C6	2.52	0.44
40:BG:8:GLU:H	40:BG:8:GLU:CD	2.21	0.44
47:BN:23:ARG:CZ	47:BN:30:ALA:HB2	2.48	0.44
59:BZ:107:VAL:HG13	59:BZ:135:PHE:HD2	1.83	0.44
59:BZ:125:ALA:C	59:BZ:132:ARG:HH12	2.21	0.44
1:CA:493:G:H2'	1:CA:494:G:O4'	2.18	0.44
1:CA:651:G:OP2	32:C8:21:LYS:HE3	2.18	0.44
1:CA:848:G:O6	1:CA:928:G:H2'	2.17	0.44
1:CA:1235:G:C6	1:CA:1236:G:N1	2.85	0.44
1:CA:1495:A:H2'	1:CA:1496:A:H8	1.82	0.44
1:CA:1996:C:H4'	1:CA:1997:G:OP1	2.17	0.44
3:CC:24:ASP:OD1	3:CC:24:ASP:C	2.55	0.44
20:CW:59:VAL:HG12	20:CW:60:ASN:ND2	2.33	0.44
22:CY:35:TYR:CE2	22:CY:69:ALA:HB3	2.52	0.44
23:CZ:67:LEU:HD22	23:CZ:90:VAL:HG11	1.99	0.44
34:DA:513:C:H42	34:DA:538:G:H1	1.66	0.44
34:DA:537:G:H5''	45:DL:113:ARG:NH1	2.33	0.44
34:DA:1320:C:H5'	52:DS:70:LYS:HG3	2.00	0.44
35:DB:162:ILE:O	35:DB:185:ILE:HG12	2.18	0.44
41:DH:14:ARG:O	41:DH:18:ARG:HD3	2.18	0.44
52:DS:27:GLU:HB2	52:DS:28:LYS:NZ	2.33	0.44
52:DS:40:ILE:HB	52:DS:67:VAL:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:DT:79:ARG:HD2	53:DT:83:ARG:NH1	2.33	0.44
59:DZ:654:GLY:O	59:DZ:658:ASP:HB2	2.18	0.44
1:AA:386:U:H6	1:AA:386:U:H2'	1.60	0.43
1:AA:1014:U:H2'	1:AA:1015:C:C6	2.52	0.43
1:AA:1065:U:O2'	1:AA:1067:A:H2	1.90	0.43
1:AA:1891:G:H5'	3:AC:206:LYS:CE	2.48	0.43
3:AC:60:ARG:HG3	3:AC:165:ARG:HB2	2.00	0.43
3:AC:194:ILE:HD11	3:AC:227:PRO:HB2	1.99	0.43
7:AG:43:LEU:HB3	7:AG:44:GLY:H	1.46	0.43
34:BA:1066:C:O2'	34:BA:1067:A:H5'	2.18	0.43
34:BA:1251:A:H2'	34:BA:1252:A:H8	1.81	0.43
37:BD:13:ARG:HB3	37:BD:38:TYR:O	2.18	0.43
37:BD:121:VAL:O	37:BD:134:ASP:HA	2.18	0.43
38:BE:24:ARG:HH11	38:BE:24:ARG:HG2	1.83	0.43
48:BO:5:LYS:H	48:BO:5:LYS:HD2	1.83	0.43
51:BR:59:SER:OG	51:BR:62:GLU:HG2	2.18	0.43
58:BY:58:A:O2'	58:BY:60:U:H5	2.01	0.43
59:BZ:401:SER:O	59:BZ:402:ILE:HG12	2.18	0.43
1:CA:322:A:C5	1:CA:340:A:C2	3.06	0.43
1:CA:1158:C:H4'	27:C3:32:GLN:HB2	1.99	0.43
1:CA:2124:G:O6	1:CA:2174:C:N4	2.48	0.43
1:CA:2892:A:C8	1:CA:2893:G:N7	2.86	0.43
4:CD:5:LYS:HE3	4:CD:5:LYS:HB3	1.63	0.43
7:CG:61:ALA:HA	7:CG:66:GLN:O	2.17	0.43
7:CG:96:ARG:O	7:CG:99:MET:HB3	2.18	0.43
11:CN:34:LEU:O	11:CN:49:GLY:HA3	2.17	0.43
23:CZ:10:ARG:NH2	23:CZ:26:GLY:O	2.49	0.43
23:CZ:39:VAL:HG21	23:CZ:44:PHE:HB2	2.00	0.43
27:C3:7:LYS:HB2	27:C3:34:GLU:HG3	1.99	0.43
34:DA:437:U:H5'	37:DD:155:LEU:HD21	2.00	0.43
34:DA:652:U:O4	34:DA:752:G:O2'	2.22	0.43
34:DA:685:G:N2	34:DA:686:U:C4	2.86	0.43
34:DA:881:G:P	45:DL:12:ARG:HH22	2.42	0.43
34:DA:1228:C:OP2	46:DM:111:LYS:HD3	2.18	0.43
34:DA:1324:A:O4'	34:DA:1362:C:H4'	2.18	0.43
34:DA:1410:G:H2'	34:DA:1411:C:H6	1.83	0.43
34:DA:1510:U:H2'	34:DA:1511:G:C8	2.52	0.43
35:DB:158:LEU:HA	35:DB:159:PRO:HD2	1.86	0.43
36:DC:77:ILE:HG13	36:DC:78:GLY:N	2.33	0.43
36:DC:113:ALA:HA	36:DC:116:VAL:HG23	2.00	0.43
38:DE:31:LEU:HD11	38:DE:132:ALA:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:DK:85:ARG:HG2	44:DK:111:ASP:O	2.18	0.43
56:DW:43:C:H2'	56:DW:44:G:C8	2.53	0.43
57:DX:67:C:H2'	57:DX:68:C:H5'	1.99	0.43
1:AA:1127:U:O3'	10:AL:117:THR:HB	2.18	0.43
1:AA:1485:A:H2'	1:AA:1486:G:O4'	2.18	0.43
1:AA:2867:G:N2	1:AA:2870:A:OP2	2.45	0.43
17:AT:80:SER:HA	17:AT:81:PRO:HD3	1.85	0.43
30:A6:18:ARG:HD2	30:A6:42:TRP:CG	2.53	0.43
34:BA:926:G:C6	34:BA:1505:G:C6	3.06	0.43
34:BA:1136:U:H5''	34:BA:1137:C:N3	2.33	0.43
35:BB:45:GLN:O	35:BB:49:GLU:HG3	2.18	0.43
55:BV:14:A:N6	55:BV:15:A:C6	2.87	0.43
59:BZ:-7:GLU:HA	59:BZ:-4:ALA:HB3	1.98	0.43
1:CA:300:A:H1'	1:CA:319:C:H1'	1.99	0.43
1:CA:2175:C:H1'	3:CC:218:THR:O	2.18	0.43
1:CA:2461:C:H2'	1:CA:2462:U:C6	2.54	0.43
3:CC:55:SER:C	3:CC:57:GLN:N	2.71	0.43
7:CG:116:ASP:N	7:CG:116:ASP:OD1	2.51	0.43
21:CX:32:PRO:HA	21:CX:77:LYS:HD2	2.00	0.43
28:C4:46:GLN:HG2	28:C4:48:ARG:HH21	1.83	0.43
34:DA:1029:C:H2'	34:DA:1030:C:H5''	2.00	0.43
34:DA:1434:A:H2'	34:DA:1435:G:O4'	2.18	0.43
35:DB:187:LEU:HA	35:DB:201:ILE:HB	1.99	0.43
40:DG:149:ARG:HG2	44:DK:59:TYR:CE1	2.54	0.43
41:DH:34:GLU:O	41:DH:38:ILE:HG12	2.18	0.43
41:DH:121:ASP:N	41:DH:121:ASP:OD1	2.49	0.43
43:DJ:52:GLY:HA2	43:DJ:53:PRO:HD3	1.82	0.43
46:DM:57:ARG:O	46:DM:61:GLU:HB2	2.18	0.43
49:DP:5:ARG:HB3	49:DP:67:THR:CG2	2.48	0.43
59:DZ:-53:ASP:O	59:DZ:-50:GLN:HB3	2.17	0.43
59:DZ:493:VAL:HG21	59:DZ:593:ALA:HB2	2.00	0.43
1:AA:2219:U:C5	1:AA:2236:G:C6	3.06	0.43
4:AD:275:LYS:HB3	4:AD:276:LYS:H	1.52	0.43
5:AE:12:THR:HG22	5:AE:13:ARG:N	2.32	0.43
9:AK:118:THR:O	9:AK:120:LYS:N	2.47	0.43
12:AO:122:LEU:HD13	17:AT:72:VAL:HG11	1.98	0.43
25:A1:86:SER:OG	25:A1:89:GLU:HG2	2.18	0.43
34:BA:299:G:H2'	34:BA:300:A:C8	2.54	0.43
34:BA:406:G:N2	34:BA:437:U:O2	2.51	0.43
34:BA:688:G:H2'	34:BA:689:C:C6	2.54	0.43
34:BA:925:G:H1'	34:BA:1502:A:C4	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BA:1020:U:H2'	34:BA:1021:G:H8	1.83	0.43
34:BA:1058:G:N2	43:BJ:53:PRO:HG3	2.33	0.43
35:BB:121:LEU:HD13	35:BB:121:LEU:HA	1.85	0.43
37:BD:120:LEU:HA	37:BD:120:LEU:HD23	1.70	0.43
38:BE:76:ILE:HB	38:BE:77:PRO:HD2	2.01	0.43
46:BM:14:ARG:HB2	46:BM:17:VAL:HG23	2.00	0.43
46:BM:73:GLU:O	46:BM:77:ASN:ND2	2.48	0.43
59:BZ:289:ILE:H	59:BZ:289:ILE:HG13	1.50	0.43
1:CA:724:U:H2'	1:CA:725:G:O4'	2.18	0.43
1:CA:945:A:C4	1:CA:2448:A:C2	3.06	0.43
1:CA:1557:C:H5''	1:CA:1558:A:OP2	2.17	0.43
1:CA:2086:U:H2'	1:CA:2087:G:C8	2.52	0.43
1:CA:2110:G:H4'	1:CA:2111:C:OP2	2.17	0.43
1:CA:2132:U:C2	3:CC:6:LYS:CE	3.01	0.43
8:CH:154:PRO:HB3	8:CH:163:TYR:CZ	2.53	0.43
34:DA:60:A:H4'	34:DA:61:G:O5'	2.19	0.43
34:DA:620:C:C2	37:DD:135:LEU:HG	2.53	0.43
34:DA:1051:C:H2'	34:DA:1052:U:C6	2.53	0.43
34:DA:1342:C:O2'	42:DI:124:GLN:HG2	2.17	0.43
36:DC:178:LEU:HD13	36:DC:178:LEU:HA	1.85	0.43
45:DL:31:PRO:HB2	45:DL:32:PHE:CD2	2.53	0.43
46:DM:25:ILE:HD11	46:DM:66:LEU:HD23	1.99	0.43
58:DY:39:PSU:C2	58:DY:40:C:C4	3.07	0.43
58:DY:65:G:H2'	58:DY:66:U:C6	2.53	0.43
1:AA:85:C:O2'	1:AA:86:C:H5'	2.18	0.43
1:AA:278:G:OP1	25:A1:76:ARG:HD2	2.18	0.43
1:AA:1617:A:H2'	1:AA:1618:A:C8	2.53	0.43
1:AA:1922:A:N1	1:AA:1992:A:C6	2.87	0.43
1:AA:2453:C:OP2	1:AA:2598:C:O2'	2.36	0.43
2:AB:28:C:H2'	2:AB:29:A:O4'	2.18	0.43
7:AG:137:GLU:HB3	7:AG:139:LEU:HD12	2.01	0.43
16:AS:36:TYR:N	16:AS:36:TYR:CD1	2.86	0.43
17:AT:24:PRO:HA	17:AT:49:VAL:HG22	2.01	0.43
22:AY:20:TYR:CE1	22:AY:43:ASN:HA	2.53	0.43
28:A4:6:HIS:HA	28:A4:7:PRO:HD3	1.79	0.43
29:A5:38:ALA:CB	29:A5:48:GLU:HG3	2.49	0.43
34:BA:235:C:H5'	50:BQ:70:ARG:HG2	2.00	0.43
34:BA:761:G:C6	34:BA:762:C:C4	3.06	0.43
34:BA:1116:C:O2'	42:BI:108:VAL:HG21	2.18	0.43
34:BA:1434:A:H2'	34:BA:1435:G:O4'	2.18	0.43
35:BB:68:ILE:HG12	35:BB:161:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:BC:58:GLU:HB2	36:BC:65:ALA:CB	2.48	0.43
36:BC:100:ALA:O	36:BC:101:LEU:HB2	2.19	0.43
39:BF:55:ASP:HA	39:BF:56:PRO:HD3	1.85	0.43
44:BK:43:SER:HB3	44:BK:68:ALA:HB2	2.00	0.43
46:BM:70:LEU:O	46:BM:74:VAL:HG23	2.19	0.43
52:BS:50:ALA:HB1	52:BS:57:HIS:HB3	1.99	0.43
56:BW:7:A:H5'	56:BW:8:4SU:H5	1.99	0.43
56:BW:39:PSU:H2'	56:BW:40:C:C6	2.53	0.43
58:BY:53:G:H1	58:BY:61:C:H42	1.64	0.43
1:CA:652(C):G:H5''	1:CA:652(D):C:OP2	2.19	0.43
1:CA:1144:G:H2'	1:CA:1145:C:H6	1.81	0.43
1:CA:1719:G:C6	1:CA:1720:U:C4	3.07	0.43
2:CB:8:U:H6	2:CB:8:U:H5''	1.83	0.43
6:CF:60:SER:OG	6:CF:61:GLY:N	2.51	0.43
7:CG:145:THR:HG22	7:CG:148:MET:CG	2.47	0.43
12:CO:120:GLU:HG2	12:CO:122:LEU:HG	1.99	0.43
17:CT:120:ARG:HA	17:CT:123:GLN:HG3	2.00	0.43
34:DA:35:G:H2'	34:DA:36:C:C6	2.53	0.43
34:DA:961:U:H2'	34:DA:962:C:O4'	2.19	0.43
34:DA:1187:G:H4'	42:DI:111:ARG:HH11	1.84	0.43
34:DA:1321:C:H5''	34:DA:1322:C:H2'	2.00	0.43
35:DB:25:ASN:HA	35:DB:26:PRO:HD3	1.82	0.43
43:DJ:39:PRO:HA	43:DJ:70:ARG:HD3	2.00	0.43
59:DZ:74:TRP:HE1	59:DZ:274:ASP:N	2.17	0.43
59:DZ:169:GLY:HA3	59:DZ:173:THR:O	2.18	0.43
1:AA:438:G:C5	13:AP:72:PRO:HB3	2.53	0.43
1:AA:1604:C:H5''	1:AA:1605:A:OP2	2.19	0.43
1:AA:2784:C:H2'	1:AA:2785:C:C6	2.53	0.43
5:AE:131:ALA:HB1	5:AE:134:ILE:HD11	2.00	0.43
22:AY:90:LEU:HB2	22:AY:94:LYS:O	2.18	0.43
23:AZ:146:ILE:HA	23:AZ:147:GLY:HA2	1.65	0.43
31:A7:5:TRP:CD1	31:A7:7:PRO:HD3	2.53	0.43
32:A8:36:LYS:HB2	32:A8:41:ILE:HD11	1.99	0.43
34:BA:950:U:H2'	34:BA:951:G:C8	2.53	0.43
34:BA:1029:C:N4	34:BA:1030(A):G:N3	2.66	0.43
34:BA:1131:G:O5'	34:BA:1131:G:H8	2.01	0.43
34:BA:1189:C:OP1	43:BJ:51:ARG:NH2	2.51	0.43
35:BB:192:SER:O	35:BB:194:PRO:HD3	2.18	0.43
1:CA:141:A:C8	1:CA:1408:C:O2'	2.69	0.43
1:CA:1071:G:H1'	1:CA:1089:G:H2'	2.00	0.43
1:CA:1837:C:O2'	1:CA:1927:A:N3	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CB:24:G:N7	2:CB:56:G:H2'	2.33	0.43
3:CC:54:ARG:HE	3:CC:57:GLN:HG2	1.83	0.43
4:CD:3:VAL:HG13	4:CD:17:THR:HB	2.00	0.43
4:CD:146:GLU:HB2	4:CD:189:CYS:CB	2.49	0.43
8:CH:126:PRO:HB2	8:CH:127:GLU:H	1.64	0.43
13:CP:100:LEU:HD23	13:CP:100:LEU:HA	1.77	0.43
19:CV:1:MET:HG3	19:CV:43:GLU:OE2	2.18	0.43
23:CZ:75:ASN:O	23:CZ:84:GLU:HG2	2.18	0.43
28:C4:34:GLU:HG2	46:DM:3:ARG:CB	2.48	0.43
34:DA:189:G:H2'	34:DA:189(A):C:C6	2.54	0.43
34:DA:394:G:H2'	34:DA:395:C:C6	2.54	0.43
34:DA:1074:G:C6	34:DA:1075:C:C4	3.07	0.43
34:DA:1316:G:H22	34:DA:1319:A:C5'	2.31	0.43
34:DA:1399:C:C2	34:DA:1502:A:N6	2.87	0.43
34:DA:1465:C:H2'	34:DA:1466:C:O4'	2.19	0.43
38:DE:42:GLY:HA2	38:DE:65:ASN:O	2.19	0.43
43:DJ:50:ILE:HD11	43:DJ:57:LYS:HE2	1.99	0.43
50:DQ:6:LEU:O	50:DQ:58:GLU:HA	2.19	0.43
59:DZ:428:LEU:HD13	59:DZ:440:VAL:HG11	2.01	0.43
59:DZ:438:PHE:CE2	59:DZ:440:VAL:HG23	2.50	0.43
1:AA:861:C:H4'	1:AA:1270:C:O2	2.19	0.43
1:AA:1549:U:H2'	1:AA:1550:C:C6	2.53	0.43
1:AA:2316:G:H22	1:AA:2324:U:H3	1.66	0.43
1:AA:2649:U:H5''	5:AE:82:ARG:HH21	1.83	0.43
1:AA:2724:U:O2'	1:AA:2726:A:H5'	2.19	0.43
1:AA:2724:U:OP1	1:AA:2727:G:H4'	2.18	0.43
6:AF:124:LEU:O	6:AF:193:VAL:HA	2.19	0.43
23:AZ:120:ILE:HG13	23:AZ:171:ILE:C	2.39	0.43
23:AZ:150:LEU:HB3	23:AZ:171:ILE:HD11	2.01	0.43
23:AZ:155:LEU:HD12	23:AZ:155:LEU:HA	1.76	0.43
32:A8:37:SER:OG	32:A8:39:LYS:N	2.52	0.43
34:BA:486:U:H2'	34:BA:487:A:H8	1.84	0.43
34:BA:1324:A:O4'	34:BA:1362:C:H4'	2.18	0.43
36:BC:44:GLU:HA	36:BC:52:LEU:HD13	1.99	0.43
43:BJ:70:ARG:HA	43:BJ:70:ARG:HD3	1.88	0.43
50:BQ:92:ARG:HA	50:BQ:92:ARG:HD3	1.83	0.43
59:BZ:7:ASN:HB3	59:BZ:10:LYS:HE2	1.99	0.43
59:BZ:131:PRO:HG2	59:BZ:281:PRO:HG2	2.00	0.43
59:BZ:411:VAL:HB	59:BZ:459:LEU:HD13	2.01	0.43
59:BZ:637:ARG:C	59:BZ:639:ASN:H	2.21	0.43
1:CA:671:C:H2'	1:CA:672:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:729:G:C6	4:CD:208:LYS:HB2	2.52	0.43
1:CA:1056:G:H5''	1:CA:1057:A:O4'	2.17	0.43
1:CA:1754:C:H5''	17:CT:113:LYS:HE3	1.99	0.43
1:CA:2218:U:O4'	25:C1:52:ARG:NH2	2.51	0.43
2:CB:22:U:H3	2:CB:61:G:H1	1.66	0.43
7:CG:52:ILE:O	7:CG:53:LEU:HD23	2.18	0.43
13:CP:55:ARG:HA	65:CP:308:HOH:O	2.19	0.43
23:CZ:18:LEU:HD13	23:CZ:18:LEU:HA	1.78	0.43
24:C0:53:MET:HG3	24:C0:59:LEU:CD2	2.46	0.43
34:DA:89:C:H2'	34:DA:90:U:O4'	2.18	0.43
34:DA:1291:G:OP1	40:DG:37:ASN:ND2	2.51	0.43
36:DC:16:ARG:HD2	36:DC:16:ARG:HA	1.66	0.43
39:DF:79:LEU:HD23	39:DF:79:LEU:HA	1.83	0.43
43:DJ:46:ARG:NH2	43:DJ:64:GLU:OE1	2.52	0.43
47:DN:23:ARG:HD2	47:DN:28:GLY:O	2.19	0.43
59:DZ:319:ASP:HA	59:DZ:320:PRO:HD3	1.84	0.43
59:DZ:459:LEU:HD23	59:DZ:459:LEU:HA	1.83	0.43
1:AA:310:C:H2'	1:AA:311:C:H6	1.83	0.43
1:AA:2478:C:OP1	33:A9:4:ARG:HB3	2.19	0.43
6:AF:199:TRP:O	6:AF:203:GLN:HG2	2.18	0.43
8:AH:98:LEU:HD12	8:AH:98:LEU:HA	1.84	0.43
11:AN:15:LEU:HD22	11:AN:16:ILE:N	2.33	0.43
20:AW:1:MET:HA	20:AW:1:MET:HE3	2.01	0.43
22:AY:28:LYS:HB3	22:AY:28:LYS:HE3	1.79	0.43
27:A3:23:LEU:HD12	27:A3:23:LEU:HA	1.81	0.43
34:BA:194:C:H2'	34:BA:195:A:H5''	2.01	0.43
34:BA:448:A:C4	34:BA:487:A:C2	3.07	0.43
34:BA:548:G:C6	34:BA:549:C:C4	3.06	0.43
34:BA:757:U:O2'	34:BA:879:C:O2	2.28	0.43
34:BA:1284:C:H3'	34:BA:1285:A:C8	2.53	0.43
34:BA:1437:C:H2'	34:BA:1438:G:C8	2.54	0.43
36:BC:59:ARG:O	43:BJ:92:THR:HG22	2.18	0.43
38:BE:143:ARG:NH1	41:BH:77:GLU:OE2	2.52	0.43
53:BT:97:ALA:N	53:BT:98:PRO:HD3	2.33	0.43
58:BY:25:C:C2	58:BY:26:A:C8	3.07	0.43
59:BZ:114:VAL:HG12	59:BZ:115:GLU:N	2.32	0.43
59:BZ:330:VAL:HB	59:BZ:371:ALA:HA	2.01	0.43
59:BZ:519:ARG:NH2	59:BZ:678:GLU:H	2.16	0.43
1:CA:41:C:H2'	1:CA:42:G:O4'	2.19	0.43
1:CA:57:C:H2'	1:CA:58:G:O4'	2.19	0.43
1:CA:597:U:H2'	1:CA:598:G:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1110:G:N3	1:CA:1110:G:C2'	2.82	0.43
1:CA:1452:A:O2'	1:CA:1453:U:H2'	2.19	0.43
1:CA:1628:G:H2'	1:CA:1629:U:H6	1.84	0.43
1:CA:1857:G:C6	1:CA:1858:G:N1	2.87	0.43
1:CA:2692:C:O2'	1:CA:2693:A:H5'	2.19	0.43
4:CD:16:MET:HE1	4:CD:208:LYS:HD3	2.01	0.43
8:CH:148:ILE:O	8:CH:151:ILE:HB	2.19	0.43
23:CZ:70:LEU:HD23	23:CZ:70:LEU:HA	1.79	0.43
34:DA:539:A:OP2	45:DL:115:LYS:NZ	2.48	0.43
34:DA:632:A:OP2	34:DA:632:A:H8	2.02	0.43
34:DA:735:C:O2'	34:DA:736:C:H5'	2.18	0.43
36:DC:110:ASN:HB3	36:DC:141:VAL:HA	2.01	0.43
36:DC:173:VAL:O	36:DC:175:LEU:HD12	2.18	0.43
45:DL:7:ILE:O	45:DL:11:VAL:HG23	2.18	0.43
46:DM:14:ARG:HB3	46:DM:16:ASP:OD1	2.18	0.43
56:DW:76:F3N:H5''	56:DW:76:F3N:O	2.17	0.43
59:DZ:123:ARG:HD2	59:DZ:675:HIS:ND1	2.34	0.43
59:DZ:160:ARG:HH21	59:DZ:253:LEU:HA	1.84	0.43
59:DZ:309:LEU:HA	59:DZ:333:GLY:HA3	2.01	0.43
59:DZ:552:SER:HB3	59:DZ:591:LYS:HZ2	1.83	0.43
1:AA:142:G:H1'	21:AX:37:THR:CG2	2.49	0.43
1:AA:313:A:H2'	1:AA:314:G:O4'	2.18	0.43
1:AA:733:G:N2	1:AA:835:A:H61	2.17	0.43
4:AD:8:PRO:HB3	4:AD:14:ARG:HB2	1.99	0.43
5:AE:49:LEU:HD12	5:AE:49:LEU:HA	1.78	0.43
8:AH:86:GLU:OE2	8:AH:132:ARG:NH2	2.52	0.43
22:AY:49:VAL:HG11	22:AY:61:ILE:HD13	1.99	0.43
28:A4:10:VAL:N	28:A4:26:SER:O	2.37	0.43
34:BA:377:G:OP1	49:BP:5:ARG:HD2	2.19	0.43
34:BA:872:A:C5	34:BA:874:G:C8	3.06	0.43
34:BA:1279:A:N1	36:BC:26:LYS:NZ	2.67	0.43
59:BZ:69:VAL:HG11	59:BZ:374:LEU:HD22	2.01	0.43
59:BZ:486:THR:O	59:BZ:599:PRO:HA	2.18	0.43
1:CA:443:A:H5''	1:CA:444:C:OP1	2.19	0.43
1:CA:574:C:N3	5:CE:145:LYS:NZ	2.61	0.43
1:CA:2328:A:H2'	1:CA:2329:G:H8	1.83	0.43
3:CC:195:ARG:HH11	3:CC:195:ARG:HG3	1.83	0.43
6:CF:140:LEU:HD13	6:CF:170:LEU:HD21	2.00	0.43
11:CN:43:THR:HB	11:CN:46:VAL:CG2	2.49	0.43
16:CS:67:ARG:O	16:CS:71:ARG:HG3	2.18	0.43
16:CS:69:VAL:O	16:CS:72:ALA:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:CU:104:GLN:NE2	18:CU:105:VAL:HG23	2.34	0.43
25:C1:50:ARG:HG2	25:C1:59:THR:HB	2.01	0.43
28:C4:59:PHE:HA	28:C4:60:GLN:C	2.39	0.43
34:DA:152:A:N6	34:DA:170:U:C2	2.86	0.43
34:DA:707:C:H2'	34:DA:708:C:C6	2.52	0.43
34:DA:1097:C:H2'	34:DA:1098:C:C6	2.54	0.43
35:DB:71:VAL:O	35:DB:165:VAL:HG23	2.19	0.43
39:DF:82:ARG:HD2	39:DF:82:ARG:HA	1.70	0.43
40:DG:29:LYS:HB3	40:DG:105:VAL:HG21	2.00	0.43
46:DM:50:GLU:O	46:DM:54:VAL:HG22	2.19	0.43
47:DN:24:CYS:HA	47:DN:38:GLY:O	2.18	0.43
59:DZ:87:HIS:O	59:DZ:89:ASP:N	2.47	0.43
59:DZ:228:MET:O	59:DZ:232:LEU:HD22	2.18	0.43
1:AA:275:C:H2'	1:AA:276:C:C6	2.53	0.43
1:AA:313:A:N6	1:AA:375:G:H1'	2.33	0.43
1:AA:694:G:N2	1:AA:696:C:O2	2.31	0.43
1:AA:2163:G:N7	1:AA:2173:G:N2	2.67	0.43
5:AE:28:ALA:HB3	5:AE:93:VAL:HG13	2.00	0.43
5:AE:79:ARG:HD3	5:AE:79:ARG:HA	1.84	0.43
12:AO:1:MET:HE3	12:AO:32:TYR:CD1	2.54	0.43
12:AO:69:ILE:HD11	12:AO:105:GLU:OE1	2.18	0.43
14:AQ:56:ARG:HA	14:AQ:56:ARG:HD2	1.45	0.43
34:BA:872:A:C4	34:BA:874:G:N7	2.87	0.43
37:BD:166:LYS:N	37:BD:168:ARG:HH12	2.17	0.43
39:BF:19:LEU:HD11	39:BF:59:TYR:CZ	2.54	0.43
59:BZ:536:LYS:H	59:BZ:536:LYS:HD2	1.83	0.43
1:CA:982:C:O5'	1:CA:982:C:H6	2.02	0.43
1:CA:1095:A:H2'	1:CA:1096:A:C8	2.54	0.43
1:CA:1668:A:H4'	1:CA:1669:A:O5'	2.18	0.43
1:CA:2468:G:C6	1:CA:2481:G:C4	3.07	0.43
3:CC:60:ARG:HG3	3:CC:165:ARG:HB2	2.01	0.43
6:CF:57:VAL:HG13	6:CF:59:TYR:CD2	2.53	0.43
23:CZ:45:ASP:CG	23:CZ:49:ARG:HH11	2.22	0.43
34:DA:735:C:H2'	34:DA:736:C:H6	1.84	0.43
34:DA:1206:G:C6	34:DA:1207:G:C5	3.07	0.43
34:DA:1356:G:N2	34:DA:1367:C:O2	2.51	0.43
35:DB:94:ASN:HA	35:DB:94:ASN:HD22	1.56	0.43
35:DB:102:LEU:HD23	35:DB:182:ILE:HD12	2.00	0.43
39:DF:96:PRO:HB3	51:DR:30:ASP:OD2	2.19	0.43
59:DZ:-58:LEU:HB3	59:DZ:-55:LEU:HB2	2.01	0.43
59:DZ:38:ARG:HH12	59:DZ:270:GLN:HE22	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:DZ:324:ARG:HD3	59:DZ:380:LEU:O	2.19	0.43
1:AA:613:A:H2'	1:AA:614:C:O4'	2.19	0.43
1:AA:933:C:OP1	1:AA:933:C:H4'	2.18	0.43
1:AA:1384:G:N7	21:AX:62:LYS:NZ	2.59	0.43
1:AA:1975:A:H2	1:AA:2561:G:N3	2.17	0.43
1:AA:2569:G:H2'	1:AA:2570:C:C6	2.54	0.43
3:AC:6:LYS:N	3:AC:9:ARG:HH12	2.17	0.43
7:AG:77:ILE:O	7:AG:82:LEU:N	2.49	0.43
12:AO:10:VAL:HG21	12:AO:16:ALA:HB3	2.01	0.43
14:AQ:2:LEU:HB2	14:AQ:70:PRO:HG3	2.01	0.43
14:AQ:39:PRO:HA	14:AQ:97:VAL:O	2.19	0.43
30:A6:50:ARG:HE	30:A6:50:ARG:HB2	1.65	0.43
34:BA:1437:C:H2'	34:BA:1438:G:H8	1.84	0.43
36:BC:78:GLY:HA3	36:BC:83:ARG:H	1.83	0.43
37:BD:173:TRP:HB2	37:BD:187:ARG:O	2.19	0.43
38:BE:64:ARG:HE	38:BE:64:ARG:HB3	1.70	0.43
42:BI:81:ILE:HA	42:BI:84:ALA:HB3	2.00	0.43
48:BO:32:LEU:O	48:BO:35:ARG:N	2.51	0.43
49:BP:8:ARG:C	49:BP:9:PHE:HD1	2.22	0.43
52:BS:20:LEU:HD21	52:BS:43:GLU:HG2	2.00	0.43
53:BT:56:MET:HE1	53:BT:85:MET:HG2	2.01	0.43
59:BZ:146:LEU:HD22	59:BZ:150:ILE:HD11	2.00	0.43
1:CA:25:U:H2'	1:CA:26:G:O4'	2.19	0.43
1:CA:171:G:H2'	1:CA:172:C:C6	2.54	0.43
1:CA:289:A:N6	1:CA:351:G:O2'	2.49	0.43
1:CA:571:A:O2'	19:CV:78:LYS:HE2	2.18	0.43
1:CA:699:A:C2	1:CA:1633:G:N3	2.86	0.43
1:CA:699:A:H2'	1:CA:700:G:O4'	2.19	0.43
1:CA:760:G:H2'	1:CA:761:A:O4'	2.19	0.43
1:CA:867:C:N4	1:CA:868:U:O4	2.52	0.43
1:CA:1064:C:H4'	10:CL:89:HIS:HB3	2.00	0.43
1:CA:2290:G:C2	1:CA:2343:C:O2	2.72	0.43
1:CA:2489:G:C6	1:CA:2490:G:N1	2.87	0.43
3:CC:31:LYS:H	3:CC:31:LYS:HG2	1.57	0.43
4:CD:94:LEU:HD22	4:CD:95:LEU:N	2.33	0.43
5:CE:195:LEU:HD21	65:CE:3111:HOH:O	2.19	0.43
13:CP:39:LYS:HB2	13:CP:45:LEU:CG	2.40	0.43
34:DA:73:G:C6	34:DA:76:C:C4	3.07	0.43
34:DA:612:C:O2	34:DA:629:G:N2	2.52	0.43
34:DA:833:U:H2'	34:DA:834:C:C6	2.54	0.43
34:DA:1004:A:N6	34:DA:1037:C:C2	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:DM:80:ARG:O	46:DM:84:ILE:HG12	2.19	0.43
53:DT:44:ALA:HB1	53:DT:91:LEU:HB2	2.00	0.43
57:DX:23:C:H2'	57:DX:24:U:H6	1.83	0.43
59:DZ:-62:LEU:N	59:DZ:-62:LEU:HD12	2.34	0.43
59:DZ:420:ASP:OD1	59:DZ:423:LYS:HB2	2.19	0.43
1:AA:553:A:N1	1:AA:2064:A:H2'	2.33	0.42
1:AA:589:U:H2'	1:AA:590:A:O4'	2.19	0.42
1:AA:866:A:H8	1:AA:866:A:C5'	2.31	0.42
1:AA:1003:U:OP2	14:AQ:14:ARG:HD3	2.19	0.42
1:AA:1692:G:H5''	1:AA:1693:C:H5'	2.01	0.42
1:AA:2203:G:O2'	1:AA:2204:G:OP1	2.30	0.42
1:AA:2589:A:H5'	29:A5:3:LYS:HD2	2.00	0.42
3:AC:11:LEU:HD11	3:AC:35:THR:HG23	2.01	0.42
3:AC:195:ARG:HG3	3:AC:195:ARG:NH1	2.34	0.42
12:AO:104:ARG:HH12	17:AT:43:GLN:NE2	2.17	0.42
23:AZ:89:PHE:HE2	23:AZ:96:VAL:HG23	1.84	0.42
34:BA:445:G:C6	34:BA:490:G:C6	3.07	0.42
34:BA:908:A:H2'	34:BA:909:A:C8	2.54	0.42
34:BA:1513:A:H2'	34:BA:1514:C:C6	2.53	0.42
35:BB:24:TRP:CE3	35:BB:26:PRO:HA	2.54	0.42
35:BB:173:ALA:O	35:BB:176:GLU:N	2.52	0.42
50:BQ:41:LYS:HZ3	50:BQ:92:ARG:HH21	1.66	0.42
57:BX:2:G:H2'	57:BX:3:C:C6	2.54	0.42
59:BZ:88:VAL:HG22	59:BZ:120:THR:HG21	2.01	0.42
59:BZ:201:ILE:H	59:BZ:201:ILE:HG13	1.67	0.42
1:CA:528:A:OP2	11:CN:114:ARG:NH1	2.51	0.42
1:CA:639:U:H2'	1:CA:640:C:H6	1.81	0.42
1:CA:830:G:H4'	1:CA:831:G:OP2	2.17	0.42
1:CA:1027:A:C2	1:CA:2488:A:H5'	2.54	0.42
1:CA:1570:A:H2'	1:CA:1571:A:C8	2.54	0.42
3:CC:11:LEU:HD11	3:CC:35:THR:HG23	2.01	0.42
4:CD:106:ILE:HD13	4:CD:106:ILE:HG21	1.80	0.42
32:C8:57:ARG:O	32:C8:60:LEU:N	2.49	0.42
34:DA:7:G:H5'	34:DA:298:A:O4'	2.19	0.42
34:DA:253:U:H2'	34:DA:254:G:C8	2.54	0.42
34:DA:1438:G:H2'	34:DA:1439:C:C6	2.53	0.42
35:DB:70:PHE:CE1	35:DB:163:PHE:HD2	2.37	0.42
50:DQ:31:LEU:HD23	50:DQ:32:TYR:CZ	2.54	0.42
59:DZ:295:GLU:H	59:DZ:295:GLU:HG3	1.48	0.42
1:AA:180:A:H2'	1:AA:181:C:C6	2.54	0.42
1:AA:733:G:P	31:A7:11:LYS:HZ3	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:101:ILE:HG22	7:AG:105:LYS:HE2	2.01	0.42
16:AS:78:LEU:HD21	16:AS:83:LYS:HG3	2.01	0.42
34:BA:991:U:C4	34:BA:1212:U:H1'	2.54	0.42
34:BA:1123:A:H61	34:BA:1149:C:N4	2.14	0.42
34:BA:1149:C:H2'	34:BA:1150:U:H6	1.84	0.42
34:BA:1492:A:H4'	45:BL:47:LYS:HE3	2.01	0.42
34:BA:1504:G:OP1	34:BA:1507:A:H4'	2.19	0.42
35:BB:215:LEU:HA	35:BB:215:LEU:HD23	1.79	0.42
41:BH:88:LYS:O	41:BH:92:ARG:HD3	2.19	0.42
52:BS:27:GLU:HA	52:BS:28:LYS:HA	1.91	0.42
59:BZ:639:ASN:N	59:BZ:640:ALA:HB3	2.33	0.42
1:CA:746:A:H2'	1:CA:2612:C:H5''	2.00	0.42
1:CA:1154:G:H8	1:CA:1154:G:O5'	2.02	0.42
1:CA:1805:U:O2	4:CD:50:THR:HB	2.18	0.42
1:CA:2529:G:O6	33:C9:31:LYS:NZ	2.52	0.42
13:CP:55:ARG:HG2	13:CP:56:SER:N	2.34	0.42
16:CS:3:ARG:O	16:CS:4:LEU:HD23	2.19	0.42
17:CT:99:LEU:HD22	17:CT:101:PHE:HE1	1.84	0.42
22:CY:76:CYS:SG	22:CY:78:ALA:HB3	2.59	0.42
23:CZ:97:GLU:H	23:CZ:97:GLU:HG2	1.55	0.42
34:DA:67:C:H4'	34:DA:172:A:O4'	2.18	0.42
34:DA:814:A:N7	34:DA:816:A:C4	2.87	0.42
34:DA:872:A:C4	34:DA:874:G:N7	2.87	0.42
34:DA:1048:G:OP1	47:DN:3:ARG:NH2	2.52	0.42
34:DA:1221:G:H4'	52:DS:53:ASN:O	2.19	0.42
35:DB:47:THR:HG23	35:DB:202:PRO:HG2	2.01	0.42
36:DC:47:LEU:HB3	36:DC:52:LEU:HB3	2.00	0.42
40:DG:52:GLU:H	40:DG:52:GLU:HG2	1.60	0.42
41:DH:21:LYS:O	41:DH:65:TYR:OH	2.30	0.42
43:DJ:23:ILE:HD13	43:DJ:23:ILE:HA	1.84	0.42
46:DM:17:VAL:O	46:DM:20:THR:OG1	2.35	0.42
56:DW:54:5MU:C4	56:DW:55:PSU:C2	3.07	0.42
1:AA:268:G:O2'	1:AA:269:G:H8	2.02	0.42
1:AA:2284:U:H5''	1:AA:2285:A:OP1	2.19	0.42
1:AA:2566:U:H2'	1:AA:2567:U:C6	2.54	0.42
3:AC:195:ARG:HG3	3:AC:195:ARG:HH11	1.83	0.42
19:AV:49:THR:O	19:AV:49:THR:CG2	2.67	0.42
30:A6:12:GLU:HA	30:A6:19:ARG:HA	2.00	0.42
34:BA:1002:G:H2'	34:BA:1003:G:O4'	2.20	0.42
34:BA:1072:G:C6	34:BA:1073:U:C4	3.08	0.42
34:BA:1148:U:H2'	34:BA:1149:C:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:BD:194:LEU:HD12	37:BD:195:ALA:N	2.34	0.42
39:BF:10:LEU:HD23	39:BF:61:LEU:HD23	2.01	0.42
41:BH:8:ASP:O	41:BH:11:THR:N	2.46	0.42
50:BQ:89:LEU:HA	50:BQ:89:LEU:HD23	1.61	0.42
59:BZ:13:ARG:NH1	59:BZ:247:ARG:NH2	2.55	0.42
59:BZ:438:PHE:HB3	59:BZ:458:HIS:CE1	2.54	0.42
59:BZ:509:HIS:NE2	59:BZ:511:LYS:HE2	2.35	0.42
1:CA:637:A:H5''	13:CP:117:GLU:HG2	2.01	0.42
1:CA:1141:U:H4'	1:CA:1142(A):A:O4'	2.19	0.42
1:CA:1239:G:H2'	1:CA:1240:U:O4'	2.19	0.42
1:CA:2439:A:C8	1:CA:2439:A:H5'	2.55	0.42
6:CF:33:LEU:HA	6:CF:33:LEU:HD12	1.61	0.42
7:CG:31:VAL:HG22	7:CG:32:PRO:HD2	2.01	0.42
7:CG:33:ARG:NH1	7:CG:33:ARG:HB2	2.34	0.42
8:CH:15:VAL:HG23	8:CH:28:GLY:HA3	2.00	0.42
11:CN:91:LEU:HA	11:CN:91:LEU:HD23	1.74	0.42
17:CT:30:VAL:HG13	17:CT:86:ILE:HG12	2.02	0.42
27:C3:8:LEU:HD23	27:C3:8:LEU:HA	1.79	0.42
34:DA:1326:C:H2'	34:DA:1327:C:H6	1.84	0.42
36:DC:56:ASP:C	36:DC:57:ILE:HD12	2.40	0.42
37:DD:11:LEU:O	37:DD:15:GLU:HG2	2.18	0.42
39:DF:94:GLN:HE22	51:DR:72:ARG:HH12	1.67	0.42
53:DT:90:GLN:O	53:DT:93:GLU:HG3	2.19	0.42
57:DX:47:U:H3'	57:DX:48:C:C5'	2.50	0.42
59:DZ:114:VAL:HG23	59:DZ:152:THR:HB	2.01	0.42
59:DZ:160:ARG:HD3	59:DZ:256:THR:OG1	2.20	0.42
59:DZ:193:GLY:O	59:DZ:196:ILE:HG22	2.18	0.42
1:AA:734:C:H5''	31:A7:2:LYS:HE2	2.02	0.42
1:AA:1137:G:C6	1:AA:1147:U:C2	3.07	0.42
1:AA:1346:U:H4'	1:AA:1347:A:H5''	2.01	0.42
1:AA:2402:U:O2'	1:AA:2403:G:H5'	2.19	0.42
1:AA:2407:C:H2'	1:AA:2408:G:O4'	2.19	0.42
7:AG:60:LEU:HA	7:AG:60:LEU:HD13	1.67	0.42
8:AH:7:LEU:HD12	8:AH:7:LEU:HA	1.89	0.42
17:AT:39:ARG:HH22	34:BA:345:C:H5	1.66	0.42
34:BA:254:G:OP1	50:BQ:67:LYS:O	2.37	0.42
34:BA:690:G:C6	34:BA:691:G:C6	3.07	0.42
34:BA:1100:C:O2'	34:BA:1102:A:OP1	2.38	0.42
34:BA:1272:G:H2'	34:BA:1273:G:O4'	2.18	0.42
34:BA:1292:U:H2'	34:BA:1293:G:C8	2.55	0.42
34:BA:1521:G:H2'	34:BA:1522:U:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BB:50:GLU:O	35:BB:54:THR:N	2.50	0.42
35:BB:200:ILE:H	35:BB:200:ILE:HG12	1.47	0.42
37:BD:52:SER:O	37:BD:56:VAL:HG23	2.20	0.42
37:BD:147:ALA:HA	37:BD:182:LYS:HA	2.01	0.42
42:BI:127:LYS:O	42:BI:128:ARG:HG2	2.19	0.42
59:BZ:-29:LEU:H	59:BZ:-29:LEU:HD23	1.84	0.42
59:BZ:417:THR:HA	59:BZ:418:LYS:CB	2.49	0.42
1:CA:1022:G:H22	1:CA:1142(A):A:H2	1.62	0.42
1:CA:1354:A:H2'	1:CA:1355:G:O4'	2.19	0.42
1:CA:1514:U:H2'	1:CA:1515:G:H8	1.84	0.42
1:CA:2130:U:OP1	3:CC:6:LYS:HG2	2.20	0.42
1:CA:2243:U:H2'	1:CA:2244:U:H6	1.83	0.42
65:CA:4673:HOH:O	5:CE:135:HIS:NE2	2.30	0.42
3:CC:27:ALA:O	3:CC:30:VAL:CG2	2.64	0.42
10:CL:90:LYS:HD3	10:CL:93:ARG:NH2	2.33	0.42
26:C2:21:LEU:HA	26:C2:21:LEU:HD23	1.81	0.42
31:C7:19:ARG:HG2	31:C7:19:ARG:HH11	1.83	0.42
34:DA:189(L):G:H2'	34:DA:190:U:C6	2.54	0.42
34:DA:229:U:H2'	34:DA:230:G:O4'	2.19	0.42
34:DA:575:G:C6	34:DA:821:G:N7	2.87	0.42
34:DA:991:U:H3'	34:DA:1212:U:C4	2.54	0.42
34:DA:1303:C:N4	34:DA:1304:G:C6	2.87	0.42
35:DB:105:PHE:O	35:DB:107:THR:N	2.52	0.42
37:DD:64:LEU:HB2	37:DD:198:VAL:HG11	2.01	0.42
37:DD:191:ARG:HD2	37:DD:191:ARG:HA	1.73	0.42
42:DI:17:VAL:HA	42:DI:63:ILE:HG12	2.02	0.42
46:DM:29:ARG:HG3	46:DM:64:TRP:CH2	2.54	0.42
1:AA:485:U:H5''	31:A7:40:TRP:CD2	2.54	0.42
1:AA:579:G:H2'	1:AA:580:U:C6	2.55	0.42
1:AA:1271:G:O3'	19:AV:84:LYS:HE2	2.19	0.42
1:AA:2267:G:H21	24:A0:9:SER:HB3	1.84	0.42
1:AA:2595:G:N3	56:BW:76:F3N:C2	2.82	0.42
2:AB:66:A:N6	2:AB:108:U:H2'	2.35	0.42
11:AN:85:ILE:HA	11:AN:86:PRO:HD3	1.81	0.42
19:AV:28:GLU:HG3	19:AV:29:PRO:HD2	2.01	0.42
21:AX:24:GLY:O	21:AX:83:VAL:HG22	2.19	0.42
34:BA:342:C:O2'	34:BA:343:U:H5'	2.19	0.42
34:BA:924:C:H2'	34:BA:925:G:H8	1.85	0.42
34:BA:1055:A:C5	34:BA:1206:G:C2	3.07	0.42
43:BJ:61:GLU:OE1	47:BN:49:HIS:HE1	2.03	0.42
50:BQ:87:LYS:HA	50:BQ:87:LYS:HD3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:BY:38:A:H2'	58:BY:39:PSU:O4'	2.20	0.42
59:BZ:73:PHE:CZ	59:BZ:78:ARG:NH1	2.79	0.42
59:BZ:247:ARG:HG3	59:BZ:247:ARG:NH1	2.34	0.42
59:BZ:422:GLU:H	59:BZ:422:GLU:HG3	1.61	0.42
1:CA:253:C:OP2	32:C8:5:LYS:NZ	2.44	0.42
1:CA:924:C:H2'	1:CA:925:C:C6	2.54	0.42
1:CA:1404:C:H2'	1:CA:1405:U:H6	1.85	0.42
1:CA:2126:A:N6	1:CA:2163:C:H5'	2.34	0.42
2:CB:78:A:C2	2:CB:100:A:C4	3.07	0.42
4:CD:16:MET:CE	4:CD:208:LYS:HD3	2.50	0.42
6:CF:31:HIS:O	6:CF:34:TRP:HB3	2.20	0.42
11:CN:34:LEU:HD12	11:CN:34:LEU:HA	1.61	0.42
11:CN:43:THR:HA	11:CN:44:PRO:HD3	1.82	0.42
15:CR:18:LEU:HD23	15:CR:18:LEU:HA	1.64	0.42
23:CZ:100:VAL:HA	23:CZ:101:PRO:HD3	1.90	0.42
24:C0:72:ARG:HE	24:C0:75:LEU:HD12	1.85	0.42
26:C2:22:GLU:OE2	26:C2:68:ARG:NH2	2.52	0.42
30:C6:8:LYS:HD3	32:C8:34:TRP:CG	2.54	0.42
33:C9:14:CYS:HA	33:C9:27:CYS:HB2	2.02	0.42
34:DA:1074:G:O2'	34:DA:1101:A:N1	2.44	0.42
42:DI:8:GLY:O	42:DI:14:VAL:HA	2.19	0.42
1:AA:726:C:H2'	1:AA:727:G:H8	1.85	0.42
1:AA:2150:C:H2'	1:AA:2151:C:H6	1.84	0.42
1:AA:2595:G:N3	56:BW:76:F3N:H2	2.35	0.42
10:AL:101:TRP:O	10:AL:105:LEU:HD12	2.19	0.42
34:BA:155:C:N4	34:BA:167:G:O6	2.53	0.42
34:BA:162:A:C8	34:BA:163:C:H1'	2.55	0.42
34:BA:836:G:OP2	51:BR:61:LYS:HE3	2.19	0.42
34:BA:1002:G:C2	34:BA:1003:G:H1'	2.55	0.42
37:BD:158:ILE:H	37:BD:158:ILE:HG12	1.61	0.42
41:BH:49:GLU:HG2	41:BH:62:TYR:HE1	1.85	0.42
45:BL:24:VAL:HB	45:BL:27:LEU:HD22	2.01	0.42
45:BL:27:LEU:HD12	45:BL:27:LEU:HA	1.84	0.42
47:BN:33:VAL:HA	47:BN:40:CYS:HA	2.02	0.42
51:BR:45:SER:OG	51:BR:47:THR:HG22	2.20	0.42
59:BZ:-34:ARG:O	59:BZ:-32:LEU:N	2.52	0.42
59:BZ:100:VAL:HG12	59:BZ:100:VAL:O	2.19	0.42
1:CA:18:C:H2'	1:CA:19:C:H6	1.83	0.42
1:CA:315:G:H2'	1:CA:316:C:C6	2.55	0.42
1:CA:330:A:H2	1:CA:1210:A:HO2'	1.65	0.42
1:CA:686:G:N2	1:CA:788:A:H61	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:794:G:H2'	1:CA:795:C:C6	2.55	0.42
1:CA:814:C:H2'	1:CA:815:C:H6	1.85	0.42
1:CA:862:G:O2'	2:CB:78:A:N3	2.53	0.42
1:CA:956:G:N2	1:CA:959:A:H3'	2.34	0.42
1:CA:1104:C:H2'	1:CA:1105:U:C6	2.55	0.42
1:CA:1473:G:H2'	1:CA:1474:C:O4'	2.19	0.42
1:CA:2756:U:H1'	1:CA:2757:A:H5''	2.01	0.42
3:CC:195:ARG:HG3	3:CC:195:ARG:NH1	2.35	0.42
7:CG:86:MET:HA	7:CG:87:PRO:HD2	1.93	0.42
7:CG:136:ARG:HD2	7:CG:137:GLU:HG3	2.01	0.42
12:CO:98:VAL:CG1	12:CO:117:LEU:HB3	2.48	0.42
13:CP:84:ASN:OD1	13:CP:117:GLU:HB2	2.19	0.42
13:CP:85:LEU:HD23	13:CP:88:LEU:HD12	2.01	0.42
25:C1:80:LEU:HD23	25:C1:82:LEU:HD21	2.01	0.42
34:DA:26:A:O2'	37:DD:209:ARG:NH2	2.53	0.42
34:DA:165:C:H2'	34:DA:166:G:H8	1.84	0.42
34:DA:923:A:N6	34:DA:1392:G:O6	2.52	0.42
36:DC:22:TRP:HB2	36:DC:23:TYR:H	1.69	0.42
40:DG:26:PHE:CD1	40:DG:62:PHE:CE1	3.07	0.42
40:DG:28:ASN:HD21	40:DG:36:LYS:NZ	2.16	0.42
40:DG:79:ARG:HB3	40:DG:80:VAL:H	1.42	0.42
56:DW:37:MIA:H2'	56:DW:38:A:O4'	2.19	0.42
59:DZ:31:ARG:HA	59:DZ:31:ARG:HE	1.83	0.42
59:DZ:285:ASP:OD2	59:DZ:285:ASP:N	2.53	0.42
59:DZ:443:HIS:HA	59:DZ:444:PRO:HD2	1.79	0.42
1:AA:1634:C:H2'	1:AA:1635:C:C6	2.53	0.42
1:AA:1911:A:N1	1:AA:2246:G:H1'	2.34	0.42
1:AA:2289:G:OP2	24:A0:10:THR:HG21	2.20	0.42
3:AC:225:ILE:O	3:AC:227:PRO:HD3	2.19	0.42
5:AE:178:GLU:H	5:AE:178:GLU:CD	2.21	0.42
6:AF:181:LEU:HA	6:AF:181:LEU:HD12	1.81	0.42
14:AQ:31:ASP:OD2	14:AQ:107:ALA:HA	2.20	0.42
17:AT:18:ASP:OD2	17:AT:18:ASP:N	2.53	0.42
17:AT:53:ARG:CZ	17:AT:53:ARG:HB3	2.49	0.42
24:A0:56:ASP:O	24:A0:57:PHE:HB2	2.19	0.42
34:BA:134:A:N6	49:BP:25:ARG:NH1	2.68	0.42
34:BA:1092:A:N3	34:BA:1183:A:N6	2.67	0.42
34:BA:1456:G:H1'	53:BT:39:LYS:HZ3	1.85	0.42
34:BA:1486:G:H2'	34:BA:1487:G:O4'	2.20	0.42
38:BE:152:ARG:HA	41:BH:64:LYS:HZ2	1.84	0.42
51:BR:46:GLU:H	51:BR:46:GLU:HG3	1.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:BW:19:G:H4'	56:BW:20:U:OP1	2.19	0.42
59:BZ:21:ILE:HD12	59:BZ:87:HIS:NE2	2.35	0.42
1:CA:86:C:P	22:CY:32:PRO:HG2	2.60	0.42
1:CA:590:A:H2'	1:CA:591:C:O4'	2.19	0.42
1:CA:610:G:N2	1:CA:619:G:H1'	2.34	0.42
1:CA:910:A:H2'	1:CA:2264:C:O2'	2.20	0.42
1:CA:1070:A:H5'	1:CA:1072:C:OP2	2.19	0.42
1:CA:1615:C:C5	1:CA:1617:C:C4	3.07	0.42
1:CA:1889:A:N1	1:CA:2234:G:H1'	2.34	0.42
2:CB:11:C:OP2	2:CB:12:C:N4	2.33	0.42
3:CC:6:LYS:N	3:CC:9:ARG:HH12	2.17	0.42
7:CG:33:ARG:HB2	7:CG:33:ARG:CZ	2.50	0.42
9:CK:56:ASN:HA	9:CK:83:TYR:HA	2.02	0.42
13:CP:2:LYS:HE2	13:CP:2:LYS:HB2	1.84	0.42
34:DA:784:C:H2'	34:DA:785:G:C8	2.54	0.42
34:DA:1041:A:H5'	34:DA:1042:G:OP2	2.20	0.42
34:DA:1418:A:H5''	34:DA:1419:G:OP2	2.19	0.42
35:DB:55:PHE:HD1	35:DB:58:ILE:HD12	1.83	0.42
36:DC:32:LEU:O	36:DC:36:ASP:HB2	2.19	0.42
38:DE:100:VAL:HG12	38:DE:107:ARG:HH21	1.85	0.42
59:DZ:630:GLN:CG	59:DZ:646:PHE:HB2	2.50	0.42
1:AA:645:G:H2'	1:AA:645:G:N3	2.33	0.42
1:AA:1117:G:O2'	1:AA:1135:G:OP2	2.30	0.42
1:AA:2200:C:H2'	1:AA:2201:C:C6	2.55	0.42
1:AA:2703:C:O3'	1:AA:2881:C:H4'	2.20	0.42
3:AC:54:ARG:HE	3:AC:57:GLN:HG2	1.83	0.42
8:AH:33:LEU:HD21	8:AH:136:ILE:HG13	2.01	0.42
11:AN:4:TYR:CE2	18:AU:100:VAL:HG11	2.54	0.42
13:AP:65:ARG:HG3	13:AP:66:GLY:N	2.34	0.42
16:AS:110:LEU:HD12	16:AS:110:LEU:HA	1.75	0.42
23:AZ:98:MET:O	23:AZ:125:LEU:HD12	2.18	0.42
23:AZ:107:THR:HA	23:AZ:108:PRO:HD3	1.71	0.42
34:BA:1028:C:H2'	34:BA:1029:C:H4'	2.02	0.42
34:BA:1054:C:C4	56:BW:34:G:H1'	2.55	0.42
34:BA:1250:A:H4'	42:BI:68:GLY:N	2.35	0.42
36:BC:8:ILE:HG22	47:BN:49:HIS:O	2.19	0.42
37:BD:116:GLN:NE2	37:BD:157:LEU:HD11	2.35	0.42
38:BE:31:LEU:HD23	38:BE:45:PHE:CD1	2.55	0.42
40:BG:103:TRP:CH2	40:BG:141:VAL:HG21	2.55	0.42
53:BT:99:LEU:HA	53:BT:100:ILE:O	2.19	0.42
57:BX:39:C:O2'	58:BY:35:A:O2'	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:BZ:2:LYS:HA	59:BZ:5:LEU:HB2	2.00	0.42
59:BZ:111:SER:O	59:BZ:148:LEU:HD21	2.20	0.42
59:BZ:268:GLY:HA2	59:BZ:271:LEU:HD13	2.02	0.42
1:CA:373:U:H1'	1:CA:423:A:N3	2.34	0.42
1:CA:572:A:H5''	1:CA:573:G:OP2	2.19	0.42
1:CA:1155:A:H5''	18:CU:55:ARG:NH1	2.26	0.42
1:CA:1810:A:H2'	1:CA:1811:G:O4'	2.18	0.42
1:CA:2112:G:C5	1:CA:2113:U:H1'	2.55	0.42
1:CA:2712:U:H2'	1:CA:2714:G:H5''	2.01	0.42
3:CC:20:VAL:O	3:CC:21:TYR:CB	2.59	0.42
3:CC:225:ILE:O	3:CC:227:PRO:HD3	2.19	0.42
15:CR:12:ARG:HG3	15:CR:12:ARG:HH11	1.84	0.42
17:CT:41:ARG:NH1	34:DA:346:G:OP1	2.49	0.42
18:CU:76:TYR:HH	18:CU:92:ARG:NH1	2.18	0.42
22:CY:68:HIS:CE1	22:CY:70:SER:HB3	2.55	0.42
23:CZ:40:ASP:OD2	23:CZ:42:VAL:HG12	2.20	0.42
34:DA:685:G:C2	34:DA:686:U:C4	3.08	0.42
34:DA:1144:G:N2	34:DA:1146:A:H62	2.18	0.42
44:DK:84:VAL:HG11	44:DK:91:ARG:HD2	2.00	0.42
49:DP:36:ILE:HD12	49:DP:56:ALA:HB2	2.02	0.42
50:DQ:52:LYS:HB2	50:DQ:52:LYS:HE3	1.83	0.42
53:DT:57:ARG:HH12	53:DT:100:ILE:CD1	2.33	0.42
59:DZ:280:LEU:HA	59:DZ:281:PRO:HD3	1.92	0.42
59:DZ:286:ILE:O	59:DZ:286:ILE:HG12	2.19	0.42
1:AA:233:A:C2	1:AA:244:A:C4	3.07	0.42
1:AA:330:U:H2'	1:AA:331:G:O4'	2.20	0.42
1:AA:540:A:H2	1:AA:1306:G:N3	2.17	0.42
1:AA:800:C:H2'	1:AA:801:C:H6	1.85	0.42
1:AA:1764:G:C6	1:AA:1765:U:C4	3.08	0.42
1:AA:1831:C:OP2	4:AD:183:ARG:NH2	2.53	0.42
1:AA:2022:G:OP1	15:AR:5:LYS:NZ	2.49	0.42
1:AA:2340:A:H2'	1:AA:2341:G:C8	2.54	0.42
1:AA:2408:G:H5'	25:A1:25:LYS:HE2	2.02	0.42
5:AE:49:LEU:HD22	5:AE:81:ILE:HG13	2.01	0.42
33:A9:17:ILE:HD12	33:A9:17:ILE:HA	1.72	0.42
34:BA:106:C:O2	34:BA:379:C:H4'	2.20	0.42
34:BA:158:G:N2	34:BA:163:C:O2	2.50	0.42
34:BA:342:C:N3	34:BA:348:G:N2	2.68	0.42
34:BA:1368:G:OP2	42:BI:112:LYS:HG3	2.20	0.42
40:BG:45:ASP:O	40:BG:49:ILE:HG13	2.20	0.42
40:BG:78:ARG:HG2	40:BG:79:ARG:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:BT:81:LYS:O	53:BT:85:MET:HG3	2.19	0.42
1:CA:86:C:H4'	1:CA:104:U:H1'	2.02	0.42
1:CA:814:C:O2'	1:CA:815:C:H5'	2.20	0.42
1:CA:2258:C:O2'	1:CA:2427:C:OP2	2.34	0.42
1:CA:2285:C:OP2	30:C6:6:ARG:NH1	2.52	0.42
1:CA:2628:C:H1'	1:CA:2781:A:H2'	2.01	0.42
1:CA:2689:U:P	1:CA:2719:G:H22	2.43	0.42
3:CC:48:LEU:CD2	3:CC:59:VAL:HG21	2.50	0.42
4:CD:132:PRO:HD3	4:CD:190:TYR:CZ	2.55	0.42
5:CE:24:THR:HG23	5:CE:184:VAL:HG13	2.00	0.42
5:CE:36:ARG:HG2	5:CE:47:VAL:HG12	2.01	0.42
8:CH:42:ARG:HH12	8:CH:53:GLU:HB2	1.84	0.42
8:CH:88:LEU:HD22	8:CH:165:ALA:HA	2.00	0.42
11:CN:120:LEU:HD22	11:CN:122:VAL:HG23	2.01	0.42
13:CP:47:ASP:HA	13:CP:48:PRO:HD3	1.87	0.42
15:CR:51:LEU:HD23	15:CR:51:LEU:HA	1.74	0.42
17:CT:118:ARG:HG2	34:DA:1442(A):G:C8	2.55	0.42
26:C2:2:LYS:HE3	26:C2:2:LYS:HB3	1.92	0.42
34:DA:232:G:H1'	34:DA:262:A:N1	2.35	0.42
34:DA:688:G:H2'	34:DA:689:C:C6	2.55	0.42
34:DA:992:U:H3	34:DA:1044:A:N6	2.12	0.42
34:DA:1004:A:H62	34:DA:1037:C:C2'	2.30	0.42
35:DB:184:VAL:N	35:DB:198:ASP:OD2	2.50	0.42
57:DX:47:U:N3	57:DX:50:U:OP1	2.52	0.42
57:DX:58:A:H4'	57:DX:59:A:OP1	2.18	0.42
59:DZ:463:VAL:HA	59:DZ:466:LEU:HB2	2.02	0.42
1:AA:1091:A:C8	1:AA:1093:G:C2	3.08	0.42
1:AA:1500:A:O2'	1:AA:1501:U:H2'	2.20	0.42
1:AA:1938:A:H2'	1:AA:1939:U:O4'	2.20	0.42
1:AA:1944:G:H2'	1:AA:1945:U:C6	2.54	0.42
1:AA:2554:A:H4'	1:AA:2555:G:C8	2.55	0.42
5:AE:51:PHE:CE2	5:AE:52:LEU:HG	2.55	0.42
17:AT:45:PHE:CE1	17:AT:65:LYS:HD3	2.55	0.42
22:AY:55:TYR:H	22:AY:55:TYR:HD1	1.68	0.42
22:AY:90:LEU:HD12	22:AY:90:LEU:HA	1.75	0.42
23:AZ:104:PHE:HB3	23:AZ:141:VAL:HG21	2.01	0.42
25:A1:23:LYS:HB2	25:A1:23:LYS:HE3	1.90	0.42
25:A1:85:LEU:HA	25:A1:85:LEU:HD23	1.75	0.42
32:A8:52:LYS:N	32:A8:53:PRO:HD2	2.35	0.42
34:BA:864:A:H2'	34:BA:865:A:C8	2.55	0.42
39:BF:4:TYR:HD1	39:BF:92:LYS:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:BH:64:LYS:HB3	41:BH:79:VAL:HG21	2.01	0.42
53:BT:14:LYS:O	53:BT:18:GLN:HG3	2.20	0.42
59:BZ:94:VAL:HB	59:BZ:98:MET:HB2	2.02	0.42
1:CA:503:A:H4'	1:CA:504:U:H5''	2.02	0.42
1:CA:748:G:O6	20:CW:90:ARG:NH1	2.52	0.42
1:CA:857:C:OP2	24:C0:77:ARG:NH2	2.52	0.42
1:CA:1268:A:H2'	1:CA:1269:A:O4'	2.20	0.42
1:CA:1312:U:OP2	21:CX:63:LYS:NZ	2.36	0.42
1:CA:1651:G:H2'	1:CA:1652:A:O4'	2.20	0.42
1:CA:1713:U:H2'	1:CA:1714:G:C8	2.55	0.42
1:CA:2335:A:C8	1:CA:2337:G:C5	3.07	0.42
1:CA:2583:G:N3	56:DW:76:F3N:H2	2.35	0.42
3:CC:42:VAL:O	3:CC:216:THR:C	2.59	0.42
7:CG:136:ARG:HD2	7:CG:136:ARG:C	2.40	0.42
9:CK:4:LYS:HA	9:CK:5:ARG:HA	1.86	0.42
12:CO:15:GLY:O	12:CO:47:ILE:HG13	2.20	0.42
16:CS:63:THR:HG23	16:CS:64:GLU:N	2.35	0.42
21:CX:5:TYR:CE2	26:C2:30:ARG:HB3	2.54	0.42
21:CX:5:TYR:HB3	26:C2:33:MET:HB2	2.02	0.42
23:CZ:145:GLU:HG2	23:CZ:146:ILE:HD12	2.01	0.42
23:CZ:150:LEU:HB3	23:CZ:171:ILE:HD11	2.02	0.42
34:DA:834:C:C4	34:DA:835:U:C4	3.08	0.42
34:DA:1263:C:H2'	34:DA:1264:C:C6	2.55	0.42
36:DC:18:TRP:HE3	36:DC:18:TRP:H	1.68	0.42
38:DE:24:ARG:NH1	55:DV:24:A:OP2	2.52	0.42
38:DE:139:LEU:C	38:DE:141:GLN:N	2.72	0.42
44:DK:72:ALA:HB1	44:DK:77:MET:HB2	2.01	0.42
45:DL:32:PHE:CB	45:DL:84:LEU:HD11	2.46	0.42
45:DL:84:LEU:HD13	45:DL:85:ILE:N	2.35	0.42
46:DM:82:MET:HE3	46:DM:92:HIS:HB3	2.01	0.42
53:DT:55:ILE:HA	53:DT:55:ILE:HD13	1.82	0.42
57:DX:72:A:H2'	57:DX:73:A:C8	2.55	0.42
1:AA:1185:C:O3'	11:AN:25:ARG:NH1	2.53	0.41
1:AA:1715:A:H4'	1:AA:1716:A:O5'	2.20	0.41
1:AA:1961:U:OP1	1:AA:2616:U:O2'	2.34	0.41
1:AA:2132:G:C6	1:AA:2142:G:C8	3.08	0.41
1:AA:2348:A:N6	24:A0:43:THR:HG21	2.33	0.41
1:AA:2429:C:OP1	13:AP:65:ARG:NH2	2.53	0.41
2:AB:88:C:H2'	2:AB:89:G:O4'	2.19	0.41
3:AC:48:LEU:CD2	3:AC:59:VAL:HG21	2.50	0.41
11:AN:115:ARG:HA	11:AN:118:LYS:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AS:74:ALA:HA	16:AS:110:LEU:HD22	2.02	0.41
17:AT:32:TYR:HD2	17:AT:34:VAL:HG23	1.85	0.41
19:AV:97:LYS:HA	19:AV:97:LYS:HD2	1.46	0.41
22:AY:76:CYS:HA	22:AY:77:PRO:HD3	1.89	0.41
31:A7:31:LEU:HD22	31:A7:42:LEU:HD13	2.00	0.41
34:BA:99:U:H2'	34:BA:100:C:C6	2.55	0.41
34:BA:107:G:H2'	34:BA:108:G:O4'	2.20	0.41
34:BA:109:A:H2'	34:BA:326:G:H21	1.83	0.41
34:BA:392:G:H2'	34:BA:393:A:C8	2.55	0.41
34:BA:567:G:H2'	34:BA:568:G:O4'	2.19	0.41
34:BA:955:U:O2'	52:BS:83:HIS:CD2	2.73	0.41
37:BD:202:LEU:HD23	37:BD:202:LEU:HA	1.74	0.41
38:BE:83:GLU:HG2	38:BE:88:LYS:HB2	2.02	0.41
39:BF:2:ARG:CZ	39:BF:69:GLU:HG2	2.50	0.41
52:BS:31:ILE:HD12	52:BS:49:ILE:HG12	2.01	0.41
53:BT:63:ILE:HG22	53:BT:77:ALA:HB1	2.02	0.41
1:CA:403:U:H4'	1:CA:404:C:H5'	2.01	0.41
1:CA:623:G:H2'	1:CA:624:C:C6	2.55	0.41
1:CA:687:C:H1'	31:C7:4:THR:HG22	2.02	0.41
1:CA:1816:G:C8	4:CD:62:TYR:CE2	3.09	0.41
1:CA:2378:A:H4'	16:CS:23:ARG:NH1	2.35	0.41
3:CC:60:ARG:NH2	3:CC:165:ARG:HH21	2.18	0.41
5:CE:51:PHE:CE2	5:CE:52:LEU:HD13	2.55	0.41
11:CN:58:ASP:OD2	11:CN:59:LYS:HE3	2.20	0.41
13:CP:3:LEU:HD12	13:CP:3:LEU:HA	1.88	0.41
13:CP:46:LYS:HE3	13:CP:46:LYS:HB3	1.87	0.41
18:CU:104:GLN:CD	18:CU:104:GLN:H	2.21	0.41
34:DA:114:U:O2'	34:DA:115:G:H5'	2.20	0.41
34:DA:519:C:H2'	34:DA:520:A:O4'	2.20	0.41
34:DA:519:C:H2'	34:DA:520:A:C8	2.55	0.41
34:DA:918:A:H2'	34:DA:919:A:O4'	2.20	0.41
34:DA:1018:C:H2'	34:DA:1019:C:O4'	2.20	0.41
34:DA:1328:C:H2'	34:DA:1329:A:O4'	2.20	0.41
34:DA:1429:C:H2'	34:DA:1430:C:C6	2.55	0.41
35:DB:214:ILE:H	35:DB:214:ILE:HG12	1.64	0.41
37:DD:28:SER:HB2	37:DD:29:PRO:HD2	2.01	0.41
40:DG:104:LEU:HD13	40:DG:104:LEU:HA	1.73	0.41
41:DH:97:VAL:HG21	41:DH:128:GLY:HA2	2.02	0.41
57:DX:49:G:N2	57:DX:66:C:O2	2.53	0.41
1:AA:696:C:P	1:AA:696:C:H6	2.43	0.41
1:AA:1042:A:H4'	18:AU:91:ASP:OD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1403:U:H2'	1:AA:1404:G:O4'	2.20	0.41
1:AA:2431:U:H2'	1:AA:2432:C:C6	2.56	0.41
1:AA:2481:A:H5'	1:AA:2482:G:OP2	2.20	0.41
3:AC:42:VAL:O	3:AC:216:THR:C	2.59	0.41
5:AE:144:ARG:HB3	5:AE:145:LYS:H	1.45	0.41
12:AO:1:MET:HE3	12:AO:32:TYR:CE1	2.55	0.41
12:AO:19:ILE:HB	12:AO:41:ALA:HB1	2.01	0.41
13:AP:3:LEU:HD12	13:AP:3:LEU:HA	1.75	0.41
15:AR:100:LEU:HD11	15:AR:113:LEU:HD23	2.02	0.41
21:AX:41:ASN:O	21:AX:45:THR:HG23	2.20	0.41
30:A6:19:ARG:HD2	30:A6:19:ARG:N	2.35	0.41
34:BA:62:U:H5''	34:BA:385:C:H1'	2.02	0.41
34:BA:143:A:H2	34:BA:220:G:H1	1.66	0.41
34:BA:382:A:H2'	34:BA:383:A:C8	2.55	0.41
34:BA:1152:A:H5'	43:BJ:13:HIS:ND1	2.35	0.41
34:BA:1352:C:OP1	54:BU:3:LYS:NZ	2.46	0.41
34:BA:1516:G:H2'	34:BA:1518:A:OP2	2.20	0.41
35:BB:145:LEU:HD12	35:BB:149:LEU:HD12	2.01	0.41
38:BE:127:ASN:HA	38:BE:128:PRO:HD3	1.79	0.41
45:BL:39:VAL:HG11	45:BL:41:ARG:NH1	2.35	0.41
51:BR:40:LEU:O	51:BR:43:PHE:N	2.38	0.41
59:BZ:6:GLU:O	59:BZ:10:LYS:N	2.53	0.41
59:BZ:264:LEU:HB2	64:BZ:702:GDP:C6	2.55	0.41
59:BZ:414:GLU:C	59:BZ:416:LYS:H	2.22	0.41
1:CA:443:A:H1'	1:CA:1201:C:O4'	2.19	0.41
1:CA:590:A:OP1	6:CF:95:ARG:NH1	2.49	0.41
1:CA:815:C:H2'	1:CA:816:C:H6	1.84	0.41
1:CA:888:C:P	46:DM:93:ARG:HD3	2.59	0.41
1:CA:1469:A:H2'	1:CA:1470:G:O4'	2.20	0.41
1:CA:2127:G:OP1	1:CA:2127:G:H4'	2.20	0.41
1:CA:2137:C:H2'	1:CA:2138:C:C6	2.55	0.41
1:CA:2183:C:H2'	1:CA:2184:G:C8	2.52	0.41
1:CA:2206:G:H3'	1:CA:2207:G:H8	1.75	0.41
5:CE:48:GLN:OE1	5:CE:78:LEU:HG	2.21	0.41
6:CF:64:ILE:HD12	6:CF:65:TRP:CZ3	2.55	0.41
16:CS:87:PHE:CE1	16:CS:102:ALA:HB2	2.55	0.41
18:CU:79:PHE:O	18:CU:83:LEU:HD22	2.20	0.41
18:CU:86:ALA:O	19:CV:49:THR:HG23	2.20	0.41
19:CV:82:ARG:O	19:CV:83:ARG:HD3	2.20	0.41
23:CZ:8:TYR:HB2	23:CZ:38:TYR:CZ	2.55	0.41
23:CZ:102:LEU:HD11	23:CZ:121:HIS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:CZ:157:LEU:HB3	23:CZ:161:VAL:HG13	2.02	0.41
30:C6:40:CYS:SG	30:C6:42:TRP:HB2	2.59	0.41
34:DA:730:G:O2'	34:DA:766:A:H5'	2.20	0.41
34:DA:1049:U:C6	34:DA:1201:A:H5'	2.55	0.41
34:DA:1090:U:H2'	34:DA:1091:U:H6	1.86	0.41
34:DA:1119:C:H2'	34:DA:1120:G:C8	2.54	0.41
36:DC:184:TYR:HD1	36:DC:201:TYR:CE2	2.38	0.41
43:DJ:38:ILE:HG12	43:DJ:71:LEU:O	2.20	0.41
46:DM:88:ARG:HG2	46:DM:98:VAL:HG12	2.03	0.41
56:DW:9:A:H8	56:DW:11:C:H41	1.67	0.41
1:AA:50:G:H4'	1:AA:51:A:H5'	2.01	0.41
1:AA:469:A:C6	6:AF:45:ARG:HD2	2.55	0.41
1:AA:733:G:OP1	31:A7:11:LYS:NZ	2.50	0.41
1:AA:1067:A:C8	1:AA:1067:A:C3'	3.03	0.41
1:AA:1098:C:H2'	1:AA:1099:C:H6	1.84	0.41
1:AA:2124:U:H2'	1:AA:2125:C:C6	2.54	0.41
1:AA:2164:C:H2'	1:AA:2165:C:C6	2.55	0.41
4:AD:260:ARG:NH2	4:AD:264:LYS:HD3	2.35	0.41
5:AE:108:SER:O	5:AE:162:ALA:HA	2.20	0.41
7:AG:11:TYR:HA	7:AG:15:VAL:HB	2.01	0.41
8:AH:84:SER:HA	8:AH:133:VAL:O	2.20	0.41
15:AR:21:TYR:OH	15:AR:43:GLU:HG2	2.20	0.41
16:AS:97:ARG:O	16:AS:100:ALA:HB3	2.20	0.41
23:AZ:129:SER:HA	23:AZ:130:PRO:HD3	1.74	0.41
34:BA:78:G:H22	34:BA:92:C:H42	1.67	0.41
34:BA:243:A:C2	34:BA:246:A:C8	3.09	0.41
34:BA:715:A:H2'	34:BA:716:A:C8	2.55	0.41
34:BA:1118:C:H1'	34:BA:1179:A:C4	2.56	0.41
34:BA:1250:A:H2'	34:BA:1251:A:C8	2.56	0.41
38:BE:74:GLY:HA3	38:BE:116:THR:HG22	2.01	0.41
44:BK:33:THR:HA	44:BK:39:PRO:HA	2.02	0.41
52:BS:48:THR:HA	52:BS:60:VAL:O	2.19	0.41
59:BZ:257:PRO:HB2	59:BZ:259:PHE:CE1	2.55	0.41
59:BZ:358:MET:HE1	59:BZ:363:ARG:NH1	2.36	0.41
1:CA:271(F):C:H2'	1:CA:271(G):C:O4'	2.20	0.41
1:CA:583:G:OP2	18:CU:10:ARG:HD2	2.20	0.41
1:CA:863:A:H2'	1:CA:864:G:H8	1.84	0.41
1:CA:1082:U:H5''	10:CL:122:ALA:HB1	2.02	0.41
1:CA:1107:G:C2	1:CA:1108:U:C4	3.08	0.41
1:CA:1401:G:H2'	1:CA:1402:C:O4'	2.21	0.41
1:CA:1638:C:H5''	1:CA:2710:C:O2'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1647:G:H3'	1:CA:1647:G:OP2	2.20	0.41
1:CA:1656:C:H2'	1:CA:1657:C:C6	2.56	0.41
1:CA:2536:G:C6	1:CA:2537:U:C4	3.09	0.41
9:CK:118:THR:O	9:CK:120:LYS:N	2.51	0.41
13:CP:36:LYS:O	13:CP:40:SER:HB3	2.20	0.41
13:CP:87:ASP:HB3	13:CP:105:LEU:HD22	2.02	0.41
20:CW:53:SER:O	20:CW:56:ALA:HB3	2.20	0.41
22:CY:98:VAL:HG23	22:CY:99:CYS:O	2.20	0.41
23:CZ:67:LEU:HA	23:CZ:68:PRO:HD3	1.73	0.41
26:C2:49:LYS:HE2	26:C2:49:LYS:HB3	1.89	0.41
34:DA:64:G:H4'	34:DA:65:U:C3'	2.49	0.41
34:DA:137:C:H2'	34:DA:138:G:H8	1.84	0.41
34:DA:391:G:C6	34:DA:392:G:C5	3.08	0.41
34:DA:1106:G:H4'	36:DC:171:GLY:O	2.20	0.41
34:DA:1130:A:H5'	42:DI:18:PHE:CE2	2.55	0.41
34:DA:1314:C:OP2	52:DS:4:SER:OG	2.12	0.41
37:DD:60:GLU:OE1	37:DD:199:ASN:N	2.52	0.41
40:DG:26:PHE:HB2	40:DG:101:LEU:HD22	2.01	0.41
50:DQ:15:MET:HE1	50:DQ:43:LEU:HD13	2.01	0.41
1:AA:170:A:H2'	1:AA:171:A:C8	2.55	0.41
1:AA:659:C:H2'	1:AA:660:C:C6	2.55	0.41
1:AA:2147:G:OP1	3:AC:71:LYS:NZ	2.52	0.41
1:AA:2173:G:H2'	1:AA:2174:G:C8	2.56	0.41
7:AG:43:LEU:HD12	7:AG:43:LEU:HA	1.81	0.41
7:AG:97:ASP:O	7:AG:101:ILE:HG13	2.20	0.41
8:AH:56:SER:OG	8:AH:61:HIS:ND1	2.40	0.41
15:AR:36:THR:HG22	15:AR:37:THR:H	1.84	0.41
17:AT:109:GLU:HG2	17:AT:112:ARG:HH21	1.85	0.41
23:AZ:150:LEU:O	23:AZ:171:ILE:HG13	2.20	0.41
23:AZ:152:ALA:HA	23:AZ:155:LEU:HD22	2.02	0.41
34:BA:28:G:O2'	34:BA:296:U:OP1	2.30	0.41
34:BA:565:U:H3'	34:BA:566:G:H2'	2.01	0.41
34:BA:1220:G:N2	52:BS:54:GLY:O	2.50	0.41
34:BA:1261:A:H3'	34:BA:1262:C:H6	1.84	0.41
36:BC:131:ARG:HH11	38:BE:50:GLU:HG3	1.86	0.41
47:BN:8:GLU:OE2	47:BN:11:LYS:HD2	2.21	0.41
52:BS:65:ASN:HD22	52:BS:65:ASN:H	1.67	0.41
53:BT:53:LEU:O	53:BT:57:ARG:HG3	2.20	0.41
59:BZ:427:ALA:O	59:BZ:431:LEU:HD22	2.20	0.41
59:BZ:471:LYS:HE2	59:BZ:471:LYS:HB3	1.97	0.41
1:CA:888:C:H5''	1:CA:889:C:OP2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1652:A:O2'	1:CA:1653:G:H5'	2.20	0.41
1:CA:1804:C:O5'	1:CA:1804:C:H6	2.02	0.41
1:CA:1860:G:H4'	3:CC:206:LYS:HG3	1.76	0.41
34:DA:520:A:N1	34:DA:536:C:H1'	2.35	0.41
34:DA:546:G:P	37:DD:72:GLU:HB3	2.60	0.41
34:DA:719:C:O2'	51:DR:49:LYS:HB3	2.21	0.41
34:DA:1343:G:H2'	34:DA:1344:C:C6	2.55	0.41
35:DB:212:GLN:O	35:DB:216:SER:OG	2.35	0.41
37:DD:100:ARG:HH11	37:DD:100:ARG:HG2	1.84	0.41
39:DF:61:LEU:HD23	39:DF:63:TYR:OH	2.20	0.41
48:DO:32:LEU:HA	48:DO:32:LEU:HD23	1.75	0.41
56:DW:4:C:N4	56:DW:5:G:O6	2.53	0.41
59:DZ:165:GLN:O	59:DZ:166:LEU:HD12	2.20	0.41
59:DZ:201:ILE:HG22	59:DZ:202:PRO:O	2.20	0.41
1:AA:1400:A:C8	1:AA:1401:G:C8	3.09	0.41
1:AA:1704:C:H2'	1:AA:1705:C:C6	2.55	0.41
1:AA:1841:A:H2'	1:AA:1842:G:O4'	2.20	0.41
2:AB:41:U:C5	7:AG:70:VAL:HB	2.56	0.41
3:AC:31:LYS:H	3:AC:31:LYS:HG2	1.57	0.41
11:AN:138:LEU:HD22	11:AN:138:LEU:HA	1.74	0.41
14:AQ:31:ASP:HB2	14:AQ:32:TYR:HD2	1.85	0.41
16:AS:67:ARG:HD2	16:AS:71:ARG:NH2	2.35	0.41
23:AZ:111:VAL:HG12	23:AZ:112:ARG:N	2.35	0.41
25:A1:23:LYS:HB3	25:A1:29:GLY:HA3	2.02	0.41
28:A4:69:LYS:HE2	52:BS:20:LEU:HD13	2.02	0.41
31:A7:33:ARG:NH2	65:A7:201:HOH:O	2.54	0.41
34:BA:7:G:H5'	34:BA:298:A:O4'	2.20	0.41
34:BA:368:U:P	59:BZ:351:ARG:HH11	2.43	0.41
34:BA:1053:G:O2'	34:BA:1199:U:OP2	2.21	0.41
34:BA:1130:A:C4	34:BA:1146:A:C2	3.08	0.41
34:BA:1183:A:H3'	34:BA:1184:G:C5'	2.51	0.41
34:BA:1318:A:H2'	34:BA:1319:A:H5''	2.03	0.41
35:BB:167:PRO:HG3	35:BB:186:ALA:HB1	2.02	0.41
46:BM:4:ILE:HA	46:BM:5:ALA:HA	1.90	0.41
57:BX:19:G:H4'	57:BX:20:U:OP2	2.21	0.41
59:BZ:-20:LEU:HD22	59:BZ:-20:LEU:HA	1.70	0.41
59:BZ:78:ARG:HH11	59:BZ:78:ARG:CB	2.32	0.41
59:BZ:414:GLU:O	59:BZ:416:LYS:N	2.54	0.41
1:CA:297:C:H2'	1:CA:298:G:O4'	2.20	0.41
1:CA:620:G:N3	1:CA:620:G:H2'	2.35	0.41
1:CA:859:G:O2'	1:CA:916:G:O6	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CD:68:LYS:O	4:CD:69:ARG:HB2	2.21	0.41
13:CP:3:LEU:HD12	13:CP:6:LEU:HD12	2.02	0.41
30:C6:34:LEU:HB2	30:C6:51:GLU:HB2	2.03	0.41
34:DA:344:A:H4'	34:DA:345:C:OP2	2.21	0.41
34:DA:511:C:C2	34:DA:512:U:C5	3.08	0.41
34:DA:869:G:H8	34:DA:869:G:O5'	2.03	0.41
34:DA:1063:C:OP2	34:DA:1064:G:O2'	2.23	0.41
36:DC:33:LEU:O	36:DC:37:GLN:N	2.52	0.41
36:DC:112:SER:O	36:DC:115:LEU:HB2	2.21	0.41
37:DD:78:LEU:HB3	37:DD:93:PHE:HE1	1.86	0.41
38:DE:129:ILE:O	38:DE:132:ALA:HB3	2.20	0.41
39:DF:5:GLU:N	39:DF:91:VAL:O	2.47	0.41
40:DG:26:PHE:CZ	40:DG:30:ILE:HD11	2.56	0.41
40:DG:155:ARG:CZ	40:DG:155:ARG:HB3	2.49	0.41
41:DH:9:MET:SD	41:DH:26:VAL:HG21	2.61	0.41
45:DL:124:LYS:HA	45:DL:125:PRO:HD3	1.79	0.41
59:DZ:38:ARG:HE	59:DZ:38:ARG:HB2	1.60	0.41
1:AA:52:A:H2'	1:AA:53:G:O4'	2.20	0.41
1:AA:277:G:H2'	1:AA:278:G:C8	2.55	0.41
1:AA:2133:C:N3	1:AA:2167:C:O2'	2.48	0.41
1:AA:2140:U:OP1	1:AA:2170:G:H4'	2.20	0.41
1:AA:2202:U:C4	1:AA:2203:G:N7	2.88	0.41
1:AA:2595:G:H2'	1:AA:2596:U:O4'	2.21	0.41
4:AD:34:VAL:HA	4:AD:62:TYR:O	2.21	0.41
7:AG:126:ASP:CG	7:AG:130:ASN:HD22	2.23	0.41
7:AG:140:ILE:HG22	7:AG:141:PHE:CD1	2.56	0.41
16:AS:89:ARG:HD2	16:AS:92:TYR:O	2.21	0.41
24:A0:70:GLN:HG2	24:A0:72:ARG:HG3	2.02	0.41
34:BA:5:U:H5'	34:BA:6:G:C5	2.55	0.41
34:BA:149:A:H2'	34:BA:150:C:H6	1.84	0.41
34:BA:303:A:H2'	34:BA:304:U:O4'	2.20	0.41
34:BA:321:A:C2	34:BA:333:G:C2	3.08	0.41
34:BA:911:U:OP2	45:BL:97:ARG:NH1	2.54	0.41
34:BA:982:U:H4'	34:BA:983:A:O5'	2.21	0.41
37:BD:110:PHE:CE2	37:BD:148:VAL:HG23	2.55	0.41
41:BH:113:SER:O	41:BH:131:GLY:HA3	2.21	0.41
42:BI:23:ASN:HB2	42:BI:25:LYS:NZ	2.35	0.41
46:BM:19:LEU:HD12	46:BM:19:LEU:HA	1.85	0.41
59:BZ:88:VAL:HG23	59:BZ:117:GLN:HA	2.02	0.41
59:BZ:309:LEU:HD21	59:BZ:335:LEU:HD13	2.03	0.41
59:BZ:443:HIS:HA	59:BZ:444:PRO:HD2	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:BZ:520:GLY:H	59:BZ:562:ASP:CG	2.23	0.41
1:CA:184:C:H2'	1:CA:185:U:H6	1.86	0.41
1:CA:777:A:O2'	1:CA:778:G:H5'	2.20	0.41
1:CA:1081:U:O5'	10:CL:125:ARG:HD3	2.20	0.41
1:CA:1645:G:H5''	1:CA:1646:C:O4'	2.21	0.41
1:CA:2557:G:H2'	1:CA:2558:C:C6	2.55	0.41
2:CB:19:G:H2'	2:CB:20:C:O4'	2.21	0.41
5:CE:60:ASN:CG	5:CE:62:PRO:HD2	2.41	0.41
16:CS:39:ILE:HD13	16:CS:85:VAL:HG21	2.01	0.41
16:CS:65:VAL:O	16:CS:68:GLN:HB2	2.21	0.41
22:CY:49:VAL:HG11	22:CY:55:TYR:HD2	1.85	0.41
23:CZ:153:SER:HB3	23:CZ:167:PRO:HB3	2.03	0.41
26:C2:2:LYS:HG2	26:C2:5:GLU:OE1	2.20	0.41
34:DA:67:C:H2'	34:DA:68:G:C8	2.55	0.41
34:DA:841:U:H6	34:DA:841:U:P	2.43	0.41
34:DA:1319:A:N6	34:DA:1361:G:H21	2.18	0.41
35:DB:155:LEU:HD11	35:DB:159:PRO:HD3	2.02	0.41
38:DE:60:TYR:CE1	38:DE:64:ARG:HD3	2.54	0.41
40:DG:26:PHE:CD1	40:DG:62:PHE:HE1	2.39	0.41
41:DH:132:GLU:O	41:DH:134:ILE:N	2.54	0.41
59:DZ:346:LYS:HZ2	59:DZ:346:LYS:HG3	1.68	0.41
1:AA:381:A:H2'	1:AA:382:U:O4'	2.21	0.41
1:AA:667:G:H21	1:AA:671:A:H2	1.69	0.41
1:AA:1020:C:OP1	65:AA:4082:HOH:O	2.22	0.41
1:AA:2170:G:H2'	1:AA:2171:G:H8	1.86	0.41
1:AA:2693:C:OP2	5:AE:109:LYS:NZ	2.46	0.41
7:AG:111:LEU:HD23	7:AG:111:LEU:HA	1.89	0.41
13:AP:63:PRO:HD3	32:A8:27:THR:HG22	2.02	0.41
18:AU:112:ARG:HH11	18:AU:112:ARG:HG2	1.84	0.41
19:AV:25:LEU:HD12	19:AV:92:THR:HG21	2.02	0.41
23:AZ:104:PHE:O	23:AZ:106:GLY:N	2.54	0.41
34:BA:452:A:OP1	49:BP:43:LYS:NZ	2.30	0.41
34:BA:741:G:H2'	34:BA:742:G:O4'	2.21	0.41
34:BA:786:G:C2	34:BA:797:C:C2	3.09	0.41
34:BA:1165:C:HO2'	34:BA:1166:G:P	2.44	0.41
38:BE:96:PRO:HA	38:BE:117:ASP:OD2	2.21	0.41
41:BH:36:LEU:HD23	41:BH:36:LEU:HA	1.80	0.41
43:BJ:38:ILE:HG13	43:BJ:71:LEU:HB3	2.02	0.41
46:BM:121:LYS:NZ	56:BW:40:C:H4'	2.36	0.41
49:BP:5:ARG:O	49:BP:20:VAL:N	2.46	0.41
53:BT:29:LYS:O	53:BT:33:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:335:C:H4'	22:CY:73:ARG:NE	2.35	0.41
1:CA:623:G:C6	1:CA:624:C:C4	3.09	0.41
1:CA:652:C:C2'	1:CA:652(A):A:H5'	2.50	0.41
1:CA:1291:C:H2'	1:CA:1292:U:C6	2.56	0.41
1:CA:1668:A:O2'	1:CA:1674:G:N7	2.49	0.41
1:CA:1890:A:O5'	1:CA:1890:A:H8	2.04	0.41
1:CA:2380:C:O5'	1:CA:2380:C:H6	2.02	0.41
1:CA:2732:G:H3'	1:CA:2733:A:O4'	2.21	0.41
4:CD:148:GLU:OE1	4:CD:151:LYS:NZ	2.34	0.41
6:CF:20:LEU:HD23	6:CF:20:LEU:HA	1.75	0.41
8:CH:106:THR:O	8:CH:106:THR:OG1	2.35	0.41
16:CS:93:LYS:HG2	16:CS:95:HIS:HB3	2.02	0.41
18:CU:76:TYR:O	18:CU:79:PHE:HB3	2.20	0.41
23:CZ:14:LYS:HA	23:CZ:15:PRO:HD3	1.79	0.41
25:C1:83:GLU:HA	25:C1:84:GLY:HA2	1.60	0.41
34:DA:255:G:H1'	50:DQ:16:GLN:NE2	2.36	0.41
34:DA:407:G:H5''	37:DD:115:ARG:HB3	2.02	0.41
34:DA:561:U:HO2'	34:DA:562:C:P	2.44	0.41
34:DA:662:G:H2'	34:DA:663:A:C8	2.56	0.41
34:DA:1151:A:O2'	34:DA:1152:A:O5'	2.36	0.41
34:DA:1373:G:H8	34:DA:1373:G:O5'	2.02	0.41
34:DA:1410:G:H2'	34:DA:1411:C:C6	2.56	0.41
34:DA:1429:C:H2'	34:DA:1430:C:H6	1.85	0.41
37:DD:15:GLU:HB3	37:DD:63:LYS:HD2	2.03	0.41
42:DI:17:VAL:HG23	42:DI:63:ILE:HG12	2.03	0.41
45:DL:52:LEU:HD12	45:DL:52:LEU:HA	1.78	0.41
47:DN:14:PRO:HB2	47:DN:16:PHE:O	2.21	0.41
57:DX:14:A:C5	57:DX:22:G:C6	3.08	0.41
59:DZ:88:VAL:HG23	59:DZ:117:GLN:HE21	1.86	0.41
1:AA:552:C:C4	1:AA:2792:U:H2'	2.55	0.41
1:AA:599:U:H2'	1:AA:600:G:C8	2.56	0.41
1:AA:2227:G:H3'	1:AA:2228:G:N7	2.36	0.41
1:AA:2287:C:O2	14:AQ:85:LYS:HE2	2.20	0.41
1:AA:2325:C:H4'	7:AG:91:ARG:HG3	2.02	0.41
3:AC:60:ARG:NH2	3:AC:165:ARG:HH21	2.18	0.41
6:AF:64:ILE:H	6:AF:64:ILE:HG13	1.59	0.41
8:AH:83:TYR:CE2	8:AH:138:LYS:HB2	2.55	0.41
17:AT:61:PHE:CE1	17:AT:76:PHE:HB2	2.56	0.41
17:AT:117:ASP:O	17:AT:121:ILE:HG13	2.21	0.41
32:A8:31:HIS:O	32:A8:32:LEU:HB2	2.20	0.41
34:BA:418:C:H2'	34:BA:419:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BA:1072:G:C5	34:BA:1073:U:C4	3.09	0.41
34:BA:1187:G:H2'	34:BA:1188:A:C8	2.56	0.41
36:BC:85:ARG:O	36:BC:89:GLU:HG2	2.21	0.41
38:BE:40:ARG:HB3	38:BE:66:MET:CE	2.51	0.41
46:BM:49:THR:O	46:BM:53:VAL:HG23	2.20	0.41
48:BO:66:LEU:HD12	48:BO:66:LEU:HA	1.76	0.41
51:BR:39:VAL:O	51:BR:42:ARG:HB2	2.20	0.41
59:BZ:171:GLU:C	59:BZ:173:THR:H	2.23	0.41
59:BZ:538:TYR:OH	59:BZ:577:SER:O	2.30	0.41
1:CA:443:A:C6	6:CF:45:ARG:HD2	2.56	0.41
1:CA:479:A:H4'	1:CA:480:A:OP1	2.20	0.41
1:CA:1125:G:H5'	33:C9:37:GLY:HA2	2.03	0.41
1:CA:1445(A):C:H2'	1:CA:1446:C:H6	1.86	0.41
1:CA:1657:C:H2'	1:CA:1658:C:H6	1.85	0.41
1:CA:1823:G:OP1	4:CD:54:ARG:NH1	2.54	0.41
3:CC:44:VAL:HG23	3:CC:176:VAL:CG2	2.51	0.41
7:CG:15:VAL:HG22	7:CG:175:LEU:HB3	2.02	0.41
12:CO:68:GLU:OE2	12:CO:78:ARG:NH1	2.51	0.41
17:CT:109:GLU:O	17:CT:113:LYS:HB2	2.21	0.41
23:CZ:30:ASN:ND2	23:CZ:90:VAL:HB	2.35	0.41
25:C1:53:VAL:O	25:C1:56:GLN:HB2	2.21	0.41
25:C1:95:LEU:O	25:C1:98:LEU:HB2	2.20	0.41
30:C6:9:LEU:HD11	30:C6:23:THR:HG23	2.02	0.41
32:C8:23:VAL:HA	32:C8:48:PHE:O	2.20	0.41
34:DA:336:C:O2'	34:DA:337:C:H5'	2.21	0.41
34:DA:694:A:H2'	34:DA:695:A:O4'	2.21	0.41
34:DA:1057:G:H2'	34:DA:1058:G:O4'	2.21	0.41
34:DA:1273:G:H5'	34:DA:1274:G:OP2	2.21	0.41
34:DA:1319:A:H61	34:DA:1361:G:H21	1.68	0.41
35:DB:91:PRO:HB3	35:DB:154:LEU:HB3	2.03	0.41
38:DE:41:VAL:HG22	38:DE:113:ALA:HA	2.02	0.41
49:DP:58:TYR:O	49:DP:61:SER:N	2.52	0.41
53:DT:63:ILE:HG21	53:DT:81:LYS:HG3	2.02	0.41
58:DY:36:A:H2'	58:DY:37:MIA:O4'	2.20	0.41
59:DZ:590:ILE:HD13	59:DZ:590:ILE:HA	1.83	0.41
59:DZ:641:GLN:HE21	59:DZ:641:GLN:HB2	1.63	0.41
59:DZ:655:TYR:CZ	59:DZ:659:LEU:HG	2.56	0.41
1:AA:139:A:C8	1:AA:1454:C:O2'	2.67	0.41
1:AA:354:A:O2'	1:AA:355:A:C8	2.72	0.41
1:AA:505:A:N3	1:AA:507:G:H5''	2.35	0.41
1:AA:841:G:H2'	1:AA:842:C:H6	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:926:G:H8	1:AA:926:G:O5'	2.02	0.41
1:AA:1401:G:P	4:AD:38:LYS:HE2	2.61	0.41
1:AA:1572:G:C6	1:AA:1573:G:C2	3.08	0.41
1:AA:1756:U:H2'	1:AA:1757:C:C6	2.56	0.41
1:AA:1815:A:H4'	1:AA:1816:A:C5'	2.51	0.41
1:AA:1957:G:H1'	1:AA:1986:G:N2	2.36	0.41
1:AA:2356:U:O2'	30:A6:36:LEU:HD22	2.21	0.41
3:AC:11:LEU:HD22	3:AC:11:LEU:H	1.86	0.41
3:AC:206:LYS:HB3	3:AC:206:LYS:HZ3	1.85	0.41
4:AD:33:LEU:HD23	4:AD:33:LEU:HA	1.94	0.41
12:AO:17:ARG:N	12:AO:45:GLU:O	2.40	0.41
18:AU:47:TYR:HA	18:AU:50:ARG:NH2	2.35	0.41
19:AV:71:LEU:HD23	19:AV:71:LEU:HA	1.94	0.41
33:A9:3:VAL:C	33:A9:4:ARG:HG3	2.40	0.41
34:BA:443:C:H2'	34:BA:444:C:H6	1.86	0.41
34:BA:501:C:H1'	34:BA:549:C:H1'	2.03	0.41
34:BA:509:A:H3'	34:BA:509:A:C8	2.55	0.41
34:BA:973:G:OP1	43:BJ:57:LYS:HE3	2.20	0.41
34:BA:981:U:OP1	47:BN:6:LEU:HD11	2.21	0.41
34:BA:1142:G:H2'	34:BA:1143:G:O4'	2.21	0.41
34:BA:1169:A:N6	34:BA:1170:A:N1	2.69	0.41
34:BA:1304:G:C6	34:BA:1305:G:N1	2.89	0.41
35:BB:21:ARG:HB3	35:BB:39:ILE:HA	2.02	0.41
35:BB:204:ASN:OD1	35:BB:205:ASP:N	2.54	0.41
36:BC:108:ASN:HA	36:BC:109:PRO:HD2	1.91	0.41
37:BD:167:GLY:H	37:BD:168:ARG:NH2	2.19	0.41
38:BE:85:GLY:O	38:BE:86:ALA:HB3	2.21	0.41
44:BK:56:GLY:O	44:BK:89:ALA:HB3	2.21	0.41
46:BM:78:ILE:O	46:BM:82:MET:HG3	2.21	0.41
49:BP:7:ALA:O	49:BP:9:PHE:CD1	2.73	0.41
53:BT:18:GLN:O	53:BT:22:ARG:HG3	2.21	0.41
59:BZ:125:ALA:CB	59:BZ:132:ARG:NH1	2.84	0.41
59:BZ:291:GLY:HA3	59:BZ:301:ILE:HD11	2.01	0.41
59:BZ:603:GLU:HG2	59:BZ:679:VAL:HG12	2.03	0.41
1:CA:1002:G:H2'	1:CA:1003:G:O4'	2.21	0.41
1:CA:1485:G:H2'	1:CA:1486:A:O4'	2.20	0.41
1:CA:2404:C:O3'	13:CP:77:ARG:NH2	2.54	0.41
1:CA:2544:G:H1'	1:CA:2646:C:H4'	2.03	0.41
1:CA:2630:G:H2'	1:CA:2631:G:H8	1.86	0.41
1:CA:2801(A):A:H1'	1:CA:2895:U:H1'	2.03	0.41
1:CA:2876:G:OP1	17:CT:3:ARG:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CC:11:LEU:HD22	3:CC:11:LEU:H	1.86	0.41
3:CC:16:ASP:HA	3:CC:17:PRO:HD2	1.90	0.41
6:CF:103:LYS:HA	6:CF:106:ARG:HG3	2.01	0.41
6:CF:197:ASP:O	6:CF:200:GLU:HB2	2.21	0.41
11:CN:91:LEU:O	11:CN:95:PRO:HB3	2.20	0.41
13:CP:93:GLY:H	13:CP:123:LEU:HD21	1.86	0.41
18:CU:76:TYR:CZ	18:CU:80:ILE:HG13	2.55	0.41
19:CV:1:MET:HG2	19:CV:41:GLY:O	2.20	0.41
20:CW:10:VAL:HG21	20:CW:103:ILE:HD12	2.01	0.41
21:CX:4:ALA:HB1	21:CX:42:ALA:HA	2.01	0.41
32:C8:26:LYS:HG2	32:C8:48:PHE:CD1	2.56	0.41
34:DA:401:C:H1'	34:DA:622:A:H1'	2.02	0.41
34:DA:796:C:H6	34:DA:796:C:O5'	2.04	0.41
34:DA:1122:U:H2'	34:DA:1123:A:O4'	2.20	0.41
34:DA:1277:C:O2'	34:DA:1279:A:H1'	2.20	0.41
34:DA:1281:U:H5''	34:DA:1282:C:C5	2.56	0.41
37:DD:26:CYS:HA	63:DD:501:SF4:S3	2.61	0.41
37:DD:135:LEU:C	37:DD:137:SER:H	2.23	0.41
40:DG:110:GLN:HE21	40:DG:110:GLN:HB3	1.71	0.41
40:DG:120:ILE:HG22	40:DG:124:LEU:CD1	2.50	0.41
41:DH:39:LEU:HD13	41:DH:39:LEU:HA	1.96	0.41
41:DH:134:ILE:HG22	41:DH:135:CYS:SG	2.61	0.41
46:DM:20:THR:C	46:DM:22:ILE:H	2.24	0.41
46:DM:60:VAL:HG23	46:DM:64:TRP:CE3	2.56	0.41
50:DQ:89:LEU:HD23	50:DQ:89:LEU:HA	1.64	0.41
53:DT:36:LEU:HD13	53:DT:36:LEU:HA	1.57	0.41
56:DW:13:C:O2'	56:DW:14:A:P	2.79	0.41
59:DZ:164:MET:HG3	59:DZ:257:PRO:HB3	2.01	0.41
59:DZ:168:ILE:HG12	59:DZ:205:TYR:CD2	2.55	0.41
1:AA:789:G:H4'	1:AA:1723:A:H5'	2.03	0.41
1:AA:1002:A:H5'	14:AQ:76:LYS:HG2	2.03	0.41
1:AA:1712:A:H2'	1:AA:1713:G:O4'	2.20	0.41
1:AA:1772:C:H6	1:AA:1772:C:O5'	2.04	0.41
1:AA:2555:G:H2'	1:AA:2556:G:C8	2.56	0.41
3:AC:224:ARG:HE	3:AC:224:ARG:HB3	1.73	0.41
6:AF:62:ARG:HB3	6:AF:62:ARG:NH1	2.36	0.41
12:AO:66:LYS:HA	12:AO:79:PHE:O	2.21	0.41
13:AP:85:LEU:HD12	13:AP:116:GLY:O	2.20	0.41
23:AZ:138:GLU:H	23:AZ:156:LYS:HD3	1.86	0.41
34:BA:1118:C:OP1	42:BI:9:ARG:NH1	2.54	0.41
34:BA:1254:C:H2'	34:BA:1255:G:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BB:215:LEU:O	35:BB:219:VAL:HG23	2.21	0.41
37:BD:188:LEU:HD23	37:BD:188:LEU:H	1.86	0.41
59:BZ:-27:THR:O	59:BZ:-23:LEU:HB2	2.21	0.41
59:BZ:350:GLU:OE1	59:BZ:382:GLU:N	2.53	0.41
59:BZ:499:ARG:HB2	59:BZ:506:GLN:HB2	2.04	0.41
1:CA:224:G:N7	1:CA:420:C:H4'	2.36	0.41
1:CA:1019:U:OP1	1:CA:1035:U:O2'	2.26	0.41
1:CA:1405:U:H2'	1:CA:1406:U:C6	2.55	0.41
1:CA:2330:G:H2'	1:CA:2331:G:O4'	2.20	0.41
1:CA:2733:A:H2	5:CE:204:ALA:H	1.68	0.41
1:CA:2745:C:H4'	8:CH:142:GLY:O	2.20	0.41
3:CC:54:ARG:CZ	3:CC:55:SER:O	2.69	0.41
7:CG:53:LEU:HD23	7:CG:53:LEU:HA	1.83	0.41
12:CO:113:LYS:O	12:CO:117:LEU:HD12	2.21	0.41
14:CQ:85:LYS:HD3	24:C0:7:LEU:HG	2.02	0.41
20:CW:70:TYR:O	20:CW:107:LEU:HD12	2.21	0.41
22:CY:5:MET:HG2	22:CY:30:VAL:HG11	2.03	0.41
22:CY:99:CYS:SG	22:CY:102:CYS:N	2.93	0.41
34:DA:253:U:H2'	34:DA:254:G:H8	1.85	0.41
34:DA:1030(A):G:N2	34:DA:1030(C):G:H3'	2.36	0.41
34:DA:1310:G:H5'	46:DM:77:ASN:OD1	2.21	0.41
59:DZ:327:PHE:CE1	59:DZ:376:ALA:HB2	2.56	0.41
59:DZ:382:GLU:H	59:DZ:382:GLU:HG2	1.76	0.41
59:DZ:628:ARG:HD2	59:DZ:680:PRO:HG2	2.03	0.41
1:AA:100:G:H5''	26:A2:3:LEU:CD1	2.51	0.40
1:AA:253:C:O2'	1:AA:254:A:H2'	2.22	0.40
1:AA:254:A:N6	1:AA:454:U:O2'	2.46	0.40
1:AA:325:G:C4	1:AA:326:C:C5	3.09	0.40
1:AA:347:G:C8	6:AF:171:PRO:HG3	2.56	0.40
1:AA:895:G:H2'	1:AA:896:A:C8	2.56	0.40
1:AA:1117:G:N2	1:AA:1135:G:HO2'	2.18	0.40
1:AA:1855:G:OP1	4:AD:52:ARG:NH1	2.46	0.40
1:AA:1985:U:H4'	1:AA:1986:G:OP1	2.20	0.40
1:AA:2146:G:H5''	3:AC:175:PRO:HG3	2.03	0.40
1:AA:2819:A:C6	1:AA:2901:A:C8	3.09	0.40
3:AC:194:ILE:CD1	3:AC:227:PRO:CB	2.99	0.40
7:AG:125:PHE:HB3	7:AG:166:ASP:CG	2.41	0.40
7:AG:132:ASN:HA	7:AG:157:ILE:O	2.22	0.40
8:AH:98:LEU:HD13	8:AH:125:VAL:CG2	2.51	0.40
11:AN:10:GLU:OE1	11:AN:11:PRO:HD2	2.21	0.40
12:AO:47:ILE:HB	12:AO:48:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AQ:81:VAL:HB	24:A0:7:LEU:HD11	2.01	0.40
17:AT:118:ARG:HH11	17:AT:118:ARG:HG3	1.86	0.40
34:BA:435:C:H2'	34:BA:436:C:H6	1.85	0.40
34:BA:622:A:C8	34:BA:623:C:C5	3.09	0.40
34:BA:1015:A:N3	34:BA:1218:C:O2'	2.45	0.40
35:BB:84:GLU:O	35:BB:219:VAL:HG21	2.20	0.40
35:BB:87:ARG:NH2	35:BB:220:ASP:OD1	2.42	0.40
38:BE:100:VAL:O	38:BE:101:ILE:HD13	2.21	0.40
42:BI:26:VAL:HG13	42:BI:61:ALA:HB3	2.03	0.40
47:BN:13:THR:HA	47:BN:14:PRO:HD3	1.78	0.40
48:BO:27:VAL:O	48:BO:31:LEU:HG	2.21	0.40
50:BQ:27:PHE:CE2	50:BQ:36:ILE:HD11	2.55	0.40
50:BQ:29:HIS:HA	50:BQ:30:PRO:HD2	1.79	0.40
1:CA:190:A:OP2	25:C1:39:LYS:HE3	2.22	0.40
1:CA:811:U:P	13:CP:29:LYS:H	2.45	0.40
1:CA:856:C:H3'	1:CA:856:C:C6	2.56	0.40
1:CA:1283:G:N2	1:CA:1285:G:H3'	2.36	0.40
1:CA:1297:C:H2'	1:CA:1298:C:H6	1.86	0.40
1:CA:1652:A:OP1	15:CR:8:ARG:HD3	2.21	0.40
1:CA:1654:A:OP1	15:CR:1:MET:HA	2.20	0.40
1:CA:2164:C:H3'	1:CA:2165:G:O4'	2.21	0.40
1:CA:2309:A:C6	1:CA:2310:A:C6	3.09	0.40
1:CA:2494:G:O2'	14:CQ:80:GLU:HA	2.22	0.40
1:CA:2689:U:O2	1:CA:2689:U:H2'	2.21	0.40
5:CE:67:PHE:CE2	5:CE:74:PRO:HA	2.56	0.40
5:CE:179:GLU:O	5:CE:180:ASN:HB2	2.22	0.40
11:CN:128:HIS:HA	11:CN:129:PRO:HD3	1.75	0.40
16:CS:111:GLU:O	16:CS:112:PHE:HB3	2.22	0.40
32:C8:26:LYS:HG2	32:C8:48:PHE:HD1	1.86	0.40
33:C9:9:ARG:HG2	33:C9:14:CYS:HB2	2.03	0.40
34:DA:939:G:C6	34:DA:940:C:N4	2.90	0.40
34:DA:1207:G:H2'	34:DA:1208:C:C6	2.55	0.40
37:DD:173:TRP:CD1	37:DD:174:LEU:HG	2.56	0.40
43:DJ:47:PHE:CZ	47:DN:37:PHE:HE1	2.40	0.40
46:DM:20:THR:HG22	46:DM:26:GLY:O	2.21	0.40
49:DP:21:VAL:CG1	49:DP:34:GLU:HB3	2.51	0.40
51:DR:76:LEU:HA	51:DR:76:LEU:HD12	1.56	0.40
59:DZ:221:ALA:HB1	59:DZ:228:MET:HB2	2.02	0.40
1:AA:1445:C:N4	65:AA:4432:HOH:O	2.53	0.40
1:AA:1686:U:H4'	1:AA:2711:C:H4'	2.03	0.40
1:AA:2108:U:H2'	1:AA:2109:G:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:2650:G:P	5:AE:82:ARG:HH22	2.44	0.40
5:AE:120:TRP:CE3	5:AE:155:LYS:HE2	2.56	0.40
6:AF:200:GLU:O	6:AF:203:GLN:HB2	2.22	0.40
12:AO:98:VAL:HG22	12:AO:118:ALA:HA	2.04	0.40
13:AP:106:LEU:HA	13:AP:106:LEU:HD23	1.80	0.40
13:AP:144:GLU:HA	13:AP:145:PRO:HD3	1.84	0.40
16:AS:74:ALA:HB2	16:AS:105:ALA:HA	2.03	0.40
17:AT:23:ARG:HG3	17:AT:120:ARG:NH1	2.35	0.40
22:AY:92:ASN:N	22:AY:92:ASN:ND2	2.67	0.40
23:AZ:102:LEU:HD12	23:AZ:102:LEU:HA	1.79	0.40
23:AZ:150:LEU:C	23:AZ:151:HIS:HD1	2.25	0.40
34:BA:375:U:C2	34:BA:376:G:C8	3.10	0.40
38:BE:143:ARG:NH1	41:BH:77:GLU:OE1	2.54	0.40
46:BM:60:VAL:HG13	46:BM:64:TRP:CZ3	2.55	0.40
47:BN:27:CYS:SG	47:BN:29:ARG:HB2	2.61	0.40
56:BW:52:G:H2'	56:BW:53:G:O4'	2.21	0.40
59:BZ:188:TYR:CE1	59:BZ:196:ILE:HD12	2.56	0.40
1:CA:248:G:H2'	65:CA:3866:HOH:O	2.20	0.40
1:CA:947:G:H2'	1:CA:948:G:C8	2.57	0.40
1:CA:1627:G:OP2	65:CA:4545:HOH:O	2.22	0.40
1:CA:1721:G:H5'	1:CA:1722:A:OP2	2.22	0.40
1:CA:2203:U:H2'	1:CA:2205:C:C6	2.56	0.40
1:CA:2626:C:H2'	1:CA:2627:G:O4'	2.21	0.40
4:CD:218:ARG:HB3	4:CD:219:PRO:HD2	2.03	0.40
5:CE:75:VAL:HG13	5:CE:77:ILE:H	1.86	0.40
14:CQ:65:PHE:HB2	14:CQ:105:GLU:HB2	2.03	0.40
22:CY:30:VAL:O	22:CY:32:PRO:HD3	2.22	0.40
34:DA:338:A:H2'	34:DA:339:C:O4'	2.21	0.40
34:DA:555:C:H2'	34:DA:556:C:C6	2.56	0.40
34:DA:1014:A:H2'	34:DA:1015:A:N9	2.36	0.40
35:DB:149:LEU:O	35:DB:153:ARG:N	2.47	0.40
40:DG:139:GLU:O	40:DG:143:ARG:N	2.53	0.40
57:DX:8:4SU:O2	57:DX:21:A:H2	2.05	0.40
1:AA:96:C:OP1	26:A2:2:LYS:HE2	2.22	0.40
1:AA:174:U:H4'	1:AA:207:A:H4'	2.03	0.40
1:AA:438:G:OP2	1:AA:2418:U:O2'	2.36	0.40
1:AA:1824:C:H2'	1:AA:1825:U:C6	2.57	0.40
1:AA:2221:A:H3'	1:AA:2222:C:H6	1.86	0.40
1:AA:2603:C:P	4:AD:239:ARG:HG3	2.62	0.40
3:AC:54:ARG:CZ	3:AC:55:SER:O	2.69	0.40
4:AD:223:GLY:HA3	4:AD:231:HIS:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AH:41:MET:HE1	8:AH:65:HIS:HA	2.03	0.40
10:AL:84:LEU:HD21	10:AL:96:VAL:HB	2.03	0.40
14:AQ:37:LEU:HA	14:AQ:37:LEU:HD23	1.65	0.40
14:AQ:109:VAL:HG13	14:AQ:113:GLN:HB2	2.03	0.40
21:AX:65:ARG:HB2	21:AX:70:LEU:HD22	2.04	0.40
22:AY:5:MET:HE2	22:AY:5:MET:HB2	1.90	0.40
25:A1:20:ARG:HD3	25:A1:20:ARG:HH11	1.71	0.40
34:BA:708:C:H2'	34:BA:709:G:C8	2.56	0.40
34:BA:986:A:H2'	34:BA:987:G:O4'	2.21	0.40
34:BA:1316:G:O2'	47:BN:18:VAL:HG11	2.20	0.40
34:BA:1510:U:H2'	34:BA:1511:G:C8	2.57	0.40
36:BC:18:TRP:H	36:BC:18:TRP:HE3	1.68	0.40
38:BE:8:GLU:HG3	38:BE:34:VAL:HG23	2.03	0.40
41:BH:6:ILE:H	41:BH:6:ILE:HG12	1.53	0.40
46:BM:56:LEU:O	46:BM:60:VAL:HG23	2.22	0.40
56:BW:24:G:C5	56:BW:25:C:C4	3.10	0.40
58:BY:20:U:H4'	58:BY:21:A:OP1	2.20	0.40
1:CA:527:C:C5	1:CA:2779:U:H2'	2.57	0.40
1:CA:1093:G:H1'	1:CA:1099:G:N2	2.37	0.40
1:CA:1301:A:C8	1:CA:1303:G:C8	3.09	0.40
1:CA:1826:G:H4'	4:CD:242:ARG:CZ	2.51	0.40
1:CA:2178:C:HO2'	3:CC:169:THR:HB	1.80	0.40
1:CA:2306:C:C4	1:CA:2307:G:C6	3.10	0.40
1:CA:2667:C:N3	8:CH:110:SER:OG	2.54	0.40
1:CA:2787:C:O2'	1:CA:2810:A:O2'	2.29	0.40
2:CB:79:C:H2'	2:CB:80:U:O4'	2.21	0.40
4:CD:26:LYS:HE2	4:CD:28:GLU:O	2.21	0.40
6:CF:155:LEU:CD2	6:CF:186:ILE:HG13	2.50	0.40
14:CQ:18:LYS:HB2	14:CQ:18:LYS:HE3	1.75	0.40
15:CR:84:ALA:HB3	15:CR:85:PRO:HD3	2.03	0.40
22:CY:49:VAL:HG21	22:CY:61:ILE:HG23	2.03	0.40
26:C2:53:LEU:O	26:C2:57:ILE:HG13	2.21	0.40
33:C9:17:ILE:HD12	33:C9:18:ARG:H	1.86	0.40
34:DA:684:A:H1'	44:DK:38:ASN:HB3	2.04	0.40
34:DA:790:A:OP1	57:DX:38:A:O2'	2.37	0.40
34:DA:1073:U:O2'	35:DB:104:ASN:OD1	2.35	0.40
34:DA:1090:U:H2'	34:DA:1091:U:C6	2.56	0.40
34:DA:1104:G:O5'	35:DB:111:ARG:HD2	2.21	0.40
34:DA:1229:A:H2'	34:DA:1230:C:H6	1.85	0.40
34:DA:1237:C:OP1	34:DA:1238:A:H1'	2.21	0.40
35:DB:193:ASP:HA	35:DB:194:PRO:HD2	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:DD:196:LEU:O	37:DD:198:VAL:N	2.48	0.40
39:DF:100:ASN:HD21	51:DR:23:LYS:HG2	1.86	0.40
40:DG:36:LYS:O	40:DG:39:ALA:HB3	2.22	0.40
51:DR:21:LYS:HE2	51:DR:21:LYS:HB2	1.85	0.40
56:DW:32:PSU:C2	56:DW:33:U:C4	3.09	0.40
1:AA:461:U:H1'	1:AA:462:C:H5	1.86	0.40
1:AA:632:A:H2'	1:AA:633:G:O4'	2.22	0.40
1:AA:704:U:H2'	1:AA:705:C:H6	1.86	0.40
1:AA:1249:A:H61	1:AA:1286:U:H2'	1.86	0.40
1:AA:2203:G:HO2'	1:AA:2204:G:P	2.44	0.40
1:AA:2225:U:O4'	4:AD:151:LYS:HE2	2.21	0.40
1:AA:2247:G:H2'	1:AA:2248:C:C6	2.56	0.40
1:AA:2367:C:O3'	24:A0:24:LYS:HE3	2.21	0.40
2:AB:43:C:O2'	7:AG:95:ARG:HD2	2.22	0.40
5:AE:21:VAL:HG23	5:AE:185:LYS:HD2	2.04	0.40
5:AE:52:LEU:O	5:AE:76:ARG:N	2.54	0.40
6:AF:139:PHE:HB2	6:AF:166:ALA:HB1	2.03	0.40
6:AF:140:LEU:HD12	6:AF:140:LEU:HA	1.75	0.40
7:AG:161:THR:HG22	7:AG:163:ALA:N	2.33	0.40
9:AK:23:SER:HA	9:AK:117:LEU:O	2.21	0.40
11:AN:121:LYS:HG2	11:AN:130:HIS:CE1	2.57	0.40
34:BA:619:U:N3	37:BD:134:ASP:OD2	2.42	0.40
34:BA:954:G:H2'	34:BA:955:U:O4'	2.21	0.40
34:BA:1330:U:C2'	34:BA:1331:G:H5'	2.51	0.40
34:BA:1350:A:N7	42:BI:118:LYS:NZ	2.70	0.40
35:BB:71:VAL:HG22	35:BB:93:VAL:CG2	2.52	0.40
36:BC:56:ASP:HB2	36:BC:67:THR:HB	2.03	0.40
38:BE:48:ALA:HB3	38:BE:54:ALA:HB2	2.03	0.40
38:BE:51:VAL:HB	38:BE:52:PRO:HD3	2.04	0.40
41:BH:112:LEU:HB3	41:BH:133:LEU:HA	2.03	0.40
46:BM:80:ARG:NH2	52:BS:69:HIS:CE1	2.90	0.40
48:BO:43:LEU:HA	48:BO:43:LEU:HD23	1.78	0.40
50:BQ:9:VAL:H	50:BQ:9:VAL:HG23	1.57	0.40
50:BQ:81:ARG:HA	50:BQ:81:ARG:HD2	1.90	0.40
59:BZ:404:VAL:HA	59:BZ:405:PRO:HD3	1.80	0.40
59:BZ:462:ILE:O	59:BZ:466:LEU:HB2	2.21	0.40
1:CA:1913:A:H4'	1:CA:1914:C:O5'	2.20	0.40
1:CA:1913:A:C8	34:DA:1494:G:H4'	2.57	0.40
1:CA:2280:G:N3	1:CA:2388:A:H2	2.19	0.40
13:CP:39:LYS:CB	13:CP:45:LEU:HG	2.41	0.40
14:CQ:32:TYR:CZ	14:CQ:133:ARG:HD3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:CS:110:LEU:HA	16:CS:110:LEU:HD12	1.74	0.40
19:CV:35:LEU:HA	19:CV:36:PRO:HD3	1.94	0.40
22:CY:79:CYS:O	22:CY:81:LYS:HG3	2.21	0.40
23:CZ:120:ILE:HD11	23:CZ:171:ILE:C	2.42	0.40
34:DA:186:C:H2'	34:DA:187:C:C6	2.56	0.40
34:DA:499:A:H4'	34:DA:500:G:OP1	2.20	0.40
35:DB:16:HIS:CD2	35:DB:17:PHE:N	2.90	0.40
35:DB:105:PHE:C	35:DB:107:THR:H	2.25	0.40
35:DB:223:ILE:H	35:DB:223:ILE:HG13	1.74	0.40
36:DC:181:ASN:OD1	36:DC:204:LEU:HD12	2.21	0.40
37:DD:97:LEU:HD23	37:DD:97:LEU:HA	1.93	0.40
38:DE:36:ASP:C	38:DE:38:GLN:H	2.24	0.40
39:DF:100:ASN:ND2	51:DR:23:LYS:HE3	2.37	0.40
40:DG:59:LEU:O	40:DG:63:LYS:HE2	2.21	0.40
41:DH:51:VAL:HG12	41:DH:52:ASP:H	1.86	0.40
41:DH:84:ARG:HD2	41:DH:86:ILE:HD13	2.03	0.40
42:DI:4:TYR:CG	42:DI:88:TYR:HB2	2.57	0.40
43:DJ:29:ARG:HA	43:DJ:29:ARG:HD3	1.83	0.40
59:DZ:105:ILE:HG22	59:DZ:280:LEU:HD11	2.03	0.40
59:DZ:116:PRO:O	59:DZ:117:GLN:HG3	2.22	0.40
59:DZ:355:LEU:HD12	59:DZ:355:LEU:HA	1.93	0.40
1:AA:863:C:H2'	1:AA:864:C:H6	1.86	0.40
1:AA:955:A:H2'	1:AA:958:C:H5	1.86	0.40
1:AA:2371:C:H2'	1:AA:2372:A:O4'	2.22	0.40
5:AE:21:VAL:HA	5:AE:22:PRO:HD3	1.89	0.40
6:AF:129:PHE:HB3	6:AF:132:VAL:CG1	2.52	0.40
6:AF:150:GLY:HA2	6:AF:172:TRP:CE3	2.56	0.40
18:AU:104:GLN:H	18:AU:104:GLN:NE2	2.20	0.40
22:AY:54:LYS:HA	22:AY:55:TYR:HA	1.95	0.40
34:BA:45:U:O5'	34:BA:45:U:H6	2.04	0.40
34:BA:185:A:H1'	53:BT:81:LYS:HZ1	1.86	0.40
34:BA:456:C:H42	34:BA:475:G:H1	1.68	0.40
34:BA:1082:G:H2'	34:BA:1083:U:O4'	2.22	0.40
34:BA:1106:G:H5''	36:BC:172:ARG:HG2	2.04	0.40
34:BA:1250:A:C2	34:BA:1370:G:H1'	2.56	0.40
34:BA:1417:G:H22	34:BA:1482:G:H2'	1.86	0.40
36:BC:20:SER:HB3	36:BC:22:TRP:NE1	2.37	0.40
36:BC:33:LEU:HD11	47:BN:53:LEU:HD23	2.03	0.40
36:BC:113:ALA:HB3	36:BC:114:PRO:HD3	2.04	0.40
37:BD:61:LYS:HA	37:BD:203:VAL:HG22	2.03	0.40
37:BD:110:PHE:H	37:BD:110:PHE:HD1	1.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:277:C:H1'	1:CA:278:A:P	2.62	0.40
1:CA:307:G:H2'	1:CA:309:G:OP2	2.21	0.40
1:CA:1171:G:N2	1:CA:1179:C:C2	2.89	0.40
1:CA:1341:U:O2	21:CX:80:ILE:HD12	2.22	0.40
1:CA:1740:G:H2'	1:CA:1741:A:C8	2.57	0.40
1:CA:2576:G:H1'	65:CA:3997:HOH:O	2.21	0.40
2:CB:101:G:H2'	2:CB:102:A:O4'	2.21	0.40
4:CD:242:ARG:N	4:CD:242:ARG:HD3	2.36	0.40
6:CF:36:VAL:HG12	6:CF:40:GLN:OE1	2.21	0.40
6:CF:148:LEU:HD11	6:CF:193:VAL:HG21	2.03	0.40
14:CQ:118:LEU:HD23	14:CQ:118:LEU:HA	1.93	0.40
18:CU:61:TRP:CD2	18:CU:93:LYS:HA	2.56	0.40
22:CY:13:VAL:O	22:CY:24:VAL:HA	2.21	0.40
34:DA:188:C:H2'	34:DA:189:G:C8	2.53	0.40
34:DA:643:C:H5'	41:DH:31:PHE:CD1	2.57	0.40
34:DA:719:C:N4	51:DR:71:LYS:HE2	2.37	0.40
34:DA:865:A:H5'	34:DA:1078:U:O4	2.21	0.40
34:DA:976:G:N2	34:DA:1362:C:H2'	2.37	0.40
34:DA:1125:U:O2'	34:DA:1126:U:H2'	2.21	0.40
34:DA:1132:C:H2'	34:DA:1133:G:H8	1.86	0.40
34:DA:1222:G:C2	34:DA:1223:C:C2	3.09	0.40
34:DA:1409:C:H2'	34:DA:1410:G:H8	1.86	0.40
35:DB:97:TRP:CH2	35:DB:102:LEU:HD13	2.57	0.40
36:DC:8:ILE:HG13	36:DC:16:ARG:HG2	2.02	0.40
36:DC:140:ARG:NH1	36:DC:141:VAL:HG23	2.36	0.40
37:DD:38:TYR:CE1	37:DD:45:GLN:HG3	2.57	0.40
37:DD:203:VAL:O	37:DD:206:PHE:HB3	2.22	0.40
39:DF:50:TYR:CE2	51:DR:77:GLY:HA2	2.56	0.40
41:DH:40:ALA:O	41:DH:43:GLY:N	2.46	0.40
42:DI:111:ARG:O	42:DI:113:LYS:HD2	2.20	0.40
49:DP:55:ARG:O	49:DP:58:TYR:HB3	2.21	0.40
53:DT:56:MET:HE2	53:DT:88:VAL:HG21	2.03	0.40
58:DY:8:4SU:H1'	58:DY:48:C:O2	2.21	0.40
59:DZ:71:THR:HG22	59:DZ:80:ASN:OD1	2.22	0.40
59:DZ:160:ARG:HB3	59:DZ:256:THR:H	1.87	0.40
59:DZ:659:LEU:HD23	59:DZ:659:LEU:HA	1.87	0.40
59:DZ:682:GLN:O	59:DZ:686:LYS:HB3	2.21	0.40

All (17) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:9:ARG:NH2	59:DZ:504:ARG:NH1[3_654]	0.73	1.47
59:BZ:504:ARG:NH2	3:CC:9:ARG:NE[2_655]	1.08	1.12
59:BZ:504:ARG:NH1	3:CC:9:ARG:NH1[2_655]	1.09	1.11
3:AC:6:LYS:O	59:DZ:501:THR:O[3_654]	1.74	0.46
59:BZ:504:ARG:NH1	3:CC:9:ARG:NE[2_655]	1.80	0.40
59:BZ:504:ARG:CZ	3:CC:9:ARG:CZ[2_655]	1.83	0.37
3:AC:9:ARG:CZ	59:DZ:504:ARG:NH1[3_654]	1.85	0.35
59:BZ:502:GLY:CA	3:CC:9:ARG:CB[2_655]	1.85	0.35
59:BZ:504:ARG:CZ	3:CC:9:ARG:CD[2_655]	1.85	0.35
3:AC:9:ARG:NH2	59:DZ:504:ARG:CZ[3_654]	1.86	0.34
59:BZ:504:ARG:NH2	3:CC:9:ARG:CZ[2_655]	1.91	0.29
59:BZ:504:ARG:NH1	3:CC:9:ARG:CD[2_655]	2.04	0.16
59:BZ:504:ARG:NH2	3:CC:9:ARG:CD[2_655]	2.07	0.13
1:AA:2154:U:O4	59:DZ:501:THR:OG1[3_654]	2.08	0.12
1:AA:2158:C:O2'	34:DA:1000:U:O2'[3_654]	2.08	0.12
3:AC:9:ARG:CB	59:DZ:502:GLY:CA[3_654]	2.10	0.10
59:BZ:502:GLY:N	3:CC:9:ARG:CB[2_655]	2.17	0.03

### 5.3 Torsion angles [i](#)

#### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AC	133/228 (58%)	90 (68%)	25 (19%)	18 (14%)	0	0
3	CC	133/228 (58%)	90 (68%)	25 (19%)	18 (14%)	0	0
4	AD	273/276 (99%)	248 (91%)	22 (8%)	3 (1%)	14	41
4	CD	273/276 (99%)	245 (90%)	25 (9%)	3 (1%)	14	41
5	AE	202/206 (98%)	189 (94%)	12 (6%)	1 (0%)	29	61
5	CE	202/206 (98%)	189 (94%)	10 (5%)	3 (2%)	10	33
6	AF	201/210 (96%)	185 (92%)	16 (8%)	0	100	100
6	CF	201/210 (96%)	189 (94%)	8 (4%)	4 (2%)	7	24
7	AG	179/182 (98%)	159 (89%)	14 (8%)	6 (3%)	3	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	CG	179/182 (98%)	154 (86%)	19 (11%)	6 (3%)	3	13
8	AH	172/180 (96%)	160 (93%)	11 (6%)	1 (1%)	25	56
8	CH	172/180 (96%)	153 (89%)	13 (8%)	6 (4%)	3	12
9	AK	128/173 (74%)	74 (58%)	26 (20%)	28 (22%)	0	0
9	CK	128/173 (74%)	80 (62%)	28 (22%)	20 (16%)	0	0
10	AL	64/147 (44%)	47 (73%)	13 (20%)	4 (6%)	1	3
10	CL	64/147 (44%)	44 (69%)	17 (27%)	3 (5%)	2	7
11	AN	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
11	CN	138/140 (99%)	126 (91%)	10 (7%)	2 (1%)	11	34
12	AO	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	19	49
12	CO	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	19	49
13	AP	147/150 (98%)	133 (90%)	12 (8%)	2 (1%)	11	34
13	CP	147/150 (98%)	129 (88%)	15 (10%)	3 (2%)	7	24
14	AQ	139/141 (99%)	128 (92%)	11 (8%)	0	100	100
14	CQ	139/141 (99%)	123 (88%)	13 (9%)	3 (2%)	6	22
15	AR	116/118 (98%)	109 (94%)	6 (5%)	1 (1%)	17	46
15	CR	116/118 (98%)	104 (90%)	11 (10%)	1 (1%)	17	46
16	AS	108/112 (96%)	99 (92%)	8 (7%)	1 (1%)	17	46
16	CS	108/112 (96%)	89 (82%)	17 (16%)	2 (2%)	8	26
17	AT	129/146 (88%)	119 (92%)	10 (8%)	0	100	100
17	CT	129/146 (88%)	120 (93%)	9 (7%)	0	100	100
18	AU	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
18	CU	114/118 (97%)	108 (95%)	6 (5%)	0	100	100
19	AV	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	15	44
19	CV	99/101 (98%)	90 (91%)	7 (7%)	2 (2%)	7	24
20	AW	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
20	CW	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
21	AX	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	14	41
21	CX	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	14	41
22	AY	105/110 (96%)	95 (90%)	9 (9%)	1 (1%)	15	44
22	CY	105/110 (96%)	90 (86%)	11 (10%)	4 (4%)	3	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	AZ	169/206 (82%)	136 (80%)	28 (17%)	5 (3%)	4	15
23	CZ	172/206 (84%)	144 (84%)	25 (14%)	3 (2%)	9	29
24	A0	81/85 (95%)	74 (91%)	6 (7%)	1 (1%)	13	39
24	C0	81/85 (95%)	76 (94%)	5 (6%)	0	100	100
25	A1	95/98 (97%)	86 (90%)	9 (10%)	0	100	100
25	C1	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	14	41
26	A2	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
26	C2	68/72 (94%)	64 (94%)	4 (6%)	0	100	100
27	A3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	C3	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	8	28
28	A4	67/71 (94%)	44 (66%)	16 (24%)	7 (10%)	0	1
28	C4	67/71 (94%)	49 (73%)	13 (19%)	5 (8%)	1	2
29	A5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
29	C5	57/60 (95%)	57 (100%)	0	0	100	100
30	A6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
30	C6	51/54 (94%)	45 (88%)	6 (12%)	0	100	100
31	A7	46/49 (94%)	46 (100%)	0	0	100	100
31	C7	46/49 (94%)	44 (96%)	0	2 (4%)	2	8
32	A8	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
32	C8	62/65 (95%)	58 (94%)	2 (3%)	2 (3%)	4	13
33	A9	35/37 (95%)	35 (100%)	0	0	100	100
33	C9	35/37 (95%)	35 (100%)	0	0	100	100
35	BB	229/256 (90%)	187 (82%)	29 (13%)	13 (6%)	1	5
35	DB	229/256 (90%)	177 (77%)	37 (16%)	15 (7%)	1	3
36	BC	204/239 (85%)	171 (84%)	25 (12%)	8 (4%)	3	10
36	DC	204/239 (85%)	171 (84%)	30 (15%)	3 (2%)	10	33
37	BD	206/209 (99%)	186 (90%)	16 (8%)	4 (2%)	8	26
37	DD	206/209 (99%)	180 (87%)	20 (10%)	6 (3%)	4	15
38	BE	146/162 (90%)	128 (88%)	13 (9%)	5 (3%)	3	13
38	DE	146/162 (90%)	128 (88%)	12 (8%)	6 (4%)	3	9
39	BF	98/101 (97%)	89 (91%)	7 (7%)	2 (2%)	7	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	DF	98/101 (97%)	91 (93%)	6 (6%)	1 (1%)	15	44
40	BG	153/156 (98%)	142 (93%)	9 (6%)	2 (1%)	12	36
40	DG	153/156 (98%)	132 (86%)	19 (12%)	2 (1%)	12	36
41	BH	135/138 (98%)	120 (89%)	12 (9%)	3 (2%)	6	22
41	DH	135/138 (98%)	121 (90%)	12 (9%)	2 (2%)	10	33
42	BI	125/128 (98%)	111 (89%)	10 (8%)	4 (3%)	4	13
42	DI	125/128 (98%)	111 (89%)	12 (10%)	2 (2%)	9	31
43	BJ	95/105 (90%)	81 (85%)	9 (10%)	5 (5%)	2	6
43	DJ	94/105 (90%)	77 (82%)	10 (11%)	7 (7%)	1	2
44	BK	112/129 (87%)	102 (91%)	8 (7%)	2 (2%)	8	28
44	DK	112/129 (87%)	98 (88%)	10 (9%)	4 (4%)	3	11
45	BL	120/132 (91%)	106 (88%)	13 (11%)	1 (1%)	19	49
45	DL	120/132 (91%)	109 (91%)	11 (9%)	0	100	100
46	BM	121/126 (96%)	101 (84%)	17 (14%)	3 (2%)	5	19
46	DM	120/126 (95%)	98 (82%)	13 (11%)	9 (8%)	1	2
47	BN	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	9	29
47	DN	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	9	29
48	BO	86/89 (97%)	77 (90%)	7 (8%)	2 (2%)	6	21
48	DO	86/89 (97%)	72 (84%)	12 (14%)	2 (2%)	6	21
49	BP	80/88 (91%)	66 (82%)	12 (15%)	2 (2%)	5	19
49	DP	80/88 (91%)	66 (82%)	13 (16%)	1 (1%)	12	36
50	BQ	97/105 (92%)	87 (90%)	9 (9%)	1 (1%)	15	44
50	DQ	97/105 (92%)	85 (88%)	12 (12%)	0	100	100
51	BR	66/88 (75%)	61 (92%)	4 (6%)	1 (2%)	10	33
51	DR	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
52	BS	82/93 (88%)	73 (89%)	9 (11%)	0	100	100
52	DS	81/93 (87%)	67 (83%)	12 (15%)	2 (2%)	5	19
53	BT	94/106 (89%)	78 (83%)	10 (11%)	6 (6%)	1	3
53	DT	94/106 (89%)	78 (83%)	12 (13%)	4 (4%)	2	8
54	BU	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
54	DU	21/27 (78%)	19 (90%)	1 (5%)	1 (5%)	2	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
59	BZ	722/758 (95%)	598 (83%)	92 (13%)	32 (4%)	2	8
59	DZ	726/758 (96%)	594 (82%)	97 (13%)	35 (5%)	2	7
All	All	13220/14444 (92%)	11544 (87%)	1298 (10%)	378 (3%)	4	15

All (378) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	42	VAL
3	AC	47	LYS
3	AC	68	GLY
3	AC	180	SER
3	AC	181	PHE
4	AD	275	LYS
7	AG	43	LEU
7	AG	47	LYS
7	AG	50	ALA
7	AG	126	ASP
9	AK	56	ASN
9	AK	71	LEU
9	AK	74	LEU
9	AK	75	GLN
9	AK	77	PRO
9	AK	80	VAL
9	AK	85	ASP
9	AK	104	ILE
9	AK	105	PRO
9	AK	107	VAL
9	AK	128	LEU
10	AL	115	LEU
16	AS	59	LYS
28	A4	45	GLY
28	A4	49	PHE
28	A4	59	PHE
28	A4	62	ARG
35	BB	17	PHE
35	BB	125	PRO
35	BB	231	GLU
36	BC	65	ALA
36	BC	66	VAL
37	BD	42	GLN
38	BE	98	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
40	BG	79	ARG
40	BG	80	VAL
41	BH	133	LEU
42	BI	41	VAL
42	BI	44	VAL
42	BI	54	ASP
43	BJ	79	ARG
53	BT	10	LEU
53	BT	100	ILE
59	BZ	-57	GLU
59	BZ	-33	GLY
59	BZ	88	VAL
59	BZ	97	SER
59	BZ	98	MET
59	BZ	171	GLU
59	BZ	183	MET
59	BZ	404	VAL
59	BZ	405	PRO
59	BZ	472	VAL
59	BZ	481	VAL
3	CC	42	VAL
3	CC	47	LYS
3	CC	68	GLY
3	CC	180	SER
3	CC	181	PHE
6	CF	130	ALA
7	CG	14	GLU
7	CG	51	ARG
7	CG	81	LYS
8	CH	92	ILE
8	CH	126	PRO
8	CH	143	GLN
8	CH	144	VAL
9	CK	69	PRO
9	CK	70	GLU
9	CK	71	LEU
9	CK	74	LEU
9	CK	75	GLN
9	CK	77	PRO
9	CK	80	VAL
9	CK	85	ASP
9	CK	105	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	CK	107	VAL
10	CL	87	GLY
13	CP	38	GLN
21	CX	94	GLY
28	C4	62	ARG
28	C4	63	TYR
31	C7	46	VAL
35	DB	10	LEU
35	DB	17	PHE
36	DC	98	ASN
40	DG	55	GLY
42	DI	54	ASP
43	DJ	56	HIS
43	DJ	79	ARG
46	DM	4	ILE
48	DO	19	PRO
53	DT	10	LEU
53	DT	100	ILE
59	DZ	-65	LYS
59	DZ	-57	GLU
59	DZ	85	PRO
59	DZ	117	GLN
59	DZ	160	ARG
59	DZ	183	MET
59	DZ	290	LYS
59	DZ	472	VAL
3	AC	53	ARG
3	AC	161	ARG
3	AC	179	ALA
4	AD	3	VAL
9	AK	91	LYS
9	AK	93	LEU
9	AK	125	LEU
9	AK	132	ASP
10	AL	82	ALA
15	AR	2	ARG
19	AV	79	VAL
21	AX	94	GLY
23	AZ	105	VAL
28	A4	63	TYR
35	BB	10	LEU
35	BB	19	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	BC	101	LEU
37	BD	179	GLU
39	BF	70	ASP
43	BJ	31	GLY
43	BJ	56	HIS
50	BQ	49	GLU
53	BT	47	GLY
59	BZ	85	PRO
59	BZ	92	ILE
59	BZ	114	VAL
59	BZ	400	GLU
59	BZ	402	ILE
59	BZ	418	LYS
59	BZ	688	ILE
3	CC	53	ARG
3	CC	161	ARG
3	CC	179	ALA
4	CD	3	VAL
6	CF	195	ASP
7	CG	96	ARG
9	CK	84	GLU
9	CK	93	LEU
23	CZ	105	VAL
28	C4	11	PRO
28	C4	45	GLY
35	DB	106	LYS
35	DB	123	ALA
36	DC	95	THR
37	DD	10	ARG
38	DE	140	ARG
40	DG	80	VAL
41	DH	133	LEU
43	DJ	75	ILE
44	DK	49	GLY
44	DK	117	ASN
46	DM	67	GLU
46	DM	106	ASN
52	DS	12	ASP
53	DT	46	GLU
54	DU	3	LYS
59	DZ	39	ILE
59	DZ	92	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
59	DZ	402	ILE
59	DZ	403	GLU
59	DZ	404	VAL
59	DZ	479	PRO
59	DZ	481	VAL
59	DZ	600	VAL
3	AC	30	VAL
3	AC	43	GLU
3	AC	52	PRO
3	AC	69	LEU
3	AC	184	GLU
3	AC	202	PRO
3	AC	209	PHE
4	AD	125	ILE
7	AG	51	ARG
9	AK	20	ALA
9	AK	22	GLY
9	AK	39	ALA
9	AK	69	PRO
9	AK	101	PRO
10	AL	89	HIS
12	AO	5	GLN
13	AP	36	LYS
22	AY	54	LYS
23	AZ	65	GLN
36	BC	51	GLY
43	BJ	77	PRO
44	BK	105	VAL
46	BM	67	GLU
46	BM	113	PRO
48	BO	19	PRO
48	BO	86	GLY
51	BR	41	LYS
53	BT	71	THR
53	BT	102	GLY
59	BZ	115	GLU
59	BZ	170	ARG
59	BZ	315	LYS
59	BZ	320	PRO
3	CC	30	VAL
3	CC	43	GLU
3	CC	52	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	CC	69	LEU
3	CC	184	GLU
3	CC	202	PRO
3	CC	209	PHE
4	CD	239	ARG
5	CE	52	LEU
6	CF	21	ALA
7	CG	52	ILE
9	CK	86	PRO
9	CK	128	LEU
9	CK	132	ASP
10	CL	89	HIS
11	CN	23	LEU
13	CP	122	PRO
16	CS	89	ARG
19	CV	24	LYS
23	CZ	31	ARG
23	CZ	114	GLY
25	C1	3	LYS
28	C4	46	GLN
31	C7	45	ALA
35	DB	8	LYS
35	DB	16	HIS
35	DB	121	LEU
35	DB	125	PRO
35	DB	213	LEU
37	DD	47	ARG
43	DJ	36	GLY
43	DJ	55	LYS
43	DJ	77	PRO
44	DK	105	VAL
46	DM	5	ALA
46	DM	6	GLY
46	DM	101	GLN
46	DM	108	ARG
48	DO	88	ARG
52	DS	24	ALA
53	DT	102	GLY
59	DZ	-25	SER
59	DZ	20	HIS
59	DZ	170	ARG
59	DZ	400	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
59	DZ	418	LYS
59	DZ	598	ASP
59	DZ	599	PRO
59	DZ	651	GLU
3	AC	16	ASP
5	AE	52	LEU
9	AK	33	PRO
9	AK	86	PRO
9	AK	114	GLY
10	AL	81	ALA
24	A0	57	PHE
35	BB	9	GLU
35	BB	16	HIS
35	BB	131	PRO
36	BC	50	ALA
38	BE	86	ALA
41	BH	51	VAL
42	BI	96	LEU
44	BK	49	GLY
59	BZ	172	ASP
59	BZ	469	GLU
59	BZ	596	LYS
59	BZ	641	GLN
59	BZ	671	MET
3	CC	16	ASP
4	CD	125	ILE
5	CE	74	PRO
8	CH	119	GLU
9	CK	91	LYS
9	CK	104	ILE
11	CN	2	LYS
15	CR	45	ARG
16	CS	84	GLN
19	CV	79	VAL
22	CY	78	ALA
27	C3	59	VAL
32	C8	57	ARG
35	DB	20	GLU
35	DB	131	PRO
37	DD	22	LYS
37	DD	171	GLY
38	DE	96	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
38	DE	104	ALA
38	DE	107	ARG
42	DI	34	ASN
43	DJ	78	ASN
46	DM	35	GLU
47	DN	27	CYS
49	DP	53	VAL
59	DZ	-33	GLY
59	DZ	416	LYS
59	DZ	471	LYS
59	DZ	559	PRO
3	AC	21	TYR
9	AK	120	LYS
9	AK	123	GLU
23	AZ	152	ALA
35	BB	56	ARG
35	BB	195	ASP
36	BC	129	ALA
36	BC	156	ARG
37	BD	178	VAL
46	BM	19	LEU
47	BN	58	LYS
49	BP	49	LEU
59	BZ	322	VAL
59	BZ	324	ARG
59	BZ	416	LYS
59	BZ	479	PRO
3	CC	21	TYR
6	CF	60	SER
7	CG	47	LYS
9	CK	119	ALA
10	CL	112	MET
22	CY	43	ASN
22	CY	102	CYS
35	DB	83	MET
37	DD	136	PRO
44	DK	106	LYS
59	DZ	180	VAL
59	DZ	473	ASP
59	DZ	477	GLY
3	AC	221	PRO
8	AH	148	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	AK	31	GLY
9	AK	119	ALA
28	A4	47	GLN
37	BD	109	GLY
38	BE	68	GLU
39	BF	39	LYS
49	BP	41	PRO
59	BZ	415	PRO
3	CC	221	PRO
8	CH	80	SER
9	CK	101	PRO
13	CP	29	LYS
14	CQ	115	MET
22	CY	51	VAL
35	DB	21	ARG
35	DB	202	PRO
36	DC	108	ASN
37	DD	5	ILE
59	DZ	199	ILE
7	AG	32	PRO
13	AP	122	PRO
23	AZ	158	PRO
35	BB	183	PRO
35	BB	234	PRO
38	BE	69	VAL
43	BJ	75	ILE
53	BT	96	GLY
59	DZ	116	PRO
35	BB	202	PRO
32	C8	58	ILE
46	DM	85	GLY
9	AK	68	LEU
23	AZ	167	PRO
28	A4	41	PRO
45	BL	125	PRO
14	CQ	27	VAL
35	DB	232	PRO
59	DZ	88	VAL
59	DZ	688	ILE
9	CK	68	LEU
14	CQ	88	GLY
38	DE	69	VAL

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Mol	Chain	Res	Type
41	DH	83	ILE
36	BC	81	GLY
38	BE	85	GLY
41	BH	90	GLY
12	CO	110	GLY
38	DE	105	VAL
39	DF	40	VAL
5	CE	30	PRO

### 5.3.2 Protein sidechains [i](#)

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	
3	AC	111/180 (62%)	103 (93%)	8 (7%)	14	38
3	CC	111/180 (62%)	103 (93%)	8 (7%)	14	38
4	AD	215/218 (99%)	189 (88%)	26 (12%)	5	15
4	CD	216/218 (99%)	181 (84%)	35 (16%)	2	7
5	AE	164/166 (99%)	140 (85%)	24 (15%)	3	9
5	CE	164/166 (99%)	139 (85%)	25 (15%)	3	8
6	AF	160/166 (96%)	134 (84%)	26 (16%)	2	7
6	CF	159/166 (96%)	135 (85%)	24 (15%)	3	9
7	AG	143/156 (92%)	119 (83%)	24 (17%)	2	6
7	CG	142/156 (91%)	108 (76%)	34 (24%)	0	2
8	AH	144/148 (97%)	128 (89%)	16 (11%)	6	19
8	CH	144/148 (97%)	125 (87%)	19 (13%)	4	12
10	AL	50/111 (45%)	45 (90%)	5 (10%)	7	22
10	CL	50/111 (45%)	45 (90%)	5 (10%)	7	22
11	AN	118/119 (99%)	94 (80%)	24 (20%)	1	4
11	CN	118/119 (99%)	98 (83%)	20 (17%)	2	6
12	AO	100/100 (100%)	83 (83%)	17 (17%)	2	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	CO	100/100 (100%)	83 (83%)	17 (17%)	2	6
13	AP	116/116 (100%)	97 (84%)	19 (16%)	2	7
13	CP	115/116 (99%)	99 (86%)	16 (14%)	3	11
14	AQ	111/111 (100%)	90 (81%)	21 (19%)	1	5
14	CQ	111/111 (100%)	95 (86%)	16 (14%)	3	10
15	AR	101/101 (100%)	79 (78%)	22 (22%)	1	3
15	CR	101/101 (100%)	84 (83%)	17 (17%)	2	6
16	AS	87/88 (99%)	71 (82%)	16 (18%)	1	5
16	CS	85/88 (97%)	67 (79%)	18 (21%)	1	3
17	AT	115/127 (91%)	97 (84%)	18 (16%)	2	8
17	CT	113/127 (89%)	93 (82%)	20 (18%)	2	5
18	AU	93/94 (99%)	77 (83%)	16 (17%)	2	6
18	CU	93/94 (99%)	82 (88%)	11 (12%)	5	16
19	AV	80/82 (98%)	65 (81%)	15 (19%)	1	5
19	CV	80/82 (98%)	67 (84%)	13 (16%)	2	7
20	AW	90/92 (98%)	80 (89%)	10 (11%)	6	19
20	CW	90/92 (98%)	79 (88%)	11 (12%)	5	15
21	AX	77/78 (99%)	73 (95%)	4 (5%)	23	55
21	CX	77/78 (99%)	70 (91%)	7 (9%)	9	27
22	AY	85/91 (93%)	73 (86%)	12 (14%)	3	10
22	CY	85/91 (93%)	70 (82%)	15 (18%)	2	5
23	AZ	145/179 (81%)	117 (81%)	28 (19%)	1	4
23	CZ	145/179 (81%)	125 (86%)	20 (14%)	3	11
24	A0	65/67 (97%)	63 (97%)	2 (3%)	40	74
24	C0	65/67 (97%)	60 (92%)	5 (8%)	13	35
25	A1	80/83 (96%)	72 (90%)	8 (10%)	7	22
25	C1	80/83 (96%)	69 (86%)	11 (14%)	3	11
26	A2	65/67 (97%)	54 (83%)	11 (17%)	2	6
26	C2	65/67 (97%)	55 (85%)	10 (15%)	2	8
27	A3	51/52 (98%)	44 (86%)	7 (14%)	3	11
27	C3	50/52 (96%)	38 (76%)	12 (24%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	A4	60/63 (95%)	49 (82%)	11 (18%)	1	5
28	C4	53/63 (84%)	39 (74%)	14 (26%)	0	1
29	A5	50/52 (96%)	43 (86%)	7 (14%)	3	11
29	C5	50/52 (96%)	44 (88%)	6 (12%)	5	15
30	A6	51/52 (98%)	40 (78%)	11 (22%)	1	3
30	C6	50/52 (96%)	43 (86%)	7 (14%)	3	11
31	A7	41/42 (98%)	35 (85%)	6 (15%)	3	9
31	C7	41/42 (98%)	36 (88%)	5 (12%)	5	15
32	A8	54/55 (98%)	47 (87%)	7 (13%)	4	13
32	C8	54/55 (98%)	49 (91%)	5 (9%)	9	26
33	A9	34/34 (100%)	31 (91%)	3 (9%)	10	29
33	C9	34/34 (100%)	29 (85%)	5 (15%)	3	9
35	BB	192/220 (87%)	144 (75%)	48 (25%)	0	2
35	DB	187/220 (85%)	157 (84%)	30 (16%)	2	7
36	BC	143/188 (76%)	124 (87%)	19 (13%)	4	12
36	DC	141/188 (75%)	115 (82%)	26 (18%)	1	5
37	BD	170/181 (94%)	146 (86%)	24 (14%)	3	10
37	DD	174/181 (96%)	148 (85%)	26 (15%)	3	9
38	BE	113/123 (92%)	104 (92%)	9 (8%)	12	34
38	DE	114/123 (93%)	96 (84%)	18 (16%)	2	8
39	BF	84/90 (93%)	71 (84%)	13 (16%)	2	8
39	DF	86/90 (96%)	75 (87%)	11 (13%)	4	13
40	BG	119/127 (94%)	98 (82%)	21 (18%)	2	5
40	DG	120/127 (94%)	112 (93%)	8 (7%)	16	43
41	BH	114/119 (96%)	98 (86%)	16 (14%)	3	11
41	DH	114/119 (96%)	92 (81%)	22 (19%)	1	4
42	BI	91/99 (92%)	72 (79%)	19 (21%)	1	3
42	DI	89/99 (90%)	71 (80%)	18 (20%)	1	4
43	BJ	66/92 (72%)	58 (88%)	8 (12%)	5	15
43	DJ	69/92 (75%)	58 (84%)	11 (16%)	2	7
44	BK	83/99 (84%)	71 (86%)	12 (14%)	3	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	DK	83/99 (84%)	74 (89%)	9 (11%)	6	19
45	BL	97/109 (89%)	90 (93%)	7 (7%)	14	38
45	DL	97/109 (89%)	86 (89%)	11 (11%)	6	18
46	BM	95/101 (94%)	82 (86%)	13 (14%)	3	11
46	DM	92/101 (91%)	76 (83%)	16 (17%)	2	6
47	BN	49/50 (98%)	39 (80%)	10 (20%)	1	4
47	DN	49/50 (98%)	40 (82%)	9 (18%)	1	5
48	BO	78/80 (98%)	64 (82%)	14 (18%)	2	5
48	DO	78/80 (98%)	68 (87%)	10 (13%)	4	13
49	BP	69/74 (93%)	56 (81%)	13 (19%)	1	5
49	DP	68/74 (92%)	61 (90%)	7 (10%)	7	21
50	BQ	94/97 (97%)	81 (86%)	13 (14%)	3	11
50	DQ	94/97 (97%)	82 (87%)	12 (13%)	4	13
51	BR	59/77 (77%)	47 (80%)	12 (20%)	1	4
51	DR	59/77 (77%)	51 (86%)	8 (14%)	3	11
52	BS	70/80 (88%)	61 (87%)	9 (13%)	4	13
52	DS	67/80 (84%)	60 (90%)	7 (10%)	7	21
53	BT	70/82 (85%)	59 (84%)	11 (16%)	2	8
53	DT	71/82 (87%)	58 (82%)	13 (18%)	1	5
54	BU	18/22 (82%)	16 (89%)	2 (11%)	6	19
54	DU	18/22 (82%)	16 (89%)	2 (11%)	6	19
59	BZ	604/636 (95%)	489 (81%)	115 (19%)	1	4
59	DZ	607/636 (95%)	505 (83%)	102 (17%)	2	6
All	All	10652/11672 (91%)	9013 (85%)	1639 (15%)	2	8

All (1639) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	AC	28	ARG
3	AC	32	GLU
3	AC	48	LEU
3	AC	50	ILE
3	AC	53	ARG
3	AC	54	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	AC	203	GLU
3	AC	208	THR
4	AD	12	SER
4	AD	13	ARG
4	AD	38	LYS
4	AD	61	LEU
4	AD	88	ARG
4	AD	94	LEU
4	AD	99	ASP
4	AD	103	ARG
4	AD	106	ILE
4	AD	113	VAL
4	AD	122	ASP
4	AD	126	GLN
4	AD	138	VAL
4	AD	142	VAL
4	AD	155	LEU
4	AD	175	LEU
4	AD	183	ARG
4	AD	193	VAL
4	AD	211	ARG
4	AD	229	VAL
4	AD	242	ARG
4	AD	253	GLN
4	AD	257	LEU
4	AD	259	THR
4	AD	260	ARG
4	AD	274	ARG
5	AE	1	MET
5	AE	9	VAL
5	AE	21	VAL
5	AE	34	VAL
5	AE	47	VAL
5	AE	48	GLN
5	AE	49	LEU
5	AE	75	VAL
5	AE	78	LEU
5	AE	82	ARG
5	AE	93	VAL
5	AE	97	LYS
5	AE	111	ARG
5	AE	116	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	AE	119	ARG
5	AE	136	ARG
5	AE	144	ARG
5	AE	154	LYS
5	AE	163	GLU
5	AE	170	LEU
5	AE	175	VAL
5	AE	179	GLU
5	AE	181	LEU
5	AE	183	LEU
6	AF	12	LEU
6	AF	17	ARG
6	AF	19	GLU
6	AF	24	LEU
6	AF	33	LEU
6	AF	53	THR
6	AF	57	VAL
6	AF	64	ILE
6	AF	74	ARG
6	AF	82	ILE
6	AF	88	VAL
6	AF	95	ARG
6	AF	106	ARG
6	AF	110	LEU
6	AF	125	LEU
6	AF	132	VAL
6	AF	137	LYS
6	AF	140	LEU
6	AF	158	THR
6	AF	161	GLU
6	AF	162	LEU
6	AF	170	LEU
6	AF	183	VAL
6	AF	192	LEU
6	AF	195	ASP
6	AF	197	ASP
7	AG	5	VAL
7	AG	7	LEU
7	AG	21	ARG
7	AG	28	VAL
7	AG	31	VAL
7	AG	41	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	AG	43	LEU
7	AG	45	GLU
7	AG	58	GLN
7	AG	60	LEU
7	AG	79	ASN
7	AG	82	LEU
7	AG	84	LYS
7	AG	86	MET
7	AG	91	ARG
7	AG	128	ARG
7	AG	140	ILE
7	AG	146	TYR
7	AG	153	ARG
7	AG	159	VAL
7	AG	170	ARG
7	AG	174	GLU
7	AG	175	LEU
7	AG	181	ARG
8	AH	3	ARG
8	AH	6	ARG
8	AH	13	LYS
8	AH	24	VAL
8	AH	25	LYS
8	AH	49	VAL
8	AH	57	ASP
8	AH	62	LYS
8	AH	69	ARG
8	AH	71	LEU
8	AH	97	ARG
8	AH	116	GLU
8	AH	122	THR
8	AH	125	VAL
8	AH	134	SER
8	AH	139	GLN
10	AL	77	LEU
10	AL	86	LYS
10	AL	100	THR
10	AL	105	LEU
10	AL	106	GLU
11	AN	5	VAL
11	AN	9	VAL
11	AN	15	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	AN	21	LYS
11	AN	28	THR
11	AN	33	LEU
11	AN	34	LEU
11	AN	39	ARG
11	AN	48	MET
11	AN	61	ARG
11	AN	62	VAL
11	AN	67	LEU
11	AN	73	THR
11	AN	84	LYS
11	AN	87	LEU
11	AN	88	GLU
11	AN	97	ARG
11	AN	99	LEU
11	AN	120	LEU
11	AN	133	GLN
11	AN	136	GLU
11	AN	137	LYS
11	AN	138	LEU
11	AN	140	VAL
12	AO	8	LEU
12	AO	10	VAL
12	AO	17	ARG
12	AO	20	MET
12	AO	24	VAL
12	AO	28	SER
12	AO	35	VAL
12	AO	47	ILE
12	AO	52	VAL
12	AO	53	LYS
12	AO	80	ASP
12	AO	82	ASN
12	AO	91	LEU
12	AO	92	GLU
12	AO	94	ARG
12	AO	98	VAL
12	AO	113	LYS
13	AP	21	ARG
13	AP	42	SER
13	AP	55	ARG
13	AP	59	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
13	AP	70	GLN
13	AP	74	GLU
13	AP	77	ARG
13	AP	83	VAL
13	AP	98	GLU
13	AP	99	LEU
13	AP	106	LEU
13	AP	112	LEU
13	AP	126	VAL
13	AP	135	LEU
13	AP	138	LEU
13	AP	139	LYS
13	AP	147	LEU
13	AP	148	LEU
13	AP	149	GLU
14	AQ	2	LEU
14	AQ	7	MET
14	AQ	8	LYS
14	AQ	16	ARG
14	AQ	21	THR
14	AQ	22	LYS
14	AQ	35	VAL
14	AQ	42	ILE
14	AQ	45	GLN
14	AQ	54	MET
14	AQ	59	ARG
14	AQ	60	ARG
14	AQ	75	THR
14	AQ	76	LYS
14	AQ	85	LYS
14	AQ	98	LYS
14	AQ	109	VAL
14	AQ	110	THR
14	AQ	115	MET
14	AQ	133	ARG
14	AQ	134	ARG
15	AR	6	SER
15	AR	9	LYS
15	AR	18	LEU
15	AR	27	SER
15	AR	28	LEU
15	AR	29	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
15	AR	33	ARG
15	AR	36	THR
15	AR	44	LEU
15	AR	45	ARG
15	AR	54	LEU
15	AR	57	ARG
15	AR	59	ASP
15	AR	60	LEU
15	AR	63	ARG
15	AR	65	LEU
15	AR	67	LEU
15	AR	79	LEU
15	AR	91	GLN
15	AR	96	ARG
15	AR	102	GLU
15	AR	111	LEU
16	AS	3	ARG
16	AS	14	VAL
16	AS	19	LYS
16	AS	20	ARG
16	AS	25	ARG
16	AS	36	TYR
16	AS	46	VAL
16	AS	48	LEU
16	AS	49	VAL
16	AS	50	SER
16	AS	57	LYS
16	AS	69	VAL
16	AS	83	LYS
16	AS	85	VAL
16	AS	93	LYS
16	AS	110	LEU
17	AT	6	LEU
17	AT	13	ARG
17	AT	17	THR
17	AT	23	ARG
17	AT	28	VAL
17	AT	40	THR
17	AT	49	VAL
17	AT	59	THR
17	AT	65	LYS
17	AT	67	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	AT	74	ARG
17	AT	78	LEU
17	AT	85	LYS
17	AT	96	ARG
17	AT	108	ARG
17	AT	118	ARG
17	AT	125	ARG
17	AT	128	GLU
18	AU	5	LYS
18	AU	8	VAL
18	AU	13	LYS
18	AU	16	LYS
18	AU	19	LYS
18	AU	36	ARG
18	AU	52	ARG
18	AU	60	LEU
18	AU	74	LEU
18	AU	77	SER
18	AU	83	LEU
18	AU	92	ARG
18	AU	95	LEU
18	AU	103	PRO
18	AU	104	GLN
18	AU	112	ARG
19	AV	18	LEU
19	AV	20	LEU
19	AV	21	ARG
19	AV	28	GLU
19	AV	35	LEU
19	AV	43	GLU
19	AV	46	VAL
19	AV	51	VAL
19	AV	62	LEU
19	AV	72	VAL
19	AV	79	VAL
19	AV	85	LYS
19	AV	92	THR
19	AV	95	LEU
19	AV	100	ARG
20	AW	4	LYS
20	AW	11	ARG
20	AW	12	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
20	AW	15	ARG
20	AW	19	LEU
20	AW	24	ILE
20	AW	51	LEU
20	AW	63	ASP
20	AW	98	LYS
20	AW	107	LEU
21	AX	2	LYS
21	AX	57	LEU
21	AX	65	ARG
21	AX	70	LEU
22	AY	7	VAL
22	AY	23	ARG
22	AY	31	LEU
22	AY	47	LYS
22	AY	55	TYR
22	AY	73	ARG
22	AY	85	VAL
22	AY	90	LEU
22	AY	91	GLU
22	AY	92	ASN
22	AY	106	LEU
22	AY	107	ASP
23	AZ	5	LEU
23	AZ	6	LYS
23	AZ	18	LEU
23	AZ	31	ARG
23	AZ	33	LEU
23	AZ	41	LEU
23	AZ	50	GLN
23	AZ	58	VAL
23	AZ	72	ARG
23	AZ	76	LEU
23	AZ	84	GLU
23	AZ	86	VAL
23	AZ	91	LEU
23	AZ	98	MET
23	AZ	102	LEU
23	AZ	117	LEU
23	AZ	120	ILE
23	AZ	126	VAL
23	AZ	128	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
23	AZ	129	SER
23	AZ	141	VAL
23	AZ	146	ILE
23	AZ	148	ASP
23	AZ	149	SER
23	AZ	154	ASP
23	AZ	155	LEU
23	AZ	161	VAL
23	AZ	170	THR
24	A0	20	ARG
24	A0	55	ARG
25	A1	21	ARG
25	A1	30	VAL
25	A1	40	ARG
25	A1	46	LEU
25	A1	52	ARG
25	A1	59	THR
25	A1	83	GLU
25	A1	95	LEU
26	A2	3	LEU
26	A2	28	LYS
26	A2	30	ARG
26	A2	32	LEU
26	A2	45	SER
26	A2	53	LEU
26	A2	59	ARG
26	A2	62	THR
26	A2	65	ASN
26	A2	68	ARG
26	A2	70	GLN
27	A3	3	ARG
27	A3	8	LEU
27	A3	23	LEU
27	A3	29	ARG
27	A3	54	VAL
27	A3	58	VAL
27	A3	60	GLU
28	A4	1	MET
28	A4	3	GLU
28	A4	5	ILE
28	A4	34	GLU
28	A4	46	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
28	A4	49	PHE
28	A4	50	VAL
28	A4	55	ARG
28	A4	56	VAL
28	A4	59	PHE
28	A4	63	TYR
29	A5	6	VAL
29	A5	16	ARG
29	A5	26	THR
29	A5	29	THR
29	A5	40	LYS
29	A5	55	ARG
29	A5	56	LYS
30	A6	3	SER
30	A6	4	GLU
30	A6	6	ARG
30	A6	7	ILE
30	A6	9	LEU
30	A6	14	THR
30	A6	33	LYS
30	A6	35	GLU
30	A6	44	ARG
30	A6	48	VAL
30	A6	50	ARG
31	A7	1	MET
31	A7	9	ARG
31	A7	10	ARG
31	A7	41	ARG
31	A7	43	THR
31	A7	46	VAL
32	A8	6	THR
32	A8	30	ARG
32	A8	31	HIS
32	A8	32	LEU
32	A8	37	SER
32	A8	41	ILE
32	A8	46	ARG
33	A9	4	ARG
33	A9	17	ILE
33	A9	19	ARG
35	BB	8	LYS
35	BB	11	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
35	BB	15	VAL
35	BB	17	PHE
35	BB	19	HIS
35	BB	20	GLU
35	BB	21	ARG
35	BB	23	ARG
35	BB	24	TRP
35	BB	35	GLU
35	BB	37	ASN
35	BB	45	GLN
35	BB	48	MET
35	BB	58	ILE
35	BB	60	ASP
35	BB	67	THR
35	BB	75	LYS
35	BB	76	GLN
35	BB	78	GLN
35	BB	80	ILE
35	BB	84	GLU
35	BB	87	ARG
35	BB	93	VAL
35	BB	96	ARG
35	BB	97	TRP
35	BB	111	ARG
35	BB	112	VAL
35	BB	113	HIS
35	BB	126	GLU
35	BB	137	ARG
35	BB	145	LEU
35	BB	147	LYS
35	BB	150	SER
35	BB	153	ARG
35	BB	156	LYS
35	BB	160	ASP
35	BB	167	PRO
35	BB	168	THR
35	BB	169	LYS
35	BB	170	GLU
35	BB	178	ARG
35	BB	187	LEU
35	BB	195	ASP
35	BB	196	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
35	BB	200	ILE
35	BB	208	ILE
35	BB	221	LEU
35	BB	230	VAL
36	BC	3	ASN
36	BC	28	GLN
36	BC	29	TYR
36	BC	37	GLN
36	BC	38	ARG
36	BC	44	GLU
36	BC	45	LYS
36	BC	49	SER
36	BC	52	LEU
36	BC	70	VAL
36	BC	77	ILE
36	BC	82	GLU
36	BC	118	GLN
36	BC	131	ARG
36	BC	188	LEU
36	BC	196	LEU
36	BC	202	ILE
36	BC	206	GLU
36	BC	207	VAL
37	BD	5	ILE
37	BD	15	GLU
37	BD	19	LEU
37	BD	28	SER
37	BD	31	CYS
37	BD	49	ARG
37	BD	57	ARG
37	BD	58	LEU
37	BD	65	ARG
37	BD	85	LYS
37	BD	86	LYS
37	BD	100	ARG
37	BD	108	LEU
37	BD	115	ARG
37	BD	118	ARG
37	BD	127	THR
37	BD	134	ASP
37	BD	135	LEU
37	BD	141	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
37	BD	157	LEU
37	BD	158	ILE
37	BD	168	ARG
37	BD	188	LEU
37	BD	190	ASP
38	BE	10	MET
38	BE	13	ILE
38	BE	41	VAL
38	BE	47	LYS
38	BE	78	HIS
38	BE	79	GLU
38	BE	87	SER
38	BE	120	THR
38	BE	150	ARG
39	BF	28	ARG
39	BF	40	VAL
39	BF	45	LEU
39	BF	55	ASP
39	BF	69	GLU
39	BF	70	ASP
39	BF	71	ARG
39	BF	72	VAL
39	BF	73	ASN
39	BF	75	LEU
39	BF	82	ARG
39	BF	89	MET
39	BF	91	VAL
40	BG	8	GLU
40	BG	12	LEU
40	BG	21	VAL
40	BG	31	MET
40	BG	38	LEU
40	BG	50	ILE
40	BG	51	GLN
40	BG	56	GLN
40	BG	73	MET
40	BG	76	ARG
40	BG	78	ARG
40	BG	79	ARG
40	BG	91	VAL
40	BG	104	LEU
40	BG	113	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
40	BG	114	ARG
40	BG	131	LYS
40	BG	138	LYS
40	BG	139	GLU
40	BG	140	ASP
40	BG	155	ARG
41	BH	2	LEU
41	BH	6	ILE
41	BH	18	ARG
41	BH	21	LYS
41	BH	23	SER
41	BH	37	ARG
41	BH	51	VAL
41	BH	60	ARG
41	BH	63	LEU
41	BH	68	ARG
41	BH	78	GLN
41	BH	83	ILE
41	BH	99	GLU
41	BH	115	SER
41	BH	121	ASP
41	BH	122	ARG
42	BI	3	GLN
42	BI	7	THR
42	BI	17	VAL
42	BI	23	ASN
42	BI	27	THR
42	BI	56	LEU
42	BI	64	THR
42	BI	65	VAL
42	BI	75	ASP
42	BI	78	LYS
42	BI	81	ILE
42	BI	87	GLN
42	BI	97	LYS
42	BI	102	LEU
42	BI	104	ARG
42	BI	109	VAL
42	BI	111	ARG
42	BI	121	ARG
42	BI	128	ARG
43	BJ	5	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
43	BJ	7	LYS
43	BJ	16	LEU
43	BJ	23	ILE
43	BJ	44	VAL
43	BJ	49	VAL
43	BJ	67	THR
43	BJ	92	THR
44	BK	25	TYR
44	BK	41	THR
44	BK	48	ILE
44	BK	63	LEU
44	BK	83	ILE
44	BK	84	VAL
44	BK	96	ARG
44	BK	98	LEU
44	BK	104	GLN
44	BK	105	VAL
44	BK	109	VAL
44	BK	114	VAL
45	BL	23	LYS
45	BL	27	LEU
45	BL	42	THR
45	BL	60	LEU
45	BL	86	ARG
45	BL	89	ARG
45	BL	97	ARG
46	BM	4	ILE
46	BM	17	VAL
46	BM	19	LEU
46	BM	20	THR
46	BM	43	THR
46	BM	56	LEU
46	BM	63	THR
46	BM	64	TRP
46	BM	70	LEU
46	BM	102	ARG
46	BM	109	THR
46	BM	110	ARG
46	BM	121	LYS
47	BN	3	ARG
47	BN	6	LEU
47	BN	7	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
47	BN	9	LYS
47	BN	18	VAL
47	BN	32	SER
47	BN	33	VAL
47	BN	41	ARG
47	BN	44	LEU
47	BN	60	SER
48	BO	3	ILE
48	BO	5	LYS
48	BO	6	GLU
48	BO	22	THR
48	BO	26	GLU
48	BO	34	LEU
48	BO	35	ARG
48	BO	38	ARG
48	BO	39	LEU
48	BO	41	GLU
48	BO	66	LEU
48	BO	83	GLU
48	BO	87	ILE
48	BO	88	ARG
49	BP	1	MET
49	BP	6	LEU
49	BP	11	SER
49	BP	19	ILE
49	BP	20	VAL
49	BP	27	LYS
49	BP	36	ILE
49	BP	50	LYS
49	BP	60	LEU
49	BP	62	VAL
49	BP	67	THR
49	BP	69	THR
49	BP	71	ARG
50	BQ	6	LEU
50	BQ	36	ILE
50	BQ	45	HIS
50	BQ	60	ILE
50	BQ	63	ARG
50	BQ	68	ARG
50	BQ	72	ARG
50	BQ	78	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	BQ	86	GLU
50	BQ	90	ILE
50	BQ	91	ARG
50	BQ	92	ARG
50	BQ	97	SER
51	BR	31	LEU
51	BR	32	ARG
51	BR	35	ARG
51	BR	37	VAL
51	BR	38	GLU
51	BR	45	SER
51	BR	46	GLU
51	BR	47	THR
51	BR	55	ARG
51	BR	65	ILE
51	BR	68	LYS
51	BR	76	LEU
52	BS	12	ASP
52	BS	28	LYS
52	BS	37	ARG
52	BS	38	SER
52	BS	62	ILE
52	BS	65	ASN
52	BS	78	ARG
52	BS	81	ARG
52	BS	85	LYS
53	BT	8	ARG
53	BT	13	LEU
53	BT	24	LEU
53	BT	43	LEU
53	BT	45	GLN
53	BT	56	MET
53	BT	58	LYS
53	BT	60	GLU
53	BT	62	LEU
53	BT	84	LEU
53	BT	100	ILE
54	BU	9	ARG
54	BU	10	ARG
59	BZ	-64	VAL
59	BZ	-42	TYR
59	BZ	-29	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
59	BZ	-23	LEU
59	BZ	-20	LEU
59	BZ	-19	GLU
59	BZ	-10	ARG
59	BZ	-6	ARG
59	BZ	-1	GLU
59	BZ	0	ARG
59	BZ	4	ILE
59	BZ	7	ASN
59	BZ	12	LEU
59	BZ	13	ARG
59	BZ	15	ILE
59	BZ	21	ILE
59	BZ	30	GLU
59	BZ	33	LEU
59	BZ	69	VAL
59	BZ	71	THR
59	BZ	75	LYS
59	BZ	76	ASP
59	BZ	78	ARG
59	BZ	87	HIS
59	BZ	89	ASP
59	BZ	92	ILE
59	BZ	99	ARG
59	BZ	102	ASP
59	BZ	105	ILE
59	BZ	112	GLN
59	BZ	130	VAL
59	BZ	132	ARG
59	BZ	139	MET
59	BZ	146	LEU
59	BZ	148	LEU
59	BZ	152	THR
59	BZ	156	ARG
59	BZ	160	ARG
59	BZ	166	LEU
59	BZ	170	ARG
59	BZ	172	ASP
59	BZ	196	ILE
59	BZ	198	GLU
59	BZ	203	GLU
59	BZ	207	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
59	BZ	208	GLN
59	BZ	222	ASP
59	BZ	238	THR
59	BZ	239	GLU
59	BZ	240	GLU
59	BZ	247	ARG
59	BZ	255	ILE
59	BZ	267	LYS
59	BZ	269	VAL
59	BZ	282	SER
59	BZ	284	LEU
59	BZ	286	ILE
59	BZ	289	ILE
59	BZ	298	VAL
59	BZ	312	LEU
59	BZ	328	ILE
59	BZ	329	ARG
59	BZ	331	TYR
59	BZ	336	THR
59	BZ	349	LYS
59	BZ	352	VAL
59	BZ	354	ARG
59	BZ	356	LEU
59	BZ	362	HIS
59	BZ	363	ARG
59	BZ	368	GLU
59	BZ	369	LEU
59	BZ	374	LEU
59	BZ	381	LYS
59	BZ	382	GLU
59	BZ	389	LEU
59	BZ	397	VAL
59	BZ	399	LEU
59	BZ	402	ILE
59	BZ	406	GLU
59	BZ	420	ASP
59	BZ	421	GLN
59	BZ	422	GLU
59	BZ	431	LEU
59	BZ	433	GLU
59	BZ	437	THR
59	BZ	442	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
59	BZ	446	THR
59	BZ	457	LEU
59	BZ	464	ASP
59	BZ	468	ARG
59	BZ	473	ASP
59	BZ	484	ARG
59	BZ	485	GLU
59	BZ	486	THR
59	BZ	504	ARG
59	BZ	506	GLN
59	BZ	512	ILE
59	BZ	572	TYR
59	BZ	600	VAL
59	BZ	614	GLU
59	BZ	630	GLN
59	BZ	634	MET
59	BZ	644	ARG
59	BZ	647	VAL
59	BZ	651	GLU
59	BZ	659	LEU
59	BZ	660	ARG
59	BZ	669	PHE
59	BZ	670	VAL
59	BZ	679	VAL
59	BZ	681	LYS
59	BZ	683	VAL
59	BZ	684	GLN
59	BZ	686	LYS
3	CC	28	ARG
3	CC	32	GLU
3	CC	48	LEU
3	CC	50	ILE
3	CC	53	ARG
3	CC	54	ARG
3	CC	203	GLU
3	CC	208	THR
4	CD	3	VAL
4	CD	5	LYS
4	CD	12	SER
4	CD	13	ARG
4	CD	14	ARG
4	CD	26	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	CD	32	SER
4	CD	54	ARG
4	CD	61	LEU
4	CD	71	ASP
4	CD	89	SER
4	CD	94	LEU
4	CD	99	ASP
4	CD	101	GLU
4	CD	103	ARG
4	CD	106	ILE
4	CD	111	LEU
4	CD	113	VAL
4	CD	134	ARG
4	CD	138	VAL
4	CD	141	VAL
4	CD	142	VAL
4	CD	165	ILE
4	CD	211	ARG
4	CD	212	SER
4	CD	217	ARG
4	CD	221	VAL
4	CD	229	VAL
4	CD	242	ARG
4	CD	257	LEU
4	CD	259	THR
4	CD	260	ARG
4	CD	262	ARG
4	CD	270	ILE
4	CD	276	LYS
5	CE	12	THR
5	CE	21	VAL
5	CE	34	VAL
5	CE	40	GLU
5	CE	45	THR
5	CE	49	LEU
5	CE	58	ARG
5	CE	61	ARG
5	CE	75	VAL
5	CE	77	ILE
5	CE	78	LEU
5	CE	79	ARG
5	CE	82	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	CE	89	ASP
5	CE	111	ARG
5	CE	116	VAL
5	CE	119	ARG
5	CE	144	ARG
5	CE	154	LYS
5	CE	170	LEU
5	CE	175	VAL
5	CE	181	LEU
5	CE	184	VAL
5	CE	195	LEU
5	CE	202	LYS
6	CF	17	ARG
6	CF	19	GLU
6	CF	24	LEU
6	CF	32	LEU
6	CF	40	GLN
6	CF	50	SER
6	CF	53	THR
6	CF	57	VAL
6	CF	70	THR
6	CF	74	ARG
6	CF	77	ASP
6	CF	88	VAL
6	CF	95	ARG
6	CF	106	ARG
6	CF	107	LYS
6	CF	110	LEU
6	CF	135	LYS
6	CF	140	LEU
6	CF	158	THR
6	CF	169	ASN
6	CF	175	THR
6	CF	186	ILE
6	CF	192	LEU
6	CF	200	GLU
7	CG	3	LEU
7	CG	4	ASP
7	CG	5	VAL
7	CG	16	ARG
7	CG	18	GLU
7	CG	28	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	CG	31	VAL
7	CG	33	ARG
7	CG	35	GLU
7	CG	43	LEU
7	CG	49	ASP
7	CG	60	LEU
7	CG	70	VAL
7	CG	71	THR
7	CG	79	ASN
7	CG	80	PHE
7	CG	91	ARG
7	CG	111	LEU
7	CG	115	ARG
7	CG	116	ASP
7	CG	128	ARG
7	CG	130	ASN
7	CG	133	LEU
7	CG	136	ARG
7	CG	139	LEU
7	CG	143	GLU
7	CG	145	THR
7	CG	148	MET
7	CG	152	LEU
7	CG	153	ARG
7	CG	159	VAL
7	CG	162	THR
7	CG	165	THR
7	CG	170	ARG
8	CH	3	ARG
8	CH	27	LYS
8	CH	33	LEU
8	CH	41	MET
8	CH	44	VAL
8	CH	69	ARG
8	CH	84	SER
8	CH	88	LEU
8	CH	98	LEU
8	CH	106	THR
8	CH	110	SER
8	CH	111	HIS
8	CH	122	THR
8	CH	124	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	CH	129	THR
8	CH	136	ILE
8	CH	139	GLN
8	CH	147	ASN
8	CH	171	LEU
10	CL	86	LYS
10	CL	93	ARG
10	CL	96	VAL
10	CL	112	MET
10	CL	117	THR
11	CN	2	LYS
11	CN	3	THR
11	CN	5	VAL
11	CN	12	ARG
11	CN	33	LEU
11	CN	34	LEU
11	CN	43	THR
11	CN	46	VAL
11	CN	48	MET
11	CN	82	LEU
11	CN	87	LEU
11	CN	97	ARG
11	CN	99	LEU
11	CN	104	LYS
11	CN	119	ARG
11	CN	120	LEU
11	CN	127	ASP
11	CN	133	GLN
11	CN	138	LEU
11	CN	140	VAL
12	CO	1	MET
12	CO	5	GLN
12	CO	10	VAL
12	CO	14	THR
12	CO	24	VAL
12	CO	28	SER
12	CO	66	LYS
12	CO	69	ILE
12	CO	77	ILE
12	CO	78	ARG
12	CO	85	VAL
12	CO	86	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	CO	92	GLU
12	CO	98	VAL
12	CO	108	GLU
12	CO	113	LYS
12	CO	117	LEU
13	CP	2	LYS
13	CP	3	LEU
13	CP	38	GLN
13	CP	40	SER
13	CP	42	SER
13	CP	45	LEU
13	CP	55	ARG
13	CP	56	SER
13	CP	64	LYS
13	CP	65	ARG
13	CP	75	ILE
13	CP	83	VAL
13	CP	95	VAL
13	CP	106	LEU
13	CP	131	SER
13	CP	148	LEU
14	CQ	1	MET
14	CQ	3	MET
14	CQ	7	MET
14	CQ	8	LYS
14	CQ	12	GLN
14	CQ	16	ARG
14	CQ	21	THR
14	CQ	35	VAL
14	CQ	45	GLN
14	CQ	60	ARG
14	CQ	75	THR
14	CQ	109	VAL
14	CQ	110	THR
14	CQ	115	MET
14	CQ	128	LYS
14	CQ	131	ILE
15	CR	1	MET
15	CR	18	LEU
15	CR	27	SER
15	CR	28	LEU
15	CR	29	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
15	CR	36	THR
15	CR	44	LEU
15	CR	60	LEU
15	CR	65	LEU
15	CR	67	LEU
15	CR	75	LEU
15	CR	79	LEU
15	CR	86	ARG
15	CR	96	ARG
15	CR	100	LEU
15	CR	111	LEU
15	CR	114	VAL
16	CS	3	ARG
16	CS	13	ARG
16	CS	14	VAL
16	CS	19	LYS
16	CS	20	ARG
16	CS	25	ARG
16	CS	35	ILE
16	CS	36	TYR
16	CS	49	VAL
16	CS	58	LEU
16	CS	64	GLU
16	CS	67	ARG
16	CS	68	GLN
16	CS	69	VAL
16	CS	78	LEU
16	CS	80	LEU
16	CS	103	GLU
16	CS	110	LEU
17	CT	6	LEU
17	CT	8	LYS
17	CT	28	VAL
17	CT	34	VAL
17	CT	49	VAL
17	CT	51	ARG
17	CT	53	ARG
17	CT	59	THR
17	CT	64	ARG
17	CT	74	ARG
17	CT	78	LEU
17	CT	85	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	CT	89	VAL
17	CT	93	ARG
17	CT	96	ARG
17	CT	113	LYS
17	CT	115	ARG
17	CT	118	ARG
17	CT	123	GLN
17	CT	124	ASP
18	CU	6	THR
18	CU	8	VAL
18	CU	13	LYS
18	CU	31	SER
18	CU	60	LEU
18	CU	74	LEU
18	CU	83	LEU
18	CU	92	ARG
18	CU	101	ARG
18	CU	104	GLN
18	CU	108	GLU
19	CV	1	MET
19	CV	6	LYS
19	CV	15	GLU
19	CV	18	LEU
19	CV	19	LYS
19	CV	51	VAL
19	CV	52	VAL
19	CV	61	VAL
19	CV	62	LEU
19	CV	66	ARG
19	CV	73	SER
19	CV	79	VAL
19	CV	95	LEU
20	CW	11	ARG
20	CW	15	ARG
20	CW	17	VAL
20	CW	19	LEU
20	CW	23	LEU
20	CW	37	ARG
20	CW	51	LEU
20	CW	63	ASP
20	CW	100	THR
20	CW	101	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
20	CW	107	LEU
21	CX	35	THR
21	CX	45	THR
21	CX	57	LEU
21	CX	60	ARG
21	CX	76	ARG
21	CX	87	GLN
21	CX	92	LEU
22	CY	2	ARG
22	CY	6	HIS
22	CY	7	VAL
22	CY	9	LYS
22	CY	21	LYS
22	CY	23	ARG
22	CY	37	VAL
22	CY	43	ASN
22	CY	47	LYS
22	CY	49	VAL
22	CY	50	ARG
22	CY	70	SER
22	CY	73	ARG
22	CY	91	GLU
22	CY	102	CYS
23	CZ	5	LEU
23	CZ	18	LEU
23	CZ	33	LEU
23	CZ	41	LEU
23	CZ	56	VAL
23	CZ	61	LEU
23	CZ	66	SER
23	CZ	71	VAL
23	CZ	86	VAL
23	CZ	91	LEU
23	CZ	102	LEU
23	CZ	107	THR
23	CZ	120	ILE
23	CZ	128	VAL
23	CZ	129	SER
23	CZ	136	PHE
23	CZ	144	LEU
23	CZ	146	ILE
23	CZ	154	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
23	CZ	170	THR
24	C0	3	HIS
24	C0	19	LYS
24	C0	20	ARG
24	C0	36	ILE
24	C0	44	ARG
25	C1	21	ARG
25	C1	35	THR
25	C1	40	ARG
25	C1	51	VAL
25	C1	52	ARG
25	C1	59	THR
25	C1	80	LEU
25	C1	86	SER
25	C1	89	GLU
25	C1	95	LEU
25	C1	97	LEU
26	C2	2	LYS
26	C2	19	VAL
26	C2	32	LEU
26	C2	40	SER
26	C2	41	ILE
26	C2	44	LEU
26	C2	53	LEU
26	C2	66	GLU
26	C2	67	LYS
26	C2	70	GLN
27	C3	3	ARG
27	C3	5	LYS
27	C3	6	VAL
27	C3	8	LEU
27	C3	18	ASP
27	C3	23	LEU
27	C3	24	LYS
27	C3	30	ARG
27	C3	31	LEU
27	C3	34	GLU
27	C3	54	VAL
27	C3	56	VAL
28	C4	1	MET
28	C4	3	GLU
28	C4	5	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
28	C4	10	VAL
28	C4	34	GLU
28	C4	36	CYS
28	C4	41	PRO
28	C4	50	VAL
28	C4	56	VAL
28	C4	58	ARG
28	C4	61	ARG
28	C4	63	TYR
28	C4	68	ARG
28	C4	69	LYS
29	C5	6	VAL
29	C5	16	ARG
29	C5	29	THR
29	C5	35	GLU
29	C5	40	LYS
29	C5	48	GLU
30	C6	5	VAL
30	C6	6	ARG
30	C6	23	THR
30	C6	27	LYS
30	C6	28	ARG
30	C6	44	ARG
30	C6	48	VAL
31	C7	1	MET
31	C7	9	ARG
31	C7	14	LYS
31	C7	39	ARG
31	C7	43	THR
32	C8	14	VAL
32	C8	26	LYS
32	C8	30	ARG
32	C8	31	HIS
32	C8	34	TRP
33	C9	4	ARG
33	C9	17	ILE
33	C9	19	ARG
33	C9	26	ILE
33	C9	35	ARG
35	DB	7	VAL
35	DB	10	LEU
35	DB	15	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
35	DB	23	ARG
35	DB	24	TRP
35	DB	51	LEU
35	DB	60	ASP
35	DB	67	THR
35	DB	80	ILE
35	DB	95	GLN
35	DB	97	TRP
35	DB	108	ILE
35	DB	115	LEU
35	DB	117	GLU
35	DB	128	GLU
35	DB	135	GLN
35	DB	154	LEU
35	DB	155	LEU
35	DB	157	ARG
35	DB	158	LEU
35	DB	162	ILE
35	DB	163	PHE
35	DB	179	LYS
35	DB	185	ILE
35	DB	187	LEU
35	DB	189	ASP
35	DB	212	GLN
35	DB	215	LEU
35	DB	217	ARG
35	DB	224	GLN
36	DC	3	ASN
36	DC	15	THR
36	DC	16	ARG
36	DC	21	ARG
36	DC	22	TRP
36	DC	29	TYR
36	DC	30	ARG
36	DC	47	LEU
36	DC	48	TYR
36	DC	52	LEU
36	DC	72	LYS
36	DC	91	LEU
36	DC	104	GLN
36	DC	105	GLU
36	DC	108	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	DC	115	LEU
36	DC	116	VAL
36	DC	127	ARG
36	DC	128	PHE
36	DC	140	ARG
36	DC	152	ILE
36	DC	153	VAL
36	DC	154	SER
36	DC	190	ARG
36	DC	191	THR
36	DC	195	VAL
37	DD	3	ARG
37	DD	10	ARG
37	DD	25	ARG
37	DD	31	CYS
37	DD	34	GLU
37	DD	47	ARG
37	DD	53	ASP
37	DD	57	ARG
37	DD	58	LEU
37	DD	61	LYS
37	DD	63	LYS
37	DD	65	ARG
37	DD	73	ARG
37	DD	96	LEU
37	DD	102	ASP
37	DD	107	ARG
37	DD	108	LEU
37	DD	127	THR
37	DD	135	LEU
37	DD	137	SER
37	DD	150	GLU
37	DD	155	LEU
37	DD	187	ARG
37	DD	188	LEU
37	DD	194	LEU
37	DD	208	SER
38	DE	10	MET
38	DE	16	THR
38	DE	18	ARG
38	DE	31	LEU
38	DE	41	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
38	DE	47	LYS
38	DE	53	LEU
38	DE	71	LEU
38	DE	75	THR
38	DE	78	HIS
38	DE	82	VAL
38	DE	87	SER
38	DE	89	ILE
38	DE	91	LEU
38	DE	107	ARG
38	DE	117	ASP
38	DE	120	THR
38	DE	150	ARG
39	DF	7	ASN
39	DF	10	LEU
39	DF	21	LEU
39	DF	27	GLN
39	DF	28	ARG
39	DF	69	GLU
39	DF	72	VAL
39	DF	75	LEU
39	DF	82	ARG
39	DF	87	ARG
39	DF	93	SER
40	DG	32	ARG
40	DG	57	GLU
40	DG	75	VAL
40	DG	98	SER
40	DG	104	LEU
40	DG	114	ARG
40	DG	115	ARG
40	DG	155	ARG
41	DH	2	LEU
41	DH	3	THR
41	DH	24	THR
41	DH	26	VAL
41	DH	37	ARG
41	DH	39	LEU
41	DH	51	VAL
41	DH	52	ASP
41	DH	60	ARG
41	DH	63	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
41	DH	65	TYR
41	DH	78	GLN
41	DH	84	ARG
41	DH	85	ARG
41	DH	98	LYS
41	DH	111	ILE
41	DH	112	LEU
41	DH	119	LEU
41	DH	120	THR
41	DH	125	ARG
41	DH	127	LEU
41	DH	133	LEU
42	DI	23	ASN
42	DI	27	THR
42	DI	31	GLN
42	DI	41	VAL
42	DI	53	VAL
42	DI	64	THR
42	DI	65	VAL
42	DI	85	LEU
42	DI	89	ASN
42	DI	92	TYR
42	DI	102	LEU
42	DI	104	ARG
42	DI	108	VAL
42	DI	109	VAL
42	DI	113	LYS
42	DI	124	GLN
42	DI	125	TYR
42	DI	128	ARG
43	DJ	6	ILE
43	DJ	21	GLN
43	DJ	30	SER
43	DJ	34	VAL
43	DJ	43	ARG
43	DJ	46	ARG
43	DJ	59	SER
43	DJ	67	THR
43	DJ	72	VAL
43	DJ	85	LEU
43	DJ	96	ILE
44	DK	14	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
44	DK	18	ARG
44	DK	30	VAL
44	DK	33	THR
44	DK	54	ARG
44	DK	92	GLU
44	DK	109	VAL
44	DK	120	ARG
44	DK	126	ARG
45	DL	33	ARG
45	DL	42	THR
45	DL	47	LYS
45	DL	52	LEU
45	DL	53	ARG
45	DL	75	HIS
45	DL	89	ARG
45	DL	92	ASP
45	DL	102	ARG
45	DL	104	VAL
45	DL	114	LYS
46	DM	3	ARG
46	DM	8	GLU
46	DM	11	ARG
46	DM	15	VAL
46	DM	27	LYS
46	DM	29	ARG
46	DM	52	GLU
46	DM	66	LEU
46	DM	70	LEU
46	DM	73	GLU
46	DM	77	ASN
46	DM	90	LEU
46	DM	92	HIS
46	DM	106	ASN
46	DM	110	ARG
46	DM	121	LYS
47	DN	3	ARG
47	DN	13	THR
47	DN	15	LYS
47	DN	18	VAL
47	DN	22	THR
47	DN	29	ARG
47	DN	33	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
47	DN	44	LEU
47	DN	46	GLU
48	DO	3	ILE
48	DO	4	THR
48	DO	5	LYS
48	DO	7	GLU
48	DO	22	THR
48	DO	38	ARG
48	DO	39	LEU
48	DO	48	LYS
48	DO	66	LEU
48	DO	68	ARG
49	DP	1	MET
49	DP	2	VAL
49	DP	4	ILE
49	DP	5	ARG
49	DP	45	THR
49	DP	60	LEU
49	DP	62	VAL
50	DQ	6	LEU
50	DQ	50	LYS
50	DQ	52	LYS
50	DQ	63	ARG
50	DQ	69	LYS
50	DQ	72	ARG
50	DQ	74	LEU
50	DQ	79	SER
50	DQ	86	GLU
50	DQ	91	ARG
50	DQ	96	GLU
50	DQ	98	LEU
51	DR	32	ARG
51	DR	37	VAL
51	DR	41	LYS
51	DR	42	ARG
51	DR	53	ARG
51	DR	65	ILE
51	DR	76	LEU
51	DR	85	LEU
52	DS	6	LYS
52	DS	12	ASP
52	DS	22	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	DS	33	THR
52	DS	65	ASN
52	DS	78	ARG
52	DS	83	HIS
53	DT	10	LEU
53	DT	24	LEU
53	DT	36	LEU
53	DT	46	GLU
53	DT	56	MET
53	DT	61	SER
53	DT	62	LEU
53	DT	71	THR
53	DT	79	ARG
53	DT	80	ARG
53	DT	84	LEU
53	DT	89	ARG
53	DT	93	GLU
54	DU	10	ARG
54	DU	15	ARG
59	DZ	-55	LEU
59	DZ	-53	ASP
59	DZ	-47	ASP
59	DZ	-29	LEU
59	DZ	-20	LEU
59	DZ	-13	GLN
59	DZ	-10	ARG
59	DZ	-6	ARG
59	DZ	-5	LYS
59	DZ	7	ASN
59	DZ	8	ASP
59	DZ	9	LEU
59	DZ	12	LEU
59	DZ	15	ILE
59	DZ	21	ILE
59	DZ	25	LYS
59	DZ	26	THR
59	DZ	30	GLU
59	DZ	31	ARG
59	DZ	33	LEU
59	DZ	70	THR
59	DZ	75	LYS
59	DZ	92	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
59	DZ	100	VAL
59	DZ	105	ILE
59	DZ	112	GLN
59	DZ	117	GLN
59	DZ	121	VAL
59	DZ	132	ARG
59	DZ	146	LEU
59	DZ	163	VAL
59	DZ	170	ARG
59	DZ	196	ILE
59	DZ	204	GLU
59	DZ	207	ASP
59	DZ	215	LYS
59	DZ	228	MET
59	DZ	232	LEU
59	DZ	236	GLU
59	DZ	240	GLU
59	DZ	255	ILE
59	DZ	264	LEU
59	DZ	277	VAL
59	DZ	285	ASP
59	DZ	286	ILE
59	DZ	292	THR
59	DZ	297	GLU
59	DZ	299	VAL
59	DZ	302	HIS
59	DZ	312	LEU
59	DZ	322	VAL
59	DZ	326	THR
59	DZ	328	ILE
59	DZ	341	VAL
59	DZ	355	LEU
59	DZ	363	ARG
59	DZ	369	LEU
59	DZ	377	VAL
59	DZ	382	GLU
59	DZ	385	THR
59	DZ	396	ARG
59	DZ	399	LEU
59	DZ	403	GLU
59	DZ	421	GLN
59	DZ	422	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
59	DZ	426	GLN
59	DZ	437	THR
59	DZ	442	THR
59	DZ	443	HIS
59	DZ	446	THR
59	DZ	471	LYS
59	DZ	473	ASP
59	DZ	475	ASN
59	DZ	488	THR
59	DZ	504	ARG
59	DZ	512	ILE
59	DZ	536	LYS
59	DZ	537	GLU
59	DZ	547	GLU
59	DZ	572	TYR
59	DZ	578	SER
59	DZ	598	ASP
59	DZ	600	VAL
59	DZ	601	ILE
59	DZ	602	LEU
59	DZ	612	THR
59	DZ	614	GLU
59	DZ	623	ASP
59	DZ	624	LEU
59	DZ	625	ASN
59	DZ	630	GLN
59	DZ	631	ILE
59	DZ	649	LEU
59	DZ	651	GLU
59	DZ	659	LEU
59	DZ	660	ARG
59	DZ	668	SER
59	DZ	675	HIS
59	DZ	679	VAL
59	DZ	681	LYS
59	DZ	686	LYS
59	DZ	689	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (154) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	AC	67	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	AC	189	ASN
3	AC	200	HIS
4	AD	126	GLN
4	AD	253	GLN
5	AE	85	ASN
6	AF	169	ASN
6	AF	203	GLN
7	AG	40	ASN
7	AG	41	GLN
7	AG	132	ASN
11	AN	131	GLN
13	AP	38	GLN
15	AR	71	GLN
16	AS	95	HIS
18	AU	94	ASN
21	AX	31	HIS
21	AX	82	GLN
22	AY	92	ASN
23	AZ	34	ASN
26	A2	9	GLN
27	A3	32	GLN
33	A9	36	GLN
35	BB	40	HIS
35	BB	45	GLN
36	BC	6	HIS
36	BC	118	GLN
36	BC	136	GLN
36	BC	162	GLN
36	BC	176	HIS
36	BC	181	ASN
37	BD	45	GLN
37	BD	119	GLN
37	BD	123	HIS
37	BD	125	HIS
37	BD	160	GLN
37	BD	161	ASN
38	BE	56	GLN
38	BE	141	GLN
39	BF	73	ASN
40	BG	28	ASN
40	BG	51	GLN
40	BG	64	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
40	BG	97	GLN
42	BI	23	ASN
42	BI	89	ASN
42	BI	124	GLN
43	BJ	56	HIS
44	BK	104	GLN
45	BL	78	GLN
47	BN	49	HIS
48	BO	9	GLN
48	BO	28	GLN
49	BP	13	HIS
50	BQ	16	GLN
52	BS	65	ASN
52	BS	69	HIS
53	BT	26	ASN
53	BT	45	GLN
53	BT	75	ASN
59	BZ	-50	GLN
59	BZ	-13	GLN
59	BZ	77	HIS
59	BZ	112	GLN
59	BZ	154	GLN
59	BZ	208	GLN
59	BZ	362	HIS
59	BZ	475	ASN
59	BZ	500	GLN
59	BZ	573	HIS
59	BZ	641	GLN
59	BZ	675	HIS
59	BZ	677	GLN
59	BZ	682	GLN
3	CC	67	HIS
3	CC	189	ASN
3	CC	200	HIS
4	CD	87	ASN
4	CD	96	HIS
4	CD	164	GLN
4	CD	253	GLN
6	CF	69	HIS
6	CF	75	HIS
6	CF	169	ASN
6	CF	203	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	CG	40	ASN
10	CL	116	ASN
11	CN	133	GLN
13	CP	38	GLN
14	CQ	45	GLN
15	CR	13	HIS
15	CR	31	HIS
16	CS	95	HIS
18	CU	104	GLN
18	CU	117	GLN
20	CW	60	ASN
21	CX	31	HIS
23	CZ	132	ASN
33	C9	36	GLN
35	DB	16	HIS
35	DB	45	GLN
35	DB	76	GLN
35	DB	94	ASN
36	DC	3	ASN
36	DC	28	GLN
36	DC	37	GLN
36	DC	104	GLN
36	DC	123	GLN
37	DD	123	HIS
37	DD	125	HIS
37	DD	160	GLN
39	DF	7	ASN
39	DF	27	GLN
39	DF	94	GLN
39	DF	100	ASN
40	DG	28	ASN
40	DG	51	GLN
40	DG	96	GLN
40	DG	97	GLN
40	DG	110	GLN
41	DH	15	ASN
42	DI	31	GLN
42	DI	58	HIS
42	DI	73	GLN
42	DI	89	ASN
42	DI	124	GLN
43	DJ	13	HIS

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Mol	Chain	Res	Type
43	DJ	21	GLN
43	DJ	62	HIS
43	DJ	68	HIS
44	DK	93	GLN
45	DL	49	ASN
45	DL	78	GLN
45	DL	99	HIS
46	DM	40	ASN
46	DM	92	HIS
48	DO	28	GLN
50	DQ	16	GLN
52	DS	23	ASN
52	DS	69	HIS
52	DS	83	HIS
53	DT	75	ASN
59	DZ	-50	GLN
59	DZ	7	ASN
59	DZ	117	GLN
59	DZ	165	GLN
59	DZ	270	GLN
59	DZ	302	HIS
59	DZ	421	GLN
59	DZ	509	HIS
59	DZ	630	GLN
59	DZ	641	GLN
59	DZ	664	GLN
59	DZ	677	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2866/2915 (98%)	477 (16%)	41 (1%)
1	CA	2860/2915 (98%)	517 (18%)	37 (1%)
2	AB	119/121 (98%)	11 (9%)	0
2	CB	119/121 (98%)	19 (15%)	0
34	BA	1494/1521 (98%)	265 (17%)	21 (1%)
34	DA	1501/1521 (98%)	284 (18%)	23 (1%)
55	BV	12/24 (50%)	3 (25%)	0
55	DV	11/24 (45%)	1 (9%)	0
56	BW	70/76 (92%)	18 (25%)	1 (1%)
56	DW	67/76 (88%)	22 (32%)	2 (2%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
57	BX	74/77 (96%)	10 (13%)	0
57	DX	74/77 (96%)	13 (17%)	0
58	BY	71/76 (93%)	20 (28%)	2 (2%)
58	DY	69/76 (90%)	19 (27%)	0
All	All	9407/9620 (97%)	1679 (17%)	127 (1%)

All (1679) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	12	U
1	AA	13	A
1	AA	34	C
1	AA	45	C
1	AA	62	U
1	AA	70	A
1	AA	71	U
1	AA	73	A
1	AA	74	G
1	AA	83	A
1	AA	91	G
1	AA	94	G
1	AA	99	G
1	AA	116	A
1	AA	117	A
1	AA	118	U
1	AA	120	G
1	AA	137	G
1	AA	149	A
1	AA	185	A
1	AA	186	A
1	AA	188	A
1	AA	189	U
1	AA	190	C
1	AA	194	G
1	AA	203	G
1	AA	204	G
1	AA	205	A
1	AA	210	A
1	AA	211	A
1	AA	217	A
1	AA	218	A
1	AA	222	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	AA	237	G
1	AA	239	G
1	AA	262	C
1	AA	269	G
1	AA	271	U
1	AA	272	U
1	AA	273	G
1	AA	274	U
1	AA	276	C
1	AA	279	G
1	AA	289	G
1	AA	299	G
1	AA	303	C
1	AA	311	C
1	AA	335	A
1	AA	348	A
1	AA	353	G
1	AA	354	A
1	AA	376	G
1	AA	387	G
1	AA	407	U
1	AA	413	G
1	AA	423	G
1	AA	434	G
1	AA	438	G
1	AA	439	A
1	AA	455	A
1	AA	469	A
1	AA	470	C
1	AA	474	U
1	AA	477	C
1	AA	482	C
1	AA	483	A
1	AA	496	A
1	AA	501	U
1	AA	505	A
1	AA	507	G
1	AA	519	G
1	AA	529	U
1	AA	530	A
1	AA	534	C
1	AA	551	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	AA	553	A
1	AA	555	G
1	AA	556	C
1	AA	557	A
1	AA	558	G
1	AA	569	G
1	AA	573	G
1	AA	574	G
1	AA	586	G
1	AA	596	G
1	AA	598	A
1	AA	609	A
1	AA	616	G
1	AA	626	A
1	AA	627	G
1	AA	630	U
1	AA	633	G
1	AA	639	G
1	AA	641	G
1	AA	644	G
1	AA	659	C
1	AA	662	A
1	AA	670	C
1	AA	671	A
1	AA	692	C
1	AA	693	G
1	AA	697	C
1	AA	716	G
1	AA	717	A
1	AA	733	G
1	AA	762	G
1	AA	777	C
1	AA	785	G
1	AA	787	U
1	AA	793	A
1	AA	794	U
1	AA	811	A
1	AA	812	G
1	AA	822	G
1	AA	823	G
1	AA	829	A
1	AA	831	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	AA	832	G
1	AA	837	C
1	AA	839	G
1	AA	852	G
1	AA	859	C
1	AA	866	A
1	AA	867	A
1	AA	874	U
1	AA	875	U
1	AA	877	G
1	AA	888	A
1	AA	906	G
1	AA	924	U
1	AA	927	G
1	AA	931	C
1	AA	932	C
1	AA	933	C
1	AA	934	A
1	AA	935	C
1	AA	936	C
1	AA	937	A
1	AA	938	G
1	AA	939	C
1	AA	940	C
1	AA	942	A
1	AA	943	C
1	AA	945	A
1	AA	946	A
1	AA	953	U
1	AA	956	A
1	AA	957	A
1	AA	960	C
1	AA	972	A
1	AA	977	G
1	AA	986	A
1	AA	990	A
1	AA	991	G
1	AA	1003	U
1	AA	1004	A
1	AA	1006	C
1	AA	1019	G
1	AA	1020	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	AA	1029	A
1	AA	1036	A
1	AA	1042	A
1	AA	1051	C
1	AA	1054	C
1	AA	1058	U
1	AA	1059	C
1	AA	1068	G
1	AA	1072	U
1	AA	1077	G
1	AA	1079	U
1	AA	1084	C
1	AA	1092	A
1	AA	1093	G
1	AA	1096	A
1	AA	1099	C
1	AA	1100	A
1	AA	1101	G
1	AA	1105	G
1	AA	1106	U
1	AA	1107	U
1	AA	1108	G
1	AA	1111	U
1	AA	1112	U
1	AA	1116	A
1	AA	1121	C
1	AA	1122	C
1	AA	1125	C
1	AA	1126	C
1	AA	1129	U
1	AA	1134	A
1	AA	1136	U
1	AA	1139	G
1	AA	1154	U
1	AA	1155	C
1	AA	1156	G
1	AA	1174	A
1	AA	1180	C
1	AA	1181	G
1	AA	1184	G
1	AA	1196	C
1	AA	1197	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	AA	1210	G
1	AA	1217	G
1	AA	1218	G
1	AA	1219	A
1	AA	1220	U
1	AA	1221	G
1	AA	1222	A
1	AA	1223	C
1	AA	1255	A
1	AA	1256	U
1	AA	1265	A
1	AA	1287	A
1	AA	1290	G
1	AA	1294	G
1	AA	1299	A
1	AA	1302	G
1	AA	1317	G
1	AA	1318	A
1	AA	1322	A
1	AA	1346	U
1	AA	1347	A
1	AA	1349	G
1	AA	1367	A
1	AA	1391	C
1	AA	1405	A
1	AA	1406	A
1	AA	1411	A
1	AA	1425	A
1	AA	1430	A
1	AA	1431	G
1	AA	1462	G
1	AA	1463	C
1	AA	1466	U
1	AA	1467	G
1	AA	1468	G
1	AA	1473	A
1	AA	1474	C
1	AA	1491	A
1	AA	1496	A
1	AA	1497	G
1	AA	1500	A
1	AA	1502	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	AA	1508	G
1	AA	1514	C
1	AA	1518	A
1	AA	1525	G
1	AA	1529	G
1	AA	1539	C
1	AA	1554	A
1	AA	1555	C
1	AA	1556	A
1	AA	1578	C
1	AA	1587	U
1	AA	1589	A
1	AA	1590	C
1	AA	1605	A
1	AA	1607	G
1	AA	1613	A
1	AA	1616	A
1	AA	1625	U
1	AA	1627	A
1	AA	1628	G
1	AA	1630	A
1	AA	1631	C
1	AA	1632	A
1	AA	1654	A
1	AA	1655	A
1	AA	1656	A
1	AA	1695	C
1	AA	1721	G
1	AA	1743	G
1	AA	1747	A
1	AA	1764	G
1	AA	1767	A
1	AA	1776	G
1	AA	1787	G
1	AA	1788	U
1	AA	1793	A
1	AA	1794	G
1	AA	1795	G
1	AA	1804	A
1	AA	1811	A
1	AA	1813	C
1	AA	1822	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	AA	1831	C
1	AA	1833	A
1	AA	1847	G
1	AA	1850	A
1	AA	1870	G
1	AA	1878	A
1	AA	1889	G
1	AA	1890	A
1	AA	1892	G
1	AA	1898	A
1	AA	1900	G
1	AA	1911	A
1	AA	1922	A
1	AA	1928	G
1	AA	1935	A
1	AA	1941	A
1	AA	1951	G
1	AA	1952	G
1	AA	1953	U
1	AA	1956	C
1	AA	1960	A
1	AA	1977	U
1	AA	1985	U
1	AA	1987	C
1	AA	1989	C
1	AA	1992	A
1	AA	1993	A
1	AA	1994	A
1	AA	2003	A
1	AA	2014	G
1	AA	2015	U
1	AA	2019	G
1	AA	2028	C
1	AA	2042	A
1	AA	2045	G
1	AA	2053	A
1	AA	2055	A
1	AA	2065	C
1	AA	2073	A
1	AA	2077	C
1	AA	2078	G
1	AA	2082	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	AA	2083	G
1	AA	2084	A
1	AA	2091	G
1	AA	2123	G
1	AA	2132	G
1	AA	2133	C
1	AA	2141	A
1	AA	2143	G
1	AA	2144	U
1	AA	2149	G
1	AA	2152	U
1	AA	2153	G
1	AA	2154	U
1	AA	2155	G
1	AA	2156	A
1	AA	2157	A
1	AA	2158	C
1	AA	2159	C
1	AA	2160	C
1	AA	2162	C
1	AA	2163	G
1	AA	2164	C
1	AA	2165	C
1	AA	2169	G
1	AA	2173	G
1	AA	2175	G
1	AA	2179	G
1	AA	2180	A
1	AA	2181	G
1	AA	2182	G
1	AA	2188	G
1	AA	2190	G
1	AA	2191	A
1	AA	2194	U
1	AA	2195	A
1	AA	2196	C
1	AA	2198	A
1	AA	2199	C
1	AA	2200	C
1	AA	2203	G
1	AA	2204	G
1	AA	2205	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	AA	2206	G
1	AA	2210	C
1	AA	2211	U
1	AA	2213	G
1	AA	2214	G
1	AA	2220	A
1	AA	2221	A
1	AA	2227	G
1	AA	2228	G
1	AA	2229	A
1	AA	2237	A
1	AA	2251	G
1	AA	2252	C
1	AA	2280	A
1	AA	2285	A
1	AA	2287	C
1	AA	2295	C
1	AA	2298	A
1	AA	2299	A
1	AA	2317	A
1	AA	2319	G
1	AA	2320	G
1	AA	2324	U
1	AA	2332	A
1	AA	2337	G
1	AA	2346	G
1	AA	2348	A
1	AA	2352	G
1	AA	2359	C
1	AA	2362	C
1	AA	2366	G
1	AA	2373	A
1	AA	2391	G
1	AA	2395	G
1	AA	2397	C
1	AA	2418	U
1	AA	2426	G
1	AA	2436	C
1	AA	2437	A
1	AA	2441	G
1	AA	2442	A
1	AA	2443	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	AA	2446	A
1	AA	2447	A
1	AA	2451	A
1	AA	2452	C
1	AA	2453	C
1	AA	2459	G
1	AA	2460	A
1	AA	2461	U
1	AA	2471	A
1	AA	2488	A
1	AA	2490	A
1	AA	2506	G
1	AA	2514	G
1	AA	2517	G
1	AA	2530	A
1	AA	2541	G
1	AA	2566	U
1	AA	2567	U
1	AA	2578	A
1	AA	2579	G
1	AA	2585	C
1	AA	2594	G
1	AA	2614	A
1	AA	2621	U
1	AA	2623	U
1	AA	2624	C
1	AA	2640	C
1	AA	2641	A
1	AA	2642	G
1	AA	2644	A
1	AA	2653	G
1	AA	2658	C
1	AA	2666	A
1	AA	2675	G
1	AA	2701	U
1	AA	2702	C
1	AA	2714	U
1	AA	2715	C
1	AA	2725	A
1	AA	2726	A
1	AA	2727	G
1	AA	2739	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	AA	2740	G
1	AA	2746	A
1	AA	2752	U
1	AA	2768	C
1	AA	2771	A
1	AA	2774	G
1	AA	2778	A
1	AA	2779	G
1	AA	2791	A
1	AA	2803	A
1	AA	2804	C
1	AA	2813	G
1	AA	2828	G
1	AA	2830	A
1	AA	2831	A
1	AA	2843	G
1	AA	2845	A
1	AA	2847	G
1	AA	2871	G
1	AA	2882	G
1	AA	2883	A
1	AA	2890	C
1	AA	2902	G
1	AA	2903	G
2	AB	2	C
2	AB	9	G
2	AB	12	C
2	AB	21	G
2	AB	45	A
2	AB	47	C
2	AB	56	G
2	AB	67	G
2	AB	73	A
2	AB	110	G
2	AB	116	G
34	BA	5	U
34	BA	7	G
34	BA	9	G
34	BA	29	G
34	BA	30	U
34	BA	32	A
34	BA	39	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	BA	47	C
34	BA	48	C
34	BA	50	A
34	BA	51	A
34	BA	58	C
34	BA	61	G
34	BA	69	G
34	BA	77	G
34	BA	79	G
34	BA	91	C
34	BA	97	G
34	BA	101	A
34	BA	115	G
34	BA	116	A
34	BA	121	C
34	BA	129(A)	G
34	BA	131	C
34	BA	139	G
34	BA	161	A
34	BA	163	C
34	BA	174	C
34	BA	182	U
34	BA	189(D)	C
34	BA	189(F)	U
34	BA	195	A
34	BA	197	A
34	BA	199	G
34	BA	202	U
34	BA	204	U
34	BA	216	G
34	BA	222	U
34	BA	247	G
34	BA	251	G
34	BA	266	G
34	BA	267	C
34	BA	289	G
34	BA	301	G
34	BA	321	A
34	BA	328	C
34	BA	332	G
34	BA	342	C
34	BA	343	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	BA	346	G
34	BA	347	G
34	BA	348	G
34	BA	351	G
34	BA	352	C
34	BA	353	A
34	BA	354	G
34	BA	355	C
34	BA	365	U
34	BA	367	U
34	BA	372	C
34	BA	373	A
34	BA	383	A
34	BA	384	G
34	BA	388	G
34	BA	397	A
34	BA	398	C
34	BA	406	G
34	BA	412	A
34	BA	413	G
34	BA	424	G
34	BA	429	U
34	BA	439	A
34	BA	442	C
34	BA	452	A
34	BA	470	C
34	BA	485	G
34	BA	496	A
34	BA	498	U
34	BA	505	G
34	BA	509	A
34	BA	510	A
34	BA	511	C
34	BA	513	C
34	BA	518	C
34	BA	524	G
34	BA	527	G
34	BA	531	U
34	BA	532	A
34	BA	533	A
34	BA	536	C
34	BA	547	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	BA	559	A
34	BA	561	U
34	BA	572	A
34	BA	573	A
34	BA	576	G
34	BA	577	G
34	BA	596	C
34	BA	607	A
34	BA	616	G
34	BA	618	C
34	BA	630	G
34	BA	631	G
34	BA	632	A
34	BA	634	C
34	BA	653	A
34	BA	661	G
34	BA	665	A
34	BA	666	G
34	BA	667	G
34	BA	671	G
34	BA	673	G
34	BA	687	A
34	BA	688	G
34	BA	695	A
34	BA	723	U
34	BA	724	G
34	BA	728	A
34	BA	731	G
34	BA	749	C
34	BA	755	G
34	BA	765	G
34	BA	786	G
34	BA	788	U
34	BA	792	A
34	BA	793	U
34	BA	794	A
34	BA	815	A
34	BA	817	C
34	BA	828	A
34	BA	832	C
34	BA	840	C
34	BA	841	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	BA	848	C
34	BA	851	G
34	BA	859	A
34	BA	860	A
34	BA	874	G
34	BA	875	C
34	BA	876	G
34	BA	902	G
34	BA	908	A
34	BA	914	A
34	BA	926	G
34	BA	927	G
34	BA	932	C
34	BA	934	C
34	BA	935	A
34	BA	942	G
34	BA	960	U
34	BA	961	U
34	BA	968	A
34	BA	969	A
34	BA	971	G
34	BA	972	C
34	BA	974	A
34	BA	975	A
34	BA	976	G
34	BA	977	A
34	BA	982	U
34	BA	992	U
34	BA	993	G
34	BA	1000	U
34	BA	1003	G
34	BA	1004	A
34	BA	1005	A
34	BA	1008	C
34	BA	1009	G
34	BA	1016	A
34	BA	1019	C
34	BA	1022	G
34	BA	1023	G
34	BA	1025	U
34	BA	1027	C
34	BA	1028	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	BA	1030	C
34	BA	1030(A)	G
34	BA	1030(C)	G
34	BA	1031	G
34	BA	1033	G
34	BA	1045	C
34	BA	1054	C
34	BA	1065	U
34	BA	1066	C
34	BA	1068	G
34	BA	1070	U
34	BA	1081	G
34	BA	1094	G
34	BA	1095	U
34	BA	1101	A
34	BA	1108	G
34	BA	1123	A
34	BA	1124	G
34	BA	1125	U
34	BA	1126	U
34	BA	1134	G
34	BA	1136	U
34	BA	1137	C
34	BA	1138	G
34	BA	1139	G
34	BA	1140	C
34	BA	1141	C
34	BA	1145	C
34	BA	1146	A
34	BA	1152	A
34	BA	1159	U
34	BA	1166	G
34	BA	1183	A
34	BA	1184	G
34	BA	1187	G
34	BA	1189	C
34	BA	1196	U
34	BA	1197	G
34	BA	1202	G
34	BA	1212	U
34	BA	1213	A
34	BA	1227	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	BA	1236	A
34	BA	1238	A
34	BA	1240	U
34	BA	1253	G
34	BA	1256	A
34	BA	1257	U
34	BA	1258	G
34	BA	1260	C
34	BA	1270	C
34	BA	1273	G
34	BA	1278	U
34	BA	1279	A
34	BA	1280	A
34	BA	1286	A
34	BA	1287	A
34	BA	1299	A
34	BA	1300	G
34	BA	1302	U
34	BA	1321	C
34	BA	1335	C
34	BA	1336	C
34	BA	1338	G
34	BA	1340	A
34	BA	1347	G
34	BA	1353	G
34	BA	1359	C
34	BA	1360	A
34	BA	1363	C
34	BA	1364	U
34	BA	1370	G
34	BA	1397	C
34	BA	1419	G
34	BA	1442	G
34	BA	1442(A)	G
34	BA	1447	A
34	BA	1452	C
34	BA	1492	A
34	BA	1494	G
34	BA	1502	A
34	BA	1503	A
34	BA	1504	G
34	BA	1506	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	BA	1516	G
34	BA	1517	G
34	BA	1519	A
34	BA	1529	G
34	BA	1530	G
34	BA	1531	A
55	BV	13	A
55	BV	23	A
55	BV	24	A
56	BW	3	C
56	BW	8	4SU
56	BW	9	A
56	BW	13	C
56	BW	14	A
56	BW	19	G
56	BW	20	U
56	BW	21	A
56	BW	24	G
56	BW	45	U
56	BW	46	7MG
56	BW	47	U
56	BW	48	C
56	BW	49	C
56	BW	64	A
56	BW	68	C
56	BW	73	A
56	BW	74	C
57	BX	13	C
57	BX	19	G
57	BX	21	A
57	BX	34	C
57	BX	42	G
57	BX	47	U
57	BX	49	G
57	BX	56	C
57	BX	58	A
57	BX	68	C
58	BY	5	G
58	BY	6	G
58	BY	9	A
58	BY	13	C
58	BY	14	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
58	BY	20	U
58	BY	21	A
58	BY	26	A
58	BY	36	A
58	BY	41	C
58	BY	42	C
58	BY	44	G
58	BY	45	U
58	BY	46	7MG
58	BY	47	U
58	BY	48	C
58	BY	57	G
58	BY	59	U
58	BY	60	U
58	BY	68	C
1	CA	12	U
1	CA	13	A
1	CA	34	C
1	CA	36	G
1	CA	41	C
1	CA	45	C
1	CA	64	A
1	CA	71	A
1	CA	74	A
1	CA	75	G
1	CA	84	A
1	CA	90	U
1	CA	95	G
1	CA	100	G
1	CA	102	G
1	CA	118	A
1	CA	119	A
1	CA	120	U
1	CA	141	A
1	CA	154(A)	C
1	CA	157	U
1	CA	173	G
1	CA	196	A
1	CA	205	G
1	CA	214	G
1	CA	215	G
1	CA	216	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	CA	221	A
1	CA	222	A
1	CA	225	A
1	CA	228	A
1	CA	229	A
1	CA	248	G
1	CA	250	G
1	CA	271(I)	G
1	CA	271(K)	U
1	CA	271(L)	U
1	CA	271(M)	G
1	CA	271(N)	U
1	CA	271(O)	C
1	CA	272(A)	U
1	CA	272(B)	G
1	CA	277	C
1	CA	278	A
1	CA	283	A
1	CA	294	A
1	CA	299	A
1	CA	304	G
1	CA	311	A
1	CA	329	G
1	CA	330	A
1	CA	338	G
1	CA	342	G
1	CA	345	A
1	CA	352	G
1	CA	357	A
1	CA	362	U
1	CA	363	G
1	CA	363(B)	G
1	CA	363(C)	G
1	CA	363(F)	A
1	CA	386	G
1	CA	395	U
1	CA	407	G
1	CA	411	G
1	CA	412	A
1	CA	422	A
1	CA	428	A
1	CA	443	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	CA	444	C
1	CA	455	C
1	CA	456	C
1	CA	457	A
1	CA	470	A
1	CA	471	A
1	CA	481	G
1	CA	501	A
1	CA	504	U
1	CA	505	A
1	CA	509	C
1	CA	528	A
1	CA	529	A
1	CA	530	G
1	CA	531	C
1	CA	532	A
1	CA	533	G
1	CA	545	G
1	CA	563	G
1	CA	573	G
1	CA	575	A
1	CA	586	A
1	CA	587	C
1	CA	588	U
1	CA	599	G
1	CA	603	A
1	CA	604	G
1	CA	606	U
1	CA	607	U
1	CA	614(B)	G
1	CA	614(C)	A
1	CA	615	G
1	CA	616	G
1	CA	627	A
1	CA	631	A
1	CA	637	A
1	CA	645	C
1	CA	646	A
1	CA	652(A)	A
1	CA	652(B)	A
1	CA	652(C)	G
1	CA	652(U)	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	CA	668	G
1	CA	669	G
1	CA	686	G
1	CA	709	U
1	CA	730	C
1	CA	752	A
1	CA	753	C
1	CA	764	A
1	CA	765	G
1	CA	774	A
1	CA	775	G
1	CA	776	G
1	CA	782	A
1	CA	784	A
1	CA	785	G
1	CA	790	C
1	CA	792	G
1	CA	805	G
1	CA	812	C
1	CA	819	A
1	CA	827	U
1	CA	828	U
1	CA	857	C
1	CA	859	G
1	CA	866	A
1	CA	879	G
1	CA	880	G
1	CA	884	C
1	CA	886	C
1	CA	887	A
1	CA	888	C
1	CA	889	C
1	CA	890	A
1	CA	893	C
1	CA	896	A
1	CA	897	C
1	CA	898	C
1	CA	900	A
1	CA	901	A
1	CA	902	C
1	CA	910	A
1	CA	917	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	CA	931	G
1	CA	932	G
1	CA	938	G
1	CA	941	A
1	CA	945	A
1	CA	946	G
1	CA	958	U
1	CA	959	A
1	CA	961	C
1	CA	968	G
1	CA	974	G
1	CA	975	C
1	CA	983	A
1	CA	996	A
1	CA	1002	G
1	CA	1005	C
1	CA	1012	U
1	CA	1013	C
1	CA	1016	G
1	CA	1022	G
1	CA	1033	U
1	CA	1036	G
1	CA	1038	C
1	CA	1039	G
1	CA	1042	G
1	CA	1046	A
1	CA	1047	G
1	CA	1048	A
1	CA	1053	C
1	CA	1054	A
1	CA	1055	G
1	CA	1058	G
1	CA	1059	G
1	CA	1060	U
1	CA	1061	U
1	CA	1062	G
1	CA	1063	G
1	CA	1064	C
1	CA	1069	A
1	CA	1070	A
1	CA	1073	A
1	CA	1076	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	CA	1081	U
1	CA	1083	U
1	CA	1088	A
1	CA	1090	U
1	CA	1100	C
1	CA	1101	U
1	CA	1107	G
1	CA	1109	C
1	CA	1110	G
1	CA	1111	A
1	CA	1112	G
1	CA	1113	U
1	CA	1116	C
1	CA	1119	C
1	CA	1128	A
1	CA	1135	C
1	CA	1136	G
1	CA	1139	G
1	CA	1151	G
1	CA	1155	A
1	CA	1204	A
1	CA	1210	A
1	CA	1211	U
1	CA	1220	A
1	CA	1241	A
1	CA	1252	G
1	CA	1253	A
1	CA	1256	G
1	CA	1271	G
1	CA	1272	A
1	CA	1273	U
1	CA	1287	A
1	CA	1300	U
1	CA	1301	A
1	CA	1308	A
1	CA	1314	C
1	CA	1327	C
1	CA	1342	A
1	CA	1359	A
1	CA	1360	A
1	CA	1365	A
1	CA	1368	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	CA	1370	C
1	CA	1379	A
1	CA	1384	A
1	CA	1385	G
1	CA	1386	C
1	CA	1395	A
1	CA	1416	G
1	CA	1417	C
1	CA	1419	A
1	CA	1420	U
1	CA	1421	G
1	CA	1427	A
1	CA	1428	C
1	CA	1436	G
1	CA	1437	C
1	CA	1445	A
1	CA	1449	A
1	CA	1450	G
1	CA	1455	G
1	CA	1459	G
1	CA	1465	G
1	CA	1467	C
1	CA	1471	A
1	CA	1482	G
1	CA	1490	A
1	CA	1493	C
1	CA	1494	A
1	CA	1496	A
1	CA	1497	U
1	CA	1509	C
1	CA	1509(A)	A
1	CA	1525	G
1	CA	1531	C
1	CA	1532	C
1	CA	1533	G
1	CA	1542	A
1	CA	1547	C
1	CA	1554	A
1	CA	1558	A
1	CA	1559	G
1	CA	1560	G
1	CA	1566	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	CA	1569	A
1	CA	1578	U
1	CA	1582	C
1	CA	1584	C
1	CA	1586	A
1	CA	1608	A
1	CA	1609	A
1	CA	1616	A
1	CA	1648	C
1	CA	1654	A
1	CA	1674	G
1	CA	1676	A
1	CA	1696	G
1	CA	1700	A
1	CA	1701	A
1	CA	1703	G
1	CA	1722	A
1	CA	1739	U
1	CA	1756	G
1	CA	1763	G
1	CA	1764	G
1	CA	1773	A
1	CA	1780	A
1	CA	1791	A
1	CA	1800	C
1	CA	1801	G
1	CA	1812	A
1	CA	1816	G
1	CA	1829	A
1	CA	1835	G
1	CA	1847	A
1	CA	1848	A
1	CA	1866	C
1	CA	1877	A
1	CA	1878	G
1	CA	1883	G
1	CA	1889	A
1	CA	1900	A
1	CA	1906	G
1	CA	1913	A
1	CA	1914	C
1	CA	1929	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	CA	1930	G
1	CA	1934	C
1	CA	1952	A
1	CA	1955	U
1	CA	1963	U
1	CA	1967	C
1	CA	1970	A
1	CA	1971	A
1	CA	1972	A
1	CA	1983	C
1	CA	1992	G
1	CA	1993	U
1	CA	1997	G
1	CA	2005	A
1	CA	2020	A
1	CA	2023	G
1	CA	2031	A
1	CA	2032	G
1	CA	2033	A
1	CA	2038	G
1	CA	2043	C
1	CA	2046	G
1	CA	2055	C
1	CA	2056	G
1	CA	2060	A
1	CA	2061	G
1	CA	2062	A
1	CA	2063	C
1	CA	2069	G
1	CA	2082	A
1	CA	2096	U
1	CA	2102	U
1	CA	2106	G
1	CA	2110	G
1	CA	2111	C
1	CA	2112	G
1	CA	2113	U
1	CA	2115	G
1	CA	2116	G
1	CA	2117	A
1	CA	2119	A
1	CA	2122	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	CA	2124	G
1	CA	2126	A
1	CA	2127	G
1	CA	2130	U
1	CA	2131	G
1	CA	2132	U
1	CA	2133	G
1	CA	2134	A
1	CA	2135	A
1	CA	2136	C
1	CA	2137	C
1	CA	2142	C
1	CA	2144	U
1	CA	2146	C
1	CA	2148	G
1	CA	2150	U
1	CA	2153	G
1	CA	2154	G
1	CA	2157	G
1	CA	2158	A
1	CA	2161	C
1	CA	2162	G
1	CA	2164	C
1	CA	2165	G
1	CA	2166	G
1	CA	2167	U
1	CA	2168	G
1	CA	2169	A
1	CA	2170	A
1	CA	2172	U
1	CA	2173	A
1	CA	2178	C
1	CA	2181	G
1	CA	2185	C
1	CA	2186	G
1	CA	2188	C
1	CA	2189	U
1	CA	2192	G
1	CA	2198	A
1	CA	2206	G
1	CA	2207	G
1	CA	2208	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	CA	2218	U
1	CA	2225	A
1	CA	2238	G
1	CA	2239	G
1	CA	2240	C
1	CA	2248	C
1	CA	2268	A
1	CA	2269	A
1	CA	2275	C
1	CA	2278	A
1	CA	2279	G
1	CA	2283	C
1	CA	2287	A
1	CA	2289	G
1	CA	2294	C
1	CA	2305	A
1	CA	2308	G
1	CA	2312	U
1	CA	2319	G
1	CA	2320	A
1	CA	2321	G
1	CA	2325	G
1	CA	2334	G
1	CA	2336	A
1	CA	2343	C
1	CA	2347	C
1	CA	2350	C
1	CA	2354	G
1	CA	2376	A
1	CA	2383	G
1	CA	2385	C
1	CA	2406	U
1	CA	2410	G
1	CA	2423	U
1	CA	2424	C
1	CA	2425	A
1	CA	2428	G
1	CA	2429	G
1	CA	2430	A
1	CA	2435	A
1	CA	2439	A
1	CA	2440	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	CA	2441	C
1	CA	2448	A
1	CA	2452	C
1	CA	2474	C
1	CA	2476	A
1	CA	2491	U
1	CA	2492	U
1	CA	2494	G
1	CA	2498	C
1	CA	2502	G
1	CA	2505	G
1	CA	2506	U
1	CA	2518	A
1	CA	2520	C
1	CA	2529	G
1	CA	2554	U
1	CA	2564	A
1	CA	2566	A
1	CA	2567	G
1	CA	2573	C
1	CA	2582	G
1	CA	2602	A
1	CA	2611	U
1	CA	2612	C
1	CA	2629	A
1	CA	2630	G
1	CA	2632	A
1	CA	2636	U
1	CA	2654	A
1	CA	2663	G
1	CA	2669	G
1	CA	2673	G
1	CA	2689	U
1	CA	2690	C
1	CA	2703	C
1	CA	2712(A)	A
1	CA	2713	A
1	CA	2718	G
1	CA	2721	A
1	CA	2726	U
1	CA	2733	A
1	CA	2739	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	CA	2744	G
1	CA	2748	A
1	CA	2751	G
1	CA	2757	A
1	CA	2758	A
1	CA	2761	G
1	CA	2764	A
1	CA	2765	A
1	CA	2766	G
1	CA	2778	A
1	CA	2793	G
1	CA	2794	C
1	CA	2802	G
1	CA	2808	U
1	CA	2818	G
1	CA	2820	A
1	CA	2821	A
1	CA	2833	G
1	CA	2835	A
1	CA	2839	G
1	CA	2872	G
1	CA	2876	G
1	CA	2880	C
1	CA	2892	A
1	CA	2893	G
1	CA	2894	G
1	CA	2896	C
1	CA	2897	U
2	CB	2	C
2	CB	7	G
2	CB	8	U
2	CB	12	C
2	CB	13	A
2	CB	15	A
2	CB	25	A
2	CB	28	C
2	CB	30	C
2	CB	32	C
2	CB	42	C
2	CB	52	A
2	CB	56	G
2	CB	58	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	CB	73	A
2	CB	85	G
2	CB	95	C
2	CB	106	G
2	CB	110	G
34	DA	5	U
34	DA	9	G
34	DA	22	G
34	DA	26	A
34	DA	32	A
34	DA	39	G
34	DA	47	C
34	DA	48	C
34	DA	50	A
34	DA	51	A
34	DA	60	A
34	DA	61	G
34	DA	65	U
34	DA	66	G
34	DA	73	G
34	DA	80	G
34	DA	88	A
34	DA	89	C
34	DA	97	G
34	DA	98	G
34	DA	101	A
34	DA	116	A
34	DA	121	C
34	DA	122	G
34	DA	129(A)	G
34	DA	131	C
34	DA	144	G
34	DA	151	A
34	DA	163	C
34	DA	180	U
34	DA	182	U
34	DA	189(E)	U
34	DA	189(F)	U
34	DA	189(K)	U
34	DA	195	A
34	DA	197	A
34	DA	201	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	DA	203	U
34	DA	204	U
34	DA	216	G
34	DA	221	C
34	DA	231	G
34	DA	247	G
34	DA	251	G
34	DA	258	G
34	DA	266	G
34	DA	267	C
34	DA	269	C
34	DA	281	G
34	DA	289	G
34	DA	301	G
34	DA	317	G
34	DA	321	A
34	DA	328	C
34	DA	332	G
34	DA	344	A
34	DA	352	C
34	DA	353	A
34	DA	354	G
34	DA	355	C
34	DA	367	U
34	DA	372	C
34	DA	373	A
34	DA	384	G
34	DA	398	C
34	DA	406	G
34	DA	410	G
34	DA	412	A
34	DA	413	G
34	DA	423	G
34	DA	424	G
34	DA	429	U
34	DA	430	A
34	DA	439	A
34	DA	442	C
34	DA	452	A
34	DA	461	A
34	DA	485	G
34	DA	496	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	DA	498	U
34	DA	505	G
34	DA	509	A
34	DA	510	A
34	DA	511	C
34	DA	513	C
34	DA	518	C
34	DA	527	G
34	DA	531	U
34	DA	532	A
34	DA	533	A
34	DA	547	A
34	DA	559	A
34	DA	561	U
34	DA	563	A
34	DA	564	C
34	DA	571	U
34	DA	572	A
34	DA	573	A
34	DA	576	G
34	DA	577	G
34	DA	581	G
34	DA	596	C
34	DA	601	C
34	DA	607	A
34	DA	620	C
34	DA	630	G
34	DA	632	A
34	DA	651	C
34	DA	653	A
34	DA	654	G
34	DA	665	A
34	DA	671	G
34	DA	687	A
34	DA	688	G
34	DA	695	A
34	DA	703	G
34	DA	720	C
34	DA	723	U
34	DA	724	G
34	DA	731	G
34	DA	749	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	DA	753	A
34	DA	755	G
34	DA	777	A
34	DA	792	A
34	DA	793	U
34	DA	794	A
34	DA	802	A
34	DA	817	C
34	DA	819	A
34	DA	821	G
34	DA	828	A
34	DA	829	G
34	DA	833	U
34	DA	836	G
34	DA	840	C
34	DA	841	U
34	DA	848	C
34	DA	851	G
34	DA	853	G
34	DA	859	A
34	DA	874	G
34	DA	902	G
34	DA	914	A
34	DA	916	G
34	DA	922	G
34	DA	926	G
34	DA	927	G
34	DA	934	C
34	DA	935	A
34	DA	960	U
34	DA	961	U
34	DA	968	A
34	DA	969	A
34	DA	971	G
34	DA	972	C
34	DA	974	A
34	DA	975	A
34	DA	976	G
34	DA	977	A
34	DA	984	C
34	DA	989	C
34	DA	991	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	DA	992	U
34	DA	993	G
34	DA	999	C
34	DA	1002	G
34	DA	1003	G
34	DA	1005	A
34	DA	1006	C
34	DA	1017	G
34	DA	1022	G
34	DA	1023	G
34	DA	1024	G
34	DA	1025	U
34	DA	1026	G
34	DA	1027	C
34	DA	1028	C
34	DA	1030	C
34	DA	1030(A)	G
34	DA	1030(B)	C
34	DA	1030(C)	G
34	DA	1038	C
34	DA	1041	A
34	DA	1046	A
34	DA	1052	U
34	DA	1054	C
34	DA	1065	U
34	DA	1066	C
34	DA	1081	G
34	DA	1089	G
34	DA	1094	G
34	DA	1095	U
34	DA	1100	C
34	DA	1101	A
34	DA	1117	G
34	DA	1121	U
34	DA	1122	U
34	DA	1124	G
34	DA	1125	U
34	DA	1129	C
34	DA	1130	A
34	DA	1136	U
34	DA	1137	C
34	DA	1138	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	DA	1139	G
34	DA	1146	A
34	DA	1152	A
34	DA	1154	G
34	DA	1157	A
34	DA	1159	U
34	DA	1166	G
34	DA	1181	G
34	DA	1183	A
34	DA	1184	G
34	DA	1196	U
34	DA	1202	G
34	DA	1211	U
34	DA	1212	U
34	DA	1213	A
34	DA	1220	G
34	DA	1227	A
34	DA	1228	C
34	DA	1238	A
34	DA	1240	U
34	DA	1241	G
34	DA	1253	G
34	DA	1254	C
34	DA	1256	A
34	DA	1257	U
34	DA	1258	G
34	DA	1260	C
34	DA	1273	G
34	DA	1275	A
34	DA	1278	U
34	DA	1279	A
34	DA	1280	A
34	DA	1281	U
34	DA	1282	C
34	DA	1285	A
34	DA	1287	A
34	DA	1299	A
34	DA	1300	G
34	DA	1305	G
34	DA	1317	C
34	DA	1319	A
34	DA	1322	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	DA	1338	G
34	DA	1340	A
34	DA	1346	A
34	DA	1347	G
34	DA	1353	G
34	DA	1358	U
34	DA	1360	A
34	DA	1363	C
34	DA	1368	G
34	DA	1370	G
34	DA	1379	G
34	DA	1381	U
34	DA	1397	C
34	DA	1401	G
34	DA	1419	G
34	DA	1442	G
34	DA	1442(A)	G
34	DA	1442(B)	A
34	DA	1446	U
34	DA	1447	A
34	DA	1452	C
34	DA	1456	G
34	DA	1487	G
34	DA	1492	A
34	DA	1493	A
34	DA	1494	G
34	DA	1497	G
34	DA	1502	A
34	DA	1503	A
34	DA	1504	G
34	DA	1506	U
34	DA	1517	G
34	DA	1520	G
34	DA	1529	G
34	DA	1530	G
34	DA	1531	A
34	DA	1532	U
55	DV	24	A
56	DW	3	C
56	DW	7	A
56	DW	8	4SU
56	DW	9	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
56	DW	13	C
56	DW	14	A
56	DW	15	G
56	DW	19	G
56	DW	22	G
56	DW	23	A
56	DW	46	7MG
56	DW	47	U
56	DW	48	C
56	DW	49	C
56	DW	50	U
56	DW	61	C
56	DW	62	C
56	DW	67	C
56	DW	68	C
56	DW	70	G
56	DW	73	A
56	DW	74	C
57	DX	13	C
57	DX	18	G
57	DX	19	G
57	DX	20	U
57	DX	21	A
57	DX	22	G
57	DX	30	G
57	DX	47	U
57	DX	48	C
57	DX	59	A
57	DX	61	C
57	DX	68	C
57	DX	75	C
58	DY	9	A
58	DY	13	C
58	DY	14	A
58	DY	19	G
58	DY	26	A
58	DY	34	G
58	DY	39	PSU
58	DY	45	U
58	DY	46	7MG
58	DY	47	U
58	DY	48	C

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Mol	Chain	Res	Type
58	DY	49	C
58	DY	54	5MU
58	DY	55	PSU
58	DY	57	G
58	DY	58	A
58	DY	59	U
58	DY	65	G
58	DY	70	G

All (127) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	185	A
1	AA	188	A
1	AA	271	U
1	AA	302	A
1	AA	334	A
1	AA	572	A
1	AA	641	G
1	AA	716	G
1	AA	793	A
1	AA	811	A
1	AA	821	A
1	AA	945	A
1	AA	1019	G
1	AA	1098	C
1	AA	1154	U
1	AA	1188	A
1	AA	1219	A
1	AA	1220	U
1	AA	1221	G
1	AA	1255	A
1	AA	1286	U
1	AA	1321	A
1	AA	1347	A
1	AA	1425	A
1	AA	1442	U
1	AA	1466	U
1	AA	1654	A
1	AA	1655	A
1	AA	1793	A
1	AA	2014	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	AA	2148	A
1	AA	2203	G
1	AA	2209	G
1	AA	2320	G
1	AA	2345	A
1	AA	2418	U
1	AA	2442	A
1	AA	2451	A
1	AA	2623	U
1	AA	2701	U
1	AA	2902	G
34	BA	115	G
34	BA	243	A
34	BA	266	G
34	BA	347	G
34	BA	353	A
34	BA	509	A
34	BA	560	U
34	BA	687	A
34	BA	748	C
34	BA	793	U
34	BA	839	U
34	BA	913	A
34	BA	991	U
34	BA	1065	U
34	BA	1067	A
34	BA	1165	C
34	BA	1201	A
34	BA	1285	A
34	BA	1335	C
34	BA	1442	G
34	BA	1530	G
56	BW	13	C
58	BY	19	G
58	BY	58	A
1	CA	195	A
1	CA	196	A
1	CA	249	C
1	CA	271(K)	U
1	CA	271(M)	G
1	CA	277	C
1	CA	310	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	CA	529	A
1	CA	685	A
1	CA	752	A
1	CA	764	A
1	CA	774	A
1	CA	776	G
1	CA	856	C
1	CA	900	A
1	CA	1057	A
1	CA	1063	G
1	CA	1210	A
1	CA	1301	A
1	CA	1420	U
1	CA	1427	A
1	CA	1558	A
1	CA	1608	A
1	CA	1653	G
1	CA	1913	A
1	CA	1992	G
1	CA	1997	G
1	CA	2110	G
1	CA	2126	A
1	CA	2318	G
1	CA	2406	U
1	CA	2439	A
1	CA	2581	G
1	CA	2611	U
1	CA	2689	U
1	CA	2726	U
1	CA	2756	U
34	DA	60	A
34	DA	65	U
34	DA	115	G
34	DA	243	A
34	DA	266	G
34	DA	353	A
34	DA	429	U
34	DA	509	A
34	DA	532	A
34	DA	560	U
34	DA	687	A
34	DA	748	C

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Mol	Chain	Res	Type
34	DA	793	U
34	DA	840	C
34	DA	913	A
34	DA	991	U
34	DA	992	U
34	DA	1064	G
34	DA	1065	U
34	DA	1183	A
34	DA	1201	A
34	DA	1442	G
34	DA	1492	A
56	DW	13	C
56	DW	14	A

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

40 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
57	4SU	DX	8	57	18,21,22	1.78	4 (22%)	26,30,33	2.36	4 (15%)
56	MIA	BW	37	56	24,31,32	2.33	3 (12%)	26,44,47	2.76	9 (34%)
56	PSU	BW	39	56	18,21,22	1.35	4 (22%)	22,30,33	1.96	4 (18%)
58	PSU	DY	32	58	18,21,22	1.34	2 (11%)	22,30,33	1.80	3 (13%)
56	7MG	BW	46	56	22,26,27	1.36	3 (13%)	29,39,42	2.48	7 (24%)
57	31H	BX	76	60,57	28,34,35	1.29	4 (14%)	23,47,50	1.60	3 (13%)
56	PSU	BW	55	56	18,21,22	1.41	3 (16%)	22,30,33	1.92	4 (18%)
56	PSU	BW	32	60,56	18,21,22	1.34	2 (11%)	22,30,33	1.79	3 (13%)
57	PSU	DX	55	57	18,21,22	1.37	2 (11%)	22,30,33	1.75	3 (13%)
58	4SU	DY	8	58	18,21,22	1.74	4 (22%)	26,30,33	2.31	5 (19%)
57	5MU	BX	54	60,57	19,22,23	1.54	5 (26%)	28,32,35	2.02	7 (25%)
58	4SU	BY	8	58	18,21,22	1.75	4 (22%)	26,30,33	2.16	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
58	MIA	BY	37	58	18,24,32	1.18	2 (11%)	18,35,47	1.42	3 (16%)
58	MIA	DY	37	58	18,24,32	1.07	2 (11%)	18,35,47	1.31	2 (11%)
58	PSU	BY	32	58	18,21,22	1.37	3 (16%)	22,30,33	1.76	4 (18%)
56	F3N	BW	76	56,1	30,36,37	1.37	6 (20%)	29,51,54	1.27	1 (3%)
56	4SU	DW	8	56	18,21,22	1.68	5 (27%)	26,30,33	2.14	5 (19%)
58	7MG	DY	46	58	22,26,27	1.28	4 (18%)	29,39,42	2.68	8 (27%)
57	5MU	DX	54	57	19,22,23	1.43	5 (26%)	28,32,35	2.20	8 (28%)
56	F3N	DW	76	56,1	30,36,37	1.46	6 (20%)	29,51,54	1.36	2 (6%)
57	PSU	BX	55	57	18,21,22	1.26	2 (11%)	22,30,33	1.96	4 (18%)
58	PSU	BY	39	58	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
58	PSU	DY	39	58	18,21,22	1.41	2 (11%)	22,30,33	1.84	4 (18%)
56	MIA	DW	37	56	18,24,32	1.11	2 (11%)	18,35,47	1.24	2 (11%)
58	7MG	BY	46	58	22,26,27	1.28	3 (13%)	29,39,42	2.57	7 (24%)
58	5MU	DY	54	58	19,22,23	1.44	6 (31%)	28,32,35	2.05	5 (17%)
56	PSU	DW	55	56	18,21,22	1.39	2 (11%)	22,30,33	1.83	3 (13%)
58	5MU	BY	54	58	19,22,23	1.52	5 (26%)	28,32,35	2.16	9 (32%)
57	31H	DX	76	60,57	28,34,35	1.29	4 (14%)	23,47,50	1.59	3 (13%)
56	5MU	BW	54	56	19,22,23	1.50	4 (21%)	28,32,35	2.02	8 (28%)
56	PSU	DW	39	56	18,21,22	1.27	2 (11%)	22,30,33	1.79	3 (13%)
56	7MG	DW	46	56	22,26,27	1.32	3 (13%)	29,39,42	2.45	8 (27%)
58	PSU	BY	55	58	18,21,22	1.35	2 (11%)	22,30,33	1.81	3 (13%)
56	PSU	DW	32	56	18,21,22	1.39	3 (16%)	22,30,33	1.86	3 (13%)
57	5MC	BX	32	57	18,22,23	1.12	2 (11%)	26,32,35	1.27	3 (11%)
57	4SU	BX	8	57	18,21,22	1.40	3 (16%)	26,30,33	2.20	5 (19%)
56	4SU	BW	8	56	18,21,22	1.71	4 (22%)	26,30,33	2.13	5 (19%)
56	5MU	DW	54	56	19,22,23	1.41	5 (26%)	28,32,35	2.00	8 (28%)
57	5MC	DX	32	57	18,22,23	1.10	1 (5%)	26,32,35	1.36	4 (15%)
58	PSU	DY	55	58	18,21,22	1.43	2 (11%)	22,30,33	1.89	3 (13%)

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	4SU	DX	8	57	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	MIA	BW	37	56	-	3/11/33/34	0/3/3/3
56	PSU	BW	39	56	-	0/7/25/26	0/2/2/2
58	PSU	DY	32	58	-	0/7/25/26	0/2/2/2
56	7MG	BW	46	56	-	3/7/37/38	0/3/3/3
57	31H	BX	76	60,57	-	9/18/40/41	0/3/3/3
56	PSU	BW	55	56	-	0/7/25/26	0/2/2/2
56	PSU	BW	32	60,56	-	0/7/25/26	0/2/2/2
57	PSU	DX	55	57	-	1/7/25/26	0/2/2/2
58	4SU	DY	8	58	-	1/7/25/26	0/2/2/2
57	5MU	BX	54	60,57	-	0/7/25/26	0/2/2/2
58	4SU	BY	8	58	-	1/7/25/26	0/2/2/2
58	MIA	BY	37	58	-	2/3/25/34	0/3/3/3
58	MIA	DY	37	58	-	2/3/25/34	0/3/3/3
58	PSU	BY	32	58	-	0/7/25/26	0/2/2/2
56	F3N	BW	76	56,1	-	1/15/37/38	0/4/4/4
56	4SU	DW	8	56	-	0/7/25/26	0/2/2/2
58	7MG	DY	46	58	-	3/7/37/38	0/3/3/3
57	5MU	DX	54	57	-	0/7/25/26	0/2/2/2
56	F3N	DW	76	56,1	-	0/15/37/38	0/4/4/4
57	PSU	BX	55	57	-	0/7/25/26	0/2/2/2
58	PSU	BY	39	58	-	0/7/25/26	0/2/2/2
58	PSU	DY	39	58	-	2/7/25/26	0/2/2/2
56	MIA	DW	37	56	-	0/3/25/34	0/3/3/3
58	7MG	BY	46	58	-	5/7/37/38	0/3/3/3
58	5MU	DY	54	58	-	2/7/25/26	0/2/2/2
56	PSU	DW	55	56	-	0/7/25/26	0/2/2/2
58	5MU	BY	54	58	-	1/7/25/26	0/2/2/2
57	31H	DX	76	60,57	-	9/18/40/41	0/3/3/3
56	5MU	BW	54	56	-	0/7/25/26	0/2/2/2
56	PSU	DW	39	56	-	0/7/25/26	0/2/2/2
56	7MG	DW	46	56	-	2/7/37/38	0/3/3/3
58	PSU	BY	55	58	-	1/7/25/26	0/2/2/2
56	PSU	DW	32	56	-	0/7/25/26	0/2/2/2
57	5MC	BX	32	57	-	0/7/25/26	0/2/2/2
57	4SU	BX	8	57	-	0/7/25/26	0/2/2/2
56	4SU	BW	8	56	-	0/7/25/26	0/2/2/2
56	5MU	DW	54	56	-	0/7/25/26	0/2/2/2
57	5MC	DX	32	57	-	0/7/25/26	0/2/2/2
58	PSU	DY	55	58	-	2/7/25/26	0/2/2/2



All (132) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	BW	37	MIA	C2-S10	-7.54	1.69	1.75
56	BW	37	MIA	C13-C14	7.36	1.53	1.32
57	DX	8	4SU	C4-S4	-4.62	1.59	1.68
58	BY	8	4SU	C4-S4	-4.49	1.59	1.68
58	DY	8	4SU	C4-S4	-4.41	1.60	1.68
56	BW	8	4SU	C4-S4	-4.39	1.60	1.68
56	DW	8	4SU	C4-S4	-4.28	1.60	1.68
56	DW	55	PSU	C6-C5	3.99	1.40	1.35
56	DW	76	F3N	CB-CG	-3.95	1.41	1.51
56	DW	32	PSU	C6-C5	3.77	1.39	1.35
57	BX	8	4SU	C4-S4	-3.73	1.61	1.68
57	DX	55	PSU	C6-C5	3.73	1.39	1.35
58	DY	39	PSU	C6-C5	3.70	1.39	1.35
58	BY	32	PSU	C6-C5	3.69	1.39	1.35
58	DY	32	PSU	C6-C5	3.65	1.39	1.35
56	BW	76	F3N	CB-CG	-3.64	1.42	1.51
56	BW	55	PSU	C6-C5	3.63	1.39	1.35
57	DX	32	5MC	C6-C5	3.62	1.40	1.34
56	BW	32	PSU	C6-C5	3.60	1.39	1.35
56	BW	54	5MU	C4-C5	3.57	1.50	1.44
58	BY	39	PSU	C6-C5	3.52	1.39	1.35
57	DX	8	4SU	C4-N3	-3.49	1.33	1.37
56	DW	76	F3N	O4'-C1'	3.49	1.46	1.41
56	BW	46	7MG	C4-N9	-3.48	1.33	1.37
58	BY	55	PSU	C6-C5	3.48	1.39	1.35
56	DW	46	7MG	C4-N9	-3.41	1.33	1.37
56	BW	39	PSU	C6-C5	3.36	1.39	1.35
58	BY	54	5MU	C2-N1	3.33	1.43	1.38
58	DY	55	PSU	C6-C5	3.28	1.39	1.35
57	BX	54	5MU	C4-C5	3.18	1.50	1.44
57	BX	76	31H	C5-C4	-3.16	1.32	1.40
58	DY	46	7MG	C5-C4	3.15	1.48	1.38
57	DX	76	31H	C5-C4	-3.14	1.32	1.40
57	BX	54	5MU	C6-C5	3.13	1.39	1.34
57	BX	55	PSU	C6-C5	3.07	1.38	1.35
58	BY	8	4SU	C4-N3	-3.04	1.34	1.37
56	DW	8	4SU	C4-N3	-3.03	1.34	1.37
56	BW	54	5MU	C6-C5	3.03	1.39	1.34
57	BX	32	5MC	C6-C5	3.02	1.39	1.34
58	BY	54	5MU	C6-C5	3.02	1.39	1.34
57	BX	32	5MC	C6-N1	-3.01	1.32	1.38
56	BW	8	4SU	C4-N3	-2.99	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	BY	46	7MG	C5-C4	2.98	1.47	1.38
56	BW	46	7MG	C5-C4	2.96	1.47	1.38
56	DW	39	PSU	C6-C5	2.95	1.38	1.35
57	DX	76	31H	C3'-N3'	2.94	1.50	1.45
56	DW	54	5MU	C4-C5	2.94	1.49	1.44
57	BX	76	31H	C3'-N3'	2.93	1.50	1.45
56	DW	54	5MU	C6-C5	2.89	1.39	1.34
56	DW	46	7MG	C5-C4	2.87	1.47	1.38
58	BY	37	MIA	C5-C4	2.87	1.48	1.40
58	DY	8	4SU	C4-N3	-2.85	1.34	1.37
58	DY	8	4SU	C2-N1	2.81	1.43	1.38
58	BY	8	4SU	C5-C4	-2.80	1.39	1.42
57	DX	8	4SU	C5-C4	-2.80	1.39	1.42
58	DY	55	PSU	C4-N3	-2.74	1.33	1.38
57	BX	54	5MU	C4-N3	-2.73	1.33	1.38
56	DW	37	MIA	C5-C4	2.73	1.48	1.40
57	DX	54	5MU	C4-N3	-2.73	1.33	1.38
58	DY	37	MIA	C5-C4	2.72	1.48	1.40
57	DX	8	4SU	C2-N3	-2.70	1.33	1.38
58	DY	8	4SU	C5-C4	-2.67	1.39	1.42
58	DY	54	5MU	C4-N3	-2.66	1.33	1.38
57	DX	76	31H	C6-C5	-2.66	1.33	1.43
56	BW	55	PSU	C4-N3	-2.65	1.33	1.38
57	BX	76	31H	C6-C5	-2.64	1.33	1.43
58	DY	54	5MU	C6-C5	2.63	1.38	1.34
56	DW	37	MIA	C2-N3	2.62	1.36	1.32
56	BW	8	4SU	C5-C4	-2.61	1.39	1.42
58	BY	46	7MG	C4-N9	-2.59	1.34	1.37
58	BY	37	MIA	C2-N3	2.58	1.36	1.32
57	DX	54	5MU	C6-N1	-2.58	1.33	1.38
56	BW	32	PSU	C4-N3	-2.53	1.34	1.38
56	DW	76	F3N	C3'-N3'	2.51	1.49	1.45
57	DX	54	5MU	C4-C5	2.49	1.48	1.44
58	DY	54	5MU	C2-N1	2.48	1.42	1.38
56	BW	37	MIA	C5-C4	2.47	1.47	1.40
58	BY	55	PSU	C4-N3	-2.47	1.34	1.38
58	BY	39	PSU	C4-N3	-2.45	1.34	1.38
58	BY	54	5MU	C4-N3	-2.45	1.34	1.38
56	BW	76	F3N	C2'-C3'	-2.45	1.49	1.53
58	BY	32	PSU	C4-N3	-2.44	1.34	1.38
58	BY	54	5MU	C4-C5	2.44	1.48	1.44
56	BW	76	F3N	O4'-C1'	2.43	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	DW	55	PSU	C4-N3	-2.42	1.34	1.38
56	DW	76	F3N	C6-C5	-2.41	1.34	1.43
57	BX	55	PSU	C4-N3	-2.41	1.34	1.38
58	DY	37	MIA	C2-N3	2.39	1.36	1.32
57	DX	55	PSU	C4-N3	-2.39	1.34	1.38
58	DY	54	5MU	C4-C5	2.38	1.48	1.44
56	DW	8	4SU	C5-C4	-2.37	1.39	1.42
56	DW	32	PSU	C4-N3	-2.36	1.34	1.38
57	DX	54	5MU	C2-N3	-2.35	1.33	1.38
56	DW	76	F3N	C5-C4	-2.35	1.34	1.40
58	DY	46	7MG	C6-N1	-2.33	1.34	1.38
57	DX	54	5MU	C6-C5	2.33	1.38	1.34
58	BY	8	4SU	C2-N1	2.33	1.42	1.38
58	DY	32	PSU	C4-N3	-2.33	1.34	1.38
56	DW	39	PSU	C4-N3	-2.31	1.34	1.38
56	BW	76	F3N	C5-C4	-2.31	1.34	1.40
56	DW	54	5MU	C4-N3	-2.24	1.34	1.38
56	BW	76	F3N	C6-C5	-2.24	1.35	1.43
56	DW	46	7MG	C6-N1	-2.23	1.34	1.38
58	BY	46	7MG	C6-N1	-2.23	1.34	1.38
58	DY	54	5MU	C6-N1	-2.21	1.34	1.38
57	BX	8	4SU	C2-N3	-2.21	1.34	1.38
56	DW	8	4SU	C2-N1	2.19	1.42	1.38
57	BX	54	5MU	C6-N1	-2.18	1.34	1.38
56	BW	39	PSU	C2-N1	-2.15	1.33	1.36
56	DW	76	F3N	C5-N7	-2.15	1.31	1.39
56	BW	54	5MU	C4-N3	-2.14	1.34	1.38
56	BW	46	7MG	C6-N1	-2.13	1.34	1.38
57	BX	8	4SU	C4-N3	-2.12	1.35	1.37
57	BX	76	31H	C5-N7	-2.12	1.32	1.39
57	DX	76	31H	C5-N7	-2.11	1.32	1.39
56	BW	54	5MU	C6-N1	-2.10	1.34	1.38
56	BW	8	4SU	C2-N1	2.10	1.41	1.38
56	DW	32	PSU	C4-C5	2.09	1.50	1.44
56	BW	55	PSU	C2-N3	-2.08	1.33	1.37
58	BY	32	PSU	C4-C5	2.07	1.50	1.44
56	BW	76	F3N	C5-N7	-2.07	1.32	1.39
56	BW	39	PSU	C4-C5	2.06	1.50	1.44
58	DY	54	5MU	C2-N3	-2.06	1.34	1.38
56	DW	8	4SU	C6-C5	2.04	1.39	1.35
56	DW	54	5MU	C6-N1	-2.04	1.34	1.38
57	BX	54	5MU	C2-N1	2.02	1.41	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	DW	54	5MU	C2-N1	2.02	1.41	1.38
58	DY	46	7MG	C8-N9	2.02	1.47	1.46
58	DY	39	PSU	C4-N3	-2.01	1.35	1.38
56	BW	39	PSU	C4-N3	-2.01	1.35	1.38
58	BY	54	5MU	C6-N1	-2.00	1.34	1.38
58	DY	46	7MG	C4-N9	-2.00	1.35	1.37

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	DY	46	7MG	N9-C4-N3	9.67	139.93	125.47
58	BY	46	7MG	N9-C4-N3	8.99	138.92	125.47
56	BW	46	7MG	N9-C4-N3	8.53	138.23	125.47
56	BW	37	MIA	C12-C13-C14	-8.46	110.68	127.14
56	DW	46	7MG	N9-C4-N3	8.27	137.84	125.47
57	DX	8	4SU	C4-N3-C2	-7.24	120.31	127.34
57	BX	8	4SU	C4-N3-C2	-7.07	120.47	127.34
56	DW	8	4SU	C4-N3-C2	-6.55	120.98	127.34
57	DX	8	4SU	C5-C4-N3	6.50	120.72	114.69
58	DY	8	4SU	C4-N3-C2	-6.44	121.08	127.34
56	BW	8	4SU	C4-N3-C2	-6.43	121.09	127.34
58	BY	8	4SU	C4-N3-C2	-6.11	121.41	127.34
58	BY	39	PSU	N1-C2-N3	5.89	121.81	115.13
58	DY	46	7MG	C5-C4-N3	-5.86	116.96	128.13
57	BX	55	PSU	N1-C2-N3	5.84	121.75	115.13
56	BW	32	PSU	N1-C2-N3	5.82	121.73	115.13
56	DW	32	PSU	N1-C2-N3	5.81	121.71	115.13
57	BX	54	5MU	N3-C2-N1	5.79	122.58	114.89
58	DY	55	PSU	N1-C2-N3	5.77	121.67	115.13
56	DW	55	PSU	N1-C2-N3	5.68	121.56	115.13
58	BY	55	PSU	N1-C2-N3	5.64	121.53	115.13
56	DW	76	F3N	N3-C2-N1	-5.64	119.87	128.68
56	BW	76	F3N	N3-C2-N1	-5.63	119.87	128.68
58	DY	8	4SU	C5-C4-N3	5.59	119.88	114.69
58	BY	46	7MG	C5-C4-N3	-5.57	117.52	128.13
57	BX	76	31H	N3-C2-N1	-5.57	119.97	128.68
56	BW	8	4SU	C5-C4-N3	5.56	119.85	114.69
58	DY	39	PSU	N1-C2-N3	5.56	121.43	115.13
57	DX	76	31H	N3-C2-N1	-5.55	120.00	128.68
58	DY	32	PSU	N1-C2-N3	5.55	121.42	115.13
56	BW	55	PSU	N1-C2-N3	5.54	121.41	115.13
56	BW	46	7MG	N9-C8-N7	-5.52	95.49	103.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	DX	54	5MU	C4-N3-C2	-5.49	120.25	127.35
57	DX	55	PSU	N1-C2-N3	5.48	121.34	115.13
58	BY	8	4SU	C5-C4-N3	5.44	119.73	114.69
56	DW	39	PSU	N1-C2-N3	5.39	121.24	115.13
56	DW	46	7MG	N9-C8-N7	-5.33	95.76	103.38
58	BY	32	PSU	N1-C2-N3	5.31	121.15	115.13
56	DW	8	4SU	C5-C4-N3	5.25	119.56	114.69
58	BY	46	7MG	N9-C8-N7	-5.24	95.88	103.38
56	BW	39	PSU	N1-C2-N3	5.20	121.02	115.13
58	BY	54	5MU	N3-C2-N1	5.15	121.73	114.89
57	BX	8	4SU	C5-C4-N3	5.11	119.42	114.69
56	DW	46	7MG	C5-C4-N3	-5.06	118.48	128.13
58	DY	54	5MU	C4-N3-C2	-5.00	120.88	127.35
57	BX	54	5MU	C4-N3-C2	-4.94	120.96	127.35
56	BW	46	7MG	C5-C4-N3	-4.92	118.76	128.13
58	DY	46	7MG	N9-C8-N7	-4.91	96.36	103.38
57	DX	54	5MU	C5-C4-N3	4.90	119.50	115.31
58	BY	54	5MU	C4-N3-C2	-4.89	121.02	127.35
56	BW	37	MIA	C11-S10-C2	-4.88	98.62	102.27
56	DW	54	5MU	C4-N3-C2	-4.84	121.09	127.35
56	BW	54	5MU	N3-C2-N1	4.82	121.29	114.89
56	BW	37	MIA	C5-C6-N1	-4.79	116.83	120.81
58	DY	54	5MU	N3-C2-N1	4.78	121.23	114.89
56	BW	54	5MU	C4-N3-C2	-4.74	121.22	127.35
57	DX	54	5MU	N3-C2-N1	4.68	121.10	114.89
58	DY	8	4SU	C5-C4-S4	-4.54	118.62	124.47
57	BX	8	4SU	N3-C2-N1	4.48	120.84	114.89
58	BY	46	7MG	C2-N3-C4	4.46	120.25	112.30
57	DX	54	5MU	C5-C6-N1	-4.46	118.75	123.34
56	DW	54	5MU	N3-C2-N1	4.46	120.81	114.89
58	DY	46	7MG	C2-N3-C4	4.44	120.22	112.30
56	DW	8	4SU	N3-C2-N1	4.33	120.63	114.89
58	DY	54	5MU	C5-C4-N3	4.29	118.97	115.31
57	DX	8	4SU	N3-C2-N1	4.28	120.57	114.89
57	BX	55	PSU	C4-N3-C2	-4.27	120.18	126.34
56	DW	46	7MG	C2-N3-C4	4.26	119.90	112.30
56	BW	39	PSU	O2-C2-N1	-4.26	118.10	122.79
58	BY	54	5MU	O4-C4-C5	-4.22	120.01	124.90
56	BW	54	5MU	O2-C2-N1	-4.21	117.19	122.79
56	DW	54	5MU	C5-C4-N3	4.18	118.88	115.31
58	DY	39	PSU	O2-C2-N1	-4.12	118.25	122.79
56	BW	46	7MG	C2-N3-C4	4.09	119.58	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	BY	54	5MU	C5-C4-N3	4.00	118.73	115.31
56	BW	39	PSU	C6-C5-C4	-3.99	115.41	118.20
58	BY	8	4SU	C5-C4-S4	-3.97	119.36	124.47
58	DY	55	PSU	C4-N3-C2	-3.92	120.69	126.34
56	BW	8	4SU	N3-C2-N1	3.91	120.08	114.89
58	DY	8	4SU	N3-C2-N1	3.88	120.04	114.89
56	BW	8	4SU	C5-C4-S4	-3.87	119.48	124.47
57	DX	55	PSU	C4-N3-C2	-3.85	120.79	126.34
56	BW	55	PSU	C4-N3-C2	-3.84	120.80	126.34
56	BW	37	MIA	C15-C14-C13	-3.84	111.55	122.65
58	BY	8	4SU	N3-C2-N1	3.83	119.97	114.89
56	BW	37	MIA	C16-C14-C13	-3.81	111.63	122.65
57	DX	54	5MU	O4-C4-C5	-3.81	120.49	124.90
58	DY	54	5MU	C5-C6-N1	-3.75	119.48	123.34
58	DY	54	5MU	O4-C4-C5	-3.73	120.57	124.90
57	DX	8	4SU	C5-C4-S4	-3.72	119.67	124.47
58	BY	39	PSU	C4-N3-C2	-3.72	120.98	126.34
57	DX	32	5MC	C5-C4-N3	-3.71	117.67	121.67
58	DY	8	4SU	C1'-N1-C2	3.70	124.26	117.57
56	DW	8	4SU	C5-C4-S4	-3.69	119.72	124.47
56	DW	32	PSU	C4-N3-C2	-3.68	121.04	126.34
58	DY	32	PSU	C4-N3-C2	-3.67	121.05	126.34
57	BX	32	5MC	C5-C4-N3	-3.65	117.73	121.67
58	DY	55	PSU	O2-C2-N1	-3.65	118.77	122.79
56	DW	39	PSU	C4-N3-C2	-3.64	121.09	126.34
56	BW	55	PSU	C6-C5-C4	-3.63	115.66	118.20
58	BY	32	PSU	C4-N3-C2	-3.61	121.13	126.34
57	BX	8	4SU	C5-C4-S4	-3.59	119.84	124.47
58	BY	55	PSU	C4-N3-C2	-3.58	121.18	126.34
58	BY	37	MIA	N3-C2-N1	-3.55	123.14	128.68
56	BW	37	MIA	C2-N3-C4	3.55	120.21	115.32
56	BW	39	PSU	C4-N3-C2	-3.53	121.26	126.34
56	DW	37	MIA	N3-C2-N1	-3.52	123.17	128.68
56	DW	54	5MU	O4-C4-C5	-3.52	120.82	124.90
56	BW	54	5MU	C5-C6-N1	-3.51	119.73	123.34
56	DW	55	PSU	C4-N3-C2	-3.51	121.28	126.34
56	DW	54	5MU	C5-C6-N1	-3.50	119.74	123.34
58	DY	37	MIA	N3-C2-N1	-3.48	123.23	128.68
56	DW	39	PSU	O2-C2-N1	-3.47	118.97	122.79
56	BW	54	5MU	C5-C4-N3	3.47	118.27	115.31
56	BW	32	PSU	C4-N3-C2	-3.46	121.35	126.34
57	BX	32	5MC	C5-C6-N1	-3.43	119.81	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	DX	32	5MC	C5-C6-N1	-3.38	119.86	123.34
58	BY	8	4SU	C1'-N1-C2	3.35	123.63	117.57
58	BY	55	PSU	O2-C2-N1	-3.33	119.13	122.79
58	BY	54	5MU	C1'-N1-C2	3.31	123.56	117.57
58	BY	39	PSU	O2-C2-N1	-3.31	119.15	122.79
56	DW	32	PSU	O2-C2-N1	-3.30	119.16	122.79
56	BW	37	MIA	C2-N1-C6	3.30	123.09	117.19
58	DY	32	PSU	O2-C2-N1	-3.27	119.19	122.79
56	DW	55	PSU	O2-C2-N1	-3.21	119.26	122.79
58	DY	39	PSU	C4-N3-C2	-3.17	121.78	126.34
57	BX	54	5MU	O2-C2-N1	-3.15	118.60	122.79
57	BX	54	5MU	C5-C4-N3	3.14	117.99	115.31
57	BX	54	5MU	C5-C6-N1	-3.14	120.11	123.34
56	BW	37	MIA	C4-C5-N7	-3.12	106.15	109.40
56	DW	54	5MU	O2-C2-N1	-3.11	118.65	122.79
56	BW	54	5MU	C5M-C5-C4	3.11	122.19	118.77
57	BX	55	PSU	O2-C2-N1	-3.05	119.44	122.79
57	BX	76	31H	CA-N-CN	-2.98	118.25	122.82
57	DX	76	31H	CA-N-CN	-2.94	118.30	122.82
57	DX	32	5MC	O2-C2-N3	-2.93	117.56	122.33
56	DW	46	7MG	C5-C6-N1	2.90	116.11	110.99
58	BY	37	MIA	C4-C5-N7	-2.90	106.38	109.40
58	BY	46	7MG	C5-C6-N1	2.84	115.99	110.99
56	DW	76	F3N	O4'-C4'-C3'	2.75	108.01	104.06
58	DY	46	7MG	C5-C6-N1	2.75	115.83	110.99
58	BY	54	5MU	C5-C6-N1	-2.74	120.52	123.34
56	BW	32	PSU	O2-C2-N1	-2.74	119.78	122.79
56	DW	54	5MU	C5M-C5-C4	2.67	121.70	118.77
58	BY	32	PSU	O2-C2-N1	-2.66	119.86	122.79
56	BW	46	7MG	C5-C6-N1	2.63	115.63	110.99
57	BX	55	PSU	C5-C6-N1	-2.59	118.23	122.11
58	BY	32	PSU	C6-C5-C4	-2.58	116.39	118.20
57	DX	76	31H	O4'-C1'-C2'	-2.57	103.16	106.93
56	BW	46	7MG	C5-C4-N9	-2.57	103.00	106.35
57	BX	76	31H	O4'-C1'-C2'	-2.57	103.17	106.93
58	DY	37	MIA	C4-C5-N7	-2.56	106.73	109.40
57	BX	32	5MC	N4-C4-N3	2.53	123.09	118.48
57	BX	8	4SU	O2-C2-N1	-2.51	119.44	122.79
58	BY	54	5MU	O2-C2-N3	-2.50	116.84	121.50
58	DY	39	PSU	C6-C5-C4	-2.50	116.45	118.20
58	DY	46	7MG	C5-C4-N9	-2.50	103.11	106.35
56	DW	37	MIA	C4-C5-N7	-2.46	106.84	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BX	54	5MU	C5M-C5-C4	2.45	121.47	118.77
56	BW	54	5MU	C5M-C5-C6	-2.42	119.62	122.85
57	BX	54	5MU	C5M-C5-C6	-2.41	119.63	122.85
56	BW	54	5MU	O4-C4-C5	-2.39	122.13	124.90
57	DX	54	5MU	C5M-C5-C4	2.39	121.40	118.77
58	BY	54	5MU	C1'-N1-C6	-2.37	117.17	121.12
57	DX	55	PSU	O2-C2-N1	-2.34	120.21	122.79
56	BW	55	PSU	O2-C2-N1	-2.28	120.28	122.79
58	BY	37	MIA	C2-N1-C6	2.28	122.65	118.75
57	DX	54	5MU	O2-C2-N1	-2.23	119.82	122.79
56	BW	37	MIA	N3-C2-N1	-2.20	122.93	126.98
56	BW	46	7MG	O6-C6-C5	-2.19	122.16	127.54
56	BW	8	4SU	C1'-N1-C2	2.15	121.46	117.57
58	BY	46	7MG	C5-C4-N9	-2.14	103.56	106.35
58	DY	46	7MG	O6-C6-C5	-2.14	122.30	127.54
56	DW	8	4SU	O2-C2-N1	-2.11	119.98	122.79
57	DX	32	5MC	N1-C2-N3	2.09	122.62	118.81
57	DX	54	5MU	C5M-C5-C6	-2.09	120.06	122.85
56	DW	54	5MU	C5M-C5-C6	-2.08	120.07	122.85
58	BY	46	7MG	O6-C6-C5	-2.08	122.44	127.54
56	DW	46	7MG	C5-C4-N9	-2.07	103.66	106.35
58	DY	46	7MG	CM7-N7-C5	2.06	131.72	126.40
58	BY	54	5MU	C6-N1-C2	-2.04	119.23	121.30
56	DW	46	7MG	O6-C6-C5	-2.02	122.59	127.54
56	DW	46	7MG	CM7-N7-C5	2.00	131.57	126.40

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	BW	37	MIA	N1-C2-S10-C11
56	BW	37	MIA	N3-C2-S10-C11
56	BW	37	MIA	C12-C13-C14-C16
57	BX	76	31H	C3'-C4'-C5'-O5'
57	BX	76	31H	C4'-C5'-O5'-P
57	BX	76	31H	C-CA-CB-CG
57	BX	76	31H	N-CA-CB-CG
57	BX	76	31H	OCN-CN-N-CA
58	BY	46	7MG	C4'-C5'-O5'-P
57	DX	76	31H	C3'-C4'-C5'-O5'
57	DX	76	31H	C4'-C5'-O5'-P
57	DX	76	31H	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
57	DX	76	31H	N-CA-CB-CG
57	DX	76	31H	OCN-CN-N-CA
58	DY	37	MIA	C3'-C4'-C5'-O5'
58	DY	39	PSU	C3'-C4'-C5'-O5'
58	DY	46	7MG	O4'-C4'-C5'-O5'
58	DY	46	7MG	C3'-C4'-C5'-O5'
58	DY	54	5MU	O4'-C4'-C5'-O5'
58	DY	55	PSU	O4'-C1'-C5-C6
58	DY	54	5MU	C3'-C4'-C5'-O5'
57	BX	76	31H	O4'-C4'-C5'-O5'
58	BY	46	7MG	C3'-C4'-C5'-O5'
57	DX	76	31H	O4'-C4'-C5'-O5'
58	DY	37	MIA	O4'-C4'-C5'-O5'
58	DY	39	PSU	O4'-C4'-C5'-O5'
58	BY	37	MIA	C3'-C4'-C5'-O5'
56	BW	46	7MG	C3'-C4'-C5'-O5'
56	BW	46	7MG	O4'-C4'-C5'-O5'
58	BY	46	7MG	C2'-C1'-N9-C8
58	BY	37	MIA	O4'-C4'-C5'-O5'
57	BX	76	31H	O-C-CA-N
57	DX	76	31H	O-C-CA-N
58	BY	46	7MG	O4'-C4'-C5'-O5'
56	BW	46	7MG	C4'-C5'-O5'-P
56	DW	46	7MG	C2'-C1'-N9-C8
58	DY	55	PSU	O4'-C4'-C5'-O5'
57	BX	76	31H	N3'-C-CA-N
57	DX	76	31H	N3'-C-CA-N
58	BY	55	PSU	O4'-C1'-C5-C4
57	DX	55	PSU	O4'-C1'-C5-C4
56	DW	46	7MG	O4'-C1'-N9-C8
58	BY	46	7MG	O4'-C1'-N9-C8
58	BY	8	4SU	C2'-C1'-N1-C2
58	BY	54	5MU	C2'-C1'-N1-C2
58	DY	8	4SU	C2'-C1'-N1-C2
58	DY	46	7MG	C2'-C1'-N9-C8
56	BW	76	F3N	C4'-C5'-O5'-P
57	BX	76	31H	CB-CG-SD-CE
57	DX	76	31H	CB-CG-SD-CE

There are no ring outliers.

21 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	DX	8	4SU	1	0
56	BW	39	PSU	1	0
56	BW	55	PSU	1	0
57	DX	55	PSU	1	0
58	DY	8	4SU	1	0
58	BY	8	4SU	1	0
58	DY	37	MIA	2	0
56	BW	76	F3N	2	0
56	DW	76	F3N	4	0
57	BX	55	PSU	1	0
58	BY	39	PSU	1	0
58	DY	39	PSU	1	0
56	DW	37	MIA	1	0
56	DW	55	PSU	1	0
57	DX	76	31H	3	0
56	DW	46	7MG	2	0
56	DW	32	PSU	1	0
57	BX	32	5MC	2	0
56	BW	8	4SU	1	0
56	DW	54	5MU	1	0
58	DY	55	PSU	3	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2073 ligands modelled in this entry, 2069 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
64	GDP	BZ	702	60	24,30,30	1.03	1 (4%)	30,47,47	1.42	5 (16%)
64	GDP	DZ	702	60	24,30,30	1.01	1 (4%)	30,47,47	1.41	4 (13%)
63	SF4	BD	501	37	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
63	SF4	DD	501	37	0,12,12	-	-	-		

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
64	GDP	BZ	702	60	-	0/12/32/32	0/3/3/3
64	GDP	DZ	702	60	-	2/12/32/32	0/3/3/3
63	SF4	BD	501	37	-	-	0/6/5/5
63	SF4	DD	501	37	-	-	0/6/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	DZ	702	GDP	C6-N1	-2.98	1.33	1.37
64	BZ	702	GDP	C2'-C1'	-2.21	1.50	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	DZ	702	GDP	O4'-C1'-C2'	-3.40	101.96	106.93
64	DZ	702	GDP	PA-O3A-PB	-3.35	121.33	132.83
64	BZ	702	GDP	PA-O3A-PB	-3.02	122.48	132.83
64	BZ	702	GDP	O6-C6-N1	2.97	124.16	120.65
64	BZ	702	GDP	O6-C6-C5	-2.66	119.17	124.37
64	DZ	702	GDP	O3'-C3'-C4'	-2.42	104.06	111.05
64	BZ	702	GDP	O4'-C1'-C2'	-2.08	103.89	106.93
64	DZ	702	GDP	C5-C6-N1	2.05	117.57	113.95
64	BZ	702	GDP	C8-N7-C5	2.00	106.80	102.99

There are no chirality outliers.

All (2) torsion outliers are listed below:

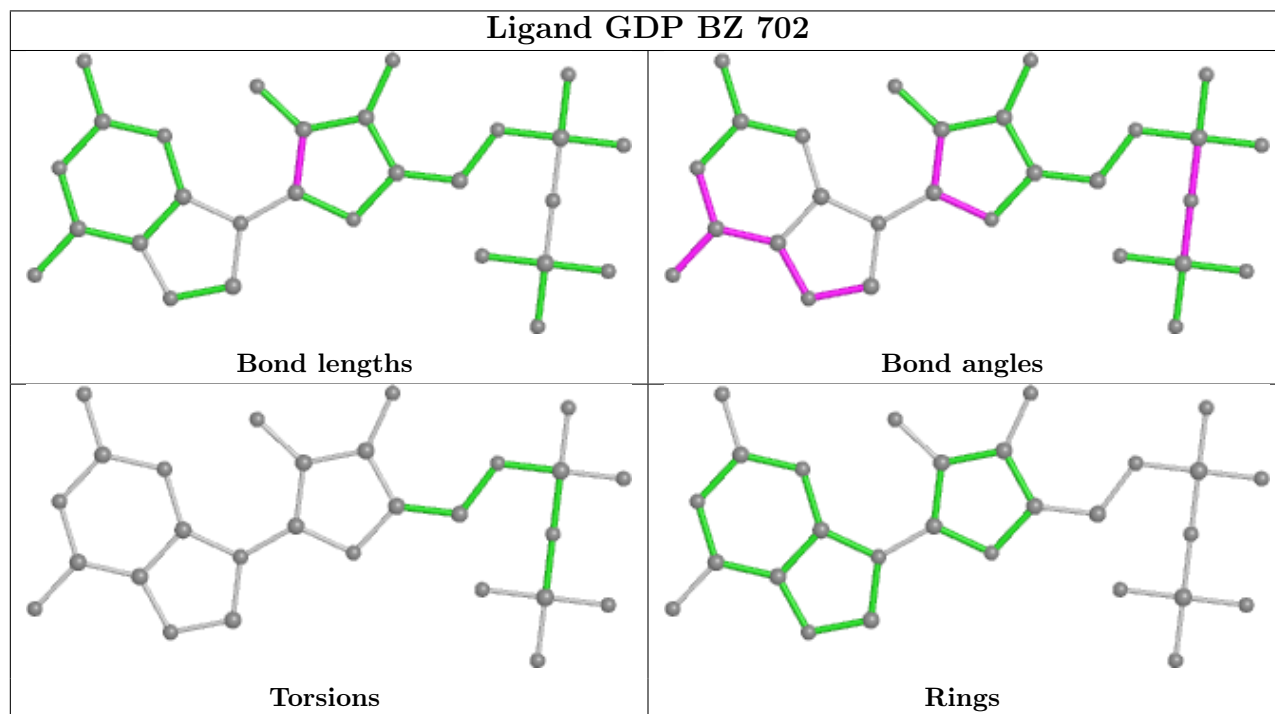
Mol	Chain	Res	Type	Atoms
64	DZ	702	GDP	PA-O3A-PB-O2B
64	DZ	702	GDP	C5'-O5'-PA-O1A

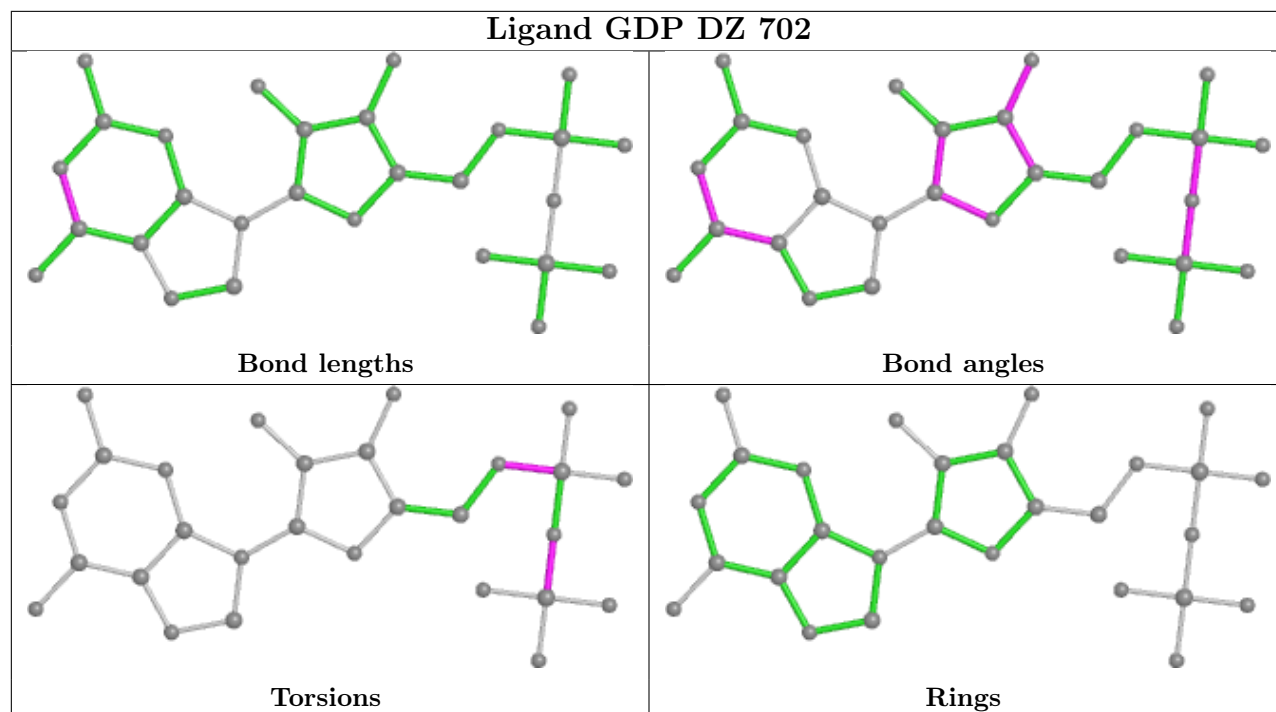
There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
64	BZ	702	GDP	6	0
64	DZ	702	GDP	7	0
63	BD	501	SF4	1	0
63	DD	501	SF4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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 i

### 6.1 Protein, DNA and RNA chains i

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	2872/2915 (98%)	-0.17	64 (2%) 62 52	16, 36, 153, 292	0
1	CA	2868/2915 (98%)	-0.05	119 (4%) 37 27	25, 54, 187, 320	0
2	AB	120/121 (99%)	-0.44	0 100 100	26, 52, 72, 110	0
2	CB	120/121 (99%)	-0.13	0 100 100	55, 87, 110, 177	0
3	AC	137/228 (60%)	4.00	113 (82%) 0 0	95, 162, 210, 232	0
3	CC	137/228 (60%)	5.74	125 (91%) 0 0	115, 183, 225, 239	0
4	AD	275/276 (99%)	-0.47	2 (0%) 87 84	16, 35, 59, 113	0
4	CD	275/276 (99%)	-0.34	1 (0%) 92 91	19, 46, 73, 142	0
5	AE	204/206 (99%)	-0.47	0 100 100	8, 36, 67, 101	0
5	CE	204/206 (99%)	-0.28	0 100 100	25, 53, 88, 136	0
6	AF	203/210 (96%)	-0.41	1 (0%) 91 88	12, 37, 91, 175	0
6	CF	203/210 (96%)	-0.29	0 100 100	23, 63, 114, 164	0
7	AG	181/182 (99%)	-0.23	3 (1%) 70 63	41, 71, 110, 179	0
7	CG	181/182 (99%)	0.30	8 (4%) 34 24	74, 106, 143, 190	0
8	AH	174/180 (96%)	-0.35	2 (1%) 80 75	30, 51, 81, 174	0
8	CH	174/180 (96%)	0.62	12 (6%) 16 10	45, 94, 139, 208	0
9	AK	130/173 (75%)	1.28	27 (20%) 1 0	62, 125, 191, 235	0
9	CK	130/173 (75%)	2.90	71 (54%) 0 0	104, 173, 211, 231	0
10	AL	66/147 (44%)	4.16	50 (75%) 0 0	134, 182, 226, 242	0
10	CL	66/147 (44%)	5.90	53 (80%) 0 0	115, 198, 249, 257	0
11	AN	140/140 (100%)	-0.53	0 100 100	17, 34, 76, 106	0
11	CN	140/140 (100%)	-0.10	1 (0%) 87 84	33, 59, 97, 139	0
12	AO	122/122 (100%)	-0.33	0 100 100	20, 40, 66, 95	0
12	CO	122/122 (100%)	-0.30	0 100 100	33, 52, 83, 102	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AP	149/150 (99%)	-0.30	0 100 100	14, 44, 83, 127	0
13	CP	149/150 (99%)	0.21	4 (2%) 54 44	29, 66, 112, 154	0
14	AQ	141/141 (100%)	-0.37	0 100 100	17, 39, 66, 97	0
14	CQ	141/141 (100%)	-0.33	0 100 100	33, 62, 91, 156	0
15	AR	118/118 (100%)	-0.48	0 100 100	17, 32, 57, 96	0
15	CR	118/118 (100%)	-0.27	0 100 100	29, 52, 78, 97	0
16	AS	110/112 (98%)	-0.16	0 100 100	32, 54, 81, 102	0
16	CS	110/112 (98%)	0.27	4 (3%) 42 32	53, 82, 112, 143	0
17	AT	131/146 (89%)	-0.30	2 (1%) 73 68	23, 44, 94, 160	0
17	CT	131/146 (89%)	-0.31	0 100 100	37, 58, 99, 155	0
18	AU	116/118 (98%)	-0.57	0 100 100	15, 28, 48, 110	0
18	CU	116/118 (98%)	-0.28	1 (0%) 84 80	36, 52, 82, 123	0
19	AV	101/101 (100%)	-0.56	1 (0%) 82 77	19, 34, 63, 119	0
19	CV	101/101 (100%)	-0.03	1 (0%) 82 77	33, 72, 108, 138	0
20	AW	112/113 (99%)	-0.45	0 100 100	15, 29, 56, 134	0
20	CW	112/113 (99%)	-0.23	1 (0%) 84 80	27, 48, 86, 149	0
21	AX	95/96 (98%)	-0.44	1 (1%) 80 75	22, 38, 69, 125	0
21	CX	95/96 (98%)	0.03	4 (4%) 36 26	40, 61, 93, 134	0
22	AY	107/110 (97%)	-0.29	1 (0%) 84 80	25, 48, 92, 129	0
22	CY	107/110 (97%)	0.67	7 (6%) 18 11	43, 78, 114, 172	0
23	AZ	171/206 (83%)	0.07	11 (6%) 19 12	33, 73, 144, 235	0
23	CZ	174/206 (84%)	0.83	21 (12%) 4 2	60, 107, 174, 243	0
24	A0	83/85 (97%)	-0.31	2 (2%) 59 49	18, 38, 68, 147	0
24	C0	83/85 (97%)	0.31	6 (7%) 15 8	37, 62, 96, 135	0
25	A1	97/98 (98%)	-0.22	2 (2%) 63 54	23, 44, 85, 108	0
25	C1	97/98 (98%)	-0.10	1 (1%) 82 77	33, 54, 107, 119	0
26	A2	70/72 (97%)	-0.28	2 (2%) 51 41	22, 47, 74, 149	0
26	C2	70/72 (97%)	0.02	1 (1%) 75 70	51, 78, 99, 121	0
27	A3	59/60 (98%)	-0.28	1 (1%) 70 63	18, 34, 63, 112	0
27	C3	59/60 (98%)	0.60	5 (8%) 10 5	43, 62, 108, 167	0
28	A4	69/71 (97%)	0.48	9 (13%) 3 2	60, 100, 186, 194	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	C4	69/71 (97%)	0.96	11 (15%) 1 1	89, 138, 197, 212	0
29	A5	59/60 (98%)	-0.56	0 100 100	15, 30, 55, 84	0
29	C5	59/60 (98%)	-0.24	1 (1%) 70 63	29, 46, 77, 112	0
30	A6	53/54 (98%)	-0.39	0 100 100	24, 42, 67, 91	0
30	C6	53/54 (98%)	-0.09	1 (1%) 66 59	43, 63, 88, 103	0
31	A7	48/49 (97%)	-0.27	2 (4%) 36 26	14, 26, 63, 126	0
31	C7	48/49 (97%)	-0.10	1 (2%) 63 54	26, 38, 83, 105	0
32	A8	64/65 (98%)	-0.44	0 100 100	17, 32, 46, 72	0
32	C8	64/65 (98%)	-0.24	0 100 100	36, 51, 70, 101	0
33	A9	37/37 (100%)	-0.12	0 100 100	23, 39, 60, 80	0
33	C9	37/37 (100%)	0.24	1 (2%) 54 44	42, 66, 96, 108	0
34	BA	1497/1521 (98%)	0.01	40 (2%) 54 44	32, 76, 169, 302	0
34	DA	1503/1521 (98%)	0.10	42 (2%) 53 43	40, 83, 174, 317	0
35	BB	231/256 (90%)	0.48	18 (7%) 13 7	61, 108, 167, 197	0
35	DB	231/256 (90%)	0.82	30 (12%) 3 2	77, 129, 184, 232	0
36	BC	206/239 (86%)	0.32	9 (4%) 34 24	60, 103, 138, 194	0
36	DC	206/239 (86%)	0.90	23 (11%) 5 3	77, 127, 170, 196	0
37	BD	208/209 (99%)	0.06	3 (1%) 75 70	51, 82, 121, 168	0
37	DD	208/209 (99%)	-0.02	3 (1%) 75 70	47, 80, 112, 165	0
38	BE	148/162 (91%)	-0.08	0 100 100	48, 73, 111, 140	0
38	DE	148/162 (91%)	0.19	4 (2%) 54 44	46, 89, 128, 151	0
39	BF	100/101 (99%)	-0.22	0 100 100	45, 80, 116, 137	0
39	DF	100/101 (99%)	-0.18	0 100 100	49, 80, 104, 121	0
40	BG	155/156 (99%)	0.27	13 (8%) 11 5	59, 88, 132, 174	0
40	DG	155/156 (99%)	0.67	17 (10%) 5 3	67, 103, 142, 192	0
41	BH	137/138 (99%)	0.08	1 (0%) 87 84	45, 76, 106, 135	0
41	DH	137/138 (99%)	0.37	6 (4%) 34 24	55, 88, 127, 170	0
42	BI	127/128 (99%)	0.59	9 (7%) 16 9	50, 101, 140, 166	0
42	DI	127/128 (99%)	1.30	28 (22%) 0 0	66, 118, 159, 201	0
43	BJ	97/105 (92%)	0.80	14 (14%) 2 1	53, 113, 158, 199	0
43	DJ	96/105 (91%)	1.45	25 (26%) 0 0	70, 134, 181, 195	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	BK	114/129 (88%)	-0.26	0 100 100	45, 72, 112, 129	0
44	DK	114/129 (88%)	-0.02	1 (0%) 84 80	44, 80, 118, 139	0
45	BL	122/132 (92%)	-0.22	0 100 100	38, 63, 88, 113	0
45	DL	122/132 (92%)	-0.02	2 (1%) 72 66	37, 72, 94, 141	0
46	BM	123/126 (97%)	0.53	9 (7%) 15 8	55, 95, 129, 222	0
46	DM	122/126 (96%)	0.88	16 (13%) 3 2	71, 125, 153, 188	0
47	BN	60/61 (98%)	0.56	5 (8%) 11 6	65, 95, 123, 138	0
47	DN	60/61 (98%)	1.69	20 (33%) 0 0	84, 123, 166, 208	0
48	BO	88/89 (98%)	-0.05	2 (2%) 60 51	39, 68, 110, 142	0
48	DO	88/89 (98%)	0.25	0 100 100	43, 78, 112, 127	0
49	BP	82/88 (93%)	0.34	1 (1%) 79 73	54, 76, 109, 134	0
49	DP	82/88 (93%)	0.18	2 (2%) 59 49	53, 70, 96, 131	0
50	BQ	99/105 (94%)	-0.08	0 100 100	43, 69, 97, 110	0
50	DQ	99/105 (94%)	0.09	0 100 100	51, 74, 103, 123	0
51	BR	68/88 (77%)	0.47	4 (5%) 22 14	48, 73, 112, 135	0
51	DR	68/88 (77%)	0.47	4 (5%) 22 14	46, 78, 116, 135	0
52	BS	84/93 (90%)	1.05	15 (17%) 1 1	67, 110, 163, 180	0
52	DS	83/93 (89%)	1.86	39 (46%) 0 0	92, 141, 187, 229	0
53	BT	96/106 (90%)	0.24	1 (1%) 82 77	53, 77, 115, 169	0
53	DT	96/106 (90%)	0.28	1 (1%) 82 77	52, 77, 117, 132	0
54	BU	23/27 (85%)	0.77	3 (13%) 3 2	56, 89, 104, 114	0
54	DU	23/27 (85%)	1.72	8 (34%) 0 0	79, 109, 130, 142	0
55	BV	13/24 (54%)	1.80	5 (38%) 0 0	49, 87, 172, 178	0
55	DV	12/24 (50%)	2.83	8 (66%) 0 0	63, 120, 171, 199	0
56	BW	66/76 (86%)	2.57	35 (53%) 0 0	64, 169, 230, 256	0
56	DW	64/76 (84%)	3.63	47 (73%) 0 0	92, 197, 239, 263	0
57	BX	71/77 (92%)	-0.05	1 (1%) 75 70	34, 78, 124, 188	0
57	DX	71/77 (92%)	0.18	2 (2%) 53 43	34, 100, 148, 162	0
58	BY	67/76 (88%)	0.92	11 (16%) 1 1	39, 159, 224, 266	0
58	DY	66/76 (86%)	1.34	15 (22%) 0 0	57, 178, 229, 251	0
59	BZ	728/758 (96%)	1.08	151 (20%) 1 0	41, 107, 195, 257	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
59	DZ	730/758 (96%)	1.54	227 (31%) 0 0	38, 116, 213, 248	0
All	All	22848/24064 (94%)	0.24	1677 (7%) 15 8	8, 68, 177, 320	0

All (1677) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
59	BZ	503	GLY	25.5
10	CL	137	GLU	19.3
3	CC	174	ALA	18.6
10	CL	138	VAL	16.1
59	BZ	502	GLY	15.3
3	CC	172	ILE	14.2
3	CC	176	VAL	14.2
10	AL	135	GLY	14.2
3	CC	69	LEU	13.9
59	DZ	688	ILE	13.8
46	DM	123	ALA	13.3
59	DZ	419	ALA	13.3
9	CK	50	ARG	13.1
59	BZ	472	VAL	12.9
10	CL	133	SER	12.9
56	DW	71	G	12.8
34	DA	1030(B)	C	12.7
59	DZ	426	GLN	12.6
3	CC	177	GLY	12.6
3	CC	162	ILE	12.6
59	DZ	422	GLU	12.4
9	AK	49	ALA	12.2
59	DZ	417	THR	12.1
59	DZ	425	SER	12.1
3	CC	41	THR	11.9
10	CL	82	ALA	11.8
3	CC	59	VAL	11.7
40	DG	83	ALA	11.5
10	CL	114	ASP	11.4
59	BZ	419	ALA	11.2
3	CC	163	GLU	11.2
3	CC	164	PHE	11.1
3	AC	159	ALA	10.9
10	CL	126	MET	10.9
3	CC	28	ARG	10.8
3	CC	180	SER	10.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
59	DZ	404	VAL	10.7
9	CK	49	ALA	10.6
3	CC	160	GLY	10.6
59	DZ	684	GLN	10.5
10	AL	86	LYS	10.4
40	DG	82	GLY	10.4
10	CL	125	ARG	10.2
10	AL	134	MET	10.1
3	CC	175	PRO	10.0
56	DW	72	C	10.0
10	AL	92	GLY	9.9
56	DW	70	G	9.8
3	AC	174	ALA	9.8
10	CL	94	GLU	9.7
10	CL	95	LYS	9.7
3	CC	67	HIS	9.6
59	DZ	421	GLN	9.6
59	DZ	444	PRO	9.6
59	DZ	487	ILE	9.6
3	CC	171	ALA	9.6
10	CL	105	LEU	9.5
9	CK	53	VAL	9.5
9	AK	50	ARG	9.5
10	AL	131	ALA	9.5
3	CC	68	GLY	9.4
3	AC	57	GLN	9.4
3	AC	219	MET	9.4
3	CC	35	THR	9.4
3	CC	61	GLY	9.3
9	CK	96	PHE	9.3
59	DZ	593	ALA	9.3
9	AK	48	GLY	9.2
59	DZ	521	SER	9.2
59	BZ	91	THR	9.2
3	AC	44	VAL	9.2
59	DZ	594	VAL	9.1
59	DZ	420	ASP	9.1
10	CL	84	LEU	9.0
59	DZ	472	VAL	9.0
10	CL	83	GLY	8.9
59	BZ	684	GLN	8.9
3	CC	44	VAL	8.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
43	DJ	10	GLY	8.9
59	DZ	634	MET	8.8
3	AC	203	GLU	8.8
59	DZ	488	THR	8.7
3	CC	70	GLY	8.6
10	CL	115	LEU	8.6
1	CA	1087	G	8.5
46	DM	124	PRO	8.4
9	CK	97	ALA	8.4
10	CL	88	ALA	8.3
3	CC	10	ALA	8.3
10	CL	127	ILE	8.3
10	AL	138	VAL	8.3
59	DZ	473	ASP	8.3
34	BA	1030(B)	C	8.3
22	CY	1	MET	8.3
59	DZ	432	ALA	8.2
3	CC	182	PRO	8.2
59	DZ	418	LYS	8.2
3	CC	219	MET	8.2
10	CL	131	ALA	8.2
23	CZ	144	LEU	8.2
56	BW	72	C	8.1
9	AK	51	LEU	8.1
3	CC	159	ALA	8.0
1	CA	1065	U	8.0
3	CC	56	ASP	8.0
59	BZ	531	GLY	7.9
10	CL	98	ARG	7.9
59	DZ	428	LEU	7.9
47	DN	17	LYS	7.8
59	BZ	501	THR	7.8
3	CC	66	PRO	7.8
3	CC	60	ARG	7.8
3	CC	170	GLY	7.8
3	CC	58	ASN	7.8
59	DZ	462	ILE	7.7
3	CC	37	LYS	7.7
59	DZ	503	GLY	7.7
9	AK	88	ALA	7.7
10	CL	135	GLY	7.7
3	CC	221	PRO	7.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	CA	1078	U	7.7
10	CL	130	SER	7.7
10	AL	89	HIS	7.6
9	CK	51	LEU	7.6
55	DV	24	A	7.6
34	BA	1002	G	7.6
10	AL	136	VAL	7.6
46	BM	124	PRO	7.5
56	DW	3	C	7.5
3	CC	166	ASN	7.5
56	BW	71	G	7.5
10	CL	129	GLY	7.5
3	AC	176	VAL	7.5
3	CC	48	LEU	7.5
34	DA	1001(A)	G	7.5
9	CK	89	ALA	7.5
1	CA	2146	C	7.5
3	CC	57	GLN	7.5
10	CL	107	ILE	7.4
56	DW	73	A	7.4
9	CK	116	ILE	7.4
59	DZ	681	LYS	7.4
59	BZ	685	GLU	7.4
59	BZ	481	VAL	7.4
3	CC	36	ALA	7.3
9	CK	99	SER	7.3
10	AL	87	GLY	7.3
59	BZ	471	LYS	7.3
56	DW	6	G	7.3
3	AC	65	LEU	7.3
9	CK	115	GLN	7.2
59	DZ	416	LYS	7.2
3	CC	63	VAL	7.2
34	DA	1036	G	7.2
3	AC	32	GLU	7.2
3	CC	40	GLU	7.2
59	BZ	90	PHE	7.2
3	CC	183	PRO	7.2
59	DZ	430	ARG	7.2
10	CL	99	ILE	7.1
10	CL	113	PRO	7.1
3	AC	170	GLY	7.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
10	CL	122	ALA	7.1
3	AC	221	PRO	7.1
10	AL	83	GLY	7.1
3	CC	42	VAL	7.0
3	CC	217	THR	7.0
9	CK	25	PHE	7.0
46	BM	123	ALA	7.0
59	DZ	639	ASN	7.0
3	CC	173	HIS	7.0
3	CC	178	LYS	7.0
35	DB	232	PRO	7.0
9	AK	53	VAL	7.0
3	AC	161	ARG	7.0
34	DA	1030(A)	G	6.9
3	CC	199	ALA	6.9
59	DZ	465	ARG	6.9
59	DZ	464	ASP	6.9
59	DZ	499	ARG	6.8
3	AC	52	PRO	6.8
59	DZ	486	THR	6.8
10	CL	123	ALA	6.8
3	AC	59	VAL	6.8
3	CC	179	ALA	6.8
59	BZ	504	ARG	6.8
10	CL	108	ALA	6.8
59	DZ	504	ARG	6.8
3	CC	190	ILE	6.8
9	CK	90	ALA	6.7
59	DZ	429	ALA	6.7
3	AC	192	ALA	6.7
1	CA	2173	A	6.7
59	DZ	415	PRO	6.7
10	CL	80	LYS	6.7
3	CC	46	ALA	6.7
28	A4	57	GLU	6.7
59	DZ	424	LEU	6.6
1	CA	1066	U	6.6
3	AC	190	ILE	6.6
40	BG	82	GLY	6.6
56	DW	5	G	6.6
3	CC	200	HIS	6.6
10	AL	94	GLU	6.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	CC	210	LEU	6.6
10	AL	91	PRO	6.6
46	DM	122	LYS	6.6
10	CL	81	ALA	6.6
3	AC	56	ASP	6.5
59	DZ	626	ALA	6.5
3	CC	220	GLY	6.5
56	BW	73	A	6.5
59	DZ	463	VAL	6.5
3	CC	192	ALA	6.5
34	BA	1036	G	6.5
1	CA	1088	A	6.4
59	DZ	427	ALA	6.4
9	CK	101	PRO	6.4
3	AC	49	GLY	6.4
56	DW	7	A	6.4
56	DW	69	G	6.3
59	DZ	500	GLN	6.3
59	BZ	89	ASP	6.3
3	CC	12	LEU	6.3
3	CC	71	LYS	6.3
3	AC	34	ALA	6.3
59	DZ	89	ASP	6.2
3	CC	184	GLU	6.2
1	CA	2155	G	6.2
42	BI	19	LEU	6.2
10	CL	110	GLN	6.2
59	DZ	90	PHE	6.2
3	AC	48	LEU	6.2
9	CK	84	GLU	6.2
3	CC	24	ASP	6.2
3	AC	172	ILE	6.2
59	DZ	562	ASP	6.2
28	C4	57	GLU	6.2
59	BZ	422	GLU	6.1
10	AL	96	VAL	6.1
59	DZ	467	LYS	6.1
10	AL	78	ILE	6.1
59	BZ	477	GLY	6.1
3	AC	166	ASN	6.1
3	CC	189	ASN	6.1
59	BZ	538	TYR	6.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
9	AK	90	ALA	6.0
1	CA	1067	A	6.0
3	AC	33	LEU	6.0
3	CC	187	ALA	6.0
9	CK	43	ALA	6.0
3	CC	208	THR	6.0
23	AZ	112	ARG	6.0
10	CL	101	TRP	6.0
3	CC	188	ASP	6.0
59	DZ	585	ALA	6.0
25	C1	2	SER	6.0
3	CC	52	PRO	6.0
10	AL	120	LEU	6.0
3	AC	197	LEU	5.9
9	AK	89	ALA	5.9
3	AC	175	PRO	5.9
3	AC	14	LYS	5.9
56	BW	3	C	5.9
9	CK	85	ASP	5.9
42	DI	30	GLY	5.9
1	AA	2168	C	5.8
56	DW	15	G	5.8
3	CC	216	THR	5.8
55	BV	24	A	5.8
3	AC	28	ARG	5.8
9	CK	98	LYS	5.8
59	DZ	614	GLU	5.8
56	DW	4	C	5.8
9	CK	44	LEU	5.7
56	DW	2	C	5.7
3	CC	5	GLY	5.7
10	CL	109	LYS	5.7
59	BZ	424	LEU	5.7
59	DZ	640	ALA	5.7
3	CC	4	HIS	5.7
35	DB	132	LYS	5.7
56	BW	70	G	5.7
59	DZ	538	TYR	5.7
10	CL	97	GLY	5.7
59	DZ	461	ILE	5.7
27	C3	60	GLU	5.7
59	DZ	435	ASP	5.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	CC	165	ARG	5.6
3	CC	161	ARG	5.6
34	DA	1257	U	5.6
56	DW	18	G	5.6
28	C4	68	ARG	5.6
9	AK	105	PRO	5.6
10	CL	93	ARG	5.6
3	AC	64	SER	5.6
59	BZ	505	GLY	5.6
3	CC	211	ARG	5.6
59	BZ	681	LYS	5.5
34	DA	1030(C)	G	5.5
22	AY	1	MET	5.5
59	BZ	639	ASN	5.5
1	AA	932	C	5.5
3	CC	203	GLU	5.5
34	BA	1001(A)	G	5.5
59	BZ	93	GLU	5.5
1	CA	2111	C	5.5
3	AC	164	PHE	5.5
3	CC	65	LEU	5.5
3	AC	218	THR	5.5
59	DZ	470	PHE	5.5
3	AC	69	LEU	5.4
40	DG	156	TRP	5.4
10	CL	124	ALA	5.4
59	DZ	685	GLU	5.4
56	BW	20	U	5.4
1	CA	2139	C	5.4
3	AC	60	ARG	5.4
1	AA	2167	C	5.4
1	CA	229	A	5.4
9	CK	31	GLY	5.4
59	DZ	522	GLY	5.4
3	AC	200	HIS	5.4
9	CK	100	ASN	5.4
1	AA	1221	G	5.4
56	BW	15	G	5.4
59	DZ	501	THR	5.4
1	CA	1090	U	5.4
10	AL	93	ARG	5.4
10	CL	75	SER	5.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	CA	2145	C	5.3
59	DZ	595	GLN	5.3
10	CL	96	VAL	5.3
1	AA	942	A	5.3
3	CC	39	ASP	5.3
3	AC	171	ALA	5.3
59	BZ	421	GLN	5.3
59	DZ	506	GLN	5.3
3	AC	26	ALA	5.3
59	BZ	231	TYR	5.3
10	AL	95	LYS	5.3
59	DZ	468	ARG	5.3
3	AC	23	ILE	5.3
59	DZ	559	PRO	5.3
10	CL	112	MET	5.2
10	CL	85	GLU	5.2
59	BZ	415	PRO	5.2
1	CA	1091	G	5.2
3	CC	197	LEU	5.2
3	CC	34	ALA	5.2
10	AL	124	ALA	5.2
59	DZ	569	ASP	5.2
3	AC	13	GLU	5.2
23	CZ	106	GLY	5.2
40	DG	81	GLY	5.2
34	BA	1003	G	5.2
52	DS	30	LEU	5.2
59	BZ	530	VAL	5.2
59	DZ	474	ALA	5.2
9	CK	105	PRO	5.2
1	AA	935	C	5.1
3	AC	160	GLY	5.1
36	BC	2	GLY	5.1
3	AC	30	VAL	5.1
3	AC	204	GLY	5.1
59	DZ	670	VAL	5.1
47	DN	38	GLY	5.1
59	BZ	426	GLN	5.1
3	AC	162	ILE	5.1
59	BZ	435	ASP	5.1
3	CC	204	GLY	5.1
59	DZ	612	THR	5.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
10	CL	111	LYS	5.1
59	DZ	528	ALA	5.1
9	CK	125	LEU	5.1
3	CC	31	LYS	5.1
9	CK	39	ALA	5.1
59	DZ	683	VAL	5.1
1	AA	2160	C	5.1
59	DZ	491	VAL	5.1
3	CC	185	LYS	5.1
59	BZ	473	ASP	5.1
59	DZ	655	TYR	5.1
10	CL	136	VAL	5.0
56	DW	22	G	5.0
59	BZ	444	PRO	5.0
55	DV	14	A	5.0
1	AA	2165	C	5.0
59	BZ	432	ALA	5.0
59	DZ	686	LYS	5.0
3	AC	50	ILE	5.0
59	DZ	471	LYS	5.0
34	DA	1030(D)	A	5.0
3	AC	194	ILE	5.0
3	CC	50	ILE	4.9
3	CC	33	LEU	4.9
10	AL	100	THR	4.9
10	AL	85	GLU	4.9
59	DZ	680	PRO	4.9
59	DZ	520	GLY	4.9
25	A1	2	SER	4.9
56	DW	14	A	4.9
1	CA	2156	G	4.9
3	CC	62	THR	4.8
1	AA	1555	C	4.8
59	DZ	405	PRO	4.8
59	DZ	664	GLN	4.8
3	AC	9	ARG	4.8
23	CZ	107	THR	4.8
35	BB	136	VAL	4.8
3	CC	32	GLU	4.8
52	DS	71	LEU	4.8
46	DM	121	LYS	4.8
59	BZ	227	ILE	4.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	CC	38	PHE	4.8
42	DI	7	THR	4.8
10	AL	132	ARG	4.8
52	DS	64	GLU	4.8
59	DZ	413	ILE	4.8
34	DA	1033	G	4.8
36	DC	64	VAL	4.8
59	DZ	541	ALA	4.8
52	DS	35	SER	4.7
34	DA	1001	A	4.7
59	BZ	597	GLY	4.7
23	CZ	156	LYS	4.7
34	BA	1030(A)	G	4.7
59	DZ	662	LYS	4.7
1	CA	2140	C	4.7
3	CC	181	PHE	4.7
3	CC	8	TYR	4.7
28	C4	56	VAL	4.7
56	BW	14	A	4.7
23	AZ	114	GLY	4.7
10	CL	79	ARG	4.7
47	DN	25	VAL	4.7
1	AA	931	C	4.7
1	AA	2166	U	4.7
59	BZ	454	MET	4.7
59	DZ	616	TYR	4.7
59	BZ	418	LYS	4.7
9	CK	77	PRO	4.7
9	CK	57	THR	4.6
3	CC	6	LYS	4.6
3	AC	24	ASP	4.6
1	CA	2147	G	4.6
3	CC	14	LYS	4.6
46	DM	82	MET	4.6
59	BZ	576	ASP	4.6
3	AC	195	ARG	4.6
59	BZ	540	PRO	4.6
59	DZ	543	GLN	4.6
1	CA	2154	G	4.6
43	DJ	71	LEU	4.6
3	AC	27	ALA	4.6
59	DZ	584	ILE	4.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	AC	211	ARG	4.6
1	CA	1086	A	4.6
55	DV	23	A	4.6
1	CA	1089	G	4.6
3	CC	45	HIS	4.6
3	CC	167	ASP	4.6
1	CA	1509	C	4.6
59	DZ	494	GLU	4.6
40	BG	80	VAL	4.5
59	BZ	449	THR	4.5
56	BW	2	C	4.5
1	AA	2131	U	4.5
10	CL	78	ILE	4.5
3	AC	40	GLU	4.5
3	AC	71	LYS	4.5
3	AC	198	GLU	4.5
1	CA	2148	G	4.5
9	CK	103	GLY	4.5
34	DA	1035	A	4.5
59	DZ	615	GLU	4.5
46	BM	121	LYS	4.5
1	AA	2138	G	4.5
34	DA	1002	G	4.5
59	DZ	87	HIS	4.5
10	AL	127	ILE	4.4
3	CC	43	GLU	4.4
59	DZ	476	VAL	4.4
1	CA	2159	G	4.4
10	AL	102	GLU	4.4
46	BM	122	LYS	4.4
1	CA	2112	G	4.4
3	CC	9	ARG	4.4
35	DB	139	LYS	4.4
1	AA	2147	G	4.4
59	DZ	682	GLN	4.4
36	DC	188	LEU	4.4
10	AL	79	ARG	4.4
56	BW	44	G	4.4
56	DW	56	C	4.4
56	DW	31	A	4.4
23	CZ	114	GLY	4.4
34	BA	202	U	4.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
35	DB	135	GLN	4.4
47	BN	2	ALA	4.4
9	CK	86	PRO	4.4
9	CK	65	GLU	4.4
34	DA	1532	U	4.4
1	CA	885	C	4.4
9	CK	118	THR	4.4
3	AC	186	LEU	4.4
10	AL	84	LEU	4.4
59	DZ	635	GLU	4.4
59	DZ	530	VAL	4.4
56	DW	13	C	4.3
59	DZ	551	GLN	4.3
9	AK	54	ALA	4.3
9	CK	119	ALA	4.3
43	DJ	9	ARG	4.3
56	BW	69	G	4.3
56	DW	23	A	4.3
59	BZ	594	VAL	4.3
59	DZ	689	LYS	4.3
59	BZ	413	ILE	4.3
59	DZ	489	LYS	4.3
23	AZ	107	THR	4.3
40	DG	79	ARG	4.3
55	BV	12	A	4.3
59	BZ	468	ARG	4.3
58	BY	20	U	4.3
10	AL	111	LYS	4.3
34	BA	1030(D)	A	4.3
34	BA	1031	G	4.3
23	AZ	144	LEU	4.3
52	DS	12	ASP	4.3
9	AK	131	MET	4.3
3	AC	213	VAL	4.3
3	AC	58	ASN	4.3
56	DW	58	A	4.3
59	DZ	598	ASP	4.3
10	AL	99	ILE	4.3
59	DZ	663	THR	4.3
40	BG	79	ARG	4.3
34	BA	1035	A	4.3
28	A4	56	VAL	4.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
10	AL	98	ARG	4.3
9	CK	37	THR	4.2
3	AC	70	GLY	4.2
9	CK	56	ASN	4.2
35	DB	228	GLY	4.2
59	BZ	430	ARG	4.2
59	DZ	407	PRO	4.2
52	BS	71	LEU	4.2
59	BZ	428	LEU	4.2
3	CC	215	VAL	4.2
9	CK	24	PHE	4.2
43	BJ	98	ILE	4.2
3	AC	43	GLU	4.2
3	AC	163	GLU	4.2
36	DC	189	ALA	4.2
34	BA	1030(C)	G	4.2
3	CC	202	PRO	4.2
36	DC	196	LEU	4.2
56	DW	67	C	4.2
43	DJ	74	ILE	4.2
56	BW	1	G	4.2
1	AA	2163	G	4.2
34	DA	1026	G	4.2
1	CA	888	C	4.2
1	CA	1079	C	4.2
3	AC	167	ASP	4.2
10	AL	137	GLU	4.1
34	DA	1021	G	4.1
59	DZ	540	PRO	4.1
59	DZ	597	GLY	4.1
35	DB	187	LEU	4.1
55	DV	22	U	4.1
59	BZ	457	LEU	4.1
8	CH	49	VAL	4.1
10	CL	92	GLY	4.1
10	CL	128	ALA	4.1
34	DA	1531	A	4.1
47	DN	2	ALA	4.1
59	DZ	455	GLY	4.1
59	DZ	529	ILE	4.1
59	BZ	433	GLU	4.1
10	AL	82	ALA	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	CA	2141	G	4.1
59	DZ	433	GLU	4.1
56	DW	59	U	4.1
59	BZ	500	GLN	4.1
59	DZ	575	VAL	4.1
1	AA	934	A	4.1
52	DS	6	LYS	4.1
43	DJ	47	PHE	4.1
3	CC	198	GLU	4.1
46	DM	120	LYS	4.1
9	AK	104	ILE	4.1
59	DZ	539	ILE	4.1
59	BZ	641	GLN	4.1
3	AC	31	LYS	4.1
10	AL	114	ASP	4.1
52	DS	32	LYS	4.1
46	DM	119	GLY	4.1
59	DZ	454	MET	4.1
35	BB	135	GLN	4.1
3	AC	206	LYS	4.1
3	CC	53	ARG	4.0
10	CL	132	ARG	4.0
56	DW	60	U	4.1
58	DY	53	G	4.1
59	DZ	581	ALA	4.0
59	DZ	638	GLY	4.0
10	CL	104	VAL	4.0
59	DZ	676	TYR	4.0
59	DZ	660	ARG	4.0
59	DZ	436	PRO	4.0
59	DZ	586	GLY	4.0
34	DA	1032	G	4.0
3	CC	13	GLU	4.0
3	AC	177	GLY	4.0
9	AK	99	SER	4.0
59	BZ	411	VAL	4.0
40	BG	83	ALA	4.0
59	DZ	408	VAL	4.0
59	DZ	505	GLY	4.0
10	AL	88	ALA	4.0
59	DZ	617	MET	4.0
3	AC	180	SER	4.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
9	CK	46	GLN	4.0
34	BA	204	U	4.0
3	CC	226	ASN	4.0
59	BZ	577	SER	4.0
3	AC	29	LEU	4.0
3	AC	188	ASP	3.9
3	AC	224	ARG	3.9
3	AC	4	HIS	3.9
59	DZ	502	GLY	3.9
3	CC	186	LEU	3.9
3	AC	220	GLY	3.9
40	BG	85	TYR	3.9
56	DW	19	G	3.9
3	AC	182	PRO	3.9
42	DI	27	THR	3.9
59	DZ	630	GLN	3.9
3	CC	64	SER	3.9
59	DZ	469	GLU	3.9
3	CC	196	ALA	3.9
59	DZ	448	GLN	3.9
59	DZ	40	HIS	3.9
59	BZ	423	LYS	3.9
59	DZ	460	GLU	3.9
59	BZ	470	PHE	3.9
3	AC	66	PRO	3.9
52	DS	26	GLY	3.9
59	DZ	523	PHE	3.9
59	DZ	458	HIS	3.9
47	DN	34	TYR	3.9
52	BS	40	ILE	3.9
36	DC	87	LEU	3.9
59	DZ	567	LEU	3.9
42	DI	42	ARG	3.8
58	DY	35	A	3.8
9	CK	129	PRO	3.8
1	CA	1082	U	3.8
55	BV	23	A	3.8
10	AL	81	ALA	3.8
59	DZ	446	THR	3.8
36	DC	39	ILE	3.8
23	CZ	108	PRO	3.8
1	CA	2131	G	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	CA	652(B)	A	3.8
1	CA	887	A	3.8
23	AZ	113	ALA	3.8
59	DZ	645	ALA	3.8
16	CS	58	LEU	3.8
56	DW	49	C	3.8
59	DZ	434	GLU	3.8
59	DZ	457	LEU	3.8
42	DI	9	ARG	3.8
58	DY	34	G	3.8
3	CC	22	THR	3.8
59	DZ	527	ASN	3.8
59	DZ	423	LYS	3.8
59	DZ	447	GLY	3.8
10	AL	107	ILE	3.8
51	BR	22	VAL	3.8
59	DZ	601	ILE	3.8
43	DJ	40	LEU	3.8
10	AL	90	LYS	3.8
9	CK	52	PHE	3.8
28	A4	55	ARG	3.8
3	AC	189	ASN	3.8
47	DN	39	LEU	3.8
59	DZ	517	LEU	3.8
24	C0	3	HIS	3.8
1	CA	2160	G	3.8
59	BZ	194	THR	3.8
34	BA	1030	C	3.8
35	DB	136	VAL	3.8
59	BZ	602	LEU	3.7
59	BZ	616	TYR	3.7
1	CA	1104	C	3.7
9	CK	76	GLY	3.7
46	DM	98	VAL	3.7
3	AC	41	THR	3.7
9	CK	23	SER	3.7
34	BA	1034	G	3.7
3	CC	213	VAL	3.7
59	DZ	631	ILE	3.7
59	DZ	519	ARG	3.7
1	CA	1103	A	3.7
1	CA	2144	U	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
36	BC	190	ARG	3.7
3	AC	46	ALA	3.7
56	BW	6	G	3.7
23	AZ	115	GLY	3.7
1	CA	2113	U	3.7
1	AA	1114	G	3.7
3	AC	191	ARG	3.7
3	AC	202	PRO	3.7
3	AC	209	PHE	3.7
52	BS	80	TYR	3.7
28	A4	52	THR	3.7
1	CA	1094	U	3.7
1	CA	2114	A	3.7
9	AK	97	ALA	3.7
1	CA	1083	U	3.7
1	CA	2142	C	3.7
59	BZ	634	MET	3.7
36	DC	190	ARG	3.7
59	BZ	578	SER	3.7
59	DZ	623	ASP	3.6
9	CK	88	ALA	3.6
40	DG	80	VAL	3.6
1	CA	1026	U	3.6
1	AA	2134	G	3.6
1	AA	2183	C	3.6
35	DB	133	LYS	3.6
59	DZ	512	ILE	3.6
59	DZ	666	ARG	3.6
59	DZ	641	GLN	3.6
59	BZ	436	PRO	3.6
1	AA	1143	U	3.6
10	CL	86	LYS	3.6
3	AC	187	ALA	3.6
46	BM	2	ALA	3.6
3	AC	68	GLY	3.6
59	BZ	642	VAL	3.6
59	BZ	670	VAL	3.6
40	DG	78	ARG	3.6
1	CA	1081	U	3.6
1	CA	1095	A	3.6
3	AC	10	ALA	3.6
35	DB	121	LEU	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
59	DZ	431	LEU	3.6
3	AC	67	HIS	3.6
56	DW	24	G	3.6
59	DZ	160	ARG	3.6
59	DZ	578	SER	3.6
59	BZ	434	GLU	3.6
51	DR	23	LYS	3.6
56	BW	19	G	3.6
59	DZ	600	VAL	3.6
56	BW	13	C	3.5
55	DV	13	A	3.5
56	BW	21	A	3.5
1	CA	2138	C	3.5
23	AZ	147	GLY	3.5
3	CC	225	ILE	3.5
59	DZ	438	PHE	3.5
36	DC	187	ALA	3.5
1	CA	2116	G	3.5
3	AC	193	PHE	3.5
9	CK	42	GLN	3.5
59	DZ	596	LYS	3.5
44	DK	25	TYR	3.5
56	DW	28	G	3.5
58	DY	57	G	3.5
3	AC	25	GLU	3.5
9	CK	106	GLN	3.5
59	DZ	514	VAL	3.5
4	AD	276	LYS	3.5
56	DW	29	G	3.5
59	BZ	489	LYS	3.5
59	DZ	637	ARG	3.5
3	AC	38	PHE	3.5
56	DW	45	U	3.5
59	DZ	443	HIS	3.5
24	C0	75	LEU	3.5
10	AL	139	VAL	3.5
1	CA	1060	U	3.5
43	DJ	72	VAL	3.5
59	BZ	638	GLY	3.4
9	CK	45	LYS	3.4
59	DZ	629	GLY	3.4
21	CX	68	ARG	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
56	BW	45	U	3.4
1	CA	1058	G	3.4
59	BZ	671	MET	3.4
46	DM	78	ILE	3.4
59	BZ	612	THR	3.4
3	CC	209	PHE	3.4
59	BZ	420	ASP	3.4
59	DZ	654	GLY	3.4
34	DA	1034	G	3.4
23	CZ	115	GLY	3.4
7	CG	2	PRO	3.4
10	AL	115	LEU	3.4
35	DB	131	PRO	3.4
43	BJ	72	VAL	3.4
56	BW	23	A	3.4
52	BS	48	THR	3.4
1	CA	2132	U	3.4
43	DJ	27	ALA	3.4
58	BY	35	A	3.4
56	BW	5	G	3.4
56	DW	10	G	3.4
1	AA	2161	C	3.4
10	CL	134	MET	3.4
59	DZ	437	THR	3.4
9	AK	101	PRO	3.3
1	CA	1068	G	3.3
1	CA	1102	C	3.3
55	DV	21	C	3.3
56	BW	22	G	3.3
58	DY	19	G	3.3
40	BG	78	ARG	3.3
36	DC	197	GLY	3.3
43	DJ	6	ILE	3.3
1	CA	652(U)	G	3.3
22	CY	55	TYR	3.3
43	DJ	73	ASP	3.3
3	AC	15	VAL	3.3
3	AC	173	HIS	3.3
28	C4	67	TYR	3.3
3	AC	165	ARG	3.3
40	DG	8	GLU	3.3
28	A4	50	VAL	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
59	BZ	463	VAL	3.3
59	BZ	414	GLU	3.3
56	BW	7	A	3.3
9	CK	54	ALA	3.3
56	BW	65	G	3.3
52	BS	84	GLY	3.3
1	CA	883	G	3.3
1	CA	2125	G	3.3
40	BG	156	TRP	3.3
1	AA	2141	A	3.3
43	BJ	10	GLY	3.3
34	BA	1029	C	3.3
56	DW	48	C	3.3
59	DZ	642	VAL	3.3
10	AL	133	SER	3.2
58	DY	56	C	3.2
59	BZ	412	ALA	3.2
59	BZ	689	LYS	3.2
36	DC	159	GLY	3.2
1	AA	698	G	3.2
59	BZ	425	SER	3.2
36	DC	32	LEU	3.2
40	BG	81	GLY	3.2
42	BI	8	GLY	3.2
59	BZ	537	GLU	3.2
59	DZ	513	LYS	3.2
59	BZ	474	ALA	3.2
3	AC	208	THR	3.2
59	DZ	459	LEU	3.2
3	CC	214	TYR	3.2
35	BB	133	LYS	3.2
21	CX	1	MET	3.2
59	DZ	624	LEU	3.2
59	BZ	546	ILE	3.2
59	DZ	561	VAL	3.2
11	CN	8	GLN	3.2
59	DZ	677	GLN	3.2
34	BA	1026	G	3.2
10	CL	118	THR	3.2
58	DY	36	A	3.2
3	CC	201	LYS	3.2
35	DB	164	VAL	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	CC	25	GLU	3.2
9	CK	78	SER	3.2
10	AL	76	TYR	3.2
10	AL	101	TRP	3.2
59	DZ	587	SER	3.2
56	BW	4	C	3.2
1	CA	652(C)	G	3.2
34	DA	1031	G	3.2
41	DH	99	GLU	3.2
35	DB	140	HIS	3.2
35	DB	229	VAL	3.2
1	CA	1098	A	3.1
34	DA	1004	A	3.1
9	CK	26	LEU	3.1
23	CZ	149	SER	3.1
59	DZ	475	ASN	3.1
59	BZ	459	LEU	3.1
1	CA	886	C	3.1
9	CK	122	VAL	3.1
59	DZ	560	VAL	3.1
40	BG	154	TYR	3.1
40	DG	154	TYR	3.1
52	DS	80	TYR	3.1
59	DZ	572	TYR	3.1
3	CC	222	SER	3.1
10	AL	122	ALA	3.1
43	DJ	89	ASP	3.1
59	BZ	493	VAL	3.1
34	BA	1028	C	3.1
3	AC	178	LYS	3.1
9	CK	73	GLY	3.1
23	CZ	96	VAL	3.1
59	BZ	541	ALA	3.1
42	BI	4	TYR	3.1
59	DZ	568	TYR	3.1
1	AA	1113	A	3.1
1	CA	1077	A	3.1
24	C0	8	GLY	3.1
27	C3	59	VAL	3.1
37	DD	23	GLY	3.1
56	DW	50	U	3.1
59	DZ	537	GLU	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	AC	21	TYR	3.1
28	C4	32	TYR	3.1
52	DS	44	MET	3.1
35	DB	214	ILE	3.1
43	DJ	38	ILE	3.1
59	BZ	535	PRO	3.1
36	DC	198	VAL	3.1
1	AA	1141	A	3.1
46	DM	92	HIS	3.1
59	BZ	491	VAL	3.1
59	BZ	615	GLU	3.1
34	BA	1257	U	3.1
1	CA	884	C	3.1
34	DA	1042	G	3.1
58	DY	18	G	3.1
35	BB	233	SER	3.0
3	CC	193	PHE	3.0
35	DB	122	PHE	3.0
1	AA	2162	C	3.0
21	CX	69	TYR	3.0
59	DZ	599	PRO	3.0
21	CX	92	LEU	3.0
59	DZ	627	ARG	3.0
34	BA	1001	A	3.0
34	DA	1043	C	3.0
28	C4	50	VAL	3.0
59	BZ	447	GLY	3.0
23	CZ	50	GLN	3.0
56	DW	68	C	3.0
43	BJ	5	ARG	3.0
56	DW	12	U	3.0
59	BZ	438	PHE	3.0
59	DZ	515	GLU	3.0
1	AA	2174	G	3.0
56	DW	30	G	3.0
56	BW	49	C	3.0
3	CC	206	LYS	3.0
59	DZ	235	GLU	3.0
1	AA	2176	G	3.0
34	DA	204	U	3.0
59	DZ	91	THR	3.0
59	DZ	687	LEU	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
10	AL	97	GLY	3.0
46	DM	102	ARG	3.0
9	CK	4	LYS	3.0
1	CA	1093	G	3.0
56	DW	57	G	3.0
34	DA	1040	U	3.0
34	BA	1039	C	3.0
59	BZ	442	THR	3.0
59	DZ	576	ASP	3.0
59	DZ	580	MET	3.0
43	DJ	26	ALA	3.0
3	AC	210	LEU	3.0
24	C0	7	LEU	3.0
28	C4	59	PHE	3.0
42	DI	18	PHE	3.0
34	DA	1003	G	3.0
47	DN	35	ARG	3.0
58	DY	52	G	3.0
1	CA	2143	C	3.0
35	DB	48	MET	3.0
59	DZ	613	PRO	2.9
52	DS	29	ARG	2.9
52	DS	61	TYR	2.9
1	CA	2168	G	2.9
43	BJ	73	ASP	2.9
43	DJ	98	ILE	2.9
36	DC	91	LEU	2.9
9	CK	30	GLN	2.9
1	AA	2164	C	2.9
52	DS	4	SER	2.9
56	BW	68	C	2.9
3	AC	185	LYS	2.9
4	CD	262	ARG	2.9
59	BZ	499	ARG	2.9
38	DE	31	LEU	2.9
59	BZ	613	PRO	2.9
10	AL	110	GLN	2.9
9	AK	37	THR	2.9
1	CA	2157	G	2.9
3	AC	181	PHE	2.9
34	BA	1033	G	2.9
43	DJ	85	LEU	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	AA	2135	U	2.9
59	BZ	680	PRO	2.9
59	BZ	494	GLU	2.9
9	CK	132	ASP	2.9
1	CA	1080	C	2.9
1	CA	2804	C	2.9
3	AC	212	SER	2.9
59	DZ	481	VAL	2.9
59	DZ	618	GLY	2.9
1	AA	218	A	2.9
1	AA	2153	G	2.9
1	CA	1085	A	2.9
34	BA	1447	A	2.9
1	AA	2159	C	2.9
23	AZ	143	GLY	2.9
28	C4	44	THR	2.9
23	CZ	169	GLU	2.9
37	BD	179	GLU	2.9
1	CA	882	G	2.9
1	CA	2110	G	2.9
1	CA	2149	G	2.9
9	CK	47	ASN	2.9
59	BZ	688	ILE	2.9
3	CC	49	GLY	2.9
28	C4	49	PHE	2.9
52	DS	39	THR	2.9
59	BZ	417	THR	2.9
59	BZ	640	ALA	2.9
3	CC	54	ARG	2.9
1	CA	896	A	2.9
43	BJ	38	ILE	2.9
51	DR	21	LYS	2.9
46	BM	24	GLY	2.9
28	A4	66	SER	2.9
1	CA	2167	U	2.9
10	CL	119	ASP	2.9
22	CY	46	LYS	2.9
42	DI	36	TYR	2.9
26	A2	70	GLN	2.8
22	CY	63	LYS	2.8
59	BZ	658	ASP	2.8
35	DB	203	GLY	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
54	DU	6	ARG	2.8
59	BZ	495	GLY	2.8
59	DZ	542	VAL	2.8
9	CK	74	LEU	2.8
1	CA	1059	G	2.8
34	BA	723	U	2.8
56	BW	56	C	2.8
46	DM	64	TRP	2.8
49	DP	48	TRP	2.8
59	BZ	458	HIS	2.8
3	AC	61	GLY	2.8
42	DI	54	ASP	2.8
59	BZ	665	GLY	2.8
46	DM	42	ALA	2.8
1	AA	2180	A	2.8
1	CA	2153	G	2.8
42	DI	66	ARG	2.8
23	AZ	146	ILE	2.8
47	DN	36	PHE	2.8
52	DS	82	GLY	2.8
36	BC	91	LEU	2.8
59	BZ	635	GLU	2.8
1	CA	2158	A	2.8
56	DW	21	A	2.8
52	DS	48	THR	2.8
25	A1	98	LEU	2.8
35	BB	78	GLN	2.8
59	BZ	429	ALA	2.8
7	AG	51	ARG	2.8
31	A7	47	ARG	2.8
1	AA	1072	U	2.8
7	CG	182	LYS	2.8
1	AA	34	C	2.8
34	DA	1027	C	2.8
59	DZ	411	VAL	2.8
57	DX	70	G	2.8
40	BG	4	ARG	2.8
1	AA	1142	A	2.8
56	BW	67	C	2.8
47	DN	4	LYS	2.8
52	DS	81	ARG	2.8
59	BZ	232	LEU	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
59	DZ	555	LEU	2.8
1	CA	1536	C	2.8
1	AA	2177	G	2.8
8	CH	29	PRO	2.8
52	DS	31	ILE	2.8
23	CZ	139	VAL	2.8
36	DC	204	LEU	2.8
1	CA	652(T)	C	2.8
23	CZ	152	ALA	2.8
52	DS	65	ASN	2.7
53	BT	9	ASN	2.7
3	AC	53	ARG	2.7
8	CH	13	LYS	2.7
9	CK	19	ARG	2.7
10	CL	102	GLU	2.7
59	BZ	523	PHE	2.7
9	CK	58	LEU	2.7
34	DA	1030	C	2.7
1	CA	1046	A	2.7
3	CC	23	ILE	2.7
59	BZ	431	LEU	2.7
1	AA	2178	G	2.7
57	DX	4	G	2.7
9	AK	83	TYR	2.7
16	CS	57	LYS	2.7
59	DZ	532	GLY	2.7
3	CC	227	PRO	2.7
7	AG	49	ASP	2.7
35	DB	138	LEU	2.7
41	DH	61	VAL	2.7
6	AF	17	ARG	2.7
9	CK	126	ALA	2.7
59	BZ	596	LYS	2.7
1	CA	1074	G	2.7
23	CZ	162	GLU	2.7
28	C4	52	THR	2.7
38	DE	144	THR	2.7
59	BZ	507	TYR	2.7
59	DZ	678	GLU	2.7
1	CA	645	C	2.7
1	CA	2803	C	2.7
35	DB	115	LEU	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
42	DI	17	VAL	2.7
43	BJ	71	LEU	2.7
47	DN	61	TRP	2.7
51	DR	58	LEU	2.7
59	DZ	608	VAL	2.7
36	BC	126	ARG	2.7
59	DZ	573	HIS	2.7
52	BS	27	GLU	2.7
26	C2	1	MET	2.7
1	AA	2169	G	2.7
34	BA	163	C	2.7
3	CC	191	ARG	2.7
36	BC	204	LEU	2.7
52	BS	20	LEU	2.7
52	DS	67	VAL	2.7
59	DZ	492	ASP	2.7
59	DZ	510	VAL	2.7
36	BC	193	TYR	2.7
3	AC	12	LEU	2.7
3	CC	20	VAL	2.7
24	A0	3	HIS	2.7
47	BN	11	LYS	2.7
28	A4	68	ARG	2.7
41	DH	122	ARG	2.7
1	CA	898	C	2.7
7	CG	19	LEU	2.7
42	DI	26	VAL	2.7
59	BZ	408	VAL	2.7
59	DZ	493	VAL	2.7
56	DW	44	G	2.7
3	CC	26	ALA	2.7
41	DH	128	GLY	2.7
3	AC	55	SER	2.7
43	BJ	35	SER	2.7
40	DG	4	ARG	2.7
54	DU	24	ARG	2.7
3	AC	216	THR	2.7
3	CC	29	LEU	2.7
52	DS	16	LEU	2.7
59	BZ	575	VAL	2.7
59	DZ	619	ASP	2.7
52	DS	42	PRO	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	CC	7	ARG	2.7
47	DN	13	THR	2.6
52	DS	13	ASP	2.6
59	DZ	554	PRO	2.6
59	DZ	412	ALA	2.6
42	BI	12	GLU	2.6
58	BY	47	U	2.6
43	BJ	29	ARG	2.6
1	CA	652(D)	C	2.6
34	DA	1038	C	2.6
56	DW	47	U	2.6
34	BA	1024	G	2.6
9	CK	107	VAL	2.6
40	BG	84	ASN	2.6
55	BV	13	A	2.6
59	DZ	531	GLY	2.6
59	DZ	611	THR	2.6
23	CZ	138	GLU	2.6
37	BD	163	GLU	2.6
59	DZ	236	GLU	2.6
59	BZ	498	ILE	2.6
1	CA	1061	U	2.6
3	CC	195	ARG	2.6
42	DI	4	TYR	2.6
41	DH	54	ASP	2.6
59	DZ	477	GLY	2.6
1	CA	2166	G	2.6
59	BZ	346	LYS	2.6
54	DU	17	THR	2.6
59	BZ	677	GLN	2.6
40	DG	16	LEU	2.6
3	AC	47	LYS	2.6
3	CC	47	LYS	2.6
42	BI	17	VAL	2.6
59	BZ	522	GLY	2.6
59	BZ	579	GLU	2.6
1	CA	2115	G	2.6
56	BW	24	G	2.6
59	BZ	653	PHE	2.6
1	CA	2118	U	2.6
47	DN	49	HIS	2.6
59	BZ	455	GLY	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
59	BZ	514	VAL	2.6
3	AC	217	THR	2.6
47	DN	50	LYS	2.6
1	CA	1092	C	2.6
52	DS	34	TRP	2.6
42	DI	87	GLN	2.6
1	CA	1105	U	2.6
9	CK	36	GLU	2.6
13	CP	92	GLU	2.6
59	DZ	83	ASP	2.6
40	DG	7	ALA	2.6
42	DI	8	GLY	2.5
1	CA	2169	A	2.5
52	BS	83	HIS	2.5
1	AA	696	C	2.5
3	AC	39	ASP	2.5
3	AC	201	LYS	2.5
28	C4	69	LYS	2.5
1	AA	930	G	2.5
35	DB	226	ARG	2.5
42	DI	5	TYR	2.5
51	BR	24	ALA	2.5
10	CL	91	PRO	2.5
59	BZ	630	GLN	2.5
35	DB	118	LEU	2.5
36	DC	206	GLU	2.5
35	BB	139	LYS	2.5
35	DB	19	HIS	2.5
59	BZ	393	ASP	2.5
58	BY	56	C	2.5
3	AC	36	ALA	2.5
10	AL	116	ASN	2.5
19	CV	101	GLY	2.5
3	CC	224	ARG	2.5
23	CZ	150	LEU	2.5
42	DI	19	LEU	2.5
54	DU	14	TRP	2.5
48	BO	88	ARG	2.5
3	AC	63	VAL	2.5
1	AA	2139	A	2.5
1	CA	34	C	2.5
1	CA	1057	A	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	CA	2170	A	2.5
8	AH	2	SER	2.5
33	C9	37	GLY	2.5
43	DJ	77	PRO	2.5
54	DU	16	GLY	2.5
59	DZ	508	GLY	2.5
59	DZ	590	ILE	2.5
9	AK	27	VAL	2.5
27	C3	6	VAL	2.5
52	BS	19	VAL	2.5
59	BZ	437	THR	2.5
59	DZ	440	VAL	2.5
43	BJ	7	LYS	2.5
34	DA	1037	C	2.5
56	DW	11	C	2.5
59	DZ	414	GLU	2.5
34	BA	1044	A	2.5
46	BM	119	GLY	2.5
1	CA	879	G	2.5
35	BB	140	HIS	2.5
59	BZ	598	ASP	2.5
28	A4	53	GLU	2.5
38	DE	81	GLU	2.5
54	DU	10	ARG	2.5
8	CH	2	SER	2.5
1	AA	2803	A	2.5
1	CA	2134	A	2.5
43	BJ	8	LEU	2.5
56	DW	36	A	2.5
59	BZ	475	ASN	2.5
59	DZ	588	MET	2.5
13	CP	149	GLU	2.5
40	BG	8	GLU	2.5
56	BW	57	G	2.5
35	BB	123	ALA	2.5
42	DI	15	ALA	2.5
9	AK	77	PRO	2.5
46	BM	34	LEU	2.5
56	DW	41	C	2.5
34	DA	1020	U	2.5
59	BZ	617	MET	2.5
7	CG	181	ARG	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
9	CK	121	ASP	2.5
3	AC	35	THR	2.5
3	AC	196	ALA	2.5
3	CC	27	ALA	2.5
1	CA	1072	C	2.5
1	CA	614(A)	U	2.5
27	A3	60	GLU	2.5
36	DC	89	GLU	2.5
41	BH	122	ARG	2.5
42	DI	128	ARG	2.5
8	CH	57	ASP	2.5
9	AK	72	ASP	2.5
59	BZ	619	ASP	2.5
3	AC	179	ALA	2.5
9	CK	67	GLY	2.5
19	AV	101	GLY	2.5
42	DI	67	GLY	2.5
52	DS	25	LYS	2.5
59	DZ	511	LYS	2.5
3	AC	11	LEU	2.5
10	AL	105	LEU	2.5
58	BY	6	G	2.5
23	AZ	108	PRO	2.4
1	CA	1075	C	2.4
42	DI	75	ASP	2.4
21	AX	94	GLY	2.4
56	DW	9	A	2.4
42	BI	46	ALA	2.4
59	BZ	-4	ALA	2.4
9	CK	40	LEU	2.4
36	DC	19	GLU	2.4
58	BY	34	G	2.4
59	DZ	552	SER	2.4
3	CC	223	VAL	2.4
34	BA	1037	C	2.4
10	AL	118	THR	2.4
42	DI	64	THR	2.4
59	BZ	229	LEU	2.4
59	BZ	450	ILE	2.4
43	DJ	39	PRO	2.4
59	DZ	490	PRO	2.4
34	DA	1022	G	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
59	BZ	586	GLY	2.4
7	AG	50	ALA	2.4
9	CK	104	ILE	2.4
23	CZ	46	LYS	2.4
58	DY	58	A	2.4
3	AC	223	VAL	2.4
59	BZ	545	GLY	2.4
59	BZ	595	GLN	2.4
1	AA	1109	G	2.4
1	CA	878	A	2.4
34	BA	161	A	2.4
51	DR	22	VAL	2.4
59	DZ	636	PRO	2.4
34	BA	841	U	2.4
35	DB	227	GLY	2.4
36	DC	63	ASN	2.4
42	DI	105	ASP	2.4
59	DZ	393	ASP	2.4
1	AA	2181	G	2.4
34	DA	80	G	2.4
58	DY	24	G	2.4
59	DZ	570	GLY	2.4
59	DZ	556	ILE	2.4
59	BZ	509	HIS	2.4
1	AA	1105	G	2.4
34	BA	1032	G	2.4
54	BU	15	ARG	2.4
59	BZ	628	ARG	2.4
9	CK	114	GLY	2.4
59	BZ	588	MET	2.4
1	AA	943	C	2.4
46	BM	115	LYS	2.4
52	DS	10	PHE	2.4
10	AL	104	VAL	2.4
49	BP	38	TYR	2.4
56	BW	47	U	2.4
56	BW	60	U	2.4
58	BY	33	U	2.4
34	DA	1261	A	2.4
58	DY	21	A	2.4
49	DP	19	ILE	2.4
8	CH	123	PHE	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
52	DS	47	HIS	2.3
35	BB	229	VAL	2.3
59	BZ	570	GLY	2.3
4	AD	275	LYS	2.3
51	BR	23	LYS	2.3
3	CC	55	SER	2.3
1	AA	697	C	2.3
35	BB	228	GLY	2.3
47	DN	16	PHE	2.3
56	DW	61	C	2.3
59	BZ	87	HIS	2.3
8	CH	44	VAL	2.3
59	BZ	448	GLN	2.3
31	A7	48	LYS	2.3
55	DV	20	U	2.3
17	AT	1	MET	2.3
8	CH	105	LEU	2.3
9	CK	117	LEU	2.3
56	BW	18	G	2.3
10	AL	129	GLY	2.3
55	BV	14	A	2.3
58	BY	36	A	2.3
7	CG	49	ASP	2.3
43	DJ	46	ARG	2.3
9	CK	32	LEU	2.3
35	BB	222	ILE	2.3
42	DI	29	ASN	2.3
22	CY	45	VAL	2.3
34	BA	1006	C	2.3
35	DB	137	ARG	2.3
1	AA	1220	U	2.3
56	DW	66	U	2.3
58	DY	47	U	2.3
35	DB	222	ILE	2.3
59	BZ	446	THR	2.3
59	BZ	611	THR	2.3
59	DZ	449	THR	2.3
59	DZ	497	PHE	2.3
1	CA	2135	A	2.3
1	CA	2152	G	2.3
23	CZ	140	ASP	2.3
34	BA	1137	C	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
55	DV	15	A	2.3
59	DZ	535	PRO	2.3
10	AL	112	MET	2.3
24	C0	2	ALA	2.3
3	CC	194	ILE	2.3
59	BZ	590	ILE	2.3
36	BC	171	GLY	2.3
51	BR	29	PHE	2.3
54	DU	9	ARG	2.3
23	AZ	141	VAL	2.3
8	CH	119	GLU	2.3
1	AA	2191	A	2.3
9	AK	102	LYS	2.3
7	CG	77	ILE	2.3
9	CK	48	GLY	2.3
46	DM	88	ARG	2.3
59	BZ	539	ILE	2.3
59	DZ	498	ILE	2.3
9	CK	108	LYS	2.3
47	DN	8	GLU	2.3
3	AC	183	PRO	2.3
34	DA	723	U	2.3
37	BD	3	ARG	2.3
38	DE	21	ALA	2.3
1	CA	1847	A	2.3
34	DA	994	A	2.3
59	DZ	227	ILE	2.3
1	CA	2123	G	2.3
35	BB	122	PHE	2.3
58	BY	19	G	2.3
59	DZ	525	PHE	2.3
23	CZ	170	THR	2.3
26	A2	12	GLU	2.3
59	BZ	476	VAL	2.3
36	DC	6	HIS	2.3
9	AK	74	LEU	2.3
59	DZ	466	LEU	2.3
52	BS	61	TYR	2.3
47	DN	32	SER	2.2
59	BZ	401	SER	2.2
52	DS	78	ARG	2.2
59	BZ	492	ASP	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	AC	168	LYS	2.2
36	DC	81	GLY	2.2
45	DL	64	TYR	2.2
8	CH	46	GLU	2.2
58	DY	61	C	2.2
59	BZ	506	GLN	2.2
1	AA	2187	G	2.2
10	CL	100	THR	2.2
42	DI	115	GLY	2.2
59	BZ	672	PHE	2.2
59	DZ	558	PHE	2.2
59	DZ	582	PHE	2.2
40	DG	85	TYR	2.2
34	BA	1027	C	2.2
40	DG	86	GLN	2.2
52	DS	79	THR	2.2
59	DZ	566	THR	2.2
1	AA	2190	G	2.2
35	BB	232	PRO	2.2
3	AC	8	TYR	2.2
59	BZ	340	TYR	2.2
59	DZ	-10	ARG	2.2
1	CA	2119	A	2.2
43	DJ	65	LEU	2.2
40	BG	153	HIS	2.2
52	DS	17	GLU	2.2
59	BZ	669	PHE	2.2
1	AA	2173	G	2.2
58	DY	22	G	2.2
59	DZ	671	MET	2.2
1	CA	652(V)	C	2.2
35	DB	165	VAL	2.2
35	DB	38	GLY	2.2
16	CS	3	ARG	2.2
28	A4	62	ARG	2.2
34	DA	1044	A	2.2
47	BN	17	LYS	2.2
52	DS	40	ILE	2.2
34	DA	79	G	2.2
42	BI	41	VAL	2.2
20	CW	112	GLY	2.2
59	DZ	189	GLY	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
24	A0	7	LEU	2.2
52	DS	37	ARG	2.2
54	BU	9	ARG	2.2
59	DZ	7	ASN	2.2
9	AK	52	PHE	2.2
56	DW	51	U	2.2
1	AA	2195	A	2.2
27	C3	2	PRO	2.2
42	DI	103	THR	2.2
59	BZ	529	ILE	2.2
59	DZ	516	PRO	2.2
59	DZ	643	ILE	2.2
42	DI	124	GLN	2.2
1	CA	881	G	2.2
37	DD	179	GLU	2.2
34	BA	91	C	2.2
43	DJ	99	LYS	2.2
46	DM	91	ARG	2.2
46	DM	93	ARG	2.2
34	BA	203	U	2.2
34	DA	202	U	2.2
59	BZ	687	LEU	2.2
30	C6	54	ILE	2.2
59	DZ	509	HIS	2.2
59	DZ	550	MET	2.2
1	CA	2117	A	2.2
34	BA	1531	A	2.2
45	DL	69	TYR	2.2
47	DN	31	ARG	2.2
52	DS	28	LYS	2.2
59	DZ	545	GLY	2.2
1	AA	933	C	2.2
35	BB	37	ASN	2.2
47	DN	37	PHE	2.2
40	DG	120	ILE	2.2
52	DS	56	GLN	2.2
3	CC	218	THR	2.2
31	C7	47	ARG	2.2
1	AA	1144	A	2.2
34	BA	1004	A	2.2
35	BB	148	TYR	2.2
36	DC	194	GLY	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
42	DI	59	PHE	2.1
34	DA	1029	C	2.1
58	BY	45	U	2.1
35	DB	95	GLN	2.1
1	AA	2146	G	2.1
8	CH	32	GLU	2.1
10	AL	75	SER	2.1
23	CZ	153	SER	2.1
47	BN	51	GLY	2.1
1	AA	2148	A	2.1
34	DA	1005	A	2.1
34	DA	1447	A	2.1
9	CK	64	LYS	2.1
59	DZ	589	ALA	2.1
43	DJ	70	ARG	2.1
1	AA	694	G	2.1
1	CA	1062	G	2.1
35	DB	7	VAL	2.1
36	DC	195	VAL	2.1
22	CY	90	LEU	2.1
43	DJ	7	LYS	2.1
40	DG	42	ILE	2.1
1	AA	2133	C	2.1
1	CA	2161	C	2.1
56	BW	48	C	2.1
43	BJ	34	VAL	2.1
3	AC	169	THR	2.1
22	CY	4	LYS	2.1
34	DA	1017	G	2.1
13	CP	88	LEU	2.1
59	DZ	212	TYR	2.1
35	BB	45	GLN	2.1
1	CA	1084	A	2.1
53	DT	40	ALA	2.1
8	AH	174	GLY	2.1
47	DN	33	VAL	2.1
54	DU	2	GLY	2.1
56	BW	25	C	2.1
3	CC	169	THR	2.1
54	BU	17	THR	2.1
59	DZ	659	LEU	2.1
1	CA	1963	U	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
42	DI	61	ALA	2.1
59	BZ	528	ALA	2.1
1	CA	1073	A	2.1
8	CH	113	VAL	2.1
52	BS	4	SER	2.1
52	DS	38	SER	2.1
16	CS	29	PHE	2.1
18	CU	89	GLU	2.1
59	DZ	233	GLU	2.1
56	BW	59	U	2.1
59	BZ	593	ALA	2.1
59	DZ	450	ILE	2.1
1	CA	1063	G	2.1
27	C3	5	LYS	2.1
1	AA	1878	A	2.1
3	AC	42	VAL	2.1
23	CZ	141	VAL	2.1
34	BA	160	A	2.1
35	BB	165	VAL	2.1
59	DZ	652	MET	2.1
35	BB	137	ARG	2.1
9	CK	38	HIS	2.1
52	BS	21	GLU	2.1
9	CK	130	THR	2.1
1	AA	271	U	2.1
59	BZ	532	GLY	2.1
37	DD	47	ARG	2.1
56	DW	34	G	2.1
35	DB	124	SER	2.1
42	BI	106	ALA	2.1
43	BJ	100	THR	2.1
57	BX	47	U	2.1
17	AT	37	GLY	2.1
13	CP	95	VAL	2.1
29	C5	60	VAL	2.1
48	BO	6	GLU	2.1
52	DS	60	VAL	2.1
1	CA	2833	G	2.1
34	DA	1024	G	2.1
40	DG	18	TYR	2.0
52	DS	62	ILE	2.0
9	AK	130	THR	2.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
34	BA	1446	U	2.0
59	DZ	93	GLU	2.0
59	DZ	536	LYS	2.0
3	CC	30	VAL	2.0
59	DZ	533	VAL	2.0
59	BZ	466	LEU	2.0
1	CA	2137	C	2.0
1	CA	2165	G	2.0
52	BS	49	ILE	2.0
52	DS	49	ILE	2.0
59	BZ	464	ASP	2.0
9	AK	31	GLY	2.0
9	CK	102	LYS	2.0
36	BC	89	GLU	2.0
43	BJ	97	GLU	2.0
52	BS	85	LYS	2.0
59	BZ	657	THR	2.0
59	DZ	225	GLU	2.0
41	DH	129	VAL	2.0
52	BS	41	VAL	2.0
42	BI	50	LEU	2.0
43	DJ	69	ASN	2.0
59	DZ	229	LEU	2.0
52	DS	83	HIS	2.0
36	DC	62	ASP	2.0
1	CA	897	C	2.0
43	DJ	35	SER	2.0
1	CA	899	A	2.0
1	CA	2802	G	2.0
58	BY	5	G	2.0
43	DJ	100	THR	2.0
9	CK	131	MET	2.0
24	C0	63	VAL	2.0
7	CG	51	ARG	2.0
59	BZ	544	LYS	2.0
9	AK	73	GLY	2.0
9	AK	103	GLY	2.0
59	BZ	409	ILE	2.0
36	BC	189	ALA	2.0
47	BN	59	ALA	2.0
59	BZ	667	GLY	2.0
1	AA	2130	C	2.0

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Mol	Chain	Res	Type	RSRZ
34	BA	1005	A	2.0
7	CG	43	LEU	2.0
47	DN	15	LYS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å <sup>2</sup> )	Q<0.9
58	5MU	BY	54	21/22	0.30	0.33	217,217,217,217	0
58	PSU	DY	55	20/21	0.51	0.54	222,222,222,222	0
56	PSU	DW	55	20/21	0.52	0.44	190,190,190,190	0
56	4SU	DW	8	20/21	0.58	0.49	225,225,225,225	0
58	4SU	DY	8	20/21	0.62	0.21	193,193,193,193	0
56	4SU	BW	8	20/21	0.64	0.28	200,200,200,200	0
58	7MG	DY	46	24/25	0.64	0.24	206,206,206,206	0
58	PSU	BY	55	20/21	0.64	0.24	205,205,205,205	0
56	7MG	DW	46	24/25	0.65	0.34	244,244,244,244	0
58	MIA	DY	37	22/30	0.68	0.29	156,156,156,156	0
58	7MG	BY	46	24/25	0.71	0.21	200,200,200,200	0
58	4SU	BY	8	20/21	0.71	0.21	191,191,191,191	0
56	PSU	BW	55	20/21	0.72	0.31	113,113,113,113	0
58	5MU	DY	54	21/22	0.72	0.36	200,200,200,200	0
56	7MG	BW	46	24/25	0.72	0.27	203,203,203,203	0
58	PSU	DY	32	20/21	0.82	0.20	154,154,154,154	0
58	PSU	DY	39	20/21	0.84	0.21	138,138,138,138	0
58	PSU	BY	32	20/21	0.84	0.20	126,126,126,126	0
58	MIA	BY	37	22/30	0.85	0.18	118,118,118,118	0
57	31H	DX	76	32/33	0.87	0.31	58,58,58,58	4
56	5MU	DW	54	21/22	0.87	0.22	118,118,118,118	0
56	PSU	DW	39	20/21	0.89	0.24	118,118,118,118	0
56	5MU	BW	54	21/22	0.89	0.25	89,89,89,89	0
56	PSU	DW	32	20/21	0.89	0.36	139,139,139,139	0
56	MIA	BW	37	29/30	0.90	0.30	95,95,95,95	1
56	MIA	DW	37	22/30	0.90	0.27	116,116,116,116	0
56	PSU	BW	39	20/21	0.90	0.23	96,96,96,96	0
57	4SU	DX	8	20/21	0.90	0.14	96,96,96,96	0
57	PSU	DX	55	20/21	0.91	0.13	95,95,95,95	0
56	F3N	DW	76	33/34	0.91	0.35	75,75,75,75	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	PSU	BY	39	20/21	0.91	0.17	106,106,106,106	0
56	PSU	BW	32	20/21	0.92	0.21	110,110,110,110	0
57	4SU	BX	8	20/21	0.93	0.14	70,70,70,70	1
57	5MU	BX	54	21/22	0.93	0.17	85,85,85,85	0
57	5MC	DX	32	21/22	0.93	0.20	86,86,86,86	0
57	31H	BX	76	32/33	0.94	0.26	58,58,58,58	4
57	PSU	BX	55	20/21	0.94	0.13	74,74,74,74	0
57	5MU	DX	54	21/22	0.94	0.18	108,108,108,108	0
57	5MC	BX	32	21/22	0.95	0.17	65,65,65,65	0
56	F3N	BW	76	33/34	0.96	0.25	54,54,54,54	1

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	BA	1800	1/1	0.10	0.56	116,116,116,116	0
60	MG	CA	3543	1/1	0.17	0.55	114,114,114,114	0
60	MG	DA	1686	1/1	0.22	0.36	102,102,102,102	0
60	MG	CA	3491	1/1	0.26	0.61	99,99,99,99	0
60	MG	AA	3108	1/1	0.31	0.41	88,88,88,88	0
60	MG	CA	3527	1/1	0.34	0.38	83,83,83,83	0
60	MG	AA	3203	1/1	0.35	1.03	125,125,125,125	0
60	MG	CA	3206	1/1	0.37	0.65	109,109,109,109	0
60	MG	CA	3073	1/1	0.38	0.73	94,94,94,94	0
60	MG	CA	3550	1/1	0.39	0.36	88,88,88,88	0
60	MG	AA	3805	1/1	0.39	1.54	117,117,117,117	0
60	MG	CA	3653	1/1	0.41	0.51	102,102,102,102	0
60	MG	CA	3478	1/1	0.41	0.29	91,91,91,91	0
60	MG	AA	3136	1/1	0.42	0.46	74,74,74,74	0
60	MG	AA	3490	1/1	0.43	0.52	87,87,87,87	0
60	MG	DA	1715	1/1	0.43	0.46	87,87,87,87	0
60	MG	AA	3770	1/1	0.44	0.80	57,57,57,57	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
60	MG	CA	3098	1/1	0.45	1.04	90,90,90,90	0
60	MG	CA	3514	1/1	0.46	0.16	68,68,68,68	0
60	MG	AA	3040	1/1	0.47	0.13	93,93,93,93	0
60	MG	CB	3008	1/1	0.47	0.26	87,87,87,87	0
60	MG	CA	3031	1/1	0.48	0.73	102,102,102,102	0
60	MG	CA	3177	1/1	0.49	0.65	98,98,98,98	0
60	MG	CA	3139	1/1	0.50	0.53	83,83,83,83	0
60	MG	CA	3597	1/1	0.50	0.48	108,108,108,108	0
60	MG	DA	1615	1/1	0.51	0.52	87,87,87,87	0
60	MG	BK	3101	1/1	0.51	0.57	95,95,95,95	0
60	MG	CA	3481	1/1	0.51	0.24	86,86,86,86	0
60	MG	CA	3079	1/1	0.52	0.57	82,82,82,82	0
60	MG	CA	3042	1/1	0.52	0.89	84,84,84,84	0
60	MG	BA	1740	1/1	0.52	0.12	89,89,89,89	0
60	MG	AA	3736	1/1	0.53	0.37	74,74,74,74	0
60	MG	AA	3246	1/1	0.54	0.60	86,86,86,86	0
60	MG	CA	3581	1/1	0.54	0.22	100,100,100,100	0
60	MG	AA	3327	1/1	0.55	0.23	36,36,36,36	0
60	MG	BA	1779	1/1	0.55	0.33	82,82,82,82	0
60	MG	CA	3502	1/1	0.56	0.14	66,66,66,66	0
60	MG	AA	3225	1/1	0.56	0.89	91,91,91,91	0
60	MG	CA	3578	1/1	0.57	0.12	96,96,96,96	0
60	MG	CA	3070	1/1	0.57	0.57	78,78,78,78	0
60	MG	CA	3588	1/1	0.57	0.19	78,78,78,78	0
60	MG	AA	3271	1/1	0.58	0.29	81,81,81,81	0
60	MG	BA	1803	1/1	0.58	0.22	79,79,79,79	0
60	MG	CQ	201	1/1	0.58	0.76	85,85,85,85	0
60	MG	DA	1764	1/1	0.58	0.41	94,94,94,94	0
60	MG	CA	3090	1/1	0.59	0.46	98,98,98,98	0
60	MG	BA	1624	1/1	0.59	0.21	75,75,75,75	0
60	MG	BA	1709	1/1	0.59	0.27	96,96,96,96	0
60	MG	AA	3051	1/1	0.59	0.69	84,84,84,84	0
60	MG	DX	3001	1/1	0.59	0.41	75,75,75,75	0
60	MG	CA	3376	1/1	0.60	0.17	94,94,94,94	0
60	MG	DA	1671	1/1	0.60	0.65	77,77,77,77	0
60	MG	AA	3694	1/1	0.60	0.17	49,49,49,49	0
60	MG	DA	1753	1/1	0.61	0.26	85,85,85,85	0
60	MG	AA	3739	1/1	0.61	0.42	90,90,90,90	0
60	MG	AA	3242	1/1	0.61	0.20	69,69,69,69	0
60	MG	AA	3725	1/1	0.62	0.27	42,42,42,42	0
60	MG	CA	3575	1/1	0.62	0.47	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
60	MG	CA	3085	1/1	0.62	0.53	82,82,82,82	0
60	MG	CA	3049	1/1	0.62	0.29	63,63,63,63	0
60	MG	CA	3613	1/1	0.64	0.31	42,42,42,42	0
60	MG	CA	3622	1/1	0.64	0.17	106,106,106,106	0
60	MG	AA	3026	1/1	0.64	0.38	69,69,69,69	0
60	MG	CA	3101	1/1	0.64	0.11	86,86,86,86	0
60	MG	CA	3111	1/1	0.64	0.20	82,82,82,82	0
60	MG	BW	101	1/1	0.64	0.47	82,82,82,82	0
60	MG	AA	3579	1/1	0.65	0.14	66,66,66,66	0
60	MG	AA	3150	1/1	0.65	0.32	63,63,63,63	0
60	MG	BA	1706	1/1	0.65	0.25	82,82,82,82	0
60	MG	CA	3239	1/1	0.65	0.32	76,76,76,76	0
60	MG	DA	1623	1/1	0.65	0.38	70,70,70,70	0
60	MG	DA	1651	1/1	0.65	0.26	86,86,86,86	0
60	MG	DA	1610	1/1	0.66	0.29	59,59,59,59	0
60	MG	CA	3092	1/1	0.66	0.49	74,74,74,74	0
60	MG	CA	3506	1/1	0.66	0.25	120,120,120,120	0
60	MG	CA	3592	1/1	0.66	0.23	87,87,87,87	0
60	MG	CA	3212	1/1	0.66	0.10	78,78,78,78	0
60	MG	CA	3016	1/1	0.66	0.48	69,69,69,69	0
60	MG	AA	3070	1/1	0.66	0.35	68,68,68,68	0
60	MG	AA	3625	1/1	0.66	0.30	88,88,88,88	0
60	MG	AA	3664	1/1	0.66	0.21	94,94,94,94	0
60	MG	CA	3063	1/1	0.66	0.71	74,74,74,74	0
60	MG	CA	3526	1/1	0.67	0.13	69,69,69,69	0
60	MG	BA	1691	1/1	0.67	0.34	98,98,98,98	0
60	MG	CA	3199	1/1	0.67	0.58	92,92,92,92	0
60	MG	CA	3482	1/1	0.67	0.29	89,89,89,89	0
60	MG	BA	1703	1/1	0.67	0.22	65,65,65,65	0
60	MG	CB	3006	1/1	0.67	0.19	82,82,82,82	0
60	MG	DA	1739	1/1	0.67	0.43	85,85,85,85	0
60	MG	AA	3599	1/1	0.67	0.43	113,113,113,113	0
60	MG	AA	3692	1/1	0.67	0.48	86,86,86,86	0
60	MG	AA	3324	1/1	0.67	0.10	69,69,69,69	0
60	MG	CA	3348	1/1	0.68	0.14	78,78,78,78	0
60	MG	AA	3263	1/1	0.68	0.44	75,75,75,75	0
60	MG	BA	1674	1/1	0.68	0.08	78,78,78,78	0
60	MG	BA	1722	1/1	0.68	0.29	86,86,86,86	0
60	MG	BX	112	1/1	0.68	0.21	78,78,78,78	0
60	MG	DA	1676	1/1	0.68	0.29	69,69,69,69	0
60	MG	DA	1734	1/1	0.69	0.28	75,75,75,75	0
60	MG	CA	3089	1/1	0.69	0.71	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
60	MG	AA	3192	1/1	0.69	0.42	69,69,69,69	0
60	MG	DA	1762	1/1	0.69	0.16	86,86,86,86	0
60	MG	DA	1704	1/1	0.69	0.31	83,83,83,83	0
60	MG	CA	3244	1/1	0.69	0.32	70,70,70,70	0
60	MG	DA	1608	1/1	0.70	0.50	79,79,79,79	0
60	MG	BA	1763	1/1	0.70	0.08	75,75,75,75	0
60	MG	AA	3537	1/1	0.70	0.12	90,90,90,90	0
60	MG	CA	3152	1/1	0.70	0.17	67,67,67,67	0
60	MG	CA	3664	1/1	0.70	0.31	69,69,69,69	0
60	MG	CA	3590	1/1	0.70	0.53	78,78,78,78	0
60	MG	CA	3234	1/1	0.70	0.35	96,96,96,96	0
60	MG	AA	3648	1/1	0.70	0.17	80,80,80,80	0
60	MG	BY	3002	1/1	0.71	0.17	83,83,83,83	0
60	MG	CA	3245	1/1	0.71	0.30	53,53,53,53	0
60	MG	AA	3766	1/1	0.71	0.22	69,69,69,69	0
60	MG	AA	3015	1/1	0.71	0.46	74,74,74,74	0
60	MG	AA	3773	1/1	0.71	0.20	77,77,77,77	0
60	MG	AA	3783	1/1	0.71	0.38	68,68,68,68	0
60	MG	AA	3632	1/1	0.71	0.26	97,97,97,97	0
60	MG	AA	3828	1/1	0.71	0.55	68,68,68,68	0
60	MG	AA	3249	1/1	0.71	0.45	64,64,64,64	0
60	MG	AA	3183	1/1	0.72	0.97	89,89,89,89	0
60	MG	AA	3571	1/1	0.72	0.11	53,53,53,53	0
60	MG	BA	1737	1/1	0.72	0.27	87,87,87,87	0
60	MG	AQ	3002	1/1	0.72	0.31	79,79,79,79	0
60	MG	CA	3303	1/1	0.72	0.28	52,52,52,52	0
60	MG	CA	3311	1/1	0.72	0.29	54,54,54,54	0
60	MG	AA	3689	1/1	0.72	0.16	84,84,84,84	0
60	MG	CA	3374	1/1	0.72	0.15	74,74,74,74	0
60	MG	BA	1767	1/1	0.72	0.27	73,73,73,73	0
60	MG	DA	1765	1/1	0.72	0.26	66,66,66,66	0
60	MG	BA	1770	1/1	0.72	0.12	62,62,62,62	0
60	MG	CA	3529	1/1	0.73	0.31	69,69,69,69	0
60	MG	CA	3616	1/1	0.73	0.34	62,62,62,62	0
60	MG	CA	3535	1/1	0.73	0.19	74,74,74,74	0
60	MG	AB	3014	1/1	0.73	0.23	70,70,70,70	0
60	MG	CA	3282	1/1	0.73	0.38	75,75,75,75	0
60	MG	AA	3059	1/1	0.73	0.52	62,62,62,62	0
60	MG	BA	1790	1/1	0.73	0.32	87,87,87,87	0
60	MG	CE	303	1/1	0.73	0.39	55,55,55,55	0
60	MG	DA	1743	1/1	0.73	0.13	83,83,83,83	0
60	MG	CA	3059	1/1	0.73	0.38	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	A0	104	1/1	0.73	0.80	81,81,81,81	0
60	MG	BA	1699	1/1	0.73	0.19	70,70,70,70	0
60	MG	CA	3411	1/1	0.73	0.24	49,49,49,49	0
60	MG	CA	3475	1/1	0.73	0.17	55,55,55,55	0
60	MG	AA	3755	1/1	0.74	0.23	77,77,77,77	0
60	MG	AA	3088	1/1	0.74	0.53	42,42,42,42	0
60	MG	AA	3221	1/1	0.74	0.16	72,72,72,72	0
60	MG	CA	3241	1/1	0.74	0.19	69,69,69,69	0
60	MG	AD	307	1/1	0.74	0.20	54,54,54,54	0
60	MG	CF	306	1/1	0.74	0.94	85,85,85,85	0
60	MG	CA	3194	1/1	0.74	0.55	87,87,87,87	0
60	MG	CA	3195	1/1	0.74	0.18	36,36,36,36	0
60	MG	CA	3542	1/1	0.74	0.20	82,82,82,82	0
60	MG	DA	1611	1/1	0.74	0.23	80,80,80,80	0
60	MG	AA	3347	1/1	0.74	0.32	63,63,63,63	0
60	MG	AA	3578	1/1	0.74	0.37	71,71,71,71	0
60	MG	CA	3642	1/1	0.74	0.11	75,75,75,75	0
60	MG	AA	3582	1/1	0.75	0.36	78,78,78,78	0
60	MG	AA	3234	1/1	0.75	0.42	58,58,58,58	0
60	MG	AA	3245	1/1	0.75	0.22	79,79,79,79	0
60	MG	CA	3524	1/1	0.75	0.29	87,87,87,87	0
60	MG	BA	1804	1/1	0.75	0.47	94,94,94,94	0
60	MG	AA	3751	1/1	0.75	0.20	76,76,76,76	0
60	MG	CA	3183	1/1	0.75	0.43	83,83,83,83	0
60	MG	AA	3713	1/1	0.75	0.52	48,48,48,48	0
60	MG	CA	3247	1/1	0.75	0.16	45,45,45,45	0
60	MG	CA	3619	1/1	0.75	0.36	78,78,78,78	0
60	MG	AA	3763	1/1	0.75	0.25	66,66,66,66	0
60	MG	CA	3067	1/1	0.75	0.60	82,82,82,82	0
60	MG	DW	3001	1/1	0.75	0.80	90,90,90,90	0
60	MG	CA	3652	1/1	0.75	0.23	79,79,79,79	0
60	MG	CA	3298	1/1	0.76	0.21	68,68,68,68	0
60	MG	AA	3480	1/1	0.76	0.13	78,78,78,78	0
60	MG	CA	3505	1/1	0.76	0.26	66,66,66,66	0
60	MG	AF	304	1/1	0.76	0.43	69,69,69,69	0
60	MG	CA	3511	1/1	0.76	0.34	66,66,66,66	0
60	MG	AA	3700	1/1	0.76	0.21	48,48,48,48	0
60	MG	CA	3113	1/1	0.76	0.47	75,75,75,75	0
60	MG	CA	3083	1/1	0.76	0.22	80,80,80,80	0
60	MG	AA	3638	1/1	0.76	0.36	72,72,72,72	0
60	MG	AA	3487	1/1	0.76	0.10	66,66,66,66	0
60	MG	BA	1646	1/1	0.76	0.52	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	BA	1670	1/1	0.76	0.30	76,76,76,76	0
60	MG	CA	3631	1/1	0.76	0.29	88,88,88,88	0
60	MG	CA	3094	1/1	0.76	0.35	92,92,92,92	0
60	MG	CA	3273	1/1	0.77	0.21	42,42,42,42	0
60	MG	AX	102	1/1	0.77	0.37	78,78,78,78	0
60	MG	AA	3002	1/1	0.77	0.24	53,53,53,53	0
60	MG	CA	3103	1/1	0.77	0.19	80,80,80,80	0
60	MG	AA	3548	1/1	0.77	0.13	69,69,69,69	0
60	MG	BA	1627	1/1	0.77	0.21	63,63,63,63	0
60	MG	AB	3019	1/1	0.77	0.18	61,61,61,61	0
60	MG	CA	3091	1/1	0.77	0.40	60,60,60,60	0
60	MG	DA	1620	1/1	0.77	0.23	68,68,68,68	0
60	MG	BA	1657	1/1	0.77	0.47	72,72,72,72	0
60	MG	DA	1631	1/1	0.77	0.22	55,55,55,55	0
60	MG	CA	3032	1/1	0.77	0.43	67,67,67,67	0
60	MG	CA	3096	1/1	0.77	0.28	75,75,75,75	0
60	MG	AA	3164	1/1	0.78	0.21	106,106,106,106	0
60	MG	BA	1786	1/1	0.78	0.33	79,79,79,79	0
60	MG	CA	3431	1/1	0.78	0.17	80,80,80,80	0
60	MG	DA	1634	1/1	0.78	0.34	66,66,66,66	0
60	MG	CA	3467	1/1	0.78	0.44	99,99,99,99	0
60	MG	CA	3645	1/1	0.78	0.13	78,78,78,78	0
60	MG	CA	3018	1/1	0.78	0.18	59,59,59,59	0
60	MG	A2	3001	1/1	0.78	0.25	62,62,62,62	0
60	MG	DA	1702	1/1	0.78	0.27	58,58,58,58	0
60	MG	BA	1621	1/1	0.78	0.66	78,78,78,78	0
60	MG	AA	3152	1/1	0.78	0.41	80,80,80,80	0
60	MG	BA	1752	1/1	0.78	0.07	48,48,48,48	0
60	MG	DA	1735	1/1	0.78	0.10	75,75,75,75	0
60	MG	CB	3012	1/1	0.78	0.16	74,74,74,74	0
60	MG	CA	3187	1/1	0.78	0.32	70,70,70,70	0
60	MG	CA	3057	1/1	0.78	0.71	77,77,77,77	0
60	MG	AA	3732	1/1	0.78	0.18	63,63,63,63	0
60	MG	CA	3509	1/1	0.78	0.19	52,52,52,52	0
60	MG	BN	503	1/1	0.78	0.23	61,61,61,61	0
60	MG	DE	201	1/1	0.78	0.31	93,93,93,93	0
60	MG	BA	1629	1/1	0.78	0.25	71,71,71,71	0
60	MG	AA	3541	1/1	0.78	0.20	61,61,61,61	0
60	MG	BW	102	1/1	0.79	0.20	75,75,75,75	0
60	MG	AA	3210	1/1	0.79	0.55	106,106,106,106	0
60	MG	CA	3633	1/1	0.79	0.19	85,85,85,85	0
60	MG	AA	3793	1/1	0.79	0.35	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3202	1/1	0.79	0.32	67,67,67,67	0
60	MG	CA	3015	1/1	0.79	0.48	66,66,66,66	0
60	MG	AA	3146	1/1	0.79	0.20	53,53,53,53	0
60	MG	AZ	5001	1/1	0.79	0.11	67,67,67,67	0
60	MG	CA	3474	1/1	0.79	0.14	72,72,72,72	0
60	MG	CA	3080	1/1	0.79	0.58	78,78,78,78	0
60	MG	A0	101	1/1	0.79	0.23	88,88,88,88	0
60	MG	CA	3122	1/1	0.79	0.33	95,95,95,95	0
60	MG	AA	3161	1/1	0.79	0.57	89,89,89,89	0
60	MG	CA	3483	1/1	0.79	0.17	67,67,67,67	0
60	MG	CA	3087	1/1	0.79	0.41	107,107,107,107	0
60	MG	CA	3155	1/1	0.79	0.48	69,69,69,69	0
60	MG	AA	3640	1/1	0.79	0.49	74,74,74,74	0
60	MG	CA	3291	1/1	0.79	0.17	74,74,74,74	0
60	MG	AA	3093	1/1	0.79	0.86	81,81,81,81	0
60	MG	AA	3744	1/1	0.79	0.15	79,79,79,79	0
60	MG	BA	1671	1/1	0.80	0.36	71,71,71,71	0
60	MG	DA	1602	1/1	0.80	0.22	65,65,65,65	0
60	MG	CA	3445	1/1	0.80	0.36	70,70,70,70	0
60	MG	AA	3486	1/1	0.80	0.21	34,34,34,34	0
60	MG	CA	3222	1/1	0.80	0.70	81,81,81,81	0
60	MG	BA	1689	1/1	0.80	0.29	65,65,65,65	0
60	MG	CA	3235	1/1	0.80	0.37	78,78,78,78	0
60	MG	AA	3110	1/1	0.80	0.48	57,57,57,57	0
60	MG	AA	3649	1/1	0.80	0.07	78,78,78,78	0
60	MG	CA	3599	1/1	0.80	0.09	75,75,75,75	0
60	MG	AA	3165	1/1	0.80	0.41	64,64,64,64	0
60	MG	BA	1808	1/1	0.80	0.16	80,80,80,80	0
60	MG	AA	3182	1/1	0.80	0.27	73,73,73,73	0
60	MG	CA	3249	1/1	0.80	0.18	67,67,67,67	0
60	MG	AA	3605	1/1	0.80	0.11	66,66,66,66	0
60	MG	AA	3159	1/1	0.80	0.41	66,66,66,66	0
60	MG	AD	306	1/1	0.80	0.22	108,108,108,108	0
60	MG	BX	106	1/1	0.80	0.17	85,85,85,85	0
60	MG	CA	3521	1/1	0.80	0.34	59,59,59,59	0
60	MG	AA	3444	1/1	0.80	0.10	52,52,52,52	0
60	MG	CA	3659	1/1	0.80	0.35	72,72,72,72	0
60	MG	BA	1630	1/1	0.80	0.19	61,61,61,61	0
60	MG	BA	1757	1/1	0.80	0.35	63,63,63,63	0
60	MG	AD	309	1/1	0.80	0.34	58,58,58,58	0
60	MG	CB	3010	1/1	0.80	0.16	67,67,67,67	0
60	MG	AA	3702	1/1	0.80	0.44	45,45,45,45	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3407	1/1	0.80	0.28	41,41,41,41	0
60	MG	AA	3061	1/1	0.80	0.77	64,64,64,64	0
60	MG	CA	3043	1/1	0.81	0.19	75,75,75,75	0
60	MG	AA	3351	1/1	0.81	0.10	80,80,80,80	0
60	MG	CA	3296	1/1	0.81	0.14	61,61,61,61	0
60	MG	AA	3753	1/1	0.81	0.15	59,59,59,59	0
60	MG	BV	101	1/1	0.81	0.16	78,78,78,78	0
60	MG	AB	3005	1/1	0.81	0.17	70,70,70,70	0
60	MG	CA	3329	1/1	0.81	0.22	59,59,59,59	0
60	MG	AA	3585	1/1	0.81	0.15	60,60,60,60	0
60	MG	DA	1638	1/1	0.81	0.28	60,60,60,60	0
60	MG	CA	3628	1/1	0.81	0.12	76,76,76,76	0
60	MG	CA	3371	1/1	0.81	0.61	70,70,70,70	0
60	MG	AA	3758	1/1	0.81	0.35	70,70,70,70	0
60	MG	BA	1622	1/1	0.81	0.63	64,64,64,64	0
60	MG	CA	3387	1/1	0.81	0.40	73,73,73,73	0
60	MG	AA	3089	1/1	0.81	0.39	58,58,58,58	0
60	MG	BA	1788	1/1	0.81	0.17	79,79,79,79	0
60	MG	AA	3657	1/1	0.81	0.11	73,73,73,73	0
60	MG	CA	3151	1/1	0.81	0.21	66,66,66,66	0
60	MG	CA	3462	1/1	0.81	0.34	63,63,63,63	0
60	MG	AA	3321	1/1	0.81	0.08	45,45,45,45	0
60	MG	CA	3555	1/1	0.81	0.08	59,59,59,59	0
60	MG	AA	3018	1/1	0.81	0.66	55,55,55,55	0
60	MG	CA	3576	1/1	0.81	0.35	91,91,91,91	0
60	MG	CE	305	1/1	0.81	0.26	37,37,37,37	0
60	MG	CA	3156	1/1	0.81	1.42	92,92,92,92	0
60	MG	AA	3204	1/1	0.81	0.45	83,83,83,83	0
60	MG	AA	3098	1/1	0.81	0.29	65,65,65,65	0
60	MG	CA	3167	1/1	0.82	0.32	68,68,68,68	0
60	MG	CA	3169	1/1	0.82	0.28	65,65,65,65	0
60	MG	BX	103	1/1	0.82	0.08	88,88,88,88	0
60	MG	CA	3532	1/1	0.82	0.16	59,59,59,59	0
60	MG	AA	3005	1/1	0.82	0.20	63,63,63,63	0
60	MG	CA	3538	1/1	0.82	0.31	58,58,58,58	0
60	MG	AA	3127	1/1	0.82	0.45	83,83,83,83	0
60	MG	AA	3716	1/1	0.82	0.20	63,63,63,63	0
60	MG	AA	3639	1/1	0.82	0.23	74,74,74,74	0
60	MG	AA	3048	1/1	0.82	0.16	39,39,39,39	0
60	MG	DA	1614	1/1	0.82	0.15	71,71,71,71	0
60	MG	BA	1787	1/1	0.82	0.13	64,64,64,64	0
60	MG	CA	3030	1/1	0.82	0.43	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3027	1/1	0.82	0.55	85,85,85,85	0
60	MG	AA	3408	1/1	0.82	0.26	41,41,41,41	0
60	MG	CA	3459	1/1	0.82	0.12	46,46,46,46	0
60	MG	CA	3226	1/1	0.82	0.37	56,56,56,56	0
60	MG	BA	1601	1/1	0.82	0.19	66,66,66,66	0
60	MG	DA	1661	1/1	0.82	0.14	74,74,74,74	0
60	MG	AA	3829	1/1	0.82	0.40	89,89,89,89	0
60	MG	AA	3440	1/1	0.82	0.18	63,63,63,63	0
60	MG	DA	1677	1/1	0.82	0.38	67,67,67,67	0
60	MG	CA	3240	1/1	0.82	0.14	49,49,49,49	0
60	MG	DA	1700	1/1	0.82	0.21	66,66,66,66	0
60	MG	CA	3051	1/1	0.82	0.18	52,52,52,52	0
60	MG	AA	3056	1/1	0.82	0.49	72,72,72,72	0
60	MG	CA	3112	1/1	0.82	0.47	76,76,76,76	0
60	MG	CA	3487	1/1	0.82	0.29	64,64,64,64	0
60	MG	AA	3279	1/1	0.82	0.55	62,62,62,62	0
60	MG	DA	1737	1/1	0.82	0.40	73,73,73,73	0
60	MG	CA	3496	1/1	0.82	0.55	58,58,58,58	0
60	MG	AA	3299	1/1	0.82	0.18	64,64,64,64	0
60	MG	AA	3300	1/1	0.82	0.30	43,43,43,43	0
60	MG	DA	1757	1/1	0.82	0.12	77,77,77,77	0
60	MG	CA	3280	1/1	0.82	0.17	43,43,43,43	0
60	MG	CA	3281	1/1	0.82	0.20	74,74,74,74	0
60	MG	BA	1755	1/1	0.82	0.18	92,92,92,92	0
60	MG	DD	502	1/1	0.82	0.50	64,64,64,64	0
60	MG	CA	3071	1/1	0.82	0.31	53,53,53,53	0
60	MG	AA	3243	1/1	0.82	0.29	79,79,79,79	0
60	MG	CA	3077	1/1	0.82	0.28	62,62,62,62	0
60	MG	AA	3688	1/1	0.83	0.16	76,76,76,76	0
60	MG	C3	101	1/1	0.83	0.46	91,91,91,91	0
60	MG	BA	1672	1/1	0.83	0.22	61,61,61,61	0
60	MG	CA	3560	1/1	0.83	0.16	103,103,103,103	0
60	MG	AH	201	1/1	0.83	1.23	83,83,83,83	0
60	MG	AA	3479	1/1	0.83	0.14	66,66,66,66	0
60	MG	AA	3181	1/1	0.83	0.40	55,55,55,55	0
60	MG	AA	3767	1/1	0.83	0.29	75,75,75,75	0
60	MG	CA	3583	1/1	0.83	0.28	114,114,114,114	0
60	MG	AA	3265	1/1	0.83	0.36	64,64,64,64	0
60	MG	CA	3129	1/1	0.83	0.30	76,76,76,76	0
60	MG	CA	3132	1/1	0.83	0.19	67,67,67,67	0
60	MG	AA	3346	1/1	0.83	0.23	32,32,32,32	0
60	MG	CA	3146	1/1	0.83	0.31	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3250	1/1	0.83	0.17	69,69,69,69	0
60	MG	AA	3612	1/1	0.83	0.20	60,60,60,60	0
60	MG	DA	1673	1/1	0.83	0.40	68,68,68,68	0
60	MG	BA	1712	1/1	0.83	0.60	68,68,68,68	0
60	MG	AA	3489	1/1	0.83	0.32	39,39,39,39	0
60	MG	AA	3105	1/1	0.83	0.18	77,77,77,77	0
60	MG	AA	3036	1/1	0.83	0.21	63,63,63,63	0
60	MG	AA	3538	1/1	0.83	0.20	62,62,62,62	0
60	MG	AA	3230	1/1	0.83	0.34	55,55,55,55	0
60	MG	AA	3413	1/1	0.83	0.15	34,34,34,34	0
60	MG	DA	1718	1/1	0.83	0.11	66,66,66,66	0
60	MG	CA	3646	1/1	0.83	0.10	90,90,90,90	0
60	MG	BA	1758	1/1	0.83	0.18	56,56,56,56	0
60	MG	AA	3208	1/1	0.83	0.27	55,55,55,55	0
60	MG	BA	1766	1/1	0.83	0.16	81,81,81,81	0
60	MG	CA	3660	1/1	0.83	0.14	65,65,65,65	0
60	MG	DA	1749	1/1	0.83	0.23	72,72,72,72	0
60	MG	AA	3650	1/1	0.83	0.29	62,62,62,62	0
60	MG	AA	3443	1/1	0.83	0.21	58,58,58,58	0
60	MG	BA	1776	1/1	0.83	0.10	64,64,64,64	0
60	MG	CA	3533	1/1	0.83	0.14	63,63,63,63	0
60	MG	CA	3377	1/1	0.83	0.14	53,53,53,53	0
60	MG	AA	3252	1/1	0.83	0.37	76,76,76,76	0
60	MG	CA	3213	1/1	0.83	0.34	62,62,62,62	0
60	MG	DE	202	1/1	0.83	0.17	92,92,92,92	0
60	MG	DT	3001	1/1	0.83	0.25	59,59,59,59	0
60	MG	CF	301	1/1	0.83	0.45	61,61,61,61	0
60	MG	CA	3218	1/1	0.83	0.88	63,63,63,63	0
60	MG	DA	1621	1/1	0.84	0.08	69,69,69,69	0
60	MG	CA	3011	1/1	0.84	0.25	75,75,75,75	0
60	MG	CA	3498	1/1	0.84	0.34	68,68,68,68	0
60	MG	AA	3151	1/1	0.84	0.32	63,63,63,63	0
60	MG	AA	3442	1/1	0.84	0.13	73,73,73,73	0
60	MG	DA	1648	1/1	0.84	0.46	66,66,66,66	0
60	MG	AA	3654	1/1	0.84	0.25	81,81,81,81	0
60	MG	DA	1655	1/1	0.84	0.22	72,72,72,72	0
60	MG	BA	1696	1/1	0.84	0.14	84,84,84,84	0
60	MG	AA	3337	1/1	0.84	0.22	52,52,52,52	0
60	MG	CA	3341	1/1	0.84	0.19	35,35,35,35	0
60	MG	AA	3109	1/1	0.84	0.35	75,75,75,75	0
60	MG	CA	3355	1/1	0.84	0.13	71,71,71,71	0
60	MG	BA	1602	1/1	0.84	0.20	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3747	1/1	0.84	0.33	65,65,65,65	0
60	MG	AA	3615	1/1	0.84	0.39	65,65,65,65	0
60	MG	BA	1715	1/1	0.84	0.21	90,90,90,90	0
60	MG	CA	3383	1/1	0.84	0.34	66,66,66,66	0
60	MG	AA	3624	1/1	0.84	0.27	56,56,56,56	0
60	MG	AA	3543	1/1	0.84	0.17	84,84,84,84	0
60	MG	CA	3115	1/1	0.84	0.54	71,71,71,71	0
60	MG	AA	3175	1/1	0.84	0.33	50,50,50,50	1
60	MG	CA	3545	1/1	0.84	0.11	93,93,93,93	0
60	MG	AA	3202	1/1	0.84	0.12	46,46,46,46	0
60	MG	CA	3068	1/1	0.84	0.19	73,73,73,73	0
60	MG	CA	3069	1/1	0.84	0.28	66,66,66,66	0
60	MG	BA	1638	1/1	0.84	0.64	83,83,83,83	0
60	MG	AA	3764	1/1	0.84	0.38	48,48,48,48	0
60	MG	BX	102	1/1	0.84	0.10	78,78,78,78	0
60	MG	AA	3369	1/1	0.84	0.19	59,59,59,59	0
60	MG	DA	1767	1/1	0.84	0.56	88,88,88,88	0
60	MG	CA	3261	1/1	0.84	0.12	50,50,50,50	0
60	MG	CA	3584	1/1	0.84	0.27	91,91,91,91	0
60	MG	BX	105	1/1	0.84	0.09	87,87,87,87	0
60	MG	AA	3163	1/1	0.84	0.27	73,73,73,73	0
60	MG	AA	3768	1/1	0.84	0.35	67,67,67,67	0
60	MG	AA	3266	1/1	0.84	0.28	55,55,55,55	0
60	MG	BA	1733	1/1	0.85	0.09	57,57,57,57	0
60	MG	BA	1618	1/1	0.85	0.52	54,54,54,54	0
60	MG	CA	3081	1/1	0.85	0.41	69,69,69,69	0
60	MG	AA	3316	1/1	0.85	0.20	64,64,64,64	0
60	MG	AA	3580	1/1	0.85	0.14	26,26,26,26	0
60	MG	CA	3357	1/1	0.85	0.17	34,34,34,34	0
60	MG	CA	3366	1/1	0.85	0.24	60,60,60,60	0
60	MG	CA	3086	1/1	0.85	0.15	65,65,65,65	0
60	MG	AB	3010	1/1	0.85	0.09	56,56,56,56	1
60	MG	AA	3524	1/1	0.85	0.30	41,41,41,41	0
60	MG	CA	3548	1/1	0.85	0.12	53,53,53,53	0
60	MG	AA	3121	1/1	0.85	0.30	63,63,63,63	0
60	MG	BA	1759	1/1	0.85	0.14	60,60,60,60	0
60	MG	AB	3021	1/1	0.85	0.14	75,75,75,75	0
60	MG	CA	3573	1/1	0.85	0.12	82,82,82,82	0
60	MG	CA	3388	1/1	0.85	0.18	97,97,97,97	0
60	MG	CA	3397	1/1	0.85	0.10	80,80,80,80	0
60	MG	DA	1642	1/1	0.85	0.17	67,67,67,67	0
60	MG	CA	3219	1/1	0.85	0.32	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3410	1/1	0.85	0.19	72,72,72,72	0
60	MG	AA	3237	1/1	0.85	0.08	51,51,51,51	0
60	MG	CA	3412	1/1	0.85	0.21	52,52,52,52	0
60	MG	AA	3106	1/1	0.85	0.19	43,43,43,43	0
60	MG	CA	3589	1/1	0.85	0.16	67,67,67,67	0
60	MG	BA	1656	1/1	0.85	0.19	83,83,83,83	0
60	MG	AA	3412	1/1	0.85	0.16	58,58,58,58	0
60	MG	CA	3236	1/1	0.85	0.30	80,80,80,80	0
60	MG	AE	301	1/1	0.85	0.40	65,65,65,65	0
60	MG	CA	3607	1/1	0.85	0.18	76,76,76,76	0
60	MG	AF	301	1/1	0.85	0.20	49,49,49,49	0
60	MG	AA	3655	1/1	0.85	0.20	55,55,55,55	0
60	MG	AA	3544	1/1	0.85	0.17	16,16,16,16	0
60	MG	DA	1719	1/1	0.85	0.22	87,87,87,87	0
60	MG	CA	3055	1/1	0.85	0.29	77,77,77,77	0
60	MG	AA	3661	1/1	0.85	0.17	78,78,78,78	0
60	MG	CA	3058	1/1	0.85	0.44	74,74,74,74	0
60	MG	DA	1738	1/1	0.85	0.25	100,100,100,100	0
60	MG	AA	3160	1/1	0.85	0.48	96,96,96,96	0
60	MG	CA	3634	1/1	0.85	0.21	82,82,82,82	0
60	MG	DA	1748	1/1	0.85	0.18	78,78,78,78	0
60	MG	CA	3490	1/1	0.85	0.41	81,81,81,81	0
60	MG	AA	3789	1/1	0.85	0.21	71,71,71,71	0
60	MG	CA	3142	1/1	0.85	0.25	73,73,73,73	0
60	MG	DA	1758	1/1	0.85	0.35	80,80,80,80	0
60	MG	CA	3275	1/1	0.85	0.13	73,73,73,73	0
60	MG	AA	3745	1/1	0.85	0.28	42,42,42,42	0
60	MG	CA	3503	1/1	0.85	0.09	67,67,67,67	0
60	MG	AA	3795	1/1	0.85	0.28	26,26,26,26	1
60	MG	AA	3028	1/1	0.85	0.30	40,40,40,40	1
60	MG	AA	3806	1/1	0.85	0.55	56,56,56,56	0
60	MG	CA	3293	1/1	0.85	0.31	82,82,82,82	0
60	MG	AA	3441	1/1	0.85	0.18	62,62,62,62	0
60	MG	BA	1603	1/1	0.85	0.20	65,65,65,65	0
60	MG	BA	1609	1/1	0.85	0.20	77,77,77,77	0
60	MG	AE	304	1/1	0.86	0.53	70,70,70,70	0
60	MG	BA	1688	1/1	0.86	0.30	71,71,71,71	0
60	MG	CA	3497	1/1	0.86	0.18	85,85,85,85	0
60	MG	AA	3029	1/1	0.86	0.20	50,50,50,50	0
60	MG	AA	3595	1/1	0.86	0.18	60,60,60,60	0
60	MG	AG	202	1/1	0.86	0.08	69,69,69,69	0
60	MG	CE	301	1/1	0.86	0.61	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3265	1/1	0.86	0.19	66,66,66,66	0
60	MG	CE	304	1/1	0.86	0.74	74,74,74,74	0
60	MG	BX	111	1/1	0.86	0.14	67,67,67,67	0
60	MG	AA	3378	1/1	0.86	0.21	24,24,24,24	0
60	MG	AN	3001	1/1	0.86	0.47	64,64,64,64	0
60	MG	CA	3001	1/1	0.86	0.17	81,81,81,81	0
60	MG	CQ	203	1/1	0.86	0.28	62,62,62,62	0
60	MG	C0	102	1/1	0.86	0.08	56,56,56,56	0
60	MG	CA	3517	1/1	0.86	0.21	75,75,75,75	0
60	MG	CA	3005	1/1	0.86	0.18	69,69,69,69	0
60	MG	CA	3114	1/1	0.86	0.20	59,59,59,59	0
60	MG	DA	1609	1/1	0.86	0.18	49,49,49,49	0
60	MG	AQ	3001	1/1	0.86	0.26	56,56,56,56	0
60	MG	AA	3671	1/1	0.86	0.58	31,31,31,31	1
60	MG	AA	3177	1/1	0.86	0.21	43,43,43,43	0
60	MG	AA	3180	1/1	0.86	0.25	53,53,53,53	0
60	MG	CA	3021	1/1	0.86	0.33	91,91,91,91	0
60	MG	AA	3025	1/1	0.86	0.44	60,60,60,60	0
60	MG	CA	3338	1/1	0.86	0.14	58,58,58,58	0
60	MG	DA	1624	1/1	0.86	0.07	83,83,83,83	0
60	MG	CA	3540	1/1	0.86	0.24	71,71,71,71	0
60	MG	AA	3621	1/1	0.86	0.12	34,34,34,34	0
60	MG	A0	105	1/1	0.86	0.08	52,52,52,52	0
60	MG	AA	3425	1/1	0.86	0.17	40,40,40,40	0
60	MG	A4	502	1/1	0.86	0.18	81,81,81,81	0
60	MG	AA	3429	1/1	0.86	0.22	58,58,58,58	0
60	MG	AA	3708	1/1	0.86	0.30	71,71,71,71	0
60	MG	DA	1658	1/1	0.86	0.13	89,89,89,89	0
60	MG	AA	3631	1/1	0.86	0.39	74,74,74,74	0
60	MG	DA	1662	1/1	0.86	0.10	51,51,51,51	0
60	MG	BA	1607	1/1	0.86	0.11	64,64,64,64	0
60	MG	AA	3434	1/1	0.86	0.27	58,58,58,58	0
60	MG	CA	3382	1/1	0.86	0.18	70,70,70,70	0
60	MG	BA	1617	1/1	0.86	0.16	64,64,64,64	0
60	MG	CA	3386	1/1	0.86	0.14	79,79,79,79	0
60	MG	CA	3191	1/1	0.86	0.28	61,61,61,61	0
60	MG	AA	3438	1/1	0.86	0.21	75,75,75,75	0
60	MG	CA	3394	1/1	0.86	0.26	54,54,54,54	0
60	MG	AA	3727	1/1	0.86	0.16	64,64,64,64	0
60	MG	CA	3401	1/1	0.86	0.07	75,75,75,75	0
60	MG	AA	3132	1/1	0.86	0.45	43,43,43,43	0
60	MG	DA	1722	1/1	0.86	0.19	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	DA	1729	1/1	0.86	0.10	82,82,82,82	0
60	MG	CA	3201	1/1	0.86	0.32	70,70,70,70	0
60	MG	AA	3250	1/1	0.86	0.45	46,46,46,46	1
60	MG	BA	1784	1/1	0.86	0.18	59,59,59,59	0
60	MG	AB	3006	1/1	0.86	0.22	84,84,84,84	0
60	MG	AA	3646	1/1	0.86	0.28	82,82,82,82	0
60	MG	CA	3617	1/1	0.86	0.38	41,41,41,41	0
60	MG	CA	3075	1/1	0.86	0.15	51,51,51,51	0
60	MG	AA	3024	1/1	0.86	0.13	60,60,60,60	0
60	MG	AB	3018	1/1	0.86	0.13	76,76,76,76	0
60	MG	CA	3629	1/1	0.86	0.14	74,74,74,74	0
60	MG	BA	1642	1/1	0.86	0.18	59,59,59,59	0
60	MG	DA	1761	1/1	0.86	0.08	68,68,68,68	0
60	MG	AA	3140	1/1	0.86	0.90	66,66,66,66	0
60	MG	DA	1763	1/1	0.86	0.15	61,61,61,61	0
60	MG	AA	3195	1/1	0.86	0.20	55,55,55,55	0
60	MG	CA	3637	1/1	0.86	0.24	78,78,78,78	0
60	MG	CA	3640	1/1	0.86	0.24	47,47,47,47	0
60	MG	AA	3652	1/1	0.86	0.44	87,87,87,87	0
60	MG	BA	1669	1/1	0.86	0.17	70,70,70,70	0
60	MG	AA	3171	1/1	0.86	0.51	71,71,71,71	0
60	MG	CA	3486	1/1	0.86	0.14	48,48,48,48	0
60	MG	AA	3238	1/1	0.86	0.13	68,68,68,68	0
60	MG	AA	3756	1/1	0.86	0.24	57,57,57,57	0
60	MG	CA	3562	1/1	0.87	0.17	69,69,69,69	0
60	MG	CA	3013	1/1	0.87	0.32	52,52,52,52	0
60	MG	AA	3200	1/1	0.87	0.28	73,73,73,73	0
60	MG	AA	3111	1/1	0.87	0.31	47,47,47,47	0
60	MG	BA	1632	1/1	0.87	0.23	60,60,60,60	0
60	MG	AA	3016	1/1	0.87	0.31	44,44,44,44	0
60	MG	AF	303	1/1	0.87	0.56	54,54,54,54	0
60	MG	CA	3464	1/1	0.87	0.61	78,78,78,78	0
60	MG	DA	1628	1/1	0.87	0.20	69,69,69,69	0
60	MG	DA	1630	1/1	0.87	0.27	51,51,51,51	0
60	MG	AA	3258	1/1	0.87	0.26	32,32,32,32	0
60	MG	AA	3542	1/1	0.87	0.10	47,47,47,47	0
60	MG	CA	3035	1/1	0.87	0.36	47,47,47,47	0
60	MG	BA	1774	1/1	0.87	0.09	79,79,79,79	0
60	MG	AA	3062	1/1	0.87	0.36	60,60,60,60	0
60	MG	CA	3276	1/1	0.87	0.17	32,32,32,32	0
60	MG	CA	3045	1/1	0.87	0.23	68,68,68,68	0
60	MG	DA	1657	1/1	0.87	0.14	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3485	1/1	0.87	0.24	76,76,76,76	0
60	MG	BA	1661	1/1	0.87	0.45	59,59,59,59	0
60	MG	BA	1782	1/1	0.87	0.29	72,72,72,72	0
60	MG	DA	1664	1/1	0.87	0.24	49,49,49,49	0
60	MG	DA	1668	1/1	0.87	0.27	68,68,68,68	0
60	MG	DA	1670	1/1	0.87	0.25	74,74,74,74	0
60	MG	BA	1666	1/1	0.87	0.34	70,70,70,70	0
60	MG	AA	3780	1/1	0.87	0.35	51,51,51,51	1
60	MG	CA	3494	1/1	0.87	0.17	58,58,58,58	0
60	MG	AA	3130	1/1	0.87	0.33	59,59,59,59	0
60	MG	AA	3017	1/1	0.87	0.11	71,71,71,71	0
60	MG	DA	1695	1/1	0.87	0.18	79,79,79,79	0
60	MG	AA	3268	1/1	0.87	0.23	80,80,80,80	0
60	MG	AA	3644	1/1	0.87	0.21	74,74,74,74	0
60	MG	BA	1681	1/1	0.87	0.66	69,69,69,69	0
60	MG	AA	3575	1/1	0.87	0.16	63,63,63,63	0
60	MG	CA	3184	1/1	0.87	0.26	43,43,43,43	0
60	MG	AA	3270	1/1	0.87	0.20	92,92,92,92	0
60	MG	DA	1720	1/1	0.87	0.12	61,61,61,61	0
60	MG	BD	502	1/1	0.87	0.42	56,56,56,56	0
60	MG	AA	3447	1/1	0.87	0.19	44,44,44,44	0
60	MG	CA	3361	1/1	0.87	0.14	70,70,70,70	0
60	MG	BA	1694	1/1	0.87	0.23	78,78,78,78	0
60	MG	AA	3738	1/1	0.87	0.14	73,73,73,73	0
60	MG	CA	3663	1/1	0.87	0.26	74,74,74,74	0
60	MG	AA	3362	1/1	0.87	0.21	69,69,69,69	0
60	MG	AA	3158	1/1	0.87	0.37	50,50,50,50	0
60	MG	DA	1746	1/1	0.87	0.28	67,67,67,67	0
60	MG	CA	3528	1/1	0.87	0.07	51,51,51,51	1
60	MG	AA	3010	1/1	0.87	0.29	68,68,68,68	0
60	MG	AA	3589	1/1	0.87	0.33	31,31,31,31	1
60	MG	AB	3015	1/1	0.87	0.12	51,51,51,51	0
60	MG	CA	3384	1/1	0.87	0.20	52,52,52,52	0
60	MG	CA	3536	1/1	0.87	0.13	95,95,95,95	0
60	MG	AB	3016	1/1	0.87	0.14	47,47,47,47	0
60	MG	BX	107	1/1	0.87	0.11	69,69,69,69	0
60	MG	AA	3656	1/1	0.87	0.24	62,62,62,62	1
60	MG	CO	201	1/1	0.87	0.16	72,72,72,72	0
60	MG	CA	3390	1/1	0.87	0.21	42,42,42,42	0
60	MG	AA	3291	1/1	0.87	0.13	84,84,84,84	0
60	MG	AA	3297	1/1	0.87	0.08	56,56,56,56	0
60	MG	AA	3247	1/1	0.87	0.43	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3552	1/1	0.87	0.09	60,60,60,60	0
60	MG	AA	3509	1/1	0.87	0.26	51,51,51,51	0
60	MG	AA	3678	1/1	0.87	0.13	62,62,62,62	0
60	MG	BA	1724	1/1	0.88	0.31	60,60,60,60	0
60	MG	BA	1732	1/1	0.88	0.25	65,65,65,65	0
60	MG	AA	3802	1/1	0.88	0.27	55,55,55,55	0
60	MG	CA	3210	1/1	0.88	0.23	44,44,44,44	0
60	MG	AA	3353	1/1	0.88	0.11	68,68,68,68	0
60	MG	BA	1739	1/1	0.88	0.18	52,52,52,52	0
60	MG	BA	1633	1/1	0.88	0.36	65,65,65,65	0
60	MG	AA	3107	1/1	0.88	0.17	51,51,51,51	0
60	MG	DA	1617	1/1	0.88	0.18	47,47,47,47	0
60	MG	DA	1618	1/1	0.88	0.09	51,51,51,51	0
60	MG	AA	3824	1/1	0.88	0.33	53,53,53,53	0
60	MG	CA	3569	1/1	0.88	0.17	71,71,71,71	0
60	MG	CA	3409	1/1	0.88	0.32	63,63,63,63	0
60	MG	BX	113	1/1	0.88	0.21	78,78,78,78	0
60	MG	CA	3230	1/1	0.88	0.11	64,64,64,64	0
60	MG	BY	3001	1/1	0.88	0.07	78,78,78,78	0
60	MG	BA	1645	1/1	0.88	0.77	58,58,58,58	0
60	MG	CA	3442	1/1	0.88	0.13	70,70,70,70	0
60	MG	AA	3364	1/1	0.88	0.24	57,57,57,57	0
60	MG	CA	3587	1/1	0.88	0.13	72,72,72,72	0
60	MG	CA	3457	1/1	0.88	0.22	60,60,60,60	0
60	MG	BA	1649	1/1	0.88	0.34	56,56,56,56	0
60	MG	CA	3007	1/1	0.88	0.24	75,75,75,75	0
60	MG	AA	3033	1/1	0.88	0.41	48,48,48,48	0
60	MG	CA	3242	1/1	0.88	0.33	48,48,48,48	0
60	MG	CA	3598	1/1	0.88	0.21	66,66,66,66	0
60	MG	CA	3097	1/1	0.88	0.17	79,79,79,79	0
60	MG	AB	3001	1/1	0.88	0.18	80,80,80,80	0
60	MG	AA	3637	1/1	0.88	0.19	54,54,54,54	0
60	MG	AA	3455	1/1	0.88	0.23	80,80,80,80	0
60	MG	AA	3228	1/1	0.88	0.32	63,63,63,63	0
60	MG	AB	3011	1/1	0.88	0.18	47,47,47,47	0
60	MG	AA	3388	1/1	0.88	0.16	55,55,55,55	0
60	MG	AA	3078	1/1	0.88	0.26	54,54,54,54	0
60	MG	A8	5001	1/1	0.88	0.31	66,66,66,66	0
60	MG	DA	1688	1/1	0.88	0.20	46,46,46,46	0
60	MG	CA	3630	1/1	0.88	0.21	91,91,91,91	0
60	MG	AA	3156	1/1	0.88	0.23	46,46,46,46	0
60	MG	CA	3039	1/1	0.88	0.39	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3041	1/1	0.88	0.47	67,67,67,67	0
60	MG	DA	1712	1/1	0.88	0.17	67,67,67,67	0
60	MG	CA	3135	1/1	0.88	0.11	73,73,73,73	0
60	MG	CA	3136	1/1	0.88	0.21	112,112,112,112	0
60	MG	CA	3138	1/1	0.88	0.28	67,67,67,67	0
60	MG	CA	3643	1/1	0.88	0.33	83,83,83,83	0
60	MG	CA	3500	1/1	0.88	0.47	56,56,56,56	0
60	MG	AA	3248	1/1	0.88	0.49	79,79,79,79	0
60	MG	CA	3648	1/1	0.88	0.60	78,78,78,78	0
60	MG	AA	3236	1/1	0.88	0.10	61,61,61,61	0
60	MG	BA	1789	1/1	0.88	0.11	68,68,68,68	0
60	MG	CA	3658	1/1	0.88	0.19	62,62,62,62	0
60	MG	CA	3305	1/1	0.88	0.31	64,64,64,64	0
60	MG	DA	1742	1/1	0.88	0.25	52,52,52,52	0
60	MG	CA	3309	1/1	0.88	0.11	50,50,50,50	0
60	MG	CA	3510	1/1	0.88	0.17	71,71,71,71	0
60	MG	DA	1747	1/1	0.88	0.11	67,67,67,67	0
60	MG	AA	3769	1/1	0.88	0.46	48,48,48,48	1
60	MG	BA	1793	1/1	0.88	0.10	68,68,68,68	0
60	MG	DA	1751	1/1	0.88	0.25	84,84,84,84	0
60	MG	BA	1799	1/1	0.88	0.07	69,69,69,69	0
60	MG	AA	3329	1/1	0.88	0.23	82,82,82,82	0
60	MG	CB	3011	1/1	0.88	0.27	51,51,51,51	0
60	MG	BA	1613	1/1	0.88	0.07	92,92,92,92	0
60	MG	AA	3598	1/1	0.88	0.20	57,57,57,57	0
60	MG	AA	3087	1/1	0.88	0.32	62,62,62,62	0
60	MG	CA	3181	1/1	0.88	0.31	68,68,68,68	0
60	MG	CA	3064	1/1	0.88	0.20	72,72,72,72	0
60	MG	BA	1813	1/1	0.88	0.17	66,66,66,66	0
60	MG	AA	3285	1/1	0.88	0.22	72,72,72,72	0
60	MG	AA	3439	1/1	0.88	0.18	43,43,43,43	0
60	MG	AE	305	1/1	0.88	0.43	44,44,44,44	0
60	MG	DJ	5001	1/1	0.88	0.17	94,94,94,94	0
60	MG	AA	3287	1/1	0.88	0.20	25,25,25,25	0
60	MG	CR	202	1/1	0.88	0.39	61,61,61,61	0
60	MG	AA	3199	1/1	0.88	0.22	61,61,61,61	0
60	MG	AA	3482	1/1	0.89	0.26	46,46,46,46	0
60	MG	CA	3530	1/1	0.89	0.15	68,68,68,68	0
60	MG	CA	3153	1/1	0.89	0.31	54,54,54,54	0
60	MG	CR	201	1/1	0.89	0.36	63,63,63,63	0
60	MG	AA	3063	1/1	0.89	0.17	46,46,46,46	0
60	MG	AA	3778	1/1	0.89	0.10	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3054	1/1	0.89	0.13	50,50,50,50	0
60	MG	AA	3154	1/1	0.89	0.16	64,64,64,64	0
60	MG	CA	3539	1/1	0.89	0.31	72,72,72,72	0
60	MG	CA	3170	1/1	0.89	0.36	68,68,68,68	0
60	MG	CA	3175	1/1	0.89	0.14	59,59,59,59	0
60	MG	AN	3003	1/1	0.89	0.07	52,52,52,52	0
60	MG	AA	3604	1/1	0.89	0.23	44,44,44,44	1
60	MG	AA	3187	1/1	0.89	0.17	29,29,29,29	0
60	MG	CA	3549	1/1	0.89	0.18	29,29,29,29	0
60	MG	CA	3379	1/1	0.89	0.22	62,62,62,62	0
60	MG	AU	201	1/1	0.89	0.53	72,72,72,72	0
60	MG	AU	203	1/1	0.89	0.24	55,55,55,55	0
60	MG	CA	3557	1/1	0.89	0.26	76,76,76,76	0
60	MG	BA	1807	1/1	0.89	0.20	72,72,72,72	0
60	MG	AW	3002	1/1	0.89	0.18	59,59,59,59	0
60	MG	AA	3608	1/1	0.89	0.15	66,66,66,66	0
60	MG	AY	502	1/1	0.89	0.24	54,54,54,54	0
60	MG	CA	3200	1/1	0.89	0.15	65,65,65,65	0
60	MG	AA	3419	1/1	0.89	0.05	88,88,88,88	0
60	MG	BL	201	1/1	0.89	0.19	104,104,104,104	0
60	MG	CA	3204	1/1	0.89	0.25	88,88,88,88	0
60	MG	AA	3800	1/1	0.89	0.28	59,59,59,59	0
60	MG	AA	3491	1/1	0.89	0.30	40,40,40,40	0
60	MG	BA	1702	1/1	0.89	0.46	56,56,56,56	0
60	MG	AA	3500	1/1	0.89	0.14	27,27,27,27	0
60	MG	AA	3191	1/1	0.89	0.29	57,57,57,57	0
60	MG	CA	3418	1/1	0.89	0.31	53,53,53,53	0
60	MG	AA	3822	1/1	0.89	0.60	67,67,67,67	0
60	MG	DA	1666	1/1	0.89	0.19	45,45,45,45	0
60	MG	DA	1667	1/1	0.89	0.43	70,70,70,70	0
60	MG	CA	3596	1/1	0.89	0.10	75,75,75,75	0
60	MG	AA	3342	1/1	0.89	0.11	77,77,77,77	0
60	MG	AA	3119	1/1	0.89	0.23	41,41,41,41	0
60	MG	AA	3194	1/1	0.89	0.35	58,58,58,58	0
60	MG	CA	3606	1/1	0.89	0.27	58,58,58,58	0
60	MG	BX	110	1/1	0.89	0.14	67,67,67,67	0
60	MG	CA	3608	1/1	0.89	0.11	69,69,69,69	0
60	MG	CA	3611	1/1	0.89	0.29	64,64,64,64	0
60	MG	AA	3157	1/1	0.89	0.33	93,93,93,93	0
60	MG	CA	3614	1/1	0.89	0.28	79,79,79,79	0
60	MG	AB	3004	1/1	0.89	0.29	69,69,69,69	0
60	MG	AA	3198	1/1	0.89	0.09	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3093	1/1	0.89	0.34	77,77,77,77	0
60	MG	BA	1612	1/1	0.89	0.14	79,79,79,79	0
60	MG	CA	3477	1/1	0.89	0.24	65,65,65,65	0
60	MG	AA	3360	1/1	0.89	0.45	72,72,72,72	0
60	MG	CA	3480	1/1	0.89	0.14	61,61,61,61	0
60	MG	DA	1721	1/1	0.89	0.32	60,60,60,60	0
60	MG	AA	3740	1/1	0.89	0.25	54,54,54,54	0
60	MG	AA	3743	1/1	0.89	0.20	66,66,66,66	0
60	MG	AA	3120	1/1	0.89	0.26	54,54,54,54	0
60	MG	AA	3101	1/1	0.89	0.48	68,68,68,68	0
60	MG	AA	3559	1/1	0.89	0.21	37,37,37,37	0
60	MG	CA	3254	1/1	0.89	0.15	35,35,35,35	0
60	MG	AA	3563	1/1	0.89	0.07	37,37,37,37	1
60	MG	AA	3568	1/1	0.89	0.22	23,23,23,23	0
60	MG	AA	3303	1/1	0.89	0.21	30,30,30,30	0
60	MG	AA	3080	1/1	0.89	0.36	54,54,54,54	0
60	MG	AA	3379	1/1	0.89	0.14	40,40,40,40	1
60	MG	CA	3123	1/1	0.89	0.27	63,63,63,63	0
60	MG	AA	3473	1/1	0.89	0.15	57,57,57,57	0
60	MG	DA	1750	1/1	0.89	0.18	86,86,86,86	0
60	MG	AA	3476	1/1	0.89	0.10	50,50,50,50	0
60	MG	CA	3287	1/1	0.89	0.35	43,43,43,43	0
60	MG	CA	3133	1/1	0.89	0.20	72,72,72,72	0
60	MG	CA	3033	1/1	0.89	0.13	47,47,47,47	0
60	MG	AA	3477	1/1	0.89	0.15	47,47,47,47	0
60	MG	CA	3036	1/1	0.89	0.26	65,65,65,65	0
60	MG	CA	3302	1/1	0.89	0.11	67,67,67,67	0
60	MG	AA	3381	1/1	0.89	0.12	34,34,34,34	0
60	MG	AA	3095	1/1	0.89	0.16	58,58,58,58	0
60	MG	CD	302	1/1	0.89	0.43	51,51,51,51	0
60	MG	CA	3144	1/1	0.89	0.29	84,84,84,84	0
60	MG	CA	3523	1/1	0.89	0.09	77,77,77,77	0
60	MG	BA	1785	1/1	0.89	0.19	69,69,69,69	0
60	MG	CA	3312	1/1	0.89	0.38	52,52,52,52	0
60	MG	DK	202	1/1	0.89	0.23	80,80,80,80	0
60	MG	CE	306	1/1	0.89	0.09	69,69,69,69	0
60	MG	CA	3317	1/1	0.89	0.16	61,61,61,61	0
60	MG	AA	3592	1/1	0.89	0.27	67,67,67,67	0
60	MG	CF	303	1/1	0.90	0.28	63,63,63,63	0
60	MG	CA	3323	1/1	0.90	0.16	32,32,32,32	0
60	MG	AA	3445	1/1	0.90	0.06	59,59,59,59	0
60	MG	CA	3333	1/1	0.90	0.20	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3534	1/1	0.90	0.12	58,58,58,58	0
60	MG	AA	3622	1/1	0.90	0.13	52,52,52,52	0
60	MG	CA	3062	1/1	0.90	0.09	41,41,41,41	0
60	MG	AA	3046	1/1	0.90	0.36	47,47,47,47	0
60	MG	AA	3273	1/1	0.90	0.27	57,57,57,57	0
60	MG	C5	101	1/1	0.90	0.43	64,64,64,64	0
60	MG	CA	3065	1/1	0.90	0.15	56,56,56,56	0
60	MG	AA	3721	1/1	0.90	0.20	21,21,21,21	0
60	MG	BA	1673	1/1	0.90	0.72	63,63,63,63	0
60	MG	CA	3544	1/1	0.90	0.18	74,74,74,74	0
60	MG	AA	3724	1/1	0.90	0.31	37,37,37,37	0
60	MG	DA	1613	1/1	0.90	0.25	50,50,50,50	0
60	MG	AA	3630	1/1	0.90	0.15	66,66,66,66	0
60	MG	AA	3812	1/1	0.90	0.20	78,78,78,78	0
60	MG	AA	3460	1/1	0.90	0.30	81,81,81,81	0
60	MG	CA	3074	1/1	0.90	0.31	64,64,64,64	0
60	MG	AA	3728	1/1	0.90	0.27	75,75,75,75	0
60	MG	BM	201	1/1	0.90	0.06	60,60,60,60	0
60	MG	AA	3402	1/1	0.90	0.33	53,53,53,53	0
60	MG	AA	3021	1/1	0.90	0.20	49,49,49,49	0
60	MG	DA	1626	1/1	0.90	0.41	63,63,63,63	0
60	MG	BA	1698	1/1	0.90	0.31	57,57,57,57	0
60	MG	DA	1629	1/1	0.90	0.80	79,79,79,79	0
60	MG	AA	3550	1/1	0.90	0.21	47,47,47,47	0
60	MG	A6	101	1/1	0.90	0.21	69,69,69,69	0
60	MG	AA	3019	1/1	0.90	0.26	53,53,53,53	0
60	MG	DA	1636	1/1	0.90	0.32	77,77,77,77	0
60	MG	CA	3215	1/1	0.90	0.43	50,50,50,50	0
60	MG	AA	3235	1/1	0.90	0.28	42,42,42,42	0
60	MG	CA	3404	1/1	0.90	0.11	46,46,46,46	0
60	MG	CA	3088	1/1	0.90	0.43	85,85,85,85	0
60	MG	CA	3220	1/1	0.90	0.50	89,89,89,89	0
60	MG	BA	1708	1/1	0.90	0.27	55,55,55,55	0
60	MG	AA	3288	1/1	0.90	0.13	39,39,39,39	0
60	MG	CA	3228	1/1	0.90	0.71	68,68,68,68	0
60	MG	AA	3092	1/1	0.90	0.23	41,41,41,41	0
60	MG	BA	1604	1/1	0.90	0.16	85,85,85,85	0
60	MG	CA	3437	1/1	0.90	0.25	41,41,41,41	0
60	MG	BA	1719	1/1	0.90	0.27	75,75,75,75	0
60	MG	AA	3572	1/1	0.90	0.16	51,51,51,51	0
60	MG	CA	3603	1/1	0.90	0.28	93,93,93,93	0
60	MG	AA	3483	1/1	0.90	0.18	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
60	MG	DA	1672	1/1	0.90	0.16	61,61,61,61	0
60	MG	CA	3458	1/1	0.90	0.14	28,28,28,28	0
60	MG	AA	3294	1/1	0.90	0.19	56,56,56,56	0
60	MG	CA	3460	1/1	0.90	0.28	57,57,57,57	0
60	MG	AA	3752	1/1	0.90	0.63	75,75,75,75	0
60	MG	AA	3079	1/1	0.90	0.10	27,27,27,27	0
60	MG	AA	3488	1/1	0.90	0.09	56,56,56,56	0
60	MG	CA	3108	1/1	0.90	0.18	84,84,84,84	0
60	MG	BA	1619	1/1	0.90	0.13	54,54,54,54	0
60	MG	AA	3055	1/1	0.90	0.17	61,61,61,61	0
60	MG	DA	1707	1/1	0.90	0.09	79,79,79,79	0
60	MG	CA	3626	1/1	0.90	0.09	52,52,52,52	0
60	MG	DA	1714	1/1	0.90	0.39	82,82,82,82	0
60	MG	AD	303	1/1	0.90	0.13	46,46,46,46	0
60	MG	BA	1623	1/1	0.90	0.25	67,67,67,67	0
60	MG	CA	3257	1/1	0.90	0.14	45,45,45,45	0
60	MG	AA	3096	1/1	0.90	0.22	54,54,54,54	0
60	MG	BA	1625	1/1	0.90	0.24	53,53,53,53	0
60	MG	CA	3267	1/1	0.90	0.24	110,110,110,110	0
60	MG	DA	1724	1/1	0.90	0.19	74,74,74,74	0
60	MG	DA	1725	1/1	0.90	0.13	78,78,78,78	0
60	MG	CA	3271	1/1	0.90	0.11	59,59,59,59	0
60	MG	BA	1762	1/1	0.90	0.07	57,57,57,57	0
60	MG	CA	3127	1/1	0.90	0.15	68,68,68,68	0
60	MG	AA	3081	1/1	0.90	0.20	38,38,38,38	0
60	MG	AA	3494	1/1	0.90	0.14	66,66,66,66	0
60	MG	AA	3498	1/1	0.90	0.17	56,56,56,56	0
60	MG	AA	3307	1/1	0.90	0.12	35,35,35,35	0
60	MG	CA	3283	1/1	0.90	0.23	57,57,57,57	0
60	MG	CA	3286	1/1	0.90	0.21	62,62,62,62	0
60	MG	CA	3655	1/1	0.90	0.47	69,69,69,69	0
60	MG	AA	3504	1/1	0.90	0.14	44,44,44,44	0
60	MG	CA	3288	1/1	0.90	0.34	39,39,39,39	0
60	MG	AA	3377	1/1	0.90	0.15	19,19,19,19	0
60	MG	CA	3662	1/1	0.90	0.37	60,60,60,60	0
60	MG	BA	1640	1/1	0.90	0.19	56,56,56,56	0
60	MG	CA	3295	1/1	0.90	0.30	55,55,55,55	0
60	MG	AA	3516	1/1	0.90	0.27	38,38,38,38	0
60	MG	CB	3007	1/1	0.90	0.14	57,57,57,57	0
60	MG	CA	3143	1/1	0.90	0.23	62,62,62,62	0
60	MG	AA	3142	1/1	0.90	0.27	50,50,50,50	0
60	MG	AA	3530	1/1	0.90	0.10	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3519	1/1	0.90	0.20	68,68,68,68	0
60	MG	CB	3013	1/1	0.90	0.12	90,90,90,90	0
60	MG	DA	1768	1/1	0.90	0.10	57,57,57,57	0
60	MG	AA	3698	1/1	0.90	0.31	51,51,51,51	1
60	MG	CD	303	1/1	0.90	0.14	70,70,70,70	0
60	MG	AA	3226	1/1	0.90	0.27	51,51,51,51	0
60	MG	AN	3002	1/1	0.90	0.20	76,76,76,76	0
60	MG	AA	3784	1/1	0.90	0.15	69,69,69,69	0
60	MG	CA	3314	1/1	0.90	0.15	41,41,41,41	0
60	MG	BA	1662	1/1	0.90	0.17	45,45,45,45	0
60	MG	CA	3322	1/1	0.90	0.28	41,41,41,41	0
60	MG	CA	3263	1/1	0.91	0.12	50,50,50,50	0
60	MG	AA	3141	1/1	0.91	0.20	46,46,46,46	0
60	MG	BA	1801	1/1	0.91	0.12	55,55,55,55	0
60	MG	CA	3268	1/1	0.91	0.21	46,46,46,46	0
60	MG	AA	3004	1/1	0.91	0.14	30,30,30,30	0
60	MG	CF	302	1/1	0.91	0.32	64,64,64,64	0
60	MG	BA	1643	1/1	0.91	0.09	56,56,56,56	0
60	MG	BA	1644	1/1	0.91	0.27	72,72,72,72	0
60	MG	AA	3125	1/1	0.91	0.35	74,74,74,74	0
60	MG	CA	3095	1/1	0.91	0.09	92,92,92,92	0
60	MG	CA	3515	1/1	0.91	0.11	72,72,72,72	0
60	MG	BA	1809	1/1	0.91	0.18	74,74,74,74	0
60	MG	AA	3289	1/1	0.91	0.19	47,47,47,47	0
60	MG	BA	1647	1/1	0.91	0.09	57,57,57,57	0
60	MG	BF	3001	1/1	0.91	0.15	49,49,49,49	0
60	MG	AA	3179	1/1	0.91	0.23	62,62,62,62	0
60	MG	C7	101	1/1	0.91	0.43	47,47,47,47	0
60	MG	AA	3066	1/1	0.91	0.20	63,63,63,63	0
60	MG	DA	1605	1/1	0.91	0.29	59,59,59,59	0
60	MG	AD	305	1/1	0.91	0.55	75,75,75,75	0
60	MG	BA	1658	1/1	0.91	0.55	68,68,68,68	0
60	MG	AA	3254	1/1	0.91	0.29	47,47,47,47	0
60	MG	AA	3257	1/1	0.91	0.22	18,18,18,18	0
60	MG	AA	3201	1/1	0.91	0.32	71,71,71,71	0
60	MG	BA	1667	1/1	0.91	0.15	69,69,69,69	0
60	MG	BA	1668	1/1	0.91	0.18	72,72,72,72	0
60	MG	BX	104	1/1	0.91	0.20	67,67,67,67	0
60	MG	AA	3466	1/1	0.91	0.17	48,48,48,48	0
60	MG	AA	3380	1/1	0.91	0.18	75,75,75,75	0
60	MG	AA	3104	1/1	0.91	0.25	55,55,55,55	0
60	MG	DA	1622	1/1	0.91	0.15	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3561	1/1	0.91	0.17	64,64,64,64	0
60	MG	CA	3315	1/1	0.91	0.21	44,44,44,44	0
60	MG	AA	3562	1/1	0.91	0.06	45,45,45,45	0
60	MG	AA	3069	1/1	0.91	0.08	32,32,32,32	0
60	MG	AA	3394	1/1	0.91	0.13	22,22,22,22	0
60	MG	BA	1683	1/1	0.91	0.24	50,50,50,50	0
60	MG	BA	1684	1/1	0.91	0.21	64,64,64,64	0
60	MG	CA	3335	1/1	0.91	0.16	38,38,38,38	0
60	MG	DA	1635	1/1	0.91	0.44	61,61,61,61	0
60	MG	CA	3551	1/1	0.91	0.15	76,76,76,76	0
60	MG	AA	3309	1/1	0.91	0.18	72,72,72,72	0
60	MG	DA	1639	1/1	0.91	0.10	59,59,59,59	0
60	MG	DA	1640	1/1	0.91	0.35	73,73,73,73	0
60	MG	AA	3765	1/1	0.91	0.20	62,62,62,62	0
60	MG	AA	3481	1/1	0.91	0.06	53,53,53,53	0
60	MG	CA	3349	1/1	0.91	0.15	36,36,36,36	0
60	MG	AA	3014	1/1	0.91	0.17	45,45,45,45	0
60	MG	AA	3240	1/1	0.91	0.51	39,39,39,39	0
60	MG	AA	3269	1/1	0.91	0.54	78,78,78,78	0
60	MG	CA	3363	1/1	0.91	0.18	55,55,55,55	0
60	MG	AA	3058	1/1	0.91	0.12	38,38,38,38	0
60	MG	CA	3162	1/1	0.91	0.27	57,57,57,57	0
60	MG	CA	3372	1/1	0.91	0.29	63,63,63,63	0
60	MG	AU	202	1/1	0.91	0.28	65,65,65,65	0
60	MG	CA	3168	1/1	0.91	0.23	65,65,65,65	0
60	MG	AA	3667	1/1	0.91	0.14	45,45,45,45	0
60	MG	AA	3777	1/1	0.91	0.32	58,58,58,58	0
60	MG	AA	3420	1/1	0.91	0.13	26,26,26,26	0
60	MG	AA	3421	1/1	0.91	0.12	73,73,73,73	0
60	MG	DA	1675	1/1	0.91	0.13	61,61,61,61	0
60	MG	AA	3782	1/1	0.91	0.17	70,70,70,70	0
60	MG	AA	3679	1/1	0.91	0.18	64,64,64,64	0
60	MG	AA	3683	1/1	0.91	0.10	40,40,40,40	0
60	MG	CA	3037	1/1	0.91	0.19	65,65,65,65	0
60	MG	DA	1689	1/1	0.91	0.24	68,68,68,68	0
60	MG	DA	1691	1/1	0.91	0.18	66,66,66,66	0
60	MG	DA	1694	1/1	0.91	0.27	60,60,60,60	0
60	MG	CA	3389	1/1	0.91	0.09	55,55,55,55	0
60	MG	BA	1720	1/1	0.91	0.14	51,51,51,51	0
60	MG	AA	3785	1/1	0.91	0.21	54,54,54,54	0
60	MG	CA	3396	1/1	0.91	0.14	59,59,59,59	0
60	MG	DA	1705	1/1	0.91	0.17	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	BA	1723	1/1	0.91	0.27	61,61,61,61	0
60	MG	AA	3788	1/1	0.91	0.17	64,64,64,64	0
60	MG	CA	3402	1/1	0.91	0.16	46,46,46,46	0
60	MG	AA	3687	1/1	0.91	0.11	48,48,48,48	0
60	MG	DA	1716	1/1	0.91	0.27	56,56,56,56	0
60	MG	AA	3587	1/1	0.91	0.17	44,44,44,44	0
60	MG	CA	3050	1/1	0.91	0.65	55,55,55,55	0
60	MG	AA	3794	1/1	0.91	0.20	47,47,47,47	0
60	MG	BA	1738	1/1	0.91	0.23	55,55,55,55	0
60	MG	AA	3209	1/1	0.91	0.26	64,64,64,64	0
60	MG	AA	3797	1/1	0.91	0.30	60,60,60,60	0
60	MG	AA	3690	1/1	0.91	0.11	58,58,58,58	0
60	MG	CA	3214	1/1	0.91	0.28	50,50,50,50	0
60	MG	AA	3167	1/1	0.91	0.29	69,69,69,69	0
60	MG	BA	1605	1/1	0.91	0.11	76,76,76,76	0
60	MG	AA	3804	1/1	0.91	0.38	70,70,70,70	0
60	MG	AA	3277	1/1	0.91	0.19	48,48,48,48	0
60	MG	AA	3495	1/1	0.91	0.20	58,58,58,58	0
60	MG	AA	3811	1/1	0.91	0.59	65,65,65,65	0
60	MG	AA	3435	1/1	0.91	0.27	54,54,54,54	0
60	MG	AA	3813	1/1	0.91	0.21	68,68,68,68	0
60	MG	AA	3499	1/1	0.91	0.11	46,46,46,46	0
60	MG	CA	3470	1/1	0.91	0.10	55,55,55,55	0
60	MG	CA	3650	1/1	0.91	0.17	42,42,42,42	0
60	MG	AA	3705	1/1	0.91	0.44	29,29,29,29	1
60	MG	AA	3827	1/1	0.91	0.29	39,39,39,39	0
60	MG	CA	3238	1/1	0.91	0.34	73,73,73,73	0
60	MG	AA	3437	1/1	0.91	0.20	25,25,25,25	0
60	MG	AA	3170	1/1	0.91	0.57	44,44,44,44	1
60	MG	CA	3076	1/1	0.91	0.32	48,48,48,48	0
60	MG	AA	3715	1/1	0.91	0.09	62,62,62,62	0
60	MG	AA	3507	1/1	0.91	0.25	53,53,53,53	0
60	MG	CA	3484	1/1	0.91	0.26	56,56,56,56	0
60	MG	CB	3001	1/1	0.91	0.21	68,68,68,68	0
60	MG	BA	1628	1/1	0.91	0.30	59,59,59,59	0
60	MG	CA	3246	1/1	0.91	0.28	79,79,79,79	0
60	MG	AA	3613	1/1	0.91	0.12	96,96,96,96	0
60	MG	AA	3614	1/1	0.91	0.13	66,66,66,66	0
60	MG	AA	3280	1/1	0.91	0.20	63,63,63,63	0
60	MG	AA	3618	1/1	0.91	0.13	39,39,39,39	0
60	MG	CA	3495	1/1	0.91	0.18	64,64,64,64	0
60	MG	BA	1634	1/1	0.91	0.21	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3260	1/1	0.91	0.14	59,59,59,59	0
60	MG	AA	3512	1/1	0.91	0.13	32,32,32,32	0
61	K	AA	3814	1/1	0.91	0.27	87,87,87,87	0
60	MG	AA	3260	1/1	0.92	0.43	67,67,67,67	0
60	MG	CD	301	1/1	0.92	0.35	61,61,61,61	0
60	MG	AA	3501	1/1	0.92	0.16	45,45,45,45	0
60	MG	BA	1806	1/1	0.92	0.17	63,63,63,63	0
60	MG	AA	3693	1/1	0.92	0.19	47,47,47,47	0
60	MG	AA	3261	1/1	0.92	0.27	53,53,53,53	0
60	MG	AA	3262	1/1	0.92	0.59	70,70,70,70	0
60	MG	AA	3609	1/1	0.92	0.21	57,57,57,57	0
60	MG	AA	3295	1/1	0.92	0.16	24,24,24,24	0
60	MG	CA	3499	1/1	0.92	0.21	68,68,68,68	0
60	MG	AA	3215	1/1	0.92	0.18	48,48,48,48	0
60	MG	AA	3370	1/1	0.92	0.16	43,43,43,43	0
60	MG	AA	3798	1/1	0.92	0.10	34,34,34,34	0
60	MG	AA	3712	1/1	0.92	0.20	50,50,50,50	0
60	MG	BA	1679	1/1	0.92	0.20	51,51,51,51	0
60	MG	CQ	202	1/1	0.92	0.25	56,56,56,56	0
60	MG	CA	3507	1/1	0.92	0.14	99,99,99,99	0
60	MG	BT	3001	1/1	0.92	0.27	47,47,47,47	0
60	MG	CA	3102	1/1	0.92	0.34	50,50,50,50	0
60	MG	C0	101	1/1	0.92	0.07	50,50,50,50	0
60	MG	CA	3278	1/1	0.92	0.24	38,38,38,38	0
60	MG	AA	3217	1/1	0.92	0.16	50,50,50,50	0
60	MG	CA	3105	1/1	0.92	0.12	47,47,47,47	0
60	MG	AA	3525	1/1	0.92	0.21	45,45,45,45	0
60	MG	AA	3619	1/1	0.92	0.12	39,39,39,39	0
60	MG	BX	101	1/1	0.92	0.30	63,63,63,63	0
60	MG	DA	1607	1/1	0.92	0.83	63,63,63,63	0
60	MG	BA	1687	1/1	0.92	0.59	73,73,73,73	0
60	MG	AA	3450	1/1	0.92	0.27	71,71,71,71	0
60	MG	CA	3525	1/1	0.92	0.07	30,30,30,30	0
60	MG	A5	102	1/1	0.92	0.25	46,46,46,46	0
60	MG	CA	3119	1/1	0.92	0.69	63,63,63,63	0
60	MG	AA	3810	1/1	0.92	0.34	49,49,49,49	0
60	MG	AA	3452	1/1	0.92	0.07	53,53,53,53	0
60	MG	CA	3125	1/1	0.92	0.48	58,58,58,58	0
60	MG	CA	3126	1/1	0.92	0.54	71,71,71,71	0
60	MG	AA	3139	1/1	0.92	0.25	64,64,64,64	0
60	MG	AA	3540	1/1	0.92	0.20	28,28,28,28	0
60	MG	AA	3458	1/1	0.92	0.20	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3729	1/1	0.92	0.07	40,40,40,40	0
60	MG	AA	3222	1/1	0.92	0.26	58,58,58,58	0
60	MG	AA	3735	1/1	0.92	0.27	30,30,30,30	0
60	MG	BA	1608	1/1	0.92	0.35	52,52,52,52	0
60	MG	AA	3305	1/1	0.92	0.16	38,38,38,38	0
60	MG	BA	1710	1/1	0.92	0.10	83,83,83,83	0
60	MG	AA	3049	1/1	0.92	0.14	35,35,35,35	0
60	MG	AA	3113	1/1	0.92	0.23	41,41,41,41	0
60	MG	CA	3330	1/1	0.92	0.27	37,37,37,37	0
60	MG	BA	1717	1/1	0.92	0.15	77,77,77,77	0
60	MG	CA	3334	1/1	0.92	0.09	56,56,56,56	0
60	MG	CA	3149	1/1	0.92	0.22	58,58,58,58	0
60	MG	CA	3150	1/1	0.92	0.12	52,52,52,52	0
60	MG	BA	1614	1/1	0.92	0.18	70,70,70,70	0
60	MG	CA	3342	1/1	0.92	0.17	84,84,84,84	0
60	MG	DA	1650	1/1	0.92	0.31	48,48,48,48	0
60	MG	CA	3346	1/1	0.92	0.30	48,48,48,48	0
60	MG	DA	1654	1/1	0.92	0.40	48,48,48,48	0
60	MG	AA	3310	1/1	0.92	0.17	37,37,37,37	0
60	MG	CA	3566	1/1	0.92	0.24	47,47,47,47	0
60	MG	AA	3552	1/1	0.92	0.14	73,73,73,73	0
60	MG	CA	3572	1/1	0.92	0.22	82,82,82,82	0
60	MG	CA	3350	1/1	0.92	0.07	74,74,74,74	0
60	MG	CA	3351	1/1	0.92	0.13	50,50,50,50	0
60	MG	CA	3154	1/1	0.92	0.22	68,68,68,68	0
60	MG	AA	3401	1/1	0.92	0.22	26,26,26,26	0
60	MG	CA	3022	1/1	0.92	0.62	76,76,76,76	0
60	MG	CA	3023	1/1	0.92	0.19	56,56,56,56	0
60	MG	CA	3165	1/1	0.92	0.52	58,58,58,58	0
60	MG	BA	1620	1/1	0.92	0.09	60,60,60,60	0
60	MG	BA	1731	1/1	0.92	0.06	65,65,65,65	0
60	MG	AA	3313	1/1	0.92	0.17	31,31,31,31	0
60	MG	AA	3746	1/1	0.92	0.43	62,62,62,62	0
60	MG	BA	1736	1/1	0.92	0.09	66,66,66,66	0
60	MG	DA	1678	1/1	0.92	0.40	66,66,66,66	0
60	MG	CA	3595	1/1	0.92	0.26	67,67,67,67	0
60	MG	AA	3043	1/1	0.92	0.29	39,39,39,39	0
60	MG	AA	3145	1/1	0.92	0.32	41,41,41,41	1
60	MG	AA	3567	1/1	0.92	0.14	69,69,69,69	0
60	MG	BA	1626	1/1	0.92	0.25	72,72,72,72	0
60	MG	CA	3601	1/1	0.92	0.36	61,61,61,61	0
60	MG	DA	1698	1/1	0.92	0.15	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3274	1/1	0.92	0.49	48,48,48,48	1
60	MG	CA	3188	1/1	0.92	0.27	55,55,55,55	0
60	MG	CA	3190	1/1	0.92	0.30	77,77,77,77	0
60	MG	AA	3484	1/1	0.92	0.23	48,48,48,48	0
60	MG	CA	3610	1/1	0.92	0.45	94,94,94,94	0
60	MG	DA	1710	1/1	0.92	0.23	56,56,56,56	0
60	MG	AB	3023	1/1	0.92	0.26	63,63,63,63	0
60	MG	CA	3393	1/1	0.92	0.35	47,47,47,47	0
60	MG	CA	3048	1/1	0.92	0.30	48,48,48,48	0
60	MG	AA	3325	1/1	0.92	0.11	78,78,78,78	0
60	MG	BA	1631	1/1	0.92	0.09	44,44,44,44	0
60	MG	BA	1761	1/1	0.92	0.18	74,74,74,74	0
60	MG	CA	3620	1/1	0.92	0.22	41,41,41,41	0
60	MG	AA	3231	1/1	0.92	0.49	87,87,87,87	0
60	MG	AA	3278	1/1	0.92	0.35	58,58,58,58	0
60	MG	CA	3205	1/1	0.92	0.31	66,66,66,66	0
60	MG	AA	3659	1/1	0.92	0.10	56,56,56,56	0
60	MG	CA	3209	1/1	0.92	0.27	101,101,101,101	0
60	MG	DA	1733	1/1	0.92	0.09	73,73,73,73	0
60	MG	BA	1636	1/1	0.92	0.27	66,66,66,66	0
60	MG	AA	3332	1/1	0.92	0.18	55,55,55,55	0
60	MG	BA	1773	1/1	0.92	0.24	69,69,69,69	0
60	MG	CA	3636	1/1	0.92	0.32	60,60,60,60	0
60	MG	CA	3419	1/1	0.92	0.18	55,55,55,55	0
60	MG	DA	1741	1/1	0.92	0.32	81,81,81,81	0
60	MG	AD	310	1/1	0.92	0.49	63,63,63,63	0
60	MG	AA	3233	1/1	0.92	0.28	85,85,85,85	0
60	MG	AA	3581	1/1	0.92	0.26	48,48,48,48	0
60	MG	CA	3644	1/1	0.92	0.17	60,60,60,60	0
60	MG	CA	3066	1/1	0.92	0.42	69,69,69,69	0
60	MG	AA	3072	1/1	0.92	0.08	20,20,20,20	0
60	MG	CA	3221	1/1	0.92	0.56	60,60,60,60	0
60	MG	AA	3674	1/1	0.92	0.09	56,56,56,56	0
60	MG	DA	1752	1/1	0.92	0.32	73,73,73,73	0
60	MG	AA	3492	1/1	0.92	0.12	41,41,41,41	0
60	MG	DA	1754	1/1	0.92	0.23	77,77,77,77	0
60	MG	AA	3147	1/1	0.92	0.51	52,52,52,52	0
60	MG	AA	3099	1/1	0.92	0.08	48,48,48,48	0
60	MG	CA	3656	1/1	0.92	0.55	75,75,75,75	0
60	MG	CA	3232	1/1	0.92	0.24	69,69,69,69	0
60	MG	CA	3072	1/1	0.92	0.43	54,54,54,54	0
60	MG	BA	1650	1/1	0.92	0.22	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	BA	1652	1/1	0.92	0.10	65,65,65,65	0
60	MG	AA	3497	1/1	0.92	0.10	36,36,36,36	0
60	MG	BA	1791	1/1	0.92	0.18	58,58,58,58	0
60	MG	BA	1792	1/1	0.92	0.07	61,61,61,61	0
60	MG	CB	3002	1/1	0.92	0.13	78,78,78,78	0
60	MG	AA	3137	1/1	0.92	0.36	55,55,55,55	0
60	MG	BA	1798	1/1	0.92	0.38	62,62,62,62	0
60	MG	CA	3243	1/1	0.92	0.35	55,55,55,55	0
60	MG	CB	3009	1/1	0.92	0.16	66,66,66,66	0
60	MG	AA	3352	1/1	0.92	0.18	64,64,64,64	0
60	MG	BA	1659	1/1	0.92	0.33	68,68,68,68	0
60	MG	BA	1660	1/1	0.92	0.32	55,55,55,55	0
60	MG	AA	3591	1/1	0.93	0.23	61,61,61,61	0
60	MG	AA	3448	1/1	0.93	0.27	74,74,74,74	0
60	MG	CA	3292	1/1	0.93	0.15	56,56,56,56	0
60	MG	BA	1735	1/1	0.93	0.14	58,58,58,58	0
60	MG	AA	3511	1/1	0.93	0.26	84,84,84,84	0
60	MG	AA	3681	1/1	0.93	0.21	52,52,52,52	0
60	MG	CA	3140	1/1	0.93	0.55	54,54,54,54	0
60	MG	CA	3512	1/1	0.93	0.12	58,58,58,58	0
60	MG	CG	3001	1/1	0.93	0.19	66,66,66,66	0
60	MG	BA	1635	1/1	0.93	0.29	62,62,62,62	0
60	MG	AA	3772	1/1	0.93	0.53	37,37,37,37	0
60	MG	CA	3029	1/1	0.93	0.11	68,68,68,68	0
60	MG	AA	3596	1/1	0.93	0.21	39,39,39,39	0
60	MG	CQ	204	1/1	0.93	0.28	74,74,74,74	0
60	MG	CA	3520	1/1	0.93	0.10	27,27,27,27	0
60	MG	CA	3148	1/1	0.93	0.15	41,41,41,41	0
60	MG	BA	1745	1/1	0.93	0.09	46,46,46,46	0
60	MG	AA	3684	1/1	0.93	0.17	47,47,47,47	0
60	MG	AA	3382	1/1	0.93	0.13	29,29,29,29	0
60	MG	AA	3513	1/1	0.93	0.22	37,37,37,37	0
60	MG	AA	3600	1/1	0.93	0.39	70,70,70,70	0
60	MG	DA	1601	1/1	0.93	0.17	59,59,59,59	0
60	MG	AA	3601	1/1	0.93	0.28	44,44,44,44	0
60	MG	CA	3326	1/1	0.93	0.21	54,54,54,54	0
60	MG	BA	1760	1/1	0.93	0.18	68,68,68,68	0
60	MG	CA	3531	1/1	0.93	0.13	67,67,67,67	0
60	MG	CA	3040	1/1	0.93	0.18	63,63,63,63	0
60	MG	AA	3114	1/1	0.93	0.34	55,55,55,55	0
60	MG	AA	3392	1/1	0.93	0.17	31,31,31,31	0
60	MG	AP	202	1/1	0.93	0.26	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3044	1/1	0.93	0.14	64,64,64,64	0
60	MG	CA	3339	1/1	0.93	0.33	75,75,75,75	0
60	MG	AA	3393	1/1	0.93	0.17	18,18,18,18	0
60	MG	AA	3032	1/1	0.93	0.54	62,62,62,62	0
60	MG	DA	1619	1/1	0.93	0.36	50,50,50,50	0
60	MG	BA	1653	1/1	0.93	0.23	62,62,62,62	0
60	MG	AA	3461	1/1	0.93	0.22	57,57,57,57	0
60	MG	AA	3138	1/1	0.93	0.14	58,58,58,58	0
60	MG	CA	3053	1/1	0.93	0.19	71,71,71,71	0
60	MG	AA	3333	1/1	0.93	0.15	33,33,33,33	0
60	MG	CA	3353	1/1	0.93	0.13	48,48,48,48	0
60	MG	CA	3185	1/1	0.93	0.32	47,47,47,47	0
60	MG	AW	3001	1/1	0.93	0.19	46,46,46,46	0
60	MG	CA	3056	1/1	0.93	0.34	83,83,83,83	0
60	MG	BA	1781	1/1	0.93	0.14	63,63,63,63	0
60	MG	DA	1632	1/1	0.93	0.21	77,77,77,77	0
60	MG	DA	1633	1/1	0.93	0.58	67,67,67,67	0
60	MG	AA	3406	1/1	0.93	0.14	52,52,52,52	0
60	MG	AA	3153	1/1	0.93	0.27	47,47,47,47	0
60	MG	AA	3341	1/1	0.93	0.14	74,74,74,74	0
60	MG	CA	3563	1/1	0.93	0.29	30,30,30,30	0
60	MG	CA	3197	1/1	0.93	0.28	48,48,48,48	0
60	MG	BA	1664	1/1	0.93	0.57	64,64,64,64	0
60	MG	CA	3571	1/1	0.93	0.14	52,52,52,52	0
60	MG	AA	3211	1/1	0.93	0.59	53,53,53,53	0
60	MG	AA	3545	1/1	0.93	0.06	64,64,64,64	0
60	MG	AA	3623	1/1	0.93	0.10	58,58,58,58	0
60	MG	AA	3547	1/1	0.93	0.06	50,50,50,50	0
60	MG	A1	101	1/1	0.93	0.10	58,58,58,58	0
60	MG	AA	3808	1/1	0.93	0.16	47,47,47,47	0
60	MG	CA	3582	1/1	0.93	0.15	60,60,60,60	0
60	MG	AA	3417	1/1	0.93	0.19	16,16,16,16	0
60	MG	BA	1794	1/1	0.93	0.15	63,63,63,63	0
60	MG	AA	3627	1/1	0.93	0.14	53,53,53,53	0
60	MG	DA	1665	1/1	0.93	0.15	57,57,57,57	0
60	MG	AA	3213	1/1	0.93	0.60	49,49,49,49	0
60	MG	CA	3391	1/1	0.93	0.10	67,67,67,67	0
60	MG	BA	1675	1/1	0.93	0.19	50,50,50,50	0
60	MG	BA	1676	1/1	0.93	0.24	39,39,39,39	0
60	MG	CA	3593	1/1	0.93	0.11	62,62,62,62	0
60	MG	AA	3168	1/1	0.93	0.20	60,60,60,60	0
60	MG	BA	1680	1/1	0.93	0.08	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	DA	1674	1/1	0.93	0.28	60,60,60,60	0
60	MG	A9	502	1/1	0.93	0.28	52,52,52,52	0
60	MG	BA	1682	1/1	0.93	0.11	71,71,71,71	0
60	MG	AA	3821	1/1	0.93	0.13	59,59,59,59	0
60	MG	CA	3406	1/1	0.93	0.08	54,54,54,54	0
60	MG	DA	1684	1/1	0.93	0.29	54,54,54,54	0
60	MG	CA	3602	1/1	0.93	0.07	49,49,49,49	0
60	MG	DA	1687	1/1	0.93	0.25	60,60,60,60	0
60	MG	AA	3083	1/1	0.93	0.67	48,48,48,48	1
60	MG	CA	3604	1/1	0.93	0.20	54,54,54,54	0
60	MG	CA	3084	1/1	0.93	0.39	73,73,73,73	0
60	MG	CA	3229	1/1	0.93	0.21	48,48,48,48	0
60	MG	BA	1812	1/1	0.93	0.16	47,47,47,47	0
60	MG	DA	1697	1/1	0.93	0.21	67,67,67,67	0
60	MG	BA	1685	1/1	0.93	0.11	41,41,41,41	0
60	MG	DA	1699	1/1	0.93	0.20	79,79,79,79	0
60	MG	CA	3414	1/1	0.93	0.18	50,50,50,50	0
60	MG	CA	3417	1/1	0.93	0.18	58,58,58,58	0
60	MG	AA	3219	1/1	0.93	0.22	38,38,38,38	0
60	MG	AA	3428	1/1	0.93	0.14	36,36,36,36	0
60	MG	CA	3420	1/1	0.93	0.26	50,50,50,50	0
60	MG	CA	3425	1/1	0.93	0.15	45,45,45,45	0
60	MG	CA	3428	1/1	0.93	0.36	50,50,50,50	0
60	MG	CA	3621	1/1	0.93	0.22	55,55,55,55	0
60	MG	CA	3429	1/1	0.93	0.23	80,80,80,80	0
60	MG	CA	3623	1/1	0.93	0.58	71,71,71,71	0
60	MG	AA	3006	1/1	0.93	0.29	56,56,56,56	0
60	MG	CA	3434	1/1	0.93	0.17	67,67,67,67	0
60	MG	CA	3435	1/1	0.93	0.16	55,55,55,55	0
60	MG	CA	3237	1/1	0.93	0.34	70,70,70,70	0
60	MG	CA	3441	1/1	0.93	0.16	37,37,37,37	0
60	MG	BA	1690	1/1	0.93	0.19	59,59,59,59	0
60	MG	AA	3354	1/1	0.93	0.29	56,56,56,56	0
60	MG	DA	1726	1/1	0.93	0.16	58,58,58,58	0
60	MG	CA	3635	1/1	0.93	0.30	77,77,77,77	0
60	MG	DA	1730	1/1	0.93	0.39	65,65,65,65	0
60	MG	CA	3453	1/1	0.93	0.08	43,43,43,43	0
60	MG	AA	3834	1/1	0.93	0.29	49,49,49,49	0
60	MG	AA	3123	1/1	0.93	0.49	55,55,55,55	0
60	MG	AB	3003	1/1	0.93	0.12	40,40,40,40	0
60	MG	AA	3570	1/1	0.93	0.14	22,22,22,22	0
60	MG	AA	3223	1/1	0.93	0.17	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3272	1/1	0.93	0.40	74,74,74,74	0
60	MG	AA	3365	1/1	0.93	0.40	55,55,55,55	0
60	MG	BA	1707	1/1	0.93	0.24	57,57,57,57	0
60	MG	CA	3473	1/1	0.93	0.24	48,48,48,48	0
60	MG	AA	3577	1/1	0.93	0.13	65,65,65,65	0
60	MG	AA	3176	1/1	0.93	0.21	70,70,70,70	0
60	MG	CA	3654	1/1	0.93	0.63	76,76,76,76	0
60	MG	CA	3104	1/1	0.93	0.15	64,64,64,64	0
60	MG	AA	3073	1/1	0.93	0.22	61,61,61,61	0
60	MG	CA	3106	1/1	0.93	0.27	45,45,45,45	0
60	MG	AA	3054	1/1	0.93	0.28	26,26,26,26	0
60	MG	AA	3251	1/1	0.93	0.26	50,50,50,50	0
60	MG	CA	3661	1/1	0.93	0.18	78,78,78,78	0
60	MG	AA	3068	1/1	0.93	0.34	52,52,52,52	0
60	MG	BA	1718	1/1	0.93	0.16	48,48,48,48	0
60	MG	AA	3757	1/1	0.93	0.29	67,67,67,67	0
60	MG	BX	114	1/1	0.93	0.27	57,57,57,57	0
60	MG	CA	3118	1/1	0.93	0.11	67,67,67,67	0
60	MG	CA	3489	1/1	0.93	0.18	64,64,64,64	0
60	MG	BX	115	1/1	0.93	0.20	44,44,44,44	0
60	MG	AA	3041	1/1	0.93	0.33	41,41,41,41	0
60	MG	CA	3492	1/1	0.93	0.26	60,60,60,60	0
60	MG	AA	3446	1/1	0.93	0.11	25,25,25,25	0
60	MG	CA	3124	1/1	0.93	0.38	68,68,68,68	0
60	MG	DF	3001	1/1	0.93	0.12	53,53,53,53	0
60	MG	AA	3283	1/1	0.93	0.31	48,48,48,48	0
60	MG	DK	201	1/1	0.93	0.23	55,55,55,55	0
60	MG	AA	3590	1/1	0.93	0.19	71,71,71,71	0
60	MG	BA	1730	1/1	0.93	0.21	68,68,68,68	0
60	MG	CA	3284	1/1	0.93	0.22	49,49,49,49	0
60	MG	AA	3672	1/1	0.93	0.07	71,71,71,71	0
60	MG	CA	3012	1/1	0.93	0.09	41,41,41,41	0
60	MG	AA	3787	1/1	0.94	0.27	55,55,55,55	0
60	MG	AA	3034	1/1	0.94	0.35	84,84,84,84	0
60	MG	AA	3122	1/1	0.94	0.29	39,39,39,39	0
60	MG	A0	103	1/1	0.94	0.12	67,67,67,67	0
60	MG	AA	3791	1/1	0.94	0.23	48,48,48,48	0
60	MG	AA	3526	1/1	0.94	0.15	26,26,26,26	0
60	MG	BN	502	1/1	0.94	0.29	64,64,64,64	0
60	MG	CA	3488	1/1	0.94	0.17	58,58,58,58	0
60	MG	CA	3269	1/1	0.94	0.40	64,64,64,64	0
60	MG	CD	304	1/1	0.94	0.23	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3529	1/1	0.94	0.19	12,12,12,12	1
60	MG	CE	302	1/1	0.94	0.13	31,31,31,31	0
60	MG	CA	3272	1/1	0.94	0.05	56,56,56,56	0
60	MG	AA	3343	1/1	0.94	0.07	60,60,60,60	0
60	MG	CA	3493	1/1	0.94	0.22	66,66,66,66	0
60	MG	AA	3531	1/1	0.94	0.15	61,61,61,61	0
60	MG	AA	3533	1/1	0.94	0.12	20,20,20,20	0
60	MG	BA	1693	1/1	0.94	0.14	69,69,69,69	0
60	MG	AA	3799	1/1	0.94	0.12	45,45,45,45	0
60	MG	AA	3535	1/1	0.94	0.18	37,37,37,37	0
60	MG	BA	1697	1/1	0.94	0.47	80,80,80,80	0
60	MG	AA	3474	1/1	0.94	0.14	74,74,74,74	0
60	MG	CA	3116	1/1	0.94	0.45	57,57,57,57	0
60	MG	AA	3475	1/1	0.94	0.15	73,73,73,73	0
60	MG	BA	1700	1/1	0.94	0.11	62,62,62,62	0
60	MG	BA	1701	1/1	0.94	0.21	47,47,47,47	0
60	MG	CA	3290	1/1	0.94	0.15	61,61,61,61	0
60	MG	CA	3508	1/1	0.94	0.14	74,74,74,74	0
60	MG	AA	3345	1/1	0.94	0.10	34,34,34,34	0
60	MG	AA	3707	1/1	0.94	0.43	59,59,59,59	0
60	MG	AA	3050	1/1	0.94	0.25	29,29,29,29	0
60	MG	AA	3710	1/1	0.94	0.17	55,55,55,55	0
60	MG	CA	3513	1/1	0.94	0.24	109,109,109,109	0
60	MG	C8	5001	1/1	0.94	0.29	43,43,43,43	0
60	MG	AA	3298	1/1	0.94	0.15	28,28,28,28	0
60	MG	AA	3349	1/1	0.94	0.13	34,34,34,34	0
60	MG	CA	3300	1/1	0.94	0.15	56,56,56,56	0
60	MG	DA	1606	1/1	0.94	0.16	66,66,66,66	0
60	MG	CA	3301	1/1	0.94	0.43	56,56,56,56	0
60	MG	AA	3714	1/1	0.94	0.24	44,44,44,44	0
60	MG	AA	3820	1/1	0.94	0.21	31,31,31,31	0
60	MG	CA	3134	1/1	0.94	0.18	64,64,64,64	0
60	MG	CA	3308	1/1	0.94	0.19	35,35,35,35	0
60	MG	BA	1713	1/1	0.94	0.24	61,61,61,61	0
60	MG	CA	3002	1/1	0.94	0.24	32,32,32,32	0
60	MG	AA	3214	1/1	0.94	0.08	47,47,47,47	0
60	MG	AA	3060	1/1	0.94	0.34	23,23,23,23	0
60	MG	CA	3010	1/1	0.94	0.13	49,49,49,49	0
60	MG	CA	3141	1/1	0.94	0.32	51,51,51,51	0
60	MG	BA	1615	1/1	0.94	0.30	65,65,65,65	0
60	MG	AA	3823	1/1	0.94	0.33	51,51,51,51	0
60	MG	CA	3325	1/1	0.94	0.25	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3720	1/1	0.94	0.35	78,78,78,78	0
60	MG	CA	3327	1/1	0.94	0.22	37,37,37,37	0
60	MG	CA	3145	1/1	0.94	0.33	65,65,65,65	0
60	MG	CA	3537	1/1	0.94	0.10	64,64,64,64	0
60	MG	AA	3071	1/1	0.94	0.73	55,55,55,55	0
60	MG	AA	3426	1/1	0.94	0.20	47,47,47,47	0
60	MG	AA	3549	1/1	0.94	0.12	53,53,53,53	0
60	MG	CA	3019	1/1	0.94	0.14	23,23,23,23	0
60	MG	BA	1726	1/1	0.94	0.17	59,59,59,59	0
60	MG	BA	1728	1/1	0.94	0.18	53,53,53,53	0
60	MG	AA	3830	1/1	0.94	0.30	75,75,75,75	0
60	MG	AA	3090	1/1	0.94	0.27	52,52,52,52	0
60	MG	DA	1637	1/1	0.94	0.38	61,61,61,61	0
60	MG	CA	3343	1/1	0.94	0.15	37,37,37,37	0
60	MG	AA	3835	1/1	0.94	0.23	34,34,34,34	1
60	MG	AA	3356	1/1	0.94	0.12	51,51,51,51	0
60	MG	DA	1641	1/1	0.94	0.13	55,55,55,55	0
60	MG	AA	3553	1/1	0.94	0.17	47,47,47,47	0
60	MG	CA	3554	1/1	0.94	0.16	60,60,60,60	0
60	MG	DA	1649	1/1	0.94	0.30	53,53,53,53	0
60	MG	CA	3163	1/1	0.94	0.31	41,41,41,41	0
60	MG	AA	3556	1/1	0.94	0.17	54,54,54,54	0
60	MG	CA	3034	1/1	0.94	0.15	51,51,51,51	0
60	MG	CA	3354	1/1	0.94	0.18	40,40,40,40	0
60	MG	AA	3558	1/1	0.94	0.14	72,72,72,72	0
60	MG	CA	3564	1/1	0.94	0.28	33,33,33,33	0
60	MG	DA	1659	1/1	0.94	0.35	79,79,79,79	0
60	MG	AA	3635	1/1	0.94	0.15	33,33,33,33	0
60	MG	CA	3568	1/1	0.94	0.24	71,71,71,71	0
60	MG	CA	3360	1/1	0.94	0.17	52,52,52,52	0
60	MG	CA	3570	1/1	0.94	0.09	61,61,61,61	0
60	MG	AB	3009	1/1	0.94	0.10	62,62,62,62	0
60	MG	CA	3173	1/1	0.94	0.53	72,72,72,72	0
60	MG	CA	3364	1/1	0.94	0.19	64,64,64,64	0
60	MG	CA	3574	1/1	0.94	0.11	31,31,31,31	0
60	MG	CA	3365	1/1	0.94	0.18	69,69,69,69	0
60	MG	AA	3636	1/1	0.94	0.21	71,71,71,71	0
60	MG	AA	3012	1/1	0.94	0.17	38,38,38,38	0
60	MG	BA	1751	1/1	0.94	0.30	49,49,49,49	0
60	MG	AB	3013	1/1	0.94	0.13	55,55,55,55	0
60	MG	BA	1754	1/1	0.94	0.05	75,75,75,75	0
60	MG	AA	3197	1/1	0.94	0.32	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3586	1/1	0.94	0.25	75,75,75,75	0
60	MG	DA	1682	1/1	0.94	0.30	60,60,60,60	0
60	MG	AA	3134	1/1	0.94	0.52	49,49,49,49	0
60	MG	CA	3380	1/1	0.94	0.16	37,37,37,37	0
60	MG	CA	3046	1/1	0.94	0.07	72,72,72,72	0
60	MG	AA	3173	1/1	0.94	0.26	74,74,74,74	0
60	MG	BA	1637	1/1	0.94	0.19	64,64,64,64	0
60	MG	AA	3642	1/1	0.94	0.23	60,60,60,60	0
60	MG	DA	1692	1/1	0.94	0.26	49,49,49,49	0
60	MG	DA	1693	1/1	0.94	0.15	50,50,50,50	0
60	MG	AA	3366	1/1	0.94	0.18	35,35,35,35	0
60	MG	CA	3052	1/1	0.94	0.34	46,46,46,46	0
60	MG	AB	3020	1/1	0.94	0.09	66,66,66,66	0
60	MG	AA	3493	1/1	0.94	0.22	56,56,56,56	0
60	MG	AB	3022	1/1	0.94	0.06	79,79,79,79	0
60	MG	AA	3749	1/1	0.94	0.14	30,30,30,30	0
60	MG	DA	1701	1/1	0.94	0.14	61,61,61,61	0
60	MG	CA	3203	1/1	0.94	0.32	45,45,45,45	0
60	MG	AD	302	1/1	0.94	0.39	31,31,31,31	0
60	MG	BA	1772	1/1	0.94	0.33	51,51,51,51	0
60	MG	CA	3398	1/1	0.94	0.20	57,57,57,57	0
60	MG	AA	3174	1/1	0.94	0.27	39,39,39,39	0
60	MG	CA	3207	1/1	0.94	0.48	62,62,62,62	0
60	MG	CA	3403	1/1	0.94	0.19	70,70,70,70	0
60	MG	CA	3208	1/1	0.94	0.12	24,24,24,24	0
60	MG	CA	3060	1/1	0.94	0.28	50,50,50,50	0
60	MG	DA	1717	1/1	0.94	0.17	70,70,70,70	0
60	MG	AA	3317	1/1	0.94	0.19	56,56,56,56	0
60	MG	CA	3408	1/1	0.94	0.27	35,35,35,35	0
60	MG	AA	3320	1/1	0.94	0.24	65,65,65,65	0
60	MG	BA	1651	1/1	0.94	0.12	69,69,69,69	0
60	MG	AA	3573	1/1	0.94	0.09	47,47,47,47	0
60	MG	DA	1723	1/1	0.94	0.28	53,53,53,53	0
60	MG	AA	3038	1/1	0.94	0.40	42,42,42,42	0
60	MG	CA	3413	1/1	0.94	0.25	38,38,38,38	0
60	MG	CA	3217	1/1	0.94	0.13	52,52,52,52	0
60	MG	CA	3624	1/1	0.94	0.22	76,76,76,76	0
60	MG	BA	1783	1/1	0.94	0.15	61,61,61,61	0
60	MG	AA	3322	1/1	0.94	0.19	37,37,37,37	0
60	MG	AA	3077	1/1	0.94	0.26	44,44,44,44	0
60	MG	AA	3759	1/1	0.94	0.13	29,29,29,29	0
60	MG	AA	3256	1/1	0.94	0.18	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3658	1/1	0.94	0.21	25,25,25,25	0
60	MG	AA	3503	1/1	0.94	0.14	41,41,41,41	0
60	MG	CA	3430	1/1	0.94	0.22	38,38,38,38	0
60	MG	AA	3047	1/1	0.94	0.30	40,40,40,40	0
60	MG	AA	3383	1/1	0.94	0.21	31,31,31,31	0
60	MG	CA	3638	1/1	0.94	0.48	68,68,68,68	0
60	MG	CA	3231	1/1	0.94	0.26	56,56,56,56	0
60	MG	BA	1665	1/1	0.94	0.41	68,68,68,68	0
60	MG	CA	3440	1/1	0.94	0.41	69,69,69,69	0
60	MG	AA	3064	1/1	0.94	0.22	31,31,31,31	0
60	MG	CA	3078	1/1	0.94	0.14	49,49,49,49	0
60	MG	AA	3670	1/1	0.94	0.17	66,66,66,66	0
60	MG	CA	3647	1/1	0.94	0.38	61,61,61,61	0
60	MG	CA	3452	1/1	0.94	0.17	37,37,37,37	0
60	MG	DA	1756	1/1	0.94	0.24	60,60,60,60	0
60	MG	BA	1796	1/1	0.94	0.18	75,75,75,75	0
60	MG	AA	3586	1/1	0.94	0.19	75,75,75,75	0
60	MG	AA	3771	1/1	0.94	0.18	40,40,40,40	0
60	MG	AA	3207	1/1	0.94	0.34	67,67,67,67	0
60	MG	AA	3001	1/1	0.94	0.21	39,39,39,39	0
60	MG	BA	1802	1/1	0.94	0.13	58,58,58,58	0
60	MG	CA	3657	1/1	0.94	0.24	34,34,34,34	0
60	MG	AA	3675	1/1	0.94	0.16	67,67,67,67	0
60	MG	CA	3465	1/1	0.94	0.08	64,64,64,64	0
60	MG	AA	3067	1/1	0.94	0.62	82,82,82,82	0
60	MG	CA	3469	1/1	0.94	0.58	76,76,76,76	0
60	MG	AA	3515	1/1	0.94	0.14	27,27,27,27	0
60	MG	AA	3680	1/1	0.94	0.12	70,70,70,70	0
60	MG	AA	3339	1/1	0.94	0.29	18,18,18,18	0
60	MG	AA	3593	1/1	0.94	0.14	49,49,49,49	0
60	MG	BA	1811	1/1	0.94	0.14	52,52,52,52	0
60	MG	CB	3004	1/1	0.94	0.13	70,70,70,70	0
60	MG	CB	3005	1/1	0.94	0.22	65,65,65,65	0
60	MG	AA	3518	1/1	0.94	0.18	28,28,28,28	0
60	MG	CA	3255	1/1	0.94	0.35	61,61,61,61	0
60	MG	AA	3801	1/1	0.95	0.16	39,39,39,39	0
60	MG	CA	3310	1/1	0.95	0.21	45,45,45,45	0
60	MG	BA	1711	1/1	0.95	0.37	63,63,63,63	0
60	MG	AA	3701	1/1	0.95	0.56	62,62,62,62	0
60	MG	AA	3803	1/1	0.95	0.33	37,37,37,37	0
60	MG	AA	3610	1/1	0.95	0.10	66,66,66,66	0
60	MG	AA	3704	1/1	0.95	0.17	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3319	1/1	0.95	0.07	32,32,32,32	0
60	MG	CA	3321	1/1	0.95	0.13	65,65,65,65	0
60	MG	CA	3516	1/1	0.95	0.20	58,58,58,58	0
60	MG	AA	3463	1/1	0.95	0.19	41,41,41,41	0
60	MG	CA	3518	1/1	0.95	0.18	72,72,72,72	0
60	MG	AA	3807	1/1	0.95	0.20	62,62,62,62	0
60	MG	BA	1610	1/1	0.95	0.14	112,112,112,112	0
60	MG	AA	3464	1/1	0.95	0.09	69,69,69,69	0
60	MG	CU	201	1/1	0.95	0.51	62,62,62,62	0
60	MG	CV	201	1/1	0.95	0.36	84,84,84,84	0
60	MG	CV	202	1/1	0.95	0.36	82,82,82,82	0
60	MG	AA	3539	1/1	0.95	0.23	42,42,42,42	0
60	MG	CA	3328	1/1	0.95	0.17	40,40,40,40	0
60	MG	CA	3025	1/1	0.95	0.50	32,32,32,32	1
60	MG	AA	3398	1/1	0.95	0.19	29,29,29,29	0
60	MG	AA	3711	1/1	0.95	0.37	41,41,41,41	0
60	MG	CA	3160	1/1	0.95	0.27	33,33,33,33	0
60	MG	BA	1616	1/1	0.95	0.11	69,69,69,69	0
60	MG	AA	3468	1/1	0.95	0.12	34,34,34,34	0
60	MG	DA	1604	1/1	0.95	0.12	90,90,90,90	0
60	MG	CA	3164	1/1	0.95	0.13	38,38,38,38	0
60	MG	AA	3815	1/1	0.95	0.46	72,72,72,72	0
60	MG	AA	3469	1/1	0.95	0.20	37,37,37,37	0
60	MG	AA	3472	1/1	0.95	0.24	37,37,37,37	0
60	MG	AA	3344	1/1	0.95	0.18	65,65,65,65	0
60	MG	AA	3276	1/1	0.95	0.18	64,64,64,64	0
60	MG	CA	3038	1/1	0.95	0.21	26,26,26,26	0
60	MG	AA	3719	1/1	0.95	0.09	62,62,62,62	0
60	MG	CA	3176	1/1	0.95	0.35	60,60,60,60	0
60	MG	AA	3546	1/1	0.95	0.17	36,36,36,36	0
60	MG	CA	3179	1/1	0.95	0.27	27,27,27,27	0
60	MG	CA	3180	1/1	0.95	0.17	46,46,46,46	0
60	MG	AA	3117	1/1	0.95	0.17	64,64,64,64	0
60	MG	CA	3358	1/1	0.95	0.13	41,41,41,41	0
60	MG	CA	3546	1/1	0.95	0.17	59,59,59,59	0
60	MG	AA	3722	1/1	0.95	0.17	31,31,31,31	0
60	MG	AA	3308	1/1	0.95	0.11	45,45,45,45	0
60	MG	CA	3362	1/1	0.95	0.11	20,20,20,20	0
60	MG	BA	1748	1/1	0.95	0.33	75,75,75,75	0
60	MG	DA	1627	1/1	0.95	0.36	48,48,48,48	0
60	MG	AA	3831	1/1	0.95	0.39	41,41,41,41	0
60	MG	AA	3348	1/1	0.95	0.30	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3478	1/1	0.95	0.07	70,70,70,70	0
60	MG	CA	3556	1/1	0.95	0.05	77,77,77,77	0
60	MG	AA	3551	1/1	0.95	0.17	58,58,58,58	0
60	MG	BA	1756	1/1	0.95	0.25	43,43,43,43	0
60	MG	AA	3634	1/1	0.95	0.25	63,63,63,63	0
60	MG	CA	3196	1/1	0.95	0.28	57,57,57,57	0
60	MG	AA	3220	1/1	0.95	0.19	65,65,65,65	0
60	MG	CA	3565	1/1	0.95	0.14	36,36,36,36	0
60	MG	CA	3378	1/1	0.95	0.15	63,63,63,63	0
60	MG	AA	3414	1/1	0.95	0.17	43,43,43,43	0
60	MG	AA	3554	1/1	0.95	0.07	48,48,48,48	0
60	MG	AB	3008	1/1	0.95	0.39	46,46,46,46	0
60	MG	AA	3416	1/1	0.95	0.19	31,31,31,31	0
60	MG	AA	3184	1/1	0.95	0.20	39,39,39,39	0
60	MG	AA	3418	1/1	0.95	0.17	22,22,22,22	0
60	MG	BA	1641	1/1	0.95	0.29	56,56,56,56	0
60	MG	AA	3741	1/1	0.95	0.27	47,47,47,47	0
60	MG	CA	3061	1/1	0.95	0.15	36,36,36,36	0
60	MG	AA	3742	1/1	0.95	0.20	68,68,68,68	0
60	MG	DA	1656	1/1	0.95	0.07	67,67,67,67	0
60	MG	AA	3312	1/1	0.95	0.14	25,25,25,25	0
60	MG	AA	3186	1/1	0.95	0.24	53,53,53,53	0
60	MG	AB	3017	1/1	0.95	0.07	76,76,76,76	0
60	MG	DA	1660	1/1	0.95	0.29	81,81,81,81	0
60	MG	CA	3395	1/1	0.95	0.12	60,60,60,60	0
60	MG	BA	1777	1/1	0.95	0.12	76,76,76,76	0
60	MG	DA	1663	1/1	0.95	0.10	53,53,53,53	0
60	MG	AA	3314	1/1	0.95	0.20	43,43,43,43	0
60	MG	BA	1648	1/1	0.95	0.18	28,28,28,28	0
60	MG	AA	3424	1/1	0.95	0.11	48,48,48,48	0
60	MG	AA	3315	1/1	0.95	0.21	56,56,56,56	0
60	MG	CA	3591	1/1	0.95	0.14	69,69,69,69	0
60	MG	AA	3118	1/1	0.95	0.30	59,59,59,59	0
60	MG	AA	3651	1/1	0.95	0.23	66,66,66,66	0
60	MG	AA	3190	1/1	0.95	0.18	51,51,51,51	0
60	MG	BA	1654	1/1	0.95	0.12	45,45,45,45	0
60	MG	CA	3225	1/1	0.95	0.24	73,73,73,73	0
60	MG	BA	1655	1/1	0.95	0.27	65,65,65,65	0
60	MG	CA	3227	1/1	0.95	0.25	30,30,30,30	0
60	MG	AA	3044	1/1	0.95	0.35	62,62,62,62	0
60	MG	AA	3431	1/1	0.95	0.15	25,25,25,25	0
60	MG	DA	1679	1/1	0.95	0.38	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	DA	1680	1/1	0.95	0.17	40,40,40,40	0
60	MG	AA	3433	1/1	0.95	0.28	50,50,50,50	0
60	MG	AA	3162	1/1	0.95	0.32	35,35,35,35	0
60	MG	CA	3605	1/1	0.95	0.19	72,72,72,72	0
60	MG	AA	3129	1/1	0.95	0.27	52,52,52,52	0
60	MG	AA	3267	1/1	0.95	0.31	43,43,43,43	0
60	MG	AA	3760	1/1	0.95	0.34	50,50,50,50	0
60	MG	DA	1690	1/1	0.95	0.20	74,74,74,74	0
60	MG	CA	3609	1/1	0.95	0.21	62,62,62,62	0
60	MG	AA	3761	1/1	0.95	0.19	72,72,72,72	0
60	MG	CA	3421	1/1	0.95	0.19	39,39,39,39	0
60	MG	CA	3612	1/1	0.95	0.13	59,59,59,59	0
60	MG	CA	3424	1/1	0.95	0.25	40,40,40,40	0
60	MG	DA	1696	1/1	0.95	0.26	65,65,65,65	0
60	MG	AA	3292	1/1	0.95	0.18	31,31,31,31	0
60	MG	CA	3615	1/1	0.95	0.15	33,33,33,33	0
60	MG	CA	3426	1/1	0.95	0.16	46,46,46,46	0
60	MG	CA	3427	1/1	0.95	0.29	69,69,69,69	0
60	MG	CA	3618	1/1	0.95	0.21	79,79,79,79	0
60	MG	AA	3662	1/1	0.95	0.33	60,60,60,60	0
60	MG	AA	3372	1/1	0.95	0.27	59,59,59,59	0
60	MG	AF	302	1/1	0.95	0.09	42,42,42,42	0
60	MG	DA	1706	1/1	0.95	0.19	70,70,70,70	0
60	MG	AA	3666	1/1	0.95	0.29	28,28,28,28	0
60	MG	CA	3433	1/1	0.95	0.15	45,45,45,45	0
60	MG	AA	3373	1/1	0.95	0.22	23,23,23,23	0
60	MG	DA	1713	1/1	0.95	0.15	59,59,59,59	0
60	MG	BA	1805	1/1	0.95	0.10	55,55,55,55	0
60	MG	CA	3627	1/1	0.95	0.07	59,59,59,59	0
60	MG	AA	3376	1/1	0.95	0.21	39,39,39,39	0
60	MG	AA	3293	1/1	0.95	0.14	68,68,68,68	0
60	MG	AA	3102	1/1	0.95	0.24	38,38,38,38	0
60	MG	AA	3331	1/1	0.95	0.20	61,61,61,61	0
60	MG	AA	3084	1/1	0.95	0.10	27,27,27,27	0
60	MG	AA	3676	1/1	0.95	0.17	46,46,46,46	0
60	MG	BA	1677	1/1	0.95	0.32	57,57,57,57	0
60	MG	BA	1678	1/1	0.95	0.22	52,52,52,52	0
60	MG	AA	3775	1/1	0.95	0.18	52,52,52,52	0
60	MG	AA	3133	1/1	0.95	0.47	92,92,92,92	1
60	MG	AA	3091	1/1	0.95	0.48	62,62,62,62	0
60	MG	DA	1727	1/1	0.95	0.17	65,65,65,65	0
60	MG	CA	3641	1/1	0.95	0.54	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3779	1/1	0.95	0.28	41,41,41,41	0
60	MG	CA	3463	1/1	0.95	0.43	75,75,75,75	0
60	MG	AA	3338	1/1	0.95	0.13	49,49,49,49	0
60	MG	CA	3266	1/1	0.95	0.15	67,67,67,67	0
60	MG	CA	3107	1/1	0.95	0.11	64,64,64,64	0
60	MG	AU	204	1/1	0.95	0.45	55,55,55,55	0
60	MG	CA	3109	1/1	0.95	0.18	65,65,65,65	0
60	MG	CA	3471	1/1	0.95	0.21	59,59,59,59	0
60	MG	CA	3472	1/1	0.95	0.29	49,49,49,49	0
60	MG	AA	3781	1/1	0.95	0.17	49,49,49,49	0
60	MG	AA	3449	1/1	0.95	0.20	46,46,46,46	0
60	MG	AW	3003	1/1	0.95	0.33	38,38,38,38	0
60	MG	CA	3274	1/1	0.95	0.18	64,64,64,64	0
60	MG	AA	3682	1/1	0.95	0.20	58,58,58,58	0
60	MG	CA	3479	1/1	0.95	0.16	67,67,67,67	0
60	MG	AA	3384	1/1	0.95	0.16	26,26,26,26	0
60	MG	AA	3253	1/1	0.95	0.19	42,42,42,42	0
60	MG	BA	1692	1/1	0.95	0.31	69,69,69,69	0
60	MG	AA	3454	1/1	0.95	0.16	27,27,27,27	0
60	MG	CA	3121	1/1	0.95	0.32	78,78,78,78	0
60	MG	AA	3389	1/1	0.95	0.18	46,46,46,46	0
60	MG	AA	3135	1/1	0.95	0.16	53,53,53,53	0
60	MG	AA	3602	1/1	0.95	0.21	39,39,39,39	0
60	MG	AA	3792	1/1	0.95	0.26	35,35,35,35	0
60	MG	A1	102	1/1	0.95	0.16	46,46,46,46	0
60	MG	AA	3459	1/1	0.95	0.47	65,65,65,65	0
60	MG	CA	3128	1/1	0.95	0.22	31,31,31,31	0
60	MG	AA	3302	1/1	0.95	0.34	58,58,58,58	0
60	MG	CA	3131	1/1	0.95	0.28	61,61,61,61	0
60	MG	AA	3607	1/1	0.95	0.15	39,39,39,39	0
60	MG	AA	3695	1/1	0.95	0.29	50,50,50,50	0
60	MG	BA	1704	1/1	0.95	0.26	68,68,68,68	0
60	MG	CA	3299	1/1	0.95	0.23	42,42,42,42	0
60	MG	BA	1705	1/1	0.95	0.31	61,61,61,61	0
60	MG	AA	3696	1/1	0.95	0.20	62,62,62,62	0
60	MG	A8	5002	1/1	0.95	0.25	45,45,45,45	0
60	MG	AA	3255	1/1	0.95	0.28	64,64,64,64	0
60	MG	CA	3304	1/1	0.95	0.15	48,48,48,48	0
60	MG	AA	3462	1/1	0.95	0.06	73,73,73,73	0
60	MG	CA	3009	1/1	0.95	0.05	24,24,24,24	0
62	ZN	A4	501	1/1	0.95	0.08	120,120,120,120	0
62	ZN	C4	501	1/1	0.95	0.07	163,163,163,163	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3275	1/1	0.96	0.39	56,56,56,56	0
60	MG	CA	3367	1/1	0.96	0.13	39,39,39,39	0
60	MG	CA	3369	1/1	0.96	0.17	65,65,65,65	0
60	MG	AA	3620	1/1	0.96	0.14	49,49,49,49	0
60	MG	AA	3357	1/1	0.96	0.18	52,52,52,52	0
60	MG	CA	3373	1/1	0.96	0.38	71,71,71,71	0
60	MG	AA	3358	1/1	0.96	0.06	72,72,72,72	0
60	MG	CA	3375	1/1	0.96	0.09	65,65,65,65	0
60	MG	AA	3022	1/1	0.96	0.09	19,19,19,19	0
60	MG	AA	3422	1/1	0.96	0.19	22,22,22,22	0
60	MG	CA	3216	1/1	0.96	0.25	32,32,32,32	0
60	MG	CA	3082	1/1	0.96	0.21	31,31,31,31	0
60	MG	AA	3009	1/1	0.96	0.09	26,26,26,26	0
60	MG	AA	3626	1/1	0.96	0.23	59,59,59,59	0
60	MG	AA	3131	1/1	0.96	0.29	39,39,39,39	0
60	MG	A7	101	1/1	0.96	0.10	57,57,57,57	0
60	MG	AA	3629	1/1	0.96	0.11	51,51,51,51	0
60	MG	AA	3172	1/1	0.96	0.18	50,50,50,50	0
60	MG	BB	3001	1/1	0.96	0.23	67,67,67,67	0
60	MG	CA	3558	1/1	0.96	0.20	49,49,49,49	1
60	MG	BA	1695	1/1	0.96	0.06	64,64,64,64	0
60	MG	CA	3561	1/1	0.96	0.12	62,62,62,62	0
60	MG	AA	3057	1/1	0.96	0.29	56,56,56,56	0
60	MG	AA	3809	1/1	0.96	0.25	46,46,46,46	0
60	MG	CA	3392	1/1	0.96	0.09	66,66,66,66	0
60	MG	AA	3367	1/1	0.96	0.11	52,52,52,52	0
60	MG	AA	3633	1/1	0.96	0.25	51,51,51,51	0
60	MG	AA	3368	1/1	0.96	0.31	54,54,54,54	0
60	MG	CA	3233	1/1	0.96	0.30	52,52,52,52	0
60	MG	AA	3281	1/1	0.96	0.43	38,38,38,38	0
60	MG	AA	3282	1/1	0.96	0.39	65,65,65,65	0
60	MG	AA	3816	1/1	0.96	0.25	64,64,64,64	0
60	MG	CA	3100	1/1	0.96	0.17	75,75,75,75	0
60	MG	AA	3817	1/1	0.96	0.46	40,40,40,40	0
60	MG	AA	3094	1/1	0.96	0.31	82,82,82,82	0
60	MG	CA	3405	1/1	0.96	0.15	50,50,50,50	0
60	MG	CA	3577	1/1	0.96	0.12	52,52,52,52	0
60	MG	AA	3726	1/1	0.96	0.13	74,74,74,74	0
60	MG	CA	3579	1/1	0.96	0.07	58,58,58,58	0
60	MG	CA	3580	1/1	0.96	0.12	37,37,37,37	0
60	MG	AA	3436	1/1	0.96	0.13	31,31,31,31	0
60	MG	AA	3039	1/1	0.96	0.25	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3375	1/1	0.96	0.13	16,16,16,16	0
60	MG	AA	3825	1/1	0.96	0.29	45,45,45,45	0
60	MG	DA	1644	1/1	0.96	0.18	49,49,49,49	0
60	MG	DA	1646	1/1	0.96	0.30	51,51,51,51	0
60	MG	CA	3585	1/1	0.96	0.11	44,44,44,44	0
60	MG	AA	3730	1/1	0.96	0.27	34,34,34,34	0
60	MG	AA	3566	1/1	0.96	0.19	26,26,26,26	0
60	MG	CA	3110	1/1	0.96	0.33	35,35,35,35	0
60	MG	CA	3248	1/1	0.96	0.08	58,58,58,58	0
60	MG	BX	108	1/1	0.96	0.10	78,78,78,78	0
60	MG	BX	109	1/1	0.96	0.22	55,55,55,55	0
60	MG	CA	3252	1/1	0.96	0.25	30,30,30,30	0
60	MG	CA	3253	1/1	0.96	0.38	61,61,61,61	0
60	MG	CA	3594	1/1	0.96	0.16	62,62,62,62	0
60	MG	AA	3734	1/1	0.96	0.12	23,23,23,23	0
60	MG	CA	3423	1/1	0.96	0.18	57,57,57,57	0
60	MG	AA	3326	1/1	0.96	0.14	22,22,22,22	0
60	MG	CA	3256	1/1	0.96	0.29	73,73,73,73	0
60	MG	BA	1716	1/1	0.96	0.27	71,71,71,71	0
60	MG	AA	3645	1/1	0.96	0.10	57,57,57,57	0
60	MG	CA	3117	1/1	0.96	0.13	46,46,46,46	0
60	MG	AA	3832	1/1	0.96	0.21	52,52,52,52	0
60	MG	CA	3264	1/1	0.96	0.20	54,54,54,54	0
60	MG	AA	3155	1/1	0.96	0.24	31,31,31,31	0
60	MG	AA	3647	1/1	0.96	0.14	35,35,35,35	0
60	MG	AA	3569	1/1	0.96	0.19	17,17,17,17	0
60	MG	AA	3229	1/1	0.96	0.13	33,33,33,33	0
60	MG	CA	3436	1/1	0.96	0.15	34,34,34,34	0
60	MG	AA	3013	1/1	0.96	0.14	38,38,38,38	0
60	MG	CA	3270	1/1	0.96	0.33	69,69,69,69	0
60	MG	BA	1725	1/1	0.96	0.31	52,52,52,52	0
60	MG	AA	3020	1/1	0.96	0.18	25,25,25,25	0
60	MG	CA	3443	1/1	0.96	0.31	40,40,40,40	0
60	MG	CA	3444	1/1	0.96	0.24	70,70,70,70	0
60	MG	DA	1681	1/1	0.96	0.14	44,44,44,44	0
60	MG	AA	3259	1/1	0.96	0.37	27,27,27,27	0
60	MG	DA	1683	1/1	0.96	0.42	60,60,60,60	0
60	MG	CA	3447	1/1	0.96	0.12	44,44,44,44	0
60	MG	DA	1685	1/1	0.96	0.20	49,49,49,49	0
60	MG	CA	3448	1/1	0.96	0.08	64,64,64,64	0
60	MG	AA	3653	1/1	0.96	0.12	47,47,47,47	0
60	MG	AA	3334	1/1	0.96	0.21	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3456	1/1	0.96	0.15	37,37,37,37	0
60	MG	CA	3130	1/1	0.96	0.17	57,57,57,57	0
60	MG	AA	3502	1/1	0.96	0.09	41,41,41,41	0
60	MG	AA	3748	1/1	0.96	0.18	62,62,62,62	0
60	MG	CA	3014	1/1	0.96	0.14	58,58,58,58	0
60	MG	AA	3336	1/1	0.96	0.27	52,52,52,52	0
60	MG	AA	3003	1/1	0.96	0.07	14,14,14,14	0
60	MG	AA	3385	1/1	0.96	0.20	24,24,24,24	0
60	MG	AA	3387	1/1	0.96	0.21	34,34,34,34	0
60	MG	CA	3020	1/1	0.96	0.18	38,38,38,38	0
60	MG	CA	3468	1/1	0.96	0.17	37,37,37,37	0
60	MG	AA	3754	1/1	0.96	0.09	25,25,25,25	0
60	MG	CA	3289	1/1	0.96	0.13	23,23,23,23	0
60	MG	AA	3510	1/1	0.96	0.22	13,13,13,13	0
60	MG	BA	1741	1/1	0.96	0.15	49,49,49,49	0
60	MG	CA	3024	1/1	0.96	0.62	67,67,67,67	0
60	MG	BA	1742	1/1	0.96	0.09	45,45,45,45	0
60	MG	CA	3026	1/1	0.96	0.47	55,55,55,55	0
60	MG	DA	1709	1/1	0.96	0.22	57,57,57,57	0
60	MG	BA	1744	1/1	0.96	0.13	48,48,48,48	0
60	MG	DA	1711	1/1	0.96	0.10	64,64,64,64	0
60	MG	CA	3297	1/1	0.96	0.16	55,55,55,55	0
60	MG	CA	3147	1/1	0.96	0.12	51,51,51,51	0
60	MG	AA	3205	1/1	0.96	0.31	45,45,45,45	0
60	MG	BA	1746	1/1	0.96	0.16	70,70,70,70	0
60	MG	AA	3451	1/1	0.96	0.18	43,43,43,43	0
60	MG	AA	3665	1/1	0.96	0.06	63,63,63,63	0
60	MG	AA	3206	1/1	0.96	0.19	55,55,55,55	0
60	MG	BA	1753	1/1	0.96	0.14	48,48,48,48	0
60	MG	AA	3390	1/1	0.96	0.14	23,23,23,23	0
60	MG	AA	3391	1/1	0.96	0.13	27,27,27,27	0
60	MG	AA	3762	1/1	0.96	0.26	63,63,63,63	0
60	MG	AA	3517	1/1	0.96	0.31	44,44,44,44	0
60	MG	AA	3457	1/1	0.96	0.17	18,18,18,18	0
60	MG	AA	3522	1/1	0.96	0.16	31,31,31,31	0
60	MG	AA	3594	1/1	0.96	0.26	48,48,48,48	0
60	MG	AA	3100	1/1	0.96	0.21	34,34,34,34	0
60	MG	DA	1728	1/1	0.96	0.09	53,53,53,53	0
60	MG	AA	3264	1/1	0.96	0.09	54,54,54,54	0
60	MG	AE	302	1/1	0.96	0.18	62,62,62,62	0
60	MG	DA	1732	1/1	0.96	0.11	54,54,54,54	0
60	MG	AA	3085	1/1	0.96	0.24	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3047	1/1	0.96	0.06	54,54,54,54	0
60	MG	CA	3172	1/1	0.96	0.17	41,41,41,41	0
60	MG	DA	1736	1/1	0.96	0.17	63,63,63,63	0
60	MG	AA	3528	1/1	0.96	0.19	26,26,26,26	0
60	MG	AA	3086	1/1	0.96	0.35	43,43,43,43	1
60	MG	CA	3501	1/1	0.96	0.17	78,78,78,78	0
60	MG	BA	1771	1/1	0.96	0.13	48,48,48,48	0
60	MG	AA	3239	1/1	0.96	0.21	63,63,63,63	0
60	MG	CA	3504	1/1	0.96	0.11	77,77,77,77	0
60	MG	DA	1744	1/1	0.96	0.14	57,57,57,57	0
60	MG	DA	1745	1/1	0.96	0.23	54,54,54,54	0
60	MG	AA	3052	1/1	0.96	0.20	15,15,15,15	0
60	MG	AA	3774	1/1	0.96	0.10	44,44,44,44	0
60	MG	CA	3331	1/1	0.96	0.47	62,62,62,62	0
60	MG	AA	3241	1/1	0.96	0.26	29,29,29,29	0
60	MG	AA	3776	1/1	0.96	0.12	21,21,21,21	0
60	MG	BA	1663	1/1	0.96	0.13	66,66,66,66	0
60	MG	AA	3685	1/1	0.96	0.15	58,58,58,58	0
60	MG	AA	3686	1/1	0.96	0.24	62,62,62,62	0
60	MG	AA	3534	1/1	0.96	0.20	34,34,34,34	0
60	MG	DA	1755	1/1	0.96	0.14	69,69,69,69	0
60	MG	CA	3189	1/1	0.96	0.07	40,40,40,40	0
60	MG	AA	3606	1/1	0.96	0.18	62,62,62,62	0
60	MG	CA	3344	1/1	0.96	0.18	27,27,27,27	0
60	MG	DA	1759	1/1	0.96	0.42	64,64,64,64	0
60	MG	DA	1760	1/1	0.96	0.27	53,53,53,53	0
60	MG	CA	3345	1/1	0.96	0.19	41,41,41,41	0
60	MG	AA	3407	1/1	0.96	0.19	22,22,22,22	0
60	MG	AA	3536	1/1	0.96	0.09	36,36,36,36	0
60	MG	AA	3691	1/1	0.96	0.09	51,51,51,51	0
60	MG	AA	3467	1/1	0.96	0.13	54,54,54,54	0
60	MG	AA	3035	1/1	0.96	0.22	69,69,69,69	0
60	MG	CF	305	1/1	0.96	0.20	45,45,45,45	0
60	MG	CA	3198	1/1	0.96	0.25	49,49,49,49	0
60	MG	AA	3611	1/1	0.96	0.26	57,57,57,57	0
60	MG	AA	3143	1/1	0.96	0.05	37,37,37,37	0
60	MG	CP	201	1/1	0.96	0.13	57,57,57,57	0
60	MG	CA	3356	1/1	0.96	0.24	28,28,28,28	0
60	MG	AA	3188	1/1	0.96	0.16	15,15,15,15	0
60	MG	AA	3697	1/1	0.96	0.15	71,71,71,71	0
60	MG	AW	3004	1/1	0.96	0.14	45,45,45,45	0
60	MG	AA	3074	1/1	0.96	0.37	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	BA	1797	1/1	0.96	0.15	75,75,75,75	0
60	MG	AA	3699	1/1	0.96	0.22	61,61,61,61	0
60	MG	AA	3311	1/1	0.96	0.21	46,46,46,46	0
60	MG	AA	3075	1/1	0.96	0.28	47,47,47,47	0
62	ZN	DN	501	1/1	0.96	0.07	120,120,120,120	0
64	GDP	DZ	702	28/28	0.96	0.13	69,69,69,69	0
60	MG	BA	1686	1/1	0.97	0.25	58,58,58,58	0
60	MG	DA	1625	1/1	0.97	0.12	38,38,38,38	0
60	MG	AA	3403	1/1	0.97	0.14	55,55,55,55	0
60	MG	CA	3438	1/1	0.97	0.29	45,45,45,45	0
60	MG	CA	3439	1/1	0.97	0.23	47,47,47,47	0
60	MG	AA	3404	1/1	0.97	0.10	50,50,50,50	0
60	MG	AA	3405	1/1	0.97	0.15	27,27,27,27	0
60	MG	AA	3496	1/1	0.97	0.05	43,43,43,43	0
60	MG	AA	3833	1/1	0.97	0.25	39,39,39,39	0
60	MG	CA	3171	1/1	0.97	0.43	48,48,48,48	0
60	MG	AA	3103	1/1	0.97	0.12	11,11,11,11	0
60	MG	CA	3446	1/1	0.97	0.24	37,37,37,37	0
60	MG	AA	3284	1/1	0.97	0.39	45,45,45,45	0
60	MG	BA	1606	1/1	0.97	0.28	74,74,74,74	0
60	MG	CA	3449	1/1	0.97	0.21	52,52,52,52	0
60	MG	CA	3451	1/1	0.97	0.12	78,78,78,78	0
60	MG	AA	3144	1/1	0.97	0.49	48,48,48,48	0
60	MG	AA	3453	1/1	0.97	0.11	51,51,51,51	0
60	MG	CA	3455	1/1	0.97	0.27	37,37,37,37	0
60	MG	AA	3409	1/1	0.97	0.19	51,51,51,51	0
60	MG	AA	3411	1/1	0.97	0.15	21,21,21,21	0
60	MG	DA	1647	1/1	0.97	0.14	39,39,39,39	0
60	MG	BA	1611	1/1	0.97	0.09	31,31,31,31	0
60	MG	CA	3182	1/1	0.97	0.58	45,45,45,45	0
60	MG	AA	3617	1/1	0.97	0.12	32,32,32,32	0
60	MG	AA	3555	1/1	0.97	0.16	57,57,57,57	0
60	MG	DA	1653	1/1	0.97	0.08	29,29,29,29	0
60	MG	AA	3011	1/1	0.97	0.10	27,27,27,27	0
60	MG	AA	3557	1/1	0.97	0.17	21,21,21,21	0
60	MG	CA	3316	1/1	0.97	0.19	34,34,34,34	0
60	MG	AA	3189	1/1	0.97	0.26	31,31,31,31	0
60	MG	CA	3318	1/1	0.97	0.16	31,31,31,31	0
60	MG	AB	3012	1/1	0.97	0.14	24,24,24,24	1
60	MG	CA	3320	1/1	0.97	0.25	47,47,47,47	0
60	MG	BA	1810	1/1	0.97	0.13	39,39,39,39	0
60	MG	AA	3505	1/1	0.97	0.23	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3192	1/1	0.97	0.26	47,47,47,47	0
60	MG	CA	3324	1/1	0.97	0.22	31,31,31,31	0
60	MG	AA	3560	1/1	0.97	0.20	49,49,49,49	0
60	MG	AA	3506	1/1	0.97	0.20	19,19,19,19	0
60	MG	AA	3045	1/1	0.97	0.33	58,58,58,58	0
60	MG	AA	3374	1/1	0.97	0.15	22,22,22,22	0
60	MG	BE	3001	1/1	0.97	0.08	83,83,83,83	0
60	MG	AA	3564	1/1	0.97	0.23	17,17,17,17	0
60	MG	AA	3628	1/1	0.97	0.18	62,62,62,62	0
60	MG	CA	3332	1/1	0.97	0.24	47,47,47,47	0
60	MG	AA	3565	1/1	0.97	0.21	26,26,26,26	0
60	MG	BL	202	1/1	0.97	0.14	56,56,56,56	0
60	MG	AA	3290	1/1	0.97	0.16	78,78,78,78	0
60	MG	AA	3042	1/1	0.97	0.20	43,43,43,43	0
60	MG	AA	3115	1/1	0.97	0.47	44,44,44,44	0
60	MG	AD	301	1/1	0.97	0.34	46,46,46,46	0
60	MG	AA	3318	1/1	0.97	0.16	64,64,64,64	0
60	MG	AA	3703	1/1	0.97	0.07	76,76,76,76	0
60	MG	AD	304	1/1	0.97	0.34	49,49,49,49	0
60	MG	AA	3514	1/1	0.97	0.21	32,32,32,32	0
60	MG	CA	3639	1/1	0.97	0.31	54,54,54,54	0
60	MG	AA	3232	1/1	0.97	0.22	58,58,58,58	0
60	MG	AA	3193	1/1	0.97	0.20	63,63,63,63	0
60	MG	AD	308	1/1	0.97	0.36	49,49,49,49	0
60	MG	BA	1727	1/1	0.97	0.28	53,53,53,53	0
60	MG	AA	3423	1/1	0.97	0.22	53,53,53,53	0
60	MG	BA	1729	1/1	0.97	0.13	38,38,38,38	0
60	MG	AA	3126	1/1	0.97	0.24	68,68,68,68	0
60	MG	AA	3576	1/1	0.97	0.29	49,49,49,49	0
60	MG	CA	3099	1/1	0.97	0.46	55,55,55,55	0
60	MG	CA	3649	1/1	0.97	0.19	15,15,15,15	0
60	MG	AA	3786	1/1	0.97	0.19	57,57,57,57	0
60	MG	CA	3651	1/1	0.97	0.17	41,41,41,41	0
60	MG	AE	303	1/1	0.97	0.19	23,23,23,23	0
60	MG	CA	3359	1/1	0.97	0.22	44,44,44,44	0
60	MG	CA	3224	1/1	0.97	0.18	32,32,32,32	0
60	MG	BA	1734	1/1	0.97	0.13	35,35,35,35	0
60	MG	AA	3519	1/1	0.97	0.13	39,39,39,39	0
60	MG	AA	3521	1/1	0.97	0.19	30,30,30,30	0
60	MG	AA	3643	1/1	0.97	0.14	56,56,56,56	0
60	MG	AA	3790	1/1	0.97	0.23	11,11,11,11	0
60	MG	AA	3350	1/1	0.97	0.16	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	BZ	701	1/1	0.97	0.20	58,58,58,58	0
60	MG	DA	1708	1/1	0.97	0.10	67,67,67,67	0
60	MG	CA	3368	1/1	0.97	0.12	45,45,45,45	0
60	MG	AA	3323	1/1	0.97	0.18	42,42,42,42	0
60	MG	AF	305	1/1	0.97	0.09	48,48,48,48	0
60	MG	CA	3003	1/1	0.97	0.31	49,49,49,49	0
60	MG	CA	3004	1/1	0.97	0.18	43,43,43,43	0
60	MG	AA	3717	1/1	0.97	0.23	47,47,47,47	0
60	MG	CA	3006	1/1	0.97	0.09	24,24,24,24	0
60	MG	BA	1743	1/1	0.97	0.08	60,60,60,60	0
60	MG	CA	3522	1/1	0.97	0.24	25,25,25,25	0
60	MG	CA	3008	1/1	0.97	0.39	52,52,52,52	0
60	MG	AA	3718	1/1	0.97	0.14	40,40,40,40	0
60	MG	AA	3116	1/1	0.97	0.32	36,36,36,36	0
60	MG	AA	3196	1/1	0.97	0.34	48,48,48,48	0
60	MG	CA	3381	1/1	0.97	0.22	37,37,37,37	0
60	MG	CA	3120	1/1	0.97	0.12	47,47,47,47	0
60	MG	BA	1747	1/1	0.97	0.14	53,53,53,53	0
60	MG	AA	3584	1/1	0.97	0.12	63,63,63,63	0
60	MG	BA	1750	1/1	0.97	0.10	54,54,54,54	0
60	MG	AP	201	1/1	0.97	0.31	35,35,35,35	0
60	MG	AA	3527	1/1	0.97	0.16	20,20,20,20	0
60	MG	AA	3430	1/1	0.97	0.24	23,23,23,23	0
60	MG	AA	3386	1/1	0.97	0.21	19,19,19,19	0
60	MG	DA	1731	1/1	0.97	0.20	51,51,51,51	0
60	MG	CA	3251	1/1	0.97	0.15	62,62,62,62	0
60	MG	AR	5001	1/1	0.97	0.14	34,34,34,34	0
60	MG	AA	3588	1/1	0.97	0.15	33,33,33,33	0
60	MG	AA	3128	1/1	0.97	0.46	53,53,53,53	1
60	MG	AA	3355	1/1	0.97	0.14	19,19,19,19	0
60	MG	CA	3541	1/1	0.97	0.34	58,58,58,58	0
60	MG	CF	304	1/1	0.97	0.15	46,46,46,46	0
60	MG	AA	3532	1/1	0.97	0.18	20,20,20,20	0
60	MG	AV	201	1/1	0.97	0.28	46,46,46,46	0
60	MG	CA	3258	1/1	0.97	0.17	54,54,54,54	0
60	MG	CA	3399	1/1	0.97	0.18	45,45,45,45	0
60	MG	CO	202	1/1	0.97	0.13	53,53,53,53	0
60	MG	AA	3216	1/1	0.97	0.17	68,68,68,68	0
60	MG	CA	3547	1/1	0.97	0.06	57,57,57,57	1
60	MG	CA	3028	1/1	0.97	0.64	60,60,60,60	0
60	MG	CA	3262	1/1	0.97	0.28	59,59,59,59	0
60	MG	AA	3030	1/1	0.97	0.33	44,44,44,44	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3137	1/1	0.97	0.18	64,64,64,64	0
60	MG	AA	3733	1/1	0.97	0.13	40,40,40,40	0
60	MG	CA	3553	1/1	0.97	0.14	77,77,77,77	0
60	MG	BA	1764	1/1	0.97	0.16	55,55,55,55	0
60	MG	AA	3330	1/1	0.97	0.21	33,33,33,33	0
60	MG	CY	502	1/1	0.97	0.14	53,53,53,53	0
60	MG	AX	101	1/1	0.97	0.11	37,37,37,37	0
60	MG	BA	1768	1/1	0.97	0.18	64,64,64,64	0
60	MG	AA	3359	1/1	0.97	0.18	31,31,31,31	0
60	MG	CA	3559	1/1	0.97	0.14	30,30,30,30	0
60	MG	AA	3065	1/1	0.97	0.41	51,51,51,51	0
60	MG	AA	3597	1/1	0.97	0.12	58,58,58,58	0
60	MG	AA	3663	1/1	0.97	0.20	61,61,61,61	0
60	MG	CA	3415	1/1	0.97	0.18	43,43,43,43	0
60	MG	DA	1603	1/1	0.97	0.07	52,52,52,52	0
60	MG	CA	3416	1/1	0.97	0.28	33,33,33,33	0
60	MG	A0	102	1/1	0.97	0.06	41,41,41,41	0
60	MG	AA	3169	1/1	0.97	0.26	36,36,36,36	0
60	MG	AA	3397	1/1	0.97	0.36	41,41,41,41	0
60	MG	AA	3076	1/1	0.97	0.13	6,6,6,6	0
60	MG	CA	3279	1/1	0.97	0.26	46,46,46,46	0
60	MG	BA	1780	1/1	0.97	0.07	44,44,44,44	0
60	MG	AA	3399	1/1	0.97	0.24	51,51,51,51	0
60	MG	AA	3668	1/1	0.97	0.10	25,25,25,25	0
60	MG	AA	3669	1/1	0.97	0.21	36,36,36,36	0
60	MG	AA	3400	1/1	0.97	0.07	19,19,19,19	0
60	MG	CA	3285	1/1	0.97	0.07	41,41,41,41	0
60	MG	AA	3603	1/1	0.97	0.10	68,68,68,68	0
60	MG	DZ	701	1/1	0.97	0.24	47,47,47,47	0
60	MG	CA	3157	1/1	0.97	0.23	56,56,56,56	0
60	MG	AA	3185	1/1	0.97	0.20	35,35,35,35	0
60	MG	CA	3161	1/1	0.97	0.44	45,45,45,45	0
60	MG	AA	3673	1/1	0.97	0.24	58,58,58,58	0
64	GDP	BZ	702	28/28	0.97	0.14	57,57,57,57	1
60	MG	AA	3335	1/1	0.97	0.19	14,14,14,14	0
60	MG	AA	3363	1/1	0.98	0.24	47,47,47,47	0
60	MG	AA	3410	1/1	0.98	0.13	19,19,19,19	0
60	MG	AA	3301	1/1	0.98	0.17	59,59,59,59	0
60	MG	AA	3523	1/1	0.98	0.17	35,35,35,35	0
60	MG	CA	3340	1/1	0.98	0.13	38,38,38,38	0
60	MG	DA	1612	1/1	0.98	0.13	46,46,46,46	0
60	MG	CA	3211	1/1	0.98	0.14	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3583	1/1	0.98	0.12	18,18,18,18	0
60	MG	DA	1703	1/1	0.98	0.06	59,59,59,59	0
60	MG	AA	3149	1/1	0.98	0.25	15,15,15,15	0
60	MG	DA	1616	1/1	0.98	0.41	44,44,44,44	0
60	MG	CA	3567	1/1	0.98	0.12	42,42,42,42	0
60	MG	AG	201	1/1	0.98	0.05	41,41,41,41	0
60	MG	AB	3002	1/1	0.98	0.22	55,55,55,55	0
60	MG	CA	3277	1/1	0.98	0.18	43,43,43,43	0
60	MG	CA	3347	1/1	0.98	0.14	37,37,37,37	0
60	MG	BA	1795	1/1	0.98	0.15	64,64,64,64	0
60	MG	AA	3616	1/1	0.98	0.10	33,33,33,33	0
60	MG	CA	3159	1/1	0.98	0.42	42,42,42,42	0
60	MG	CA	3422	1/1	0.98	0.18	43,43,43,43	0
60	MG	AA	3286	1/1	0.98	0.25	48,48,48,48	0
60	MG	CA	3352	1/1	0.98	0.23	40,40,40,40	0
60	MG	AA	3244	1/1	0.98	0.40	42,42,42,42	0
60	MG	AA	3723	1/1	0.98	0.16	30,30,30,30	0
60	MG	AB	3007	1/1	0.98	0.07	37,37,37,37	0
60	MG	CA	3223	1/1	0.98	0.18	46,46,46,46	0
60	MG	AA	3306	1/1	0.98	0.14	3,3,3,3	0
60	MG	AA	3470	1/1	0.98	0.13	24,24,24,24	0
60	MG	CA	3166	1/1	0.98	0.20	31,31,31,31	0
60	MG	CA	3432	1/1	0.98	0.13	29,29,29,29	0
60	MG	AA	3037	1/1	0.98	0.12	12,12,12,12	0
60	MG	CB	3003	1/1	0.98	0.13	61,61,61,61	0
60	MG	AQ	3003	1/1	0.98	0.34	37,37,37,37	0
60	MG	AA	3218	1/1	0.98	0.20	10,10,10,10	0
60	MG	AA	3371	1/1	0.98	0.07	21,21,21,21	0
60	MG	AA	3328	1/1	0.98	0.22	21,21,21,21	0
60	MG	CA	3294	1/1	0.98	0.31	40,40,40,40	0
60	MG	DA	1643	1/1	0.98	0.14	51,51,51,51	0
60	MG	AA	3395	1/1	0.98	0.14	21,21,21,21	0
60	MG	DA	1645	1/1	0.98	0.34	58,58,58,58	0
60	MG	AA	3731	1/1	0.98	0.14	34,34,34,34	0
60	MG	CA	3174	1/1	0.98	0.12	31,31,31,31	0
60	MG	AA	3053	1/1	0.98	0.15	21,21,21,21	0
60	MG	AA	3660	1/1	0.98	0.34	58,58,58,58	0
60	MG	CA	3017	1/1	0.98	0.15	28,28,28,28	0
60	MG	DA	1740	1/1	0.98	0.17	56,56,56,56	0
60	MG	CA	3178	1/1	0.98	0.21	54,54,54,54	0
60	MG	DA	1652	1/1	0.98	0.09	68,68,68,68	0
60	MG	AA	3023	1/1	0.98	0.46	40,40,40,40	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3600	1/1	0.98	0.12	60,60,60,60	0
60	MG	AA	3124	1/1	0.98	0.24	39,39,39,39	1
60	MG	AA	3007	1/1	0.98	0.10	18,18,18,18	0
60	MG	AA	3737	1/1	0.98	0.15	25,25,25,25	0
60	MG	CA	3450	1/1	0.98	0.24	38,38,38,38	0
60	MG	CA	3307	1/1	0.98	0.21	31,31,31,31	0
60	MG	BA	1765	1/1	0.98	0.29	67,67,67,67	0
60	MG	AA	3508	1/1	0.98	0.13	42,42,42,42	0
60	MG	CA	3454	1/1	0.98	0.23	43,43,43,43	0
60	MG	AA	3031	1/1	0.98	0.25	29,29,29,29	1
60	MG	CA	3186	1/1	0.98	0.07	49,49,49,49	0
60	MG	AA	3427	1/1	0.98	0.12	34,34,34,34	0
60	MG	CA	3313	1/1	0.98	0.14	54,54,54,54	0
60	MG	BA	1769	1/1	0.98	0.26	80,80,80,80	0
60	MG	CN	5001	1/1	0.98	0.10	64,64,64,64	0
60	MG	DA	1669	1/1	0.98	0.20	63,63,63,63	0
60	MG	CA	3027	1/1	0.98	0.05	29,29,29,29	0
60	MG	CA	3461	1/1	0.98	0.10	46,46,46,46	0
60	MG	BA	1721	1/1	0.98	0.26	60,60,60,60	0
60	MG	AA	3818	1/1	0.98	0.36	46,46,46,46	0
60	MG	AA	3819	1/1	0.98	0.37	46,46,46,46	0
60	MG	CA	3193	1/1	0.98	0.36	47,47,47,47	0
60	MG	DA	1766	1/1	0.98	0.07	41,41,41,41	0
60	MG	CA	3466	1/1	0.98	0.14	56,56,56,56	0
60	MG	AA	3224	1/1	0.98	0.19	26,26,26,26	0
60	MG	AA	3296	1/1	0.98	0.27	40,40,40,40	0
60	MG	AA	3485	1/1	0.98	0.17	34,34,34,34	0
60	MG	AA	3166	1/1	0.98	0.12	52,52,52,52	0
60	MG	CA	3625	1/1	0.98	0.22	46,46,46,46	0
60	MG	BA	1778	1/1	0.98	0.26	52,52,52,52	0
60	MG	CA	3259	1/1	0.98	0.17	19,19,19,19	0
60	MG	AA	3574	1/1	0.98	0.15	26,26,26,26	0
60	MG	AA	3008	1/1	0.98	0.17	28,28,28,28	0
60	MG	CA	3400	1/1	0.98	0.10	48,48,48,48	0
60	MG	CA	3476	1/1	0.98	0.22	60,60,60,60	0
60	MG	CA	3632	1/1	0.98	0.15	55,55,55,55	0
60	MG	AA	3826	1/1	0.98	0.22	56,56,56,56	0
60	MG	BA	1639	1/1	0.98	0.37	42,42,42,42	0
62	ZN	BN	501	1/1	0.98	0.09	83,83,83,83	0
62	ZN	CY	501	1/1	0.98	0.05	92,92,92,92	0
60	MG	AA	3082	1/1	0.98	0.58	57,57,57,57	1
62	ZN	C6	501	1/1	0.98	0.09	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3319	1/1	0.98	0.17	28,28,28,28	0
63	SF4	DD	501	8/8	0.98	0.11	71,71,71,71	0
60	MG	AA	3641	1/1	0.98	0.14	45,45,45,45	0
60	MG	AA	3112	1/1	0.98	0.36	44,44,44,44	0
60	MG	CA	3336	1/1	0.99	0.12	64,64,64,64	0
60	MG	CA	3337	1/1	0.99	0.13	27,27,27,27	0
60	MG	AA	3471	1/1	0.99	0.18	24,24,24,24	0
60	MG	AA	3750	1/1	0.99	0.10	26,26,26,26	0
60	MG	AA	3396	1/1	0.99	0.14	22,22,22,22	0
60	MG	AA	3415	1/1	0.99	0.20	29,29,29,29	0
60	MG	CA	3370	1/1	0.99	0.13	31,31,31,31	0
60	MG	AA	3212	1/1	0.99	0.40	43,43,43,43	0
60	MG	AA	3148	1/1	0.99	0.24	48,48,48,48	0
60	MG	AA	3097	1/1	0.99	0.25	29,29,29,29	0
60	MG	AA	3227	1/1	0.99	0.25	75,75,75,75	0
60	MG	AA	3520	1/1	0.99	0.15	34,34,34,34	0
60	MG	BA	1749	1/1	0.99	0.27	52,52,52,52	0
60	MG	AA	3796	1/1	0.99	0.24	45,45,45,45	0
60	MG	AA	3178	1/1	0.99	0.43	50,50,50,50	0
60	MG	BA	1775	1/1	0.99	0.22	47,47,47,47	0
60	MG	AA	3465	1/1	0.99	0.05	49,49,49,49	0
60	MG	AA	3361	1/1	0.99	0.17	33,33,33,33	0
60	MG	AA	3706	1/1	0.99	0.35	26,26,26,26	1
60	MG	AA	3432	1/1	0.99	0.16	24,24,24,24	0
60	MG	AA	3340	1/1	0.99	0.10	3,3,3,3	0
62	ZN	AY	501	1/1	0.99	0.06	68,68,68,68	0
60	MG	CA	3385	1/1	0.99	0.26	48,48,48,48	0
62	ZN	A6	102	1/1	0.99	0.10	47,47,47,47	0
62	ZN	A9	501	1/1	0.99	0.11	45,45,45,45	0
60	MG	AA	3709	1/1	0.99	0.47	39,39,39,39	0
60	MG	AO	5001	1/1	0.99	0.10	43,43,43,43	0
60	MG	BA	1714	1/1	0.99	0.17	44,44,44,44	0
62	ZN	C5	102	1/1	0.99	0.07	66,66,66,66	0
60	MG	AA	3456	1/1	0.99	0.13	64,64,64,64	0
62	ZN	C9	501	1/1	0.99	0.07	70,70,70,70	0
60	MG	CA	3306	1/1	0.99	0.11	39,39,39,39	0
63	SF4	BD	501	8/8	0.99	0.11	67,67,67,67	0
60	MG	AA	3677	1/1	0.99	0.20	26,26,26,26	0
60	MG	AA	3304	1/1	0.99	0.17	44,44,44,44	0
60	MG	CA	3158	1/1	0.99	0.33	54,54,54,54	0
62	ZN	A5	101	1/1	1.00	0.12	40,40,40,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.