



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2025 – 10:27 PM EST

PDB ID : 6BOK  
Title : E. coli release factor 1 (containing deletion 302-304) bound to the 70S ribosome  
Authors : Svidritskiy, E.; Korostelev, A.A.  
Deposited on : 2017-11-20  
Resolution : 3.55 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<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 : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.21  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.004 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

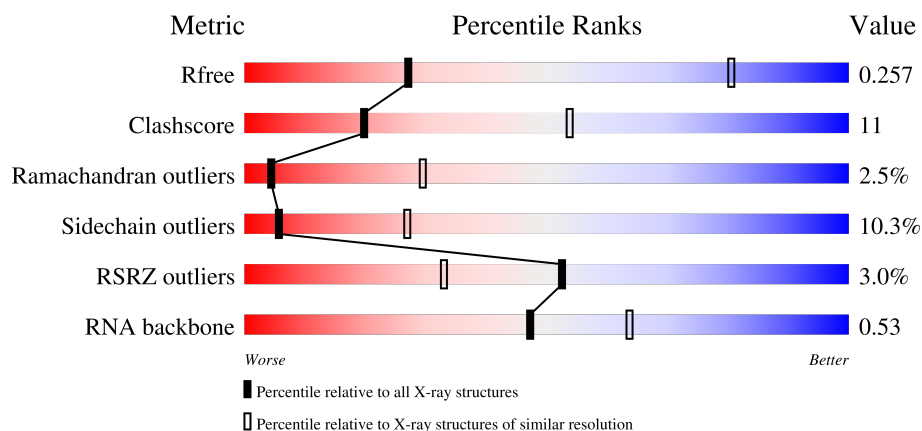
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 3.55 Å.

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





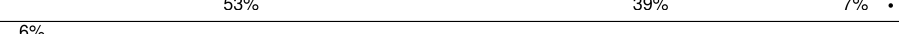
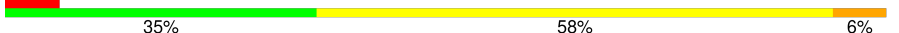
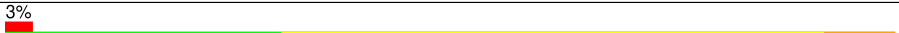
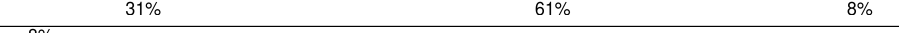

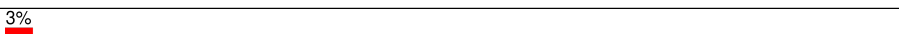


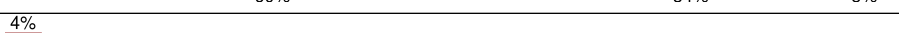


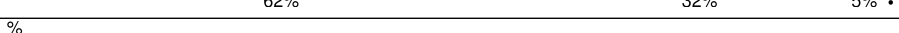


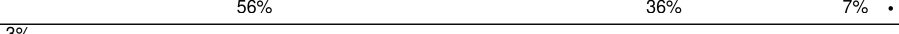








Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1261 (3.62-3.50)
Clashscore	180529	1351 (3.62-3.50)
Ramachandran outliers	177936	1336 (3.62-3.50)
Sidechain outliers	177891	1337 (3.62-3.50)
RSRZ outliers	164620	1260 (3.62-3.50)
RNA backbone	3690	1097 (4.10-3.00)

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	1507	 2% 49% 41% 9% .
1	DB	1507	 2% 49% 41% 9% .
2	B	2880	 % 43% 41% 14% .
2	EB	2880	 2% 47% 39% 12% .











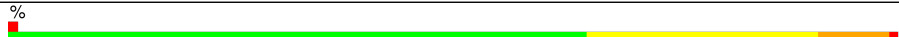


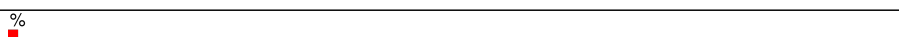
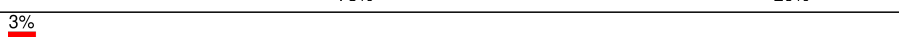
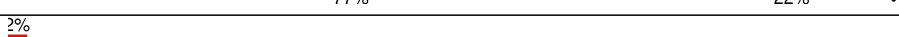



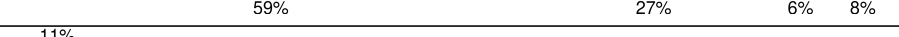





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Mol	Chain	Length	Quality of chain
3	C	120	
3	FB	120	
4	D	77	
4	GB	77	
4	IA	77	
4	LC	77	
5	E	275	
5	HB	275	
6	F	206	
6	IB	206	
7	G	205	
7	JB	205	
8	H	182	
8	KB	182	
9	I	180	
9	LB	180	
10	J	148	
10	MB	148	
11	K	140	
11	NB	140	
12	L	122	
12	OB	122	
13	M	150	
13	PB	150	
14	N	141	


















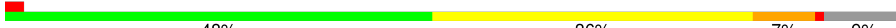







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Mol	Chain	Length	Quality of chain
14	QB	141	
15	O	118	
15	RB	118	
16	P	112	
16	SB	112	
17	Q	146	
17	TB	146	
18	R	118	
18	UB	118	
19	S	101	
19	VB	101	
20	T	113	
20	WB	113	
21	U	96	
21	XB	96	
22	V	110	
22	YB	110	
23	W	206	
23	ZB	206	
24	AC	85	
24	X	85	
25	BC	98	
25	Y	98	
26	CC	72	
26	Z	72	

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Mol	Chain	Length	Quality of chain
27	AA	60	
27	DC	60	
28	BA	71	
28	EC	71	
29	CA	60	
29	FC	60	
30	DA	54	
30	GC	54	
31	EA	49	
31	HC	49	
32	FA	65	
32	IC	65	
33	GA	37	
33	JC	37	
34	HA	27	
34	KC	27	
35	JA	256	
35	MC	256	
36	KA	239	
36	NC	239	
37	LA	209	
37	OC	209	
38	MA	162	
38	PC	162	
39	NA	101	

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Mol	Chain	Length	Quality of chain
39	QC	101	
40	OA	156	
40	RC	156	
41	PA	138	
41	SC	138	
42	QA	128	
42	TC	128	
43	RA	105	
43	UC	105	
44	SA	129	
44	VC	129	
45	TA	132	
45	WC	132	
46	UA	126	
46	XC	126	
47	VA	61	
47	YC	61	
48	WA	89	
48	ZC	89	
49	AD	88	
49	XA	88	
50	BD	105	
50	YA	105	
51	CD	88	
51	ZA	88	

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Mol	Chain	Length	Quality of chain
52	AB	93	
52	DD	93	
53	BB	106	
53	ED	106	
54	CB	27	
54	FD	27	
55	GD	365	
55	HD	365	

## 2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 299566 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1507	Total	C	N	O	P	0	0	0
			32394	14424	5998	10465	1507			
1	DB	1507	Total	C	N	O	P	0	0	0
			32394	14424	5998	10465	1507			

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	2880	Total	C	N	O	P	0	0	0
			62031	27612	11589	19950	2880			
2	EB	2880	Total	C	N	O	P	0	0	0
			62031	27612	11589	19950	2880			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	154A	C	UNK	conflict	GB 46197919
EB	154A	C	UNK	conflict	GB 46197919

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			
3	FB	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			

- Molecule 4 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	77	Total	C	N	O	P	S	0	0	0
			1642	734	297	534	76	1			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	IA	77	Total	C	N	O	P	S	0	0	0
			1642	734	297	534	76	1			
4	GB	77	Total	C	N	O	P	S	0	0	0
			1642	734	297	534	76	1			
4	LC	77	Total	C	N	O	P	S	0	0	0
			1642	734	297	534	76	1			

- Molecule 5 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			
5	HB	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			

- Molecule 6 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			
6	IB	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 7 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	202	Total	C	N	O	S	0	0	0
			1586	1011	297	275	3			
7	JB	202	Total	C	N	O	S	0	0	0
			1586	1011	297	275	3			

- Molecule 8 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	181	Total	C	N	O	S	0	0	0
			1471	940	267	260	4			
8	KB	181	Total	C	N	O	S	0	0	0
			1471	940	267	260	4			

- Molecule 9 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
9	LB	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 10 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	146	Total	C	N	O	S	0	0	0
			1137	727	201	208	1			
10	MB	146	Total	C	N	O	S	0	0	0
			1137	727	201	208	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			
11	NB	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			
12	OB	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
13	PB	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	141	Total	C	N	O	S	0	0	0
			1121	715	212	187	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	QB	141	Total	C	N	O	S	0	0	0
			1121	715	212	187	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
15	RB	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
16	P	110	Total	C	N	O	S	0	0	0
			877	553	175	149				
16	SB	110	Total	C	N	O	S	0	0	0
			877	553	175	149				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	137	Total	C	N	O	S	0	0	0
			1143	713	234	195	1			
17	TB	137	Total	C	N	O	S	0	0	0
			1143	713	234	195	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
18	UB	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
19	VB	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			
20	WB	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
21	XB	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	V	107	Total	C	N	O	S	0	0	0
			814	523	154	131	6			
22	YB	107	Total	C	N	O	S	0	0	0
			814	523	154	131	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	189	Total	C	N	O	S	0	0	0
			1495	953	266	273	3			
23	ZB	189	Total	C	N	O	S	0	0	0
			1495	953	266	273	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
24	AC	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	11	ARG	LYS	conflict	UNP Q72HR3

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Chain	Residue	Modelled	Actual	Comment	Reference
AC	11	ARG	LYS	conflict	UNP Q72HR3

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	97	Total	C	N	O	S	0	0	0
			761	478	151	131	1			
25	BC	97	Total	C	N	O	S	0	0	0
			761	478	151	131	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			
26	CC	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	AA	60	Total	C	N	O	S	0	0	0
			477	303	91	82	1			
27	DC	60	Total	C	N	O	S	0	0	0
			477	303	91	82	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BA	69	Total	C	N	O	S	0	0	0
			552	349	99	99	5			
28	EC	69	Total	C	N	O	S	0	0	0
			552	349	99	99	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	CA	59	Total	C	N	O	S	0	0	0
			460	290	90	75	5			
29	FC	59	Total	C	N	O	S	0	0	0
			460	290	90	75	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	DA	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
30	GC	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			

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

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

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

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

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

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

- Molecule 34 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	HA	11	Total	C	N	O	P	0	0	0
			220	98	44	67	11			
34	KC	11	Total	C	N	O	P	0	0	0
			220	98	44	67	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	JA	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			
35	MC	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	KA	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			
36	NC	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	LA	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
37	OC	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	MA	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
38	PC	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	NA	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
39	QC	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	OA	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	RC	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	PA	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
41	SC	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	QA	127	Total	C	N	O	S	0	0	0
			1011	639	198	174				
42	TC	127	Total	C	N	O	S	0	0	0
			1011	639	198	174				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	RA	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			
43	UC	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	SA	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			
44	VC	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	TA	122	Total	C	N	O	S	0	0	0
			958	604	193	159	2			
45	WC	122	Total	C	N	O	S	0	0	0
			958	604	193	159	2			



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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	UA	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			
46	XC	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	WA	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
48	ZC	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	XA	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			
49	AD	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	YA	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			
50	BD	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	ZA	70	Total	C	N	O	0	0	0
			574	367	112	95			
51	CD	70	Total	C	N	O	0	0	0
			574	367	112	95			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	AB	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
52	DD	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BB	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			
53	ED	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	CB	24	Total	C	N	O	0	0	0
			208	128	50	30			
54	FD	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 55 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	GD	255	Total	C	N	O	S	0	0	0
			1980	1214	374	384	8			
55	HD	255	Total	C	N	O	S	0	0	0
			1980	1214	374	384	8			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
GD	?	-	ASP	deletion	UNP B7MKB3
GD	?	-	ARG	deletion	UNP B7MKB3
GD	?	-	SER	deletion	UNP B7MKB3

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Chain	Residue	Modelled	Actual	Comment	Reference
GD	361	LEU	-	expression tag	UNP B7MKB3
GD	362	GLU	-	expression tag	UNP B7MKB3
GD	363	HIS	-	expression tag	UNP B7MKB3
GD	364	HIS	-	expression tag	UNP B7MKB3
GD	365	HIS	-	expression tag	UNP B7MKB3
GD	366	HIS	-	expression tag	UNP B7MKB3
GD	367	HIS	-	expression tag	UNP B7MKB3
GD	368	HIS	-	expression tag	UNP B7MKB3
HD	?	-	ASP	deletion	UNP B7MKB3
HD	?	-	ARG	deletion	UNP B7MKB3
HD	?	-	SER	deletion	UNP B7MKB3
HD	361	LEU	-	expression tag	UNP B7MKB3
HD	362	GLU	-	expression tag	UNP B7MKB3
HD	363	HIS	-	expression tag	UNP B7MKB3
HD	364	HIS	-	expression tag	UNP B7MKB3
HD	365	HIS	-	expression tag	UNP B7MKB3
HD	366	HIS	-	expression tag	UNP B7MKB3
HD	367	HIS	-	expression tag	UNP B7MKB3
HD	368	HIS	-	expression tag	UNP B7MKB3

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	A	160	Total Mg 160 160	0	0
56	B	514	Total Mg 514 514	0	0
56	C	23	Total Mg 23 23	0	0
56	D	6	Total Mg 6 6	0	0
56	E	4	Total Mg 4 4	0	0
56	F	1	Total Mg 1 1	0	0
56	G	4	Total Mg 4 4	0	0
56	H	1	Total Mg 1 1	0	0
56	I	3	Total Mg 3 3	0	0
56	J	5	Total Mg 5 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	K	2	Total 2	Mg 2	0	0
56	L	7	Total 7	Mg 7	0	0
56	M	4	Total 4	Mg 4	0	0
56	N	3	Total 3	Mg 3	0	0
56	O	1	Total 1	Mg 1	0	0
56	P	2	Total 2	Mg 2	0	0
56	Q	3	Total 3	Mg 3	0	0
56	R	4	Total 4	Mg 4	0	0
56	S	3	Total 3	Mg 3	0	0
56	T	2	Total 2	Mg 2	0	0
56	U	2	Total 2	Mg 2	0	0
56	V	5	Total 5	Mg 5	0	0
56	W	12	Total 12	Mg 12	0	0
56	Y	4	Total 4	Mg 4	0	0
56	Z	3	Total 3	Mg 3	0	0
56	CA	1	Total 1	Mg 1	0	0
56	EA	1	Total 1	Mg 1	0	0
56	FA	1	Total 1	Mg 1	0	0
56	HA	1	Total 1	Mg 1	0	0
56	IA	8	Total 8	Mg 8	0	0
56	JA	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	KA	1	Total 1	Mg 1	0	0
56	LA	1	Total 1	Mg 1	0	0
56	MA	3	Total 3	Mg 3	0	0
56	NA	2	Total 2	Mg 2	0	0
56	OA	3	Total 3	Mg 3	0	0
56	PA	2	Total 2	Mg 2	0	0
56	RA	2	Total 2	Mg 2	0	0
56	SA	1	Total 1	Mg 1	0	0
56	TA	3	Total 3	Mg 3	0	0
56	VA	2	Total 2	Mg 2	0	0
56	WA	3	Total 3	Mg 3	0	0
56	YA	2	Total 2	Mg 2	0	0
56	ZA	1	Total 1	Mg 1	0	0
56	AB	1	Total 1	Mg 1	0	0
56	BB	1	Total 1	Mg 1	0	0
56	DB	177	Total 177	Mg 177	0	0
56	EB	395	Total 395	Mg 395	0	0
56	FB	17	Total 17	Mg 17	0	0
56	GB	5	Total 5	Mg 5	0	0
56	HB	8	Total 8	Mg 8	0	0
56	IB	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	JB	2	Total 2	Mg 2	0	0
56	KB	1	Total 1	Mg 1	0	0
56	LB	5	Total 5	Mg 5	0	0
56	MB	2	Total 2	Mg 2	0	0
56	NB	1	Total 1	Mg 1	0	0
56	OB	3	Total 3	Mg 3	0	0
56	PB	2	Total 2	Mg 2	0	0
56	QB	3	Total 3	Mg 3	0	0
56	RB	5	Total 5	Mg 5	0	0
56	SB	1	Total 1	Mg 1	0	0
56	TB	5	Total 5	Mg 5	0	0
56	VB	1	Total 1	Mg 1	0	0
56	WB	3	Total 3	Mg 3	0	0
56	XB	2	Total 2	Mg 2	0	0
56	YB	3	Total 3	Mg 3	0	0
56	ZB	2	Total 2	Mg 2	0	0
56	AC	2	Total 2	Mg 2	0	0
56	BC	1	Total 1	Mg 1	0	0
56	DC	1	Total 1	Mg 1	0	0
56	FC	1	Total 1	Mg 1	0	0
56	HC	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	IC	2	Total 2	Mg 2	0	0
56	JC	1	Total 1	Mg 1	0	0
56	KC	1	Total 1	Mg 1	0	0
56	LC	8	Total 8	Mg 8	0	0
56	MC	3	Total 3	Mg 3	0	0
56	PC	2	Total 2	Mg 2	0	0
56	QC	2	Total 2	Mg 2	0	0
56	RC	2	Total 2	Mg 2	0	0
56	SC	1	Total 1	Mg 1	0	0
56	TC	2	Total 2	Mg 2	0	0
56	UC	1	Total 1	Mg 1	0	0
56	WC	2	Total 2	Mg 2	0	0
56	XC	2	Total 2	Mg 2	0	0
56	YC	1	Total 1	Mg 1	0	0
56	ZC	1	Total 1	Mg 1	0	0
56	AD	1	Total 1	Mg 1	0	0
56	BD	2	Total 2	Mg 2	0	0
56	CD	2	Total 2	Mg 2	0	0
56	ED	1	Total 1	Mg 1	0	0
56	GD	5	Total 5	Mg 5	0	0
56	HD	3	Total 3	Mg 3	0	0

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

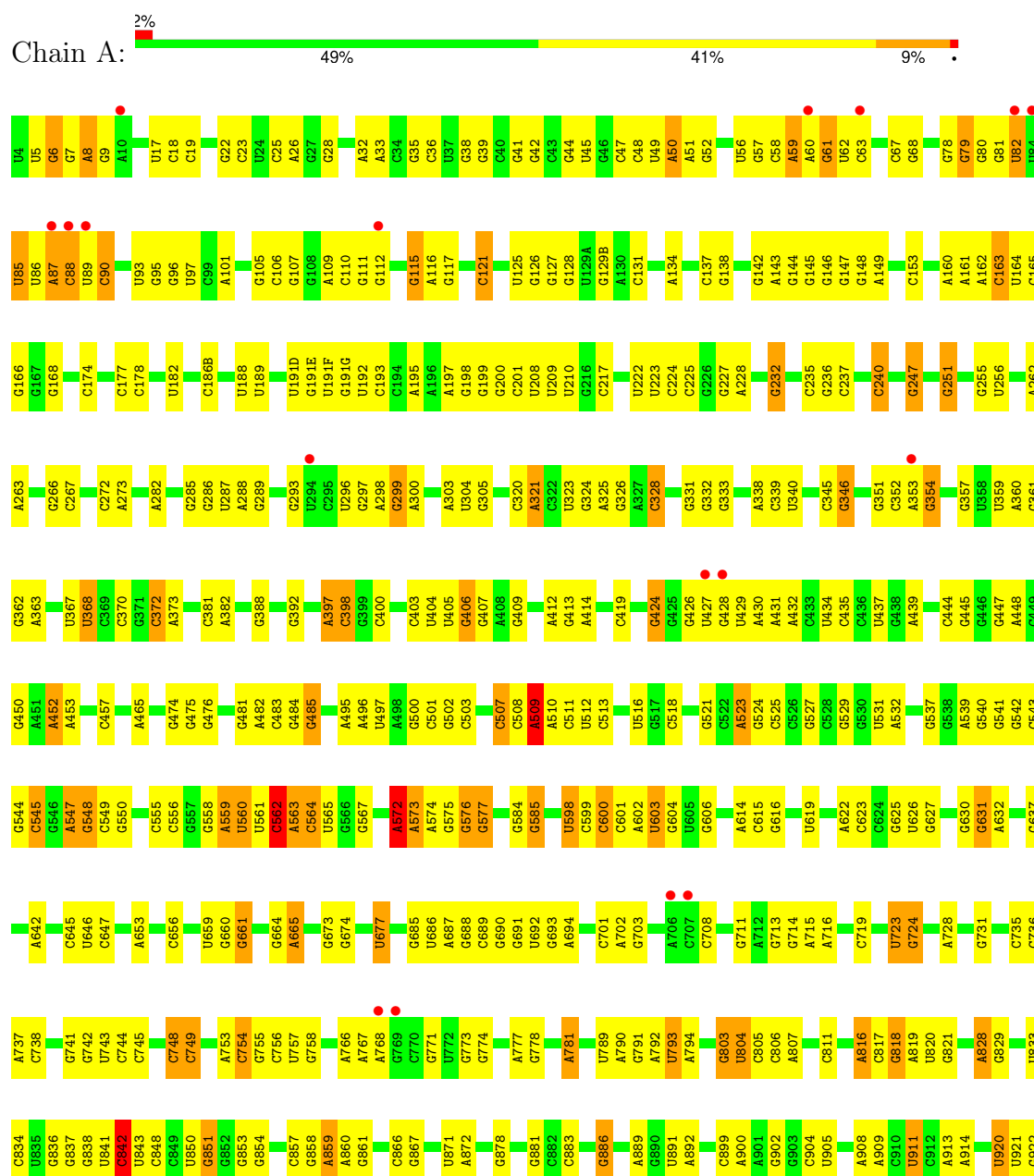
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	V	1	Total	Zn	0	0
			1	1		
57	BA	1	Total	Zn	0	0
			1	1		
57	CA	1	Total	Zn	0	0
			1	1		
57	DA	1	Total	Zn	0	0
			1	1		
57	GA	1	Total	Zn	0	0
			1	1		
57	YB	1	Total	Zn	0	0
			1	1		
57	EC	1	Total	Zn	0	0
			1	1		
57	FC	1	Total	Zn	0	0
			1	1		
57	GC	1	Total	Zn	0	0
			1	1		
57	JC	1	Total	Zn	0	0
			1	1		

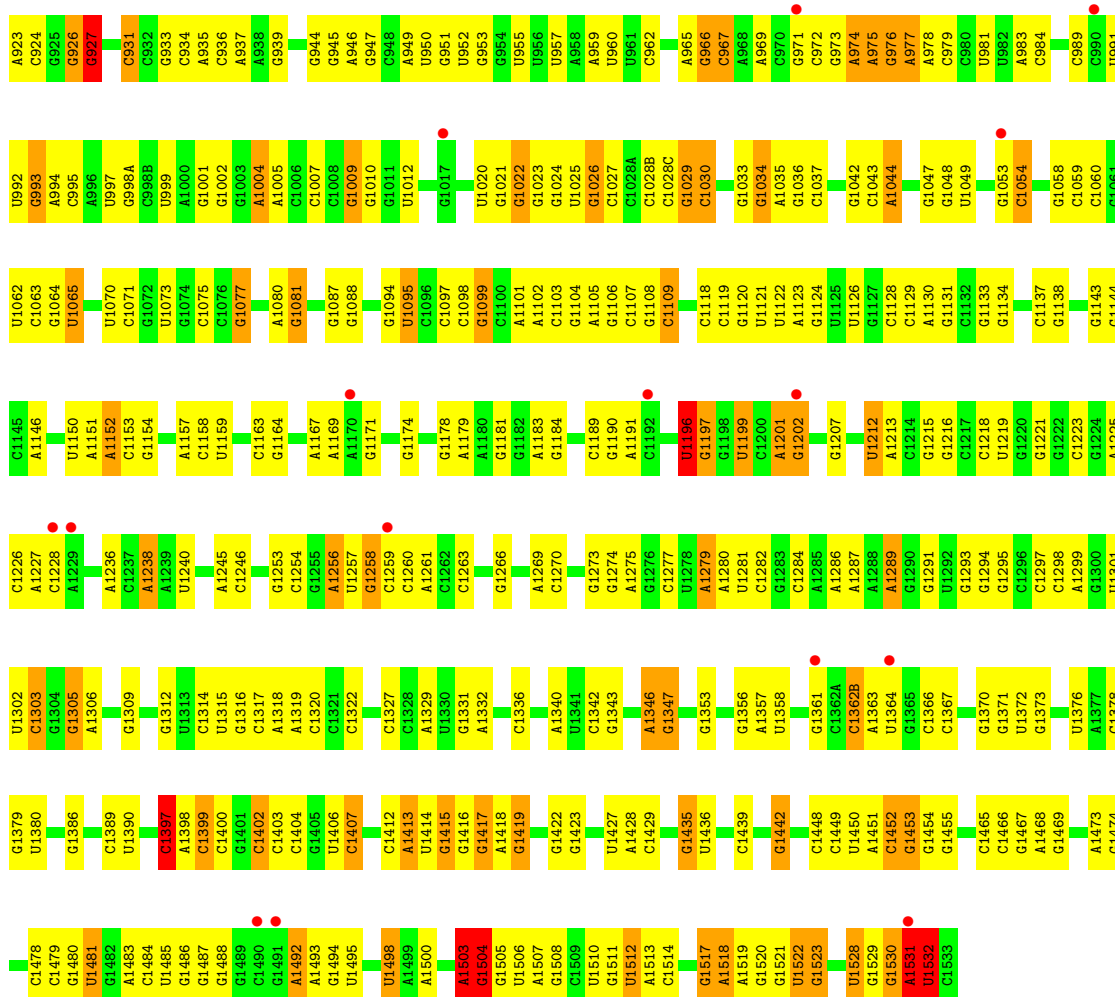


### 3 Residue-property plots

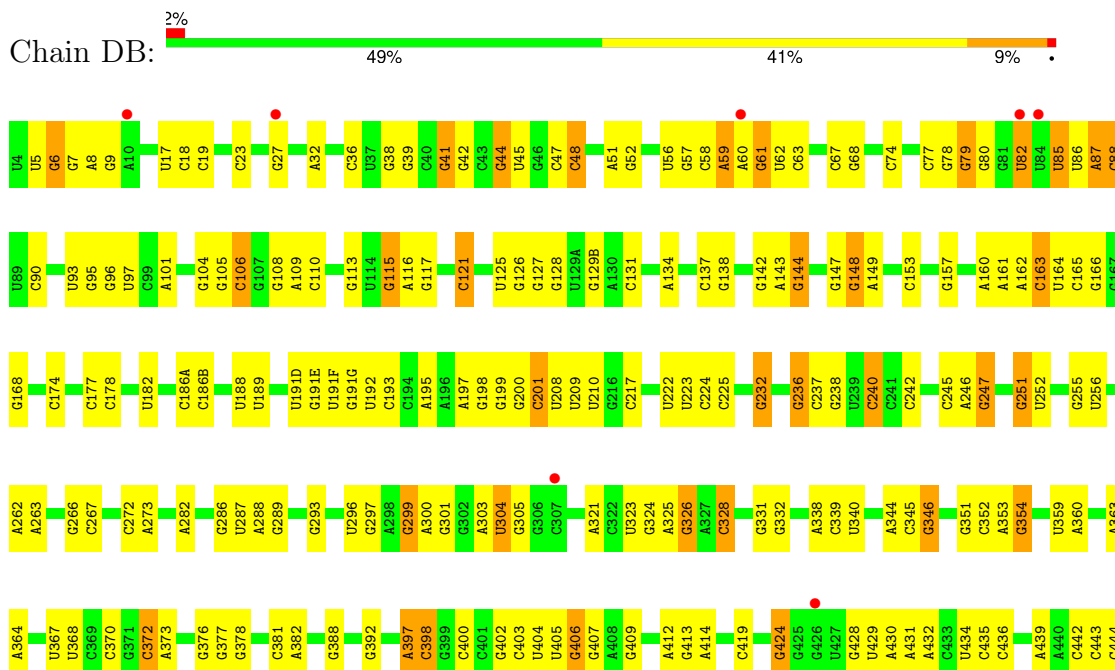
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

#### • Molecule 1: 16S ribosomal RNA

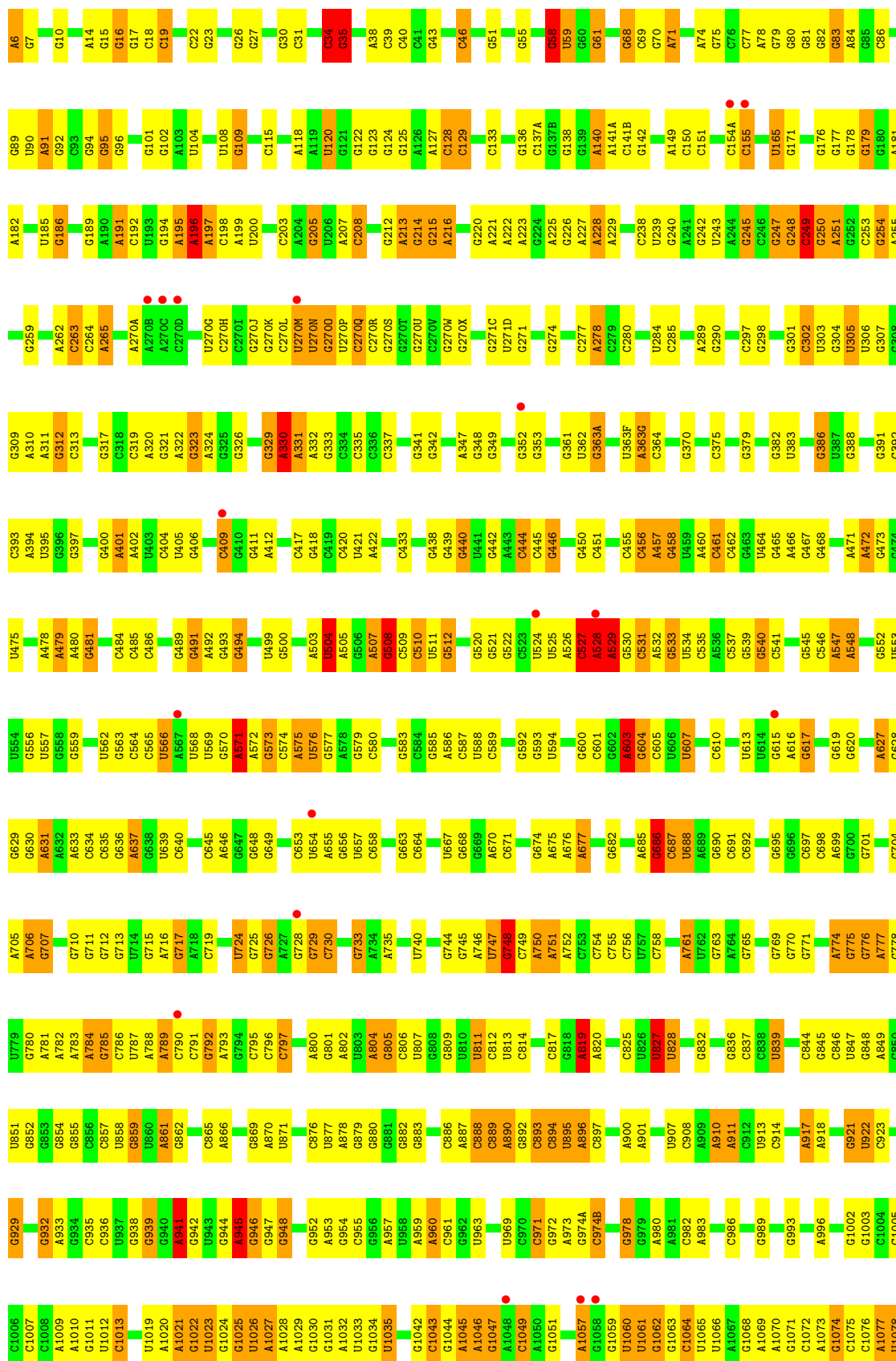




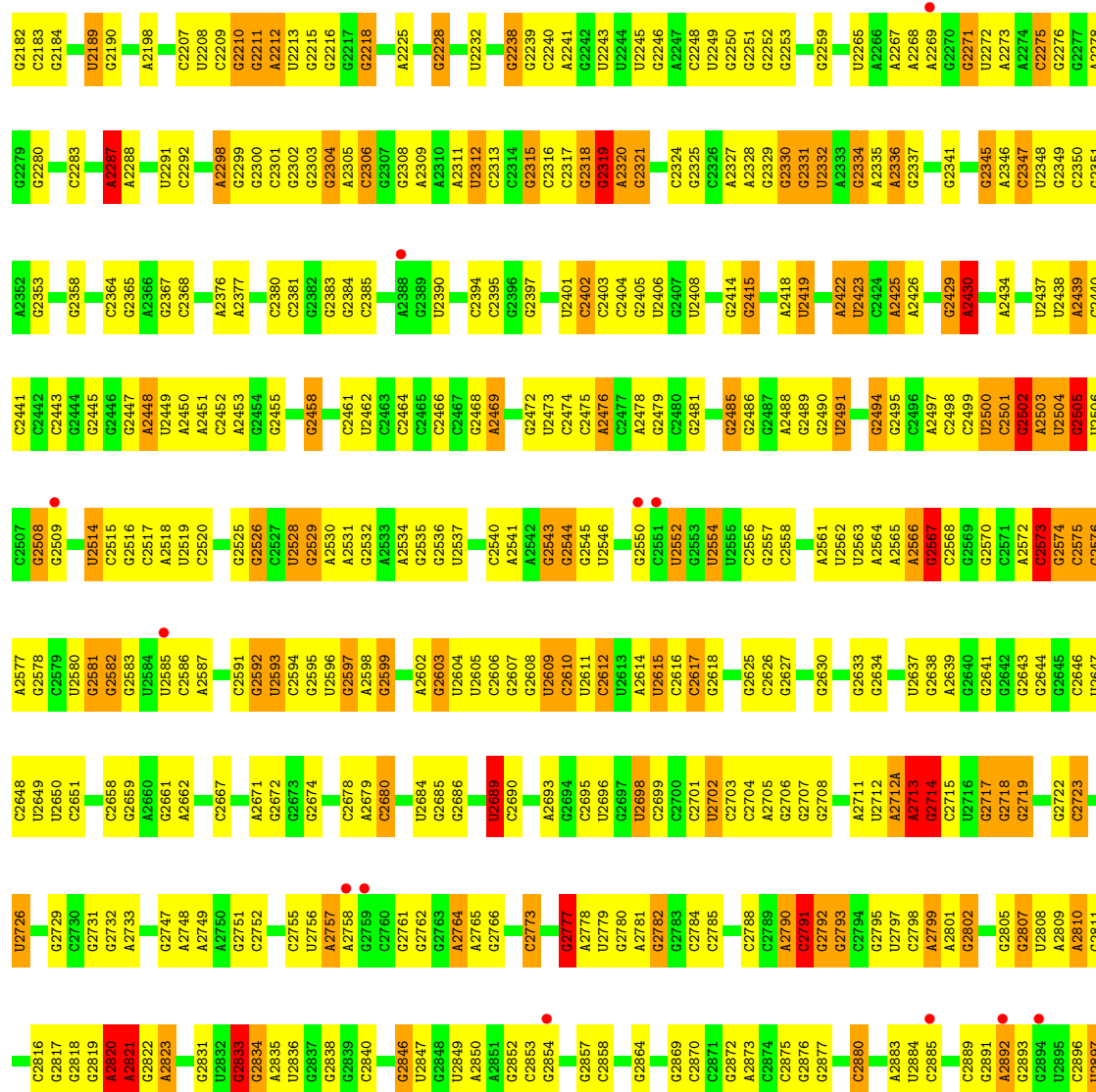
• Molecule 1: 16S ribosomal RNA



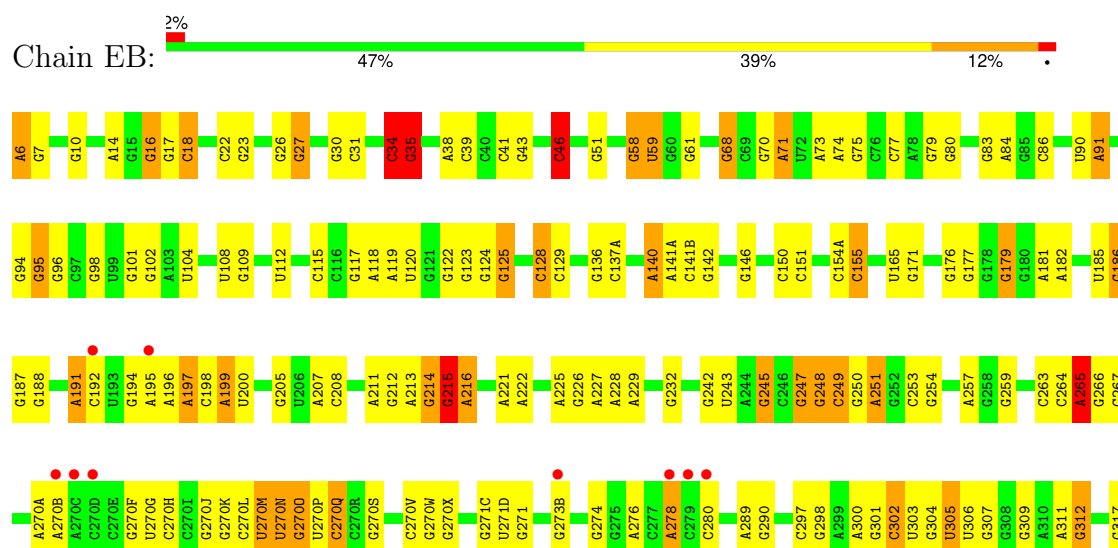


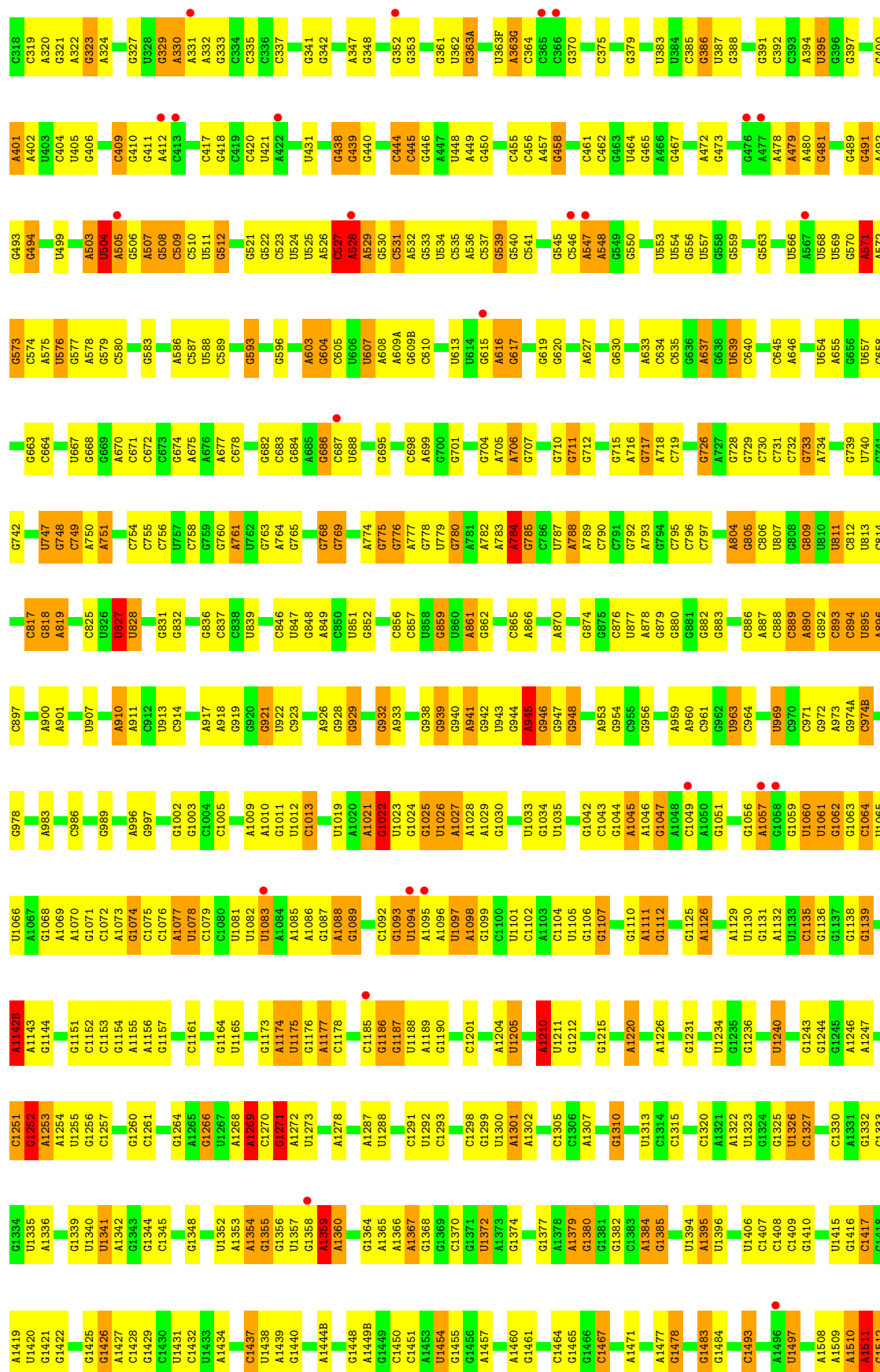


A2117	G2038	C1985	G1897	C1800	G1717	A1637	C1565	G1483	U1394	A1322	G1244	C1161	G1079
U2118	C2039	A1966	U1898	G1801	U1727	C1640	A1566	G1484	A1396	U1323	G1245	C1161	G1080
A2119	G2040	C1967	G1899	A1802	G1728	G1641	A1567	G1488	U1396	G1325	A1246	G1164	U1081
G2123	U2041	G1968	A1900	U1805	U1729	G1642	G1568	U1489	U1397	G1326	U1251	U1165	U1082
G2124	A2042	A1969	A1901	U1810	U1730	G1643	A1569	C1483	C1402	C1327	G1252	G1173	U1083
G2125	C2043	A1970	G1902	A1812	G1731	C1646	G1573	A1494	U1405	G1328	A1253	A1174	A1085
A2126	G2049	A1972	G1903	G1816	A1732	G1647	U1578	U1497	U1406	A1331	A1254	U1175	A1086
G2127	C2052	G1973	U1906	A1817	C1742	C1648	U1578	C1501	C1407	G1332	G1256	G1176	A1087
C2128	G1974	C1974	G1907	G1813	G1743	C1651	G1581	C1501	C1408	G1333	C1257	A1177	A1088
G2129	G1975	G1975	C1908	A1814	G1743	G1652	G1582	C1501	C1409	G1334	G1259	C1178	G1089
U2130	U1976	U1976	U1911	G1815	G1750	G1653	G1583	A1508	G1410	U1335	G1260	C1179	C1092
G2131	A2064	C2065	A1912	G1816	C1751	G1654	A1585	A1509	G1411	G1336	C1261	C1180	G1093
U2132	C2066	C2066	G1817	A1818	C1752	G1655	C1586	A1510	G1412	G1339	G1264	C1185	U1094
G2133	A2057	A1980	U1819	G1753	G1753	G1656	A1587	A1511	G1413	U1340	A1265	C1185	A1095
A2134	G2058	G1981	A1820	C1754	C1754	C1657	A1588	G1512	U1419	U1341	G1266	G1187	A1096
A2135	A2059	C1982	U1915	A1821	G1755	U1659	C1589	C1513	U1420	G1342	U1267	U1188	U1097
G2136	A2060	C1983	A1916	G1822	U1756	U1660	U1590	U1516	G1421	G1343	A1268	A1189	A1098
C2137	G2061	G1984	U1917	G1823	U1757	G1661	G1591	G1517	G1422	G1344	A1269	G1190	G1099
C2138	A2062	C2063	A1918	G1824	G1758	G1662	G1592	C1518	G1425	G1345	G1270	U1101	C1100
C2139	G1989	C2064	A1919	G1825	A1759	A1664	G1593	G1518	G1426	G1346	G1271	G1193	G1104
G2140	G1992	C2065	C1920	G1826	A1760	G1667	G1594	G1519	G1427	U1273	A1272	G1196	U1105
G2141	U1993	U1993	G1827	G1827	C1761	G1668	C1598	U1520	A1427	U1274	A1273	C1203	G1106
C2142	G2067	C2067	A1828	A1829	G1763	G1669	C1599	G1521	C1428	A1349	A1275	G1202	G1107
U2144	U2068	G1997	C1838	C1838	G1764	G1670	U1602	U1523	G1429	U1352	A1276	G1203	G1110
C2145	G2069	G1998	G1839	G1839	C1765	U1671	U1603	G1524	A1434	A1353	G1277	A1204	G1111
G2146	G2070	C2001	G1840	G1840	U1672	C1672	A1603	G1525	A1449	A1354	G1278	U1205	A1111
G2147	A2071	G2002	U1841	U1841	U1673	C1604	C1604	G1526	C1450	G1355	A1278	G1206	G1112
C2148	G2072	G2003	G1842	G1842	U1674	C1605	C1605	G1527	U1438	G1356	U1282	U1113	U1113
G2149	C2073	G2004	G1930	G1930	C1675	A1608	A1608	G1530	U1357	U1357	A1286	G1209	G1125
U2150	G2080	A2005	U1931	G1845	A1676	G1681	A1610	C1531	G1441	A1359	A1287	G1212	A1126
G2151	C2083	C2006	A1932	G1846	C1773	G1682	A1611	C1532	A1448	A1360	U1288	G1215	A1127
G2152	G2084	C2007	G1933	A1847	U1774	U1688	C1612	G1534	A1498	G1364	C1291	G1216	A1128
G2153	C2085	C2008	C1934	G1857	U1775	A1689	G1613	U1535	G1449	A1365	U1292	G1217	A1129
C2154	G2086	G2009	G1935	G1858	G1776	C1689	A1614	G1536	C1450	A1366	C1293	G1218	U1130
G2155	U2086	G2010	A1936	G1859	U1777	U1692	C1617	G1537	U1454	G1368	C1297	C1219	C1135
G2156	G2087	U2011	A1937	G1860	U1778	U1693	A1618	G1538	G1455	U1291	C1298	A1220	G1136
G2157	U2091	A2013	U1939	U1864	C1781	G1694	C1617	G1539	G1455	G1371	C1299	G1221	G1137
G2158	G2159	A2014	U1940	U1865	C1782	G1695	A1618	G1540	G1461	U1372	U1300	C1221A	G1138
C2161	G2093	C2020	C1941	U1866	U1780	G1696	G1622	G1541	G1462	G1374	A1301	C1224	G1139
G2162	G2094	A2020	C1942	C1870	A1784	G1697	G1623	G1542	U1464	G1377	G1304	A1225	A1143
C2163	G2095	C2021	U1946	A1871	A1785	A1698	G1624	G1543	G1465	A1378	A1307	A1226	G1144
G2164	U2096	U2022	C1947	A1872	A1786	G1699	G1625	C1544	G1466	A1379	C1304	G1227	G1149
G2165	G2097	G2023	U1947	G1878	A1787	A1700	G1626	C1544	G1467	G1380	G1310	G1231	G1152
G2166	C2097	C2026	U1951	C1879	C1788	A1701	G1627	C1550	G1468	G1381	G1310	U1234	C1153
U2167	G2100	G2027	A1952	G1882	U1789	G1702	G1628	C1551	G1469	G1382	G1310	G1235	G1154
G2168	C2107	U2028	A1953	G1883	C1790	G1703	U1629	G1552	A1469	G1383	G1314	G1236	A1155
A2169	C2108	G2029	A2030	G1954	A1791	G1705	G1630	A1553	G1470	C1384	C1315	U1240	A1156
A2170	U2109	A2031	U1955	A1889	G1792	U1706	C1630B	A1554	A1471	G1385	C1315	C1320	G1157
A2171	G2110	A2031	U1955	A1890	G1792	U1706	A1631	C1557	G1471	G1385	C1315	U1240	C1158
U2172	G2111	A2031	U1955	A1891	G1792	U1706	A1631	C1557	G1471	G1385	C1315	U1240	C1158
A2173	C2112	G2032	A1960	G1891	C1795	G1708	A1633	C1557	G1471	G1385	C1315	U1240	C1158
C2174	G2113	U2034	C1961	C1892	U1796	G1708	A1633	C1557	G1471	G1385	C1315	U1240	C1158
C2175	U2113	U2034	C1961	C1892	U1796	G1708	A1633	C1557	G1471	G1385	C1315	U1240	C1158
A2176	G2115	G2036	U1963	C1895	C1797	G1708	A1633	C1557	G1471	G1385	C1315	U1240	C1158
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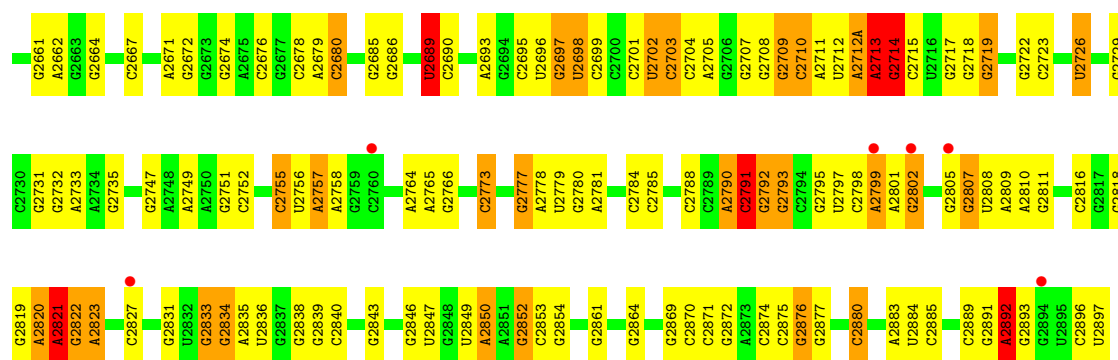
- Molecule 2: 23S ribosomal RNA





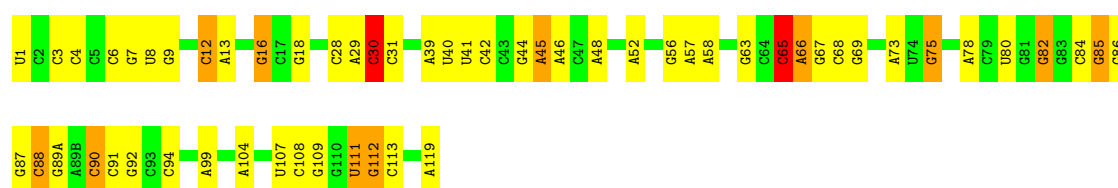
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G2582	C2507	G2337	A2267	A2435	G2166	C2097		A1936	G1840	C1765	U1671	G1592	U1517
G2583	G2436	G2338	A2268	G2436	U2167		A2020	A1937	G1841	U1766	U1672	G1593	
G2584	G2509	G2339	A2269	U2437	G2168	G2100	U2022	A1938	G1842	C1767	U1673	U1520	G1518
U2585	U2514	A2345	A2270	A2438	A2169	C2107	G2023	U1939	G1845	U1674	U1602	U1521	G1519
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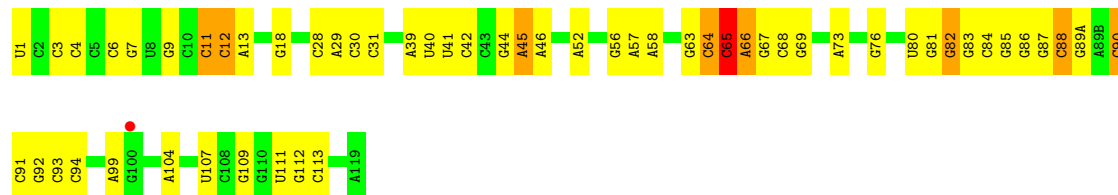
- Molecule 3: 5S ribosomal RNA

Chain C: 52% 37% 9% .



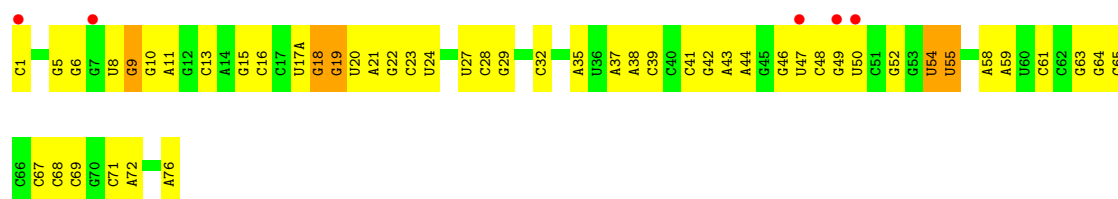
- Molecule 3: 5S ribosomal RNA

Chain FB: 53% 39% 7% .



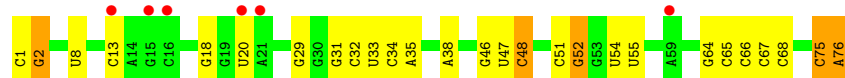
- Molecule 4: 16S ribosomal RNA

Chain D: 6% 35% 58% 6%

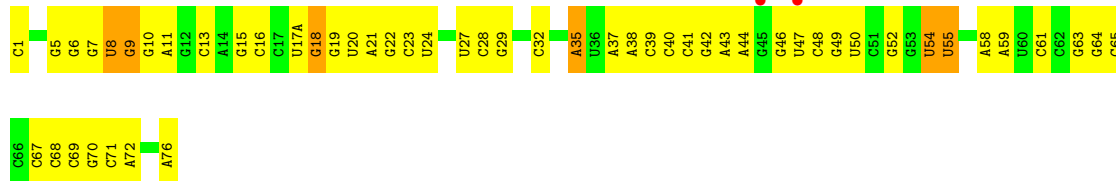


- Molecule 4: 16S ribosomal RNA

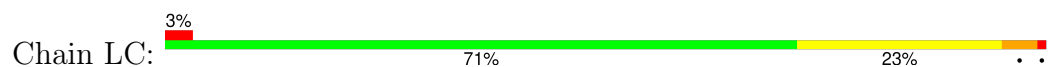
Chain IA: 8% 65% 29% 6%



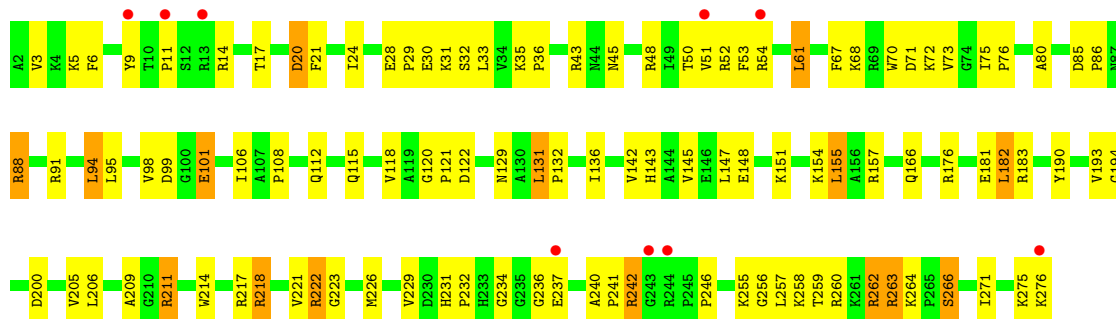
- Molecule 4: 16S ribosomal RNA



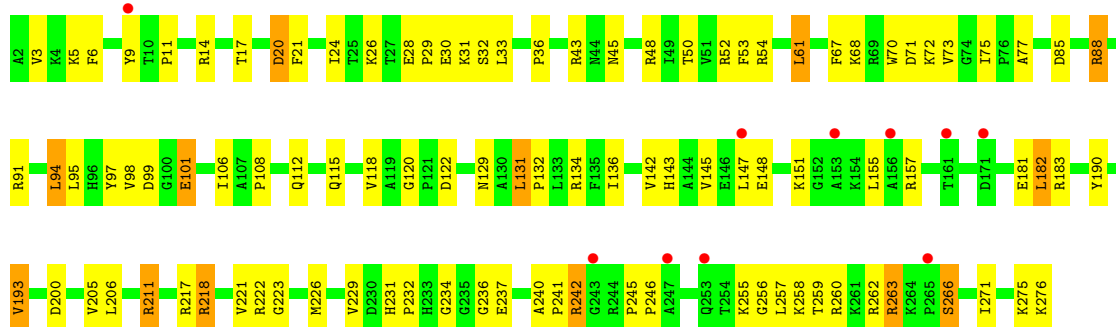
• Molecule 4: 16S ribosomal RNA



• Molecule 5: 50S ribosomal protein L2



• Molecule 5: 50S ribosomal protein L2

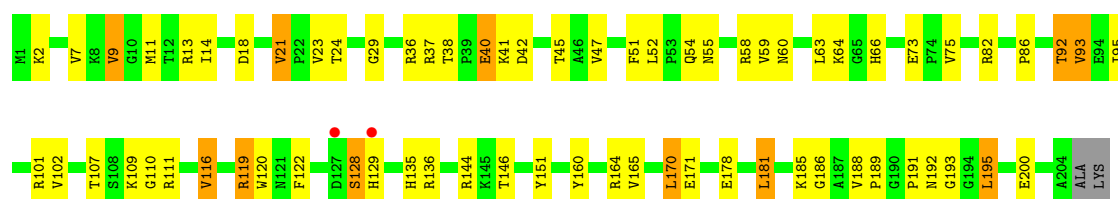


• Molecule 6: 50S ribosomal protein L3

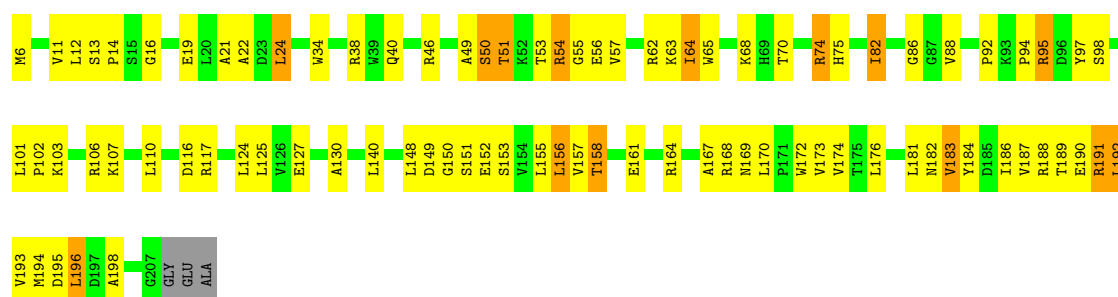
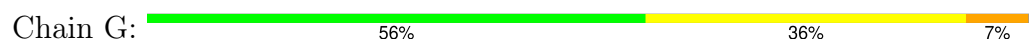




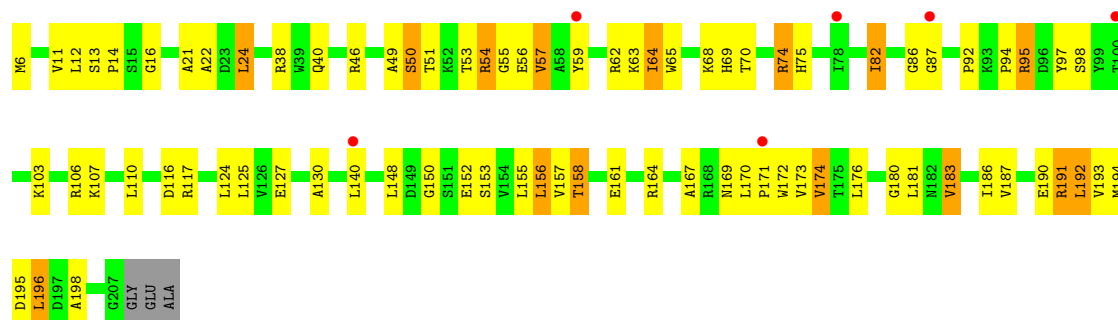
- Molecule 6: 50S ribosomal protein L3



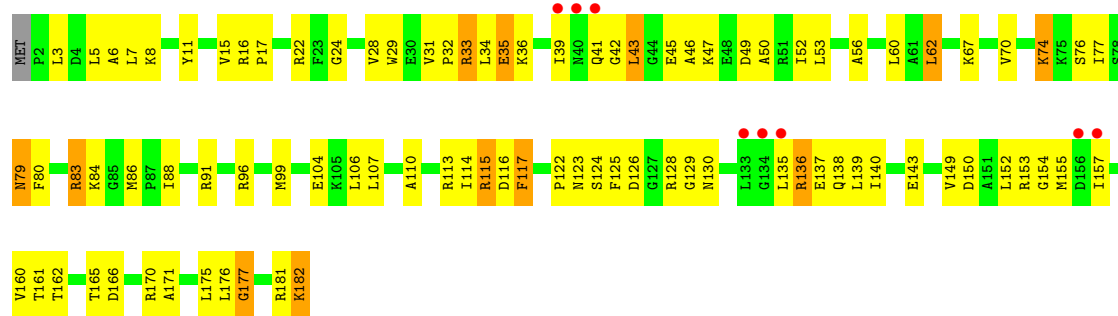
- Molecule 7: 50S ribosomal protein L4



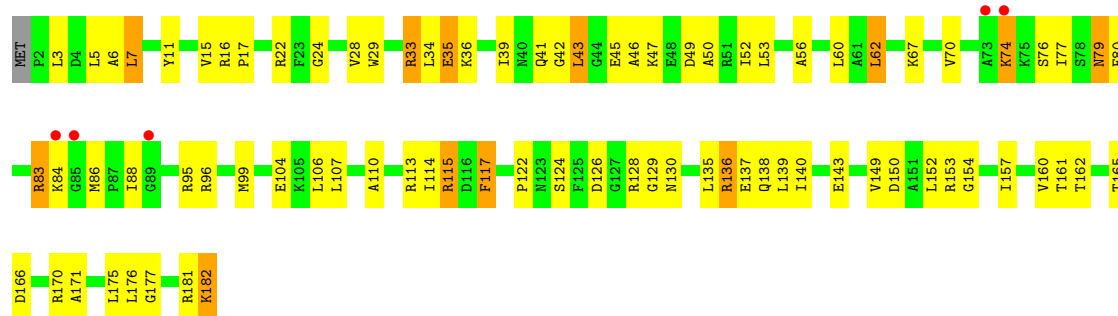
- Molecule 7: 50S ribosomal protein L4



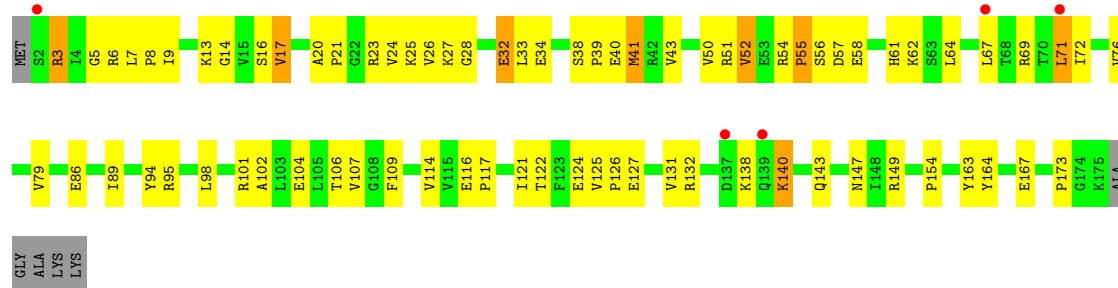
- Molecule 8: 50S ribosomal protein L5



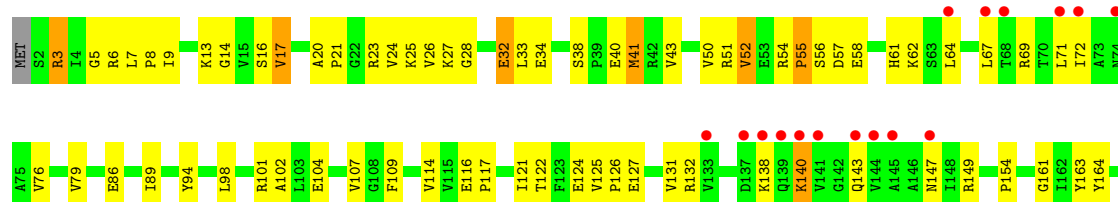
• Molecule 8: 50S ribosomal protein L5

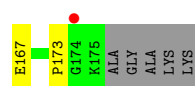


• Molecule 9: 50S ribosomal protein L6

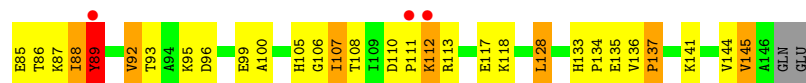
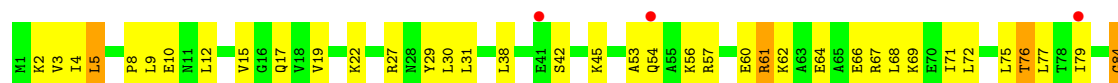


• Molecule 9: 50S ribosomal protein L6

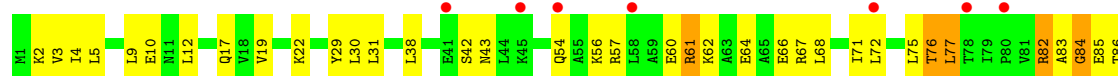




- Molecule 10: 50S ribosomal protein L9



- Molecule 10: 50S ribosomal protein L9



- Molecule 11: 50S ribosomal protein L13

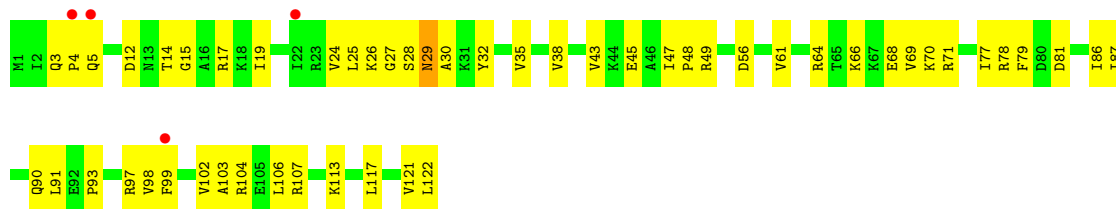


- Molecule 11: 50S ribosomal protein L13

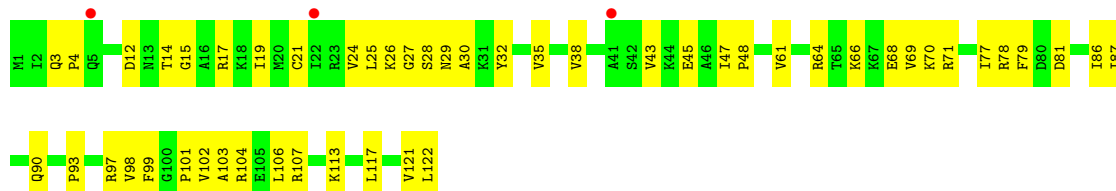


- Molecule 12: 50S ribosomal protein L14

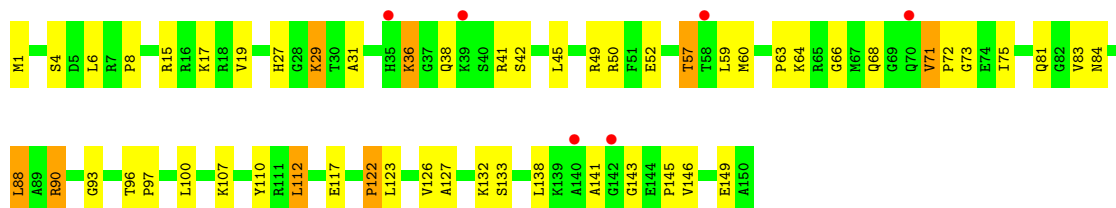




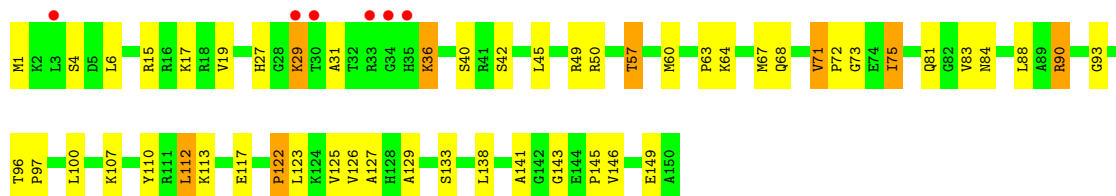
• Molecule 12: 50S ribosomal protein L14



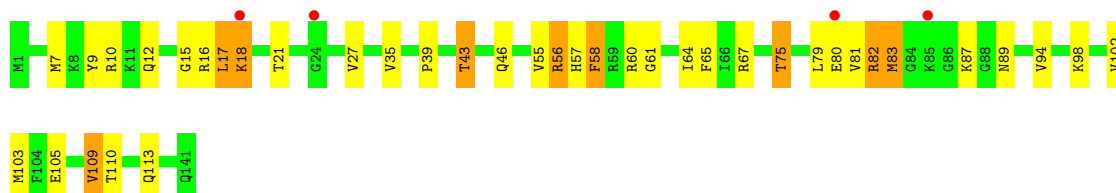
• Molecule 13: 50S ribosomal protein L15



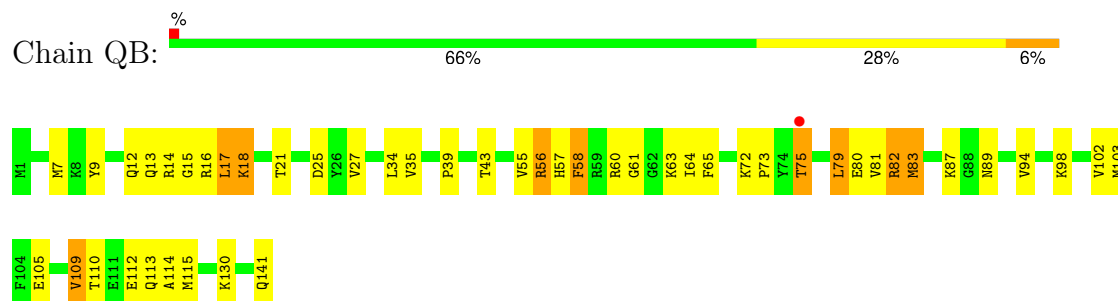
• Molecule 13: 50S ribosomal protein L15



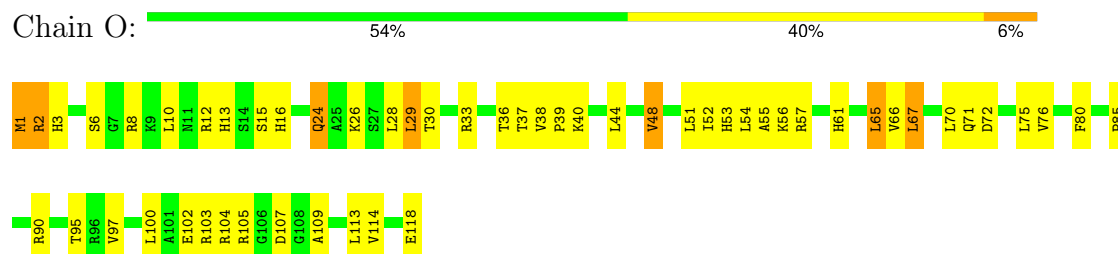
• Molecule 14: 50S ribosomal protein L16



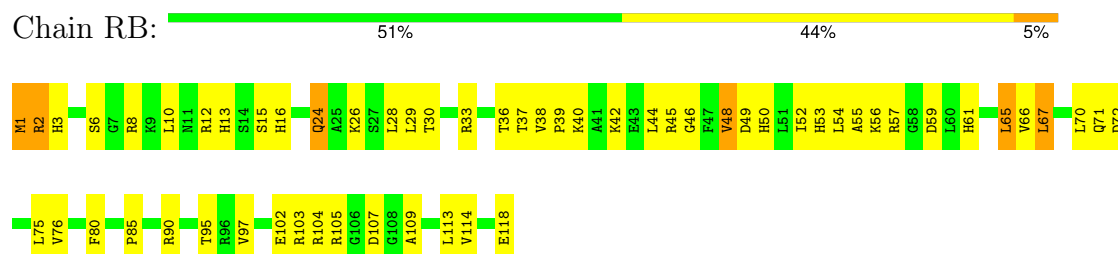
- Molecule 14: 50S ribosomal protein L16



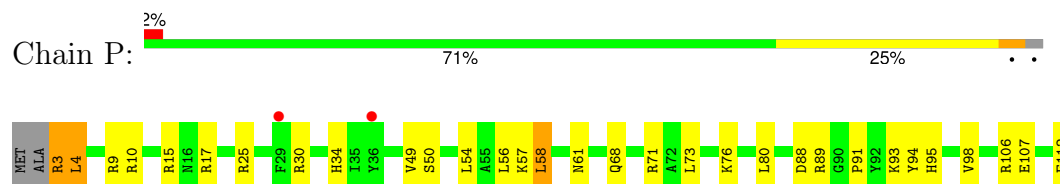
- Molecule 15: 50S ribosomal protein L17



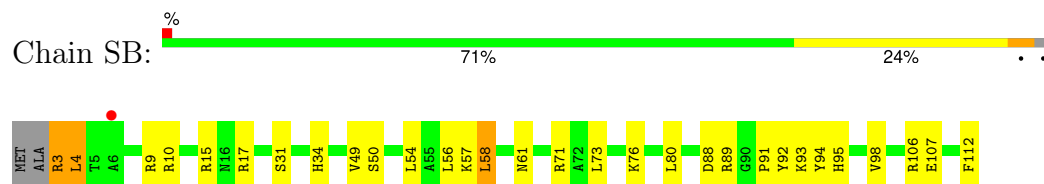
- Molecule 15: 50S ribosomal protein L17



- Molecule 16: 50S ribosomal protein L18

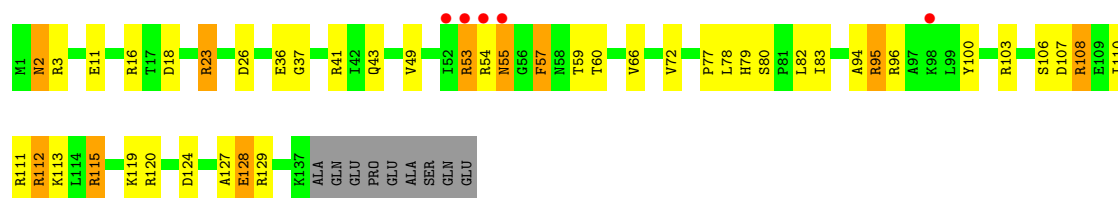


- Molecule 16: 50S ribosomal protein L18

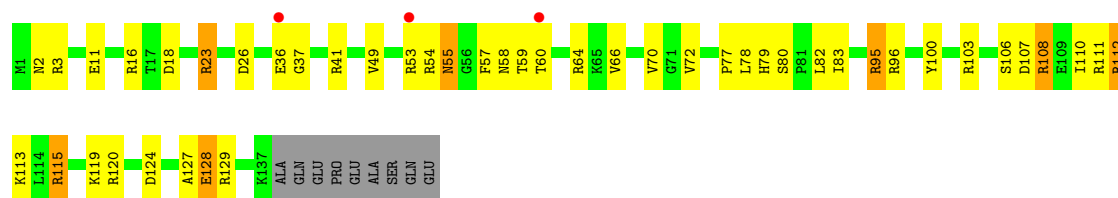


- Molecule 17: 50S ribosomal protein L19

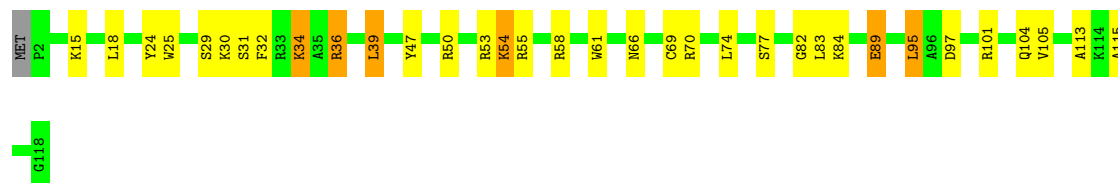




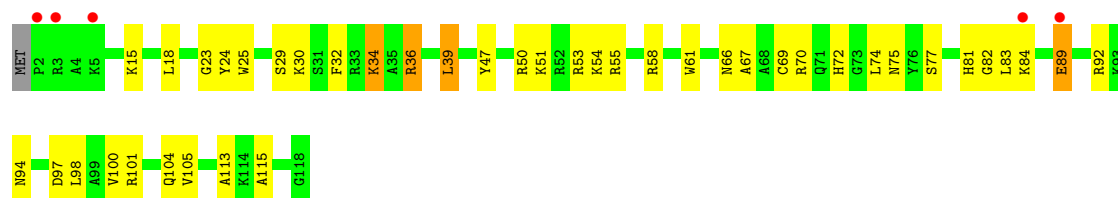
- Molecule 17: 50S ribosomal protein L19



- Molecule 18: 50S ribosomal protein L20



- Molecule 18: 50S ribosomal protein L20



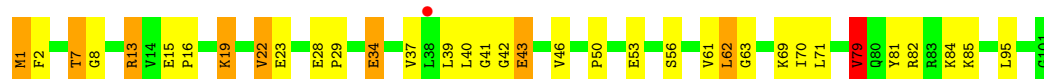
- Molecule 19: 50S ribosomal protein L21



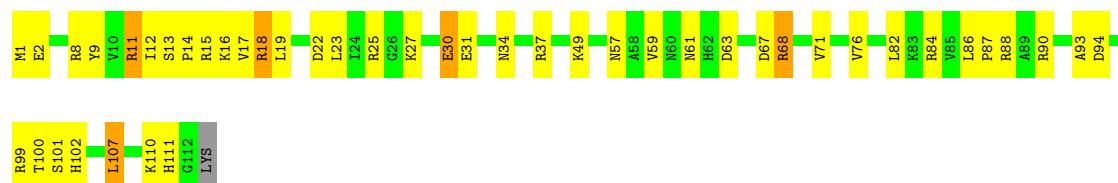
- Molecule 19: 50S ribosomal protein L21







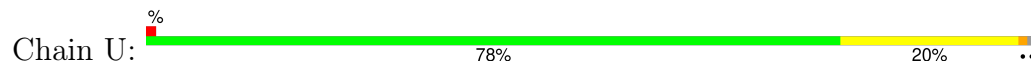
- Molecule 20: 50S ribosomal protein L22



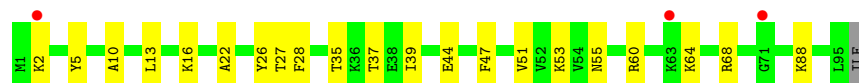
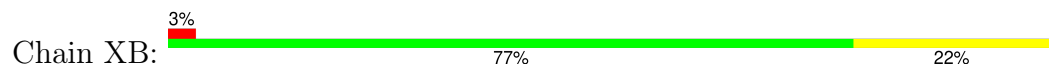
- Molecule 20: 50S ribosomal protein L22



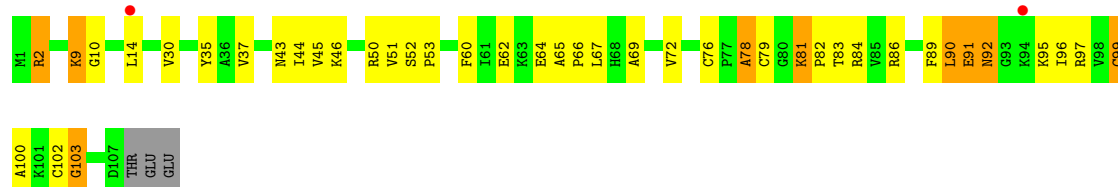
- Molecule 21: 50S ribosomal protein L23



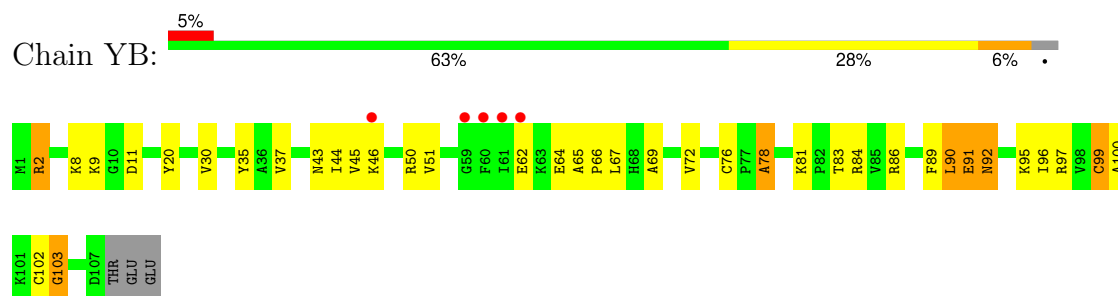
- Molecule 21: 50S ribosomal protein L23



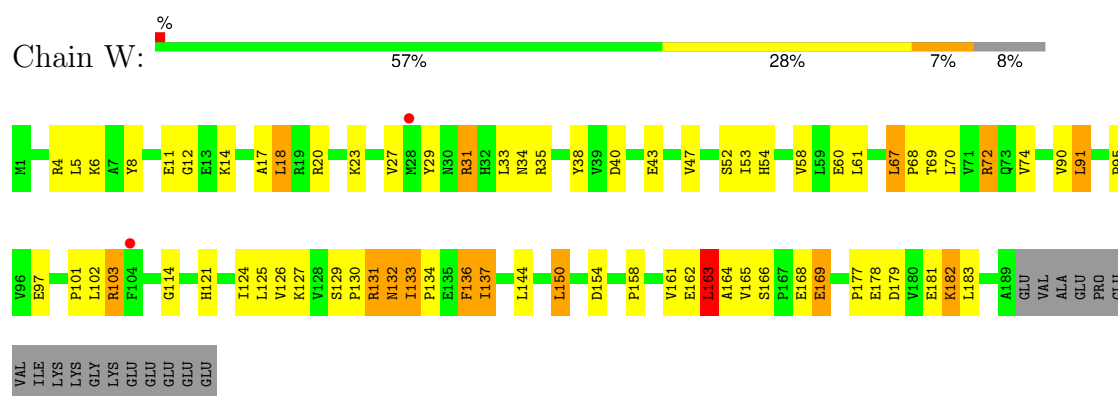
- Molecule 22: 50S ribosomal protein L24



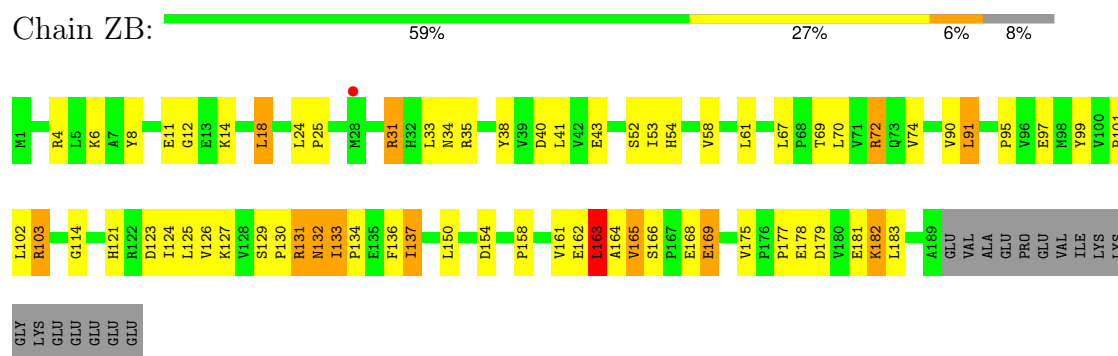
- Molecule 22: 50S ribosomal protein L24



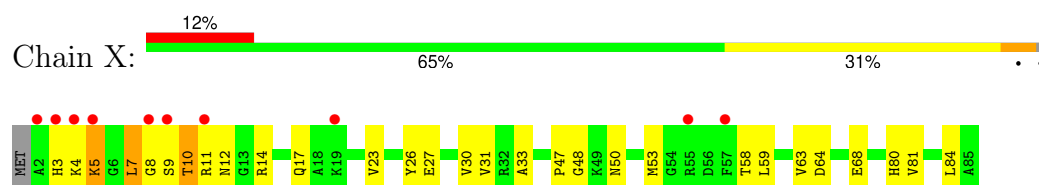
- Molecule 23: 50S ribosomal protein L25



- Molecule 23: 50S ribosomal protein L25



- Molecule 24: 50S ribosomal protein L27

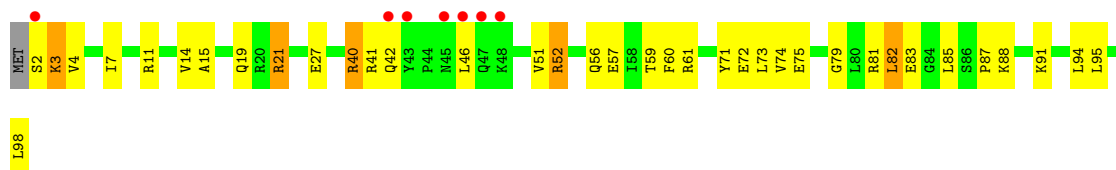


- Molecule 24: 50S ribosomal protein L27

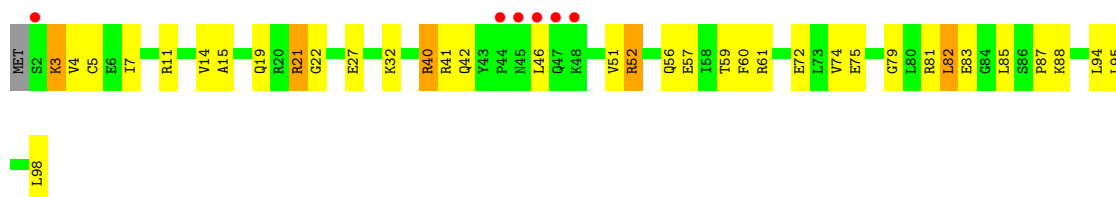




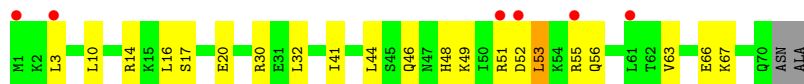
- Molecule 25: 50S ribosomal protein L28



- 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



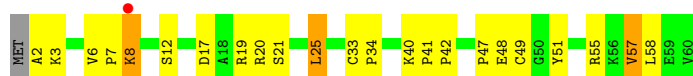
- Molecule 28: 50S ribosomal protein L31



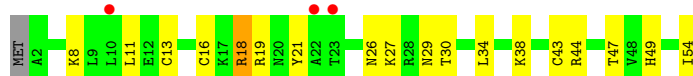
- Molecule 29: 50S ribosomal protein L32



- Molecule 29: 50S ribosomal protein L32



- Molecule 30: 50S ribosomal protein L33



- Molecule 30: 50S ribosomal protein L33

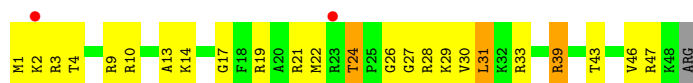


- Molecule 31: 50S ribosomal protein L34





- Molecule 31: 50S ribosomal protein L34



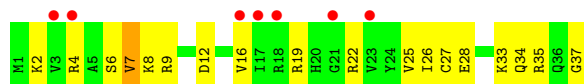
- Molecule 32: 50S ribosomal protein L35



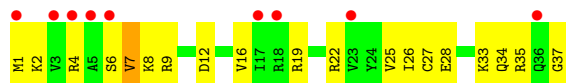
- Molecule 32: 50S ribosomal protein L35



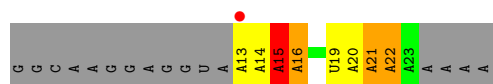
- Molecule 33: 50S ribosomal protein L36



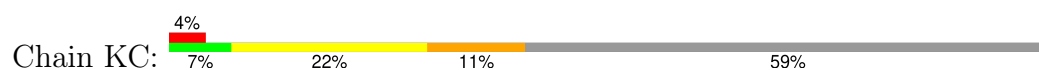
- Molecule 33: 50S ribosomal protein L36



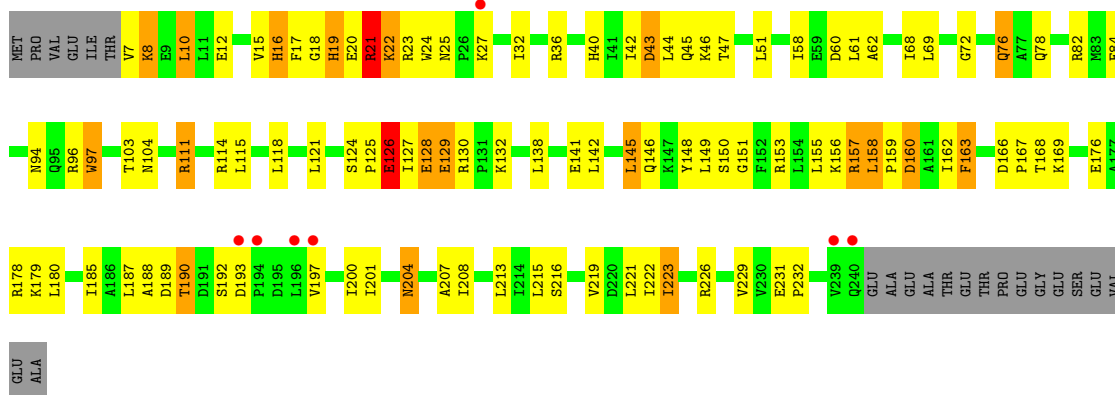
- Molecule 34: mRNA



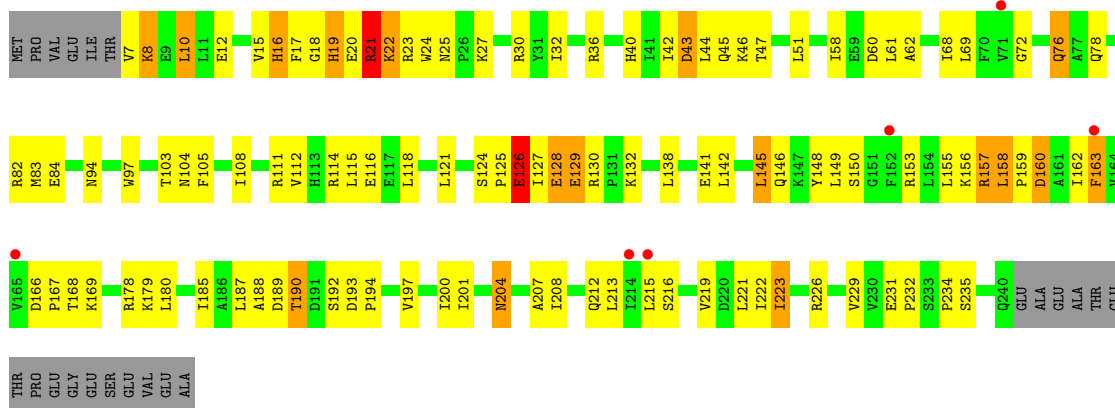
- Molecule 34: mRNA



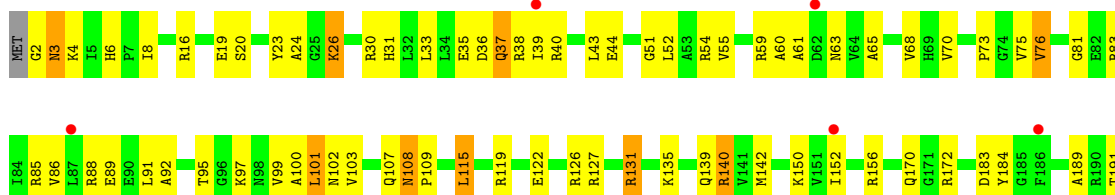
• Molecule 35: 30S ribosomal protein S2

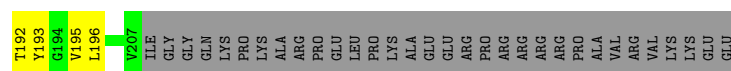


• Molecule 35: 30S ribosomal protein S2

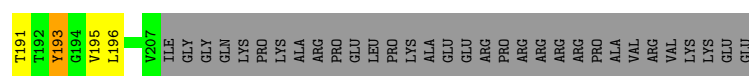


• Molecule 36: 30S ribosomal protein S3

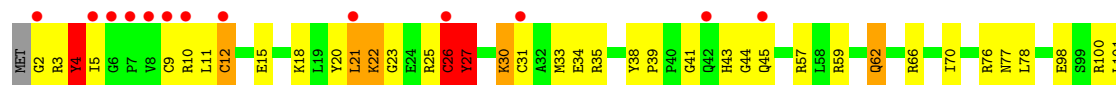




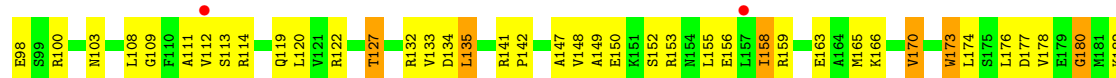
• Molecule 36: 30S ribosomal protein S3



• Molecule 37: 30S ribosomal protein S4

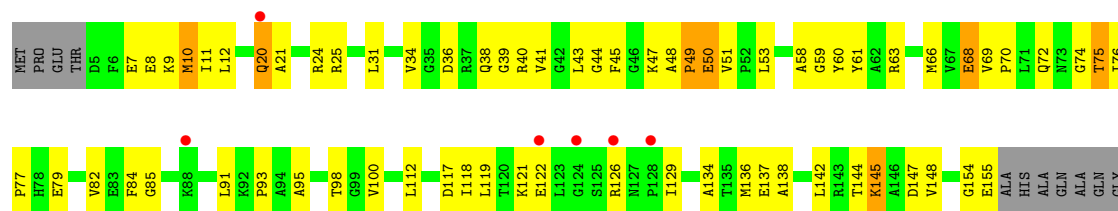


• Molecule 37: 30S ribosomal protein S4

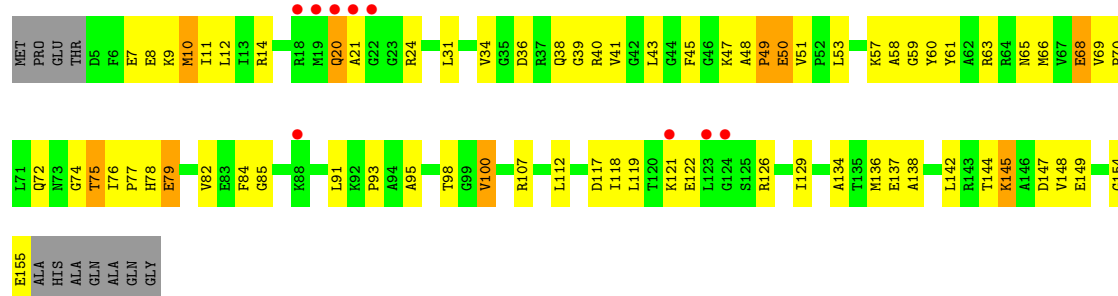


• Molecule 38: 30S ribosomal protein S5

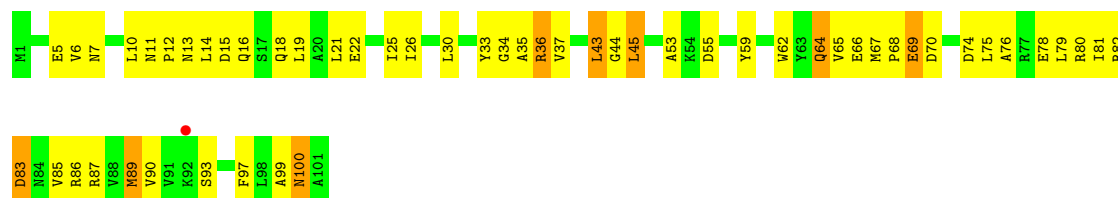




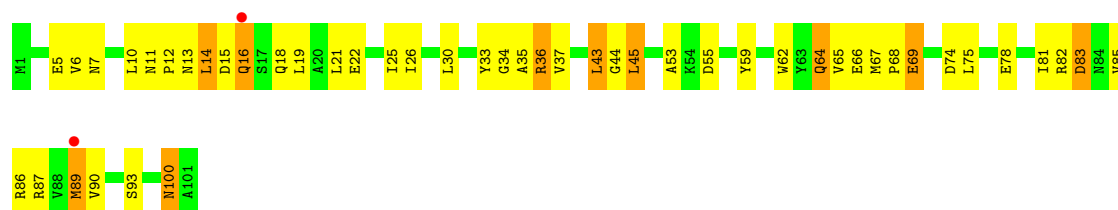
• Molecule 38: 30S ribosomal protein S5



• Molecule 39: 30S ribosomal protein S6



• Molecule 39: 30S ribosomal protein S6



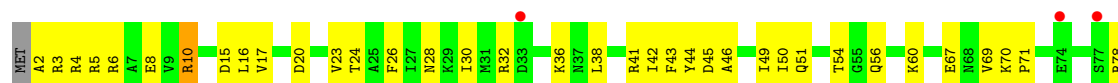
• Molecule 40: 30S ribosomal protein S7







- Molecule 40: 30S ribosomal protein S7



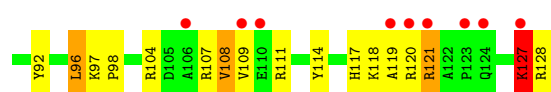
- Molecule 41: 30S ribosomal protein S8



- Molecule 41: 30S ribosomal protein S8

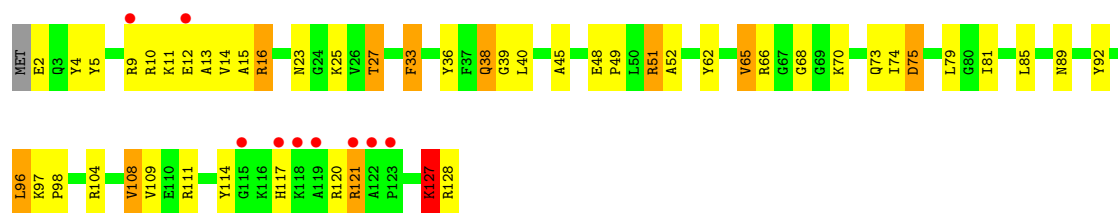


- Molecule 42: 30S ribosomal protein S9

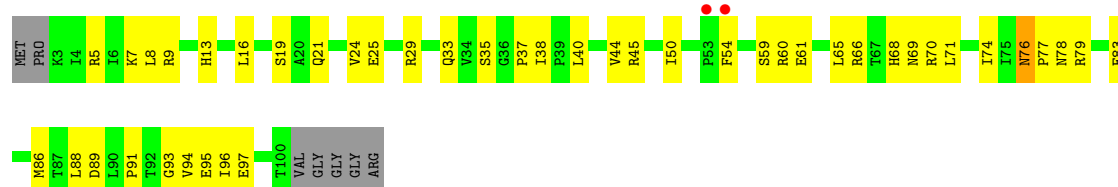


- Molecule 42: 30S ribosomal protein S9

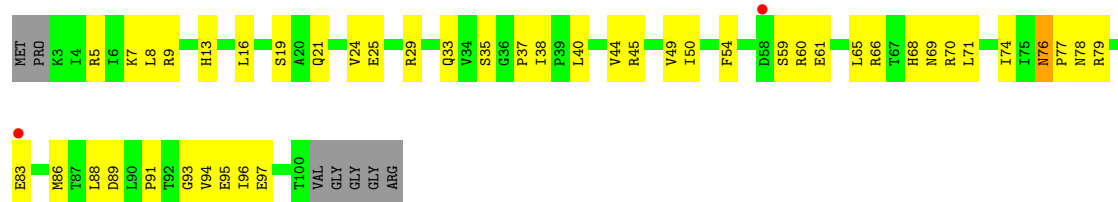




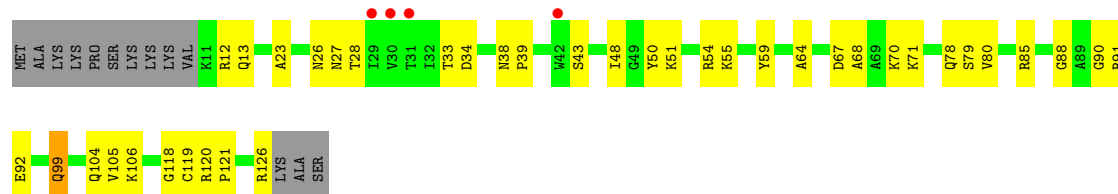
• Molecule 43: 30S ribosomal protein S10



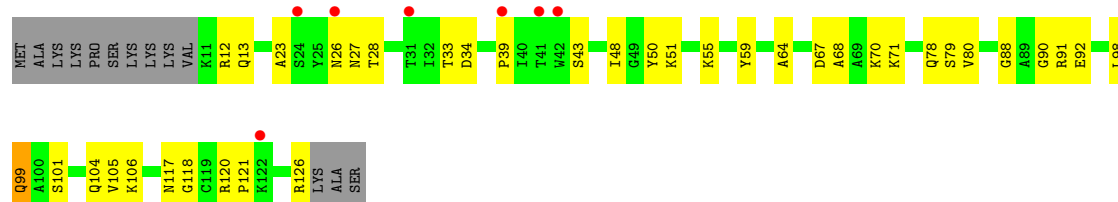
• Molecule 43: 30S ribosomal protein S10



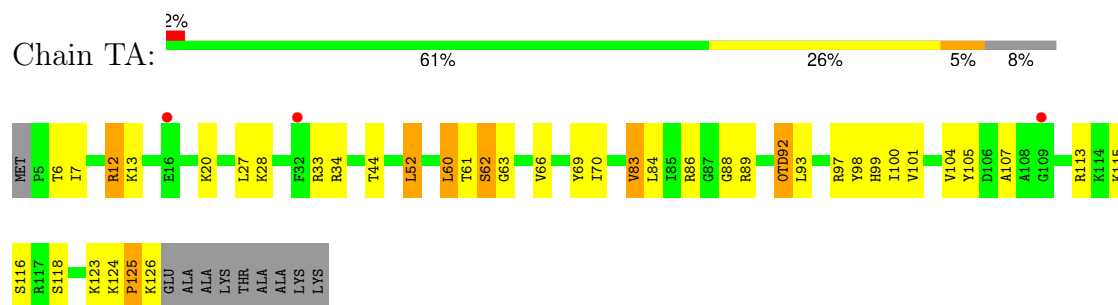
• Molecule 44: 30S ribosomal protein S11



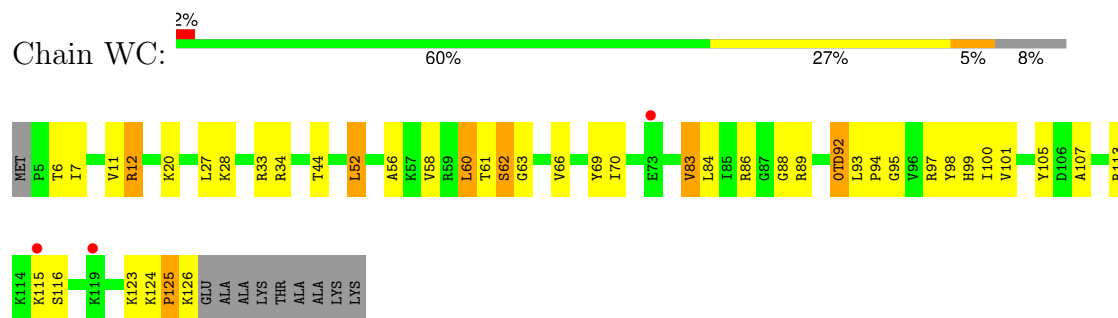
• Molecule 44: 30S ribosomal protein S11



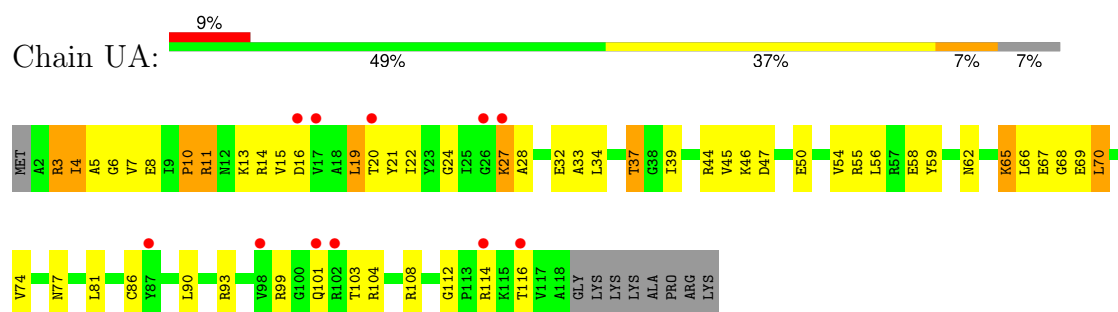
- Molecule 45: 30S ribosomal protein S12



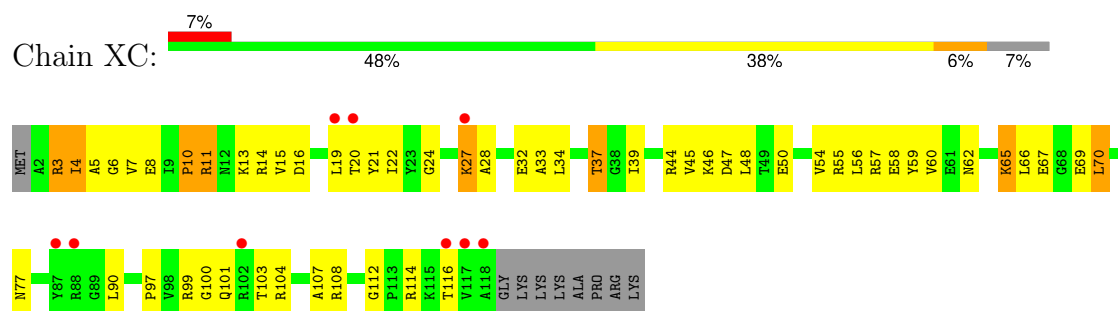
- Molecule 45: 30S ribosomal protein S12



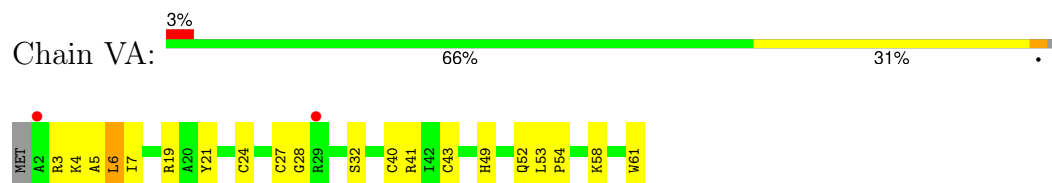
- Molecule 46: 30S ribosomal protein S13



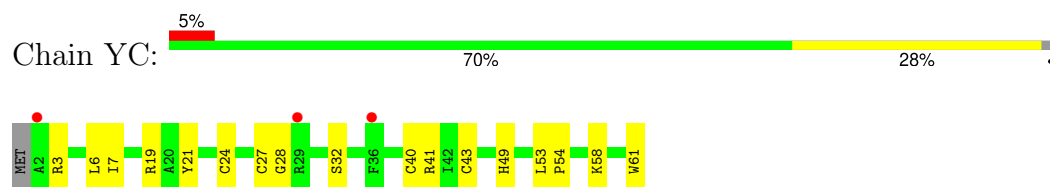
- Molecule 46: 30S ribosomal protein S13



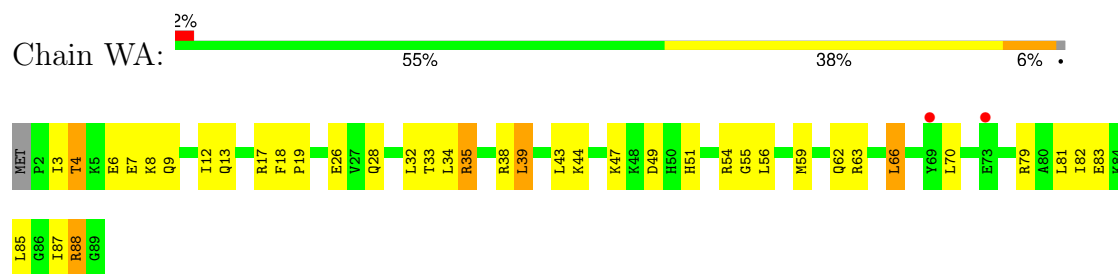
- Molecule 47: 30S ribosomal protein S14 type Z



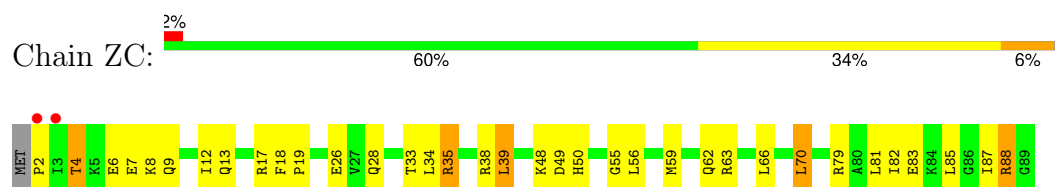
- Molecule 47: 30S ribosomal protein S14 type Z



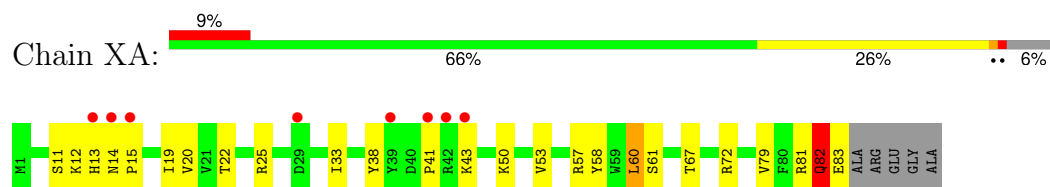
- Molecule 48: 30S ribosomal protein S15



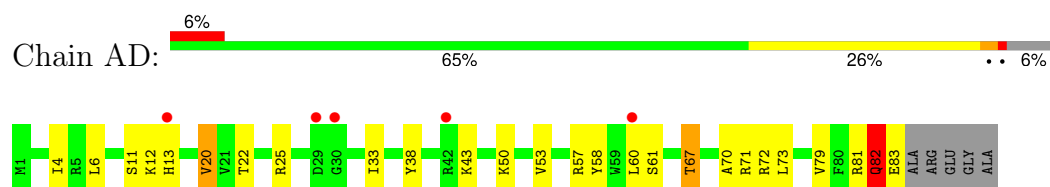
- Molecule 48: 30S ribosomal protein S15



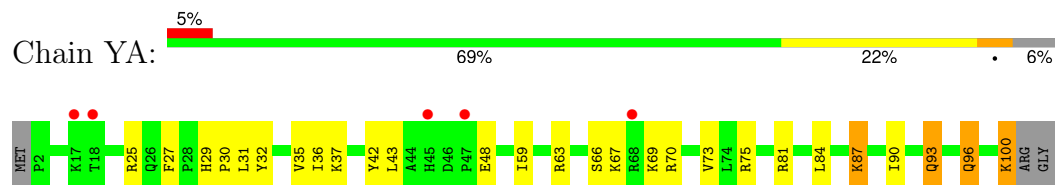
- Molecule 49: 30S ribosomal protein S16



- Molecule 49: 30S ribosomal protein S16

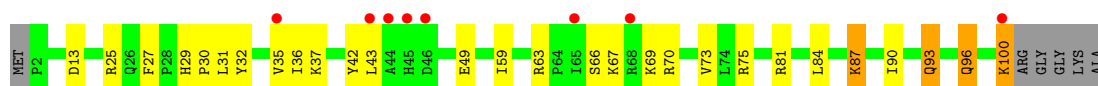


- Molecule 50: 30S ribosomal protein S17

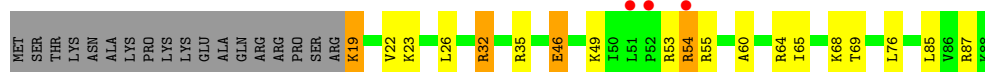


- Molecule 50: 30S ribosomal protein S17

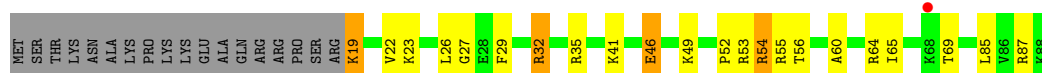




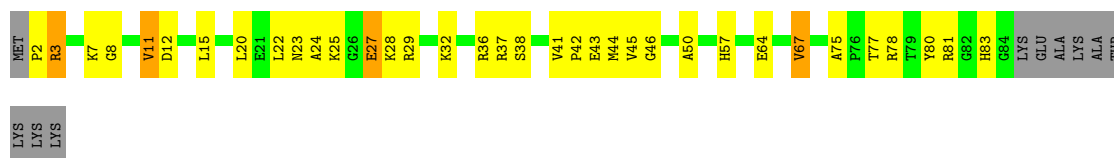
- Molecule 51: 30S ribosomal protein S18



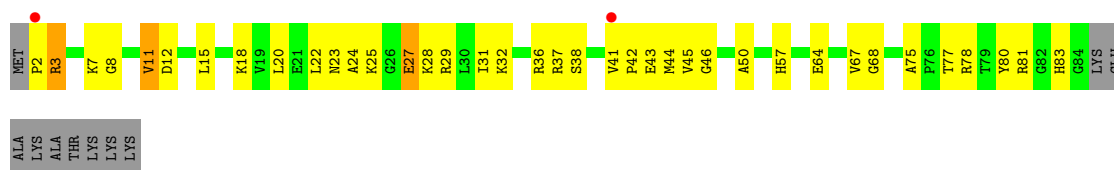
- Molecule 51: 30S ribosomal protein S18



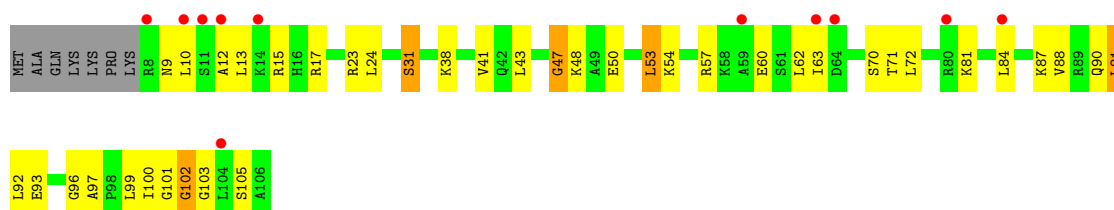
- Molecule 52: 30S ribosomal protein S19



- Molecule 52: 30S ribosomal protein S19



- Molecule 53: 30S ribosomal protein S20



- Molecule 53: 30S ribosomal protein S20

Chain ED:

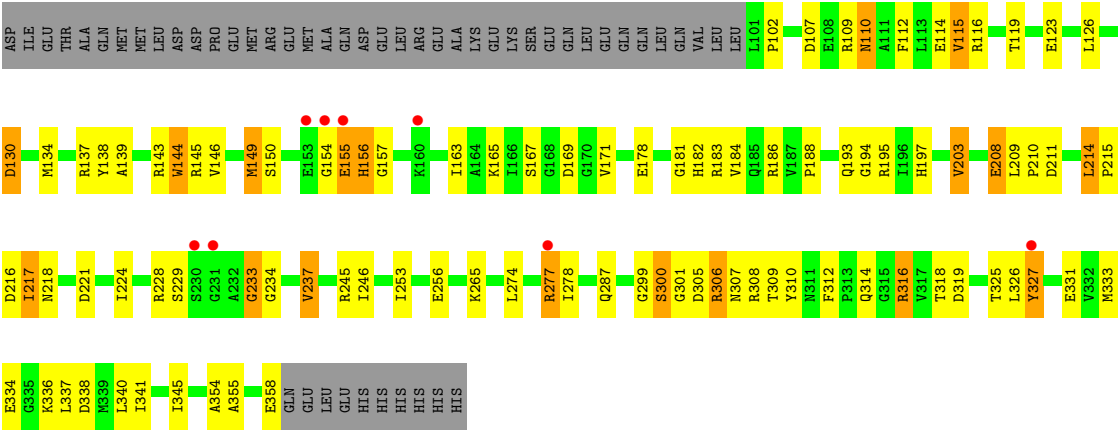
Chain CB:

Chain FD:

Chain GD:

Chain HD:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.82Å 450.45Å 615.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.55 50.00 – 3.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-3.55) 99.8 (50.00-3.55)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 3.58Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	(Not available) , (Not available) 0.221 , 0.257	Depositor DCC
$R_{free}$ test set	684222 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	124.9	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 83.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	299566	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.52% 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: 5MC, PSU, M2G, 2MG, UR3, OMG, 2MU, 7MG, 5MU, MA6, 2MA, 0TD, ZN, 4SU, MG, 4OC

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	A	0.66	8/35961 (0.0%)	1.15	147/56125 (0.3%)
1	DB	0.69	5/35961 (0.0%)	1.18	176/56125 (0.3%)
2	B	1.01	76/69214 (0.1%)	1.49	1088/108048 (1.0%)
2	EB	0.88	60/69214 (0.1%)	1.38	770/108048 (0.7%)
3	C	0.69	0/2881	1.20	18/4494 (0.4%)
3	FB	0.61	0/2881	1.09	11/4494 (0.2%)
4	D	0.47	0/1744	0.88	0/2719
4	GB	0.48	0/1744	0.88	0/2719
4	IA	0.74	0/1744	1.17	7/2719 (0.3%)
4	LC	0.70	1/1744 (0.1%)	1.12	5/2719 (0.2%)
5	E	0.78	4/2195 (0.2%)	0.74	0/2955
5	HB	0.70	3/2195 (0.1%)	0.72	0/2955
6	F	0.63	0/1596	0.67	0/2153
6	IB	0.57	0/1596	0.65	0/2153
7	G	0.70	0/1621	0.69	0/2194
7	JB	0.61	0/1621	0.65	0/2194
8	H	0.44	0/1496	0.57	0/2013
8	KB	0.40	0/1496	0.56	0/2013
9	I	0.52	0/1356	0.56	0/1834
9	LB	0.38	0/1356	0.52	0/1834
10	J	0.51	0/1152	0.58	0/1559
10	MB	0.47	0/1152	0.58	0/1559
11	K	0.62	0/1148	0.66	0/1547
11	NB	0.51	0/1148	0.63	0/1547
12	L	0.67	0/942	0.68	0/1268
12	OB	0.67	0/942	0.67	0/1268
13	M	0.64	0/1162	0.69	0/1544
13	PB	0.56	0/1162	0.67	0/1544
14	N	0.67	0/1142	0.63	0/1525
14	QB	0.60	0/1142	0.63	0/1525
15	O	0.60	0/982	0.72	0/1312
15	RB	0.57	0/982	0.68	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	P	0.45	0/887	0.58	0/1180
16	SB	0.40	0/887	0.53	0/1180
17	Q	0.61	0/1157	0.65	0/1544
17	TB	0.58	0/1157	0.65	0/1544
18	R	0.67	0/982	0.68	0/1306
18	UB	0.57	0/982	0.65	0/1306
19	S	0.65	0/790	0.67	0/1057
19	VB	0.56	0/790	0.65	0/1057
20	T	0.74	0/901	0.73	0/1209
20	WB	0.65	0/901	0.69	0/1209
21	U	0.76	0/764	0.69	0/1025
21	XB	0.63	0/764	0.65	0/1025
22	V	0.64	0/827	0.66	0/1103
22	YB	0.60	0/827	0.65	0/1103
23	W	0.49	0/1527	0.58	0/2073
23	ZB	0.43	0/1527	0.55	0/2073
24	AC	0.61	0/671	0.71	0/892
24	X	0.71	0/671	0.73	0/892
25	BC	0.65	0/768	0.71	0/1021
25	Y	0.70	0/768	0.72	0/1021
26	CC	0.57	0/594	0.60	0/785
26	Z	0.68	0/594	0.64	0/785
27	AA	0.60	0/482	0.62	0/646
27	DC	0.57	0/482	0.63	0/646
28	BA	0.42	0/565	0.46	0/761
28	EC	0.39	0/565	0.46	0/761
29	CA	0.60	0/474	0.63	0/640
29	FC	0.55	0/474	0.64	0/640
30	DA	0.41	0/460	0.50	0/613
30	GC	0.40	0/460	0.48	0/613
31	EA	0.79	0/426	0.89	3/561 (0.5%)
31	HC	0.69	0/426	0.78	1/561 (0.2%)
32	FA	0.74	1/525 (0.2%)	0.68	0/691
32	IC	0.61	0/525	0.66	0/691
33	GA	0.45	0/310	0.53	0/407
33	JC	0.46	0/310	0.53	0/407
34	HA	1.01	0/247	1.24	3/382 (0.8%)
34	KC	1.01	0/247	1.14	0/382
35	JA	0.41	0/1935	0.55	0/2609
35	MC	0.41	0/1935	0.54	0/2609
36	KA	0.41	0/1636	0.53	0/2205
36	NC	0.40	0/1636	0.53	0/2205
37	LA	0.51	1/1733 (0.1%)	0.60	1/2318 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
37	OC	0.58	1/1733 (0.1%)	0.62	1/2318 (0.0%)
38	MA	0.48	0/1171	0.61	0/1576
38	PC	0.51	0/1171	0.63	0/1576
39	NA	0.53	0/856	0.59	0/1154
39	QC	0.50	0/856	0.59	0/1154
40	OA	0.42	0/1276	0.51	0/1709
40	RC	0.44	0/1276	0.52	0/1709
41	PA	0.45	0/1136	0.59	0/1527
41	SC	0.46	0/1136	0.60	0/1527
42	QA	0.36	0/1029	0.49	0/1378
42	TC	0.36	0/1029	0.49	0/1378
43	RA	0.38	0/807	0.49	0/1085
43	UC	0.38	0/807	0.49	0/1085
44	SA	0.52	0/879	0.61	0/1187
44	VC	0.50	0/879	0.61	0/1187
45	TA	0.55	0/963	0.63	0/1287
45	WC	0.56	0/963	0.63	0/1287
46	UA	0.38	0/943	0.53	0/1265
46	XC	0.38	0/943	0.52	0/1265
47	VA	0.42	0/501	0.54	0/664
47	YC	0.39	0/501	0.53	0/664
48	WA	0.50	0/745	0.56	0/992
48	ZC	0.51	0/745	0.56	0/992
49	AD	0.49	0/716	0.58	0/963
49	XA	0.40	0/716	0.55	0/963
50	BD	0.53	0/836	0.58	0/1117
50	YA	0.52	0/836	0.59	0/1117
51	CD	0.50	0/579	0.55	0/768
51	ZA	0.52	0/579	0.57	0/768
52	AB	0.36	0/680	0.51	0/915
52	DD	0.35	0/680	0.51	0/915
53	BB	0.40	0/764	0.52	0/1006
53	ED	0.44	0/764	0.55	0/1006
54	CB	0.35	0/212	0.46	0/277
54	FD	0.36	0/212	0.46	0/277
55	GD	0.54	0/2012	0.62	0/2713
55	HD	0.48	0/2012	0.60	0/2713
All	All	0.77	160/322204 (0.0%)	1.18	2231/481240 (0.5%)

All (160) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1762	A	N9-C4	14.42	1.46	1.37
2	EB	1762	A	N9-C4	13.35	1.45	1.37
2	B	1142(B)	A	N9-C4	-10.33	1.31	1.37
1	A	1503	A	N9-C4	9.28	1.43	1.37
1	A	1531	A	N9-C4	9.11	1.43	1.37
2	EB	1762	A	C5-C6	8.99	1.49	1.41
2	B	1762	A	N3-C4	8.96	1.40	1.34
2	EB	1142(B)	A	N9-C4	-8.80	1.32	1.37
2	B	1762	A	C5-C4	8.69	1.44	1.38
2	B	1602	U	C4-O4	8.60	1.30	1.23
37	OC	12	CYS	CB-SG	8.57	1.96	1.82
2	B	2593	U	C4-O4	8.22	1.30	1.23
2	EB	1762	A	N7-C5	8.14	1.44	1.39
1	DB	1503	A	N9-C4	8.00	1.42	1.37
2	EB	1762	A	C5-C4	7.91	1.44	1.38
2	B	1762	A	C5-C6	7.78	1.48	1.41
5	E	237	GLU	CG-CD	7.76	1.63	1.51
1	DB	1531	A	N9-C4	7.64	1.42	1.37
2	EB	2593	U	C4-O4	7.54	1.29	1.23
2	EB	1762	A	N3-C4	7.51	1.39	1.34
2	EB	1783	A	N9-C4	-7.37	1.33	1.37
2	B	2271	G	C6-O6	7.35	1.30	1.24
2	B	1762	A	N7-C5	7.34	1.43	1.39
2	EB	251	A	N3-C4	-7.34	1.30	1.34
37	LA	12	CYS	CB-SG	7.18	1.94	1.82
2	B	528	A	N9-C4	-7.18	1.33	1.37
2	EB	251	A	N9-C4	-7.08	1.33	1.37
2	EB	2430	A	N9-C4	-7.02	1.33	1.37
2	EB	1026	U	N1-C2	6.99	1.44	1.38
2	EB	1780	A	N9-C4	-6.91	1.33	1.37
2	B	1566	A	N9-C4	-6.86	1.33	1.37
2	EB	2271	G	C6-O6	6.84	1.30	1.24
2	EB	804	A	N9-C4	-6.82	1.33	1.37
2	EB	528	A	N9-C4	-6.80	1.33	1.37
2	B	1026	U	N1-C2	6.79	1.44	1.38
2	B	1671	U	C2-N3	6.79	1.42	1.37
2	EB	1981	A	N9-C4	-6.73	1.33	1.37
2	B	1021	A	N9-C4	-6.71	1.33	1.37
2	B	2249	U	C4-O4	6.68	1.28	1.23
2	EB	548	A	N9-C4	6.65	1.41	1.37
2	B	688	U	C4-O4	6.60	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1531	A	N3-C4	6.51	1.38	1.34
2	B	1783	A	N9-C4	-6.51	1.33	1.37
2	B	1671	U	C4-O4	6.50	1.28	1.23
2	B	790	C	N3-C4	6.48	1.38	1.33
2	EB	199	A	N9-C4	-6.46	1.33	1.37
2	EB	2585	U	N1-C2	6.46	1.44	1.38
2	B	330	A	N9-C4	-6.43	1.33	1.37
2	B	2585	U	N1-C2	6.42	1.44	1.38
2	EB	1671	U	C4-O4	6.40	1.28	1.23
2	B	2245	U	C4-O4	6.38	1.28	1.23
2	EB	1762	A	C6-N6	6.29	1.39	1.33
2	EB	1609	A	N9-C4	-6.28	1.34	1.37
2	B	945	A	C5-C6	-6.26	1.35	1.41
1	DB	1503	A	C5-C6	6.24	1.46	1.41
2	B	2028	U	C4-O4	6.21	1.28	1.23
2	EB	2060	A	N9-C4	-6.21	1.34	1.37
5	HB	237	GLU	CG-CD	6.18	1.61	1.51
2	B	1762	A	C6-N6	6.14	1.38	1.33
5	E	237	GLU	CB-CG	6.12	1.63	1.52
2	B	2585	U	C2-N3	6.12	1.42	1.37
2	EB	1783	A	N3-C4	-6.12	1.31	1.34
2	B	251	A	N3-C4	-6.11	1.31	1.34
2	B	761	A	N9-C4	-6.11	1.34	1.37
2	B	945	A	N9-C4	-6.07	1.34	1.37
2	B	1780	A	N9-C4	-6.06	1.34	1.37
2	EB	945	A	C5-C6	-6.04	1.35	1.41
2	B	1142(B)	A	C5-C6	-6.01	1.35	1.41
5	HB	237	GLU	CB-CG	6.00	1.63	1.52
2	EB	2053	G	C5-C6	-6.00	1.36	1.42
2	EB	1671	U	N3-C4	5.95	1.43	1.38
2	EB	1810	A	N9-C4	-5.95	1.34	1.37
2	B	1046	A	N9-C4	5.91	1.41	1.37
1	DB	1531	A	N3-C4	5.89	1.38	1.34
2	B	1618	A	C5-C6	-5.88	1.35	1.41
2	B	1609	A	N9-C4	-5.86	1.34	1.37
2	B	6	A	N9-C4	5.83	1.41	1.37
2	EB	2593	U	C2-N3	5.79	1.41	1.37
2	B	127	A	N9-C4	-5.77	1.34	1.37
2	B	1608	A	N9-C4	-5.74	1.34	1.37
2	EB	761	A	N9-C4	-5.70	1.34	1.37
2	B	2606	C	N1-C6	-5.70	1.33	1.37
2	EB	733	G	N9-C8	5.69	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1251	C	N1-C6	-5.67	1.33	1.37
2	EB	276	A	N9-C4	5.66	1.41	1.37
2	EB	945	A	N9-C4	-5.64	1.34	1.37
2	B	790	C	C2-N3	5.64	1.40	1.35
1	A	781	A	N9-C4	-5.63	1.34	1.37
2	EB	2249	U	C4-O4	5.62	1.28	1.23
2	B	1566	A	N3-C4	-5.59	1.31	1.34
2	B	123	G	N9-C8	-5.59	1.33	1.37
2	EB	1021	A	N9-C4	-5.58	1.34	1.37
1	A	1503	A	N7-C5	5.55	1.42	1.39
2	EB	2028	U	C4-O4	5.55	1.28	1.23
2	EB	1963	U	N1-C2	5.55	1.43	1.38
2	EB	1367	A	N3-C4	-5.54	1.31	1.34
2	EB	1602	U	C4-O4	5.54	1.28	1.23
2	B	460	A	N3-C4	-5.53	1.31	1.34
2	EB	1342	A	N9-C4	-5.51	1.34	1.37
2	EB	1671	U	C2-N3	5.51	1.41	1.37
5	HB	28	GLU	CG-CD	5.51	1.60	1.51
2	EB	2542	A	N9-C4	-5.50	1.34	1.37
2	B	2287	A	N9-C4	-5.49	1.34	1.37
2	EB	1132	A	N9-C4	-5.48	1.34	1.37
2	B	2764	A	N9-C4	-5.47	1.34	1.37
2	B	460	A	N9-C4	-5.46	1.34	1.37
2	EB	2629	A	N9-C4	5.46	1.41	1.37
2	B	1802	A	N9-C4	-5.46	1.34	1.37
32	FA	56	GLU	CG-CD	5.45	1.60	1.51
1	DB	1503	A	N3-C4	5.44	1.38	1.34
2	EB	1511	A	N9-C4	5.44	1.41	1.37
2	B	1271	G	C6-O6	5.43	1.29	1.24
1	A	1503	A	N3-C4	5.42	1.38	1.34
2	B	2060	A	N9-C4	-5.42	1.34	1.37
2	EB	2436	G	C2-N3	-5.42	1.28	1.32
2	B	653	C	N1-C6	5.41	1.40	1.37
4	LC	1	C	N1-C2	5.41	1.45	1.40
2	B	1142(B)	A	N3-C4	-5.36	1.31	1.34
2	B	1367	A	N9-C4	-5.36	1.34	1.37
2	B	548	A	N9-C4	5.34	1.41	1.37
2	EB	6	A	N9-C4	5.33	1.41	1.37
2	B	1187	G	C6-O6	5.31	1.28	1.24
2	B	1963	U	N1-C2	5.31	1.43	1.38
2	EB	2287	A	N9-C4	-5.31	1.34	1.37
2	B	251	A	N9-C4	-5.30	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	28	GLU	CG-CD	5.29	1.59	1.51
2	EB	734	A	N9-C4	-5.29	1.34	1.37
2	B	750	A	N9-C4	-5.28	1.34	1.37
2	B	1810	A	N9-C4	-5.28	1.34	1.37
2	B	71	A	N7-C5	-5.25	1.36	1.39
2	B	251	A	C5-C4	-5.24	1.35	1.38
2	B	1511	A	N9-C4	5.23	1.41	1.37
2	B	1221(A)	C	N3-C4	-5.22	1.30	1.33
2	B	797	C	N1-C6	-5.21	1.34	1.37
2	B	1602	U	C2-N3	5.20	1.41	1.37
2	B	1825	A	C6-N1	-5.19	1.31	1.35
2	B	790	C	C4-C5	5.17	1.47	1.43
2	B	2062	A	N7-C5	5.17	1.42	1.39
2	B	255	A	N9-C4	-5.16	1.34	1.37
2	B	69	C	N1-C6	-5.15	1.34	1.37
2	EB	330	A	N9-C4	-5.15	1.34	1.37
2	B	2593	U	C2-N3	5.15	1.41	1.37
2	B	781	A	N3-C4	-5.13	1.31	1.34
2	B	2833	G	C5-C4	5.12	1.42	1.38
2	EB	251	A	C5-C4	-5.12	1.35	1.38
2	EB	1187	G	C6-O6	5.11	1.28	1.24
1	A	1503	A	C5-C6	5.10	1.45	1.41
5	E	237	GLU	CD-OE2	5.10	1.31	1.25
1	A	1531	A	N7-C5	5.10	1.42	1.39
2	B	2061	G	C6-O6	5.09	1.28	1.24
2	EB	1654	A	N9-C4	-5.06	1.34	1.37
2	EB	2439	A	N9-C4	-5.05	1.34	1.37
2	B	530	G	C2-N3	5.04	1.36	1.32
2	EB	570	G	C6-O6	5.03	1.28	1.24
2	EB	504	U	N3-C4	5.03	1.43	1.38
2	B	917	A	N9-C4	-5.02	1.34	1.37
2	EB	1566	A	C5-C6	-5.02	1.36	1.41
2	B	819	A	N9-C4	-5.01	1.34	1.37
2	EB	706	A	N9-C4	-5.01	1.34	1.37
2	EB	503	A	N3-C4	-5.00	1.31	1.34

All (2231) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	EB	2053	G	N1-C6-O6	19.40	131.54	119.90
2	EB	2053	G	C5-C6-O6	-15.62	119.23	128.60
2	B	2053	G	N1-C6-O6	15.42	129.15	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2593	U	N3-C4-C5	-14.85	105.69	114.60
2	B	1602	U	N3-C4-C5	-14.74	105.75	114.60
2	B	450	G	C5-C6-N1	-14.31	104.35	111.50
2	B	2447	G	N1-C6-O6	14.25	128.45	119.90
2	EB	733	G	N1-C6-O6	14.10	128.36	119.90
2	B	733	G	N1-C6-O6	13.89	128.23	119.90
2	B	2502	G	N1-C6-O6	13.80	128.18	119.90
2	B	2271	G	C5-C6-N1	-13.69	104.66	111.50
2	B	2053	G	C5-C6-O6	-13.51	120.49	128.60
2	EB	2593	U	N3-C4-C5	-13.44	106.53	114.60
2	B	733	G	C5-C6-O6	-13.36	120.58	128.60
2	EB	197	A	O5'-P-OP2	-13.34	93.69	105.70
2	B	197	A	O5'-P-OP2	-13.21	93.81	105.70
2	B	733	G	C5-N7-C8	-12.87	97.86	104.30
2	B	1671	U	N3-C4-C5	-12.87	106.88	114.60
2	B	1671	U	N3-C4-O4	12.70	128.29	119.40
2	EB	733	G	C4-C5-N7	12.49	115.80	110.80
2	B	733	G	C4-C5-N7	12.40	115.76	110.80
2	B	1142(B)	A	C2-N3-C4	-12.32	104.44	110.60
2	EB	733	G	C5-C6-O6	-12.29	121.22	128.60
2	EB	733	G	C5-N7-C8	-12.29	98.15	104.30
2	B	1790	C	N3-C4-N4	-12.26	109.42	118.00
2	EB	1671	U	N3-C4-O4	12.00	127.80	119.40
1	DB	1452	C	C6-N1-C2	-11.98	115.51	120.30
2	B	2544	G	N1-C6-O6	11.81	126.98	119.90
2	EB	1187	G	C5-C6-N1	-11.59	105.70	111.50
2	EB	2271	G	C5-C6-N1	-11.50	105.75	111.50
2	B	1614	A	O5'-P-OP2	-11.41	95.43	105.70
2	B	1828	G	C8-N9-C4	-11.41	101.84	106.40
1	A	117	G	N1-C6-O6	11.33	126.70	119.90
2	B	2685	G	C5-C6-N1	-11.26	105.87	111.50
2	EB	2053	G	C4-C5-N7	11.23	115.29	110.80
2	B	2061	G	N1-C6-O6	11.15	126.59	119.90
1	DB	117	G	N1-C6-O6	11.09	126.55	119.90
2	EB	2574	G	O5'-P-OP2	-11.06	95.75	105.70
2	B	576	U	O5'-P-OP2	-11.00	95.80	105.70
2	EB	1187	G	N1-C6-O6	10.88	126.43	119.90
2	EB	2447	G	N1-C6-O6	10.88	126.43	119.90
2	B	450	G	N1-C6-O6	10.86	126.42	119.90
2	EB	2544	G	N1-C6-O6	10.86	126.42	119.90
2	B	1187	G	C5-C6-N1	-10.83	106.08	111.50
2	EB	1602	U	N3-C4-C5	-10.79	108.13	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	391	G	N1-C6-O6	10.68	126.31	119.90
2	B	733	G	N7-C8-N9	10.68	118.44	113.10
1	A	529	G	N1-C6-O6	10.68	126.31	119.90
1	DB	529	G	N1-C6-O6	10.63	126.28	119.90
2	EB	1828	G	C8-N9-C4	-10.61	102.16	106.40
2	B	1756	G	C5-C6-N1	-10.61	106.20	111.50
2	EB	2053	G	C6-C5-N7	-10.61	124.04	130.40
2	EB	733	G	N7-C8-N9	10.59	118.40	113.10
1	A	1452	C	C6-N1-C2	-10.53	116.09	120.30
2	B	1021	A	C2-N3-C4	-10.47	105.37	110.60
2	B	528	A	C5-N7-C8	-10.43	98.69	103.90
2	B	2593	U	C6-N1-C2	-10.39	114.76	121.00
2	B	2249	U	N3-C4-C5	-10.39	108.37	114.60
2	B	2397	G	N1-C6-O6	10.29	126.08	119.90
2	EB	1828	G	N9-C4-C5	10.25	109.50	105.40
2	B	1840	G	N1-C6-O6	10.24	126.04	119.90
2	B	865	C	C6-N1-C2	10.16	124.36	120.30
2	EB	450	G	C5-C6-N1	-10.14	106.43	111.50
2	B	2271	G	N1-C6-O6	10.14	125.98	119.90
2	B	783	A	O5'-P-OP1	-10.12	96.59	105.70
2	B	1381	G	N1-C6-O6	10.09	125.95	119.90
2	EB	728	G	N1-C6-O6	10.08	125.95	119.90
2	EB	1627	G	N1-C6-O6	10.08	125.95	119.90
2	B	2028	U	N3-C4-C5	-10.07	108.56	114.60
2	B	2610	C	C6-N1-C2	9.98	124.29	120.30
2	B	1936	A	N1-C6-N6	9.91	124.54	118.60
2	EB	510	C	O5'-P-OP2	-9.87	96.82	105.70
2	B	2502	G	O5'-P-OP1	-9.86	96.83	105.70
1	DB	754	C	N1-C2-O2	9.84	124.81	118.90
2	B	2447	G	C5-C6-N1	-9.83	106.58	111.50
1	A	754	C	N1-C2-O2	9.82	124.80	118.90
2	B	945	A	N1-C6-N6	9.82	124.49	118.60
2	B	2592	G	C8-N9-C4	-9.82	102.47	106.40
2	EB	945	A	N1-C6-N6	9.80	124.48	118.60
2	B	450	G	C4-C5-C6	9.78	124.67	118.80
2	B	2228	G	N1-C6-O6	9.77	125.76	119.90
2	B	2238	G	O5'-P-OP2	-9.71	96.96	105.70
2	EB	2573	C	C6-N1-C2	9.68	124.17	120.30
2	B	688	U	N3-C4-O4	9.65	126.16	119.40
2	EB	2580	U	N3-C4-C5	-9.61	108.83	114.60
2	EB	1671	U	N3-C4-C5	-9.61	108.84	114.60
2	B	2245	U	N3-C4-C5	-9.60	108.84	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	528	A	C4-C5-N7	9.60	115.50	110.70
2	EB	570	G	C5-C6-N1	-9.57	106.72	111.50
2	EB	2502	G	O5'-P-OP1	-9.55	97.10	105.70
2	EB	1828	G	C5-C6-O6	9.55	134.33	128.60
2	B	1332	G	O5'-P-OP2	-9.44	97.21	105.70
2	B	1828	G	N9-C4-C5	9.43	109.17	105.40
2	EB	397	G	N1-C6-O6	9.38	125.53	119.90
2	EB	865	C	C6-N1-C2	9.38	124.05	120.30
2	EB	2685	G	C5-C6-N1	-9.31	106.85	111.50
2	EB	2061	G	N1-C6-O6	9.30	125.48	119.90
2	B	194	G	C2-N3-C4	-9.30	107.25	111.90
2	B	2685	G	N1-C6-O6	9.29	125.47	119.90
1	A	117	G	C5-C6-O6	-9.27	123.04	128.60
2	B	2505	G	C8-N9-C4	-9.24	102.70	106.40
2	B	948	G	C5-C6-N1	-9.23	106.89	111.50
2	B	1790	C	O5'-P-OP1	-9.22	97.40	105.70
2	EB	2502	G	N1-C6-O6	9.20	125.42	119.90
2	B	761	A	C5-N7-C8	-9.19	99.31	103.90
2	B	2573	C	C6-N1-C2	9.18	123.97	120.30
2	EB	1780	A	C8-N9-C4	9.16	109.46	105.80
2	EB	2505	G	C5-C6-O6	9.16	134.09	128.60
2	B	1828	G	C5-C6-O6	9.13	134.08	128.60
2	EB	2447	G	C8-N9-C4	9.11	110.05	106.40
2	B	2593	U	N1-C2-O2	-9.11	116.42	122.80
2	B	391	G	C6-C5-N7	-9.11	124.94	130.40
1	DB	293	G	N1-C6-O6	9.10	125.36	119.90
2	EB	1762	A	C4-C5-N7	-9.09	106.16	110.70
2	EB	2593	U	C6-N1-C2	-9.09	115.55	121.00
2	B	1142(B)	A	N1-C6-N6	9.08	124.05	118.60
2	B	1602	U	C4-C5-C6	9.06	125.14	119.70
2	EB	1790	C	N3-C4-N4	-8.99	111.71	118.00
2	B	790	C	O5'-P-OP2	-8.98	97.62	105.70
2	EB	191	A	C8-N9-C4	-8.93	102.23	105.80
2	B	2556	C	N1-C2-O2	8.92	124.25	118.90
2	B	1790	C	C5-C4-N4	8.91	126.44	120.20
3	C	87	G	C8-N9-C4	8.91	109.96	106.40
4	LC	48	C	C6-N1-C2	8.90	123.86	120.30
2	EB	140	A	N7-C8-N9	8.89	118.25	113.80
2	B	330	A	C2-N3-C4	-8.87	106.16	110.60
2	B	2490	G	C5-C6-N1	-8.87	107.07	111.50
2	B	1614	A	O5'-P-OP1	8.86	121.33	110.70
2	EB	391	G	N1-C6-O6	8.85	125.21	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	G	N1-C6-O6	8.84	125.21	119.90
2	B	1814	G	C5-C6-N1	-8.84	107.08	111.50
2	B	2228	G	C5-C6-N1	-8.84	107.08	111.50
2	B	787	U	O5'-P-OP2	-8.84	97.75	105.70
2	B	1981	A	C5-N7-C8	-8.80	99.50	103.90
2	B	191	A	C8-N9-C4	-8.77	102.29	105.80
2	B	1840	G	C5-C6-N1	-8.77	107.11	111.50
2	B	1240	U	C5-C4-O4	8.75	131.15	125.90
2	EB	1960	A	C8-N9-C4	8.74	109.30	105.80
1	A	372	C	C6-N1-C2	8.73	123.79	120.30
2	EB	783	A	N1-C6-N6	-8.71	113.38	118.60
2	B	461	C	N1-C2-O2	-8.71	113.68	118.90
2	B	2502	G	C6-C5-N7	-8.70	125.18	130.40
2	EB	1624	G	N1-C6-O6	8.70	125.12	119.90
2	B	1347	G	N1-C6-O6	8.69	125.12	119.90
2	B	2544	G	C5-C6-N1	-8.69	107.15	111.50
2	EB	2238	G	O5'-P-OP2	-8.68	97.89	105.70
2	B	248	G	N1-C6-O6	8.68	125.11	119.90
2	B	2505	G	N9-C4-C5	8.67	108.87	105.40
2	B	2576	G	O5'-P-OP2	-8.67	97.89	105.70
2	B	2641	G	C8-N9-C4	8.66	109.86	106.40
2	EB	2028	U	N3-C4-C5	-8.61	109.44	114.60
2	EB	1838	C	C6-N1-C2	8.59	123.74	120.30
1	A	754	C	C2-N1-C1'	8.58	128.24	118.80
1	A	117	G	C4-C5-N7	8.56	114.23	110.80
2	EB	2249	U	N3-C4-C5	-8.55	109.47	114.60
2	B	140	A	N7-C8-N9	8.54	118.07	113.80
2	EB	1021	A	C2-N3-C4	-8.53	106.33	110.60
2	B	1602	U	C6-N1-C2	-8.52	115.89	121.00
2	B	1627	G	N1-C6-O6	8.52	125.01	119.90
37	OC	12	CYS	CA-CB-SG	8.50	129.29	114.00
2	EB	548	A	C8-N9-C4	-8.49	102.41	105.80
2	B	19	C	C6-N1-C2	8.48	123.69	120.30
2	B	2052	G	C5-C6-O6	-8.48	123.51	128.60
2	B	1992	G	N3-C4-C5	-8.48	124.36	128.60
2	B	1558	A	C2-N3-C4	-8.47	106.36	110.60
1	DB	121	C	N1-C2-O2	8.45	123.97	118.90
2	EB	1936	A	N1-C6-N6	8.45	123.67	118.60
1	DB	1503	A	C2-N3-C4	8.45	114.82	110.60
2	EB	811	U	C5-C4-O4	8.44	130.96	125.90
2	B	1142(B)	A	N3-C4-C5	8.41	132.69	126.80
2	B	2430	A	N1-C6-N6	-8.41	113.56	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2685	G	N3-C2-N2	-8.40	114.02	119.90
2	EB	1936	A	N9-C4-C5	-8.38	102.45	105.80
2	B	1187	G	N1-C6-O6	8.37	124.92	119.90
1	DB	754	C	C2-N1-C1'	8.37	128.00	118.80
2	B	1698	A	C2-N3-C4	-8.36	106.42	110.60
2	EB	2610	C	C6-N1-C2	8.36	123.64	120.30
2	B	1558	A	N1-C6-N6	8.36	123.61	118.60
1	DB	529	G	C5-C6-O6	-8.35	123.59	128.60
2	EB	1602	U	C4-C5-C6	8.34	124.70	119.70
2	B	570	G	C5-C6-N1	-8.33	107.33	111.50
1	DB	117	G	C5-C6-O6	-8.33	123.60	128.60
2	EB	1532	C	C6-N1-C2	-8.33	116.97	120.30
2	B	16	G	C5-C6-N1	-8.32	107.34	111.50
2	B	128	C	C6-N1-C2	8.31	123.62	120.30
2	B	213	A	C8-N9-C4	8.31	109.12	105.80
2	B	1441	G	C5-C6-N1	-8.29	107.35	111.50
2	B	1756	G	N1-C6-O6	8.28	124.87	119.90
2	EB	2593	U	N1-C2-O2	-8.27	117.01	122.80
1	DB	1417	G	C5-C6-N1	-8.27	107.37	111.50
2	EB	1142(B)	A	C2-N3-C4	-8.27	106.47	110.60
2	EB	450	G	C4-C5-C6	8.26	123.76	118.80
2	B	248	G	C5-C6-O6	-8.26	123.65	128.60
2	B	1845	G	N1-C6-O6	8.25	124.85	119.90
2	EB	2722	G	N1-C6-O6	8.24	124.84	119.90
2	EB	195	A	C5-N7-C8	-8.23	99.78	103.90
2	B	479	A	N1-C6-N6	-8.23	113.66	118.60
2	EB	929	G	N1-C6-O6	8.23	124.84	119.90
2	EB	2245	U	N3-C4-C5	-8.22	109.67	114.60
2	EB	570	G	C4-C5-N7	-8.21	107.52	110.80
2	B	2719	G	C5-C6-N1	-8.21	107.40	111.50
2	B	929	G	N1-C6-O6	8.20	124.82	119.90
2	EB	1624	G	C5-C6-O6	-8.19	123.69	128.60
2	B	1703	G	N1-C6-O6	8.19	124.81	119.90
2	EB	1790	C	O5'-P-OP1	-8.17	98.35	105.70
2	B	2052	G	N1-C6-O6	8.16	124.80	119.90
1	A	121	C	N1-C2-O2	8.15	123.79	118.90
2	EB	1789	A	O5'-P-OP1	-8.15	98.36	105.70
2	EB	1981	A	C5-N7-C8	-8.14	99.83	103.90
2	B	688	U	N3-C4-C5	-8.14	109.72	114.60
2	EB	140	A	C8-N9-C4	-8.13	102.55	105.80
34	HA	15	A	C8-N9-C4	8.12	109.05	105.80
2	B	2545	G	N1-C6-O6	8.12	124.77	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	EB	1628	G	N1-C6-O6	8.12	124.77	119.90
2	B	1791	A	N1-C6-N6	-8.09	113.75	118.60
2	B	140	A	C5-N7-C8	-8.08	99.86	103.90
2	B	391	G	C5-C6-O6	-8.08	123.75	128.60
2	EB	733	G	C6-C5-N7	-8.06	125.56	130.40
2	B	16	G	N1-C6-O6	8.05	124.73	119.90
2	B	568	U	N3-C4-C5	-8.01	109.80	114.60
2	B	2241	A	N1-C2-N3	8.00	133.30	129.30
2	B	1671	U	C6-N1-C2	-8.00	116.20	121.00
2	B	1936	A	N9-C4-C5	-8.00	102.60	105.80
2	B	528	A	N3-C4-C5	7.99	132.39	126.80
2	B	948	G	N1-C6-O6	7.98	124.69	119.90
2	B	2593	U	N3-C4-O4	7.98	124.99	119.40
2	B	1271	G	O5'-P-OP2	-7.98	98.52	105.70
2	B	1190	G	N1-C6-O6	7.97	124.68	119.90
2	EB	929	G	C5-C6-N1	-7.97	107.51	111.50
2	EB	1762	A	C5-N7-C8	7.97	107.89	103.90
2	B	2838	G	N1-C6-O6	7.97	124.68	119.90
2	B	375	C	O5'-P-OP2	-7.97	98.53	105.70
2	EB	2052	G	N1-C6-O6	7.97	124.68	119.90
2	B	1628	G	N1-C6-O6	7.95	124.67	119.90
2	B	1789	A	O5'-P-OP1	-7.95	98.55	105.70
2	B	1973	G	N1-C6-O6	7.94	124.66	119.90
2	B	304	G	C5-C6-N1	-7.93	107.53	111.50
2	B	2415	G	C5-C6-N1	-7.92	107.54	111.50
1	DB	945	G	N1-C6-O6	7.92	124.65	119.90
2	EB	2580	U	C6-N1-C2	-7.92	116.25	121.00
2	B	548	A	C8-N9-C4	-7.89	102.64	105.80
2	EB	2414	G	N1-C6-O6	7.89	124.63	119.90
2	B	1023	U	O5'-P-OP1	-7.87	98.62	105.70
2	EB	1841	U	N3-C4-C5	-7.86	109.88	114.60
2	B	1441	G	N1-C6-O6	7.85	124.61	119.90
2	B	379	G	N1-C6-O6	7.85	124.61	119.90
2	B	520	G	N1-C6-O6	7.84	124.61	119.90
2	EB	1240	U	C5-C4-O4	7.84	130.61	125.90
2	B	404	C	C6-N1-C2	7.84	123.43	120.30
2	B	2304	G	N3-C4-N9	-7.82	121.31	126.00
2	EB	776	G	C5-C6-N1	-7.82	107.59	111.50
2	EB	2685	G	N3-C2-N2	-7.81	114.43	119.90
2	B	1671	U	C4-C5-C6	7.81	124.39	119.70
2	EB	2593	U	N3-C4-O4	7.81	124.86	119.40
2	EB	527	C	C2-N1-C1'	7.80	127.38	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	IA	48	C	C6-N1-C2	7.80	123.42	120.30
2	B	2580	U	N3-C4-C5	-7.79	109.93	114.60
2	B	1325	G	N3-C4-N9	7.79	130.67	126.00
2	EB	528	A	N3-C4-C5	7.78	132.24	126.80
2	B	1240	U	N3-C4-C5	-7.76	109.94	114.60
1	DB	1452	C	C5-C6-N1	7.76	124.88	121.00
2	B	974(B)	C	C6-N1-C2	7.74	123.40	120.30
37	LA	12	CYS	CA-CB-SG	7.74	127.93	114.00
2	EB	2053	G	C5-N7-C8	-7.74	100.43	104.30
3	C	87	G	N7-C8-N9	-7.73	109.23	113.10
2	B	2053	G	C4-C5-N7	7.73	113.89	110.80
2	EB	2614	A	C6-N1-C2	-7.73	113.96	118.60
2	B	1271	G	C5-C6-N1	-7.72	107.64	111.50
2	EB	1298	C	O5'-P-OP1	-7.71	98.76	105.70
2	EB	2505	G	C5-C6-N1	-7.71	107.65	111.50
2	B	2505	G	C5-C6-O6	7.71	133.22	128.60
2	EB	2447	G	C5-C6-N1	-7.71	107.65	111.50
2	B	2502	G	C5-C6-N1	-7.70	107.65	111.50
1	A	1503	A	C2-N3-C4	7.69	114.45	110.60
2	B	1936	A	C4-C5-N7	7.69	114.55	110.70
2	EB	806	C	O5'-P-OP1	-7.69	98.78	105.70
2	EB	330	A	C2-N3-C4	-7.68	106.76	110.60
2	B	1240	U	C6-N1-C2	-7.68	116.39	121.00
2	EB	1756	G	N1-C6-O6	7.68	124.51	119.90
1	DB	117	G	C6-C5-N7	-7.67	125.80	130.40
2	EB	528	A	C5-N7-C8	-7.67	100.06	103.90
2	EB	2614	A	N1-C2-N3	7.66	133.13	129.30
2	B	1347	G	C5-C6-N1	-7.66	107.67	111.50
1	A	529	G	C5-C6-O6	-7.66	124.00	128.60
2	B	2449	U	C5-C4-O4	-7.66	121.31	125.90
2	EB	2276	G	N1-C6-O6	7.65	124.49	119.90
1	DB	326	G	C5-C6-N1	-7.65	107.68	111.50
2	B	2464	C	C6-N1-C2	7.64	123.36	120.30
2	EB	1635	G	OP2-P-O3'	7.64	122.00	105.20
2	B	2055	C	OP2-P-O3'	7.63	121.99	105.20
4	IA	13	C	C6-N1-C2	-7.63	117.25	120.30
2	B	409	C	O5'-P-OP1	7.61	119.83	110.70
2	B	733	G	C6-C5-N7	-7.60	125.84	130.40
2	B	2241	A	C2-N3-C4	-7.60	106.80	110.60
1	DB	117	G	C4-C5-N7	7.60	113.84	110.80
2	B	2593	U	C4-C5-C6	7.60	124.26	119.70
2	B	2022	U	N1-C2-N3	-7.59	110.34	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	804	A	C8-N9-C4	7.59	108.83	105.80
2	B	1244	G	C5-C6-N1	-7.59	107.71	111.50
2	B	945	A	C4-C5-N7	7.58	114.49	110.70
2	B	2846	G	C5-C6-N1	-7.58	107.71	111.50
2	B	1307	A	C8-N9-C4	7.57	108.83	105.80
2	EB	2447	G	N9-C4-C5	-7.57	102.37	105.40
2	B	2036	C	N1-C2-O2	-7.57	114.36	118.90
1	A	842	C	C6-N1-C2	-7.57	117.27	120.30
2	B	2773	C	C6-N1-C2	7.56	123.32	120.30
2	EB	758	C	C6-N1-C2	7.56	123.32	120.30
2	B	1602	U	N3-C4-O4	7.55	124.69	119.40
2	B	527	C	C2-N1-C1'	7.55	127.10	118.80
2	EB	577	G	N1-C6-O6	7.54	124.42	119.90
2	EB	2698	U	C6-N1-C2	-7.54	116.48	121.00
2	B	1869	G	N1-C6-O6	7.52	124.41	119.90
1	A	23	C	C6-N1-C2	-7.52	117.29	120.30
2	EB	577	G	C6-C5-N7	-7.50	125.90	130.40
2	EB	397	G	C5-C6-O6	-7.50	124.10	128.60
2	B	1142(B)	A	C5-N7-C8	-7.49	100.16	103.90
2	B	1635	G	OP2-P-O3'	7.46	121.61	105.20
2	B	1348	G	N1-C6-O6	7.46	124.37	119.90
2	EB	2059	A	O5'-P-OP2	-7.45	99.00	105.70
2	EB	2419	U	N3-C4-C5	-7.43	110.14	114.60
2	B	2494	G	N1-C6-O6	7.43	124.36	119.90
2	B	1024	G	C5-C6-O6	-7.42	124.15	128.60
2	B	1236	G	C5-C6-N1	-7.42	107.79	111.50
2	B	945	A	C2-N3-C4	-7.42	106.89	110.60
2	B	1355	G	N1-C6-O6	7.42	124.35	119.90
2	EB	1614	A	O5'-P-OP2	-7.40	99.04	105.70
1	A	112	G	N1-C6-O6	7.40	124.34	119.90
2	B	2502	G	C5-C6-O6	-7.38	124.17	128.60
2	B	1780	A	C8-N9-C4	7.38	108.75	105.80
2	B	1021	A	N1-C2-N3	7.37	132.99	129.30
2	EB	1602	U	C6-N1-C2	-7.36	116.58	121.00
2	EB	1788	C	OP1-P-O3'	7.36	121.39	105.20
2	EB	391	G	C6-C5-N7	-7.35	125.99	130.40
2	B	195	A	C5-N7-C8	-7.34	100.23	103.90
2	B	1762	A	C8-N9-C4	-7.34	102.86	105.80
2	B	1193	G	C5-C6-N1	-7.33	107.83	111.50
2	EB	512	G	O4'-C1'-N9	7.33	114.07	108.20
1	A	117	G	N9-C4-C5	-7.33	102.47	105.40
2	B	1271	G	N1-C6-O6	7.33	124.30	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1762	A	C6-N1-C2	7.32	122.99	118.60
2	B	2698	U	C6-N1-C2	-7.31	116.61	121.00
2	EB	2088	G	N1-C6-O6	7.31	124.29	119.90
2	EB	527	C	C6-N1-C1'	-7.31	112.03	120.80
2	EB	1756	G	C5-C6-N1	-7.30	107.85	111.50
2	EB	2052	G	C5-C6-O6	-7.30	124.22	128.60
2	EB	16	G	N1-C6-O6	7.29	124.28	119.90
2	B	512	G	O4'-C1'-N9	7.28	114.03	108.20
2	EB	305	U	N3-C4-C5	-7.28	110.23	114.60
2	B	2056	G	C4-C5-N7	7.28	113.71	110.80
2	EB	2641	G	C8-N9-C4	7.28	109.31	106.40
2	B	2491	U	C5-C4-O4	-7.27	121.54	125.90
2	B	921	G	C5-C6-N1	-7.26	107.87	111.50
2	B	1319	G	N1-C6-O6	7.25	124.25	119.90
2	B	2698	U	N3-C4-C5	-7.25	110.25	114.60
1	DB	372	C	C6-N1-C2	7.24	123.20	120.30
2	EB	804	A	C8-N9-C4	7.23	108.69	105.80
2	B	1664	A	C8-N9-C4	-7.23	102.91	105.80
2	B	1602	U	N1-C2-N3	7.22	119.23	114.90
2	B	1532	C	C6-N1-C2	-7.22	117.41	120.30
1	A	509	A	C8-N9-C4	-7.21	102.91	105.80
2	EB	128	C	C6-N1-C2	7.21	123.19	120.30
2	EB	1698	A	C2-N3-C4	-7.21	107.00	110.60
2	B	1024	G	C4-C5-N7	7.21	113.68	110.80
2	EB	939	G	N1-C6-O6	7.21	124.22	119.90
2	EB	1816	G	N1-C6-O6	7.20	124.22	119.90
2	B	123	G	C8-N9-C4	7.20	109.28	106.40
2	EB	1327	C	N3-C4-C5	-7.19	119.02	121.90
1	DB	351	G	OP2-P-O3'	7.18	121.00	105.20
2	B	1381	G	C5-C6-N1	-7.18	107.91	111.50
2	EB	1840	G	N1-C6-O6	7.17	124.20	119.90
2	EB	1671	U	C5-C6-N1	7.17	126.29	122.70
2	B	1964	G	C8-N9-C4	7.17	109.27	106.40
2	EB	1646	C	C6-N1-C2	7.17	123.17	120.30
2	EB	1703	G	N1-C6-O6	7.15	124.19	119.90
2	EB	2010	G	C8-N9-C4	-7.14	103.54	106.40
2	B	383	U	N3-C2-O2	-7.14	117.20	122.20
2	EB	733	G	C8-N9-C4	-7.14	103.54	106.40
2	EB	1603	A	O5'-P-OP2	-7.13	99.28	105.70
2	B	1366	A	N1-C2-N3	7.13	132.86	129.30
2	EB	2489	G	C5-C6-O6	-7.12	124.33	128.60
2	EB	2505	G	C4-C5-N7	-7.12	107.95	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	EB	450	G	N1-C6-O6	7.11	124.17	119.90
2	B	2059	A	N1-C6-N6	7.11	122.86	118.60
2	EB	569	U	N1-C2-O2	7.11	127.77	122.80
2	B	2271	G	C4-C5-C6	7.10	123.06	118.80
2	B	2061	G	C5-C6-N1	-7.10	107.95	111.50
2	B	2449	U	N3-C4-O4	7.10	124.37	119.40
2	B	2489	G	N1-C6-O6	7.10	124.16	119.90
2	B	527	C	C6-N1-C1'	-7.08	112.30	120.80
2	B	777	A	C5-N7-C8	-7.08	100.36	103.90
2	B	2232	U	N3-C4-C5	-7.08	110.35	114.60
2	EB	1271	G	O5'-P-OP2	-7.08	99.33	105.70
2	B	1154	G	N1-C6-O6	7.07	124.14	119.90
2	B	70	G	N1-C6-O6	7.07	124.14	119.90
2	B	2447	G	C6-C5-N7	-7.07	126.16	130.40
1	DB	1232	U	C5-C6-N1	7.07	126.23	122.70
2	B	2249	U	C2-N3-C4	7.06	131.24	127.00
2	EB	2061	G	O5'-P-OP1	-7.06	99.34	105.70
2	B	869	G	C5-C6-N1	-7.06	107.97	111.50
1	DB	282	A	N1-C6-N6	7.06	122.83	118.60
1	DB	608	A	C8-N9-C4	7.05	108.62	105.80
2	EB	1828	G	C5-C6-N1	-7.05	107.97	111.50
2	B	2612	C	OP1-P-OP2	-7.05	109.03	119.60
2	EB	2509	G	N1-C6-O6	7.05	124.13	119.90
1	DB	842	C	C6-N1-C2	-7.05	117.48	120.30
2	EB	528	A	C6-N1-C2	7.05	122.83	118.60
2	B	775	G	N1-C6-O6	-7.04	115.67	119.90
2	EB	1142(B)	A	N3-C4-C5	7.04	131.73	126.80
2	B	1210	A	C8-N9-C4	-7.04	102.98	105.80
2	EB	2544	G	C6-C5-N7	-7.03	126.18	130.40
2	B	2330	G	N1-C6-O6	7.02	124.11	119.90
1	A	562	C	C6-N1-C2	7.02	123.11	120.30
2	EB	2489	G	N1-C6-O6	7.01	124.11	119.90
2	EB	1190	G	N1-C6-O6	7.00	124.10	119.90
2	B	191	A	N9-C4-C5	6.99	108.60	105.80
2	EB	2053	G	N9-C4-C5	-6.99	102.60	105.40
2	EB	2218	G	N1-C6-O6	6.98	124.09	119.90
2	EB	2612	C	OP1-P-OP2	-6.98	109.13	119.60
2	EB	68	G	C5-C6-N1	-6.98	108.01	111.50
1	A	1495	U	N3-C4-C5	-6.97	110.42	114.60
1	DB	818	G	N3-C4-N9	-6.97	121.81	126.00
2	EB	2022	U	N1-C2-N3	-6.97	110.72	114.90
1	A	117	G	C6-C5-N7	-6.96	126.22	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	450	G	C6-C5-N7	-6.96	126.22	130.40
2	EB	1762	A	C5-C6-N6	6.96	129.27	123.70
2	B	1838	C	C6-N1-C2	6.96	123.08	120.30
1	DB	576	G	N1-C6-O6	6.96	124.08	119.90
2	B	2593	U	N1-C2-N3	6.96	119.07	114.90
2	EB	2358	G	N1-C6-O6	-6.95	115.73	119.90
2	EB	2838	G	N1-C6-O6	6.95	124.07	119.90
2	B	120	U	O5'-P-OP2	6.95	119.04	110.70
2	B	859	G	C8-N9-C4	6.95	109.18	106.40
1	DB	509	A	C8-N9-C4	-6.95	103.02	105.80
2	EB	568	U	N3-C4-C5	-6.95	110.43	114.60
2	EB	265	A	N1-C6-N6	6.95	122.77	118.60
2	B	520	G	C5-C6-O6	-6.94	124.43	128.60
2	B	576	U	O5'-P-OP1	6.94	119.03	110.70
2	EB	2791	C	C6-N1-C2	-6.94	117.52	120.30
2	EB	195	A	C4-C5-C6	-6.94	113.53	117.00
2	B	1823	G	N1-C6-O6	6.92	124.05	119.90
2	B	2610	C	N1-C2-N3	-6.92	114.36	119.20
2	B	865	C	N3-C4-C5	6.92	124.67	121.90
2	B	869	G	N1-C6-O6	6.91	124.05	119.90
2	B	2053	G	C6-C5-N7	-6.91	126.25	130.40
2	EB	1395	A	O4'-C1'-N9	6.91	113.73	108.20
2	B	1366	A	C8-N9-C4	-6.90	103.04	105.80
2	B	939	G	N1-C6-O6	6.90	124.04	119.90
2	B	2248	C	O5'-P-OP1	-6.90	99.49	105.70
2	B	528	A	N1-C6-N6	6.90	122.74	118.60
2	B	1255	U	N1-C2-O2	6.89	127.63	122.80
1	DB	899	C	C5-C6-N1	6.89	124.45	121.00
2	EB	571	A	O5'-P-OP2	-6.89	99.50	105.70
2	B	2592	G	N7-C8-N9	6.89	116.55	113.10
2	EB	711	G	N1-C6-O6	6.89	124.03	119.90
2	B	2419	U	N3-C4-C5	-6.89	110.47	114.60
2	B	775	G	N7-C8-N9	-6.89	109.66	113.10
2	B	1814	G	C4-C5-C6	6.89	122.93	118.80
2	B	2439	A	C2-N3-C4	-6.88	107.16	110.60
2	B	570	G	C5-C6-O6	6.88	132.72	128.60
2	B	1624	G	N1-C6-O6	6.87	124.02	119.90
2	EB	1660	C	C6-N1-C2	-6.87	117.55	120.30
2	EB	1992	G	P-O3'-C3'	6.86	127.94	119.70
2	B	2249	U	N3-C4-O4	6.86	124.20	119.40
2	EB	323	G	N1-C6-O6	6.86	124.02	119.90
2	B	575	A	C6-N1-C2	-6.86	114.48	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2597	G	O5'-P-OP1	6.86	118.93	110.70
2	B	220	G	C5-C6-N1	-6.85	108.07	111.50
2	EB	764	A	N1-C6-N6	6.85	122.71	118.60
2	B	2265	U	N3-C2-O2	-6.85	117.41	122.20
2	B	1215	G	N1-C6-O6	6.84	124.01	119.90
3	C	108	C	C6-N1-C2	6.84	123.04	120.30
2	B	770	G	C5-C6-O6	-6.84	124.49	128.60
2	B	948	G	O5'-P-OP1	6.84	118.91	110.70
1	DB	1467	G	O5'-P-OP2	-6.84	99.55	105.70
2	EB	2072	G	N9-C4-C5	-6.83	102.67	105.40
2	B	1125	G	N1-C6-O6	6.83	124.00	119.90
2	B	832	G	N1-C6-O6	6.83	124.00	119.90
2	EB	596	G	C5-C6-N1	-6.83	108.09	111.50
2	B	450	G	C4-N9-C1'	6.83	135.37	126.50
2	B	790	C	N3-C4-C5	-6.82	119.17	121.90
2	EB	2508	G	C8-N9-C4	6.82	109.13	106.40
2	B	1298	C	O5'-P-OP1	-6.82	99.56	105.70
2	EB	2436	G	N3-C2-N2	-6.82	115.13	119.90
2	B	801	G	N1-C2-N3	6.82	127.99	123.90
2	EB	827	U	O5'-P-OP1	6.82	118.88	110.70
1	DB	1522	U	C6-N1-C2	-6.82	116.91	121.00
2	EB	2505	G	N9-C4-C5	6.82	108.13	105.40
2	B	527	C	N1-C2-O2	6.81	122.99	118.90
2	B	593	G	C5-C6-N1	-6.81	108.09	111.50
2	EB	1769	G	N1-C6-O6	6.81	123.99	119.90
1	A	529	G	C6-C5-N7	-6.81	126.31	130.40
2	B	2061	G	O5'-P-OP1	-6.81	99.57	105.70
2	B	577	G	N1-C6-O6	6.81	123.98	119.90
2	EB	259	G	N1-C6-O6	6.80	123.98	119.90
2	B	2053	G	N9-C4-C5	-6.80	102.68	105.40
2	B	2430	A	N9-C4-C5	6.80	108.52	105.80
2	EB	1762	A	C5-C6-N1	-6.80	114.30	117.70
2	B	2544	G	C6-C5-N7	-6.80	126.32	130.40
4	IA	1	C	N1-C2-O2	6.80	122.98	118.90
2	B	1297	C	C6-N1-C2	-6.79	117.58	120.30
2	EB	2304	G	N3-C4-N9	-6.79	121.93	126.00
2	B	827	U	O5'-P-OP1	6.78	118.84	110.70
2	EB	526	A	O5'-P-OP2	-6.78	99.59	105.70
2	EB	528	A	C4-C5-N7	6.78	114.09	110.70
2	EB	2064	C	N1-C2-O2	-6.78	114.83	118.90
1	A	1522	U	N3-C4-C5	-6.78	110.53	114.60
2	EB	787	U	O5'-P-OP2	-6.77	99.61	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1240	U	N1-C2-N3	6.77	118.96	114.90
1	DB	1495	U	N3-C4-C5	-6.77	110.54	114.60
2	EB	795	C	C6-N1-C2	-6.77	117.59	120.30
1	DB	1504	G	O5'-P-OP1	-6.76	99.61	105.70
2	EB	2053	G	N3-C2-N2	-6.76	115.17	119.90
2	B	35	G	N1-C6-O6	6.76	123.96	119.90
2	B	2028	U	C4-C5-C6	6.76	123.76	119.70
2	EB	494	G	N1-C6-O6	6.76	123.95	119.90
2	B	559	G	N1-C6-O6	6.75	123.95	119.90
2	B	2509	G	N1-C6-O6	6.75	123.95	119.90
1	DB	144	G	N1-C6-O6	6.75	123.95	119.90
2	B	2717	G	N1-C6-O6	6.75	123.95	119.90
2	EB	2580	U	C5-C4-O4	6.75	129.95	125.90
2	EB	2714	G	O5'-P-OP2	6.74	118.79	110.70
2	B	1628	G	C5-C6-N1	-6.74	108.13	111.50
2	EB	569	U	C2-N1-C1'	6.73	125.78	117.70
2	B	761	A	C4-C5-N7	6.73	114.06	110.70
2	B	2545	G	C5-C6-N1	-6.73	108.14	111.50
2	B	1244	G	N1-C6-O6	6.73	123.94	119.90
2	B	2011	U	N1-C2-O2	-6.72	118.09	122.80
1	A	1452	C	C5-C6-N1	6.72	124.36	121.00
1	DB	1099	G	C5-C6-O6	6.72	132.63	128.60
1	A	1481	U	N3-C4-C5	-6.72	110.57	114.60
2	B	2232	U	C5-C4-O4	6.72	129.93	125.90
2	B	1869	G	N3-C4-C5	6.71	131.96	128.60
2	B	1142(B)	A	C4-C5-N7	6.71	114.06	110.70
2	EB	2037	G	N1-C6-O6	6.70	123.92	119.90
2	EB	1762	A	N9-C4-C5	6.70	108.48	105.80
2	EB	2032	G	N1-C6-O6	6.70	123.92	119.90
2	B	2072	G	C4-C5-N7	6.70	113.48	110.80
2	B	1310	G	N1-C6-O6	6.70	123.92	119.90
2	EB	409	C	O5'-P-OP1	6.69	118.73	110.70
2	EB	1142(B)	A	C5-N7-C8	-6.69	100.56	103.90
2	EB	1823	G	N1-C6-O6	6.68	123.91	119.90
2	B	2318	G	O4'-C1'-N9	6.68	113.54	108.20
2	B	945	A	C5-C6-N6	-6.67	118.36	123.70
2	B	472	A	N1-C2-N3	6.67	132.64	129.30
2	EB	140	A	C5-N7-C8	-6.67	100.56	103.90
2	B	2037	G	N1-C6-O6	6.67	123.90	119.90
2	EB	305	U	C5-C4-O4	6.66	129.90	125.90
2	B	566	U	N3-C4-C5	6.66	118.59	114.60
2	EB	695	G	C5-C6-N1	-6.66	108.17	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	82	G	C5-C6-N1	-6.66	108.17	111.50
2	EB	776	G	C5-C6-O6	6.65	132.59	128.60
2	B	733	G	C8-N9-C4	-6.65	103.74	106.40
2	EB	1310	G	N1-C6-O6	6.65	123.89	119.90
2	EB	2271	G	C4-C5-C6	6.65	122.79	118.80
2	B	2053	G	N3-C2-N2	-6.65	115.25	119.90
2	EB	534	U	N3-C4-C5	-6.65	110.61	114.60
2	EB	1840	G	C5-C6-N1	-6.65	108.18	111.50
2	B	820	A	N1-C6-N6	-6.65	114.61	118.60
2	B	1327	C	C6-N1-C2	-6.64	117.64	120.30
2	B	2820	A	C8-N9-C4	-6.64	103.14	105.80
2	B	2614	A	C6-N1-C2	-6.64	114.62	118.60
2	EB	1240	U	N3-C2-O2	-6.64	117.55	122.20
2	B	865	C	N1-C2-N3	-6.63	114.56	119.20
2	B	40	C	C6-N1-C2	6.63	122.95	120.30
2	EB	2429	G	OP2-P-O3'	6.63	119.78	105.20
2	B	461	C	C4-C5-C6	6.62	120.71	117.40
2	B	304	G	C4-C5-N7	-6.62	108.15	110.80
2	B	751	A	N1-C6-N6	-6.62	114.63	118.60
2	B	1762	A	C5-C6-N1	-6.62	114.39	117.70
2	EB	2502	G	C6-C5-N7	-6.62	126.43	130.40
2	B	2689	U	N3-C2-O2	-6.61	117.57	122.20
2	B	751	A	N9-C4-C5	6.61	108.44	105.80
2	B	122	G	N1-C6-O6	6.61	123.87	119.90
2	B	1024	G	C5-N7-C8	-6.61	101.00	104.30
2	B	2719	G	N1-C6-O6	6.61	123.87	119.90
2	B	58	G	C5-C6-N1	-6.61	108.20	111.50
2	B	1566	A	C2-N3-C4	-6.60	107.30	110.60
2	EB	197	A	C8-N9-C4	-6.60	103.16	105.80
2	EB	2544	G	C5-C6-O6	-6.60	124.64	128.60
1	DB	754	C	C6-N1-C1'	-6.59	112.89	120.80
2	EB	1698	A	C5-N7-C8	-6.59	100.60	103.90
2	B	592	G	N1-C6-O6	6.59	123.86	119.90
2	B	935	C	C6-N1-C2	6.59	122.94	120.30
2	B	2508	G	N1-C6-O6	6.59	123.85	119.90
1	DB	1303	C	C6-N1-C2	-6.59	117.66	120.30
2	EB	267	C	C6-N1-C2	6.59	122.94	120.30
1	A	1303	C	C6-N1-C2	-6.58	117.67	120.30
2	B	451	C	C6-N1-C2	6.58	122.93	120.30
2	EB	391	G	C8-N9-C1'	-6.58	118.44	127.00
2	EB	528	A	C2-N3-C4	-6.58	107.31	110.60
2	B	1992	G	P-O3'-C3'	6.58	127.59	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2782	G	N1-C6-O6	6.58	123.84	119.90
1	DB	1522	U	N3-C4-C5	-6.58	110.66	114.60
2	EB	2575	C	O5'-P-OP1	-6.58	99.78	105.70
2	EB	531	C	C6-N1-C2	6.57	122.93	120.30
2	B	248	G	C4-C5-N7	6.57	113.43	110.80
2	B	1779	U	C2-N1-C1'	6.56	125.57	117.70
2	B	35	G	C5-C6-O6	-6.55	124.67	128.60
2	B	1936	A	C5-C6-N6	-6.55	118.46	123.70
2	EB	1215	G	N1-C6-O6	6.55	123.83	119.90
1	DB	240	C	C6-N1-C2	-6.55	117.68	120.30
1	A	351	G	OP2-P-O3'	6.55	119.60	105.20
2	B	929	G	C5-C6-N1	-6.55	108.23	111.50
2	B	2641	G	N7-C8-N9	-6.55	109.83	113.10
2	B	2447	G	C8-N9-C4	6.54	109.02	106.40
2	B	2091	U	N3-C4-C5	-6.54	110.67	114.60
1	A	240	C	C6-N1-C2	-6.54	117.68	120.30
2	EB	1240	U	C6-N1-C2	-6.54	117.08	121.00
2	B	569	U	N1-C2-O2	6.54	127.38	122.80
2	B	2020	A	C6-N1-C2	-6.54	114.68	118.60
2	EB	747	U	C6-N1-C2	6.53	124.92	121.00
1	A	529	G	C4-C5-N7	6.53	113.41	110.80
2	EB	2570	G	N1-C6-O6	6.53	123.82	119.90
2	EB	943	U	O5'-P-OP1	-6.53	99.83	105.70
2	EB	2689	U	N3-C2-O2	-6.52	117.63	122.20
2	B	446	G	C8-N9-C4	6.52	109.01	106.40
2	EB	2614	A	OP1-P-O3'	6.52	119.54	105.20
2	B	1365	A	N1-C6-N6	6.52	122.51	118.60
2	B	2532	G	N1-C6-O6	6.52	123.81	119.90
2	EB	248	G	C5-C6-O6	-6.52	124.69	128.60
2	EB	783	A	N9-C4-C5	6.51	108.41	105.80
2	B	770	G	N1-C6-O6	6.51	123.81	119.90
2	B	2593	U	C2-N3-C4	6.51	130.91	127.00
2	B	1992	G	N1-C6-O6	-6.51	116.00	119.90
1	DB	568	G	C8-N9-C4	-6.50	103.80	106.40
1	DB	793	U	N1-C2-O2	-6.50	118.25	122.80
2	B	1841	U	N3-C4-C5	-6.50	110.70	114.60
2	B	1699	G	C5-C6-O6	6.49	132.50	128.60
2	B	1560	G	N1-C6-O6	6.49	123.80	119.90
2	EB	2287	A	C2-N3-C4	-6.49	107.36	110.60
2	EB	191	A	N9-C4-C5	6.49	108.39	105.80
2	EB	2271	G	N1-C6-O6	6.49	123.79	119.90
2	B	2341	G	C5-C6-N1	-6.48	108.26	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	EB	270(B)	A	C8-N9-C4	-6.48	103.21	105.80
2	EB	1699	G	C8-N9-C4	-6.48	103.81	106.40
2	B	305	U	N3-C4-C5	-6.48	110.72	114.60
2	B	2458	G	C6-C5-N7	-6.47	126.52	130.40
2	EB	1271	G	N1-C6-O6	6.47	123.78	119.90
2	EB	1780	A	N9-C4-C5	-6.47	103.21	105.80
2	EB	2593	U	C4-C5-C6	6.47	123.58	119.70
2	EB	831	G	C5-C6-N1	-6.47	108.27	111.50
1	DB	326	G	C4-C5-N7	-6.46	108.22	110.80
2	EB	304	G	C4-C5-N7	-6.45	108.22	110.80
2	EB	701	G	N1-C6-O6	6.44	123.77	119.90
2	EB	832	G	N1-C6-O6	6.44	123.76	119.90
2	EB	1231	G	C5-C6-N1	-6.44	108.28	111.50
1	A	1054	C	N3-C4-C5	-6.44	119.33	121.90
2	B	203	C	O5'-P-OP2	6.44	118.42	110.70
2	B	1698	A	N7-C8-N9	6.43	117.02	113.80
2	B	1137	G	N1-C6-O6	6.43	123.76	119.90
2	EB	2232	U	N3-C4-C5	-6.43	110.74	114.60
2	B	375	C	O5'-P-OP1	6.43	118.42	110.70
1	DB	1432	G	N1-C6-O6	6.43	123.76	119.90
2	EB	2415	G	C5-C6-N1	-6.42	108.29	111.50
1	DB	529	G	C6-C5-N7	-6.42	126.55	130.40
2	EB	122	G	N1-C6-O6	6.42	123.75	119.90
2	B	713	G	C5-C6-N1	-6.42	108.29	111.50
2	EB	2698	U	N3-C4-C5	-6.42	110.75	114.60
2	B	391	G	C4-N9-C1'	6.41	134.84	126.50
2	B	1703	G	C5-C6-N1	-6.41	108.29	111.50
1	DB	541	G	N1-C6-O6	6.41	123.75	119.90
2	B	699	A	C5-C6-N6	-6.41	118.57	123.70
2	B	2321	G	C8-N9-C4	-6.41	103.84	106.40
2	EB	123	G	N1-C6-O6	6.41	123.75	119.90
1	A	781	A	C8-N9-C4	6.41	108.36	105.80
2	B	1427	A	C8-N9-C4	6.41	108.36	105.80
2	B	1558	A	N3-C4-C5	6.41	131.28	126.80
2	EB	1633	G	C5-C6-N1	-6.41	108.30	111.50
2	EB	1780	A	C2-N3-C4	-6.40	107.40	110.60
2	EB	1936	A	C4-C5-N7	6.40	113.90	110.70
2	B	2570	G	N1-C6-O6	6.39	123.73	119.90
1	DB	242	C	C6-N1-C2	6.39	122.86	120.30
2	EB	504	U	C5-C6-N1	6.39	125.89	122.70
1	DB	789	U	C6-N1-C2	-6.39	117.17	121.00
1	DB	1069	C	C6-N1-C2	-6.39	117.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DB	562	C	C6-N1-C2	6.38	122.85	120.30
2	EB	1190	G	C5-C6-O6	-6.38	124.77	128.60
2	B	2447	G	N9-C4-C5	-6.38	102.85	105.40
2	EB	527	C	N1-C2-O2	6.38	122.73	118.90
2	EB	1783	A	C2-N3-C4	-6.38	107.41	110.60
2	B	1382	G	C5-C6-N1	-6.37	108.31	111.50
2	B	2543	G	N1-C6-O6	-6.37	116.08	119.90
2	B	528	A	N7-C8-N9	6.37	116.99	113.80
1	DB	870	U	C6-N1-C2	6.37	124.82	121.00
2	EB	570	G	C4-C5-C6	6.37	122.62	118.80
2	B	1216	G	N1-C6-O6	6.37	123.72	119.90
2	B	569	U	C2-N1-C1'	6.37	125.34	117.70
2	EB	379	G	C5-C6-N1	-6.37	108.32	111.50
2	B	2574	G	O5'-P-OP2	-6.37	99.97	105.70
2	EB	1187	G	C6-C5-N7	-6.37	126.58	130.40
4	LC	1	C	N1-C2-O2	6.37	122.72	118.90
2	EB	1326	U	OP2-P-O3'	6.36	119.20	105.20
2	EB	2709	G	C5-C6-N1	-6.36	108.32	111.50
2	B	178	G	C5-C6-N1	-6.36	108.32	111.50
1	DB	1435	G	N1-C6-O6	6.36	123.72	119.90
2	EB	2061	G	C5-C6-N1	-6.36	108.32	111.50
2	B	337	C	C5-C6-N1	-6.36	117.82	121.00
2	B	861	A	OP2-P-O3'	6.36	119.19	105.20
2	B	1558	A	N9-C4-C5	-6.36	103.26	105.80
2	B	124	G	N1-C6-O6	6.36	123.71	119.90
2	B	783	A	C8-N9-C4	-6.35	103.26	105.80
2	B	1331	A	C2-N3-C4	-6.35	107.42	110.60
1	A	773	G	N1-C6-O6	6.35	123.71	119.90
2	B	115	C	C5-C6-N1	-6.35	117.83	121.00
2	EB	1138	G	N3-C4-C5	-6.35	125.43	128.60
2	B	194	G	N1-C2-N3	6.35	127.71	123.90
2	B	688	U	C5-C6-N1	6.35	125.87	122.70
2	B	2429	G	OP2-P-O3'	6.34	119.16	105.20
2	EB	2861	G	N1-C6-O6	6.34	123.71	119.90
2	EB	576	U	O5'-P-OP2	-6.34	99.99	105.70
2	EB	945	A	C4-C5-N7	6.34	113.87	110.70
2	B	2698	U	N1-C2-N3	6.34	118.70	114.90
2	B	1259	G	C5-C6-O6	-6.34	124.80	128.60
2	EB	783	A	C8-N9-C4	-6.34	103.27	105.80
2	EB	1790	C	C5-C4-N4	6.34	124.64	120.20
2	EB	2026	C	C6-N1-C2	6.33	122.83	120.30
2	B	583	G	C8-N9-C4	-6.33	103.87	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1828	G	N1-C6-O6	-6.33	116.10	119.90
2	EB	197	A	O5'-P-OP1	6.33	118.29	110.70
2	EB	2714	G	O5'-P-OP1	-6.33	100.00	105.70
1	A	1503	A	N1-C6-N6	-6.32	114.81	118.60
2	B	186	G	N1-C6-O6	6.32	123.69	119.90
2	B	1377	G	N3-C4-C5	-6.32	125.44	128.60
2	B	1936	A	O5'-P-OP2	-6.32	100.01	105.70
2	EB	2570	G	N3-C2-N2	-6.32	115.47	119.90
2	EB	1965	C	C6-N1-C2	6.32	122.83	120.30
2	EB	2556	C	N1-C2-O2	6.32	122.69	118.90
2	B	663	G	C5-C6-N1	-6.31	108.34	111.50
2	EB	1898	U	N3-C4-C5	-6.31	110.81	114.60
2	B	687	C	N3-C4-C5	-6.31	119.38	121.90
2	EB	1828	G	N3-C4-N9	-6.31	122.22	126.00
1	DB	117	G	N9-C4-C5	-6.30	102.88	105.40
2	EB	2030	A	C8-N9-C4	6.29	108.32	105.80
2	B	526	A	O5'-P-OP2	-6.29	100.04	105.70
2	B	2452	C	N3-C4-N4	6.29	122.40	118.00
2	EB	769	G	C5-C6-O6	-6.29	124.83	128.60
2	B	1825	A	C8-N9-C4	-6.29	103.28	105.80
2	B	191	A	N1-C2-N3	6.29	132.44	129.30
2	EB	2685	G	C4-C5-N7	-6.29	108.28	110.80
2	B	839	U	C5-C4-O4	6.29	129.67	125.90
2	EB	2055	C	OP2-P-O3'	6.29	119.03	105.20
2	EB	1348	G	N1-C6-O6	6.29	123.67	119.90
1	A	1485	U	C5-C6-N1	-6.28	119.56	122.70
2	B	648	G	C5-C6-N1	-6.28	108.36	111.50
2	B	2250	G	O5'-P-OP2	-6.28	100.05	105.70
2	EB	197	A	OP2-P-O3'	6.28	119.02	105.20
2	EB	948	G	C5-C6-N1	-6.28	108.36	111.50
2	B	138	G	N1-C6-O6	6.28	123.67	119.90
2	B	1325	G	N1-C2-N2	-6.28	110.55	116.20
2	B	2838	G	C6-C5-N7	-6.28	126.63	130.40
1	DB	1099	G	N1-C6-O6	-6.27	116.14	119.90
2	EB	663	G	C5-C6-N1	-6.27	108.36	111.50
2	EB	919	G	N1-C6-O6	6.27	123.66	119.90
2	B	249	C	C6-N1-C2	6.27	122.81	120.30
2	EB	1620	G	N1-C6-O6	6.26	123.66	119.90
1	A	754	C	C6-N1-C1'	-6.26	113.28	120.80
2	B	1323	U	N3-C4-O4	6.26	123.78	119.40
2	B	1325	G	N3-C4-C5	-6.26	125.47	128.60
2	B	1366	A	C4-C5-C6	6.26	120.13	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2331	G	C5-C6-N1	-6.26	108.37	111.50
2	EB	1366	A	N1-C2-N3	6.26	132.43	129.30
2	B	1828	G	N7-C8-N9	6.26	116.23	113.10
3	C	52	A	N1-C6-N6	6.26	122.36	118.60
4	IA	29	G	N1-C6-O6	6.26	123.66	119.90
2	EB	1356	G	C5-C6-N1	-6.26	108.37	111.50
1	DB	372	C	N3-C4-C5	6.26	124.40	121.90
2	B	510	C	O5'-P-OP2	-6.26	100.07	105.70
2	B	2039	C	N3-C4-C5	-6.26	119.40	121.90
2	EB	1024	G	C4-C5-N7	6.26	113.30	110.80
2	B	761	A	N3-C4-C5	6.25	131.18	126.80
2	B	1193	G	N1-C6-O6	6.25	123.65	119.90
2	B	1898	U	C5-C4-O4	6.25	129.65	125.90
2	B	1779	U	C5-C4-O4	-6.25	122.15	125.90
1	DB	376	G	N1-C6-O6	6.25	123.65	119.90
4	IA	75	C	OP2-P-O3'	6.25	118.94	105.20
1	DB	650	G	C5-C6-N1	-6.25	108.38	111.50
2	B	2580	U	C5-C4-O4	6.24	129.65	125.90
2	B	326	G	C5-C6-N1	-6.24	108.38	111.50
2	B	1024	G	N7-C8-N9	6.24	116.22	113.10
2	B	1333	C	N3-C4-C5	6.24	124.39	121.90
2	EB	570	G	C5-C6-O6	6.24	132.34	128.60
2	B	2546	U	N3-C4-C5	-6.24	110.86	114.60
1	A	754	C	N3-C2-O2	-6.24	117.53	121.90
2	B	391	G	C8-N9-C1'	-6.23	118.90	127.00
1	DB	293	G	C6-C5-N7	-6.23	126.66	130.40
1	A	28	G	C8-N9-C4	-6.23	103.91	106.40
2	B	83	G	N1-C6-O6	6.23	123.64	119.90
2	B	1314	C	C6-N1-C2	-6.23	117.81	120.30
1	DB	27	G	N1-C6-O6	6.23	123.64	119.90
2	EB	1828	G	C4-C5-N7	-6.23	108.31	110.80
2	EB	1602	U	N1-C2-N3	6.22	118.63	114.90
2	EB	2582	G	C8-N9-C4	-6.22	103.91	106.40
2	B	383	U	N1-C2-O2	6.22	127.16	122.80
2	B	713	G	N1-C6-O6	6.22	123.63	119.90
2	EB	2773	C	C6-N1-C2	6.22	122.79	120.30
2	B	2073	C	N1-C2-N3	6.22	123.55	119.20
2	B	2599	G	N3-C4-N9	-6.22	122.27	126.00
1	A	1504	G	O5'-P-OP1	-6.21	100.11	105.70
1	A	1397	C	O4'-C1'-N1	6.21	113.17	108.20
1	DB	773	G	N1-C6-O6	6.21	123.62	119.90
2	B	1790	C	C2-N1-C1'	-6.21	111.97	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DB	804	U	C5-C4-O4	6.20	129.62	125.90
2	EB	124	G	C5-C6-N1	-6.20	108.40	111.50
2	EB	921	G	C5-C6-N1	-6.20	108.40	111.50
2	EB	1628	G	C5-C6-N1	-6.20	108.40	111.50
1	A	232	G	N1-C6-O6	6.20	123.62	119.90
2	EB	2318	G	O4'-C1'-N9	6.20	113.16	108.20
2	EB	1332	G	O5'-P-OP2	-6.20	100.12	105.70
2	B	601	C	N3-C4-C5	-6.19	119.42	121.90
2	EB	1429	G	N9-C4-C5	6.19	107.88	105.40
2	B	2502	G	C4-C5-N7	6.19	113.28	110.80
2	B	1979	C	C6-N1-C2	-6.19	117.83	120.30
2	EB	2061	G	C6-C5-N7	-6.19	126.69	130.40
2	EB	2576	G	O5'-P-OP2	-6.19	100.13	105.70
2	B	748	G	N3-C4-C5	-6.18	125.51	128.60
1	DB	529	G	C4-C5-N7	6.18	113.27	110.80
2	B	2415	G	N1-C6-O6	6.18	123.61	119.90
1	DB	880	C	C6-N1-C2	6.18	122.77	120.30
2	EB	1377	G	N3-C4-C5	-6.18	125.51	128.60
2	B	409	C	O5'-P-OP2	-6.18	100.14	105.70
2	EB	865	C	N3-C4-C5	6.18	124.37	121.90
1	DB	331	G	N7-C8-N9	6.18	116.19	113.10
1	A	886	G	C5-C6-N1	-6.17	108.41	111.50
2	B	2037	G	C5-C6-O6	-6.17	124.89	128.60
2	B	2061	G	O5'-P-OP2	6.17	118.11	110.70
1	DB	148	G	N1-C6-O6	6.17	123.60	119.90
2	EB	1142(B)	A	C4-C5-N7	6.17	113.78	110.70
2	B	1661	G	N1-C6-O6	6.17	123.60	119.90
2	EB	1558	A	C2-N3-C4	-6.17	107.52	110.60
2	EB	2822	G	O5'-P-OP1	-6.17	100.15	105.70
2	B	775	G	C8-N9-C4	6.17	108.87	106.40
2	B	1395	A	O4'-C1'-N9	6.17	113.13	108.20
2	B	2083	G	C5-C6-N1	-6.17	108.42	111.50
3	FB	87	G	C8-N9-C4	6.17	108.87	106.40
1	DB	1532	U	C2-N1-C1'	6.16	125.09	117.70
2	EB	672	C	C6-N1-C2	-6.16	117.83	120.30
2	EB	401	A	N1-C6-N6	-6.16	114.91	118.60
2	B	2726	U	C5-C6-N1	-6.15	119.62	122.70
2	B	1698	A	C5-N7-C8	-6.15	100.82	103.90
2	EB	1672	C	C6-N1-C2	-6.15	117.84	120.30
2	B	140	A	C8-N9-C4	-6.15	103.34	105.80
2	B	1698	A	C8-N9-C4	-6.14	103.34	105.80
1	A	944	G	N1-C6-O6	-6.14	116.22	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	942	G	OP2-P-O3'	6.14	118.70	105.20
2	B	1402	C	C6-N1-C2	-6.13	117.85	120.30
2	B	2086	U	N3-C2-O2	-6.13	117.91	122.20
2	B	1368	G	C5-C6-O6	-6.13	124.92	128.60
2	B	2494	G	N9-C4-C5	-6.12	102.95	105.40
2	EB	751	A	N1-C6-N6	-6.12	114.93	118.60
2	B	534	U	C5-C4-O4	6.12	129.57	125.90
2	B	197	A	OP2-P-O3'	6.12	118.66	105.20
2	B	670	A	OP1-P-O3'	6.12	118.65	105.20
2	B	783	A	OP1-P-OP2	6.12	128.77	119.60
2	B	825	C	OP1-P-O3'	6.11	118.65	105.20
2	B	1981	A	C4-C5-N7	6.11	113.76	110.70
2	B	342	G	C5-C6-O6	-6.11	124.93	128.60
2	B	1142(B)	A	C5-C6-N1	-6.11	114.64	117.70
2	EB	2010	G	N7-C8-N9	6.11	116.16	113.10
2	EB	2043	C	C6-N1-C2	-6.11	117.86	120.30
2	EB	667	U	N3-C4-O4	6.11	123.68	119.40
2	EB	2224	G	C5-C6-N1	-6.11	108.45	111.50
2	B	939	G	C5-C6-N1	-6.11	108.45	111.50
2	B	2083	G	N1-C6-O6	6.11	123.56	119.90
2	EB	948	G	N1-C6-O6	6.11	123.56	119.90
2	B	1325	G	N3-C2-N2	6.11	124.17	119.90
2	B	1992	G	C8-N9-C4	-6.11	103.96	106.40
2	EB	945	A	N9-C4-C5	-6.11	103.36	105.80
2	B	305	U	C5-C4-O4	6.10	129.56	125.90
2	B	504	U	N1-C2-O2	6.10	127.07	122.80
2	B	1186	G	O5'-P-OP1	-6.10	100.21	105.70
2	B	194	G	C5-C6-N1	-6.10	108.45	111.50
2	B	870	A	C5-C6-N6	-6.10	118.82	123.70
2	B	1602	U	C5-C4-O4	6.10	129.56	125.90
2	EB	754	C	C6-N1-C2	6.10	122.74	120.30
2	B	802	A	C4-C5-C6	6.09	120.05	117.00
2	EB	2612	C	C6-N1-C2	6.09	122.74	120.30
1	A	1413	A	N1-C6-N6	-6.09	114.94	118.60
2	B	1185	C	OP2-P-O3'	6.09	118.60	105.20
2	B	1326	U	OP2-P-O3'	6.09	118.60	105.20
2	B	1024	G	C6-C5-N7	-6.09	126.75	130.40
2	B	486	C	C6-N1-C2	6.09	122.73	120.30
2	EB	379	G	N1-C6-O6	6.08	123.55	119.90
2	EB	2593	U	N1-C2-N3	6.08	118.55	114.90
2	B	1976	U	C4-C5-C6	6.08	123.35	119.70
2	B	1753	G	N1-C6-O6	-6.08	116.25	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1259	G	N1-C6-O6	6.08	123.55	119.90
2	EB	2228	G	N1-C6-O6	6.08	123.55	119.90
2	B	109	G	C8-N9-C4	6.07	108.83	106.40
2	B	1637	A	N1-C2-N3	6.07	132.34	129.30
1	DB	1531	A	C2-N3-C4	6.07	113.64	110.60
2	EB	2059	A	C8-N9-C4	6.07	108.23	105.80
2	EB	2610	C	N1-C2-N3	-6.07	114.95	119.20
2	B	2489	G	C5-C6-O6	-6.07	124.96	128.60
1	DB	331	G	N1-C6-O6	6.07	123.54	119.90
1	DB	842	C	N1-C2-O2	6.07	122.54	118.90
2	B	208	C	C6-N1-C2	6.07	122.73	120.30
31	EA	39	ARG	NE-CZ-NH1	6.07	123.33	120.30
2	EB	2419	U	N3-C4-O4	6.07	123.65	119.40
2	B	699	A	N1-C6-N6	6.07	122.24	118.60
2	B	1470	G	C5-C6-N1	-6.07	108.47	111.50
1	DB	899	C	C2-N3-C4	6.07	122.93	119.90
2	B	945	A	N3-C4-C5	6.06	131.04	126.80
2	B	2447	G	C5-C6-O6	-6.06	124.97	128.60
1	DB	48	C	C6-N1-C2	6.06	122.72	120.30
3	C	111	U	C5-C4-O4	6.05	129.53	125.90
2	EB	1251	C	N1-C2-O2	6.05	122.53	118.90
1	DB	754	C	N3-C2-O2	-6.05	117.66	121.90
1	A	1488	G	N1-C6-O6	6.05	123.53	119.90
2	B	761	A	C2-N3-C4	-6.05	107.57	110.60
2	B	758	C	C5-C6-N1	-6.05	117.97	121.00
2	B	978	G	N1-C6-O6	6.05	123.53	119.90
2	EB	404	C	C6-N1-C2	6.05	122.72	120.30
2	B	1790	C	O5'-P-OP2	6.05	117.95	110.70
2	EB	2453	A	O5'-P-OP2	6.05	117.96	110.70
2	B	569	U	N3-C2-O2	-6.04	117.97	122.20
2	EB	1807	G	C5-C6-N1	-6.04	108.48	111.50
2	B	1623	G	N1-C6-O6	6.04	123.52	119.90
1	A	1512	U	C5-C4-O4	6.04	129.52	125.90
2	EB	1698	A	N1-C6-N6	6.04	122.22	118.60
2	EB	2603	G	C8-N9-C4	6.04	108.81	106.40
2	B	122	G	N9-C4-C5	-6.03	102.99	105.40
2	B	855	G	N1-C6-O6	6.03	123.52	119.90
2	EB	1370	C	C6-N1-C2	6.03	122.71	120.30
1	A	945	G	N1-C6-O6	6.03	123.52	119.90
2	B	330	A	C8-N9-C4	6.03	108.21	105.80
2	B	1707	G	N1-C6-O6	6.03	123.52	119.90
2	EB	718	A	N1-C6-N6	6.02	122.21	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	265	A	C5-N7-C8	-6.02	100.89	103.90
2	B	724	U	N3-C4-C5	-6.02	110.99	114.60
2	B	1771	C	N1-C2-O2	-6.02	115.29	118.90
2	B	2414	G	N1-C6-O6	6.02	123.51	119.90
2	EB	1667	G	C5-C6-O6	-6.02	124.99	128.60
1	A	282	A	N1-C6-N6	6.01	122.21	118.60
2	EB	375	C	O5'-P-OP2	-6.01	100.29	105.70
2	B	787	U	O5'-P-OP1	6.01	117.91	110.70
2	B	2061	G	C6-C5-N7	-6.01	126.79	130.40
2	EB	761	A	C5-N7-C8	-6.00	100.90	103.90
2	B	2245	U	C4-C5-C6	6.00	123.30	119.70
2	EB	194	G	C2-N3-C4	-6.00	108.90	111.90
2	EB	2397	G	N1-C6-O6	6.00	123.50	119.90
2	EB	1325	G	N3-C4-N9	6.00	129.60	126.00
2	B	751	A	O5'-P-OP2	-6.00	100.31	105.70
2	B	1651	G	C2-N3-C4	-6.00	108.90	111.90
3	FB	11	C	C6-N1-C2	6.00	122.70	120.30
2	B	1397	U	N3-C2-O2	-5.99	118.00	122.20
2	B	570	G	C4-C5-N7	-5.99	108.40	110.80
2	B	802	A	C8-N9-C4	-5.99	103.40	105.80
2	B	1762	A	C5-C6-N6	5.99	128.49	123.70
2	B	2276	G	N1-C6-O6	5.99	123.49	119.90
3	FB	82	G	C5-C6-N1	-5.99	108.50	111.50
2	B	189	G	N1-C6-O6	5.99	123.49	119.90
2	B	450	G	C8-N9-C1'	-5.99	119.22	127.00
2	EB	728	G	N9-C4-C5	-5.99	103.00	105.40
1	A	286	G	N1-C6-O6	5.99	123.49	119.90
2	B	548	A	N7-C8-N9	5.99	116.79	113.80
2	B	1371	G	C5-C6-N1	-5.99	108.51	111.50
2	B	1612	C	C6-N1-C2	5.99	122.69	120.30
2	B	2026	C	C6-N1-C2	5.98	122.69	120.30
2	B	456	C	C6-N1-C2	5.98	122.69	120.30
2	B	1788	C	OP1-P-O3'	5.98	118.35	105.20
1	DB	299	G	C5-C6-N1	-5.98	108.51	111.50
2	B	1756	G	C4-C5-C6	5.97	122.39	118.80
2	EB	2072	G	C5-C6-O6	-5.97	125.02	128.60
2	B	2610	C	N1-C2-O2	5.97	122.48	118.90
2	EB	2298	A	N1-C6-N6	-5.97	115.02	118.60
2	B	2567	G	C5-C6-N1	-5.97	108.52	111.50
1	DB	922	G	C8-N9-C4	-5.97	104.01	106.40
2	B	2528	U	C5-C4-O4	5.97	129.48	125.90
2	B	1368	G	C5-C6-N1	5.97	114.48	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1558	A	C5-C6-N1	-5.97	114.72	117.70
2	EB	304	G	N9-C4-C5	5.97	107.79	105.40
2	EB	1429	G	C8-N9-C4	-5.97	104.01	106.40
2	EB	1627	G	C5-C6-N1	-5.97	108.52	111.50
2	EB	1240	U	C4-C5-C6	5.96	123.28	119.70
2	B	1538	G	C8-N9-C4	-5.96	104.02	106.40
2	EB	2061	G	C4-C5-C6	5.96	122.38	118.80
1	A	773	G	C5-C6-O6	-5.96	125.02	128.60
2	B	1274	A	C2-N3-C4	-5.96	107.62	110.60
2	EB	1638	C	N1-C2-O2	-5.96	115.32	118.90
2	B	1277	G	N3-C2-N2	-5.96	115.73	119.90
2	B	1762	A	C4-C5-N7	-5.96	107.72	110.70
2	B	2318	G	N7-C8-N9	5.95	116.08	113.10
2	EB	1231	G	N1-C6-O6	5.95	123.47	119.90
2	EB	1695	G	N1-C6-O6	5.95	123.47	119.90
1	DB	886	G	C5-C6-N1	-5.95	108.52	111.50
2	B	697	C	C6-N1-C2	5.95	122.68	120.30
2	B	728	G	N1-C6-O6	5.95	123.47	119.90
4	IA	31	G	N1-C6-O6	5.95	123.47	119.90
2	B	1286	A	C8-N9-C4	-5.95	103.42	105.80
2	B	1627	G	C5-C6-N1	-5.95	108.53	111.50
2	EB	825	C	OP1-P-O3'	5.95	118.29	105.20
1	A	754	C	C5-C6-N1	5.95	123.97	121.00
2	B	941	A	N1-C6-N6	-5.95	115.03	118.60
2	B	208	C	C5-C6-N1	-5.95	118.03	121.00
1	A	576	G	C8-N9-C1'	-5.94	119.28	127.00
2	B	1951	U	N3-C4-C5	-5.94	111.03	114.60
1	DB	1397	C	O4'-C1'-N1	5.94	112.95	108.20
2	EB	672	C	N3-C2-O2	-5.94	117.74	121.90
2	B	1254	A	C8-N9-C4	-5.94	103.42	105.80
2	B	2614	A	OP1-P-O3'	5.94	118.27	105.20
2	EB	1240	U	N3-C4-C5	-5.94	111.04	114.60
2	B	945	A	C5-N7-C8	-5.94	100.93	103.90
2	EB	728	G	C5-C6-N1	-5.94	108.53	111.50
4	LC	2	G	C8-N9-C4	5.94	108.77	106.40
1	A	789	U	N3-C4-C5	-5.93	111.04	114.60
2	B	585	G	C8-N9-C4	-5.93	104.03	106.40
2	B	811	U	O5'-P-OP1	-5.93	100.36	105.70
2	B	1706	U	N3-C4-C5	-5.93	111.04	114.60
2	B	2010	G	C8-N9-C4	-5.93	104.03	106.40
2	B	2726	U	C6-N1-C2	5.93	124.56	121.00
2	EB	2062	A	C8-N9-C4	5.93	108.17	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	EB	1698	A	O4'-C1'-N9	5.92	112.94	108.20
2	B	1778	U	C2-N1-C1'	-5.92	110.59	117.70
2	EB	1355	G	N1-C6-O6	5.92	123.45	119.90
1	A	1531	A	C2-N3-C4	5.92	113.56	110.60
2	B	945	A	N9-C4-C5	-5.92	103.43	105.80
2	EB	1617	C	C6-N1-C2	5.92	122.67	120.30
2	EB	450	G	C6-C5-N7	-5.92	126.85	130.40
2	EB	1842	G	C8-N9-C4	5.91	108.77	106.40
2	EB	2430	A	N9-C4-C5	5.91	108.17	105.80
2	B	1698	A	O4'-C1'-N9	5.91	112.93	108.20
2	B	195	A	C4-C5-C6	-5.91	114.05	117.00
2	EB	1234	U	C5-C4-O4	5.91	129.45	125.90
2	B	1609	A	C2-N3-C4	-5.91	107.65	110.60
2	EB	2346	A	N9-C4-C5	5.91	108.16	105.80
2	B	2091	U	C4-C5-C6	5.91	123.24	119.70
2	B	1435	G	C5-C6-O6	-5.90	125.06	128.60
1	DB	232	G	C5-C6-N1	-5.90	108.55	111.50
1	DB	1199	U	C5-C4-O4	5.90	129.44	125.90
2	EB	391	G	C4-N9-C1'	5.90	134.17	126.50
2	EB	942	G	OP2-P-O3'	5.90	118.18	105.20
2	B	2580	U	C6-N1-C2	-5.90	117.46	121.00
2	B	2575	C	O5'-P-OP1	-5.90	100.39	105.70
4	LC	48	C	C5-C6-N1	-5.90	118.05	121.00
2	EB	342	G	N1-C6-O6	5.90	123.44	119.90
2	B	528	A	C6-N1-C2	5.89	122.14	118.60
2	B	2451	A	C2-N3-C4	-5.89	107.65	110.60
2	EB	34	C	C2-N3-C4	5.89	122.85	119.90
2	B	71	A	C5-N7-C8	-5.89	100.95	103.90
2	B	1240	U	C4-C5-C6	5.89	123.23	119.70
2	B	1816	G	N1-C6-O6	5.89	123.43	119.90
2	EB	1975	G	N1-C6-O6	5.89	123.43	119.90
2	B	613	U	N3-C2-O2	-5.89	118.08	122.20
2	B	685	A	C8-N9-C4	-5.89	103.44	105.80
2	B	695	G	C5-C6-N1	-5.89	108.56	111.50
2	B	1024	G	N1-C6-O6	5.89	123.43	119.90
1	DB	752	G	N1-C6-O6	5.89	123.43	119.90
2	EB	1614	A	O5'-P-OP1	5.89	117.76	110.70
2	EB	2609	U	C5-C6-N1	-5.89	119.76	122.70
2	B	1667	G	C8-N9-C4	5.88	108.75	106.40
2	B	1768	U	C5-C4-O4	5.88	129.43	125.90
2	B	1762	A	C2-N3-C4	5.88	113.54	110.60
2	EB	1706	U	N3-C4-C5	-5.88	111.07	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	533	G	C5-C6-O6	5.88	132.13	128.60
2	B	1845	G	C5-C6-O6	-5.88	125.07	128.60
2	B	464	U	N1-C2-N3	5.88	118.42	114.90
2	B	1757	U	C6-N1-C2	5.88	124.53	121.00
2	B	2049	G	C5-C6-N1	5.88	114.44	111.50
1	A	886	G	N1-C6-O6	5.87	123.42	119.90
1	DB	886	G	N1-C6-O6	5.87	123.42	119.90
2	EB	1695	G	C5-C6-O6	-5.87	125.08	128.60
2	B	1231	G	N1-C6-O6	5.87	123.42	119.90
2	B	1671	U	C5-C6-N1	5.87	125.64	122.70
2	B	2618	G	C8-N9-C4	-5.87	104.05	106.40
1	DB	286	G	N1-C6-O6	5.87	123.42	119.90
2	EB	391	G	N9-C4-C5	-5.87	103.05	105.40
2	EB	942	G	C5-C6-N1	-5.87	108.56	111.50
2	EB	1201	C	C6-N1-C2	5.87	122.65	120.30
1	A	1492	A	C8-N9-C4	-5.87	103.45	105.80
2	EB	505	A	C8-N9-C4	-5.87	103.45	105.80
2	EB	1620	G	C5-C6-N1	-5.87	108.57	111.50
2	B	530	G	N3-C2-N2	5.87	124.01	119.90
2	B	2491	U	O5'-P-OP2	5.87	117.74	110.70
2	B	1190	G	C4-C5-N7	5.87	113.15	110.80
2	B	1240	U	N3-C2-O2	-5.86	118.10	122.20
2	EB	728	G	C6-C5-N7	-5.86	126.88	130.40
2	EB	122	G	N9-C4-C5	-5.86	103.06	105.40
2	EB	450	G	C4-N9-C1'	5.86	134.12	126.50
2	B	128	C	C5-C6-N1	-5.86	118.07	121.00
1	DB	1532	U	C5-C6-N1	5.86	125.63	122.70
2	EB	198	C	O5'-P-OP1	-5.86	100.43	105.70
2	B	1270	C	C6-N1-C2	5.86	122.64	120.30
2	B	1402	C	N3-C4-C5	-5.86	119.56	121.90
1	A	576	G	N1-C6-O6	5.85	123.41	119.90
1	A	1435	G	C5-C6-N1	-5.85	108.57	111.50
2	B	391	G	N9-C4-C5	-5.85	103.06	105.40
2	B	1622	G	N1-C6-O6	5.85	123.41	119.90
2	B	2501	C	C6-N1-C2	5.85	122.64	120.30
2	B	2059	A	C5-C6-N6	-5.85	119.02	123.70
2	B	127	A	C8-N9-C4	5.85	108.14	105.80
2	B	676	A	N1-C6-N6	5.85	122.11	118.60
2	B	2715	C	N3-C4-C5	5.85	124.24	121.90
1	DB	778	G	N1-C6-O6	5.85	123.41	119.90
2	EB	2464	C	C6-N1-C2	5.85	122.64	120.30
2	EB	747	U	C5-C4-O4	-5.84	122.39	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1622	G	C5-C6-O6	-5.84	125.10	128.60
2	B	2013	A	OP2-P-O3'	5.84	118.05	105.20
2	B	2218	G	N1-C6-O6	5.84	123.40	119.90
2	B	2614	A	C5-C6-N1	5.84	120.62	117.70
2	EB	125	G	C8-N9-C4	-5.84	104.06	106.40
2	B	70	G	C6-C5-N7	-5.84	126.90	130.40
2	EB	1341	U	OP2-P-O3'	5.84	118.04	105.20
2	B	1614	A	N1-C2-N3	5.83	132.22	129.30
2	B	2550	G	O5'-P-OP1	5.83	117.70	110.70
2	B	2576	G	OP1-P-O3'	5.83	118.03	105.20
1	DB	328	C	N1-C2-O2	5.83	122.40	118.90
2	EB	2259	G	N1-C6-O6	5.83	123.40	119.90
2	EB	945	A	C2-N3-C4	-5.83	107.68	110.60
2	EB	1231	G	N3-C4-C5	5.83	131.51	128.60
2	B	1224	C	C6-N1-C2	5.83	122.63	120.30
1	DB	793	U	C5-C4-O4	5.83	129.40	125.90
1	DB	106	C	OP2-P-O3'	5.83	118.02	105.20
2	EB	2876	G	C8-N9-C4	5.83	108.73	106.40
1	A	778	G	N1-C6-O6	5.82	123.39	119.90
2	B	2593	U	C6-N1-C1'	5.82	129.35	121.20
2	B	2021	C	N3-C2-O2	-5.82	117.83	121.90
2	B	1992	G	C5-C6-N1	5.82	114.41	111.50
2	EB	2576	G	OP1-P-O3'	5.82	118.00	105.20
2	EB	1210	A	N1-C2-N3	5.82	132.21	129.30
2	B	1779	U	C6-N1-C1'	-5.82	113.06	121.20
2	EB	2447	G	N7-C8-N9	-5.82	110.19	113.10
2	EB	2218	G	C5-C6-N1	-5.81	108.59	111.50
2	EB	2580	U	C2-N3-C4	5.81	130.49	127.00
2	B	2603	G	N3-C4-C5	5.81	131.50	128.60
2	EB	1898	U	C6-N1-C2	-5.81	117.51	121.00
2	B	787	U	N1-C2-O2	-5.81	118.73	122.80
2	B	1598	C	C6-N1-C2	5.81	122.62	120.30
2	B	993	G	N3-C4-N9	-5.80	122.52	126.00
3	C	75	G	C8-N9-C4	5.80	108.72	106.40
2	B	735	A	C8-N9-C4	5.80	108.12	105.80
1	DB	1503	A	N1-C6-N6	-5.80	115.12	118.60
2	B	2240	C	C6-N1-C2	5.80	122.62	120.30
2	B	2458	G	C4-N9-C1'	5.80	134.04	126.50
1	DB	1469	G	N1-C6-O6	5.80	123.38	119.90
2	EB	2726	U	C6-N1-C2	5.80	124.48	121.00
1	DB	574	A	O5'-P-OP1	-5.80	100.48	105.70
31	HC	39	ARG	NE-CZ-NH2	-5.80	117.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1007	C	C6-N1-C2	5.79	122.62	120.30
2	B	391	G	N3-C4-N9	5.79	129.48	126.00
1	DB	364	A	N1-C2-N3	5.79	132.20	129.30
2	EB	974(B)	C	C6-N1-C2	5.79	122.62	120.30
1	A	1512	U	N3-C4-C5	-5.79	111.12	114.60
2	B	2403	C	N3-C2-O2	-5.79	117.85	121.90
4	IA	46	G	N1-C6-O6	-5.79	116.42	119.90
2	EB	1671	U	C6-N1-C2	-5.79	117.53	121.00
2	EB	2092	U	C5-C4-O4	5.79	129.37	125.90
1	A	320	C	C6-N1-C2	5.79	122.61	120.30
2	EB	1666	G	C8-N9-C4	5.79	108.72	106.40
2	B	631	A	N1-C6-N6	5.79	122.07	118.60
2	B	2072	G	N1-C6-O6	5.79	123.37	119.90
1	DB	1099	G	N9-C4-C5	5.79	107.72	105.40
2	EB	2713	A	OP2-P-O3'	5.79	117.93	105.20
2	B	2777	G	O4'-C1'-N9	-5.78	103.58	108.20
1	DB	945	G	C5-C6-O6	-5.78	125.13	128.60
1	DB	702	A	N1-C6-N6	5.78	122.06	118.60
2	EB	1647	G	O5'-P-OP2	5.78	117.63	110.70
2	EB	2424	C	C6-N1-C2	5.77	122.61	120.30
2	B	19	C	C5-C6-N1	-5.77	118.11	121.00
2	B	559	G	C5-C6-N1	-5.77	108.61	111.50
2	B	1992	G	C2-N3-C4	5.77	114.79	111.90
2	B	179	G	C5-C6-N1	-5.77	108.62	111.50
2	B	1906	G	C5-C6-N1	-5.77	108.62	111.50
2	B	1981	A	C4-C5-C6	-5.77	114.12	117.00
2	EB	539	G	C8-N9-C4	5.77	108.71	106.40
2	EB	963	U	O5'-P-OP1	-5.77	100.51	105.70
3	C	16	G	N1-C6-O6	5.77	123.36	119.90
2	EB	1698	A	N7-C8-N9	5.77	116.68	113.80
2	B	1902	C	N3-C4-C5	5.76	124.20	121.90
2	EB	945	A	C5-C6-N6	-5.76	119.09	123.70
2	EB	2072	G	C4-C5-N7	5.76	113.11	110.80
2	B	2714	G	O5'-P-OP2	5.76	117.62	110.70
2	EB	528	A	N9-C4-C5	-5.76	103.50	105.80
2	EB	409	C	O5'-P-OP2	-5.76	100.52	105.70
2	EB	613	U	O4'-C1'-N1	5.76	112.81	108.20
2	EB	2004	G	N1-C6-O6	5.76	123.36	119.90
2	B	1898	U	N3-C4-C5	-5.76	111.15	114.60
2	EB	323	G	C5-C6-O6	-5.76	125.15	128.60
2	B	610	C	N3-C4-C5	5.75	124.20	121.90
1	DB	304	U	N3-C4-C5	-5.75	111.15	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	EB	186	G	N1-C6-O6	5.75	123.35	119.90
1	A	603	U	C6-N1-C2	-5.75	117.55	121.00
2	B	2494	G	C8-N9-C4	5.75	108.70	106.40
2	EB	124	G	N1-C6-O6	5.75	123.35	119.90
2	B	196	A	C8-N9-C4	-5.75	103.50	105.80
2	EB	534	U	C6-N1-C2	-5.75	117.55	121.00
2	EB	2330	G	N1-C6-O6	5.75	123.35	119.90
1	A	1532	U	C2-N1-C1'	5.74	124.59	117.70
2	EB	211	A	C8-N9-C4	5.74	108.10	105.80
2	EB	809	G	O5'-P-OP2	-5.74	100.53	105.70
2	EB	2593	U	C2-N3-C4	5.74	130.44	127.00
2	B	802	A	N1-C2-N3	5.74	132.17	129.30
1	DB	576	G	C5-C6-N1	-5.73	108.63	111.50
2	EB	861	A	OP2-P-O3'	5.73	117.81	105.20
1	A	285	G	N1-C6-O6	5.73	123.34	119.90
2	B	1565	C	N1-C2-O2	-5.73	115.46	118.90
2	EB	68	G	N1-C6-O6	5.73	123.34	119.90
1	DB	1503	A	C5-N7-C8	5.73	106.76	103.90
2	EB	1970	A	N7-C8-N9	5.73	116.66	113.80
2	EB	2685	G	N1-C2-N2	5.73	121.35	116.20
2	EB	1271	G	C5-C6-N1	-5.72	108.64	111.50
2	B	349	G	C4-C5-N7	-5.72	108.51	110.80
2	EB	1556	C	O5'-P-OP2	-5.72	100.55	105.70
2	EB	1642	G	N1-C6-O6	5.72	123.33	119.90
2	B	422	A	C8-N9-C4	-5.72	103.51	105.80
2	B	2397	G	C5-C6-O6	-5.72	125.17	128.60
1	DB	1505	G	N1-C6-O6	5.72	123.33	119.90
2	EB	1422	G	N1-C6-O6	5.72	123.33	119.90
2	B	827	U	O5'-P-OP2	-5.72	100.56	105.70
2	B	1489	U	C5-C4-O4	5.72	129.33	125.90
2	B	1111	A	C8-N9-C4	5.71	108.09	105.80
2	B	1131	G	C4-C5-N7	5.71	113.08	110.80
2	EB	400	G	N1-C6-O6	5.71	123.33	119.90
2	EB	1186	G	O5'-P-OP1	-5.71	100.56	105.70
2	EB	1251	C	N1-C2-N3	-5.71	115.20	119.20
2	EB	2680	C	C6-N1-C2	5.71	122.58	120.30
2	B	1022	G	C4-C5-N7	-5.71	108.52	110.80
2	EB	2474	C	C6-N1-C2	5.71	122.58	120.30
2	B	304	G	N3-C2-N2	-5.71	115.90	119.90
3	C	112	G	N1-C6-O6	5.71	123.33	119.90
2	EB	1783	A	OP2-P-O3'	5.71	117.76	105.20
2	B	379	G	C5-C6-N1	-5.71	108.65	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DB	965	A	C8-N9-C4	5.71	108.08	105.80
2	EB	1790	C	O5'-P-OP2	5.71	117.55	110.70
2	B	751	A	C8-N9-C4	-5.70	103.52	105.80
1	A	293	G	C5-C6-O6	-5.70	125.18	128.60
2	B	1374	G	N1-C6-O6	5.70	123.32	119.90
4	LC	30	G	N1-C6-O6	5.70	123.32	119.90
2	B	861	A	C8-N9-C4	-5.70	103.52	105.80
2	B	2593	U	C5-C4-O4	5.70	129.32	125.90
2	EB	1828	G	N7-C8-N9	5.70	115.95	113.10
2	B	457	A	N1-C6-N6	-5.70	115.18	118.60
2	EB	2573	C	C5-C6-N1	-5.70	118.15	121.00
1	A	773	G	C8-N9-C4	5.70	108.68	106.40
2	B	2838	G	C5-C6-O6	-5.69	125.18	128.60
1	A	711	G	N1-C6-O6	5.69	123.31	119.90
3	FB	76	G	N1-C6-O6	5.69	123.31	119.90
2	B	2576	G	N1-C6-O6	5.69	123.31	119.90
2	B	2713	A	OP2-P-O3'	5.69	117.72	105.20
2	B	859	G	N7-C8-N9	-5.69	110.26	113.10
2	EB	559	G	N1-C6-O6	5.69	123.31	119.90
2	EB	2439	A	C5-N7-C8	-5.69	101.06	103.90
3	FB	65	C	C2-N1-C1'	5.69	125.06	118.80
2	B	58	G	N1-C6-O6	5.68	123.31	119.90
2	EB	859	G	C8-N9-C4	5.68	108.67	106.40
2	EB	1769	G	C5-C6-N1	-5.68	108.66	111.50
2	B	777	A	N7-C8-N9	5.68	116.64	113.80
2	B	2395	C	N1-C2-O2	-5.68	115.49	118.90
1	DB	668	G	N1-C6-O6	5.68	123.31	119.90
3	FB	99	A	OP2-P-O3'	5.68	117.70	105.20
2	B	2065	C	C6-N1-C2	5.68	122.57	120.30
2	B	2447	G	C4-C5-C6	5.68	122.21	118.80
1	A	1435	G	C2-N3-C4	-5.68	109.06	111.90
2	EB	1240	U	N1-C2-N3	5.68	118.31	114.90
2	B	1021	A	C5-N7-C8	-5.67	101.06	103.90
2	B	1131	G	O5'-P-OP2	-5.67	100.59	105.70
2	B	1842	G	N1-C6-O6	5.67	123.31	119.90
2	EB	504	U	C2-N1-C1'	5.67	124.51	117.70
2	EB	1142(B)	A	N1-C6-N6	5.67	122.00	118.60
2	B	330	A	N1-C2-N3	5.67	132.14	129.30
2	B	2052	G	C6-C5-N7	-5.67	127.00	130.40
2	B	1660	C	C6-N1-C2	-5.67	118.03	120.30
1	DB	331	G	C5-N7-C8	-5.67	101.46	104.30
2	B	1703	G	C6-C5-N7	-5.67	127.00	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	911	A	N1-C6-N6	5.67	122.00	118.60
2	EB	2082	A	N1-C6-N6	5.67	122.00	118.60
2	B	382	G	N3-C2-N2	-5.67	115.93	119.90
2	B	2693	A	N1-C6-N6	5.67	122.00	118.60
2	EB	1852	C	C6-N1-C2	-5.67	118.03	120.30
2	B	804	A	N9-C4-C5	-5.66	103.53	105.80
2	B	1193	G	C2-N3-C4	-5.66	109.07	111.90
2	B	1970	A	C8-N9-C4	-5.66	103.53	105.80
1	DB	1158	C	C2-N1-C1'	5.66	125.03	118.80
1	A	293	G	C6-C5-N7	-5.66	127.00	130.40
2	B	1355	G	C5-C6-O6	-5.66	125.20	128.60
2	EB	577	G	C4-C5-N7	5.66	113.06	110.80
2	B	1315	C	O5'-P-OP1	-5.66	100.61	105.70
2	EB	2715	C	N3-C4-C5	5.66	124.16	121.90
2	B	460	A	N1-C2-N3	5.66	132.13	129.30
2	EB	1382	G	N3-C4-N9	-5.66	122.61	126.00
2	EB	2228	G	C5-C6-N1	-5.66	108.67	111.50
1	A	1189	C	N1-C2-O2	5.65	122.29	118.90
1	A	1196	U	C5-C6-N1	5.65	125.53	122.70
2	B	613	U	O4'-C1'-N1	5.65	112.72	108.20
2	B	2346	A	N9-C4-C5	5.65	108.06	105.80
2	EB	699	A	C5-C6-N6	-5.65	119.18	123.70
2	EB	1992	G	O4'-C1'-N9	-5.65	103.68	108.20
2	B	677	A	O5'-P-OP2	-5.65	100.62	105.70
2	EB	548	A	N7-C8-N9	5.65	116.62	113.80
2	EB	1244	G	C5-C6-N1	-5.65	108.68	111.50
2	EB	2553	G	C6-C5-N7	-5.65	127.01	130.40
2	B	400	G	N1-C6-O6	5.64	123.29	119.90
2	EB	742	G	N1-C6-O6	5.64	123.29	119.90
2	EB	2271	G	C4-C5-N7	-5.64	108.54	110.80
2	B	2659	G	C5-C6-N1	-5.64	108.68	111.50
31	EA	39	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	600	C	C6-N1-C2	5.64	122.56	120.30
2	B	1348	G	N3-C4-C5	5.64	131.42	128.60
2	EB	1697	G	N1-C6-O6	5.64	123.28	119.90
2	EB	35	G	N1-C6-O6	5.64	123.28	119.90
2	EB	2458	G	C4-N9-C1'	5.64	133.83	126.50
2	B	1190	G	C5-C6-O6	-5.63	125.22	128.60
1	DB	1467	G	N7-C8-N9	-5.63	110.28	113.10
2	EB	1382	G	C5-C6-N1	-5.63	108.68	111.50
2	EB	1667	G	N9-C4-C5	-5.63	103.15	105.40
2	B	2259	G	C5-C6-O6	-5.63	125.22	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2582	G	C8-N9-C4	-5.63	104.15	106.40
2	B	1471	A	C8-N9-C4	-5.63	103.55	105.80
2	EB	2061	G	OP2-P-O3'	5.63	117.58	105.20
2	B	1149	G	C8-N9-C4	5.62	108.65	106.40
2	EB	2088	G	C6-C5-N7	-5.62	127.03	130.40
2	B	529	A	N1-C6-N6	-5.62	115.22	118.60
2	B	922	U	N3-C4-C5	-5.62	111.23	114.60
2	B	1269	A	N7-C8-N9	5.62	116.61	113.80
1	A	1467	G	O5'-P-OP2	-5.62	100.64	105.70
2	B	528	A	C2-N3-C4	-5.62	107.79	110.60
2	B	123	G	N1-C6-O6	5.62	123.27	119.90
2	EB	805	G	C8-N9-C4	-5.62	104.15	106.40
2	EB	1936	A	C8-N9-C4	5.62	108.05	105.80
2	B	575	A	N1-C2-N3	5.62	132.11	129.30
2	B	1664	A	N7-C8-N9	5.62	116.61	113.80
2	B	2570	G	C5-C6-N1	-5.62	108.69	111.50
2	EB	445	C	OP2-P-O3'	5.62	117.56	105.20
2	EB	1698	A	C5-C6-N1	-5.61	114.89	117.70
2	B	1936	A	C5-N7-C8	-5.61	101.09	103.90
2	B	1783	A	OP2-P-O3'	5.61	117.54	105.20
2	EB	726	G	O4'-C1'-N9	5.61	112.69	108.20
2	B	450	G	C2-N3-C4	-5.61	109.10	111.90
2	B	1790	C	N3-C4-C5	5.61	124.14	121.90
1	A	115	G	P-O3'-C3'	5.60	126.42	119.70
2	B	2723	C	N3-C2-O2	-5.60	117.98	121.90
2	B	663	G	C4-C5-N7	-5.60	108.56	110.80
2	B	2782	G	C5-C6-O6	-5.60	125.24	128.60
2	EB	593	G	C5-C6-N1	-5.60	108.70	111.50
2	B	2419	U	C6-N1-C2	-5.60	117.64	121.00
2	B	2698	U	C4-C5-C6	5.60	123.06	119.70
2	EB	610	C	N3-C4-C5	5.60	124.14	121.90
2	B	754	C	C6-N1-C2	5.59	122.54	120.30
2	B	2473	U	C2-N1-C1'	5.59	124.41	117.70
1	DB	603	U	C6-N1-C2	-5.59	117.64	121.00
1	A	803	G	C8-N9-C4	-5.59	104.16	106.40
2	B	1935	G	N3-C4-C5	5.59	131.40	128.60
3	C	99	A	OP2-P-O3'	5.59	117.50	105.20
2	EB	410	G	OP1-P-O3'	5.59	117.50	105.20
2	EB	1252	G	O4'-C1'-N9	-5.59	103.73	108.20
1	A	1196	U	C6-N1-C2	-5.59	117.65	121.00
1	A	804	U	C5-C4-O4	5.59	129.25	125.90
2	B	1193	G	N1-C2-N3	5.59	127.25	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2617	C	C2-N3-C4	-5.59	117.11	119.90
1	DB	74	C	C6-N1-C2	-5.59	118.06	120.30
2	EB	699	A	N1-C6-N6	5.59	121.95	118.60
2	B	466	A	OP2-P-O3'	5.58	117.48	105.20
2	B	980	A	C8-N9-C4	-5.58	103.57	105.80
2	B	2556	C	C2-N1-C1'	5.58	124.94	118.80
2	EB	1024	G	C5-C6-O6	-5.58	125.25	128.60
2	B	1869	G	C5-C6-N1	-5.58	108.71	111.50
2	B	197	A	OP1-P-O3'	-5.58	92.93	105.20
2	B	865	C	C4-C5-C6	-5.58	114.61	117.40
2	EB	678	C	O5'-P-OP2	-5.58	100.68	105.70
2	B	2505	G	C4-C5-N7	-5.58	108.57	110.80
2	EB	1757	U	C6-N1-C2	5.58	124.35	121.00
1	A	792	A	C8-N9-C4	5.58	108.03	105.80
2	B	240	G	N3-C4-C5	-5.58	125.81	128.60
2	B	2532	G	C6-C5-N7	-5.58	127.06	130.40
1	DB	1232	U	C6-N1-C2	-5.57	117.66	121.00
2	EB	1840	G	N1-C2-N3	5.57	127.24	123.90
2	B	248	G	C5-N7-C8	-5.57	101.51	104.30
2	B	220	G	N1-C6-O6	5.57	123.24	119.90
2	B	312	G	C8-N9-C4	5.57	108.63	106.40
2	B	746	A	O4'-C1'-N9	5.57	112.66	108.20
2	EB	195	A	C4-C5-N7	5.57	113.48	110.70
2	EB	2056	G	C4-C5-N7	5.57	113.03	110.80
2	EB	780	G	N1-C6-O6	5.56	123.24	119.90
2	EB	870	A	C8-N9-C4	5.56	108.03	105.80
2	B	583	G	N7-C8-N9	5.56	115.88	113.10
1	DB	475	G	N1-C6-O6	5.56	123.23	119.90
1	DB	1522	U	N1-C2-N3	5.56	118.24	114.90
2	EB	747	U	N3-C2-O2	5.56	126.09	122.20
2	EB	34	C	P-O3'-C3'	5.56	126.37	119.70
2	EB	684	G	N3-C4-C5	5.56	131.38	128.60
2	EB	1187	G	C4-C5-C6	5.56	122.14	118.80
2	EB	1657	C	OP1-P-O3'	5.56	117.43	105.20
2	EB	2009	G	N1-C6-O6	5.56	123.23	119.90
2	B	735	A	C2-N3-C4	-5.55	107.82	110.60
2	B	747	U	N3-C2-O2	5.55	126.09	122.20
3	C	30	C	C6-N1-C2	-5.55	118.08	120.30
2	EB	2603	G	N3-C4-C5	5.55	131.38	128.60
2	EB	1667	G	C4-C5-N7	5.55	113.02	110.80
2	B	2056	G	N9-C4-C5	-5.55	103.18	105.40
2	B	569	U	C6-N1-C1'	-5.55	113.44	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	695	G	N1-C6-O6	5.55	123.23	119.90
2	B	2543	G	C5-C6-O6	5.55	131.93	128.60
1	DB	927	G	C4-C5-N7	-5.55	108.58	110.80
2	EB	1940	U	N3-C4-C5	-5.55	111.27	114.60
2	EB	2430	A	N1-C6-N6	-5.55	115.27	118.60
2	B	2043	C	N3-C2-O2	-5.54	118.02	121.90
1	A	771	G	C8-N9-C4	5.54	108.62	106.40
2	EB	1642	G	C5-C6-O6	-5.54	125.27	128.60
2	B	855	G	C5-C6-N1	-5.54	108.73	111.50
2	EB	337	C	C6-N1-C2	5.54	122.52	120.30
2	EB	2032	G	C5-C6-O6	-5.54	125.28	128.60
2	B	806	C	O5'-P-OP1	-5.54	100.71	105.70
1	DB	563	A	N7-C8-N9	5.54	116.57	113.80
2	EB	122	G	C5-C6-O6	-5.54	125.28	128.60
1	DB	711	G	C8-N9-C4	5.54	108.61	106.40
2	B	804	A	N1-C6-N6	5.53	121.92	118.60
2	B	2821	A	C8-N9-C4	-5.53	103.59	105.80
2	B	520	G	C6-C5-N7	-5.53	127.08	130.40
3	C	65	C	N1-C2-O2	5.53	122.22	118.90
1	DB	293	G	C5-C6-O6	-5.53	125.28	128.60
2	EB	1384	A	C8-N9-C4	5.53	108.01	105.80
2	B	1368	G	C6-N1-C2	-5.53	121.78	125.10
2	EB	1685	C	C6-N1-C2	5.53	122.51	120.30
2	B	451	C	N1-C2-O2	5.53	122.22	118.90
2	EB	534	U	C5-C4-O4	5.53	129.22	125.90
1	DB	911	U	C5-C4-O4	5.52	129.21	125.90
2	EB	946	G	N1-C6-O6	5.52	123.21	119.90
2	EB	2544	G	C2-N3-C4	-5.52	109.14	111.90
2	EB	1700	A	O5'-P-OP2	5.52	117.32	110.70
2	EB	2255	G	N1-C6-O6	5.52	123.21	119.90
2	B	1210	A	N7-C8-N9	5.52	116.56	113.80
2	EB	1632	A	C8-N9-C4	5.52	108.01	105.80
2	EB	2061	G	O5'-P-OP2	5.52	117.32	110.70
2	EB	1695	G	C6-C5-N7	-5.52	127.09	130.40
1	A	28	G	N7-C8-N9	5.51	115.86	113.10
2	B	84	A	C8-N9-C4	5.51	108.01	105.80
2	B	698	C	C6-N1-C2	5.51	122.51	120.30
2	B	946	G	C8-N9-C4	5.51	108.61	106.40
2	B	2346	A	N1-C6-N6	-5.51	115.29	118.60
2	EB	46	C	C6-N1-C2	5.51	122.51	120.30
2	EB	569	U	C6-N1-C1'	-5.51	113.48	121.20
1	A	286	G	C5-C6-N1	-5.51	108.74	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DB	331	G	C6-C5-N7	-5.51	127.09	130.40
1	DB	757	U	C5-C4-O4	5.51	129.21	125.90
1	DB	1435	G	C5-C6-N1	-5.51	108.74	111.50
2	B	534	U	N3-C4-C5	-5.51	111.30	114.60
2	B	1558	A	C4-C5-N7	5.51	113.45	110.70
2	B	1700	A	C8-N9-C4	5.51	108.00	105.80
2	B	1913	A	C8-N9-C4	5.51	108.00	105.80
2	B	2245	U	C5-C4-O4	5.51	129.21	125.90
2	B	2332	U	C5-C4-O4	5.51	129.21	125.90
2	B	391	G	C4-C5-N7	5.51	113.00	110.80
2	B	775	G	C5-N7-C8	5.51	107.05	104.30
2	B	2397	G	C6-C5-N7	-5.51	127.10	130.40
2	EB	2272	U	C2-N3-C4	-5.51	123.70	127.00
2	B	752	A	N1-C2-N3	5.50	132.05	129.30
2	EB	2443	C	C4-C5-C6	5.50	120.15	117.40
2	EB	2458	G	C6-C5-N7	-5.50	127.10	130.40
1	A	1397	C	C6-N1-C2	-5.50	118.10	120.30
2	B	1558	A	C6-N1-C2	5.50	121.90	118.60
3	C	52	A	C5-C6-N6	-5.50	119.30	123.70
2	EB	530	G	C2-N3-C4	5.50	114.65	111.90
2	EB	1377	G	C8-N9-C4	-5.50	104.20	106.40
1	A	927	G	C8-N9-C4	-5.50	104.20	106.40
2	EB	191	A	C6-N1-C2	-5.50	115.30	118.60
2	B	1998	G	N1-C6-O6	-5.50	116.60	119.90
1	DB	576	G	C6-C5-N7	-5.49	127.10	130.40
2	EB	528	A	C5-C6-N1	-5.49	114.95	117.70
2	B	2397	G	C5-C6-N1	-5.49	108.76	111.50
2	B	2897	U	N3-C2-O2	-5.49	118.36	122.20
2	EB	2777	G	O4'-C1'-N9	-5.49	103.81	108.20
2	B	1989	G	N1-C6-O6	5.49	123.19	119.90
2	EB	747	U	O5'-P-OP1	-5.49	100.76	105.70
2	B	270(U)	G	C8-N9-C4	5.48	108.59	106.40
2	B	198	C	O5'-P-OP1	-5.48	100.77	105.70
2	B	468	G	N1-C2-N3	5.48	127.19	123.90
2	B	1790	C	C5-C6-N1	-5.48	118.26	121.00
2	B	2061	G	N9-C4-C5	-5.48	103.21	105.40
2	EB	2022	U	C6-N1-C2	5.48	124.29	121.00
2	B	1914	C	C6-N1-C2	-5.48	118.11	120.30
2	B	2491	U	N1-C2-N3	-5.48	111.61	114.90
2	EB	395	U	N1-C2-O2	-5.48	118.97	122.80
2	EB	559	G	C5-C6-N1	-5.48	108.76	111.50
2	EB	768	G	C5-C6-O6	-5.48	125.31	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	81	G	C2-N3-C4	-5.47	109.16	111.90
2	B	1131	G	N1-C6-O6	5.47	123.19	119.90
2	B	2857	G	N1-C6-O6	-5.47	116.61	119.90
2	EB	1790	C	C2-N1-C1'	-5.47	112.78	118.80
1	DB	115	G	P-O3'-C3'	5.47	126.27	119.70
2	B	1643	G	N1-C6-O6	5.47	123.18	119.90
2	EB	1354	A	N1-C6-N6	5.47	121.88	118.60
2	B	1266	G	C5-C6-O6	-5.47	125.32	128.60
1	DB	767	A	N1-C6-N6	-5.47	115.32	118.60
2	EB	1921	G	N1-C6-O6	5.47	123.18	119.90
2	B	706	A	C8-N9-C4	5.47	107.99	105.80
2	B	1646	C	OP1-P-O3'	5.47	117.23	105.20
34	HA	15	A	N7-C8-N9	-5.47	111.07	113.80
2	B	1773	A	C8-N9-C4	-5.47	103.61	105.80
2	B	2567	G	N1-C6-O6	5.47	123.18	119.90
1	DB	301	G	N1-C6-O6	5.47	123.18	119.90
1	DB	1077	G	C5-C6-N1	-5.47	108.77	111.50
2	B	16	G	C4-C5-C6	5.46	122.08	118.80
2	B	1617	C	C5-C6-N1	-5.46	118.27	121.00
2	B	1704	G	N1-C6-O6	5.46	123.18	119.90
2	EB	577	G	C5-C6-O6	-5.46	125.32	128.60
2	B	129	C	O5'-P-OP2	-5.46	100.78	105.70
2	B	2651	C	C6-N1-C2	-5.46	118.11	120.30
2	B	568	U	C5-C4-O4	5.46	129.18	125.90
2	EB	2087	G	N1-C6-O6	5.46	123.18	119.90
2	B	761	A	C4-C5-C6	-5.46	114.27	117.00
2	B	1624	G	N3-C2-N2	-5.46	116.08	119.90
2	B	165	U	N3-C2-O2	-5.46	118.38	122.20
2	B	2324	C	C6-N1-C2	5.46	122.48	120.30
2	EB	2514	U	C5-C4-O4	5.45	129.17	125.90
2	EB	874	G	C8-N9-C4	5.45	108.58	106.40
2	EB	2033	A	C8-N9-C4	5.45	107.98	105.80
2	EB	2821	A	C8-N9-C4	-5.45	103.62	105.80
2	EB	2065	C	N3-C2-O2	5.45	125.71	121.90
1	A	121	C	N3-C2-O2	-5.45	118.09	121.90
2	B	68	G	C5-C6-N1	-5.45	108.78	111.50
2	B	1566	A	N1-C2-N3	5.45	132.02	129.30
3	C	85	G	N1-C6-O6	5.45	123.17	119.90
2	EB	2318	G	N7-C8-N9	5.45	115.82	113.10
2	B	724	U	C5-C4-O4	5.44	129.17	125.90
2	EB	1215	G	C5-C6-N1	-5.44	108.78	111.50
2	B	946	G	N1-C6-O6	5.44	123.17	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	EB	18	C	C6-N1-C2	-5.44	118.12	120.30
2	EB	1372	U	N1-C2-N3	-5.44	111.64	114.90
2	B	2820	A	N7-C8-N9	5.44	116.52	113.80
2	B	391	G	C4-C5-C6	5.44	122.06	118.80
2	B	832	G	C4-N9-C1'	5.44	133.57	126.50
2	EB	997	G	C4-C5-N7	5.44	112.97	110.80
2	B	2689	U	N1-C2-O2	5.44	126.61	122.80
2	B	1264	G	OP2-P-O3'	5.43	117.16	105.20
2	EB	431	U	C6-N1-C2	-5.43	117.74	121.00
2	B	1282	U	C5-C4-O4	5.43	129.16	125.90
2	B	786	C	OP1-P-O3'	5.43	117.14	105.20
2	B	1790	C	C2-N3-C4	-5.43	117.19	119.90
2	EB	1605	C	C6-N1-C2	-5.43	118.13	120.30
2	EB	1959	G	N3-C4-C5	-5.43	125.89	128.60
2	EB	2443	C	N3-C4-C5	-5.43	119.73	121.90
2	B	1780	A	N1-C6-N6	5.43	121.86	118.60
2	B	2315	G	C8-N9-C4	5.43	108.57	106.40
2	EB	1725	G	N1-C6-O6	5.43	123.16	119.90
2	EB	2249	U	C2-N3-C4	5.43	130.26	127.00
2	B	2501	C	C2-N3-C4	-5.42	117.19	119.90
2	EB	2433	A	N1-C2-N3	5.42	132.01	129.30
2	B	1646	C	C6-N1-C2	5.42	122.47	120.30
2	B	1773	A	OP1-P-O3'	5.42	117.13	105.20
1	DB	1391	U	C5-C4-O4	5.42	129.15	125.90
2	B	1497	U	C2-N1-C1'	5.42	124.20	117.70
2	B	2582	G	N7-C8-N9	5.42	115.81	113.10
1	DB	1503	A	C4-C5-N7	-5.42	107.99	110.70
2	EB	1633	G	N1-C6-O6	5.42	123.15	119.90
2	B	2304	G	N3-C4-C5	5.42	131.31	128.60
2	B	2581	G	N3-C4-C5	-5.42	125.89	128.60
1	DB	1467	G	N1-C6-O6	-5.42	116.65	119.90
1	A	572	A	C8-N9-C4	-5.42	103.63	105.80
1	A	661	G	C5-C6-N1	-5.42	108.79	111.50
2	B	417	C	C6-N1-C2	-5.42	118.13	120.30
2	B	1814	G	N1-C6-O6	5.41	123.15	119.90
2	EB	1247	A	N1-C6-N6	5.41	121.85	118.60
2	B	1617	C	C6-N1-C2	5.41	122.47	120.30
2	B	1341	U	OP2-P-O3'	5.41	117.11	105.20
2	B	2877	G	N1-C6-O6	5.41	123.15	119.90
2	EB	327	G	C5-C6-N1	-5.41	108.79	111.50
2	B	401	A	N1-C6-N6	-5.41	115.36	118.60
2	EB	1139	G	N1-C6-O6	5.41	123.14	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	EB	2467	C	N3-C4-C5	-5.41	119.74	121.90
2	EB	2719	G	N1-C6-O6	5.41	123.14	119.90
2	B	726	G	O4'-C1'-N9	5.40	112.52	108.20
2	B	1395	A	N1-C2-N3	5.40	132.00	129.30
2	B	1637	A	C2-N3-C4	-5.40	107.90	110.60
1	DB	1490	C	C6-N1-C2	5.40	122.46	120.30
2	EB	945	A	OP2-P-O3'	5.40	117.08	105.20
2	EB	1628	G	N3-C2-N2	-5.40	116.12	119.90
1	A	523	A	N1-C6-N6	5.40	121.84	118.60
2	EB	943	U	N3-C4-C5	-5.40	111.36	114.60
1	A	331	G	C4-C5-N7	5.40	112.96	110.80
2	EB	2838	G	C6-C5-N7	-5.40	127.16	130.40
2	B	259	G	N1-C6-O6	5.40	123.14	119.90
2	B	936	C	C6-N1-C2	5.39	122.46	120.30
2	B	2447	G	C2-N3-C4	-5.39	109.20	111.90
2	EB	1845	G	N1-C6-O6	5.39	123.14	119.90
2	B	15	G	C5-C6-N1	-5.39	108.80	111.50
2	B	528	A	N9-C4-C5	-5.39	103.64	105.80
2	B	1349	A	N1-C6-N6	5.39	121.83	118.60
2	B	1635	G	OP1-P-O3'	-5.39	93.34	105.20
2	B	2544	G	C2-N3-C4	-5.39	109.20	111.90
1	DB	842	C	N3-C2-O2	-5.39	118.12	121.90
1	A	1109	C	OP2-P-O3'	5.39	117.06	105.20
2	EB	2685	G	N1-C6-O6	5.39	123.13	119.90
2	EB	391	G	C4-C5-C6	5.39	122.03	118.80
2	EB	417	C	C6-N1-C2	-5.39	118.14	120.30
2	EB	2877	G	N1-C6-O6	5.39	123.13	119.90
2	B	2304	G	C8-N9-C1'	5.38	134.00	127.00
2	EB	1142(B)	A	N9-C4-C5	-5.38	103.65	105.80
2	EB	784	A	C6-N1-C2	-5.38	115.37	118.60
2	B	393	C	O5'-P-OP2	5.38	117.16	110.70
2	B	1307	A	N7-C8-N9	-5.38	111.11	113.80
2	B	1538	G	N7-C8-N9	5.38	115.79	113.10
2	B	433	C	N3-C4-C5	5.38	124.05	121.90
2	B	922	U	C5-C4-O4	5.38	129.13	125.90
2	B	1936	A	C2-N3-C4	-5.38	107.91	110.60
2	EB	1022	G	C4-C5-N7	-5.38	108.65	110.80
1	A	728	A	N1-C2-N3	5.38	131.99	129.30
2	B	2043	C	C6-N1-C2	-5.38	118.15	120.30
2	B	2271	G	C8-N9-C1'	-5.38	120.01	127.00
1	DB	108	G	C8-N9-C4	-5.38	104.25	106.40
2	EB	775	G	N1-C6-O6	-5.38	116.67	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	EB	804	A	C2-N3-C4	-5.38	107.91	110.60
1	A	121	C	C2-N1-C1'	5.38	124.72	118.80
1	A	598	U	N3-C4-C5	-5.38	111.37	114.60
2	B	1976	U	C5-C6-N1	-5.38	120.01	122.70
2	B	2004	G	C6-C5-N7	-5.38	127.17	130.40
1	DB	635	G	N1-C6-O6	5.38	123.12	119.90
2	EB	568	U	C5-C4-O4	5.38	129.13	125.90
2	EB	2585	U	N1-C2-O2	5.38	126.56	122.80
2	B	1251	C	N1-C2-O2	5.37	122.12	118.90
2	EB	787	U	O5'-P-OP1	5.37	117.15	110.70
2	B	1632	A	C8-N9-C4	5.37	107.95	105.80
2	B	1779	U	N1-C2-O2	5.37	126.56	122.80
3	C	78	A	N1-C2-N3	5.37	131.99	129.30
2	EB	2735	G	N3-C4-C5	5.37	131.28	128.60
2	EB	1992	G	N3-C4-C5	-5.37	125.92	128.60
2	EB	960	A	N1-C6-N6	5.37	121.82	118.60
2	B	1142(B)	A	N3-C4-N9	-5.37	123.11	127.40
1	DB	576	G	C8-N9-C1'	-5.37	120.03	127.00
1	A	911	U	C5-C4-O4	5.36	129.12	125.90
1	DB	113	G	N7-C8-N9	5.36	115.78	113.10
2	B	2762	G	N1-C6-O6	5.36	123.12	119.90
2	EB	1857	G	N1-C6-O6	5.36	123.11	119.90
2	B	1348	G	C5-C6-O6	-5.36	125.39	128.60
2	B	2008	C	C5-C6-N1	-5.36	118.32	121.00
1	DB	781	A	N1-C6-N6	5.36	121.81	118.60
2	EB	247	G	N3-C4-C5	-5.36	125.92	128.60
2	EB	1185	C	OP2-P-O3'	5.36	116.99	105.20
1	A	818	G	N3-C4-N9	-5.36	122.79	126.00
2	B	562	U	OP2-P-O3'	5.36	116.98	105.20
1	DB	563	A	P-O3'-C3'	5.36	126.13	119.70
2	EB	2614	A	C4-C5-C6	5.36	119.68	117.00
1	DB	1528	U	O5'-P-OP1	5.35	117.12	110.70
2	B	123	G	N9-C4-C5	-5.35	103.26	105.40
2	B	2550	G	O5'-P-OP2	-5.35	100.88	105.70
1	DB	915	A	C8-N9-C4	5.35	107.94	105.80
1	DB	1397	C	N1-C2-O2	5.35	122.11	118.90
2	EB	2526	G	C5-C6-N1	-5.35	108.82	111.50
2	EB	1785	A	C5-N7-C8	-5.35	101.22	103.90
2	EB	2618	G	C6-N1-C2	-5.35	121.89	125.10
1	A	1523	G	C4-C5-C6	5.35	122.01	118.80
2	B	61	G	C2-N3-C4	-5.35	109.23	111.90
1	DB	508	C	N3-C2-O2	-5.34	118.16	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	EB	2609	U	O5'-P-OP2	-5.34	100.89	105.70
2	B	1778	U	N3-C2-O2	5.34	125.94	122.20
2	B	2582	G	O5'-P-OP2	5.34	117.11	110.70
1	DB	44	G	C5-C6-N1	-5.34	108.83	111.50
2	EB	2532	G	N1-C6-O6	5.34	123.10	119.90
2	B	1697	G	N1-C6-O6	5.34	123.10	119.90
2	B	1966	A	C8-N9-C4	5.34	107.94	105.80
2	EB	1236	G	C5-C6-N1	-5.34	108.83	111.50
2	EB	2249	U	N3-C4-O4	5.33	123.13	119.40
2	B	804	A	C5-C6-N6	-5.33	119.43	123.70
2	B	2609	U	C2-N3-C4	-5.33	123.80	127.00
1	DB	331	G	C4-C5-N7	5.33	112.93	110.80
1	DB	922	G	C6-C5-N7	-5.33	127.20	130.40
1	A	1415	G	C5-C6-N1	-5.33	108.83	111.50
2	B	1629	U	C6-N1-C2	-5.33	117.80	121.00
2	B	1975	G	C5-C6-O6	-5.33	125.40	128.60
2	B	2053	G	C5-N7-C8	-5.33	101.63	104.30
2	B	2643	G	C5-C6-O6	-5.33	125.40	128.60
2	B	1187	G	C6-N1-C2	5.33	128.30	125.10
2	EB	2697	G	N1-C6-O6	5.33	123.10	119.90
1	A	927	G	C5-C6-N1	-5.33	108.84	111.50
1	A	944	G	C5-C6-O6	5.33	131.80	128.60
2	B	763	G	N3-C4-C5	-5.33	125.94	128.60
2	B	1470	G	N1-C6-O6	5.33	123.10	119.90
2	B	2430	A	OP2-P-O3'	5.33	116.92	105.20
1	DB	635	G	C5-C6-N1	-5.33	108.84	111.50
2	EB	726	G	C8-N9-C4	-5.33	104.27	106.40
2	EB	1627	G	C6-C5-N7	-5.33	127.20	130.40
2	EB	1981	A	C4-C5-N7	5.33	113.36	110.70
2	EB	2850	A	N1-C2-N3	5.33	131.96	129.30
2	B	2719	G	N3-C4-C5	5.33	131.26	128.60
2	EB	827	U	O5'-P-OP2	-5.33	100.91	105.70
2	EB	2346	A	C8-N9-C4	-5.33	103.67	105.80
1	A	1199	U	C5-C4-O4	5.32	129.09	125.90
1	A	1523	G	C5-C6-N1	-5.32	108.84	111.50
2	B	2086	U	C5-C4-O4	5.32	129.09	125.90
2	B	2639	A	C8-N9-C4	5.32	107.93	105.80
2	EB	1024	G	C5-N7-C8	-5.32	101.64	104.30
2	B	2318	G	C6-C5-N7	-5.32	127.21	130.40
3	C	52	A	N9-C4-C5	-5.32	103.67	105.80
2	B	527	C	C5-C4-N4	-5.32	116.48	120.20
2	B	2067	G	C5-C6-O6	-5.32	125.41	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DB	1399	C	C6-N1-C2	-5.32	118.17	120.30
2	EB	570	G	C5-N7-C8	5.32	106.96	104.30
2	EB	663	G	C4-C5-C6	5.32	121.99	118.80
2	EB	2259	G	C4-C5-N7	5.32	112.93	110.80
2	B	1266	G	C8-N9-C4	5.32	108.53	106.40
3	C	65	C	C2-N1-C1'	5.32	124.65	118.80
3	FB	76	G	C5-C6-O6	-5.32	125.41	128.60
2	B	1126	A	O5'-P-OP1	-5.32	100.92	105.70
2	B	2474	C	C6-N1-C2	5.32	122.43	120.30
1	DB	1522	U	C4-C5-C6	5.32	122.89	119.70
2	EB	391	G	N3-C4-N9	5.32	129.19	126.00
2	B	1304	C	C5-C6-N1	-5.31	118.34	121.00
1	DB	41	G	N1-C6-O6	5.31	123.09	119.90
2	B	1269	A	C5-N7-C8	-5.31	101.24	103.90
2	EB	775	G	N7-C8-N9	-5.31	110.44	113.10
2	B	1753	G	C5-C6-O6	5.31	131.78	128.60
2	B	2491	U	C6-N1-C2	5.31	124.19	121.00
2	EB	1251	C	O5'-P-OP2	-5.31	100.92	105.70
2	EB	2088	G	C5-C6-N1	-5.31	108.85	111.50
2	EB	763	G	N1-C2-N3	5.31	127.08	123.90
2	EB	1266	G	C5-C6-O6	-5.31	125.42	128.60
2	EB	1382	G	N3-C4-C5	5.31	131.25	128.60
2	B	1895	C	N3-C4-C5	5.30	124.02	121.90
2	B	2748	A	C2-N3-C4	-5.30	107.95	110.60
1	DB	821	G	C8-N9-C4	5.30	108.52	106.40
2	EB	874	G	N3-C4-C5	5.30	131.25	128.60
2	EB	1187	G	N7-C8-N9	5.30	115.75	113.10
2	EB	2593	U	C6-N1-C1'	5.30	128.62	121.20
2	B	776	G	C5-C6-N1	-5.30	108.85	111.50
2	B	2791	C	C6-N1-C2	-5.30	118.18	120.30
2	B	600	G	C8-N9-C4	5.30	108.52	106.40
2	B	1840	G	C4-C5-C6	5.30	121.98	118.80
2	B	2072	G	C6-C5-N7	-5.30	127.22	130.40
1	DB	201	C	C6-N1-C2	-5.30	118.18	120.30
2	EB	312	G	N9-C4-C5	-5.30	103.28	105.40
2	B	1216	G	C5-C6-N1	-5.30	108.85	111.50
2	EB	788	A	C8-N9-C4	5.30	107.92	105.80
2	EB	2266	A	O5'-P-OP2	-5.30	100.93	105.70
2	EB	2439	A	OP1-P-O3'	5.30	116.86	105.20
2	B	960	A	C8-N9-C4	5.30	107.92	105.80
2	B	676	A	N9-C4-C5	-5.29	103.68	105.80
2	B	783	A	N9-C4-C5	5.29	107.92	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DB	104	G	N1-C6-O6	5.29	123.08	119.90
1	A	298	A	N1-C6-N6	-5.29	115.42	118.60
2	B	472	A	C6-N1-C2	-5.29	115.42	118.60
2	B	1627	G	C6-C5-N7	-5.29	127.22	130.40
2	B	1825	A	N1-C2-N3	5.29	131.95	129.30
2	EB	1243	G	C5-C6-N1	-5.29	108.85	111.50
2	EB	1325	G	N3-C4-C5	-5.29	125.95	128.60
2	B	613	U	C2-N1-C1'	5.29	124.05	117.70
2	EB	2852	G	N1-C6-O6	5.29	123.08	119.90
1	A	1503	A	C5-N7-C8	5.29	106.55	103.90
2	B	1857	G	C5-C6-N1	-5.29	108.86	111.50
2	B	1756	G	C2-N3-C4	-5.29	109.26	111.90
2	B	2458	G	C8-N9-C4	-5.29	104.28	106.40
2	EB	1374	G	N1-C6-O6	5.29	123.07	119.90
2	EB	1779	U	C6-N1-C1'	-5.29	113.80	121.20
1	A	357	G	N1-C6-O6	5.29	123.07	119.90
2	B	2086	U	N1-C2-N3	5.29	118.07	114.90
2	B	2061	G	OP2-P-O3'	5.28	116.83	105.20
2	B	2461	C	C6-N1-C2	5.28	122.41	120.30
2	EB	2581	G	C5-C6-O6	5.28	131.77	128.60
1	A	766	A	O5'-P-OP1	-5.28	100.95	105.70
2	EB	1307	A	C8-N9-C4	5.28	107.91	105.80
2	B	305	U	C4-C5-C6	5.28	122.87	119.70
2	B	1624	G	C2-N3-C4	-5.28	109.26	111.90
2	EB	1635	G	OP1-P-O3'	-5.28	93.58	105.20
1	A	702	A	N1-C6-N6	5.28	121.77	118.60
2	B	1377	G	N1-C2-N3	5.28	127.07	123.90
2	B	2858	C	C6-N1-C2	5.28	122.41	120.30
2	EB	2693	A	N1-C6-N6	5.28	121.77	118.60
1	A	1399	C	N3-C2-O2	-5.28	118.20	121.90
2	B	1520	U	C5-C4-O4	5.28	129.07	125.90
1	DB	1431	C	C6-N1-C2	-5.28	118.19	120.30
1	A	1528	U	O5'-P-OP1	5.28	117.03	110.70
2	B	205	G	C8-N9-C4	5.28	108.51	106.40
2	B	1762	A	N9-C4-C5	5.27	107.91	105.80
1	DB	1079	G	C4-C5-N7	-5.27	108.69	110.80
2	EB	438	G	N1-C6-O6	5.27	123.06	119.90
2	B	603	A	C8-N9-C4	5.27	107.91	105.80
2	B	1961	C	N3-C4-C5	5.27	124.01	121.90
1	DB	1532	U	C5-C4-O4	-5.27	122.74	125.90
2	EB	698	C	C5-C6-N1	-5.27	118.36	121.00
2	EB	2473	U	C2-N1-C1'	5.27	124.02	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	59	U	C6-N1-C2	-5.27	117.84	121.00
2	B	1614	A	C8-N9-C4	-5.27	103.69	105.80
2	B	2617	C	N3-C4-C5	5.26	124.01	121.90
1	DB	232	G	N1-C6-O6	5.26	123.06	119.90
1	DB	1099	G	N3-C4-N9	-5.26	122.84	126.00
1	A	1158	C	C2-N1-C1'	5.26	124.59	118.80
2	B	2318	G	C4-C5-N7	5.26	112.91	110.80
2	EB	1706	U	C4-C5-C6	5.26	122.86	119.70
1	DB	331	G	C8-N9-C4	-5.26	104.30	106.40
2	EB	2318	G	C4-C5-N7	5.26	112.91	110.80
1	A	232	G	C5-C6-N1	-5.26	108.87	111.50
1	A	507	C	C6-N1-C2	5.26	122.40	120.30
2	B	946	G	C2-N3-C4	-5.26	109.27	111.90
2	EB	1426	G	C4-C5-N7	-5.26	108.70	110.80
2	EB	1602	U	N3-C4-O4	5.26	123.08	119.40
2	B	1327	C	N3-C4-C5	-5.26	119.80	121.90
1	A	331	G	C5-N7-C8	-5.26	101.67	104.30
2	EB	216	A	O5'-P-OP2	-5.26	100.97	105.70
2	EB	2593	U	C5-C6-N1	5.26	125.33	122.70
2	B	2453	A	O5'-P-OP2	5.25	117.01	110.70
2	EB	2755	C	C5-C6-N1	5.25	123.63	121.00
2	B	1378	A	C8-N9-C4	5.25	107.90	105.80
2	EB	1970	A	C8-N9-C4	-5.25	103.70	105.80
2	B	2440	C	N3-C4-C5	-5.25	119.80	121.90
2	B	528	A	C4-C5-C6	-5.25	114.38	117.00
2	B	2587	A	C6-N1-C2	-5.25	115.45	118.60
2	B	2782	G	C6-C5-N7	-5.25	127.25	130.40
2	EB	128	C	N3-C4-C5	5.25	124.00	121.90
2	EB	2032	G	C5-N7-C8	-5.25	101.67	104.30
2	B	1629	U	N3-C4-C5	-5.25	111.45	114.60
1	DB	1488	G	N1-C6-O6	5.25	123.05	119.90
2	EB	2086	U	C5-C4-O4	5.25	129.05	125.90
1	A	576	G	C4-C5-C6	5.25	121.95	118.80
2	EB	1779	U	C5-C4-O4	-5.25	122.75	125.90
2	EB	2053	G	C2-N3-C4	-5.25	109.28	111.90
2	EB	248	G	N1-C6-O6	5.25	123.05	119.90
2	EB	701	G	C5-C6-O6	-5.24	125.45	128.60
2	EB	1646	C	OP1-P-O3'	5.24	116.73	105.20
1	A	111	G	C5-C6-N1	-5.24	108.88	111.50
1	A	691	G	N3-C4-N9	5.24	129.15	126.00
1	A	945	G	C5-C6-O6	-5.24	125.46	128.60
2	B	801	G	C6-N1-C2	-5.24	121.95	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1422	G	N1-C6-O6	5.24	123.04	119.90
2	EB	449	A	OP2-P-O3'	5.24	116.73	105.20
2	EB	1257	C	C6-N1-C2	-5.24	118.20	120.30
1	A	805	C	N3-C4-C5	5.24	124.00	121.90
2	B	649	G	N3-C4-C5	-5.24	125.98	128.60
2	B	870	A	N1-C6-N6	5.24	121.74	118.60
2	B	1319	G	C5-C6-O6	-5.24	125.46	128.60
2	B	1558	A	C8-N9-C4	5.24	107.89	105.80
2	B	1961	C	C6-N1-C2	5.24	122.40	120.30
2	B	2287	A	C2-N3-C4	-5.24	107.98	110.60
2	B	2450	A	O5'-P-OP2	-5.24	100.99	105.70
2	B	2061	G	C5-C6-O6	-5.24	125.46	128.60
2	B	2497	A	C5-N7-C8	-5.24	101.28	103.90
2	EB	1330	C	N3-C4-C5	5.24	124.00	121.90
2	B	2072	G	C5-C6-O6	-5.24	125.46	128.60
2	EB	784	A	N1-C6-N6	-5.24	115.46	118.60
2	B	465	G	C8-N9-C4	-5.23	104.31	106.40
2	B	933	A	O4'-C1'-N9	5.23	112.39	108.20
2	EB	2587	A	N1-C6-N6	5.23	121.74	118.60
2	B	2873	A	N1-C6-N6	5.23	121.74	118.60
2	EB	1573	G	C8-N9-C4	5.23	108.49	106.40
2	B	1234	U	N3-C2-O2	-5.23	118.54	122.20
1	DB	563	A	C8-N9-C4	-5.23	103.71	105.80
2	EB	1187	G	C6-N1-C2	5.23	128.24	125.10
1	A	677	U	C6-N1-C2	-5.23	117.86	121.00
2	B	1840	G	C6-C5-N7	-5.23	127.26	130.40
2	B	1960	A	C8-N9-C4	5.23	107.89	105.80
2	B	2063	C	N3-C4-C5	-5.23	119.81	121.90
2	EB	2575	C	N1-C2-O2	-5.23	115.76	118.90
1	A	842	C	N3-C4-C5	-5.23	119.81	121.90
2	B	2546	U	C5-C4-O4	5.23	129.04	125.90
2	B	564	C	C6-N1-C2	-5.22	118.21	120.30
2	B	775	G	C5-C6-O6	5.22	131.73	128.60
2	EB	2458	G	N3-C4-N9	5.22	129.13	126.00
2	B	2706	G	N1-C6-O6	5.22	123.03	119.90
2	EB	2439	A	C2-N3-C4	-5.22	107.99	110.60
2	B	265	A	N7-C8-N9	5.22	116.41	113.80
2	B	570	G	N9-C4-C5	5.22	107.49	105.40
2	B	726	G	C8-N9-C4	-5.22	104.31	106.40
2	B	1327	C	C5-C6-N1	5.22	123.61	121.00
2	EB	464	U	N3-C4-C5	-5.22	111.47	114.60
2	EB	2245	U	C4-C5-C6	5.22	122.83	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1035	U	C5-C4-O4	5.22	129.03	125.90
1	A	22	G	N1-C6-O6	5.22	123.03	119.90
1	A	331	G	N7-C8-N9	5.22	115.71	113.10
2	B	2686	G	C4-N9-C1'	5.22	133.28	126.50
2	B	2846	G	N1-C6-O6	5.22	123.03	119.90
2	EB	2598	A	C2-N3-C4	-5.22	107.99	110.60
1	A	781	A	N9-C4-C5	-5.21	103.71	105.80
2	B	1252	G	O4'-C1'-N9	-5.21	104.03	108.20
2	B	2439	A	OP1-P-O3'	5.21	116.67	105.20
2	B	2452	C	C2-N1-C1'	5.21	124.54	118.80
2	B	2567	G	C2-N3-C4	-5.21	109.29	111.90
2	EB	1003	G	N1-C6-O6	5.21	123.03	119.90
1	A	665	A	N1-C6-N6	-5.21	115.47	118.60
2	B	982	C	O4'-C1'-N1	-5.21	104.03	108.20
1	A	117	G	C5-N7-C8	-5.21	101.70	104.30
2	B	571	A	O5'-P-OP2	-5.21	101.01	105.70
2	B	2514	U	C5-C4-O4	5.21	129.03	125.90
2	EB	695	G	N1-C6-O6	5.21	123.03	119.90
2	EB	695	G	O5'-P-OP2	-5.21	101.01	105.70
2	EB	1695	G	C4-C5-N7	5.21	112.88	110.80
2	B	540	G	N1-C6-O6	5.21	123.02	119.90
1	A	899	C	C5-C6-N1	5.21	123.60	121.00
2	B	68	G	N3-C2-N2	-5.20	116.26	119.90
2	B	1297	C	C5-C6-N1	5.20	123.60	121.00
2	EB	960	A	C4-C5-N7	5.20	113.30	110.70
2	EB	2318	G	C6-C5-N7	-5.20	127.28	130.40
1	A	251	G	O4'-C1'-N9	-5.20	104.04	108.20
2	B	980	A	N7-C8-N9	5.20	116.40	113.80
2	B	1402	C	C4-C5-C6	5.20	120.00	117.40
2	EB	2514	U	N3-C4-C5	-5.20	111.48	114.60
2	B	2439	A	O4'-C1'-N9	-5.20	104.04	108.20
3	C	87	G	C5-N7-C8	5.20	106.90	104.30
2	B	1021	A	C8-N9-C4	-5.20	103.72	105.80
2	B	2319	G	N3-C4-C5	5.20	131.20	128.60
2	EB	948	G	C2-N3-C4	-5.20	109.30	111.90
1	A	562	C	N3-C4-C5	5.20	123.98	121.90
2	B	791	C	N3-C4-C5	5.20	123.98	121.90
2	B	1131	G	N3-C4-C5	5.20	131.20	128.60
1	DB	246	A	O5'-P-OP2	-5.20	101.02	105.70
2	EB	1366	A	N9-C4-C5	5.20	107.88	105.80
2	EB	2607	G	N3-C4-N9	5.20	129.12	126.00
2	B	397	G	N1-C6-O6	5.19	123.02	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1346	A	C8-N9-C4	5.19	107.88	105.80
2	B	179	G	C8-N9-C1'	-5.19	120.25	127.00
2	B	1941	C	C6-N1-C2	5.19	122.38	120.30
2	B	82	G	C5-C6-N1	-5.19	108.91	111.50
2	B	1021	A	N7-C8-N9	5.19	116.40	113.80
2	B	1633	G	C4-C5-C6	5.19	121.92	118.80
2	EB	505	A	C5-C6-N1	5.19	120.30	117.70
2	EB	1936	A	O5'-P-OP2	-5.19	101.03	105.70
2	EB	2056	G	O4'-C1'-N9	-5.19	104.05	108.20
2	B	583	G	N1-C2-N3	5.19	127.01	123.90
2	B	747	U	C6-N1-C2	5.19	124.11	121.00
2	EB	2582	G	C4-N9-C1'	5.19	133.25	126.50
2	EB	304	G	C5-C6-N1	-5.19	108.91	111.50
2	EB	933	A	O4'-C1'-N9	5.19	112.35	108.20
2	EB	1315	C	O5'-P-OP1	-5.19	101.03	105.70
2	B	1326	U	N3-C2-O2	-5.18	118.57	122.20
2	B	1618	A	C5-C6-N6	-5.18	119.55	123.70
1	DB	106	C	N1-C2-O2	-5.18	115.79	118.90
2	EB	1269	A	C8-N9-C4	-5.18	103.73	105.80
2	EB	2569	G	OP1-P-O3'	5.18	116.61	105.20
2	B	1021	A	N3-C4-N9	-5.18	123.25	127.40
2	B	1043	C	N1-C2-O2	5.18	122.01	118.90
2	B	2490	G	C5-C6-O6	5.18	131.71	128.60
2	EB	146	G	N1-C6-O6	5.18	123.01	119.90
2	B	2593	U	C5-C6-N1	5.18	125.29	122.70
2	B	1816	G	C5-C6-N1	-5.18	108.91	111.50
2	EB	2545	G	N1-C6-O6	5.18	123.01	119.90
2	B	971	C	C6-N1-C2	5.18	122.37	120.30
2	B	196	A	N7-C8-N9	5.18	116.39	113.80
2	B	1314	C	OP2-P-O3'	5.18	116.59	105.20
2	B	2306	C	C6-N1-C2	5.17	122.37	120.30
2	EB	257	A	C8-N9-C4	5.17	107.87	105.80
2	B	1359	A	N1-C6-N6	5.17	121.70	118.60
2	B	1797	C	C6-N1-C2	5.17	122.37	120.30
2	EB	387	U	O5'-P-OP2	-5.17	101.05	105.70
2	EB	1538	G	C8-N9-C4	-5.17	104.33	106.40
2	B	1349	A	N9-C4-C5	-5.17	103.73	105.80
2	B	1614	A	N7-C8-N9	5.17	116.38	113.80
2	B	2680	C	C6-N1-C2	5.17	122.37	120.30
2	B	475	U	C6-N1-C2	-5.17	117.90	121.00
2	EB	1778	U	C2-N1-C1'	-5.17	111.50	117.70
3	FB	52	A	N9-C4-C5	-5.17	103.73	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	802	A	N7-C8-N9	5.16	116.38	113.80
2	EB	1454	U	N3-C2-O2	5.16	125.81	122.20
2	B	2519	U	O5'-P-OP1	-5.16	101.05	105.70
2	EB	2686	G	C4-N9-C1'	5.16	133.21	126.50
2	B	1657	C	OP1-P-O3'	5.16	116.55	105.20
2	B	1964	G	N7-C8-N9	-5.16	110.52	113.10
2	B	2250	G	N1-C6-O6	-5.16	116.81	119.90
2	EB	2248	C	O5'-P-OP2	5.16	116.89	110.70
1	DB	108	G	N7-C8-N9	5.16	115.68	113.10
1	DB	1523	G	C4-C5-C6	5.16	121.89	118.80
2	EB	596	G	C2-N3-C4	-5.16	109.32	111.90
2	B	59	U	C5-C4-O4	5.15	128.99	125.90
2	B	1773	A	N1-C2-N3	5.15	131.88	129.30
1	A	1481	U	C4-C5-C6	5.15	122.79	119.70
2	B	508	G	C4-C5-N7	-5.15	108.74	110.80
2	B	1158	C	C6-N1-C2	5.15	122.36	120.30
2	B	1969	A	OP2-P-O3'	5.15	116.54	105.20
2	B	2718	G	N1-C6-O6	5.15	122.99	119.90
1	DB	612	C	C6-N1-C2	5.15	122.36	120.30
2	EB	195	A	N7-C8-N9	5.15	116.38	113.80
2	EB	1367	A	N1-C2-N3	5.15	131.88	129.30
1	A	50	A	N1-C6-N6	5.15	121.69	118.60
2	B	667	U	N3-C4-O4	5.15	123.00	119.40
1	DB	945	G	C6-C5-N7	-5.15	127.31	130.40
2	B	2644	G	C5-C6-N1	-5.15	108.93	111.50
2	B	140	A	C5-C6-N1	-5.14	115.13	117.70
2	B	1659	U	N3-C2-O2	5.14	125.80	122.20
2	B	2714	G	O5'-P-OP1	-5.14	101.07	105.70
1	DB	771	G	C8-N9-C4	5.14	108.46	106.40
2	EB	2437	U	N3-C4-C5	-5.14	111.51	114.60
1	A	112	G	C5-C6-N1	-5.14	108.93	111.50
2	B	2070	G	N1-C6-O6	5.14	122.98	119.90
2	EB	790	C	O5'-P-OP2	-5.14	101.07	105.70
2	B	531	C	C2-N3-C4	-5.14	117.33	119.90
2	B	1981	A	N7-C8-N9	5.14	116.37	113.80
2	EB	1538	G	N7-C8-N9	5.14	115.67	113.10
2	EB	1672	C	C2-N1-C1'	5.14	124.45	118.80
2	EB	1698	A	C6-C5-N7	-5.14	128.70	132.30
2	B	55	G	C5-C6-N1	-5.14	108.93	111.50
2	EB	754	C	C5-C6-N1	-5.14	118.43	121.00
1	A	1417	G	C5-C6-N1	-5.14	108.93	111.50
2	B	198	C	O5'-P-OP2	5.14	116.86	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1780	A	C2-N3-C4	-5.14	108.03	110.60
1	DB	793	U	N1-C2-N3	5.14	117.98	114.90
1	A	1512	U	C6-N1-C2	-5.13	117.92	121.00
2	B	213	A	N7-C8-N9	-5.13	111.23	113.80
2	B	792	G	OP2-P-O3'	5.13	116.49	105.20
2	EB	2272	U	C5-C6-N1	-5.13	120.13	122.70
2	B	761	A	N7-C8-N9	5.13	116.37	113.80
2	B	1243	G	C5-C6-N1	-5.13	108.93	111.50
1	DB	1417	G	C4-C5-C6	5.13	121.88	118.80
2	EB	59	U	C5-C4-O4	5.13	128.98	125.90
2	EB	330	A	C8-N9-C4	5.13	107.85	105.80
2	EB	728	G	C5-C6-O6	-5.13	125.52	128.60
2	EB	2490	G	C5-C6-N1	-5.13	108.94	111.50
2	EB	2599	G	N3-C4-N9	-5.13	122.92	126.00
1	A	576	G	C4-N9-C1'	5.13	133.17	126.50
2	B	259	G	C4-C5-N7	5.13	112.85	110.80
2	B	2581	G	C8-N9-C4	-5.13	104.35	106.40
1	DB	789	U	N3-C4-C5	-5.13	111.52	114.60
2	EB	404	C	N3-C4-C5	5.13	123.95	121.90
2	EB	2710	C	N3-C2-O2	-5.13	118.31	121.90
1	A	299	G	C5-C6-N1	-5.13	108.94	111.50
2	B	195	A	C4-C5-N7	5.13	113.26	110.70
2	B	648	G	N1-C6-O6	5.12	122.97	119.90
2	B	1275	A	N1-C6-N6	5.12	121.67	118.60
2	B	1900	A	N1-C2-N3	5.12	131.86	129.30
2	EB	1305	C	N1-C2-O2	-5.12	115.83	118.90
2	EB	1497	U	N1-C2-O2	5.12	126.39	122.80
1	A	677	U	N3-C2-O2	-5.12	118.61	122.20
2	B	2056	G	N3-C4-N9	5.12	129.07	126.00
2	EB	2544	G	C5-C6-N1	-5.12	108.94	111.50
2	B	1344	G	C8-N9-C4	-5.12	104.35	106.40
2	EB	465	G	C8-N9-C4	-5.12	104.35	106.40
2	EB	2582	G	OP2-P-O3'	5.12	116.47	105.20
2	B	228	A	N1-C6-N6	5.12	121.67	118.60
2	B	1667	G	N9-C4-C5	-5.12	103.35	105.40
1	A	842	C	N3-C2-O2	-5.12	118.32	121.90
2	B	2616	C	N3-C2-O2	5.12	125.48	121.90
2	EB	2430	A	C8-N9-C4	-5.12	103.75	105.80
2	B	2485	G	N1-C6-O6	5.12	122.97	119.90
1	DB	1467	G	C6-C5-N7	5.12	133.47	130.40
2	EB	670	A	OP1-P-O3'	5.12	116.45	105.20
2	EB	1231	G	C2-N3-C4	-5.12	109.34	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	EB	2560	C	N3-C4-N4	5.12	121.58	118.00
2	B	442	G	C8-N9-C4	5.11	108.44	106.40
2	B	1127	A	C8-N9-C4	5.11	107.84	105.80
1	DB	282	A	C5-C6-N6	-5.11	119.61	123.70
3	FB	65	C	N1-C2-O2	5.11	121.97	118.90
1	DB	1137	C	C6-N1-C2	-5.11	118.25	120.30
2	EB	479	A	N1-C6-N6	-5.11	115.53	118.60
2	B	746	A	C8-N9-C4	-5.11	103.76	105.80
2	B	2056	G	C5-N7-C8	-5.11	101.75	104.30
2	EB	330	A	N3-C4-C5	5.11	130.38	126.80
2	B	2298	A	N1-C6-N6	-5.11	115.53	118.60
2	EB	1969	A	OP2-P-O3'	5.11	116.44	105.20
1	A	1099	G	N9-C4-C5	5.11	107.44	105.40
2	B	2275	C	C6-N1-C2	5.11	122.34	120.30
2	B	2574	G	N1-C6-O6	5.11	122.96	119.90
2	EB	1627	G	C5-C6-O6	-5.11	125.54	128.60
2	B	687	C	C6-N1-C2	-5.11	118.26	120.30
2	B	1335	U	N1-C2-N3	5.11	117.96	114.90
2	B	1427	A	N7-C8-N9	-5.10	111.25	113.80
2	EB	179	G	C5-C6-N1	-5.10	108.95	111.50
2	B	1573	G	C8-N9-C4	5.10	108.44	106.40
2	EB	1131	G	O5'-P-OP2	-5.10	101.11	105.70
2	B	1899	G	C5-C6-N1	-5.10	108.95	111.50
2	B	1983	C	C5-C6-N1	-5.10	118.45	121.00
2	EB	1761	C	O5'-P-OP2	-5.10	101.11	105.70
2	B	1699	G	C4-C5-N7	-5.10	108.76	110.80
2	EB	1762	A	O4'-C1'-N9	5.10	112.28	108.20
3	FB	87	G	N7-C8-N9	-5.10	110.55	113.10
2	B	471	A	N1-C2-N3	5.10	131.85	129.30
2	B	701	G	N1-C6-O6	5.10	122.96	119.90
2	B	2686	G	N3-C4-N9	5.10	129.06	126.00
2	EB	805	G	N7-C8-N9	5.10	115.65	113.10
2	EB	817	C	N3-C2-O2	-5.10	118.33	121.90
2	EB	1429	G	N1-C6-O6	-5.10	116.84	119.90
2	EB	1779	U	OP1-P-O3'	5.10	116.41	105.20
2	EB	2508	G	N1-C6-O6	5.10	122.96	119.90
2	B	1186	G	N1-C6-O6	5.10	122.96	119.90
2	EB	2277	G	N1-C6-O6	5.10	122.96	119.90
2	EB	2287	A	N1-C6-N6	5.10	121.66	118.60
2	EB	2532	G	C6-C5-N7	-5.10	127.34	130.40
2	B	783	A	N1-C6-N6	-5.09	115.54	118.60
2	B	854	G	C5-C6-N1	-5.09	108.95	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2505	G	N3-C4-N9	-5.09	122.94	126.00
2	EB	2218	G	C2-N3-C4	-5.09	109.35	111.90
2	B	1348	G	C2-N3-C4	-5.09	109.35	111.90
2	EB	831	G	N3-C2-N2	-5.09	116.33	119.90
1	A	298	A	C8-N9-C4	-5.09	103.76	105.80
2	B	828	U	C5-C6-N1	-5.09	120.15	122.70
2	B	1629	U	N1-C2-N3	5.09	117.95	114.90
1	A	576	G	C5-C6-N1	-5.09	108.95	111.50
2	B	1647	G	OP1-P-O3'	5.09	116.39	105.20
2	EB	27	G	N3-C4-C5	5.09	131.15	128.60
2	EB	2502	G	C5-C6-N1	-5.09	108.95	111.50
1	A	328	C	N1-C2-O2	5.09	121.95	118.90
2	EB	2640	G	N1-C6-O6	5.09	122.95	119.90
2	B	594	U	C5-C4-O4	5.09	128.95	125.90
2	B	1328	G	N3-C4-N9	5.09	129.05	126.00
1	DB	23	C	N3-C4-C5	-5.09	119.86	121.90
1	DB	888	G	C5-C6-O6	5.09	131.65	128.60
2	EB	2243	U	O5'-P-OP1	5.09	116.80	110.70
2	EB	528	A	N1-C6-N6	5.08	121.65	118.60
2	EB	439	G	N1-C6-O6	5.08	122.95	119.90
2	EB	969	U	C5-C4-O4	5.08	128.95	125.90
2	EB	1024	G	N7-C8-N9	5.08	115.64	113.10
2	EB	2827	C	N3-C4-C5	-5.08	119.87	121.90
2	B	197	A	O5'-P-OP1	5.08	116.80	110.70
1	DB	1201	A	P-O3'-C3'	5.08	125.80	119.70
1	A	789	U	C6-N1-C2	-5.08	117.95	121.00
34	HA	15	A	N9-C4-C5	-5.08	103.77	105.80
2	EB	929	G	C6-C5-N7	-5.08	127.35	130.40
2	EB	1940	U	C6-N1-C2	-5.08	117.95	121.00
2	B	216	A	O5'-P-OP2	-5.08	101.13	105.70
2	B	1788	C	O5'-P-OP2	-5.08	101.13	105.70
2	EB	639	U	C5-C4-O4	5.08	128.94	125.90
2	EB	1779	U	C2-N1-C1'	5.08	123.79	117.70
2	EB	2505	G	C8-N9-C4	-5.08	104.37	106.40
2	B	1417	C	C4-C5-C6	5.07	119.94	117.40
2	B	2319	G	C5-N7-C8	-5.07	101.76	104.30
1	DB	899	C	C2-N1-C1'	5.07	124.38	118.80
2	EB	2271	G	N1-C2-N3	5.07	126.94	123.90
2	B	530	G	N1-C2-N3	-5.07	120.86	123.90
1	A	754	C	C2-N3-C4	5.07	122.44	119.90
2	B	832	G	C8-N9-C1'	-5.07	120.41	127.00
2	B	1753	G	C4-C5-N7	-5.07	108.77	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	EB	2232	U	C5-C4-O4	5.07	128.94	125.90
2	EB	2585	U	N3-C2-O2	-5.07	118.65	122.20
2	B	504	U	C2-N1-C1'	5.07	123.78	117.70
2	B	707	G	C5-C6-N1	-5.07	108.97	111.50
2	B	774	A	C2-N3-C4	5.07	113.13	110.60
2	B	2034	U	C5-C4-O4	-5.07	122.86	125.90
2	EB	795	C	N1-C2-N3	5.07	122.75	119.20
2	EB	1359	A	C2-N3-C4	-5.07	108.07	110.60
2	EB	1703	G	C6-C5-N7	-5.07	127.36	130.40
2	B	440	G	N1-C6-O6	5.07	122.94	119.90
2	B	871	U	N1-C2-O2	-5.07	119.25	122.80
2	B	1940	U	C6-N1-C2	-5.07	117.96	121.00
2	EB	698	C	C6-N1-C2	5.07	122.33	120.30
2	EB	1426	G	C5-C6-O6	5.07	131.64	128.60
2	EB	2028	U	C4-C5-C6	5.07	122.74	119.70
2	B	908	C	C6-N1-C2	-5.06	118.28	120.30
1	DB	650	G	N1-C6-O6	5.06	122.94	119.90
2	EB	2709	G	N1-C6-O6	5.06	122.94	119.90
1	A	576	G	C6-C5-N7	-5.06	127.36	130.40
2	B	2341	G	C8-N9-C4	-5.06	104.38	106.40
2	EB	215	G	C5-C6-O6	-5.06	125.57	128.60
2	EB	494	G	C5-C6-O6	-5.06	125.57	128.60
2	EB	683	C	C6-N1-C2	-5.06	118.28	120.30
2	EB	1698	A	C4-C5-N7	5.06	113.23	110.70
2	B	1173	G	C8-N9-C4	-5.06	104.38	106.40
2	B	1829	A	C5-C6-N1	5.06	120.23	117.70
2	B	494	G	C4-C5-N7	5.05	112.82	110.80
2	B	1632	A	C5-C6-N1	5.05	120.23	117.70
2	EB	1981	A	N3-C4-C5	5.05	130.34	126.80
2	B	1323	U	N3-C4-C5	-5.05	111.57	114.60
2	B	801	G	N1-C2-N2	-5.05	111.65	116.20
1	DB	304	U	C4-C5-C6	5.05	122.73	119.70
2	EB	577	G	OP2-P-O3'	5.05	116.31	105.20
2	EB	2250	G	C8-N9-C4	-5.05	104.38	106.40
2	B	259	G	C5-C6-O6	-5.05	125.57	128.60
2	B	1397	U	N1-C2-O2	5.05	126.33	122.80
2	B	2061	G	N3-C4-N9	5.05	129.03	126.00
1	DB	1523	G	C5-C6-N1	-5.05	108.97	111.50
2	EB	115	C	C6-N1-C2	5.05	122.32	120.30
2	EB	818	G	C4-N9-C1'	5.05	133.06	126.50
2	B	213	A	C2-N3-C4	-5.05	108.08	110.60
2	B	312	G	C5-C6-N1	-5.05	108.98	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	960	A	N1-C6-N6	5.05	121.63	118.60
1	DB	1054	C	N3-C4-C5	-5.05	119.88	121.90
2	EB	1526	G	N9-C4-C5	-5.05	103.38	105.40
2	EB	2066	C	N1-C2-O2	-5.05	115.87	118.90
2	EB	2271	G	C8-N9-C1'	-5.05	120.44	127.00
2	B	465	G	C5-C6-N1	-5.04	108.98	111.50
2	B	819	A	C5-N7-C8	-5.04	101.38	103.90
2	B	1139	G	N1-C6-O6	5.04	122.92	119.90
2	B	2358	G	N1-C6-O6	-5.04	116.88	119.90
1	DB	236	G	N1-C6-O6	5.04	122.92	119.90
1	DB	1391	U	C5-C6-N1	-5.04	120.18	122.70
2	B	789	A	OP2-P-O3'	5.04	116.29	105.20
2	B	552	G	N1-C6-O6	5.04	122.92	119.90
2	B	1381	G	C6-C5-N7	-5.04	127.38	130.40
2	B	1781	C	C6-N1-C2	5.04	122.31	120.30
2	B	2259	G	N1-C6-O6	5.04	122.92	119.90
2	B	2321	G	C4-N9-C1'	5.04	133.05	126.50
2	EB	534	U	N1-C2-N3	5.04	117.92	114.90
2	EB	1497	U	C2-N1-C1'	5.04	123.75	117.70
2	EB	2542	A	C4-C5-N7	5.04	113.22	110.70
1	DB	1520	G	C5-C6-N1	-5.04	108.98	111.50
2	B	1778	U	C5-C4-O4	5.04	128.92	125.90
2	B	2817	G	N3-C4-C5	-5.04	126.08	128.60
31	EA	28	ARG	NE-CZ-NH1	-5.04	117.78	120.30
2	EB	2013	A	OP2-P-O3'	5.04	116.28	105.20
3	FB	64	C	C6-N1-C2	5.04	122.31	120.30
2	B	254	G	C5-C6-O6	-5.03	125.58	128.60
2	B	460	A	C2-N3-C4	-5.03	108.08	110.60
2	B	724	U	C6-N1-C2	-5.03	117.98	121.00
2	B	2526	G	C5-C6-N1	-5.03	108.98	111.50
2	EB	1773	A	OP1-P-O3'	5.03	116.27	105.20
2	B	263	C	N3-C2-O2	-5.03	118.38	121.90
2	B	1926	U	N3-C2-O2	-5.03	118.68	122.20
2	EB	2491	U	O5'-P-OP2	5.03	116.74	110.70
2	EB	2892	A	C8-N9-C4	-5.03	103.79	105.80
2	B	247	G	N3-C4-N9	5.03	129.02	126.00
1	DB	240	C	N3-C4-C5	-5.03	119.89	121.90
2	EB	739	G	C8-N9-C4	5.03	108.41	106.40
2	EB	940	G	N1-C6-O6	5.03	122.92	119.90
1	A	1077	G	N1-C6-O6	5.03	122.92	119.90
1	A	585	G	N1-C6-O6	5.03	122.92	119.90
2	EB	570	G	N9-C4-C5	5.03	107.41	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	EB	1845	G	C8-N9-C4	5.03	108.41	106.40
1	A	793	U	C5-C4-O4	5.03	128.91	125.90
2	B	140	A	C2-N3-C4	-5.03	108.09	110.60
2	B	1940	U	N3-C4-C5	-5.03	111.58	114.60
2	B	2341	G	N1-C6-O6	5.03	122.92	119.90
2	B	2561	A	N1-C6-N6	5.03	121.61	118.60
2	EB	2061	G	C8-N9-C1'	-5.03	120.47	127.00
2	EB	2501	C	N1-C2-O2	-5.03	115.88	118.90
2	EB	2004	G	C6-C5-N7	-5.02	127.39	130.40
2	B	729	G	P-O3'-C3'	5.02	125.73	119.70
2	B	963	U	O5'-P-OP2	5.02	116.73	110.70
2	B	1429	G	C8-N9-C4	-5.02	104.39	106.40
2	B	1633	G	C5-C6-N1	-5.02	108.99	111.50
1	DB	1503	A	N3-C4-C5	-5.02	123.28	126.80
2	EB	188	G	C5-N7-C8	-5.02	101.79	104.30
2	EB	1797	C	C6-N1-C2	5.02	122.31	120.30
2	B	248	G	N3-C4-C5	5.02	131.11	128.60
2	B	775	G	C4-C5-N7	-5.02	108.79	110.80
2	EB	1327	C	C6-N1-C2	-5.02	118.29	120.30
1	DB	1077	G	N1-C6-O6	5.02	122.91	119.90
2	EB	1768	U	C5-C4-O4	5.01	128.91	125.90
2	EB	1971	A	O5'-P-OP2	-5.01	101.19	105.70
2	EB	2070	G	O5'-P-OP2	5.01	116.72	110.70
1	A	1523	G	C4-N9-C1'	5.01	133.02	126.50
2	B	686	G	C4-C5-N7	5.01	112.81	110.80
2	B	1435	G	C4-C5-N7	5.01	112.81	110.80
2	EB	2091	U	N3-C4-C5	-5.01	111.59	114.60
1	A	362	G	N1-C6-O6	5.01	122.91	119.90
2	B	1275	A	C8-N9-C4	5.01	107.80	105.80
2	B	1357	U	C4-C5-C6	5.01	122.71	119.70
2	EB	1622	G	C5-C6-O6	-5.01	125.59	128.60
2	EB	2431	U	C5-C4-O4	5.01	128.91	125.90
2	B	133	C	N1-C2-O2	-5.01	115.89	118.90
2	EB	2140	C	C6-N1-C2	-5.01	118.30	120.30
1	A	701	C	C6-N1-C2	5.01	122.30	120.30
2	B	2085	C	C5-C6-N1	-5.01	118.50	121.00
2	B	2573	C	C5-C6-N1	-5.01	118.50	121.00
2	EB	1621	U	OP2-P-O3'	5.01	116.22	105.20
2	B	1921	G	N1-C6-O6	5.00	122.90	119.90
2	EB	1700	A	C2-N3-C4	-5.00	108.10	110.60
2	B	34	C	P-O3'-C3'	5.00	125.70	119.70
2	B	854	G	C2-N3-C4	-5.00	109.40	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	EB	1769	G	C6-C5-N7	-5.00	127.40	130.40
2	EB	2419	U	C6-N1-C2	-5.00	118.00	121.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32394	0	16367	505	0
1	DB	32394	0	16367	492	0
2	B	62031	0	31275	829	0
2	EB	62031	0	31275	802	0
3	C	2576	0	1305	35	0
3	FB	2576	0	1305	35	0
4	D	1642	0	841	26	0
4	GB	1642	0	841	29	0
4	IA	1642	0	841	12	0
4	LC	1642	0	841	10	0
5	E	2145	0	2234	91	0
5	HB	2145	0	2234	78	0
6	F	1563	0	1629	61	0
6	IB	1563	0	1629	55	0
7	G	1586	0	1632	65	0
7	JB	1586	0	1632	61	0
8	H	1471	0	1526	67	0
8	KB	1471	0	1526	62	0
9	I	1330	0	1407	57	0
9	LB	1330	0	1407	51	0
10	J	1137	0	1225	50	0
10	MB	1137	0	1225	40	0
11	K	1121	0	1195	34	0
11	NB	1121	0	1195	31	0
12	L	932	0	994	32	0
12	OB	932	0	994	27	0
13	M	1145	0	1228	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	PB	1145	0	1228	35	0
14	N	1121	0	1179	36	0
14	QB	1121	0	1179	42	0
15	O	968	0	1033	39	0
15	RB	968	0	1033	43	0
16	P	877	0	938	28	0
16	SB	877	0	938	29	0
17	Q	1143	0	1211	37	0
17	TB	1143	0	1211	33	0
18	R	964	0	1022	25	0
18	UB	964	0	1022	30	0
19	S	779	0	852	28	0
19	VB	779	0	852	29	0
20	T	890	0	951	34	0
20	WB	890	0	951	26	0
21	U	750	0	814	14	0
21	XB	750	0	814	14	0
22	V	814	0	907	28	0
22	YB	814	0	907	25	0
23	W	1495	0	1521	51	0
23	ZB	1495	0	1521	50	0
24	AC	662	0	688	23	0
24	X	662	0	688	23	0
25	BC	761	0	837	28	0
25	Y	761	0	837	30	0
26	CC	592	0	654	16	0
26	Z	592	0	654	16	0
27	AA	477	0	529	16	0
27	DC	477	0	529	16	0
28	BA	552	0	537	23	0
28	EC	552	0	537	22	0
29	CA	460	0	484	17	0
29	FC	460	0	484	19	0
30	DA	453	0	477	11	0
30	GC	453	0	477	11	0
31	EA	418	0	467	17	0
31	HC	418	0	467	17	0
32	FA	517	0	582	17	0
32	IC	517	0	582	19	0
33	GA	307	0	338	15	0
33	JC	307	0	337	16	0
34	HA	220	0	108	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	KC	220	0	108	9	0
35	JA	1900	0	1951	69	0
35	MC	1900	0	1951	69	0
36	KA	1612	0	1677	49	0
36	NC	1612	0	1677	48	0
37	LA	1703	0	1765	74	0
37	OC	1703	0	1765	68	0
38	MA	1155	0	1213	45	0
38	PC	1155	0	1213	51	0
39	NA	843	0	857	44	0
39	QC	843	0	857	40	0
40	OA	1257	0	1296	38	0
40	RC	1257	0	1296	42	0
41	PA	1116	0	1177	49	0
41	SC	1116	0	1177	48	0
42	QA	1011	0	1043	43	0
42	TC	1011	0	1043	43	0
43	RA	794	0	840	25	0
43	UC	794	0	840	27	0
44	SA	864	0	881	25	0
44	VC	864	0	881	21	0
45	TA	958	0	1047	31	0
45	WC	958	0	1047	31	0
46	UA	933	0	992	50	0
46	XC	933	0	992	47	0
47	VA	492	0	533	20	0
47	YC	492	0	533	17	0
48	WA	734	0	771	31	0
48	ZC	734	0	771	27	0
49	AD	700	0	720	20	0
49	XA	700	0	720	20	0
50	BD	823	0	893	24	0
50	YA	823	0	893	21	0
51	CD	574	0	644	17	0
51	ZA	574	0	644	19	0
52	AB	665	0	686	28	0
52	DD	665	0	686	29	0
53	BB	762	0	859	27	0
53	ED	762	0	859	27	0
54	CB	208	0	221	4	0
54	FD	208	0	221	12	0
55	GD	1980	0	1942	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	HD	1980	0	1942	63	0
56	A	160	0	0	0	0
56	AB	1	0	0	0	0
56	AC	2	0	0	0	0
56	AD	1	0	0	0	0
56	B	514	0	0	0	0
56	BB	1	0	0	0	0
56	BC	1	0	0	0	0
56	BD	2	0	0	0	0
56	C	23	0	0	0	0
56	CA	1	0	0	0	0
56	CD	2	0	0	0	0
56	D	6	0	0	0	0
56	DB	177	0	0	0	0
56	DC	1	0	0	0	0
56	E	4	0	0	0	0
56	EA	1	0	0	0	0
56	EB	395	0	0	0	0
56	ED	1	0	0	0	0
56	F	1	0	0	0	0
56	FA	1	0	0	0	0
56	FB	17	0	0	0	0
56	FC	1	0	0	0	0
56	G	4	0	0	0	0
56	GB	5	0	0	0	0
56	GD	5	0	0	0	0
56	H	1	0	0	0	0
56	HA	1	0	0	0	0
56	HB	8	0	0	0	0
56	HC	1	0	0	0	0
56	HD	3	0	0	0	0
56	I	3	0	0	0	0
56	IA	8	0	0	0	0
56	IB	3	0	0	0	0
56	IC	2	0	0	0	0
56	J	5	0	0	0	0
56	JA	3	0	0	0	0
56	JB	2	0	0	0	0
56	JC	1	0	0	0	0
56	K	2	0	0	0	0
56	KA	1	0	0	0	0
56	KB	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	KC	1	0	0	0	0
56	L	7	0	0	0	0
56	LA	1	0	0	0	0
56	LB	5	0	0	0	0
56	LC	8	0	0	0	0
56	M	4	0	0	0	0
56	MA	3	0	0	0	0
56	MB	2	0	0	0	0
56	MC	3	0	0	0	0
56	N	3	0	0	0	0
56	NA	2	0	0	0	0
56	NB	1	0	0	0	0
56	O	1	0	0	0	0
56	OA	3	0	0	0	0
56	OB	3	0	0	0	0
56	P	2	0	0	0	0
56	PA	2	0	0	0	0
56	PB	2	0	0	0	0
56	PC	2	0	0	0	0
56	Q	3	0	0	0	0
56	QB	3	0	0	0	0
56	QC	2	0	0	0	0
56	R	4	0	0	0	0
56	RA	2	0	0	0	0
56	RB	5	0	0	0	0
56	RC	2	0	0	0	0
56	S	3	0	0	0	0
56	SA	1	0	0	0	0
56	SB	1	0	0	0	0
56	SC	1	0	0	0	0
56	T	2	0	0	0	0
56	TA	3	0	0	0	0
56	TB	5	0	0	0	0
56	TC	2	0	0	0	0
56	U	2	0	0	0	0
56	UC	1	0	0	0	0
56	V	5	0	0	0	0
56	VA	2	0	0	0	0
56	VB	1	0	0	0	0
56	W	12	0	0	0	0
56	WA	3	0	0	0	0
56	WB	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	WC	2	0	0	0	0
56	XB	2	0	0	0	0
56	XC	2	0	0	0	0
56	Y	4	0	0	0	0
56	YA	2	0	0	0	0
56	YB	3	0	0	0	0
56	YC	1	0	0	0	0
56	Z	3	0	0	0	0
56	ZA	1	0	0	0	0
56	ZB	2	0	0	0	0
56	ZC	1	0	0	0	0
57	BA	1	0	0	0	0
57	CA	1	0	0	0	0
57	DA	1	0	0	0	0
57	EC	1	0	0	0	0
57	FC	1	0	0	0	0
57	GA	1	0	0	0	0
57	GC	1	0	0	0	0
57	JC	1	0	0	0	0
57	V	1	0	0	0	0
57	YB	1	0	0	0	0
All	All	299566	0	203671	5481	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (5481) 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)
37:LA:18:LYS:NZ	37:LA:31:CYS:SG	2.10	1.23
37:OC:18:LYS:NZ	37:OC:31:CYS:SG	2.10	1.23
37:OC:12:CYS:SG	37:OC:18:LYS:NZ	2.24	1.11
10:J:60:GLU:HG3	10:J:61:ARG:HH12	1.11	1.09
10:MB:60:GLU:HG3	10:MB:61:ARG:HH12	1.19	1.05
9:I:3:ARG:HB2	9:I:3:ARG:HH11	1.15	1.04
9:LB:3:ARG:HH11	9:LB:3:ARG:HB2	1.20	1.03
37:LA:12:CYS:SG	37:LA:18:LYS:NZ	2.33	1.01
2:B:2298:A:H62	2:B:2318:G:H8	1.08	0.99
43:UC:61:GLU:OE2	47:YC:58:LYS:NZ	1.95	0.99
1:DB:363:A:OP2	45:WC:34:ARG:NH1	1.95	0.98
2:B:1043:C:H41	2:B:1112:G:H1	1.09	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:3:ARG:HB2	9:I:3:ARG:NH1	1.80	0.97
48:ZC:35:ARG:HG3	48:ZC:35:ARG:HH11	1.30	0.97
2:EB:1043:C:H41	2:EB:1112:G:H1	1.10	0.96
2:EB:2298:A:H62	2:EB:2318:G:H8	1.07	0.96
2:B:2094:G:OP1	10:J:22:LYS:NZ	1.98	0.96
1:DB:1279:A:OP2	43:UC:9:ARG:NH2	1.99	0.95
1:A:1279:A:OP2	43:RA:9:ARG:NH2	2.00	0.95
2:B:2784:C:H1'	6:F:37:ARG:HH12	1.30	0.95
48:WA:35:ARG:HH11	48:WA:35:ARG:HG3	1.31	0.95
1:A:363:A:OP2	45:TA:34:ARG:NH1	2.00	0.94
17:Q:60:THR:HG22	17:Q:77:PRO:HA	1.49	0.93
2:EB:2784:C:H1'	6:IB:37:ARG:HH12	1.32	0.93
3:C:82:G:H1	3:C:94:C:H42	1.17	0.92
2:EB:2316:C:O2'	8:KB:128:ARG:NH1	2.02	0.92
25:Y:21:ARG:HH11	25:Y:21:ARG:HG3	1.34	0.92
2:EB:1270:C:H5''	2:EB:1271:G:H5'	1.53	0.91
25:BC:21:ARG:HH11	25:BC:21:ARG:HG3	1.35	0.91
9:LB:3:ARG:HB2	9:LB:3:ARG:NH1	1.85	0.91
17:TB:60:THR:HG22	17:TB:77:PRO:HA	1.53	0.90
2:B:2316:C:O2'	8:H:128:ARG:NH1	2.03	0.90
43:RA:61:GLU:OE2	47:VA:58:LYS:NZ	2.05	0.90
15:RB:97:VAL:HG12	15:RB:114:VAL:HG22	1.54	0.90
2:B:1270:C:H5''	2:B:1271:G:H5'	1.53	0.89
50:YA:66:SER:O	50:YA:70:ARG:NH1	2.05	0.89
39:QC:36:ARG:HH12	39:QC:66:GLU:HB2	1.36	0.89
3:FB:82:G:H1	3:FB:94:C:H42	1.19	0.89
4:LC:33:U:OP2	42:TC:128:ARG:NH2	2.04	0.88
2:EB:1379:A:H4'	2:EB:1380:G:OP2	1.73	0.88
7:G:46:ARG:HG2	7:G:46:ARG:HH11	1.36	0.88
5:E:218:ARG:HG3	5:E:218:ARG:HH11	1.37	0.88
1:A:1295:G:O2'	46:UA:14:ARG:NH1	2.07	0.88
43:UC:69:ASN:O	43:UC:70:ARG:NH1	2.07	0.88
2:B:1652:A:OP1	15:O:8:ARG:NH1	2.07	0.87
7:JB:46:ARG:HH11	7:JB:46:ARG:HG2	1.37	0.87
15:O:97:VAL:HG12	15:O:114:VAL:HG22	1.57	0.87
46:UA:37:THR:HG22	46:UA:55:ARG:HH12	1.38	0.87
8:KB:56:ALA:HB2	8:KB:153:ARG:HH11	1.40	0.86
2:B:819:A:OP2	2:B:1187:G:N2	2.09	0.86
37:OC:9:CYS:HG	37:OC:31:CYS:HG	1.21	0.86
2:EB:819:A:OP2	2:EB:1187:G:N2	2.09	0.86
43:RA:69:ASN:O	43:RA:70:ARG:NH1	2.07	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EB:1652:A:OP1	15:RB:8:ARG:NH1	2.08	0.86
1:DB:1118:C:OP1	42:TC:104:ARG:NH1	2.09	0.85
1:DB:1295:G:O2'	46:XC:14:ARG:NH1	2.09	0.85
39:NA:36:ARG:HH12	39:NA:66:GLU:HB2	1.40	0.85
1:DB:1077:G:N2	1:DB:1080:A:OP2	2.10	0.85
1:A:1118:C:OP1	42:QA:104:ARG:NH1	2.10	0.85
9:I:16:SER:HB2	9:I:27:LYS:HB2	1.59	0.84
25:Y:52:ARG:NH1	25:Y:57:GLU:HB2	1.91	0.84
1:DB:1128:C:H5''	42:TC:66:ARG:HH12	1.42	0.84
7:JB:116:ASP:OD2	13:PB:1:MET:N	2.10	0.84
4:IA:33:U:OP2	42:QA:128:ARG:NH2	2.09	0.84
2:EB:1264:G:OP1	29:FC:19:ARG:NH2	2.10	0.84
46:XC:37:THR:HG22	46:XC:55:ARG:HH12	1.42	0.84
24:X:5:LYS:HD2	55:GD:265:LYS:HE3	1.57	0.84
2:B:2747:G:OP1	9:I:138:LYS:NZ	2.10	0.84
18:R:97:ASP:OD1	18:R:101:ARG:NH1	2.11	0.84
35:JA:69:LEU:HB3	35:JA:162:ILE:HG22	1.58	0.84
2:EB:617:G:OP1	7:JB:40:GLN:NE2	2.11	0.84
22:V:102:CYS:SG	22:V:103:GLY:N	2.50	0.83
37:LA:26:CYS:HA	37:LA:31:CYS:HB2	1.60	0.83
50:BD:66:SER:O	50:BD:70:ARG:NH1	2.10	0.83
2:B:1264:G:OP1	29:CA:19:ARG:NH2	2.10	0.83
7:G:117:ARG:HH12	13:M:1:MET:H2	1.24	0.83
2:EB:2809:A:OP2	2:EB:2891:G:N1	2.10	0.83
16:P:56:LEU:HB3	16:P:58:LEU:HD23	1.59	0.83
41:PA:79:VAL:HG23	41:PA:80:ILE:HG13	1.60	0.83
8:H:56:ALA:HB2	8:H:153:ARG:HH11	1.40	0.83
9:LB:16:SER:HB2	9:LB:27:LYS:HB2	1.60	0.83
5:HB:218:ARG:HH11	5:HB:218:ARG:HG3	1.42	0.82
20:WB:18:ARG:HB2	20:WB:18:ARG:HH11	1.42	0.82
46:XC:14:ARG:HG3	46:XC:44:ARG:NH1	1.94	0.82
35:JA:21:ARG:NH1	35:JA:23:ARG:HD3	1.94	0.82
41:SC:79:VAL:HG23	41:SC:80:ILE:HG13	1.61	0.82
1:A:1128:C:H5''	42:QA:66:ARG:HH12	1.43	0.82
1:DB:1353:G:OP1	54:FD:10:ARG:NH1	2.13	0.81
26:Z:14:ARG:NH1	26:Z:66:GLU:OE1	2.13	0.81
46:UA:14:ARG:HG3	46:UA:44:ARG:NH1	1.95	0.81
35:MC:69:LEU:HB3	35:MC:162:ILE:HG22	1.62	0.81
40:OA:70:LYS:HB2	40:OA:96:GLN:HG2	1.62	0.81
37:OC:26:CYS:HA	37:OC:31:CYS:HB2	1.62	0.81
36:KA:131:ARG:HH11	36:KA:135:LYS:HE3	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EB:213:A:H5''	2:EB:214:G:OP2	1.79	0.81
35:JA:189:ASP:HB3	35:JA:204:ASN:HA	1.63	0.81
2:EB:249:C:O2'	13:PB:64:LYS:NZ	2.13	0.81
2:EB:270(M):U:O2'	2:EB:270(O):G:N2	2.14	0.81
1:A:403:C:O2'	37:LA:122:ARG:NH2	2.13	0.81
1:DB:673:G:H5''	39:QC:87:ARG:NH1	1.95	0.81
2:EB:807:U:OP1	13:PB:36:LYS:NZ	2.14	0.81
6:F:36:ARG:NH1	6:F:86:PRO:O	2.14	0.81
16:SB:56:LEU:HB3	16:SB:58:LEU:HD23	1.62	0.81
11:K:49:GLY:O	11:K:119:ARG:NH1	2.15	0.80
41:PA:10:LEU:HD22	41:PA:83:ILE:HD11	1.62	0.80
51:ZA:54:ARG:HE	51:ZA:54:ARG:H	1.29	0.80
2:B:1754:C:OP1	17:Q:96:ARG:NH1	2.15	0.80
18:UB:97:ASP:OD1	18:UB:101:ARG:NH1	2.14	0.80
40:RC:70:LYS:HB2	40:RC:96:GLN:HG2	1.63	0.80
37:LA:177:ASP:OD2	37:LA:180:GLY:HA3	1.81	0.80
2:B:807:U:OP1	13:M:36:LYS:NZ	2.14	0.80
2:B:2646:C:OP2	2:B:2732:G:O2'	1.99	0.80
8:H:136:ARG:HE	8:H:136:ARG:H	1.30	0.80
8:H:115:ARG:HD2	46:UA:7:VAL:HG22	1.64	0.80
36:NC:131:ARG:HH11	36:NC:135:LYS:HE3	1.47	0.80
20:T:22:ASP:HA	20:T:25:ARG:HH12	1.46	0.80
33:GA:25:VAL:HB	33:GA:34:GLN:HB3	1.64	0.80
8:KB:136:ARG:HE	8:KB:136:ARG:H	1.28	0.80
33:JC:25:VAL:HB	33:JC:34:GLN:HB3	1.64	0.80
2:B:1379:A:H4'	2:B:1380:G:OP2	1.78	0.79
44:SA:120:ARG:HH12	44:SA:126:ARG:NH1	1.79	0.79
5:HB:275:LYS:HE3	5:HB:276:LYS:HG3	1.64	0.79
26:Z:16:LEU:O	26:Z:67:LYS:NZ	2.16	0.79
2:B:249:C:O2'	13:M:64:LYS:NZ	2.14	0.79
2:EB:2394:C:N3	4:GB:76:A:O2'	2.15	0.79
2:EB:2747:G:OP1	9:LB:138:LYS:NZ	2.14	0.79
11:NB:49:GLY:O	11:NB:119:ARG:NH1	2.15	0.79
13:M:126:VAL:HG22	13:M:146:VAL:HB	1.63	0.79
2:EB:547:A:H3'	2:EB:548:A:C8	2.17	0.79
2:EB:2646:C:OP2	2:EB:2732:G:O2'	2.01	0.79
18:UB:69:CYS:HB3	18:UB:74:LEU:HD12	1.65	0.79
7:JB:117:ARG:HH12	13:PB:1:MET:H2	1.27	0.79
41:SC:135:CYS:SG	41:SC:136:GLU:N	2.55	0.79
2:B:2795:G:H1'	2:B:2802:G:H21	1.48	0.78
37:LA:191:ARG:HH21	37:LA:200:GLU:HG2	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EB:278:A:H61	2:EB:362:U:H3	1.30	0.78
4:GB:50:U:H3	4:GB:64:G:H1	1.29	0.78
20:WB:22:ASP:HA	20:WB:25:ARG:HH12	1.47	0.78
25:BC:52:ARG:NH1	25:BC:57:GLU:HB2	1.98	0.78
2:B:547:A:H3'	2:B:548:A:C8	2.19	0.78
2:EB:1467:C:H42	2:EB:1525:G:H1	1.32	0.78
35:MC:178:ARG:HH12	41:SC:74:PRO:HB3	1.48	0.78
15:RB:54:LEU:HD23	15:RB:66:VAL:HG23	1.66	0.78
12:L:71:ARG:HH21	12:L:77:ILE:HG21	1.47	0.78
35:MC:189:ASP:HB3	35:MC:204:ASN:HA	1.65	0.78
1:A:1266:G:N2	1:A:1269:A:OP2	2.17	0.77
1:DB:409:G:OP2	37:OC:22:LYS:HE2	1.82	0.77
24:AC:5:LYS:NZ	24:AC:5:LYS:HB2	1.98	0.77
2:EB:2795:G:H1'	2:EB:2802:G:H21	1.49	0.77
2:B:213:A:H5''	2:B:214:G:OP2	1.85	0.77
2:B:1467:C:H42	2:B:1525:G:H1	1.33	0.77
37:LA:18:LYS:NZ	37:LA:31:CYS:HG	1.82	0.77
20:WB:11:ARG:HA	20:WB:100:THR:HG22	1.66	0.77
2:B:270(M):U:O2'	2:B:270(O):G:N2	2.17	0.77
1:A:1077:G:N2	1:A:1080:A:OP2	2.14	0.77
2:B:1761:C:H3'	2:B:1762:A:H5''	1.67	0.77
21:U:5:TYR:HE1	26:Z:30:ARG:HH11	1.31	0.77
6:IB:36:ARG:NH1	6:IB:86:PRO:O	2.16	0.77
6:F:37:ARG:HA	6:F:42:ASP:OD2	1.83	0.77
43:RA:8:LEU:HB2	43:RA:70:ARG:HB3	1.67	0.77
50:BD:93:GLN:O	50:BD:96:GLN:NE2	2.17	0.77
5:E:275:LYS:HE3	5:E:276:LYS:HG3	1.67	0.77
27:AA:27:GLY:HA3	27:AA:35:ARG:NH1	2.00	0.77
53:ED:100:ILE:HG12	53:ED:102:GLY:H	1.49	0.77
20:T:18:ARG:HB2	20:T:18:ARG:HH11	1.49	0.77
50:YA:93:GLN:O	50:YA:96:GLN:NE2	2.16	0.77
37:OC:191:ARG:HH21	37:OC:200:GLU:HG2	1.49	0.77
2:B:2809:A:OP2	2:B:2891:G:N1	2.13	0.76
35:JA:178:ARG:HH12	41:PA:74:PRO:HB3	1.50	0.76
37:OC:177:ASP:OD2	37:OC:180:GLY:HA3	1.85	0.76
1:DB:1266:G:N2	1:DB:1269:A:OP2	2.18	0.76
2:B:270(K):G:O6	2:B:270(Q):C:N4	2.19	0.76
20:T:18:ARG:HD3	20:T:76:VAL:HB	1.67	0.76
2:B:1434:A:H61	2:B:1558:A:H62	1.34	0.76
2:EB:1754:C:OP1	17:TB:96:ARG:NH1	2.19	0.76
3:FB:18:G:H1	3:FB:65:C:H42	1.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:WB:18:ARG:HD3	20:WB:76:VAL:HB	1.66	0.76
2:B:2469:A:H4'	14:N:56:ARG:HG2	1.67	0.76
20:T:11:ARG:HA	20:T:100:THR:HG22	1.68	0.76
2:EB:1761:C:H3'	2:EB:1762:A:H5''	1.66	0.76
16:P:3:ARG:HH11	16:P:4:LEU:H	1.34	0.76
18:R:69:CYS:HB3	18:R:74:LEU:HD12	1.65	0.76
46:UA:37:THR:HG22	46:UA:55:ARG:NH1	2.01	0.76
50:YA:90:ILE:HA	50:YA:93:GLN:HG2	1.68	0.76
24:AC:5:LYS:HD2	55:HD:265:LYS:HE3	1.68	0.76
4:D:50:U:H3	4:D:64:G:H1	1.30	0.76
35:MC:21:ARG:NH1	35:MC:23:ARG:HD3	2.00	0.75
37:OC:15:GLU:OE1	37:OC:66:ARG:NH1	2.18	0.75
41:SC:10:LEU:HD22	41:SC:83:ILE:HD11	1.66	0.75
5:E:108:PRO:HB3	5:E:143:HIS:CE1	2.21	0.75
2:EB:270(K):G:O6	2:EB:270(Q):C:N4	2.20	0.75
13:PB:126:VAL:HG22	13:PB:146:VAL:HB	1.66	0.75
42:QA:23:ASN:HD21	42:QA:25:LYS:HE2	1.50	0.75
1:DB:1503:A:N6	34:KC:13:A:OP1	2.18	0.75
27:DC:27:GLY:HA3	27:DC:35:ARG:NH1	2.01	0.75
50:BD:90:ILE:HA	50:BD:93:GLN:HG2	1.68	0.75
1:A:673:G:H5''	39:NA:87:ARG:NH1	2.01	0.75
2:B:1043:C:N4	2:B:1112:G:H1	1.83	0.75
1:DB:1124:G:H5''	43:UC:35:SER:HB2	1.67	0.75
5:HB:147:LEU:HG	5:HB:155:LEU:HD21	1.67	0.75
51:CD:54:ARG:HE	51:CD:54:ARG:H	1.31	0.75
2:B:2394:C:N3	4:D:76:A:O2'	2.18	0.75
1:DB:931:C:H42	1:DB:1386:G:H1	1.34	0.75
43:UC:8:LEU:HB2	43:UC:70:ARG:HB3	1.68	0.75
1:A:539:A:OP2	45:TA:115:LYS:HE2	1.87	0.74
2:B:918:A:N3	3:C:80:U:O2'	2.20	0.74
15:O:56:LYS:NZ	15:O:90:ARG:O	2.19	0.74
28:EC:58:ARG:HH21	52:DD:68:GLY:HA3	1.51	0.74
2:B:278:A:H61	2:B:362:U:H3	1.34	0.74
2:EB:857:C:H4'	24:AC:23:VAL:HG21	1.67	0.74
5:HB:108:PRO:HB3	5:HB:143:HIS:CE1	2.22	0.74
12:OB:71:ARG:HH21	12:OB:77:ILE:HG21	1.52	0.74
35:JA:155:LEU:HD12	35:JA:157:ARG:HH21	1.52	0.74
1:DB:957:U:H5''	52:DD:81:ARG:HH12	1.52	0.74
1:A:339:C:OP2	12:L:97:ARG:NH1	2.21	0.74
2:B:2023:G:H5'	2:B:2617:C:H4'	1.70	0.74
15:O:12:ARG:HH11	15:O:12:ARG:HG3	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:54:LEU:HD23	15:O:66:VAL:HG23	1.70	0.74
55:HD:126:LEU:HG	55:HD:157:GLY:H	1.53	0.74
53:BB:100:ILE:HG12	53:BB:102:GLY:H	1.52	0.74
6:F:128:SER:OG	6:F:129:HIS:N	2.18	0.74
24:X:5:LYS:NZ	24:X:5:LYS:HB2	2.01	0.74
15:RB:118:GLU:OE2	15:RB:118:GLU:N	2.20	0.74
16:SB:3:ARG:HH11	16:SB:4:LEU:H	1.34	0.74
48:WA:35:ARG:HG3	48:WA:35:ARG:NH1	2.03	0.73
1:A:1124:G:H5''	43:RA:35:SER:HB2	1.68	0.73
1:A:1238:A:N6	1:A:1301:U:O2	2.20	0.73
39:NA:36:ARG:HH11	39:NA:36:ARG:HB3	1.52	0.73
3:C:18:G:H1	3:C:65:C:H42	1.35	0.73
2:EB:2023:G:H5'	2:EB:2617:C:H4'	1.70	0.73
2:EB:2469:A:H4'	14:QB:56:ARG:HG2	1.70	0.73
6:IB:37:ARG:HA	6:IB:42:ASP:OD2	1.88	0.73
28:BA:62:ARG:NH1	28:BA:62:ARG:HA	2.03	0.73
37:LA:15:GLU:OE1	37:LA:66:ARG:NH1	2.21	0.73
14:QB:75:THR:HG21	14:QB:87:LYS:NZ	2.03	0.73
26:CC:14:ARG:NH1	26:CC:66:GLU:OE1	2.21	0.73
2:B:1364:G:OP2	25:Y:3:LYS:HG3	1.89	0.73
41:PA:135:CYS:SG	41:PA:136:GLU:N	2.62	0.73
1:DB:1256:A:OP2	36:NC:26:LYS:NZ	2.20	0.73
38:MA:50:GLU:HB3	38:MA:53:LEU:HD13	1.71	0.73
1:DB:539:A:OP2	45:WC:115:LYS:HE2	1.89	0.73
10:MB:72:LEU:HD23	10:MB:75:LEU:HD21	1.69	0.73
10:J:72:LEU:HD23	10:J:75:LEU:HD21	1.70	0.72
28:BA:16:CYS:HB2	28:BA:20:ASN:HB2	1.71	0.72
1:DB:452:A:OP1	49:AD:43:LYS:NZ	2.22	0.72
6:IB:128:SER:OG	6:IB:129:HIS:N	2.20	0.72
7:JB:54:ARG:HG3	7:JB:54:ARG:HH11	1.54	0.72
42:TC:23:ASN:HD21	42:TC:25:LYS:HE2	1.52	0.72
2:B:857:C:H4'	24:X:23:VAL:HG21	1.71	0.72
7:G:117:ARG:HH12	13:M:1:MET:N	1.86	0.72
35:MC:155:LEU:HD12	35:MC:157:ARG:HH21	1.55	0.72
38:PC:31:LEU:HD22	38:PC:43:LEU:HD11	1.71	0.72
38:PC:122:GLU:O	38:PC:126:ARG:NH1	2.23	0.72
7:G:53:THR:HG23	7:G:55:GLY:H	1.53	0.72
9:I:3:ARG:NH2	9:I:5:GLY:H	1.88	0.72
45:TA:60:LEU:HD21	45:TA:66:VAL:HG22	1.72	0.72
38:MA:145:LYS:NZ	38:MA:145:LYS:HB3	2.03	0.72
22:V:83:THR:OG1	22:V:84:ARG:N	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:OC:12:CYS:HG	37:OC:18:LYS:NZ	1.85	0.72
39:QC:36:ARG:HB3	39:QC:36:ARG:HH11	1.54	0.72
39:QC:36:ARG:HB3	39:QC:36:ARG:NH1	2.05	0.72
10:J:60:GLU:HG3	10:J:61:ARG:NH1	1.96	0.72
2:EB:1043:C:N4	2:EB:1112:G:H1	1.86	0.72
10:J:60:GLU:CG	10:J:61:ARG:HH12	1.96	0.72
16:P:15:ARG:NH1	16:P:88:ASP:OD2	2.23	0.72
2:EB:1083:U:H2'	2:EB:1085:A:OP2	1.89	0.72
2:B:1658:C:OP1	6:F:135:HIS:NE2	2.23	0.71
1:DB:692:U:O4	44:VC:26:ASN:ND2	2.23	0.71
52:AB:3:ARG:NH1	52:AB:7:LYS:HG3	2.05	0.71
1:DB:642:A:N3	41:SC:113:SER:OG	2.23	0.71
1:A:957:U:H5''	52:AB:81:ARG:HH12	1.55	0.71
2:EB:1434:A:H61	2:EB:1558:A:H62	1.35	0.71
2:EB:2500:U:H5''	2:EB:2501:C:OP2	1.91	0.71
45:WC:60:LEU:HD21	45:WC:66:VAL:HG22	1.72	0.71
1:A:931:C:H42	1:A:1386:G:H1	1.38	0.71
15:O:118:GLU:OE2	15:O:118:GLU:N	2.22	0.71
22:YB:102:CYS:SG	22:YB:103:GLY:N	2.64	0.71
40:RC:150:ALA:HA	44:VC:59:TYR:HB3	1.72	0.71
1:A:692:U:O4	44:SA:26:ASN:ND2	2.24	0.71
2:B:2577:A:OP2	29:CA:3:LYS:NZ	2.24	0.71
27:AA:26:LEU:O	27:AA:35:ARG:NH1	2.24	0.71
1:DB:523:A:N6	45:WC:92:OTD:OD2	2.19	0.71
16:SB:15:ARG:NH1	16:SB:88:ASP:OD2	2.23	0.71
28:EC:62:ARG:NH1	28:EC:62:ARG:HA	2.06	0.71
35:JA:32:ILE:HD11	35:JA:40:HIS:HB3	1.73	0.71
46:XC:37:THR:HG22	46:XC:55:ARG:NH1	2.05	0.71
50:BD:81:ARG:HB3	50:BD:84:LEU:HD23	1.72	0.71
1:A:1279:A:O2'	1:A:1281:U:OP2	2.04	0.71
1:A:1320:C:O2	52:AB:36:ARG:NH1	2.23	0.71
52:AB:32:LYS:HA	52:AB:50:ALA:HB3	1.71	0.71
2:EB:1658:C:OP1	6:IB:135:HIS:NE2	2.22	0.71
12:OB:35:VAL:HG11	12:OB:103:ALA:HB3	1.73	0.71
1:A:1179:A:H5''	42:QA:97:LYS:NZ	2.06	0.70
2:B:1083:U:H2'	2:B:1085:A:OP2	1.90	0.70
27:DC:26:LEU:O	27:DC:35:ARG:NH1	2.24	0.70
28:EC:16:CYS:HB2	28:EC:20:ASN:HB2	1.73	0.70
1:A:664:G:H22	1:A:741:G:H1	1.39	0.70
39:NA:36:ARG:HB3	39:NA:36:ARG:NH1	2.05	0.70
1:DB:664:G:H22	1:DB:741:G:H1	1.38	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:AD:82:GLN:OE1	49:AD:83:GLU:N	2.24	0.70
15:O:36:THR:HG22	15:O:37:THR:H	1.56	0.70
23:W:131:ARG:HB2	23:W:131:ARG:HH11	1.56	0.70
45:TA:33:ARG:HE	45:TA:62:SER:HB3	1.56	0.70
2:EB:780:G:OP1	5:HB:218:ARG:NH2	2.25	0.70
2:EB:2833:G:H4'	2:EB:2834:G:OP2	1.90	0.70
38:PC:145:LYS:HB3	38:PC:145:LYS:NZ	2.07	0.70
7:G:54:ARG:HH11	7:G:54:ARG:HG3	1.55	0.70
24:AC:9:SER:O	24:AC:10:THR:OG1	2.05	0.70
38:MA:31:LEU:HD22	38:MA:43:LEU:HD11	1.73	0.70
2:EB:918:A:N3	3:FB:80:U:O2'	2.25	0.70
36:KA:60:ALA:HB3	36:KA:63:ASN:HB2	1.73	0.70
44:VC:120:ARG:HH12	44:VC:126:ARG:NH1	1.90	0.70
2:B:1082:U:H2'	2:B:1083:U:H4'	1.73	0.70
2:B:2500:U:H5''	2:B:2501:C:OP2	1.91	0.70
42:QA:96:LEU:H	42:QA:98:PRO:HD2	1.55	0.70
5:HB:85:ASP:OD2	5:HB:88:ARG:NH1	2.25	0.70
42:TC:96:LEU:H	42:TC:98:PRO:HD2	1.56	0.70
5:E:147:LEU:HG	5:E:155:LEU:HD21	1.73	0.70
17:Q:23:ARG:HD3	17:Q:120:ARG:NH1	2.06	0.70
2:EB:1082:U:H2'	2:EB:1083:U:H4'	1.74	0.70
20:WB:13:SER:HB3	20:WB:16:LYS:HD2	1.72	0.70
23:ZB:6:LYS:HD3	23:ZB:43:GLU:OE2	1.92	0.70
7:JB:103:LYS:HG2	7:JB:106:ARG:NH1	2.07	0.70
39:NA:87:ARG:HH11	39:NA:87:ARG:HG3	1.55	0.69
2:B:386:G:H5''	2:B:388:G:H22	1.57	0.69
4:D:18:G:H1	4:D:55:PSU:H1'	1.56	0.69
8:KB:16:ARG:HH21	8:KB:28:VAL:HG12	1.57	0.69
55:GD:126:LEU:HG	55:GD:157:GLY:H	1.56	0.69
2:B:2210:G:H3'	2:B:2211:G:C8	2.28	0.69
14:N:79:LEU:HD13	14:N:80:GLU:HB2	1.73	0.69
23:W:6:LYS:HD3	23:W:43:GLU:OE2	1.92	0.69
1:A:403:C:HO2'	37:LA:122:ARG:HH21	1.39	0.69
1:A:642:A:N3	41:PA:113:SER:OG	2.25	0.69
1:A:1327:C:OP1	54:CB:12:LYS:NZ	2.25	0.69
16:P:3:ARG:HH11	16:P:4:LEU:N	1.91	0.69
1:DB:1320:C:O2	52:DD:36:ARG:NH1	2.25	0.69
5:HB:24:ILE:HD11	5:HB:91:ARG:HD2	1.74	0.69
52:DD:3:ARG:NH1	52:DD:7:LYS:HG3	2.07	0.69
13:M:57:THR:HG23	13:M:60:MET:HB2	1.73	0.69
42:TC:15:ALA:HB2	42:TC:65:VAL:HG23	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1484:C:HO2'	2:B:1960:A:HO2'	1.40	0.69
7:G:54:ARG:HG3	7:G:54:ARG:NH1	2.06	0.69
11:K:34:LEU:O	11:K:49:GLY:HA3	1.91	0.69
38:MA:122:GLU:O	38:MA:126:ARG:NH1	2.26	0.69
49:XA:82:GLN:OE1	49:XA:83:GLU:N	2.26	0.69
7:JB:53:THR:HG23	7:JB:55:GLY:H	1.56	0.69
7:JB:54:ARG:HG3	7:JB:54:ARG:NH1	2.05	0.69
38:PC:50:GLU:HB3	38:PC:53:LEU:HD13	1.73	0.69
52:DD:32:LYS:HA	52:DD:50:ALA:HB3	1.75	0.69
7:G:50:SER:HB2	7:G:94:PRO:HD3	1.75	0.69
16:SB:3:ARG:HH11	16:SB:4:LEU:N	1.91	0.69
19:VB:82:ARG:HG3	19:VB:82:ARG:HH11	1.57	0.69
39:NA:15:ASP:OD1	39:NA:18:GLN:N	2.23	0.69
21:XB:44:GLU:HG3	21:XB:51:VAL:HG23	1.75	0.69
26:CC:16:LEU:O	26:CC:67:LYS:NZ	2.26	0.69
39:QC:87:ARG:HG3	39:QC:87:ARG:HH11	1.58	0.69
1:A:523:A:N6	45:TA:92:OTD:OD2	2.24	0.68
37:LA:39:PRO:HG2	37:LA:44:GLY:HA3	1.75	0.68
1:A:1071:C:H5''	38:MA:49:PRO:HG2	1.75	0.68
40:OA:67:GLU:OE2	40:OA:70:LYS:HD3	1.93	0.68
4:GB:18:G:H1	4:GB:55:PSU:H1'	1.56	0.68
12:L:35:VAL:HG11	12:L:103:ALA:HB3	1.74	0.68
1:DB:1279:A:O2'	1:DB:1281:U:OP2	2.06	0.68
8:KB:35:GLU:HG3	8:KB:160:VAL:HG23	1.76	0.68
7:G:53:THR:HG22	7:G:56:GLU:HG3	1.75	0.68
36:NC:60:ALA:HB3	36:NC:63:ASN:HB2	1.76	0.68
48:ZC:9:GLN:HB3	48:ZC:13:GLN:HE21	1.59	0.68
4:D:9:G:N2	4:D:46:G:N7	2.42	0.68
35:JA:155:LEU:HD21	35:JA:159:PRO:HD3	1.75	0.68
1:DB:1077:G:H1	38:PC:47:LYS:HE2	1.58	0.68
2:B:1657:C:H2'	2:B:1658:C:H6	1.57	0.68
2:B:2313:C:OP2	8:H:74:LYS:NZ	2.24	0.68
9:LB:89:ILE:HG22	9:LB:94:TYR:HB3	1.75	0.68
3:C:104:A:OP1	23:W:72:ARG:NH1	2.25	0.68
5:E:108:PRO:HB3	5:E:143:HIS:HE1	1.59	0.68
12:OB:64:ARG:NH1	12:OB:81:ASP:OD1	2.27	0.68
13:PB:57:THR:HG23	13:PB:60:MET:HB2	1.76	0.68
14:QB:17:LEU:HD12	14:QB:39:PRO:HB2	1.76	0.68
5:E:24:ILE:HD11	5:E:91:ARG:HD2	1.74	0.68
36:KA:20:SER:OG	36:KA:40:ARG:NH2	2.27	0.68
42:QA:15:ALA:HB2	42:QA:65:VAL:HG23	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:607:U:OP1	7:G:103:LYS:N	2.19	0.68
4:D:49:G:N2	4:D:65:C:O2	2.27	0.68
14:N:75:THR:HG21	14:N:87:LYS:NZ	2.08	0.68
2:EB:586:A:N1	2:EB:809:G:O2'	2.22	0.68
23:ZB:95:PRO:HA	23:ZB:130:PRO:HD3	1.76	0.68
44:VC:51:LYS:HA	44:VC:55:LYS:HE3	1.76	0.68
1:A:1314:C:N4	52:AB:2:PRO:O	2.28	0.67
2:B:1434:A:H61	2:B:1558:A:N6	1.91	0.67
9:I:143:GLN:HE21	9:I:147:ASN:HD21	1.42	0.67
50:YA:81:ARG:HB3	50:YA:84:LEU:HD23	1.77	0.67
1:DB:1314:C:N4	52:DD:2:PRO:O	2.26	0.67
2:B:2137:C:O2	2:B:2154:G:N2	2.23	0.67
5:HB:218:ARG:HG3	5:HB:218:ARG:NH1	2.08	0.67
1:DB:959:A:O2'	1:DB:984:C:O2'	2.09	0.67
39:QC:33:TYR:HB2	39:QC:75:LEU:HD12	1.76	0.67
2:B:2094:G:P	10:J:22:LYS:HZ2	2.18	0.67
10:J:29:TYR:HD1	10:J:30:LEU:HD23	1.60	0.67
12:L:64:ARG:NH1	12:L:81:ASP:OD1	2.27	0.67
5:E:218:ARG:HG3	5:E:218:ARG:NH1	2.08	0.67
2:EB:2577:A:OP2	29:FC:3:LYS:NZ	2.28	0.67
1:A:1054:C:OP2	1:A:1197:G:OP2	2.12	0.67
6:IB:29:GLY:H	6:IB:93:VAL:HG22	1.60	0.67
23:ZB:131:ARG:HH11	23:ZB:131:ARG:HB2	1.59	0.67
27:AA:59:VAL:HG22	27:AA:60:GLU:H	1.60	0.67
2:EB:2849:U:O4	17:TB:23:ARG:NH2	2.28	0.67
35:MC:153:ARG:O	35:MC:156:LYS:NZ	2.25	0.67
37:LA:9:CYS:HG	37:LA:31:CYS:HG	1.40	0.67
2:B:861:A:O3'	14:N:18:LYS:NZ	2.28	0.67
23:W:95:PRO:HA	23:W:130:PRO:HD3	1.77	0.67
1:DB:1316:G:N1	1:DB:1319:A:OP2	2.24	0.67
14:QB:79:LEU:HD13	14:QB:80:GLU:HB2	1.75	0.67
39:QC:15:ASP:OD1	39:QC:18:GLN:N	2.23	0.67
1:DB:1047:G:HO2'	1:DB:1215:G:HO2'	1.38	0.66
4:GB:9:G:N2	4:GB:46:G:N7	2.43	0.66
46:XC:3:ARG:NH1	46:XC:8:GLU:HG3	2.10	0.66
2:B:2304:G:H22	2:B:2312:U:H3	1.43	0.66
2:B:2833:G:H4'	2:B:2834:G:OP2	1.94	0.66
1:DB:134:A:H61	49:AD:25:ARG:NH1	1.93	0.66
45:WC:52:LEU:HD13	55:HD:305:ASP:OD2	1.94	0.66
55:HD:224:ILE:HG12	55:HD:246:ILE:HG12	1.77	0.66
46:UA:3:ARG:NH1	46:UA:8:GLU:HG3	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DB:134:A:H61	49:AD:25:ARG:HH12	1.42	0.66
1:DB:547:A:OP2	37:OC:2:GLY:HA2	1.95	0.66
1:DB:1179:A:H5''	42:TC:97:LYS:NZ	2.11	0.66
2:EB:1310:G:H1	2:EB:1604:C:H42	1.42	0.66
5:HB:30:GLU:O	5:HB:32:SER:N	2.29	0.66
7:JB:50:SER:HB2	7:JB:94:PRO:HD3	1.77	0.66
21:XB:5:TYR:HE1	26:CC:30:ARG:HH11	1.41	0.66
28:BA:34:GLU:HG3	46:UA:3:ARG:HA	1.76	0.66
3:FB:90:C:H5'	14:QB:16:ARG:NH2	2.10	0.66
1:A:959:A:O2'	1:A:984:C:O2'	2.10	0.66
7:JB:53:THR:HG22	7:JB:56:GLU:HG3	1.77	0.66
9:LB:3:ARG:NH2	9:LB:5:GLY:H	1.94	0.66
9:LB:116:GLU:HG2	9:LB:117:PRO:HD2	1.78	0.66
35:MC:32:ILE:HD11	35:MC:40:HIS:HB3	1.78	0.66
38:PC:59:GLY:O	38:PC:63:ARG:NH1	2.28	0.66
41:PA:12:ARG:HD2	41:PA:26:VAL:HG12	1.77	0.66
48:WA:39:LEU:HD13	48:WA:56:LEU:HB2	1.77	0.66
1:DB:559:A:H4'	1:DB:560:U:H3'	1.77	0.66
1:DB:1318:A:OP1	52:DD:7:LYS:NZ	2.25	0.66
4:GB:49:G:N2	4:GB:65:C:O2	2.27	0.66
10:MB:110:ASP:HB3	10:MB:113:ARG:HB2	1.78	0.66
12:OB:12:ASP:OD2	12:OB:14:THR:HG23	1.95	0.66
22:YB:83:THR:OG1	22:YB:84:ARG:N	2.25	0.66
36:NC:20:SER:OG	36:NC:40:ARG:NH2	2.29	0.66
2:EB:309:G:N3	2:EB:329:G:O2'	2.29	0.66
9:LB:143:GLN:HE21	9:LB:147:ASN:HD21	1.44	0.66
11:NB:34:LEU:O	11:NB:49:GLY:HA3	1.96	0.66
1:A:36:C:OP1	45:TA:123:LYS:NZ	2.29	0.66
2:B:780:G:OP1	5:E:218:ARG:NH2	2.28	0.66
3:C:90:C:H5'	14:N:16:ARG:NH2	2.11	0.66
1:DB:36:C:OP1	45:WC:123:LYS:NZ	2.28	0.66
1:DB:1054:C:OP2	1:DB:1197:G:OP2	2.13	0.66
2:EB:2210:G:H3'	2:EB:2211:G:C8	2.31	0.66
1:A:955:U:OP1	55:GD:133:ARG:NH1	2.28	0.66
2:EB:1889:A:H2'	2:EB:1890:A:C8	2.30	0.66
5:HB:108:PRO:HB3	5:HB:143:HIS:HE1	1.61	0.66
52:DD:50:ALA:HB1	52:DD:57:HIS:HB3	1.78	0.66
1:A:452:A:OP1	49:XA:43:LYS:NZ	2.29	0.66
1:A:1075:C:H5''	35:JA:179:LYS:NZ	2.11	0.66
1:A:1318:A:OP1	52:AB:7:LYS:NZ	2.23	0.66
2:B:617:G:OP1	7:G:40:GLN:NE2	2.22	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:85:ASP:OD2	5:E:88:ARG:NH1	2.26	0.66
49:XA:53:VAL:HG13	49:XA:79:VAL:HG22	1.78	0.66
27:DC:59:VAL:HG22	27:DC:60:GLU:H	1.59	0.66
1:A:572:A:H5'	1:A:573:A:OP2	1.96	0.65
2:B:1889:A:H2'	2:B:1890:A:C8	2.31	0.65
5:E:30:GLU:O	5:E:32:SER:N	2.29	0.65
1:DB:656:C:H4'	48:ZC:62:GLN:HE22	1.61	0.65
48:ZC:35:ARG:HG3	48:ZC:35:ARG:NH1	2.05	0.65
2:B:2100:G:H1	2:B:2189:U:H3	1.44	0.65
2:B:2135:A:N7	2:B:2137:C:N4	2.44	0.65
40:RC:67:GLU:OE2	40:RC:70:LYS:HD3	1.96	0.65
2:B:2151:G:N2	2:B:2152:G:O6	2.28	0.65
15:RB:12:ARG:HH11	15:RB:12:ARG:HG3	1.62	0.65
20:T:110:LYS:NZ	20:T:111:HIS:O	2.28	0.65
22:V:37:VAL:HG21	22:V:72:VAL:HG21	1.78	0.65
44:SA:51:LYS:HA	44:SA:55:LYS:HE3	1.78	0.65
15:RB:36:THR:HG22	15:RB:37:THR:H	1.62	0.65
41:SC:11:THR:HG23	41:SC:14:ARG:NH1	2.09	0.65
2:B:245:G:H5'	13:M:73:GLY:HA2	1.78	0.65
2:B:1483:G:H2'	2:B:1484:G:H8	1.61	0.65
7:G:95:ARG:NH1	7:G:97:TYR:OH	2.30	0.65
22:V:90:LEU:HD12	22:V:96:ILE:HG21	1.78	0.65
31:EA:22:MET:O	31:EA:28:ARG:NH1	2.29	0.65
7:JB:46:ARG:HG2	7:JB:46:ARG:NH1	2.08	0.65
43:UC:50:ILE:HB	47:YC:41:ARG:NH1	2.11	0.65
1:A:134:A:H61	49:XA:25:ARG:HH12	1.43	0.65
2:EB:2304:G:H22	2:EB:2312:U:H3	1.45	0.65
8:KB:16:ARG:NH2	8:KB:28:VAL:O	2.29	0.65
2:EB:1805:U:O2	5:HB:50:THR:HB	1.97	0.65
10:MB:29:TYR:HD1	10:MB:30:LEU:HD23	1.59	0.65
53:ED:10:LEU:HB3	53:ED:12:ALA:H	1.62	0.65
1:A:656:C:H4'	48:WA:62:GLN:HE22	1.62	0.65
24:X:27:GLU:HG3	24:X:68:GLU:HA	1.79	0.65
53:BB:10:LEU:HB3	53:BB:12:ALA:H	1.61	0.65
2:EB:322:A:OP2	7:JB:169:ASN:HB2	1.96	0.65
2:EB:1246:A:OP1	7:JB:38:ARG:NH2	2.27	0.65
29:FC:47:PRO:HG2	29:FC:48:GLU:OE2	1.97	0.65
35:MC:155:LEU:HD21	35:MC:159:PRO:HD3	1.78	0.65
2:B:674:G:H1'	7:G:74:ARG:HD2	1.78	0.65
2:B:2390:U:OP2	32:FA:35:GLN:NE2	2.30	0.65
6:F:9:VAL:HG23	17:Q:3:ARG:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:16:ARG:HH21	8:H:28:VAL:HG12	1.60	0.65
2:EB:1011:G:OP2	18:UB:66:ASN:ND2	2.29	0.65
2:EB:2875:C:O2'	17:TB:2:ASN:OD1	2.13	0.65
12:L:12:ASP:OD2	12:L:14:THR:HG23	1.95	0.65
21:U:44:GLU:HG3	21:U:51:VAL:HG23	1.79	0.65
17:TB:16:ARG:HH12	17:TB:83:ILE:HB	1.62	0.65
2:B:2708:G:O2'	15:O:71:GLN:NE2	2.30	0.64
9:I:116:GLU:HG2	9:I:117:PRO:HD2	1.79	0.64
2:EB:2100:G:H1	2:EB:2189:U:H3	1.44	0.64
55:GD:214:LEU:O	55:GD:216:ASP:N	2.30	0.64
2:B:1310:G:H1	2:B:1604:C:H42	1.44	0.64
10:J:110:ASP:HB3	10:J:113:ARG:HB2	1.78	0.64
2:EB:1364:G:OP2	25:BC:3:LYS:HG3	1.97	0.64
19:VB:43:GLU:H	19:VB:43:GLU:CD	2.00	0.64
44:VC:67:ASP:OD2	44:VC:71:LYS:HE2	1.97	0.64
55:GD:233:GLY:HA3	55:GD:237:VAL:HB	1.77	0.64
2:B:1805:U:O2	5:E:50:THR:HB	1.98	0.64
17:Q:11:GLU:OE1	17:Q:57:PHE:HB3	1.97	0.64
44:SA:99:GLN:HG3	44:SA:105:VAL:HG21	1.79	0.64
9:LB:17:VAL:HG11	9:LB:50:VAL:HG11	1.78	0.64
44:VC:99:GLN:HG3	44:VC:105:VAL:HG21	1.78	0.64
41:PA:51:VAL:HG21	41:PA:60:ARG:HH12	1.63	0.64
41:SC:9:MET:HG3	41:SC:26:VAL:HG11	1.79	0.64
1:A:501:C:H2'	1:A:502:G:H8	1.62	0.64
1:A:542:G:OP1	37:LA:10:ARG:NH2	2.26	0.64
38:MA:40:ARG:NH1	38:MA:68:GLU:HB3	2.12	0.64
2:EB:2137:C:O2	2:EB:2154:G:N2	2.25	0.64
2:EB:2567:G:H2'	2:EB:2568:C:C6	2.32	0.64
2:B:386:G:H5''	2:B:388:G:N2	2.11	0.64
2:B:1270:C:C5'	2:B:1271:G:H5'	2.27	0.64
45:TA:70:ILE:HG12	45:TA:100:ILE:HD12	1.78	0.64
1:A:1503:A:N6	34:HA:13:A:OP1	2.31	0.64
15:O:24:GLN:HG2	15:O:44:LEU:HG	1.79	0.64
22:V:30:VAL:HG13	22:V:37:VAL:HG12	1.80	0.64
36:NC:139:GLN:HB3	36:NC:140:ARG:NH1	2.13	0.64
2:B:101:G:H4'	2:B:102:G:OP2	1.98	0.64
37:OC:39:PRO:HG2	37:OC:44:GLY:HA3	1.79	0.64
41:SC:51:VAL:HG21	41:SC:60:ARG:HH12	1.62	0.64
1:A:1179:A:H5''	42:QA:97:LYS:HZ3	1.63	0.64
2:B:1011:G:OP2	18:R:66:ASN:ND2	2.29	0.64
19:S:85:LYS:NZ	19:S:85:LYS:HB3	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:CA:47:PRO:HG2	29:CA:48:GLU:OE2	1.98	0.64
41:PA:11:THR:HG23	41:PA:14:ARG:NH1	2.13	0.64
2:EB:1270:C:C5'	2:EB:1271:G:H5'	2.26	0.64
2:EB:2135:A:N7	2:EB:2137:C:N4	2.43	0.64
24:AC:5:LYS:HB2	24:AC:5:LYS:HZ2	1.60	0.64
38:PC:82:VAL:HG21	38:PC:138:ALA:HA	1.79	0.64
55:HD:354:ALA:HB1	55:HD:358:GLU:OE2	1.97	0.64
2:B:2784:C:H1'	6:F:37:ARG:NH1	2.09	0.64
24:X:9:SER:O	24:X:10:THR:OG1	2.13	0.64
50:YA:96:GLN:NE2	50:YA:96:GLN:H	1.96	0.64
1:DB:501:C:H2'	1:DB:502:G:H8	1.63	0.64
2:EB:2785:C:OP1	6:IB:41:LYS:NZ	2.30	0.64
2:B:1800:C:OP1	5:E:264:LYS:NZ	2.20	0.63
2:B:2573:C:N4	55:GD:228:ARG:HD2	2.13	0.63
7:G:46:ARG:HG2	7:G:46:ARG:NH1	2.10	0.63
7:G:152:GLU:OE1	7:G:191:ARG:NH1	2.30	0.63
19:S:82:ARG:HH11	19:S:82:ARG:HG3	1.62	0.63
1:DB:403:C:HO2'	37:OC:122:ARG:HH21	1.45	0.63
1:DB:1054:C:N4	55:HD:194:GLY:O	2.31	0.63
1:DB:1261:A:H5''	54:FD:25:LYS:NZ	2.13	0.63
2:EB:2573:C:N4	55:HD:228:ARG:HD2	2.13	0.63
22:YB:90:LEU:HD12	22:YB:96:ILE:HG21	1.80	0.63
1:A:1128:C:H42	1:A:1144:G:H1	1.46	0.63
1:A:1256:A:OP2	36:KA:26:LYS:NZ	2.23	0.63
7:G:103:LYS:HG2	7:G:106:ARG:NH1	2.12	0.63
20:T:22:ASP:HA	20:T:25:ARG:NH1	2.13	0.63
22:YB:44:ILE:HA	22:YB:64:GLU:HA	1.80	0.63
41:SC:12:ARG:HD2	41:SC:26:VAL:HG12	1.78	0.63
55:GD:301:GLY:HA3	55:GD:306:ARG:NH1	2.13	0.63
2:B:307:G:N2	2:B:309:G:H3'	2.14	0.63
6:F:29:GLY:H	6:F:93:VAL:HG22	1.63	0.63
2:EB:2151:G:N2	2:EB:2152:G:O6	2.31	0.63
2:EB:2799:A:HO2'	2:EB:2802:G:HO2'	1.46	0.63
3:FB:85:G:H1	3:FB:91:C:H42	1.44	0.63
2:B:2327:A:H2'	2:B:2328:A:C8	2.33	0.63
41:PA:9:MET:HG3	41:PA:26:VAL:HG11	1.78	0.63
54:CB:24:ARG:HG3	54:CB:25:LYS:HG2	1.80	0.63
2:EB:77:C:H5''	26:CC:10:LEU:HD11	1.79	0.63
2:EB:2390:U:OP2	32:IC:35:GLN:NE2	2.31	0.63
38:PC:58:ALA:HA	38:PC:61:TYR:HB2	1.81	0.63
39:QC:5:GLU:HG3	39:QC:93:SER:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:A:H4'	1:A:560:U:H3'	1.79	0.63
1:A:1004:A:O2'	1:A:1036:G:N2	2.31	0.63
2:B:309:G:N3	2:B:329:G:O2'	2.31	0.63
2:B:704:G:O2'	2:B:726:G:N2	2.27	0.63
2:B:2849:U:O4	17:Q:23:ARG:NH2	2.31	0.63
2:EB:1175:U:H2'	2:EB:1176:G:H8	1.64	0.63
20:WB:22:ASP:HA	20:WB:25:ARG:NH1	2.12	0.63
24:AC:7:LEU:H	4:LC:2:G:H5'	1.63	0.63
55:GD:114:GLU:HG3	55:GD:163:ILE:HG12	1.80	0.63
40:OA:56:GLN:HB3	40:OA:60:LYS:HE3	1.80	0.63
2:B:2345:G:N3	2:B:2381:C:H2'	2.14	0.63
2:B:2349:G:OP2	32:FA:42:ARG:HD3	1.98	0.63
39:NA:33:TYR:HB2	39:NA:75:LEU:HD12	1.81	0.63
52:AB:50:ALA:HB1	52:AB:57:HIS:HB3	1.81	0.63
5:HB:142:VAL:HG23	5:HB:193:VAL:HA	1.80	0.63
24:AC:27:GLU:HG3	24:AC:68:GLU:HA	1.80	0.63
37:OC:18:LYS:HE3	37:OC:20:TYR:H	1.64	0.63
2:B:861:A:H2'	2:B:862:G:O4'	1.99	0.63
8:H:35:GLU:HG3	8:H:160:VAL:HG23	1.80	0.63
1:DB:503:C:OP2	45:WC:116:SER:OG	2.15	0.63
1:DB:572:A:H5'	1:DB:573:A:OP2	1.99	0.63
2:EB:2141:G:N2	2:EB:2151:G:O2'	2.31	0.63
2:EB:2168:G:H2'	2:EB:2170:A:OP2	1.98	0.63
45:WC:33:ARG:HE	45:WC:62:SER:HB3	1.64	0.63
1:A:1021:G:H2'	1:A:1022:G:H4'	1.81	0.63
14:N:17:LEU:HD12	14:N:39:PRO:HB2	1.81	0.63
1:DB:82:U:C2	1:DB:85:U:H5	2.17	0.63
1:A:1370:G:H5''	42:QA:12:GLU:HG3	1.81	0.62
37:LA:12:CYS:HG	37:LA:18:LYS:NZ	1.96	0.62
2:EB:1537:C:H3'	2:EB:1538:G:H8	1.62	0.62
31:HC:22:MET:O	31:HC:28:ARG:NH1	2.32	0.62
48:ZC:56:LEU:HA	48:ZC:59:MET:HE2	1.80	0.62
5:E:217:ARG:HG2	5:E:217:ARG:HH11	1.65	0.62
9:I:89:ILE:HG22	9:I:94:TYR:HB3	1.81	0.62
2:EB:1993:U:H4'	6:IB:128:SER:HB3	1.82	0.62
20:WB:110:LYS:NZ	20:WB:111:HIS:O	2.33	0.62
36:NC:44:GLU:HA	36:NC:52:LEU:HD21	1.79	0.62
55:GD:354:ALA:HB1	55:GD:358:GLU:OE2	1.99	0.62
1:A:232:G:H1'	1:A:262:A:N1	2.14	0.62
46:UA:10:PRO:HG3	46:UA:21:TYR:HD1	1.63	0.62
45:WC:70:ILE:HG12	45:WC:100:ILE:HD12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:HD:182:HIS:HB3	55:HD:310:TYR:HE1	1.63	0.62
2:B:1537:C:H3'	2:B:1538:G:H8	1.63	0.62
2:EB:861:A:O3'	14:QB:18:LYS:NZ	2.33	0.62
50:BD:96:GLN:NE2	50:BD:96:GLN:H	1.97	0.62
55:HD:214:LEU:O	55:HD:216:ASP:N	2.32	0.62
1:A:1305:G:N2	1:A:1331:G:H1'	2.14	0.62
1:DB:1071:C:H5''	38:PC:49:PRO:HG2	1.82	0.62
2:EB:386:G:H5''	2:EB:388:G:H22	1.64	0.62
2:EB:2306:C:N4	8:KB:42:GLY:O	2.32	0.62
1:A:1191:A:OP2	36:KA:3:ASN:ND2	2.32	0.62
2:B:2567:G:H2'	2:B:2568:C:C6	2.34	0.62
44:SA:67:ASP:OD2	44:SA:71:LYS:HE2	2.00	0.62
2:EB:861:A:H2'	2:EB:862:G:O4'	2.00	0.62
2:B:2141:G:N2	2:B:2151:G:O2'	2.32	0.62
2:B:2875:C:O2'	17:Q:2:ASN:OD1	2.16	0.62
9:I:17:VAL:HG11	9:I:50:VAL:HG11	1.82	0.62
28:BA:36:CYS:SG	28:BA:37:SER:N	2.72	0.62
38:MA:148:VAL:HG21	41:PA:107:LEU:HD22	1.81	0.62
1:DB:1004:A:O2'	1:DB:1036:G:N2	2.32	0.62
14:N:10:ARG:NH1	4:IA:64:G:H4'	2.15	0.62
25:Y:21:ARG:HH11	25:Y:21:ARG:CG	2.12	0.62
43:RA:7:LYS:HB3	43:RA:97:GLU:HB2	1.82	0.62
7:JB:152:GLU:OE1	7:JB:191:ARG:NH1	2.33	0.62
23:ZB:40:ASP:HB3	23:ZB:43:GLU:HB2	1.82	0.62
24:X:5:LYS:HB2	24:X:5:LYS:HZ2	1.61	0.62
1:DB:1191:A:OP2	36:NC:3:ASN:ND2	2.33	0.62
2:EB:243:U:OP1	32:IC:6:THR:OG1	2.12	0.62
2:EB:527:C:N4	2:EB:2779:U:OP2	2.32	0.62
1:A:547:A:OP2	37:LA:2:GLY:HA2	1.99	0.62
1:A:1128:C:H5''	42:QA:66:ARG:NH1	2.14	0.62
2:B:2315:G:OP1	8:H:36:LYS:NZ	2.29	0.62
19:S:43:GLU:H	19:S:43:GLU:CD	2.01	0.62
23:W:179:ASP:OD2	23:W:181:GLU:HG2	2.00	0.62
38:MA:82:VAL:HG21	38:MA:138:ALA:HA	1.81	0.62
1:DB:1376:U:O4	40:RC:10:ARG:NH1	2.32	0.62
2:EB:307:G:N2	2:EB:309:G:H3'	2.15	0.62
2:EB:2749:A:OP1	9:LB:3:ARG:NH1	2.33	0.62
7:JB:95:ARG:NH1	7:JB:97:TYR:OH	2.33	0.62
38:PC:40:ARG:NH1	38:PC:68:GLU:HB3	2.15	0.62
2:B:1688:U:O2	2:B:1700:A:H5'	1.99	0.61
1:DB:1179:A:H5''	42:TC:97:LYS:HZ3	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:JB:12:LEU:HG	7:JB:124:LEU:HD11	1.81	0.61
11:NB:12:ARG:NH1	11:NB:50:ASP:OD2	2.33	0.61
11:NB:39:ARG:HE	11:NB:48:MET:HE2	1.65	0.61
1:A:134:A:H61	49:XA:25:ARG:NH1	1.97	0.61
2:B:2168:G:H2'	2:B:2170:A:OP2	2.00	0.61
2:B:2799:A:HO2'	2:B:2802:G:HO2'	1.48	0.61
33:GA:9:ARG:NH1	33:GA:16:VAL:HG23	2.15	0.61
39:NA:5:GLU:HG3	39:NA:93:SER:HB3	1.82	0.61
1:DB:79:G:H1	1:DB:90:C:H42	1.47	0.61
1:DB:1305:G:N2	1:DB:1331:G:H1'	2.16	0.61
2:EB:2345:G:N3	2:EB:2381:C:H2'	2.15	0.61
17:TB:23:ARG:HD3	17:TB:120:ARG:NH1	2.15	0.61
1:DB:1021:G:H2'	1:DB:1022:G:H4'	1.82	0.61
2:EB:101:G:H4'	2:EB:102:G:OP2	1.99	0.61
2:EB:1434:A:H61	2:EB:1558:A:N6	1.97	0.61
2:EB:1530:G:H1	2:EB:1541:U:H3	1.47	0.61
2:EB:2615:U:C2	29:FC:7:PRO:HA	2.35	0.61
5:E:142:VAL:HG23	5:E:193:VAL:HA	1.82	0.61
1:DB:661:G:H1	1:DB:744:C:H42	1.48	0.61
1:A:1517:G:H3'	1:A:1518:MA6:H8	1.81	0.61
36:KA:44:GLU:HA	36:KA:52:LEU:HD21	1.81	0.61
1:DB:1412:C:H2'	1:DB:1413:A:C8	2.36	0.61
1:DB:1513:A:H2'	1:DB:1514:C:C6	2.35	0.61
2:EB:2690:C:N4	2:EB:2713:A:H1'	2.14	0.61
19:VB:82:ARG:HG3	19:VB:82:ARG:NH1	2.15	0.61
33:JC:9:ARG:NH1	33:JC:16:VAL:HG23	2.15	0.61
2:B:2756:U:H3'	33:GA:19:ARG:HG3	1.82	0.61
10:J:27:ARG:HD2	25:Y:71:TYR:CE2	2.36	0.61
17:Q:16:ARG:HH12	17:Q:83:ILE:HB	1.66	0.61
38:MA:10:MET:O	38:MA:12:LEU:N	2.33	0.61
38:MA:58:ALA:HA	38:MA:61:TYR:HB2	1.82	0.61
2:EB:2349:G:OP2	32:IC:42:ARG:HD3	2.00	0.61
17:TB:26:ASP:O	17:TB:49:VAL:HG12	2.00	0.61
36:NC:115:LEU:HD22	36:NC:119:ARG:HH21	1.66	0.61
1:A:191(G):G:O2'	53:BB:101:GLY:O	2.18	0.61
1:A:1513:A:H2'	1:A:1514:C:C6	2.35	0.61
2:B:363(G):A:C8	2:B:363(G):A:OP2	2.53	0.61
2:B:1175:U:H2'	2:B:1176:G:H8	1.64	0.61
5:E:17:THR:O	5:E:211:ARG:NH2	2.33	0.61
10:J:10:GLU:N	10:J:10:GLU:OE2	2.33	0.61
1:DB:232:G:H1'	1:DB:262:A:N1	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EB:637:A:H5''	13:PB:117:GLU:HG2	1.81	0.61
2:EB:2327:A:H2'	2:EB:2328:A:C8	2.36	0.61
36:NC:35:GLU:HA	36:NC:38:ARG:HD2	1.82	0.61
1:A:165:C:H2'	1:A:166:G:C8	2.36	0.61
2:B:18:C:O2'	2:B:553:U:OP1	2.19	0.61
2:B:1534:G:O2'	2:B:1538:G:N2	2.33	0.61
37:LA:111:ALA:HB2	37:LA:120:LEU:HD12	1.82	0.61
46:UA:33:ALA:O	46:UA:37:THR:OG1	2.15	0.61
1:DB:147:G:N2	1:DB:148:G:H1'	2.15	0.61
1:DB:191(F):U:O2	53:ED:105:SER:OG	2.17	0.61
2:EB:1817:G:OP1	5:HB:88:ARG:NH2	2.32	0.61
2:EB:2807:G:H1	2:EB:2893:G:H22	1.49	0.61
10:MB:10:GLU:N	10:MB:10:GLU:OE2	2.34	0.61
10:MB:95:LYS:HA	10:MB:111:PRO:HB3	1.83	0.61
15:RB:24:GLN:HG2	15:RB:44:LEU:HG	1.82	0.61
40:RC:56:GLN:HB3	40:RC:60:LYS:HE3	1.82	0.61
46:XC:10:PRO:HG3	46:XC:21:TYR:HD1	1.65	0.61
1:A:82:U:C2	1:A:85:U:H5	2.19	0.61
1:A:191(F):U:O2	53:BB:105:SER:OG	2.16	0.61
2:B:2680:C:H5'	6:F:189:PRO:HA	1.81	0.61
2:B:2816:C:O2	2:B:2883:A:O2'	2.18	0.61
6:F:171:GLU:HB3	6:F:185:LYS:HB3	1.83	0.61
48:WA:56:LEU:HA	48:WA:59:MET:HE2	1.81	0.61
1:DB:501:C:H2'	1:DB:502:G:C8	2.36	0.61
2:EB:1107:G:H8	2:EB:1107:G:OP2	1.83	0.61
2:EB:1903:G:OP2	5:HB:241:PRO:HB2	2.00	0.61
23:ZB:8:TYR:HB2	23:ZB:38:TYR:CE2	2.35	0.61
23:ZB:95:PRO:HB3	23:ZB:129:SER:HA	1.81	0.61
55:GD:182:HIS:HB3	55:GD:310:TYR:HE1	1.65	0.61
2:B:2807:G:H1	2:B:2893:G:H22	1.48	0.61
4:IA:75:C:OP2	55:GD:261:ARG:NH2	2.34	0.61
36:KA:35:GLU:HA	36:KA:38:ARG:HD2	1.82	0.61
36:KA:139:GLN:HB3	36:KA:140:ARG:NH1	2.16	0.61
38:MA:59:GLY:O	38:MA:63:ARG:NH1	2.34	0.61
1:DB:677:U:H3	1:DB:713:G:H22	1.49	0.61
2:EB:712:G:H1	2:EB:719:C:H42	1.48	0.61
20:WB:68:ARG:HH11	20:WB:111:HIS:HA	1.66	0.61
39:QC:78:GLU:O	39:QC:81:ILE:HG22	2.01	0.61
1:A:656:C:O2'	48:WA:28:GLN:OE1	2.19	0.60
2:B:2543:G:H2'	2:B:2544:G:C8	2.36	0.60
6:F:191:PRO:O	6:F:193:GLY:N	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:44:ILE:HA	22:V:64:GLU:HA	1.82	0.60
28:BA:34:GLU:OE2	46:UA:3:ARG:HG2	2.01	0.60
2:EB:1483:G:H2'	2:EB:1484:G:H8	1.65	0.60
22:YB:37:VAL:HG21	22:YB:72:VAL:HG21	1.83	0.60
33:JC:27:CYS:SG	33:JC:28:GLU:N	2.73	0.60
55:GD:183:ARG:HH21	55:GD:309:THR:HG21	1.65	0.60
1:A:1316:G:N1	1:A:1319:A:OP2	2.26	0.60
2:B:1523:U:H2'	2:B:1524:G:C8	2.36	0.60
2:B:1778:U:H2'	2:B:1784:A:N6	2.16	0.60
3:C:57:A:OP2	3:C:58:A:OP2	2.18	0.60
35:JA:128:GLU:O	35:JA:132:LYS:NZ	2.32	0.60
39:NA:78:GLU:O	39:NA:81:ILE:HG22	2.01	0.60
44:SA:79:SER:HB2	44:SA:106:LYS:HD2	1.83	0.60
46:UA:39:ILE:HG12	46:UA:55:ARG:HH22	1.66	0.60
1:DB:656:C:O2'	48:ZC:28:GLN:OE1	2.19	0.60
24:X:5:LYS:HB3	55:GD:265:LYS:NZ	2.16	0.60
1:A:1054:C:N4	55:GD:194:GLY:O	2.33	0.60
2:B:712:G:H1	2:B:719:C:H42	1.46	0.60
43:RA:5:ARG:HD3	43:RA:71:LEU:HD11	1.83	0.60
2:EB:2712:U:O2'	2:EB:2712(A):A:H5''	2.01	0.60
21:XB:26:TYR:OH	21:XB:88:LYS:HD3	2.01	0.60
31:HC:10:ARG:NH1	31:HC:14:LYS:HE3	2.16	0.60
46:XC:39:ILE:HG12	46:XC:55:ARG:HH22	1.66	0.60
48:ZC:39:LEU:HD13	48:ZC:56:LEU:HB2	1.82	0.60
1:A:200:G:H1	1:A:217:C:H42	1.50	0.60
2:B:2749:A:OP1	9:I:3:ARG:NH1	2.27	0.60
35:JA:153:ARG:O	35:JA:156:LYS:NZ	2.27	0.60
1:DB:1298:C:H2'	40:RC:114:ARG:HH12	1.67	0.60
2:EB:2597:G:H2'	2:EB:2598:A:C8	2.37	0.60
19:VB:34:GLU:HG2	19:VB:56:SER:HB2	1.83	0.60
1:A:501:C:H2'	1:A:502:G:C8	2.37	0.60
2:B:2312:U:H5'	8:H:88:ILE:HD11	1.82	0.60
12:L:79:PHE:CD1	17:Q:72:VAL:HG22	2.37	0.60
23:W:95:PRO:HB3	23:W:129:SER:HA	1.83	0.60
2:EB:1657:C:H2'	2:EB:1658:C:H6	1.66	0.60
8:KB:113:ARG:HH11	28:EC:34:GLU:HG2	1.67	0.60
14:QB:18:LYS:O	14:QB:98:LYS:NZ	2.28	0.60
23:ZB:179:ASP:OD2	23:ZB:181:GLU:HG2	2.01	0.60
55:HD:114:GLU:HG3	55:HD:163:ILE:HG12	1.82	0.60
2:B:1196:C:HO2'	2:B:1227:G:HO2'	1.49	0.60
2:B:1530:G:H1	2:B:1541:U:H3	1.47	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:72:ARG:NH2	23:W:97:GLU:O	2.33	0.60
39:NA:43:LEU:HD21	51:ZA:35:ARG:HH21	1.65	0.60
1:DB:1128:C:H5''	42:TC:66:ARG:NH1	2.14	0.60
2:EB:2312:U:H5'	8:KB:88:ILE:HD11	1.82	0.60
14:QB:35:VAL:HG22	14:QB:102:VAL:HG22	1.84	0.60
1:A:878:G:H5'	41:PA:89:PRO:HG2	1.83	0.60
2:B:527:C:N4	2:B:2779:U:OP2	2.35	0.60
2:B:1126:A:H8	2:B:1126:A:OP1	1.85	0.60
2:B:1903:G:OP2	5:E:241:PRO:HB2	2.02	0.60
25:Y:52:ARG:HH12	25:Y:57:GLU:HB2	1.65	0.60
1:A:677:U:H3	1:A:713:G:H22	1.48	0.60
2:B:796:C:H2'	2:B:797:C:C6	2.37	0.60
2:B:900:A:H2'	2:B:901:A:H8	1.67	0.60
1:DB:978:A:OP2	1:DB:1362(B):C:N4	2.34	0.60
1:DB:1517:G:H3'	1:DB:1518:MA6:H8	1.82	0.60
2:EB:2141:G:H1	2:EB:2151:G:H1'	1.67	0.60
1:A:325:A:OP2	53:BB:70:SER:HB3	2.02	0.60
1:A:927:G:H1	1:A:1390:U:H3	1.49	0.60
19:S:34:GLU:HG2	19:S:56:SER:HB2	1.83	0.60
48:WA:85:LEU:HB3	48:WA:87:ILE:HG23	1.84	0.60
1:DB:191(G):G:O2'	53:ED:101:GLY:O	2.20	0.60
1:DB:1022:G:C5	1:DB:1023:G:H1'	2.37	0.60
2:EB:572:A:H5''	2:EB:573:G:OP2	2.02	0.60
2:EB:2708:G:O2'	15:RB:71:GLN:NE2	2.35	0.60
2:EB:2784:C:H1'	6:IB:37:ARG:NH1	2.10	0.60
8:H:143:GLU:HA	28:BA:28:LYS:HD3	1.83	0.59
9:I:9:ILE:HB	9:I:50:VAL:HG23	1.83	0.59
17:Q:26:ASP:O	17:Q:49:VAL:HG12	2.02	0.59
48:WA:9:GLN:HB3	48:WA:13:GLN:HE21	1.65	0.59
2:EB:17:G:H2'	2:EB:18:C:C6	2.37	0.59
22:YB:84:ARG:O	22:YB:100:ALA:HB2	2.02	0.59
40:RC:85:TYR:HD2	40:RC:154:TYR:HE2	1.49	0.59
2:B:556:G:H2'	2:B:557:U:C6	2.37	0.59
1:DB:165:C:H2'	1:DB:166:G:C8	2.36	0.59
2:EB:1291:C:H2'	2:EB:1292:U:C6	2.37	0.59
2:EB:2287:A:O2'	2:EB:2288:A:O5'	2.20	0.59
15:RB:56:LYS:NZ	15:RB:90:ARG:O	2.30	0.59
23:ZB:72:ARG:NH2	23:ZB:97:GLU:O	2.35	0.59
39:QC:43:LEU:HD21	51:CD:35:ARG:HH21	1.65	0.59
55:HD:233:GLY:HA3	55:HD:237:VAL:HB	1.83	0.59
1:A:1022:G:C5	1:A:1023:G:H1'	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2531:A:N3	2:B:2658:C:O2'	2.31	0.59
2:B:2593:U:H2'	2:B:2594:C:C6	2.38	0.59
2:B:2648:C:H2'	2:B:2649:U:C6	2.38	0.59
3:FB:57:A:OP2	3:FB:58:A:OP2	2.20	0.59
10:MB:61:ARG:NH1	10:MB:64:GLU:OE2	2.35	0.59
41:SC:85:ARG:NH1	41:SC:87:SER:O	2.35	0.59
2:B:2142:C:N4	2:B:2148:G:O6	2.34	0.59
5:E:73:VAL:HG23	5:E:120:GLY:HA2	1.84	0.59
8:H:137:GLU:HG2	8:H:152:LEU:HD13	1.84	0.59
9:I:41:MET:N	9:I:41:MET:SD	2.75	0.59
11:K:35:ARG:HG2	11:K:35:ARG:HH11	1.67	0.59
40:OA:85:TYR:HD2	40:OA:154:TYR:HE2	1.50	0.59
2:EB:2462:U:H1'	2:EB:2491:U:O4	2.02	0.59
2:EB:2849:U:OP2	17:TB:95:ARG:NH1	2.36	0.59
2:EB:2889:C:H2'	2:EB:2891:G:O4'	2.02	0.59
31:HC:24:THR:HG23	31:HC:27:GLY:HA3	1.83	0.59
43:UC:7:LYS:HB3	43:UC:97:GLU:HB2	1.82	0.59
55:HD:183:ARG:HH21	55:HD:309:THR:HG21	1.65	0.59
2:B:566:U:H5''	13:M:29:LYS:HE3	1.84	0.59
19:S:68:LYS:HE3	19:S:69:LYS:H	1.67	0.59
36:KA:115:LEU:HD22	36:KA:119:ARG:HH21	1.67	0.59
1:DB:646:U:H2'	1:DB:647:C:C6	2.38	0.59
2:EB:245:G:O6	32:IC:8:LYS:HE3	2.03	0.59
2:EB:796:C:H2'	2:EB:797:C:C6	2.38	0.59
2:EB:2313:C:OP2	8:KB:74:LYS:NZ	2.32	0.59
1:A:1376:U:O4	40:OA:10:ARG:NH1	2.35	0.59
14:N:35:VAL:HG22	14:N:102:VAL:HG22	1.84	0.59
28:BA:40:HIS:HB3	28:BA:43:TYR:HB2	1.85	0.59
6:IB:151:TYR:HB2	11:NB:79:PRO:HD3	1.85	0.59
11:NB:10:GLU:HA	11:NB:10:GLU:OE2	2.00	0.59
46:XC:11:ARG:HA	46:XC:45:VAL:HB	1.83	0.59
55:GD:224:ILE:HG12	55:GD:246:ILE:HG12	1.83	0.59
10:J:93:THR:HG23	10:J:95:LYS:H	1.67	0.59
11:K:12:ARG:NH1	11:K:50:ASP:OD2	2.35	0.59
15:O:70:LEU:O	15:O:72:ASP:N	2.27	0.59
1:DB:966:M2G:HM13	1:DB:967:5MC:H1'	1.84	0.59
1:DB:1223:C:P	52:DD:78:ARG:HH21	2.26	0.59
5:HB:36:PRO:HA	5:HB:61:LEU:HD12	1.85	0.59
1:A:507:C:OP2	1:A:508:C:O2'	2.12	0.59
1:A:979:C:O2	47:VA:19:ARG:NH1	2.35	0.59
1:A:1080:A:H5''	1:A:1081:G:OP2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:C:H5''	26:Z:10:LEU:HD11	1.85	0.59
3:C:82:G:H1	3:C:94:C:N4	1.97	0.59
13:M:81:GLN:HB2	13:M:110:TYR:HD1	1.68	0.59
19:S:82:ARG:HG3	19:S:82:ARG:NH1	2.16	0.59
23:W:179:ASP:O	23:W:182:LYS:HB3	2.03	0.59
1:DB:927:G:H1	1:DB:1390:U:H3	1.49	0.59
2:EB:1278:A:OP1	15:RB:36:THR:HG23	2.02	0.59
2:EB:1689:A:H62	2:EB:1698:A:H2	1.51	0.59
2:EB:2319:G:H22	16:SB:3:ARG:NH1	2.01	0.59
5:HB:217:ARG:HG2	5:HB:217:ARG:HH11	1.67	0.59
35:MC:128:GLU:O	35:MC:132:LYS:NZ	2.36	0.59
37:OC:111:ALA:HB2	37:OC:120:LEU:HD12	1.83	0.59
44:VC:79:SER:HB2	44:VC:106:LYS:HD2	1.85	0.59
2:B:140:A:H8	2:B:1408:C:HO2'	1.47	0.59
2:B:1278:A:OP1	15:O:36:THR:HG23	2.03	0.59
2:B:2287:A:O2'	2:B:2288:A:O5'	2.18	0.59
2:B:2306:C:N4	8:H:42:GLY:O	2.36	0.59
20:T:14:PRO:HG3	20:T:101:SER:HB3	1.84	0.59
41:PA:87:SER:OG	41:PA:93:VAL:N	2.34	0.59
2:EB:1523:U:H2'	2:EB:1524:G:C8	2.37	0.59
2:EB:1790:C:H5''	2:EB:1791:A:OP1	2.02	0.59
53:ED:43:LEU:O	53:ED:48:LYS:HB2	2.03	0.59
1:A:1289:A:N1	1:A:1371:G:O2'	2.27	0.59
2:B:2785:C:OP1	6:F:41:LYS:NZ	2.36	0.59
3:C:85:G:H1	3:C:91:C:H42	1.49	0.59
12:L:19:ILE:HG22	12:L:43:VAL:HA	1.84	0.59
15:O:12:ARG:HG3	15:O:12:ARG:NH1	2.17	0.59
20:T:13:SER:HB3	20:T:16:LYS:HD2	1.85	0.59
1:DB:1370:G:H5''	42:TC:12:GLU:HG3	1.84	0.59
2:EB:302:C:H2'	2:EB:303:U:H6	1.67	0.59
9:LB:25:LYS:HB3	9:LB:27:LYS:NZ	2.18	0.59
35:MC:16:HIS:HE1	35:MC:42:ILE:HD12	1.66	0.59
1:DB:1128:C:H42	1:DB:1144:G:H1	1.49	0.58
1:DB:1289:A:N1	1:DB:1371:G:O2'	2.30	0.58
9:LB:9:ILE:HB	9:LB:50:VAL:HG23	1.83	0.58
17:TB:127:ALA:O	17:TB:129:ARG:N	2.34	0.58
14:N:81:VAL:HG12	24:X:5:LYS:NZ	2.18	0.58
37:LA:18:LYS:HE3	37:LA:20:TYR:H	1.68	0.58
1:DB:1269:A:N1	1:DB:1312:G:O2'	2.25	0.58
19:VB:40:LEU:HB2	19:VB:46:VAL:HB	1.85	0.58
48:ZC:85:LEU:HB3	48:ZC:87:ILE:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:DD:20:LEU:HD13	52:DD:23:ASN:HD22	1.68	0.58
1:A:147:G:N2	1:A:148:G:H1'	2.18	0.58
2:B:34:C:O2'	2:B:35:G:O5'	2.21	0.58
11:K:10:GLU:HA	11:K:10:GLU:OE2	2.02	0.58
2:EB:1778:U:H2'	2:EB:1784:A:N6	2.18	0.58
2:EB:2006:C:O2'	2:EB:2823:A:N3	2.36	0.58
1:A:886:G:H1	1:A:911:U:H3	1.50	0.58
2:B:637:A:H5''	13:M:117:GLU:HG2	1.85	0.58
2:B:2131:G:OP2	2:B:2132:U:O2'	2.16	0.58
2:B:2141:G:H1	2:B:2151:G:H1'	1.68	0.58
5:E:67:PHE:HE1	5:E:106:ILE:HD11	1.68	0.58
2:EB:2680:C:H5'	6:IB:189:PRO:HA	1.83	0.58
5:HB:67:PHE:HE1	5:HB:106:ILE:HD11	1.68	0.58
6:IB:9:VAL:HG23	17:TB:3:ARG:HB2	1.85	0.58
54:FD:18:TYR:HA	54:FD:22:ARG:HD3	1.85	0.58
1:A:1104:G:H4'	35:JA:111:ARG:HD3	1.86	0.58
1:A:1412:C:H2'	1:A:1413:A:C8	2.38	0.58
2:B:572:A:H5''	2:B:573:G:OP2	2.04	0.58
9:I:7:LEU:HD12	9:I:8:PRO:HD2	1.84	0.58
1:DB:507:C:OP2	1:DB:508:C:O2'	2.15	0.58
2:EB:386:G:H5''	2:EB:388:G:N2	2.18	0.58
2:EB:2145:C:H4'	2:EB:2146:C:OP2	2.03	0.58
2:EB:2253:G:O6	24:AC:4:LYS:HB2	2.03	0.58
13:PB:71:VAL:HG12	13:PB:72:PRO:HA	1.84	0.58
24:AC:10:THR:HG22	24:AC:12:ASN:H	1.68	0.58
25:BC:56:GLN:HB3	25:BC:87:PRO:HG3	1.86	0.58
33:JC:7:VAL:HG12	33:JC:34:GLN:HG2	1.86	0.58
49:AD:53:VAL:HG13	49:AD:79:VAL:HG22	1.86	0.58
2:B:1557:C:H5''	2:B:1558:A:OP2	2.04	0.58
2:B:1795:C:O2	5:E:255:LYS:HE3	2.03	0.58
2:B:2597:G:H2'	2:B:2598:A:C8	2.38	0.58
13:M:71:VAL:HG12	13:M:72:PRO:HA	1.86	0.58
31:EA:10:ARG:NH1	31:EA:14:LYS:HE3	2.19	0.58
2:EB:140:A:H8	2:EB:1408:C:O2'	1.86	0.58
16:SB:4:LEU:HD12	16:SB:9:ARG:HG3	1.86	0.58
2:B:1689:A:H62	2:B:1698:A:H2	1.49	0.58
2:B:2712:U:O2'	2:B:2712(A):A:H5''	2.03	0.58
41:PA:19:VAL:HG23	41:PA:21:LYS:HG2	1.85	0.58
37:OC:166:LYS:HG2	37:OC:178:VAL:HG21	1.85	0.58
38:PC:10:MET:O	38:PC:12:LEU:N	2.36	0.58
55:GD:155:GLU:HG3	55:GD:156:HIS:ND1	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1073:U:O2'	35:JA:104:ASN:ND2	2.37	0.58
1:A:1298:C:H2'	40:OA:114:ARG:HH12	1.68	0.58
2:B:1088:A:O2'	2:B:1089:G:OP2	2.14	0.58
2:B:1107:G:OP2	2:B:1107:G:H8	1.87	0.58
19:S:62:LEU:HD21	19:S:95:LEU:HB2	1.86	0.58
37:LA:12:CYS:HB3	37:LA:33:MET:HG2	1.86	0.58
38:MA:145:LYS:HB3	38:MA:145:LYS:HZ3	1.68	0.58
2:EB:2153:G:N2	2:EB:2154:G:O6	2.37	0.58
2:EB:2315:G:OP1	8:KB:36:LYS:NZ	2.28	0.58
2:EB:2377:A:H4'	16:SB:112:PHE:OXT	2.04	0.58
2:EB:2816:C:O2	2:EB:2883:A:O2'	2.20	0.58
8:KB:41:GLN:HE22	8:KB:56:ALA:HB1	1.68	0.58
25:BC:21:ARG:HH11	25:BC:21:ARG:CG	2.13	0.58
41:SC:69:ARG:NE	41:SC:75:ARG:O	2.35	0.58
42:TC:9:ARG:HB3	42:TC:14:VAL:HG13	1.84	0.58
2:B:2564:A:OP1	2:B:2648:C:H4'	2.04	0.58
23:W:8:TYR:HB2	23:W:38:TYR:CE2	2.38	0.58
1:DB:325:A:OP2	53:ED:70:SER:HB3	2.03	0.58
2:EB:2445:G:OP1	7:JB:74:ARG:NH2	2.37	0.58
4:GB:54:5MU:HN3	4:GB:58:A:H62	1.52	0.58
7:JB:161:GLU:OE2	7:JB:164:ARG:HD3	2.03	0.58
2:B:245:G:O6	32:FA:8:LYS:HE3	2.04	0.58
2:B:2153:G:N2	2:B:2154:G:O6	2.36	0.58
2:B:2445:G:OP1	7:G:74:ARG:NH2	2.36	0.58
2:EB:1688:U:O2	2:EB:1700:A:H5'	2.04	0.58
3:FB:104:A:OP1	23:ZB:72:ARG:NH1	2.31	0.58
8:KB:143:GLU:HA	28:EC:28:LYS:HD3	1.85	0.58
19:VB:85:LYS:NZ	19:VB:85:LYS:HB3	2.19	0.58
35:MC:58:ILE:O	35:MC:62:ALA:N	2.28	0.58
53:ED:38:LYS:HA	53:ED:41:VAL:HG22	1.86	0.58
55:HD:218:ASN:HB3	55:HD:221:ASP:OD2	2.04	0.58
1:A:297:G:N2	1:A:300:A:OP2	2.34	0.57
1:A:966:M2G:HM13	1:A:967:5MC:H1'	1.84	0.57
2:B:479:A:N3	2:B:481:G:H5''	2.19	0.57
2:B:1019:U:H3	2:B:1142(B):A:H62	1.51	0.57
2:B:1923:U:H2'	2:B:1924:C:C6	2.39	0.57
2:B:2139:C:H42	2:B:2153:G:H1'	1.69	0.57
2:B:2889:C:H2'	2:B:2891:G:O4'	2.03	0.57
8:KB:181:ARG:HH11	8:KB:181:ARG:HB2	1.69	0.57
19:VB:22:VAL:HG12	19:VB:23:GLU:H	1.68	0.57
22:YB:30:VAL:HG13	22:YB:37:VAL:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:UC:5:ARG:HD3	43:UC:71:LEU:HD11	1.85	0.57
2:B:784:A:C5	5:E:229:VAL:HG21	2.39	0.57
2:B:1028:A:N3	2:B:2486:G:O2'	2.29	0.57
2:B:2145:C:H4'	2:B:2146:C:OP2	2.03	0.57
2:B:2690:C:N4	2:B:2713:A:H1'	2.19	0.57
17:Q:127:ALA:O	17:Q:129:ARG:N	2.34	0.57
33:GA:35:ARG:NH1	33:GA:37:GLY:OXT	2.36	0.57
46:UA:11:ARG:HA	46:UA:45:VAL:HB	1.86	0.57
1:DB:926:G:H22	34:KC:15:A:H5''	1.69	0.57
1:DB:1080:A:H5''	1:DB:1081:G:OP2	2.04	0.57
1:DB:1130:A:H2'	1:DB:1131:G:C8	2.39	0.57
2:EB:270(J):G:H4'	25:BC:81:ARG:HE	1.69	0.57
2:EB:1060:U:N3	2:EB:1088:A:H1'	2.19	0.57
4:GB:7:G:H5''	4:GB:8:4SU:H5	1.86	0.57
6:IB:171:GLU:HB3	6:IB:185:LYS:HB3	1.85	0.57
8:KB:34:LEU:H	8:KB:34:LEU:HD12	1.68	0.57
8:KB:137:GLU:HG2	8:KB:152:LEU:HD13	1.86	0.57
1:A:79:G:H1	1:A:90:C:H42	1.50	0.57
7:G:153:SER:OG	7:G:190:GLU:HG3	2.03	0.57
1:DB:878:G:H5'	41:SC:89:PRO:HG2	1.86	0.57
2:EB:630:G:N2	2:EB:633:A:OP2	2.35	0.57
2:EB:1534:G:O2'	2:EB:1538:G:N2	2.37	0.57
23:ZB:127:LYS:H	23:ZB:164:ALA:HB2	1.70	0.57
1:A:1269:A:N1	1:A:1312:G:O2'	2.24	0.57
2:B:302:C:H2'	2:B:303:U:H6	1.69	0.57
2:B:910:A:H62	14:N:12:GLN:HA	1.69	0.57
2:B:1778:U:H2'	2:B:1784:A:H62	1.69	0.57
2:B:2564:A:C2	2:B:2647:U:H4'	2.39	0.57
2:B:2747:G:O6	2:B:2755:C:H5''	2.04	0.57
11:K:39:ARG:HE	11:K:48:MET:HE2	1.70	0.57
13:M:63:PRO:HG2	32:FA:25:MET:HB2	1.84	0.57
35:JA:58:ILE:O	35:JA:62:ALA:N	2.27	0.57
1:DB:886:G:H1	1:DB:911:U:H3	1.53	0.57
2:EB:439:G:H2'	2:EB:440:G:C8	2.39	0.57
2:EB:1795:C:O2	5:HB:255:LYS:HE3	2.04	0.57
2:EB:2142:C:N4	2:EB:2148:G:O6	2.36	0.57
2:EB:2543:G:H2'	2:EB:2544:G:C8	2.38	0.57
2:EB:2756:U:H4'	2:EB:2757:A:OP1	2.03	0.57
12:OB:68:GLU:HB3	12:OB:78:ARG:HB2	1.87	0.57
23:ZB:54:HIS:HB3	23:ZB:101:PRO:HD3	1.87	0.57
2:B:2094:G:P	10:J:22:LYS:NZ	2.76	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2253:G:O6	24:X:4:LYS:HB2	2.04	0.57
2:B:2637:U:C4	2:B:2638:G:C6	2.92	0.57
2:B:2756:U:OP2	33:GA:19:ARG:NH2	2.28	0.57
6:F:14:ILE:HG13	6:F:21:VAL:HG13	1.86	0.57
7:G:155:LEU:HD12	7:G:174:VAL:HB	1.84	0.57
8:H:113:ARG:HH11	28:BA:34:GLU:HG2	1.70	0.57
27:AA:38:GLU:HA	27:AA:38:GLU:OE2	2.05	0.57
29:CA:49:CYS:SG	29:CA:51:TYR:HB2	2.44	0.57
2:EB:245:G:H5'	13:PB:73:GLY:HA2	1.85	0.57
2:EB:394:A:N6	2:EB:395:U:O4	2.37	0.57
2:EB:1034:G:H2'	2:EB:1035:U:O4'	2.05	0.57
2:EB:2723:C:OP2	6:IB:109:LYS:NZ	2.38	0.57
35:MC:188:ALA:HB1	35:MC:192:SER:HB2	1.86	0.57
38:PC:36:ASP:OD1	38:PC:38:GLN:N	2.37	0.57
2:B:2317:C:H2'	2:B:2318:G:H5'	1.86	0.57
24:X:10:THR:HG22	24:X:12:ASN:H	1.69	0.57
28:BA:44:THR:O	28:BA:47:GLN:NE2	2.37	0.57
1:DB:523:A:H61	45:WC:92:0TD:CG	2.13	0.57
2:EB:848:G:H2'	2:EB:849:A:C8	2.39	0.57
2:EB:1796:U:H4'	5:HB:256:GLY:H	1.70	0.57
19:VB:62:LEU:HD21	19:VB:95:LEU:HB2	1.87	0.57
45:WC:28:LYS:HD3	45:WC:62:SER:HB2	1.87	0.57
1:A:1415:G:H2'	1:A:1416:G:H8	1.69	0.57
2:B:2139:C:H3'	2:B:2140:C:H6	1.68	0.57
7:G:161:GLU:OE2	7:G:164:ARG:HD3	2.05	0.57
35:JA:166:ASP:HB3	35:JA:169:LYS:HB3	1.87	0.57
42:QA:9:ARG:HB3	42:QA:14:VAL:HG13	1.87	0.57
2:EB:2131:G:OP2	2:EB:2132:U:O2'	2.18	0.57
35:MC:129:GLU:OE2	35:MC:130:ARG:HG3	2.04	0.57
41:SC:11:THR:HG23	41:SC:14:ARG:HH12	1.69	0.57
2:B:2805:G:N2	2:B:2807:G:O6	2.35	0.57
7:G:127:GLU:HG2	7:G:196:LEU:HD22	1.86	0.57
45:TA:84:LEU:HD23	45:TA:101:VAL:HG21	1.86	0.57
2:EB:674:G:H1'	7:JB:74:ARG:HD2	1.87	0.57
2:EB:1815:A:OP2	5:HB:54:ARG:NH2	2.38	0.57
17:TB:11:GLU:OE1	17:TB:57:PHE:HB3	2.05	0.57
28:EC:44:THR:O	28:EC:47:GLN:NE2	2.37	0.57
1:A:1455:G:H5''	53:BB:31:SER:HB3	1.86	0.57
2:B:851:U:H2'	2:B:852:G:C8	2.39	0.57
2:B:1291:C:H2'	2:B:1292:U:C6	2.40	0.57
2:B:1993:U:H4'	6:F:128:SER:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:41:GLN:HE22	8:H:56:ALA:HB1	1.69	0.57
17:Q:54:ARG:HA	17:Q:59:THR:OG1	2.05	0.57
33:GA:7:VAL:HG12	33:GA:34:GLN:HG2	1.86	0.57
34:HA:21:A:H2'	55:GD:197:HIS:CD2	2.40	0.57
2:EB:616:A:C4	7:JB:180:GLY:HA2	2.40	0.57
25:BC:21:ARG:HG3	25:BC:21:ARG:NH1	2.14	0.57
1:A:407:G:O4'	37:LA:119:GLN:NE2	2.38	0.57
1:A:1009:G:N2	1:A:1020:U:O2	2.36	0.57
2:B:270(J):G:H4'	25:Y:81:ARG:HE	1.69	0.57
2:B:586:A:N1	2:B:809:G:O2'	2.30	0.57
2:B:1077:A:H3'	2:B:1078:U:H4'	1.86	0.57
2:B:1817:G:OP1	5:E:88:ARG:NH2	2.37	0.57
14:N:80:GLU:HG3	55:GD:264:HIS:HD2	1.68	0.57
1:DB:200:G:H1	1:DB:217:C:H42	1.51	0.57
1:DB:397:A:H5'	1:DB:398:C:OP1	2.04	0.57
2:EB:900:A:H2'	2:EB:901:A:H8	1.70	0.57
2:EB:1173:G:H2'	2:EB:1175:U:H5''	1.86	0.57
2:EB:1557:C:H5''	2:EB:1558:A:OP2	2.05	0.57
6:IB:14:ILE:HG13	6:IB:21:VAL:HG13	1.87	0.57
8:KB:83:ARG:O	8:KB:86:MET:HB3	2.05	0.57
11:NB:35:ARG:HG2	11:NB:35:ARG:HH11	1.70	0.57
21:XB:60:ARG:NH1	31:HC:47:ARG:NH2	2.53	0.57
42:TC:114:TYR:HE1	43:UC:59:SER:HA	1.69	0.57
2:B:155:C:H41	2:B:171:G:H1	1.53	0.56
4:D:10:G:H2'	4:D:11:A:C8	2.41	0.56
5:E:112:GLN:O	5:E:115:GLN:HB3	2.04	0.56
9:I:21:PRO:HG2	9:I:23:ARG:HH12	1.70	0.56
12:L:71:ARG:NH2	12:L:122:LEU:O	2.38	0.56
44:SA:120:ARG:NH1	44:SA:126:ARG:NH1	2.52	0.56
1:DB:1261:A:H5''	54:FD:25:LYS:HZ2	1.70	0.56
2:EB:2747:G:O6	2:EB:2755:C:H5''	2.05	0.56
9:LB:7:LEU:HD12	9:LB:8:PRO:HD2	1.87	0.56
51:CD:19:LYS:NZ	51:CD:19:LYS:HB3	2.20	0.56
55:HD:155:GLU:HG3	55:HD:156:HIS:ND1	2.20	0.56
2:B:289:A:H2'	2:B:290:G:O4'	2.06	0.56
2:B:1510:A:H2'	2:B:1511:A:C8	2.40	0.56
19:S:40:LEU:HB2	19:S:46:VAL:HB	1.86	0.56
31:EA:24:THR:HG23	31:EA:27:GLY:HA3	1.87	0.56
35:JA:25:ASN:HD21	35:JA:27:LYS:HB2	1.70	0.56
2:EB:1077:A:H3'	2:EB:1078:U:H4'	1.86	0.56
6:IB:2:LYS:NZ	6:IB:95:ILE:O	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1047:G:HO2'	1:A:1215:G:HO2'	1.45	0.56
23:W:102:LEU:HD22	23:W:137:ILE:HG21	1.87	0.56
24:X:7:LEU:H	4:IA:2:G:H5'	1.71	0.56
42:QA:40:LEU:HD11	42:QA:70:LYS:HD3	1.87	0.56
1:DB:191(D):U:H2'	1:DB:191(E):G:C8	2.40	0.56
2:EB:910:A:H62	14:QB:12:GLN:HA	1.70	0.56
2:EB:1510:A:H2'	2:EB:1511:A:C8	2.41	0.56
2:EB:1923:U:H2'	2:EB:1924:C:C6	2.41	0.56
9:LB:154:PRO:HB3	9:LB:163:TYR:CZ	2.40	0.56
13:PB:93:GLY:H	13:PB:123:LEU:HD22	1.71	0.56
14:QB:43:THR:HA	14:QB:94:VAL:HG12	1.86	0.56
14:QB:55:VAL:HG11	23:ZB:183:LEU:HD21	1.87	0.56
14:QB:75:THR:HG21	14:QB:87:LYS:HZ1	1.70	0.56
22:YB:50:ARG:NH1	22:YB:50:ARG:HB2	2.20	0.56
28:EC:36:CYS:SG	28:EC:37:SER:N	2.77	0.56
35:MC:166:ASP:HB3	35:MC:169:LYS:HB3	1.87	0.56
41:SC:44:PHE:HD1	41:SC:80:ILE:HG12	1.70	0.56
41:SC:87:SER:OG	41:SC:93:VAL:N	2.34	0.56
42:TC:5:TYR:HE1	42:TC:16:ARG:HB2	1.69	0.56
55:HD:109:ARG:NH1	55:HD:210:PRO:HD3	2.20	0.56
1:A:125:U:H2'	1:A:126:G:C8	2.41	0.56
1:A:564:C:O2'	41:PA:91:ARG:NH2	2.30	0.56
1:A:661:G:H1	1:A:744:C:H42	1.54	0.56
2:B:1709:U:H2'	2:B:1710:C:C6	2.40	0.56
9:I:154:PRO:HB3	9:I:163:TYR:CZ	2.41	0.56
23:W:40:ASP:HB3	23:W:43:GLU:HB2	1.86	0.56
4:IA:76:A:H3'	55:GD:234:GLY:HA3	1.86	0.56
2:EB:2711:A:OP2	2:EB:2712(A):A:OP2	2.24	0.56
7:JB:155:LEU:HD12	7:JB:174:VAL:HB	1.88	0.56
23:ZB:179:ASP:O	23:ZB:182:LYS:HB3	2.05	0.56
40:RC:16:LEU:HD11	42:TC:45:ALA:HB2	1.87	0.56
1:A:87:A:H2	1:A:88:C:H1'	1.70	0.56
1:A:165:C:H2'	1:A:166:G:H8	1.71	0.56
1:A:1223:C:P	52:AB:78:ARG:HH21	2.29	0.56
2:B:630:G:N2	2:B:633:A:OP2	2.36	0.56
2:B:882:G:H2'	2:B:883:G:C8	2.40	0.56
2:B:1081:U:H5'	2:B:1082:U:OP2	2.06	0.56
9:I:124:GLU:HB3	9:I:132:ARG:HB3	1.88	0.56
1:DB:87:A:H2	1:DB:88:C:H1'	1.70	0.56
2:EB:2557:G:H2'	2:EB:2558:C:C6	2.41	0.56
7:JB:157:VAL:HB	7:JB:194:MET:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:MB:84:GLY:O	10:MB:86:THR:N	2.37	0.56
19:VB:8:GLY:HA3	19:VB:23:GLU:HB2	1.86	0.56
37:OC:23:GLY:HA3	37:OC:112:VAL:HG12	1.87	0.56
1:A:191(D):U:H2'	1:A:191(E):G:C8	2.41	0.56
2:B:392:C:H5''	2:B:409:C:H5''	1.87	0.56
2:B:1799:G:H8	5:E:181:GLU:OE2	1.88	0.56
2:B:2462:U:H1'	2:B:2491:U:O4	2.05	0.56
4:D:54:5MU:HN3	4:D:58:A:H62	1.54	0.56
1:DB:564:C:O2'	41:SC:91:ARG:NH2	2.29	0.56
1:DB:1427:U:H2'	1:DB:1428:A:C8	2.41	0.56
1:DB:1510:U:H2'	1:DB:1511:G:C8	2.41	0.56
2:EB:566:U:H5''	13:PB:29:LYS:HE3	1.86	0.56
7:JB:181:LEU:HD11	7:JB:186:ILE:HD11	1.87	0.56
15:RB:13:HIS:CE1	15:RB:15:SER:HB2	2.41	0.56
28:EC:40:HIS:HB3	28:EC:43:TYR:HB2	1.87	0.56
39:QC:53:ALA:HB3	39:QC:86:ARG:NH1	2.21	0.56
2:B:1034:G:H2'	2:B:1035:U:O4'	2.06	0.56
2:B:2557:G:H2'	2:B:2558:C:C6	2.40	0.56
6:F:18:ASP:HB3	17:Q:82:LEU:HD21	1.86	0.56
41:PA:51:VAL:HG11	41:PA:60:ARG:NH1	2.20	0.56
45:TA:52:LEU:HD13	55:GD:305:ASP:OD2	2.06	0.56
1:DB:165:C:H2'	1:DB:166:G:H8	1.70	0.56
1:DB:1347:G:N2	1:DB:1373:G:H2'	2.21	0.56
2:EB:535:C:O3'	18:UB:53:ARG:NH1	2.39	0.56
2:EB:1126:A:H8	2:EB:1126:A:OP1	1.89	0.56
2:EB:1538:G:C8	2:EB:1538:G:OP2	2.59	0.56
2:EB:2637:U:C4	2:EB:2638:G:C6	2.93	0.56
2:EB:2648:C:H2'	2:EB:2649:U:C6	2.41	0.56
12:OB:66:LYS:HD2	12:OB:79:PHE:O	2.06	0.56
12:OB:71:ARG:NH2	12:OB:122:LEU:O	2.39	0.56
23:ZB:14:LYS:O	23:ZB:18:LEU:HB2	2.06	0.56
55:GD:218:ASN:HB3	55:GD:221:ASP:OD2	2.06	0.56
7:G:117:ARG:NH1	13:M:1:MET:H2	2.01	0.56
13:M:81:GLN:HB2	13:M:110:TYR:CD1	2.40	0.56
21:U:26:TYR:OH	21:U:88:LYS:HD3	2.06	0.56
1:DB:17:U:H2'	1:DB:18:C:C6	2.41	0.56
2:EB:1901:A:OP2	5:HB:255:LYS:HE2	2.06	0.56
7:JB:153:SER:OG	7:JB:190:GLU:HG3	2.06	0.56
55:GD:109:ARG:NH1	55:GD:210:PRO:HD3	2.21	0.56
2:B:242:G:H5''	32:FA:64:TYR:CE2	2.41	0.56
2:B:1060:U:N3	2:B:1088:A:H1'	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:LA:150:GLU:HA	37:LA:153:ARG:NH1	2.21	0.56
43:RA:33:GLN:HE21	43:RA:76:ASN:HB2	1.70	0.56
2:EB:489:G:N7	20:WB:49:LYS:NZ	2.54	0.56
2:EB:1341:U:OP2	2:EB:1394:U:O2'	2.24	0.56
8:KB:46:ALA:HA	8:KB:49:ASP:HB2	1.86	0.56
14:QB:81:VAL:HG12	24:AC:5:LYS:NZ	2.20	0.56
17:TB:54:ARG:HA	17:TB:59:THR:OG1	2.06	0.56
1:A:646:U:H2'	1:A:647:C:C6	2.41	0.56
2:B:1246:A:OP1	7:G:38:ARG:NH2	2.34	0.56
2:B:1943:U:OP1	55:GD:277:ARG:NH2	2.35	0.56
2:B:2712:U:H1'	2:B:2712(A):A:C8	2.41	0.56
2:B:2849:U:OP2	17:Q:95:ARG:NH1	2.39	0.56
8:H:83:ARG:O	8:H:86:MET:HB3	2.06	0.56
10:J:3:VAL:HG12	10:J:38:LEU:HA	1.88	0.56
40:OA:16:LEU:HD11	42:QA:45:ALA:HB2	1.88	0.56
40:OA:50:ILE:HD11	40:OA:121:ALA:HA	1.88	0.56
6:IB:45:THR:O	6:IB:82:ARG:HD2	2.06	0.56
12:OB:19:ILE:HG22	12:OB:43:VAL:HA	1.87	0.56
1:A:664:G:H5''	51:ZA:64:ARG:NH1	2.21	0.55
1:A:1427:U:H2'	1:A:1428:A:C8	2.42	0.55
2:B:2313:C:P	8:H:74:LYS:HZ3	2.29	0.55
6:F:111:ARG:HA	15:O:1:MET:SD	2.46	0.55
45:TA:83:VAL:HG23	45:TA:107:ALA:HB2	1.88	0.55
48:WA:39:LEU:HB3	48:WA:56:LEU:HD12	1.88	0.55
1:DB:1009:G:N2	1:DB:1020:U:O2	2.35	0.55
2:EB:155:C:H41	2:EB:171:G:H1	1.54	0.55
2:EB:1799:G:H8	5:HB:181:GLU:OE2	1.89	0.55
2:EB:2808:U:O2	2:EB:2892:A:N6	2.39	0.55
35:MC:216:SER:HA	35:MC:219:VAL:HG12	1.88	0.55
2:B:17:G:H2'	2:B:18:C:C6	2.41	0.55
2:B:1044:G:O2'	2:B:1111:A:N1	2.36	0.55
2:B:2853:C:H2'	2:B:2854:G:C8	2.40	0.55
8:H:34:LEU:H	8:H:34:LEU:HD12	1.71	0.55
9:I:86:GLU:HG2	9:I:132:ARG:HG3	1.88	0.55
19:S:29:PRO:HB3	19:S:63:GLY:HA2	1.88	0.55
35:JA:188:ALA:HB1	35:JA:192:SER:HB2	1.87	0.55
52:AB:36:ARG:NH2	52:AB:75:ALA:O	2.37	0.55
1:DB:137:C:H2'	1:DB:138:G:H8	1.71	0.55
1:DB:323:U:H2'	1:DB:324:G:O4'	2.06	0.55
1:DB:509:A:N3	1:DB:543:C:O2'	2.32	0.55
1:DB:614:A:H2'	1:DB:615:C:C6	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DB:619:U:C2	37:OC:135:LEU:HD21	2.41	0.55
1:DB:833:U:H3	1:DB:853:G:H1	1.54	0.55
1:DB:881:G:OP2	45:WC:12:ARG:NH2	2.39	0.55
2:EB:503:A:H4'	2:EB:504:U:H5''	1.89	0.55
2:EB:1111:A:H2'	2:EB:1111:A:OP2	2.06	0.55
2:EB:2756:U:H3'	33:JC:19:ARG:HG3	1.87	0.55
6:IB:59:VAL:HG11	6:IB:64:LYS:HD3	1.88	0.55
2:B:630:G:OP2	32:FA:15:LYS:NZ	2.26	0.55
2:B:2756:U:H4'	2:B:2757:A:OP1	2.05	0.55
8:H:16:ARG:NH2	8:H:28:VAL:O	2.39	0.55
25:Y:21:ARG:HG3	25:Y:21:ARG:NH1	2.13	0.55
37:LA:166:LYS:HG2	37:LA:178:VAL:HG21	1.88	0.55
40:OA:15:ASP:OD2	40:OA:44:TYR:OH	2.24	0.55
51:ZA:19:LYS:HB3	51:ZA:19:LYS:NZ	2.21	0.55
1:DB:820:U:H4'	1:DB:821:G:OP2	2.07	0.55
1:DB:1036:G:H21	1:DB:1037:C:H41	1.51	0.55
2:EB:851:U:H2'	2:EB:852:G:C8	2.41	0.55
2:EB:1587:A:H2'	2:EB:1588:C:C6	2.41	0.55
2:EB:2139:C:H42	2:EB:2153:G:H1'	1.72	0.55
2:EB:2514:U:H2'	2:EB:2515:C:C6	2.42	0.55
2:EB:2593:U:H2'	2:EB:2594:C:C6	2.41	0.55
12:OB:79:PHE:CD1	17:TB:72:VAL:HG22	2.41	0.55
23:ZB:52:SER:OG	23:ZB:53:ILE:N	2.39	0.55
25:BC:40:ARG:NH2	25:BC:42:GLN:HG2	2.20	0.55
55:GD:316:ARG:HH21	55:GD:327:TYR:HB3	1.70	0.55
55:GD:338:ASP:HA	55:GD:341:ILE:HG12	1.87	0.55
1:A:978:A:OP2	1:A:1362(B):C:N4	2.38	0.55
1:A:1418:A:H5''	1:A:1419:G:OP2	2.06	0.55
2:B:1021:A:OP2	11:K:65:LYS:NZ	2.32	0.55
2:B:1045:A:H1'	2:B:1047:G:N3	2.21	0.55
2:B:1292:U:H2'	2:B:1293:C:C6	2.42	0.55
2:B:2799:A:O2'	2:B:2802:G:O2'	2.24	0.55
17:Q:106:SER:O	17:Q:110:ILE:HG13	2.07	0.55
22:V:89:PHE:HD1	22:V:95:LYS:HB3	1.72	0.55
27:AA:6:VAL:HG12	27:AA:56:VAL:HG22	1.88	0.55
1:DB:1005:A:H1'	1:DB:1026:G:C2	2.42	0.55
2:EB:607:U:OP1	7:JB:103:LYS:N	2.25	0.55
2:EB:686:G:N2	2:EB:788:A:H61	2.05	0.55
48:ZC:39:LEU:HB3	48:ZC:56:LEU:HD12	1.89	0.55
1:A:1036:G:H21	1:A:1037:C:H41	1.53	0.55
2:B:1173:G:H2'	2:B:1175:U:H5''	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1538:G:OP2	2:B:1538:G:C8	2.60	0.55
2:B:1796:U:H4'	5:E:256:GLY:H	1.71	0.55
2:B:2210:G:H3'	2:B:2211:G:N7	2.22	0.55
12:L:66:LYS:HD2	12:L:79:PHE:O	2.05	0.55
43:RA:50:ILE:HB	47:VA:41:ARG:NH1	2.21	0.55
1:DB:1448:C:H2'	1:DB:1449:C:C6	2.41	0.55
2:EB:1065:U:H5'	2:EB:1074:G:H21	1.71	0.55
2:EB:2805:G:N2	2:EB:2807:G:O6	2.31	0.55
13:PB:63:PRO:HG2	32:IC:25:MET:HB2	1.89	0.55
54:FD:24:ARG:HG3	54:FD:25:LYS:HG2	1.87	0.55
1:A:953:G:H5'	1:A:965:A:H61	1.72	0.55
1:A:1070:U:H2'	1:A:1071:C:C6	2.41	0.55
2:B:394:A:N6	2:B:395:U:O4	2.40	0.55
2:B:545:G:N2	2:B:547:A:OP2	2.39	0.55
2:B:2808:U:O2	2:B:2892:A:N6	2.40	0.55
16:P:4:LEU:HD12	16:P:9:ARG:HG3	1.87	0.55
35:JA:76:GLN:NE2	35:JA:207:ALA:O	2.40	0.55
37:LA:30:LYS:HA	37:LA:35:ARG:HD2	1.89	0.55
1:DB:616:G:H1'	1:DB:625:G:N2	2.22	0.55
2:EB:335:C:OP2	22:YB:84:ARG:HD3	2.06	0.55
2:EB:1778:U:H2'	2:EB:1784:A:H62	1.72	0.55
2:EB:1870:C:H2'	2:EB:1871:A:O4'	2.07	0.55
2:EB:2502:G:H5''	2:EB:2503:2MA:H5''	1.89	0.55
2:EB:2564:A:C2	2:EB:2647:U:H4'	2.42	0.55
4:GB:1:C:N4	4:GB:72:A:H61	2.04	0.55
8:KB:129:GLY:O	8:KB:130:ASN:ND2	2.39	0.55
16:SB:54:LEU:O	16:SB:57:LYS:NZ	2.28	0.55
30:GC:16:CYS:SG	30:GC:18:ARG:HB2	2.46	0.55
37:OC:150:GLU:HA	37:OC:153:ARG:HH11	1.70	0.55
1:A:603:U:H2'	1:A:604:G:C8	2.42	0.55
1:A:626:U:H2'	1:A:627:G:C8	2.41	0.55
1:A:820:U:H4'	1:A:821:G:OP2	2.06	0.55
2:B:363(F):U:H3'	2:B:363(G):A:C8	2.41	0.55
2:B:1681:G:O2'	2:B:1762:A:O2'	2.21	0.55
2:B:1923:U:H2'	2:B:1924:C:H6	1.70	0.55
8:H:115:ARG:HH11	8:H:140:ILE:HD11	1.71	0.55
28:BA:14:ILE:HG12	28:BA:31:ILE:HG13	1.89	0.55
46:UA:50:GLU:O	46:UA:54:VAL:HG23	2.07	0.55
1:DB:632:A:OP1	41:SC:98:LYS:NZ	2.40	0.55
1:DB:1070:U:H2'	1:DB:1071:C:C6	2.41	0.55
1:DB:1422:G:H2'	1:DB:1423:G:H8	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EB:882:G:H2'	2:EB:883:G:C8	2.40	0.55
2:EB:1009:A:OP2	2:EB:1010:A:OP2	2.25	0.55
2:EB:1407:C:H2'	2:EB:1408:C:H6	1.71	0.55
4:GB:10:G:H2'	4:GB:11:A:C8	2.41	0.55
10:MB:111:PRO:HG2	10:MB:112:LYS:HD2	1.88	0.55
55:HD:301:GLY:HA3	55:HD:306:ARG:NH1	2.21	0.55
2:B:1417:C:H42	2:B:1581:G:H1	1.54	0.55
2:B:1464:C:H2'	2:B:1465:G:C8	2.42	0.55
33:GA:7:VAL:HA	33:GA:34:GLN:NE2	2.22	0.55
39:NA:87:ARG:NH1	39:NA:87:ARG:HG3	2.20	0.55
43:RA:21:GLN:HA	43:RA:24:VAL:HG12	1.88	0.55
1:DB:953:G:H5'	1:DB:965:A:H61	1.71	0.55
1:DB:1422:G:H2'	1:DB:1423:G:C8	2.42	0.55
2:EB:1088:A:O2'	2:EB:1089:G:OP2	2.20	0.55
36:NC:36:ASP:HB2	36:NC:59:ARG:HH21	1.72	0.55
37:OC:59:ARG:NH2	37:OC:66:ARG:NH1	2.54	0.55
41:SC:19:VAL:HG23	41:SC:21:LYS:HG2	1.88	0.55
46:XC:33:ALA:O	46:XC:37:THR:OG1	2.15	0.55
46:XC:37:THR:HB	46:XC:39:ILE:HG13	1.89	0.55
1:A:56:U:H2'	1:A:57:G:C8	2.42	0.55
1:A:1373:G:O6	42:QA:11:LYS:NZ	2.39	0.55
2:B:489:G:N7	20:T:49:LYS:NZ	2.54	0.55
2:B:1341:U:OP2	2:B:1394:U:O2'	2.20	0.55
9:I:25:LYS:HB3	9:I:27:LYS:NZ	2.22	0.55
40:OA:23:VAL:HG13	40:OA:43:PHE:CE2	2.42	0.55
42:QA:114:TYR:HE1	43:RA:59:SER:HA	1.72	0.55
2:EB:363(G):A:C8	2:EB:363(G):A:OP2	2.59	0.55
2:EB:2139:C:H3'	2:EB:2140:C:H6	1.71	0.55
2:EB:2667:C:H1'	9:LB:109:PHE:HD1	1.71	0.55
9:LB:3:ARG:HG2	9:LB:6:ARG:CZ	2.36	0.55
33:JC:7:VAL:HA	33:JC:34:GLN:NE2	2.22	0.55
38:PC:84:PHE:HB2	38:PC:134:ALA:HB2	1.89	0.55
55:HD:316:ARG:HH21	55:HD:327:TYR:HB3	1.70	0.55
1:A:1347:G:N2	1:A:1373:G:H2'	2.22	0.55
1:A:1422:G:H2'	1:A:1423:G:C8	2.42	0.55
2:B:637:A:OP1	13:M:133:SER:OG	2.19	0.55
2:B:1226:A:OP1	19:S:84:LYS:NZ	2.32	0.55
2:B:1254:A:N1	7:G:82:ILE:HD11	2.22	0.55
11:K:9:VAL:HG11	11:K:48:MET:HB2	1.89	0.55
35:JA:216:SER:HA	35:JA:219:VAL:HG12	1.89	0.55
37:LA:23:GLY:HA3	37:LA:112:VAL:HG12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:LA:150:GLU:HA	37:LA:153:ARG:HH11	1.71	0.55
38:MA:50:GLU:OE2	38:MA:51:VAL:HG23	2.06	0.55
42:QA:117:HIS:HB2	42:QA:121:ARG:HD3	1.89	0.55
52:AB:11:VAL:HG23	52:AB:38:SER:HB2	1.88	0.55
54:CB:18:TYR:HA	54:CB:22:ARG:HD3	1.88	0.55
2:EB:889:C:O2'	2:EB:890:A:O4'	2.25	0.55
2:EB:1709:U:H2'	2:EB:1710:C:C6	2.42	0.55
5:HB:5:LYS:HE3	5:HB:6:PHE:H	1.72	0.55
5:HB:17:THR:O	5:HB:211:ARG:NH2	2.36	0.55
19:VB:29:PRO:HB3	19:VB:63:GLY:HA2	1.88	0.55
25:BC:22:GLY:O	25:BC:32:LYS:NZ	2.28	0.55
43:UC:33:GLN:HE21	43:UC:76:ASN:HB2	1.72	0.55
2:B:249:C:O2	32:FA:12:LYS:NZ	2.36	0.54
2:B:503:A:H4'	2:B:504:U:H5''	1.89	0.54
2:B:1592:C:H2'	2:B:1593:G:H8	1.72	0.54
2:B:2291:U:H2'	2:B:2292:C:C6	2.42	0.54
2:B:2661:G:H2'	2:B:2662:A:C8	2.42	0.54
3:C:88:C:H2'	3:C:89(A):G:O4'	2.07	0.54
19:S:22:VAL:HG12	19:S:23:GLU:H	1.72	0.54
20:T:11:ARG:NH1	20:T:99:ARG:O	2.38	0.54
41:PA:85:ARG:NH1	41:PA:87:SER:O	2.39	0.54
44:SA:12:ARG:NH2	44:SA:13:GLN:HE22	2.05	0.54
1:DB:626:U:H2'	1:DB:627:G:C8	2.43	0.54
1:DB:1379:G:O6	40:RC:2:ALA:HB3	2.06	0.54
2:EB:479:A:N3	2:EB:481:G:H5''	2.22	0.54
2:EB:556:G:H2'	2:EB:557:U:C6	2.41	0.54
2:EB:2163:C:OP1	2:EB:2165:G:N2	2.39	0.54
2:EB:2317:C:H2'	2:EB:2318:G:H5'	1.89	0.54
2:EB:2790:A:H2'	2:EB:2791:C:H5'	1.88	0.54
39:QC:87:ARG:NH1	39:QC:87:ARG:HG3	2.22	0.54
40:RC:41:ARG:HG3	40:RC:42:ILE:HD13	1.89	0.54
40:RC:50:ILE:HD11	40:RC:121:ALA:HA	1.88	0.54
1:A:1448:C:H2'	1:A:1449:C:C6	2.43	0.54
2:B:1587:A:H2'	2:B:1588:C:C6	2.42	0.54
5:E:131:LEU:HD13	5:E:136:ILE:HG12	1.90	0.54
20:T:68:ARG:HH11	20:T:111:HIS:HA	1.72	0.54
30:DA:16:CYS:SG	30:DA:18:ARG:HB2	2.48	0.54
36:KA:55:VAL:HG22	36:KA:68:VAL:HG13	1.88	0.54
53:BB:43:LEU:O	53:BB:48:LYS:HB2	2.08	0.54
1:DB:186(B):C:N3	53:ED:105:SER:HB2	2.21	0.54
1:DB:1415:G:H2'	1:DB:1416:G:H8	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EB:2718:G:O2'	2:EB:2847:U:OP1	2.18	0.54
2:EB:2747:G:P	9:LB:138:LYS:HZ2	2.30	0.54
5:HB:73:VAL:HG23	5:HB:120:GLY:HA2	1.89	0.54
16:SB:15:ARG:HG2	16:SB:15:ARG:HH11	1.71	0.54
20:WB:14:PRO:HG3	20:WB:101:SER:HB3	1.87	0.54
37:OC:150:GLU:HA	37:OC:153:ARG:NH1	2.22	0.54
40:RC:23:VAL:HG13	40:RC:43:PHE:CE2	2.41	0.54
1:A:186(B):C:N3	53:BB:105:SER:HB2	2.22	0.54
1:A:1029:G:H2'	1:A:1030:C:H5'	1.89	0.54
2:B:1790:C:H5''	2:B:1791:A:OP1	2.07	0.54
5:E:36:PRO:HA	5:E:61:LEU:HD12	1.89	0.54
6:F:92:THR:O	6:F:95:ILE:HG23	2.07	0.54
12:L:25:LEU:O	12:L:27:GLY:N	2.41	0.54
14:N:55:VAL:HG11	23:W:183:LEU:HD21	1.89	0.54
18:R:47:TYR:HA	18:R:50:ARG:NH2	2.21	0.54
22:V:84:ARG:O	22:V:100:ALA:HB2	2.06	0.54
38:MA:8:GLU:HG2	38:MA:34:VAL:HG12	1.90	0.54
42:QA:10:ARG:NH1	42:QA:75:ASP:OD1	2.41	0.54
52:AB:22:LEU:HD11	52:AB:29:ARG:HB2	1.89	0.54
1:DB:237:C:O3'	50:BD:25:ARG:NH1	2.36	0.54
2:EB:34:C:O2'	2:EB:35:G:O5'	2.24	0.54
2:EB:1915:5MU:O2'	55:HD:287:GLN:OE1	2.21	0.54
2:EB:2476:A:H2	2:EB:2481:G:H1	1.55	0.54
1:A:1380:U:O2	40:OA:3:ARG:NH1	2.40	0.54
2:B:889:C:O2'	2:B:890:A:O4'	2.26	0.54
2:B:2163:C:OP1	2:B:2165:G:N2	2.39	0.54
17:Q:120:ARG:O	17:Q:124:ASP:HB2	2.08	0.54
46:UA:7:VAL:HG12	46:UA:8:GLU:H	1.72	0.54
1:DB:933:G:N7	40:RC:3:ARG:NH2	2.53	0.54
1:DB:1373:G:O6	42:TC:11:LYS:NZ	2.41	0.54
2:EB:784:A:H5'	2:EB:785:G:OP1	2.07	0.54
2:EB:1175:U:H2'	2:EB:1176:G:C8	2.42	0.54
2:EB:1519:G:C6	2:EB:1520:U:C4	2.95	0.54
5:HB:68:LYS:HD2	5:HB:70:TRP:CZ2	2.43	0.54
18:UB:89:GLU:HB2	19:VB:50:PRO:HB3	1.89	0.54
22:YB:89:PHE:HD1	22:YB:95:LYS:HB3	1.72	0.54
52:DD:42:PRO:O	52:DD:44:MET:N	2.38	0.54
1:A:957:U:H2'	1:A:959:A:OP2	2.07	0.54
2:B:2315:G:H2'	2:B:2316:C:C6	2.42	0.54
2:B:2406:U:C2	13:M:72:PRO:HG2	2.43	0.54
7:G:12:LEU:HG	7:G:124:LEU:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:3:LEU:HD23	8:H:5:LEU:HD11	1.89	0.54
15:O:48:VAL:HG23	15:O:95:THR:HG21	1.89	0.54
40:OA:78:ARG:HG2	40:OA:79:ARG:H	1.72	0.54
42:QA:5:TYR:HE1	42:QA:16:ARG:HB2	1.71	0.54
1:DB:664:G:H5''	51:CD:64:ARG:NH1	2.23	0.54
2:EB:1019:U:H3	2:EB:1142(B):A:H62	1.56	0.54
2:EB:1357:U:H2'	2:EB:1358:G:O4'	2.08	0.54
3:FB:88:C:H2'	3:FB:89(A):G:O4'	2.08	0.54
12:OB:79:PHE:HD1	17:TB:72:VAL:HG22	1.72	0.54
1:A:287:U:H2'	1:A:288:A:H8	1.72	0.54
1:A:323:U:H2'	1:A:324:G:O4'	2.07	0.54
1:A:409:G:OP2	37:LA:22:LYS:HE2	2.07	0.54
2:B:535:C:O3'	18:R:53:ARG:NH1	2.40	0.54
2:B:635:C:O2'	2:B:639:U:OP1	2.25	0.54
2:B:1901:A:OP2	5:E:255:LYS:HE2	2.07	0.54
6:F:47:VAL:HG11	6:F:86:PRO:HD2	1.89	0.54
6:F:151:TYR:HB2	11:K:79:PRO:HD3	1.90	0.54
12:L:47:ILE:HD12	12:L:48:PRO:O	2.08	0.54
1:DB:957:U:H2'	1:DB:959:A:OP2	2.08	0.54
1:DB:1029:G:H2'	1:DB:1030:C:H5'	1.90	0.54
1:DB:1293:G:H2'	1:DB:1294:G:C8	2.42	0.54
2:EB:142:G:H1'	21:XB:37:THR:HG21	1.89	0.54
2:EB:2712:U:H1'	2:EB:2712(A):A:C8	2.42	0.54
42:TC:117:HIS:HB2	42:TC:121:ARG:HD3	1.90	0.54
55:GD:245:ARG:HG3	55:GD:256:GLU:HG3	1.89	0.54
10:J:57:ARG:O	10:J:60:GLU:HB3	2.07	0.54
12:L:68:GLU:HB3	12:L:78:ARG:HB2	1.88	0.54
12:L:107:ARG:HD3	17:Q:37:GLY:H	1.72	0.54
24:X:12:ASN:HA	24:X:14:ARG:NH2	2.22	0.54
44:SA:48:ILE:HD11	44:SA:64:ALA:HA	1.90	0.54
46:UA:44:ARG:HB2	46:UA:47:ASP:OD2	2.08	0.54
5:HB:112:GLN:O	5:HB:115:GLN:HB3	2.08	0.54
8:KB:115:ARG:HH11	8:KB:140:ILE:HD11	1.72	0.54
11:NB:67:LEU:HA	11:NB:87:LEU:HD12	1.90	0.54
35:MC:25:ASN:HD21	35:MC:27:LYS:HB2	1.73	0.54
36:NC:108:ASN:HD22	36:NC:109:PRO:HD2	1.72	0.54
1:A:1178:G:N2	1:A:1181:G:OP2	2.40	0.54
2:B:848:G:H2'	2:B:849:A:C8	2.43	0.54
2:B:1065:U:H5'	2:B:1074:G:H21	1.73	0.54
2:B:1508:A:H3'	2:B:1509:A:C8	2.42	0.54
2:B:2792:G:N1	2:B:2805:G:H1'	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:PA:11:THR:HG23	41:PA:14:ARG:HH12	1.71	0.54
41:PA:44:PHE:HD1	41:PA:80:ILE:HG12	1.72	0.54
41:PA:110:ALA:HB3	41:PA:121:ASP:HB3	1.88	0.54
1:DB:1178:G:N2	1:DB:1181:G:OP2	2.40	0.54
1:DB:1291:G:O2'	42:TC:38:GLN:OE1	2.25	0.54
2:EB:481:G:C4	2:EB:507:A:C2	2.96	0.54
2:EB:2567:G:H2'	2:EB:2568:C:H6	1.72	0.54
6:IB:2:LYS:HG3	6:IB:200:GLU:HB2	1.89	0.54
11:NB:73:THR:HB	11:NB:82:LEU:HD11	1.90	0.54
40:RC:15:ASP:OD2	40:RC:44:TYR:OH	2.26	0.54
40:RC:78:ARG:HG2	40:RC:79:ARG:H	1.73	0.54
41:SC:11:THR:HA	41:SC:14:ARG:NH1	2.21	0.54
43:UC:21:GLN:HA	43:UC:24:VAL:HG12	1.90	0.54
45:WC:83:VAL:HG23	45:WC:107:ALA:HB2	1.90	0.54
1:A:708:C:OP1	44:SA:85:ARG:NH2	2.41	0.54
1:A:754:C:O2	1:A:754:C:H2'	2.07	0.54
2:B:1789:A:H2'	2:B:1790:C:O4'	2.07	0.54
2:B:2113:U:H2'	2:B:2114:A:H8	1.73	0.54
12:L:71:ARG:HH12	12:L:104:ARG:HB3	1.73	0.54
12:L:79:PHE:HD1	17:Q:72:VAL:HG22	1.72	0.54
19:S:8:GLY:HA3	19:S:23:GLU:HB2	1.89	0.54
23:W:70:LEU:HG	23:W:91:LEU:HD21	1.90	0.54
25:Y:56:GLN:HB3	25:Y:87:PRO:HG3	1.90	0.54
36:KA:108:ASN:HD22	36:KA:109:PRO:HD2	1.72	0.54
1:DB:558:G:C8	1:DB:559:A:H2'	2.43	0.54
1:DB:1414:U:H3	1:DB:1486:G:H1	1.56	0.54
2:EB:1081:U:H5'	2:EB:1082:U:OP2	2.06	0.54
2:EB:2529:G:H5''	2:EB:2530:A:H5''	1.89	0.54
2:EB:2853:C:H2'	2:EB:2854:G:C8	2.42	0.54
6:IB:47:VAL:HG11	6:IB:86:PRO:HD2	1.89	0.54
13:PB:81:GLN:HB2	13:PB:110:TYR:CD1	2.43	0.54
42:TC:10:ARG:HG2	42:TC:11:LYS:HG3	1.90	0.54
1:A:523:A:H61	45:TA:92:OTD:CG	2.18	0.54
1:A:757:U:H2'	1:A:758:G:O4'	2.08	0.54
2:B:17:G:H4'	18:R:25:TRP:NE1	2.23	0.54
2:B:1657:C:H2'	2:B:1658:C:C6	2.42	0.54
2:B:2319:G:H22	16:P:3:ARG:NH1	2.05	0.54
8:H:46:ALA:HA	8:H:49:ASP:HB2	1.90	0.54
8:H:138:GLN:HE22	8:H:149:VAL:HG13	1.72	0.54
20:T:90:ARG:HG2	20:T:90:ARG:HH11	1.72	0.54
23:W:179:ASP:OD2	23:W:181:GLU:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:JA:168:THR:HG23	35:JA:192:SER:HA	1.90	0.54
52:AB:20:LEU:HD13	52:AB:23:ASN:HD22	1.72	0.54
1:DB:664:G:OP1	51:CD:64:ARG:NH1	2.39	0.54
2:EB:635:C:O2'	2:EB:639:U:OP1	2.24	0.54
2:EB:2756:U:OP2	33:JC:19:ARG:NH2	2.30	0.54
9:LB:41:MET:N	9:LB:41:MET:SD	2.81	0.54
11:NB:128:HIS:O	11:NB:131:GLN:NE2	2.27	0.54
12:OB:47:ILE:HD12	12:OB:48:PRO:O	2.08	0.54
1:A:59:A:H1'	1:A:354:G:N2	2.23	0.53
2:B:481:G:C4	2:B:507:A:C2	2.96	0.53
2:B:2552:2MU:H6	2:B:2552:2MU:O5'	2.08	0.53
48:WA:82:ILE:HD12	48:WA:88:ARG:HH21	1.73	0.53
1:DB:757:U:H2'	1:DB:758:G:O4'	2.07	0.53
1:DB:1005:A:H4'	1:DB:1037:C:N3	2.23	0.53
2:EB:2113:U:H2'	2:EB:2114:A:H8	1.72	0.53
6:IB:11:MET:HG2	6:IB:24:THR:HB	1.90	0.53
13:PB:81:GLN:HB2	13:PB:110:TYR:HD1	1.73	0.53
28:EC:24:THR:OG1	28:EC:25:TYR:N	2.41	0.53
37:OC:12:CYS:HB3	37:OC:33:MET:HG2	1.90	0.53
37:OC:150:GLU:H	37:OC:150:GLU:CD	2.11	0.53
1:A:1503:A:O2'	1:A:1504:G:O5'	2.25	0.53
2:B:142:G:H1'	21:U:37:THR:HG21	1.91	0.53
2:B:2563:U:H4'	12:L:28:SER:HA	1.91	0.53
6:F:116:VAL:HG13	6:F:122:PHE:HB2	1.90	0.53
19:S:13:ARG:HG3	19:S:13:ARG:NH1	2.23	0.53
23:W:132:ASN:OD1	23:W:132:ASN:N	2.42	0.53
32:FA:31:HIS:CD2	32:FA:32:LEU:HD22	2.43	0.53
33:GA:27:CYS:SG	33:GA:28:GLU:N	2.81	0.53
35:JA:129:GLU:OE2	35:JA:130:ARG:HG3	2.08	0.53
46:UA:15:VAL:O	46:UA:19:LEU:HD13	2.08	0.53
1:DB:1448:C:H2'	1:DB:1449:C:H6	1.73	0.53
2:EB:1270:C:O2'	2:EB:1648:C:OP2	2.20	0.53
2:EB:2291:U:H2'	2:EB:2292:C:C6	2.43	0.53
4:GB:5:G:H1	4:GB:68:C:H42	1.56	0.53
5:HB:52:ARG:HB2	5:HB:53:PHE:CD2	2.43	0.53
12:OB:71:ARG:HH12	12:OB:104:ARG:HB3	1.73	0.53
35:MC:16:HIS:O	35:MC:18:GLY:N	2.41	0.53
44:VC:48:ILE:HD11	44:VC:64:ALA:HA	1.89	0.53
1:A:574:A:N3	1:A:883:C:H1'	2.24	0.53
1:A:616:G:H1'	1:A:625:G:N2	2.22	0.53
1:A:933:G:N7	40:OA:3:ARG:NH2	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:C:OP2	2:B:215:G:H2'	2.09	0.53
2:B:1585:C:H4'	2:B:1586:A:OP2	2.07	0.53
2:B:2514:U:H2'	2:B:2515:C:C6	2.42	0.53
7:G:53:THR:HG22	7:G:56:GLU:CG	2.39	0.53
8:H:165:THR:OG1	8:H:166:ASP:N	2.41	0.53
13:M:122:PRO:HB3	13:M:141:ALA:O	2.07	0.53
22:V:35:TYR:CE2	22:V:69:ALA:HB3	2.43	0.53
45:TA:28:LYS:HD3	45:TA:62:SER:HB2	1.90	0.53
1:DB:407:G:O4'	37:OC:119:GLN:NE2	2.40	0.53
1:DB:1087:G:H2'	1:DB:1088:G:C8	2.43	0.53
2:EB:1022:G:H22	2:EB:1142(B):A:H2	1.56	0.53
6:IB:18:ASP:HB3	17:TB:82:LEU:HD21	1.89	0.53
7:JB:140:LEU:HD11	7:JB:170:LEU:HD11	1.90	0.53
30:GC:13:CYS:HB3	30:GC:47:THR:HG21	1.90	0.53
36:NC:18:TRP:CD1	47:YC:54:PRO:HA	2.44	0.53
37:OC:30:LYS:HA	37:OC:35:ARG:HD2	1.90	0.53
45:WC:124:LYS:HD2	45:WC:125:PRO:HD2	1.91	0.53
55:HD:130:ASP:HB3	55:HD:333:MET:HE1	1.89	0.53
1:A:1073:U:H3	1:A:1102:A:H61	1.55	0.53
2:B:1062:G:H5''	2:B:1064:C:H1'	1.90	0.53
2:B:1870:C:H2'	2:B:1871:A:O4'	2.07	0.53
20:T:82:LEU:HD23	20:T:84:ARG:CZ	2.39	0.53
51:ZA:32:ARG:HA	51:ZA:69:THR:HG21	1.90	0.53
1:DB:1455:G:H5''	53:ED:31:SER:HB3	1.91	0.53
2:EB:271(C):G:H4'	2:EB:271(D):U:H5''	1.91	0.53
2:EB:1789:A:H2'	2:EB:1790:C:O4'	2.08	0.53
3:FB:28:C:H2'	3:FB:29:A:C8	2.43	0.53
8:KB:165:THR:OG1	8:KB:166:ASP:N	2.41	0.53
10:MB:76:THR:HB	10:MB:141:LYS:HE2	1.90	0.53
25:BC:52:ARG:HH12	25:BC:57:GLU:HB2	1.73	0.53
27:DC:38:GLU:HA	27:DC:38:GLU:OE2	2.09	0.53
40:RC:38:LEU:O	40:RC:42:ILE:HG12	2.09	0.53
1:A:1510:U:H2'	1:A:1511:G:C8	2.43	0.53
2:B:888:C:C2	46:UA:93:ARG:NH1	2.76	0.53
7:G:117:ARG:NH2	7:G:189:THR:O	2.38	0.53
21:U:60:ARG:NH1	31:EA:47:ARG:NH2	2.57	0.53
39:NA:26:ILE:O	39:NA:30:LEU:HG	2.09	0.53
53:BB:38:LYS:HA	53:BB:41:VAL:HG22	1.90	0.53
2:EB:1512:G:H2'	2:EB:1513:C:C6	2.43	0.53
2:EB:2698:U:H2'	2:EB:2699:C:C6	2.43	0.53
9:LB:21:PRO:HG2	9:LB:23:ARG:HH12	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:WB:71:VAL:HA	20:WB:107:LEU:HD12	1.91	0.53
43:UC:25:GLU:O	43:UC:29:ARG:HG2	2.09	0.53
1:A:1005:A:H1'	1:A:1026:G:C2	2.43	0.53
2:B:2476:A:H2	2:B:2481:G:H1	1.57	0.53
2:B:2790:A:H2'	2:B:2791:C:H5'	1.90	0.53
23:W:54:HIS:HB3	23:W:101:PRO:HD3	1.90	0.53
28:BA:24:THR:OG1	28:BA:25:TYR:N	2.42	0.53
46:UA:37:THR:HB	46:UA:39:ILE:HG13	1.90	0.53
1:DB:59:A:H1'	1:DB:354:G:N2	2.23	0.53
1:DB:1129:C:H42	1:DB:1143:G:H1	1.57	0.53
2:EB:2552:2MU:H2'	2:EB:2554:U:OP2	2.09	0.53
19:VB:7:THR:HG23	19:VB:22:VAL:HG11	1.91	0.53
2:B:1519:G:C6	2:B:1520:U:C4	2.96	0.53
2:B:1816:G:C6	5:E:35:LYS:NZ	2.75	0.53
2:B:2320:A:H2'	2:B:2320:A:N3	2.23	0.53
42:QA:9:ARG:H	42:QA:79:LEU:HD23	1.72	0.53
1:DB:909:A:N3	1:DB:1413:A:O2'	2.40	0.53
2:EB:1483:G:H2'	2:EB:1484:G:C8	2.44	0.53
11:NB:72:TYR:HE2	11:NB:87:LEU:HD23	1.74	0.53
15:RB:12:ARG:HG3	15:RB:12:ARG:NH1	2.23	0.53
1:A:426:G:OP1	37:LA:38:TYR:OH	2.26	0.53
1:A:1226:C:H2'	46:UA:103:THR:HB	1.91	0.53
2:B:140:A:H8	2:B:1408:C:O2'	1.90	0.53
2:B:274:G:H1'	2:B:363(A):G:N2	2.24	0.53
2:B:1175:U:H2'	2:B:1176:G:C8	2.43	0.53
28:BA:56:VAL:HG22	28:BA:61:ARG:HA	1.90	0.53
42:QA:10:ARG:HG2	42:QA:11:LYS:HG3	1.90	0.53
48:WA:18:PHE:HB2	48:WA:19:PRO:HD2	1.90	0.53
1:DB:287:U:H2'	1:DB:288:A:H8	1.73	0.53
1:DB:754:C:O2	1:DB:754:C:H2'	2.08	0.53
1:DB:892:A:O2'	1:DB:1415:G:H4'	2.08	0.53
2:EB:1364:G:OP2	25:BC:61:ARG:NH1	2.41	0.53
9:LB:124:GLU:HB3	9:LB:132:ARG:HB3	1.90	0.53
35:MC:51:LEU:HD12	35:MC:201:ILE:HD12	1.91	0.53
41:SC:110:ALA:HB3	41:SC:121:ASP:HB3	1.90	0.53
1:A:983:A:H5'	1:A:984:C:OP2	2.09	0.53
2:B:140:A:C8	2:B:1408:C:O2'	2.62	0.53
2:B:2667:C:H1'	9:I:109:PHE:HD1	1.74	0.53
20:T:23:LEU:HD22	29:CA:25:LEU:HD13	1.91	0.53
39:NA:22:GLU:O	39:NA:25:ILE:HG12	2.09	0.53
43:RA:25:GLU:O	43:RA:29:ARG:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EB:141(A):A:H5''	2:EB:141(B):C:OP2	2.09	0.53
2:EB:289:A:H2'	2:EB:290:G:O4'	2.09	0.53
2:EB:847:U:OP2	2:EB:929:G:O6	2.27	0.53
2:EB:1045:A:H1'	2:EB:1047:G:N3	2.24	0.53
2:EB:1059:G:H22	2:EB:1081:U:H1'	1.74	0.53
2:EB:1291:C:H2'	2:EB:1292:U:H6	1.72	0.53
6:IB:111:ARG:HA	15:RB:1:MET:SD	2.49	0.53
39:QC:12:PRO:HG3	39:QC:55:ASP:OD2	2.08	0.53
42:TC:9:ARG:H	42:TC:79:LEU:HD23	1.73	0.53
55:HD:338:ASP:HA	55:HD:341:ILE:HG12	1.89	0.53
1:A:1273:G:H2'	1:A:1274:G:O4'	2.09	0.53
1:A:1291:G:H4'	42:QA:39:GLY:HA3	1.91	0.53
1:A:1320:C:N3	52:AB:36:ARG:HD3	2.24	0.53
2:B:363(G):A:OP2	2:B:363(G):A:H8	1.92	0.53
2:B:851:U:H2'	2:B:852:G:H8	1.74	0.53
2:B:2831:G:P	6:F:58:ARG:HH12	2.31	0.53
10:J:84:GLY:O	10:J:86:THR:N	2.41	0.53
35:JA:16:HIS:HE1	35:JA:42:ILE:HD12	1.72	0.53
35:JA:16:HIS:O	35:JA:18:GLY:N	2.41	0.53
1:DB:936:C:H2'	1:DB:937:A:O4'	2.09	0.53
2:EB:461:C:H2'	2:EB:462:C:H6	1.73	0.53
2:EB:2094:G:OP1	10:MB:22:LYS:NZ	2.42	0.53
8:KB:67:LYS:HD3	28:EC:5:ILE:HD12	1.90	0.53
8:KB:138:GLN:HE22	8:KB:149:VAL:HG13	1.73	0.53
23:ZB:132:ASN:OD1	23:ZB:132:ASN:N	2.42	0.53
2:B:207:A:H2'	2:B:208:C:O4'	2.08	0.52
2:B:2508:G:P	55:GD:228:ARG:HH22	2.31	0.52
5:E:52:ARG:HB2	5:E:53:PHE:CD2	2.44	0.52
33:GA:2:LYS:HZ1	33:GA:4:ARG:HE	1.55	0.52
36:KA:36:ASP:HB2	36:KA:59:ARG:HH21	1.73	0.52
39:NA:83:ASP:OD1	39:NA:83:ASP:N	2.41	0.52
40:OA:26:PHE:O	40:OA:30:ILE:HG13	2.09	0.52
41:PA:13:ILE:O	41:PA:17:THR:HG23	2.08	0.52
52:AB:42:PRO:O	52:AB:44:MET:N	2.40	0.52
1:DB:56:U:H2'	1:DB:57:G:C8	2.44	0.52
1:DB:979:C:O2	47:YC:19:ARG:NH1	2.42	0.52
1:DB:1226:C:H2'	46:XC:103:THR:HB	1.91	0.52
2:EB:96:G:H4'	26:CC:48:HIS:CD2	2.43	0.52
2:EB:207:A:H2'	2:EB:208:C:O4'	2.09	0.52
2:EB:576:U:OP1	2:EB:2503:2MA:OP1	2.27	0.52
2:EB:2564:A:OP1	2:EB:2648:C:H4'	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:HB:131:LEU:HD13	5:HB:136:ILE:HG12	1.90	0.52
6:IB:119:ARG:HG2	6:IB:120:TRP:CE2	2.44	0.52
35:MC:43:ASP:OD2	35:MC:46:LYS:HB2	2.09	0.52
37:OC:142:PRO:HA	37:OC:185:PHE:HD2	1.73	0.52
1:A:1414:U:H3	1:A:1486:G:H1	1.57	0.52
6:F:11:MET:HG2	6:F:24:THR:HB	1.91	0.52
7:G:116:ASP:OD2	13:M:1:MET:N	2.42	0.52
10:J:61:ARG:NH1	10:J:64:GLU:OE2	2.42	0.52
16:P:15:ARG:HG2	16:P:15:ARG:HH11	1.75	0.52
22:V:50:ARG:NH1	22:V:50:ARG:HB2	2.25	0.52
48:WA:82:ILE:HD12	48:WA:88:ARG:NH2	2.24	0.52
49:XA:53:VAL:HG12	49:XA:57:ARG:HH11	1.74	0.52
1:DB:481:G:O2'	1:DB:483:C:N4	2.37	0.52
2:EB:392:C:H5''	2:EB:409:C:H5''	1.90	0.52
7:JB:62:ARG:HG2	7:JB:63:LYS:O	2.09	0.52
9:LB:55:PRO:HD2	9:LB:61:HIS:HD2	1.74	0.52
10:MB:57:ARG:O	10:MB:60:GLU:HB3	2.08	0.52
15:RB:104:ARG:HG2	15:RB:109:ALA:HB3	1.91	0.52
38:PC:50:GLU:OE2	38:PC:51:VAL:HG23	2.09	0.52
40:RC:20:ASP:HB3	40:RC:23:VAL:HG23	1.91	0.52
1:A:603:U:H2'	1:A:604:G:H8	1.74	0.52
1:A:1129:C:H42	1:A:1143:G:H1	1.57	0.52
2:B:537:C:H2'	2:B:539:G:H8	1.73	0.52
2:B:969:U:H4'	27:AA:14:GLY:O	2.09	0.52
2:B:2718:G:O2'	2:B:2847:U:OP1	2.17	0.52
36:KA:150:LYS:HE3	36:KA:152:ILE:HD11	1.91	0.52
1:DB:973:G:H3'	1:DB:974:A:H5''	1.91	0.52
2:EB:17:G:H4'	18:UB:25:TRP:NE1	2.23	0.52
2:EB:302:C:H2'	2:EB:303:U:C6	2.44	0.52
2:EB:2031:A:C6	2:EB:2498:C:H1'	2.45	0.52
16:SB:3:ARG:NH1	16:SB:3:ARG:HA	2.23	0.52
17:TB:106:SER:O	17:TB:110:ILE:HG13	2.09	0.52
17:TB:120:ARG:O	17:TB:124:ASP:HB2	2.09	0.52
23:ZB:125:LEU:HG	23:ZB:164:ALA:HB3	1.91	0.52
28:EC:14:ILE:HG12	28:EC:31:ILE:HG13	1.92	0.52
36:NC:60:ALA:N	36:NC:63:ASN:O	2.40	0.52
46:XC:15:VAL:O	46:XC:19:LEU:HD13	2.09	0.52
1:A:44:G:H2'	1:A:45:U:O4'	2.10	0.52
1:A:1087:G:H2'	1:A:1088:G:C8	2.44	0.52
2:B:1111:A:OP2	2:B:1111:A:H2'	2.09	0.52
6:F:2:LYS:HG3	6:F:200:GLU:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:90:GLN:N	12:L:90:GLN:OE1	2.42	0.52
30:DA:13:CYS:HB3	30:DA:47:THR:HG21	1.91	0.52
38:MA:36:ASP:OD1	38:MA:38:GLN:N	2.40	0.52
1:DB:953:G:N7	46:XC:104:ARG:NH2	2.46	0.52
1:DB:1253:G:H1	1:DB:1284:C:H42	1.58	0.52
2:EB:232:G:N2	2:EB:420:C:OP1	2.30	0.52
2:EB:242:G:H5''	32:IC:64:TYR:CE2	2.44	0.52
2:EB:1538:G:H8	2:EB:1538:G:OP2	1.92	0.52
17:TB:64:ARG:HH11	17:TB:64:ARG:HG3	1.75	0.52
19:VB:13:ARG:NH1	19:VB:13:ARG:HG3	2.25	0.52
29:FC:49:CYS:SG	29:FC:51:TYR:HB2	2.50	0.52
48:ZC:4:THR:O	48:ZC:7:GLU:HB3	2.10	0.52
1:A:1005:A:H4'	1:A:1037:C:N3	2.24	0.52
1:A:1075:C:H5''	35:JA:179:LYS:HZ1	1.74	0.52
2:B:1164:G:C6	2:B:1165:U:C4	2.98	0.52
2:B:2228:G:OP2	5:E:263:ARG:NH2	2.40	0.52
2:B:2377:A:H4'	16:P:112:PHE:OXT	2.09	0.52
4:D:1:C:N4	4:D:72:A:H61	2.06	0.52
7:G:50:SER:HA	7:G:92:PRO:O	2.09	0.52
10:J:111:PRO:HG2	10:J:112:LYS:HD2	1.92	0.52
21:U:5:TYR:HE1	26:Z:30:ARG:NH1	2.04	0.52
46:UA:3:ARG:NH2	46:UA:4:ILE:HG23	2.23	0.52
2:EB:686:G:H21	2:EB:788:A:H61	1.56	0.52
2:EB:1322:A:N1	2:EB:1333:C:O2'	2.37	0.52
2:EB:2563:U:H4'	12:OB:28:SER:HA	1.90	0.52
2:EB:2792:G:N1	2:EB:2805:G:H1'	2.25	0.52
8:KB:3:LEU:HD23	8:KB:5:LEU:HD11	1.91	0.52
12:OB:87:ILE:HG22	12:OB:93:PRO:HA	1.91	0.52
28:EC:56:VAL:HG22	28:EC:61:ARG:HA	1.90	0.52
41:SC:13:ILE:O	41:SC:17:THR:HG23	2.09	0.52
48:ZC:88:ARG:NH2	48:ZC:88:ARG:HB3	2.25	0.52
1:A:224:C:H2'	1:A:225:C:C6	2.44	0.52
1:A:981:U:H5'	47:VA:21:TYR:CE2	2.44	0.52
2:B:34:C:HO2'	2:B:35:G:H8	1.54	0.52
2:B:83:G:N2	2:B:102:G:H1'	2.24	0.52
2:B:1483:G:H2'	2:B:1484:G:C8	2.42	0.52
1:DB:297:G:N2	1:DB:300:A:OP2	2.41	0.52
1:DB:957:U:OP1	52:DD:81:ARG:NH1	2.43	0.52
1:DB:1500:A:H5''	1:DB:1508:G:H5''	1.92	0.52
2:EB:312:G:H5'	2:EB:331:A:O2'	2.10	0.52
2:EB:2210:G:H3'	2:EB:2211:G:N7	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EB:2353:G:O2'	24:AC:33:ALA:O	2.21	0.52
4:GB:37:A:H2'	4:GB:38:A:C8	2.45	0.52
6:IB:92:THR:O	6:IB:95:ILE:HG23	2.10	0.52
35:MC:76:GLN:HB2	35:MC:208:ILE:HG12	1.91	0.52
51:CD:32:ARG:HA	51:CD:69:THR:HG21	1.91	0.52
1:A:614:A:H2'	1:A:615:C:C6	2.45	0.52
1:A:1373:G:H5''	40:OA:36:LYS:HB2	1.91	0.52
1:A:1379:G:O6	40:OA:2:ALA:HB3	2.08	0.52
2:B:2528:U:H3	2:B:2535:G:H1	1.57	0.52
2:B:2529:G:H5''	2:B:2530:A:H5''	1.90	0.52
5:E:183:ARG:HG2	5:E:183:ARG:HH11	1.74	0.52
6:F:45:THR:O	6:F:82:ARG:HD2	2.09	0.52
7:G:14:PRO:HD2	7:G:127:GLU:OE2	2.10	0.52
39:NA:18:GLN:HG3	39:NA:21:LEU:HD23	1.90	0.52
1:DB:833:U:H2'	1:DB:834:C:C6	2.44	0.52
2:EB:247:G:H4'	2:EB:386:G:C5	2.45	0.52
2:EB:507:A:O2'	2:EB:508:G:OP2	2.25	0.52
2:EB:1044:G:O2'	2:EB:1111:A:N1	2.36	0.52
2:EB:1464:C:H2'	2:EB:1465:G:C8	2.45	0.52
9:LB:86:GLU:HG2	9:LB:132:ARG:HG3	1.92	0.52
10:MB:60:GLU:CG	10:MB:61:ARG:HH12	2.05	0.52
38:PC:45:PHE:HE2	38:PC:47:LYS:HE3	1.75	0.52
55:GD:144:TRP:CE2	55:GD:171:VAL:HG22	2.44	0.52
2:B:302:C:H2'	2:B:303:U:C6	2.44	0.52
2:B:1173:G:H3'	2:B:1174:A:H4'	1.91	0.52
10:J:75:LEU:HD13	10:J:105:HIS:CD2	2.45	0.52
4:IA:34:C:H2'	4:IA:35:A:C8	2.45	0.52
41:PA:69:ARG:NE	41:PA:75:ARG:O	2.39	0.52
1:DB:125:U:H2'	1:DB:126:G:C8	2.44	0.52
2:EB:784:A:C5	5:HB:229:VAL:HG21	2.43	0.52
2:EB:1173:G:H3'	2:EB:1174:A:H4'	1.91	0.52
2:EB:2792:G:H2'	2:EB:2793:G:H8	1.74	0.52
23:ZB:102:LEU:HD22	23:ZB:137:ILE:HG21	1.92	0.52
44:VC:12:ARG:NH2	44:VC:13:GLN:HE22	2.08	0.52
1:A:1389:C:H2'	1:A:1390:U:O4'	2.09	0.52
2:B:445:C:O2'	2:B:446:G:H5'	2.10	0.52
2:B:1059:G:H22	2:B:1081:U:H1'	1.75	0.52
2:B:2792:G:H2'	2:B:2793:G:H8	1.74	0.52
9:I:149:ARG:NH2	9:I:167:GLU:OE1	2.39	0.52
12:L:17:ARG:HD2	12:L:45:GLU:OE1	2.09	0.52
13:M:93:GLY:H	13:M:123:LEU:HD22	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:81:VAL:HG12	24:X:5:LYS:HZ3	1.74	0.52
25:Y:40:ARG:NH2	25:Y:42:GLN:HG2	2.24	0.52
1:DB:164:U:H2'	1:DB:165:C:C6	2.45	0.52
1:DB:1049:U:OP1	47:YC:3:ARG:HB2	2.10	0.52
1:DB:1389:C:H2'	1:DB:1390:U:O4'	2.10	0.52
1:DB:1500:A:OP2	1:DB:1505:G:OP2	2.27	0.52
2:EB:637:A:H8	13:PB:117:GLU:HG3	1.74	0.52
2:EB:1508:A:H3'	2:EB:1509:A:C8	2.45	0.52
2:EB:2320:A:H2'	2:EB:2320:A:N3	2.25	0.52
2:EB:2820:A:OP2	15:RB:2:ARG:NH2	2.43	0.52
14:QB:60:ARG:NH2	23:ZB:114:GLY:HA3	2.24	0.52
36:NC:150:LYS:HE3	36:NC:152:ILE:HD11	1.92	0.52
38:PC:145:LYS:HB3	38:PC:145:LYS:HZ2	1.75	0.52
2:B:747:U:O2	2:B:2014:A:H1'	2.10	0.52
2:B:955:C:OP1	14:N:87:LYS:HE3	2.11	0.52
2:B:2418:A:H2'	2:B:2419:U:O4'	2.10	0.52
37:LA:150:GLU:H	37:LA:150:GLU:CD	2.12	0.52
44:SA:27:ASN:OD1	44:SA:28:THR:N	2.41	0.52
1:DB:444:C:H2'	1:DB:445:G:H8	1.75	0.52
1:DB:574:A:N3	1:DB:883:C:H1'	2.25	0.52
1:DB:833:U:H2'	1:DB:834:C:H6	1.74	0.52
1:DB:1453:G:H4'	1:DB:1454:G:OP2	2.09	0.52
2:EB:117:G:OP2	2:EB:119:A:O2'	2.24	0.52
2:EB:896:A:OP2	2:EB:896:A:H4'	2.09	0.52
10:MB:75:LEU:HD13	10:MB:105:HIS:CD2	2.45	0.52
27:DC:6:VAL:HG12	27:DC:56:VAL:HG22	1.91	0.52
42:TC:11:LYS:O	42:TC:13:ALA:N	2.37	0.52
1:A:397:A:H5'	1:A:398:C:OP1	2.10	0.51
1:A:632:A:OP1	41:PA:98:LYS:NZ	2.43	0.51
1:A:1293:G:H2'	1:A:1294:G:C8	2.45	0.51
2:B:1516:U:H2'	2:B:1517:G:H8	1.75	0.51
2:B:2615:U:C2	29:CA:7:PRO:HA	2.45	0.51
2:B:2853:C:H2'	2:B:2854:G:H8	1.75	0.51
18:R:32:PHE:CZ	18:R:36:ARG:NH1	2.78	0.51
18:R:58:ARG:HA	18:R:61:TRP:CE3	2.45	0.51
23:W:97:GLU:HB2	23:W:125:LEU:HD11	1.93	0.51
1:DB:603:U:H2'	1:DB:604:G:C8	2.44	0.51
2:EB:249:C:O2	32:IC:12:LYS:NZ	2.37	0.51
2:EB:2291:U:OP1	2:EB:2380:C:O2'	2.26	0.51
5:HB:129:ASN:O	5:HB:193:VAL:HG12	2.10	0.51
6:IB:191:PRO:O	6:IB:193:GLY:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:KB:79:ASN:OD1	8:KB:79:ASN:N	2.43	0.51
12:OB:14:THR:HG21	12:OB:86:ILE:HB	1.92	0.51
28:EC:49:PHE:HE1	46:XC:62:ASN:HD22	1.58	0.51
31:HC:29:LYS:O	31:HC:33:ARG:HG3	2.09	0.51
36:NC:189:ALA:HB3	36:NC:196:LEU:HB2	1.91	0.51
42:TC:27:THR:HG23	42:TC:62:TYR:HA	1.92	0.51
42:TC:40:LEU:HD11	42:TC:70:LYS:HD3	1.92	0.51
1:A:953:G:N7	46:UA:104:ARG:NH2	2.45	0.51
1:A:973:G:H3'	1:A:974:A:H5''	1.91	0.51
1:A:1087:G:H1	1:A:1098:C:H42	1.58	0.51
1:A:1498:UR3:OP2	34:HA:16:A:O2'	2.24	0.51
2:B:1728:G:H8	2:B:1732:A:H62	1.57	0.51
2:B:2701:C:H2'	2:B:2702:U:H2'	1.92	0.51
2:B:2747:G:P	9:I:138:LYS:HZ2	2.32	0.51
4:D:37:A:H2'	4:D:38:A:C8	2.46	0.51
23:W:125:LEU:HG	23:W:164:ALA:HB3	1.92	0.51
1:DB:222:U:H2'	1:DB:223:U:C6	2.45	0.51
2:EB:540:G:H2'	2:EB:541:C:C6	2.45	0.51
3:FB:112:G:H2'	3:FB:113:C:C6	2.45	0.51
32:IC:56:GLU:HA	32:IC:59:LYS:HG3	1.93	0.51
35:MC:229:VAL:HB	35:MC:231:GLU:OE2	2.10	0.51
52:DD:22:LEU:HD11	52:DD:29:ARG:HB2	1.91	0.51
52:DD:36:ARG:NH2	52:DD:75:ALA:O	2.39	0.51
1:A:1253:G:H1	1:A:1284:C:H42	1.57	0.51
2:B:479:A:HO2'	2:B:481:G:H8	1.58	0.51
3:C:3:C:H2'	3:C:4:C:H6	1.74	0.51
14:N:10:ARG:HH12	4:IA:64:G:H4'	1.73	0.51
17:Q:55:ASN:H	17:Q:59:THR:HB	1.74	0.51
23:W:127:LYS:H	23:W:164:ALA:HB2	1.75	0.51
26:Z:32:LEU:HB2	26:Z:53:LEU:HD12	1.92	0.51
35:JA:118:LEU:HD21	35:JA:138:LEU:HD22	1.92	0.51
46:UA:3:ARG:NH1	46:UA:3:ARG:HB3	2.26	0.51
52:AB:24:ALA:HB3	52:AB:25:LYS:HE2	1.91	0.51
1:DB:1073:U:H3	1:DB:1102:A:H61	1.56	0.51
1:DB:1503:A:O2'	1:DB:1504:G:O5'	2.29	0.51
2:EB:528:A:H2'	11:NB:114:ARG:NH2	2.26	0.51
2:EB:588:U:H2'	2:EB:589:C:C6	2.45	0.51
2:EB:932:G:OP1	27:DC:29:ARG:NH2	2.44	0.51
2:EB:1614:A:C2	20:WB:93:ALA:HB2	2.46	0.51
2:EB:2791:C:H4'	2:EB:2792:G:H5'	1.93	0.51
5:HB:240:ALA:HB1	5:HB:241:PRO:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:MC:76:GLN:NE2	35:MC:207:ALA:O	2.44	0.51
45:WC:84:LEU:HD23	45:WC:101:VAL:HG21	1.92	0.51
48:ZC:82:ILE:HD12	48:ZC:88:ARG:HH21	1.75	0.51
2:B:2348:U:O2'	2:B:2349:G:H5'	2.11	0.51
13:M:138:LEU:HD23	13:M:145:PRO:HB3	1.90	0.51
20:T:90:ARG:HG2	20:T:90:ARG:NH1	2.26	0.51
25:Y:51:VAL:HG21	25:Y:74:VAL:HG21	1.93	0.51
46:UA:11:ARG:HH12	46:UA:46:LYS:HD2	1.74	0.51
49:XA:22:THR:HA	49:XA:33:ILE:HG12	1.92	0.51
53:BB:54:LYS:HA	53:BB:57:ARG:HH21	1.75	0.51
1:DB:186(A):C:O2'	53:ED:85:MET:SD	2.68	0.51
1:DB:983:A:H5'	1:DB:984:C:OP2	2.11	0.51
2:EB:2552:2MU:O5'	2:EB:2552:2MU:H6	2.10	0.51
15:RB:70:LEU:O	15:RB:72:ASP:N	2.32	0.51
24:AC:7:LEU:CD1	24:AC:8:GLY:H	2.24	0.51
40:RC:26:PHE:O	40:RC:30:ILE:HG13	2.10	0.51
41:SC:51:VAL:HG11	41:SC:60:ARG:NH1	2.26	0.51
46:XC:44:ARG:HB2	46:XC:47:ASP:OD2	2.11	0.51
52:DD:11:VAL:HG23	52:DD:38:SER:HB2	1.92	0.51
1:A:1356:G:H2'	1:A:1357:A:C8	2.45	0.51
2:B:2031:A:H1'	2:B:2455:G:O2'	2.10	0.51
8:H:96:ARG:O	8:H:99:MET:HB3	2.11	0.51
23:W:14:LYS:O	23:W:18:LEU:HB2	2.11	0.51
49:XA:58:TYR:O	49:XA:61:SER:OG	2.27	0.51
2:EB:1923:U:H2'	2:EB:1924:C:H6	1.74	0.51
5:HB:17:THR:HB	5:HB:205:VAL:H	1.75	0.51
8:KB:76:SER:OG	8:KB:83:ARG:HA	2.11	0.51
23:ZB:70:LEU:HG	23:ZB:91:LEU:HD21	1.91	0.51
23:ZB:179:ASP:OD2	23:ZB:181:GLU:N	2.42	0.51
46:XC:50:GLU:O	46:XC:54:VAL:HG23	2.10	0.51
1:A:503:C:OP2	45:TA:116:SER:OG	2.21	0.51
2:B:439:G:H2'	2:B:440:G:C8	2.45	0.51
2:B:900:A:H2'	2:B:901:A:C8	2.45	0.51
2:B:1823:G:OP1	5:E:54:ARG:NH1	2.43	0.51
6:F:7:VAL:HG23	6:F:51:PHE:HE2	1.74	0.51
8:H:11:TYR:HA	8:H:15:VAL:HB	1.93	0.51
2:EB:17:G:H2'	2:EB:18:C:H6	1.74	0.51
2:EB:1299:G:H22	2:EB:1640:C:H5''	1.76	0.51
2:EB:1796:U:H2'	2:EB:1797:C:C6	2.46	0.51
2:EB:2671:A:H2'	2:EB:2672:G:C8	2.46	0.51
18:UB:83:LEU:HD12	18:UB:113:ALA:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:XB:28:PHE:CE1	21:XB:47:PHE:HE2	2.28	0.51
38:PC:118:ILE:HG12	38:PC:119:LEU:N	2.25	0.51
41:SC:112:LEU:HA	41:SC:134:ILE:HG12	1.92	0.51
46:XC:33:ALA:HA	46:XC:59:TYR:HE2	1.75	0.51
1:A:222:U:H2'	1:A:223:U:C6	2.45	0.51
1:A:444:C:H2'	1:A:445:G:H8	1.76	0.51
1:A:447:G:O6	1:A:485:G:O2'	2.21	0.51
1:A:558:G:C8	1:A:559:A:H2'	2.45	0.51
1:A:833:U:H2'	1:A:834:C:C6	2.46	0.51
1:A:1130:A:H2'	1:A:1131:G:C8	2.45	0.51
2:B:687:C:H5''	31:EA:2:LYS:HE2	1.93	0.51
2:B:1538:G:H8	2:B:1538:G:OP2	1.92	0.51
15:O:10:LEU:O	15:O:12:ARG:HG3	2.10	0.51
22:V:76:CYS:SG	22:V:78:ALA:HB3	2.50	0.51
1:DB:563:A:O2'	1:DB:564:C:OP2	2.18	0.51
1:DB:723:U:H4'	1:DB:724:G:OP2	2.10	0.51
1:DB:828:A:H2'	1:DB:829:G:O4'	2.11	0.51
1:DB:1273:G:H2'	1:DB:1274:G:O4'	2.10	0.51
2:EB:270(W):G:H2'	2:EB:270(X):G:H8	1.76	0.51
2:EB:2228:G:OP2	5:HB:263:ARG:NH2	2.44	0.51
2:EB:2328:A:H2'	2:EB:2329:G:C8	2.46	0.51
5:HB:30:GLU:HB3	5:HB:33:LEU:HD12	1.93	0.51
7:JB:53:THR:HG22	7:JB:56:GLU:CG	2.39	0.51
12:OB:107:ARG:HD3	17:TB:37:GLY:H	1.75	0.51
15:RB:48:VAL:HG23	15:RB:95:THR:HG21	1.92	0.51
46:XC:3:ARG:NH2	46:XC:4:ILE:HG23	2.25	0.51
46:XC:108:ARG:O	46:XC:112:GLY:N	2.43	0.51
55:HD:137:ARG:NH1	55:HD:334:GLU:HG3	2.25	0.51
1:A:946:A:H2'	1:A:947:G:C8	2.46	0.51
2:B:1357:U:H2'	2:B:1358:G:O4'	2.10	0.51
10:J:95:LYS:HA	10:J:111:PRO:HB3	1.91	0.51
29:CA:40:LYS:HG3	29:CA:41:PRO:O	2.10	0.51
36:KA:60:ALA:N	36:KA:63:ASN:O	2.43	0.51
46:UA:108:ARG:O	46:UA:112:GLY:N	2.44	0.51
2:EB:1532:C:H42	2:EB:1539:G:H1	1.59	0.51
2:EB:2351:G:O6	32:IC:39:LYS:HG3	2.11	0.51
2:EB:2880:C:O2'	15:RB:90:ARG:HD3	2.10	0.51
22:YB:43:ASN:HD22	22:YB:65:ALA:HB3	1.75	0.51
35:MC:168:THR:HG23	35:MC:192:SER:HA	1.91	0.51
37:OC:43:HIS:C	37:OC:45:GLN:H	2.13	0.51
48:ZC:18:PHE:HB2	48:ZC:19:PRO:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:DD:3:ARG:NH2	52:DD:7:LYS:HE2	2.25	0.51
55:HD:245:ARG:HG3	55:HD:256:GLU:HG3	1.92	0.51
1:A:262:A:C6	1:A:263:A:C6	2.99	0.51
1:A:1422:G:H2'	1:A:1423:G:H8	1.75	0.51
2:B:528:A:O2'	2:B:529:A:O5'	2.19	0.51
2:B:1915:5MU:P	55:GD:116:ARG:HH22	2.33	0.51
3:C:28:C:OP1	16:P:34:HIS:HB2	2.10	0.51
9:I:25:LYS:HG2	9:I:34:GLU:HG3	1.92	0.51
16:P:3:ARG:NH1	16:P:3:ARG:HA	2.26	0.51
1:DB:44:G:H2'	1:DB:45:U:O4'	2.11	0.51
1:DB:404:U:H2'	1:DB:405:U:H6	1.76	0.51
2:EB:270(K):G:N1	2:EB:270(Q):C:N3	2.54	0.51
2:EB:1062:G:H5''	2:EB:1064:C:H1'	1.92	0.51
2:EB:2831:G:P	6:IB:58:ARG:HH12	2.34	0.51
7:JB:127:GLU:HG2	7:JB:196:LEU:HD22	1.93	0.51
4:LC:65:C:H2'	4:LC:66:C:H6	1.76	0.51
1:A:17:U:H2'	1:A:18:C:C6	2.45	0.51
1:A:562:C:H4'	1:A:563:A:H5'	1.91	0.51
1:A:619:U:C2	37:LA:135:LEU:HD21	2.46	0.51
2:B:576:U:OP1	2:B:2503:2MA:OP1	2.27	0.51
2:B:2698:U:H2'	2:B:2699:C:C6	2.46	0.51
5:E:17:THR:HB	5:E:205:VAL:H	1.76	0.51
9:I:55:PRO:HD2	9:I:61:HIS:HD2	1.76	0.51
35:JA:76:GLN:HB2	35:JA:208:ILE:HG12	1.93	0.51
37:LA:142:PRO:HA	37:LA:185:PHE:HD2	1.76	0.51
39:NA:53:ALA:HB3	39:NA:86:ARG:NH1	2.25	0.51
41:PA:11:THR:HA	41:PA:14:ARG:NH1	2.25	0.51
46:UA:14:ARG:N	46:UA:44:ARG:HH11	2.09	0.51
2:EB:1164:G:C6	2:EB:1165:U:C4	2.99	0.51
6:IB:7:VAL:HG23	6:IB:51:PHE:HE2	1.75	0.51
10:MB:96:ASP:HA	10:MB:99:GLU:HB2	1.93	0.51
48:ZC:82:ILE:HD12	48:ZC:88:ARG:NH2	2.25	0.51
1:A:304:U:H2'	1:A:305:G:C8	2.46	0.50
1:A:850:U:H2'	1:A:851:G:C8	2.46	0.50
2:B:637:A:H8	13:M:117:GLU:HG3	1.76	0.50
2:B:2086:U:H2'	2:B:2087:G:C8	2.46	0.50
2:B:2143:C:O2'	2:B:2148:G:N2	2.43	0.50
2:B:2792:G:H1	2:B:2805:G:H1'	1.75	0.50
8:H:116:ASP:OD2	46:UA:68:GLY:HA3	2.11	0.50
8:H:181:ARG:HB2	8:H:181:ARG:HH11	1.76	0.50
11:K:72:TYR:HE2	11:K:87:LEU:HD23	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:61:LEU:HD23	23:W:67:LEU:HD23	1.92	0.50
25:Y:4:VAL:HG21	25:Y:11:ARG:NH1	2.26	0.50
35:JA:114:ARG:HE	35:JA:118:LEU:HG	1.76	0.50
36:KA:37:GLN:NE2	47:VA:52:GLN:OE1	2.43	0.50
48:WA:4:THR:O	48:WA:7:GLU:HB3	2.10	0.50
1:DB:1036:G:H21	1:DB:1037:C:N4	2.10	0.50
1:DB:1498:UR3:O2'	34:KC:17:U:OP1	2.23	0.50
2:EB:46:C:OP2	2:EB:215:G:H2'	2.11	0.50
2:EB:83:G:N2	2:EB:102:G:H1'	2.25	0.50
2:EB:274:G:H1'	2:EB:363(A):G:N2	2.26	0.50
2:EB:2531:A:N3	2:EB:2658:C:O2'	2.31	0.50
2:EB:2661:G:H2'	2:EB:2662:A:C8	2.46	0.50
7:JB:64:ILE:HD11	7:JB:75:HIS:HB2	1.93	0.50
32:IC:31:HIS:CD2	32:IC:32:LEU:HD22	2.46	0.50
39:QC:83:ASP:OD1	39:QC:83:ASP:N	2.43	0.50
45:WC:89:ARG:HA	45:WC:97:ARG:HA	1.92	0.50
46:XC:3:ARG:NH1	46:XC:3:ARG:HB3	2.27	0.50
55:GD:214:LEU:HD23	55:GD:214:LEU:H	1.77	0.50
1:A:850:U:H2'	1:A:851:G:H8	1.76	0.50
2:B:2006:C:O2'	2:B:2823:A:N3	2.43	0.50
2:B:2031:A:C6	2:B:2498:C:H1'	2.46	0.50
8:H:129:GLY:O	8:H:130:ASN:ND2	2.45	0.50
11:K:128:HIS:O	11:K:131:GLN:NE2	2.28	0.50
19:S:13:ARG:HG3	19:S:13:ARG:HH11	1.75	0.50
39:NA:12:PRO:HG3	39:NA:55:ASP:OD2	2.11	0.50
40:OA:28:ASN:OD1	40:OA:36:LYS:NZ	2.45	0.50
48:WA:35:ARG:NH1	48:WA:35:ARG:CG	2.74	0.50
1:DB:160:A:H2'	1:DB:161:A:O4'	2.11	0.50
1:DB:224:C:H2'	1:DB:225:C:C6	2.46	0.50
1:DB:512:U:H2'	1:DB:513:C:C6	2.46	0.50
1:DB:946:A:H2'	1:DB:947:G:C8	2.47	0.50
1:DB:1291:G:H4'	42:TC:39:GLY:HA3	1.93	0.50
1:DB:1380:U:O2	40:RC:3:ARG:NH1	2.44	0.50
2:EB:947:G:H2'	2:EB:948:G:H8	1.77	0.50
2:EB:1060:U:H4'	2:EB:1061:U:H3'	1.93	0.50
2:EB:2334:G:H5'	16:SB:9:ARG:HG2	1.92	0.50
13:PB:97:PRO:HA	13:PB:100:LEU:HD12	1.94	0.50
36:NC:65:ALA:HA	36:NC:100:ALA:CB	2.42	0.50
1:A:881:G:OP2	45:TA:12:ARG:NH2	2.44	0.50
2:B:588:U:H2'	2:B:589:C:C6	2.46	0.50
2:B:890:A:H2'	2:B:892:G:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2021:C:OP1	29:CA:12:SER:OG	2.23	0.50
2:B:2317:C:C2'	2:B:2318:G:H5'	2.42	0.50
2:B:2328:A:H2'	2:B:2329:G:C8	2.46	0.50
2:B:2334:G:H5'	16:P:9:ARG:HG2	1.94	0.50
4:D:5:G:H1	4:D:68:C:H42	1.59	0.50
7:G:11:VAL:HG22	7:G:125:LEU:HB2	1.92	0.50
14:N:43:THR:HA	14:N:94:VAL:HG12	1.93	0.50
37:LA:133:VAL:HG13	37:LA:135:LEU:HD22	1.93	0.50
42:QA:81:ILE:O	42:QA:85:LEU:HG	2.11	0.50
1:DB:1034:G:H2'	1:DB:1035:A:H8	1.76	0.50
2:EB:1287:A:C5	2:EB:1288:U:C4	3.00	0.50
2:EB:1932:A:H2'	2:EB:1933:G:O4'	2.11	0.50
2:EB:2780:G:H4'	2:EB:2781:A:OP2	2.11	0.50
6:IB:21:VAL:HG22	6:IB:23:VAL:HG23	1.93	0.50
8:KB:56:ALA:HB2	8:KB:153:ARG:NH1	2.20	0.50
17:TB:100:TYR:CD1	17:TB:103:ARG:NH1	2.79	0.50
20:WB:68:ARG:NH1	20:WB:111:HIS:HA	2.25	0.50
37:OC:98:GLU:HG3	37:OC:194:LEU:HD22	1.93	0.50
1:A:345:C:H3'	17:Q:41:ARG:CZ	2.41	0.50
1:A:359:U:H2'	1:A:360:A:C8	2.46	0.50
1:A:509:A:N3	1:A:543:C:O2'	2.35	0.50
1:A:790:A:OP1	4:IA:38:A:O2'	2.28	0.50
1:A:936:C:H2'	1:A:937:A:O4'	2.11	0.50
1:A:1218:C:H2'	1:A:1219:U:C6	2.46	0.50
2:B:461:C:H2'	2:B:462:C:H6	1.77	0.50
2:B:715:G:H2'	2:B:716:A:C8	2.45	0.50
2:B:1364:G:OP2	25:Y:61:ARG:NH1	2.44	0.50
2:B:2347:C:O2'	30:DA:21:TYR:OH	2.29	0.50
2:B:2791:C:H5''	2:B:2893:G:H2'	1.94	0.50
2:B:2821:A:OP2	2:B:2822:G:OP2	2.27	0.50
8:H:76:SER:OG	8:H:83:ARG:HA	2.11	0.50
19:S:7:THR:HG23	19:S:22:VAL:HG11	1.93	0.50
40:OA:26:PHE:CE2	40:OA:30:ILE:HD11	2.46	0.50
2:EB:716:A:C2	2:EB:717:G:H1'	2.46	0.50
2:EB:2141:G:H22	2:EB:2151:G:H1'	1.77	0.50
2:EB:2853:C:H2'	2:EB:2854:G:H8	1.77	0.50
3:FB:28:C:OP1	16:SB:31:SER:OG	2.25	0.50
19:VB:69:LYS:O	19:VB:70:ILE:HD13	2.11	0.50
37:OC:98:GLU:OE2	37:OC:103:ASN:ND2	2.40	0.50
1:A:137:C:H2'	1:A:138:G:H8	1.75	0.50
1:A:381:C:H2'	1:A:382:A:O4'	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:723:U:H4'	1:A:724:G:OP2	2.10	0.50
1:A:1342:C:H2'	1:A:1343:G:C8	2.47	0.50
2:B:1407:C:H2'	2:B:1408:C:H6	1.75	0.50
2:B:1717:G:H1	2:B:1742:C:H42	1.60	0.50
5:E:148:GLU:OE2	5:E:151:LYS:NZ	2.42	0.50
9:I:3:ARG:HG2	9:I:6:ARG:CZ	2.41	0.50
23:W:52:SER:OG	23:W:53:ILE:N	2.45	0.50
1:DB:381:C:H2'	1:DB:382:A:O4'	2.12	0.50
1:DB:603:U:H2'	1:DB:604:G:H8	1.76	0.50
1:DB:1320:C:N3	52:DD:36:ARG:HD3	2.26	0.50
2:EB:136:G:H2'	2:EB:137(A):C:H6	1.77	0.50
2:EB:361:G:C2	2:EB:362:U:H5	2.30	0.50
2:EB:1437:C:H2'	2:EB:1438:U:C6	2.46	0.50
11:NB:108:PRO:O	11:NB:113:GLY:HA3	2.12	0.50
17:TB:26:ASP:OD1	17:TB:120:ARG:NH2	2.35	0.50
39:QC:44:GLY:HA2	39:QC:59:TYR:CE1	2.46	0.50
46:XC:14:ARG:N	46:XC:44:ARG:HH11	2.10	0.50
49:AD:53:VAL:HG12	49:AD:57:ARG:HH11	1.75	0.50
52:DD:27:GLU:HG3	52:DD:28:LYS:HA	1.93	0.50
52:DD:44:MET:O	52:DD:46:GLY:N	2.45	0.50
53:ED:90:GLN:HA	53:ED:93:GLU:HB3	1.92	0.50
1:A:833:U:H3	1:A:853:G:H1	1.58	0.50
1:A:1317:C:O2	52:AB:37:ARG:NH2	2.44	0.50
2:B:528:A:H2'	11:K:114:ARG:NH2	2.27	0.50
2:B:748:G:H2'	2:B:750:A:N7	2.27	0.50
2:B:1754:C:OP2	17:Q:113:LYS:HE3	2.12	0.50
20:T:82:LEU:HD23	20:T:84:ARG:NH1	2.26	0.50
38:MA:84:PHE:HB2	38:MA:134:ALA:HB2	1.94	0.50
39:NA:44:GLY:HA2	39:NA:59:TYR:CE1	2.46	0.50
46:UA:24:GLY:HA2	46:UA:70:LEU:HD12	1.93	0.50
1:DB:1118:C:H1'	1:DB:1179:A:C5	2.47	0.50
1:DB:1427:U:H2'	1:DB:1428:A:H8	1.77	0.50
2:EB:2315:G:H2'	2:EB:2316:C:C6	2.47	0.50
15:RB:10:LEU:O	15:RB:12:ARG:HG3	2.12	0.50
20:WB:12:ILE:HD13	20:WB:17:VAL:HG22	1.93	0.50
33:JC:2:LYS:HZ1	33:JC:4:ARG:HE	1.58	0.50
35:MC:160:ASP:OD1	35:MC:160:ASP:N	2.45	0.50
49:AD:12:LYS:HG2	49:AD:13:HIS:CD2	2.47	0.50
2:B:270(W):G:H2'	2:B:270(X):G:H8	1.77	0.50
2:B:847:U:OP2	2:B:929:G:O6	2.29	0.50
5:E:11:PRO:O	5:E:14:ARG:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:129:ASN:O	5:E:193:VAL:HG12	2.12	0.50
35:JA:15:VAL:HG21	35:JA:213:LEU:HG	1.94	0.50
41:PA:78:GLN:HG3	41:PA:80:ILE:H	1.77	0.50
1:DB:87:A:C2	1:DB:88:C:H1'	2.47	0.50
1:DB:1218:C:H2'	1:DB:1219:U:C6	2.47	0.50
2:EB:1252:G:C2	2:EB:1253:A:C2	3.00	0.50
2:EB:2209:C:H1'	2:EB:2216:G:N2	2.26	0.50
2:EB:2840:C:H5''	15:RB:53:HIS:CD2	2.47	0.50
4:GB:15:G:H2'	4:GB:59:A:N1	2.27	0.50
23:ZB:158:PRO:O	23:ZB:161:VAL:HB	2.12	0.50
27:DC:44:ARG:O	27:DC:48:GLU:HG3	2.10	0.50
38:PC:8:GLU:HG2	38:PC:34:VAL:HG12	1.94	0.50
39:QC:67:MET:HG3	39:QC:68:PRO:HD2	1.94	0.50
52:DD:3:ARG:NH1	52:DD:8:GLY:O	2.45	0.50
55:HD:331:GLU:HB3	55:HD:336:LYS:HE2	1.93	0.50
1:A:828:A:H2'	1:A:829:G:O4'	2.12	0.50
2:B:271(C):G:H4'	2:B:271(D):U:H5''	1.92	0.50
25:Y:7:ILE:HG23	25:Y:98:LEU:HD11	1.94	0.50
45:TA:89:ARG:HA	45:TA:97:ARG:HA	1.94	0.50
1:DB:1266:G:O2'	1:DB:1268:A:N7	2.38	0.50
2:EB:458:G:O2'	31:HC:39:ARG:HD3	2.12	0.50
2:EB:1516:U:H2'	2:EB:1517:G:H8	1.75	0.50
2:EB:1942:5MC:HM53	2:EB:1943:U:C2	2.47	0.50
2:EB:2143:C:O2'	2:EB:2148:G:N2	2.41	0.50
2:EB:2821:A:OP2	2:EB:2822:G:OP2	2.28	0.50
40:RC:28:ASN:OD1	40:RC:36:LYS:NZ	2.45	0.50
2:B:2502:G:H5''	2:B:2503:2MA:H5''	1.93	0.50
2:B:2840:C:H5''	15:O:53:HIS:CD2	2.47	0.50
6:F:59:VAL:HG11	6:F:64:LYS:HD3	1.92	0.50
6:F:93:VAL:HG11	6:F:181:LEU:O	2.11	0.50
7:G:192:LEU:HD22	7:G:194:MET:HG3	1.94	0.50
28:BA:49:PHE:HE1	46:UA:62:ASN:HD22	1.60	0.50
33:GA:6:SER:O	33:GA:6:SER:OG	2.29	0.50
1:DB:981:U:H5'	47:YC:21:TYR:CE2	2.47	0.50
1:DB:1133:G:C2	1:DB:1134:G:H1'	2.46	0.50
40:RC:150:ALA:HB2	44:VC:50:TYR:CZ	2.47	0.50
41:SC:31:PHE:O	41:SC:35:ILE:HG13	2.12	0.50
55:HD:110:ASN:HB3	55:HD:167:SER:HA	1.93	0.50
1:A:105:G:C5	1:A:106:C:C4	3.00	0.49
1:A:512:U:H2'	1:A:513:C:C6	2.47	0.49
1:A:715:A:H2'	1:A:716:A:C8	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:896:A:H4'	2:B:896:A:OP2	2.11	0.49
2:B:2565:A:H5''	2:B:2566:A:OP2	2.12	0.49
2:B:2723:C:OP2	6:F:109:LYS:NZ	2.42	0.49
10:J:96:ASP:HA	10:J:99:GLU:HB2	1.93	0.49
11:K:67:LEU:HA	11:K:87:LEU:HD12	1.93	0.49
13:M:49:ARG:HB3	32:FA:61:LEU:HD21	1.94	0.49
35:JA:231:GLU:H	35:JA:232:PRO:HD2	1.78	0.49
40:OA:150:ALA:HB2	44:SA:50:TYR:OH	2.11	0.49
1:DB:237:C:H5''	50:BD:25:ARG:NH1	2.27	0.49
1:DB:262:A:C6	1:DB:263:A:C6	2.99	0.49
1:DB:977:A:H2'	1:DB:978:A:H5''	1.94	0.49
2:EB:320:A:H4'	2:EB:322:A:C8	2.46	0.49
2:EB:704:G:O2'	2:EB:726:G:N2	2.39	0.49
2:EB:882:G:H2'	2:EB:883:G:H8	1.77	0.49
2:EB:1028:A:N3	2:EB:2486:G:O2'	2.33	0.49
15:RB:37:THR:OG1	15:RB:40:LYS:HB2	2.12	0.49
22:YB:35:TYR:CE2	22:YB:69:ALA:HB3	2.47	0.49
33:JC:35:ARG:NH1	33:JC:37:GLY:OXT	2.45	0.49
49:AD:22:THR:HA	49:AD:33:ILE:HG12	1.94	0.49
1:A:87:A:C2	1:A:88:C:H1'	2.47	0.49
1:A:236:G:H5''	50:YA:42:TYR:OH	2.12	0.49
1:A:924:C:H5'	1:A:1399:C:OP2	2.12	0.49
1:A:957:U:OP1	52:AB:81:ARG:NH1	2.45	0.49
2:B:1512:G:H2'	2:B:1513:C:C6	2.47	0.49
2:B:2671:A:H2'	2:B:2672:G:C8	2.48	0.49
3:C:28:C:H2'	3:C:29:A:C8	2.47	0.49
35:JA:21:ARG:HH11	35:JA:23:ARG:HD3	1.71	0.49
38:MA:144:THR:HG22	38:MA:147:ASP:CG	2.32	0.49
1:DB:1070:U:H2'	1:DB:1071:C:H6	1.76	0.49
1:DB:1196:U:H6	1:DB:1196:U:H5'	1.77	0.49
1:DB:1356:G:H2'	1:DB:1357:A:C8	2.47	0.49
2:EB:2401:U:H3	2:EB:2415:G:H1	1.60	0.49
40:RC:26:PHE:CE2	40:RC:30:ILE:HD11	2.47	0.49
1:A:857:C:H2'	1:A:858:G:O4'	2.13	0.49
1:A:1034:G:H2'	1:A:1035:A:H8	1.77	0.49
1:A:1047:G:O2'	1:A:1215:G:O2'	2.25	0.49
1:A:1415:G:H2'	1:A:1416:G:C8	2.47	0.49
8:H:67:LYS:HD3	28:BA:5:ILE:HD12	1.93	0.49
18:R:83:LEU:HD12	18:R:113:ALA:HB2	1.93	0.49
19:S:85:LYS:HB3	19:S:85:LYS:HZ3	1.77	0.49
22:V:66:PRO:O	22:V:67:LEU:HD23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:83:GLU:OE2	25:Y:83:GLU:N	2.46	0.49
35:JA:82:ARG:HB2	35:JA:94:ASN:HD22	1.76	0.49
37:LA:108:LEU:HD22	37:LA:176:LEU:HD13	1.93	0.49
41:PA:112:LEU:HA	41:PA:134:ILE:HG12	1.94	0.49
2:EB:18:C:O2'	2:EB:553:U:OP1	2.29	0.49
2:EB:851:U:H2'	2:EB:852:G:H8	1.77	0.49
2:EB:2406:U:C2	13:PB:72:PRO:HG2	2.47	0.49
9:LB:56:SER:OG	9:LB:57:ASP:N	2.44	0.49
38:PC:45:PHE:HD2	38:PC:47:LYS:HZ1	1.59	0.49
55:HD:144:TRP:CE2	55:HD:171:VAL:HG22	2.47	0.49
2:B:1614:A:C2	20:T:93:ALA:HB2	2.47	0.49
9:I:121:ILE:HG12	9:I:140:LYS:HD2	1.95	0.49
14:N:60:ARG:NH2	23:W:114:GLY:HA3	2.26	0.49
22:V:45:VAL:O	22:V:62:GLU:HA	2.12	0.49
52:AB:27:GLU:HG3	52:AB:28:LYS:HA	1.95	0.49
1:DB:192:U:H2'	1:DB:193:C:C6	2.48	0.49
2:EB:270(N):U:H4'	2:EB:270(O):G:H5'	1.94	0.49
2:EB:945:A:C4	2:EB:2448:A:C2	3.00	0.49
3:FB:85:G:H1	3:FB:91:C:N4	2.10	0.49
8:KB:41:GLN:HG2	8:KB:154:GLY:O	2.13	0.49
8:KB:77:ILE:HG22	8:KB:80:PHE:H	1.76	0.49
8:KB:96:ARG:O	8:KB:99:MET:HB3	2.12	0.49
17:TB:55:ASN:H	17:TB:59:THR:HB	1.77	0.49
52:DD:24:ALA:HB3	52:DD:25:LYS:HE2	1.94	0.49
1:A:247:G:OP2	50:YA:100:LYS:N	2.45	0.49
1:A:1070:U:H2'	1:A:1071:C:H6	1.76	0.49
1:A:1133:G:C2	1:A:1134:G:H1'	2.47	0.49
2:B:751:A:H5'	20:T:90:ARG:HA	1.94	0.49
2:B:1027:A:C2	2:B:2488:A:H5'	2.47	0.49
2:B:1592:C:H2'	2:B:1593:G:C8	2.48	0.49
2:B:2791:C:H4'	2:B:2792:G:H5'	1.93	0.49
7:G:64:ILE:HD11	7:G:75:HIS:HB2	1.94	0.49
37:LA:127:THR:HG23	37:LA:147:ALA:HB3	1.95	0.49
53:BB:13:LEU:HB2	53:BB:17:ARG:NH1	2.28	0.49
9:LB:3:ARG:HG2	9:LB:6:ARG:NH1	2.27	0.49
9:LB:149:ARG:NH2	9:LB:167:GLU:OE1	2.41	0.49
19:VB:13:ARG:HG3	19:VB:13:ARG:HH11	1.78	0.49
29:FC:25:LEU:H	29:FC:25:LEU:HD12	1.77	0.49
38:PC:76:ILE:HG13	38:PC:93:PRO:HG3	1.95	0.49
46:XC:108:ARG:NH2	46:XC:114:ARG:HA	2.28	0.49
53:ED:47:GLY:HA2	53:ED:48:LYS:C	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:U:H2'	1:A:126:G:H8	1.76	0.49
1:A:920:U:H2'	1:A:921:U:C6	2.47	0.49
1:A:1087:G:N1	1:A:1088:G:O6	2.46	0.49
1:A:1291:G:O2'	42:QA:38:GLN:OE1	2.30	0.49
2:B:1187:G:H5''	19:S:81:TYR:CE1	2.48	0.49
2:B:1761:C:H3'	2:B:1762:A:C5'	2.41	0.49
2:B:1932:A:H2'	2:B:1933:G:O4'	2.13	0.49
2:B:2093:G:H5'	10:J:22:LYS:HD2	1.93	0.49
2:B:2141:G:H22	2:B:2151:G:H1'	1.77	0.49
2:B:2648:C:H2'	2:B:2649:U:H6	1.77	0.49
9:I:56:SER:OG	9:I:57:ASP:N	2.46	0.49
35:JA:51:LEU:HD12	35:JA:201:ILE:HD12	1.95	0.49
40:OA:38:LEU:O	40:OA:42:ILE:HG12	2.12	0.49
40:OA:71:PRO:HA	40:OA:138:LYS:HE3	1.94	0.49
44:SA:121:PRO:HG2	44:SA:126:ARG:HB2	1.94	0.49
46:UA:27:LYS:HB2	46:UA:27:LYS:NZ	2.27	0.49
1:DB:304:U:H2'	1:DB:305:G:C8	2.48	0.49
1:DB:850:U:H2'	1:DB:851:G:H8	1.77	0.49
1:DB:1095:U:OP1	1:DB:1108:G:N2	2.35	0.49
2:EB:140:A:C8	2:EB:1408:C:O2'	2.61	0.49
2:EB:1210:A:C8	2:EB:1212:G:C2	3.01	0.49
2:EB:1728:G:H8	2:EB:1732:A:H62	1.59	0.49
3:FB:3:C:H2'	3:FB:4:C:H6	1.76	0.49
4:GB:23:C:H2'	4:GB:24:U:C6	2.47	0.49
10:MB:3:VAL:HG12	10:MB:38:LEU:HA	1.94	0.49
10:MB:62:LYS:O	10:MB:66:GLU:HB2	2.13	0.49
11:NB:13:TRP:CE2	11:NB:133:GLN:HG2	2.48	0.49
20:WB:82:LEU:HD23	20:WB:84:ARG:CZ	2.43	0.49
50:BD:84:LEU:HD12	50:BD:87:LYS:HE2	1.94	0.49
53:ED:54:LYS:HA	53:ED:57:ARG:HH21	1.77	0.49
55:HD:145:ARG:HB3	55:HD:167:SER:HB2	1.95	0.49
1:A:62:U:H2'	1:A:63:C:H6	1.78	0.49
1:A:345:C:H3'	17:Q:41:ARG:NH2	2.27	0.49
2:B:1291:C:H2'	2:B:1292:U:H6	1.76	0.49
2:B:2171:A:O2'	2:B:2172:U:H5''	2.13	0.49
2:B:2267:A:H5''	2:B:2268:A:H5'	1.94	0.49
30:DA:11:LEU:HB3	30:DA:49:HIS:HB3	1.93	0.49
51:ZA:53:ARG:HH21	51:ZA:60:ALA:N	2.11	0.49
1:DB:1095:U:H5''	1:DB:1109:C:O2	2.12	0.49
2:EB:86:C:H4'	2:EB:104:U:H1'	1.95	0.49
2:EB:2689:U:P	2:EB:2719:G:H22	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:FB:12:C:OP2	3:FB:12:C:H6	1.96	0.49
8:KB:11:TYR:HA	8:KB:15:VAL:HB	1.94	0.49
9:LB:102:ALA:HA	9:LB:117:PRO:HD3	1.95	0.49
23:ZB:97:GLU:HB2	23:ZB:125:LEU:HD11	1.94	0.49
25:BC:51:VAL:HG21	25:BC:74:VAL:HG21	1.95	0.49
1:A:1118:C:H1'	1:A:1179:A:C5	2.48	0.49
2:B:1011:G:H5''	18:R:77:SER:OG	2.13	0.49
2:B:1537:C:H3'	2:B:1538:G:C8	2.46	0.49
6:F:111:ARG:HD3	6:F:160:TYR:HD2	1.77	0.49
6:F:119:ARG:HG2	6:F:120:TRP:CE2	2.47	0.49
8:H:122:PRO:HD2	8:H:181:ARG:NH1	2.28	0.49
48:WA:44:LYS:O	48:WA:47:LYS:NZ	2.39	0.49
1:DB:1009:G:H2'	1:DB:1010:G:C8	2.48	0.49
1:DB:1493:A:N3	55:HD:119:THR:HG23	2.28	0.49
2:EB:2335:A:C8	2:EB:2337:G:C5	3.01	0.49
2:EB:2348:U:O2'	2:EB:2349:G:H5'	2.13	0.49
8:KB:16:ARG:HB3	8:KB:17:PRO:HD3	1.95	0.49
15:RB:52:ILE:O	15:RB:55:ALA:N	2.46	0.49
27:DC:7:LYS:HB2	27:DC:34:GLU:HG2	1.95	0.49
38:PC:148:VAL:HG21	41:SC:107:LEU:HD22	1.95	0.49
41:SC:81:HIS:HB2	41:SC:138:TRP:CD1	2.48	0.49
45:WC:61:THR:C	45:WC:63:GLY:H	2.16	0.49
1:A:434:U:H2'	1:A:435:C:C6	2.48	0.49
1:A:1075:C:H5''	35:JA:179:LYS:HZ2	1.78	0.49
2:B:729:G:H2'	2:B:1775:U:H1'	1.95	0.49
2:B:1322:A:N1	2:B:1333:C:O2'	2.39	0.49
5:E:5:LYS:HE3	5:E:6:PHE:H	1.78	0.49
24:X:7:LEU:CD1	24:X:8:GLY:H	2.26	0.49
35:JA:58:ILE:HA	35:JA:61:LEU:HB3	1.93	0.49
38:MA:70:PRO:HB2	38:MA:77:PRO:HG3	1.93	0.49
42:QA:48:GLU:OE2	42:QA:51:ARG:HD2	2.13	0.49
1:DB:562:C:H4'	1:DB:563:A:H5'	1.94	0.49
2:EB:630:G:OP2	32:IC:15:LYS:NZ	2.27	0.49
2:EB:969:U:H4'	27:DC:14:GLY:O	2.13	0.49
3:FB:28:C:OP1	16:SB:34:HIS:HB2	2.12	0.49
17:TB:108:ARG:HH21	17:TB:112:ARG:HH22	1.60	0.49
30:GC:11:LEU:HB3	30:GC:49:HIS:HB3	1.95	0.49
36:NC:162:GLN:NE2	36:NC:163:ALA:O	2.38	0.49
55:GD:110:ASN:HB3	55:GD:167:SER:HA	1.94	0.49
1:A:164:U:H2'	1:A:165:C:C6	2.47	0.49
2:B:2112:G:O2'	4:D:19:G:O2'	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2211:G:H2'	2:B:2212:A:C2	2.48	0.49
8:H:76:SER:HB2	8:H:84:LYS:HB3	1.95	0.49
33:GA:2:LYS:HB3	33:GA:2:LYS:HE2	1.64	0.49
38:MA:45:PHE:HE2	38:MA:47:LYS:HE3	1.78	0.49
47:VA:40:CYS:SG	47:VA:43:CYS:SG	3.11	0.49
52:AB:3:ARG:NH2	52:AB:7:LYS:HE2	2.28	0.49
53:BB:90:GLN:HA	53:BB:93:GLU:HB3	1.94	0.49
1:DB:753:A:H5'	1:DB:754:C:C5	2.47	0.49
2:EB:444:C:H4'	7:JB:49:ALA:HB2	1.95	0.49
2:EB:1177:A:H2'	2:EB:1178:C:O4'	2.12	0.49
2:EB:2086:U:H2'	2:EB:2087:G:C8	2.48	0.49
2:EB:2246:G:H1'	2:EB:2426:A:C2	2.47	0.49
2:EB:2347:C:O2'	30:GC:21:TYR:OH	2.30	0.49
2:EB:2791:C:H5''	2:EB:2893:G:H2'	1.95	0.49
5:HB:183:ARG:HG2	5:HB:183:ARG:HH11	1.77	0.49
9:LB:121:ILE:HG12	9:LB:140:LYS:HD2	1.95	0.49
13:PB:49:ARG:HB3	32:IC:61:LEU:HD21	1.95	0.49
37:OC:191:ARG:HE	37:OC:200:GLU:CD	2.16	0.49
43:UC:24:VAL:HG21	43:UC:37:PRO:HD3	1.94	0.49
48:ZC:55:GLY:O	48:ZC:59:MET:HG3	2.12	0.49
53:ED:23:ARG:HH11	53:ED:24:LEU:HD22	1.77	0.49
1:A:192:U:H2'	1:A:193:C:C6	2.48	0.48
1:A:481:G:O2'	1:A:483:C:N4	2.42	0.48
1:A:977:A:H2'	1:A:978:A:H5''	1.95	0.48
1:A:1009:G:H2'	1:A:1010:G:C8	2.48	0.48
1:A:1107:C:OP1	36:KA:172:ARG:HB2	2.13	0.48
2:B:17:G:H4'	18:R:25:TRP:HE1	1.77	0.48
2:B:686:G:N2	2:B:788:A:H61	2.11	0.48
2:B:1060:U:H4'	2:B:1061:U:H3'	1.95	0.48
2:B:1252:G:C2	2:B:1253:A:C2	3.00	0.48
2:B:1784:A:H4'	2:B:1785:A:C5'	2.43	0.48
2:B:2291:U:OP1	2:B:2380:C:O2'	2.28	0.48
2:B:2552:2MU:H2'	2:B:2554:U:OP2	2.12	0.48
3:C:112:G:H2'	3:C:113:C:C6	2.48	0.48
10:J:67:ARG:HH11	10:J:68:LEU:CD1	2.25	0.48
10:J:76:THR:HB	10:J:141:LYS:HE2	1.93	0.48
12:L:87:ILE:HG22	12:L:93:PRO:HA	1.95	0.48
20:T:71:VAL:HA	20:T:107:LEU:HD12	1.94	0.48
30:DA:26:ASN:HB3	30:DA:29:ASN:HB2	1.96	0.48
39:NA:7:ASN:HB2	39:NA:89:MET:HB3	1.95	0.48
52:AB:44:MET:O	52:AB:46:GLY:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DB:359:U:H2'	1:DB:360:A:C8	2.47	0.48
1:DB:475:G:H2'	1:DB:476:G:C8	2.47	0.48
1:DB:1105:A:H2'	1:DB:1106:G:H8	1.78	0.48
2:EB:548:A:H4'	19:VB:19:LYS:HZ1	1.78	0.48
2:EB:2211:G:H2'	2:EB:2212:A:C2	2.48	0.48
5:HB:43:ARG:HA	5:HB:48:ARG:O	2.12	0.48
11:NB:138:LEU:HD23	11:NB:139:GLU:N	2.28	0.48
16:SB:10:ARG:HH21	16:SB:91:PRO:HB2	1.76	0.48
17:TB:113:LYS:O	17:TB:115:ARG:NH1	2.46	0.48
1:A:1448:C:H2'	1:A:1449:C:H6	1.76	0.48
2:B:34:C:O2'	2:B:35:G:H8	1.96	0.48
2:B:243:U:OP1	32:FA:6:THR:OG1	2.22	0.48
2:B:280:C:C2	2:B:361:G:N2	2.80	0.48
2:B:499:U:H5'	22:V:46:LYS:HD3	1.94	0.48
2:B:882:G:H2'	2:B:883:G:H8	1.78	0.48
2:B:1156:A:OP1	18:R:55:ARG:NH1	2.46	0.48
5:E:240:ALA:HB1	5:E:241:PRO:HD2	1.95	0.48
10:J:9:LEU:HD12	10:J:10:GLU:OE2	2.12	0.48
37:LA:109:GLY:HA3	37:LA:165:MET:SD	2.53	0.48
49:XA:25:ARG:HH11	49:XA:25:ARG:HG3	1.77	0.48
1:DB:62:U:H2'	1:DB:63:C:H6	1.78	0.48
1:DB:860:A:H2'	1:DB:861:G:O4'	2.13	0.48
1:DB:1295:G:HO2'	46:XC:14:ARG:NH1	2.12	0.48
1:DB:1342:C:H2'	1:DB:1343:G:C8	2.48	0.48
1:DB:1418:A:H5''	1:DB:1419:G:OP2	2.13	0.48
2:EB:1152:C:OP1	18:UB:84:LYS:HD2	2.12	0.48
2:EB:1292:U:H2'	2:EB:1293:C:C6	2.48	0.48
2:EB:1754:C:OP2	17:TB:113:LYS:HE3	2.13	0.48
5:HB:67:PHE:CE1	5:HB:106:ILE:HD11	2.48	0.48
6:IB:116:VAL:HG13	6:IB:122:PHE:HB2	1.94	0.48
10:MB:57:ARG:O	10:MB:61:ARG:NH2	2.47	0.48
13:PB:122:PRO:O	13:PB:123:LEU:HD23	2.12	0.48
37:OC:158:ILE:HG13	37:OC:159:ARG:N	2.27	0.48
39:QC:22:GLU:O	39:QC:25:ILE:HG12	2.13	0.48
46:XC:7:VAL:HG12	46:XC:8:GLU:H	1.78	0.48
48:ZC:17:ARG:HD3	48:ZC:26:GLU:OE2	2.13	0.48
1:A:563:A:O2'	1:A:564:C:OP2	2.21	0.48
1:A:664:G:OP1	51:ZA:64:ARG:NH1	2.45	0.48
1:A:748:C:H1'	1:A:749:C:OP2	2.12	0.48
1:A:926:G:H22	34:HA:15:A:H5''	1.78	0.48
2:B:945:A:C4	2:B:2448:A:C2	3.02	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2085:C:O3'	5:E:262:ARG:NH1	2.46	0.48
2:B:2161:C:H2'	2:B:2162:G:C8	2.48	0.48
2:B:2850:A:H2	15:O:61:HIS:CG	2.32	0.48
4:D:52:G:H1'	4:D:63:G:N2	2.29	0.48
7:G:157:VAL:HB	7:G:194:MET:HG2	1.94	0.48
9:I:3:ARG:CZ	9:I:5:GLY:H	2.26	0.48
11:K:73:THR:HB	11:K:82:LEU:HD11	1.95	0.48
36:KA:189:ALA:HB3	36:KA:196:LEU:HB2	1.94	0.48
45:TA:61:THR:C	45:TA:63:GLY:H	2.16	0.48
1:DB:1417:G:O2'	1:DB:1483:A:N6	2.46	0.48
2:EB:253:C:H2'	2:EB:254:G:O4'	2.13	0.48
2:EB:540:G:H2'	2:EB:541:C:H6	1.78	0.48
2:EB:947:G:H2'	2:EB:948:G:C8	2.48	0.48
2:EB:2528:U:H3	2:EB:2535:G:H1	1.59	0.48
12:OB:90:GLN:OE1	12:OB:90:GLN:N	2.46	0.48
17:TB:16:ARG:NH1	17:TB:83:ILE:HB	2.27	0.48
19:VB:2:PHE:CE2	19:VB:41:GLY:HA3	2.48	0.48
28:EC:58:ARG:NH2	52:DD:68:GLY:HA3	2.25	0.48
35:MC:155:LEU:HA	35:MC:157:ARG:HH21	1.78	0.48
36:NC:68:VAL:HB	36:NC:103:VAL:HG13	1.96	0.48
37:OC:12:CYS:SG	37:OC:26:CYS:SG	3.12	0.48
40:RC:71:PRO:HA	40:RC:138:LYS:HE3	1.94	0.48
41:SC:86:ILE:HG21	41:SC:133:LEU:HD13	1.94	0.48
2:B:639:U:H2'	2:B:640:C:C6	2.49	0.48
2:B:890:A:H2'	2:B:892:G:H8	1.78	0.48
2:B:2345:G:OP2	30:DA:38:LYS:HG2	2.12	0.48
32:FA:56:GLU:HA	32:FA:59:LYS:HG3	1.95	0.48
35:JA:145:LEU:HD23	35:JA:149:LEU:HD13	1.95	0.48
43:RA:24:VAL:HG21	43:RA:37:PRO:HD3	1.95	0.48
1:DB:444:C:H2'	1:DB:445:G:C8	2.48	0.48
1:DB:452:A:O2'	1:DB:453:A:OP2	2.26	0.48
1:DB:1097:C:H2'	1:DB:1098:C:C6	2.48	0.48
1:DB:1317:C:O2	52:DD:37:ARG:NH2	2.46	0.48
2:EB:1188:U:H4'	19:VB:79:VAL:HG22	1.95	0.48
2:EB:1761:C:H3'	2:EB:1762:A:C5'	2.40	0.48
2:EB:1902:C:OP1	5:HB:242:ARG:HD2	2.13	0.48
2:EB:2582:G:N2	2:EB:2583:G:H1'	2.29	0.48
4:GB:35:A:H61	34:KC:13:A:H62	1.61	0.48
5:HB:132:PRO:HD3	5:HB:190:TYR:CZ	2.49	0.48
8:KB:107:LEU:HD22	8:KB:177:GLY:O	2.14	0.48
16:SB:76:LYS:O	16:SB:80:LEU:HD13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:JC:2:LYS:HB3	33:JC:2:LYS:HE2	1.62	0.48
40:RC:78:ARG:HG2	40:RC:79:ARG:HG2	1.95	0.48
40:RC:115:ARG:O	40:RC:118:VAL:HB	2.13	0.48
49:AD:25:ARG:HG3	49:AD:25:ARG:HH11	1.78	0.48
55:GD:186:ARG:HB3	55:GD:312:PHE:HB2	1.94	0.48
1:A:160:A:H2'	1:A:161:A:O4'	2.13	0.48
1:A:448:A:OP2	1:A:485:G:N2	2.36	0.48
1:A:475:G:H2'	1:A:476:G:C8	2.49	0.48
1:A:555:C:H2'	1:A:556:C:C6	2.48	0.48
1:A:833:U:H2'	1:A:834:C:H6	1.77	0.48
1:A:1036:G:H21	1:A:1037:C:N4	2.11	0.48
2:B:141(A):A:H5''	2:B:141(B):C:OP2	2.13	0.48
2:B:361:G:C2	2:B:362:U:H5	2.32	0.48
2:B:784:A:C6	5:E:229:VAL:HG21	2.49	0.48
2:B:1902:C:H5'	5:E:246:PRO:HD3	1.94	0.48
2:B:2422:A:H4'	2:B:2423:U:OP1	2.13	0.48
2:B:2593:U:H2'	2:B:2594:C:H6	1.77	0.48
2:B:2649:U:H2'	2:B:2650:U:C6	2.49	0.48
4:D:15:G:H2'	4:D:59:A:N1	2.27	0.48
11:K:4:TYR:OH	11:K:6:PRO:HA	2.13	0.48
15:O:52:ILE:O	15:O:55:ALA:N	2.46	0.48
15:O:104:ARG:HG2	15:O:109:ALA:HB3	1.94	0.48
19:S:69:LYS:O	19:S:70:ILE:HD13	2.13	0.48
41:PA:114:THR:HG22	41:PA:131:GLY:HA3	1.95	0.48
48:WA:3:ILE:HG23	48:WA:7:GLU:OE2	2.14	0.48
1:DB:434:U:H2'	1:DB:435:C:C6	2.48	0.48
1:DB:1412:C:H2'	1:DB:1413:A:H8	1.78	0.48
2:EB:604:G:C6	2:EB:605:C:C4	3.02	0.48
2:EB:769:G:H5'	2:EB:1379:A:N6	2.28	0.48
2:EB:839:U:H3	2:EB:939:G:H1	1.60	0.48
2:EB:2171:A:O2'	2:EB:2172:U:H5''	2.14	0.48
2:EB:2422:A:H4'	2:EB:2423:U:OP1	2.13	0.48
5:HB:145:VAL:HB	5:HB:155:LEU:HB2	1.95	0.48
5:HB:260:ARG:NH2	5:HB:266:SER:OG	2.47	0.48
7:JB:153:SER:OG	7:JB:190:GLU:N	2.46	0.48
15:RB:26:LYS:O	15:RB:30:THR:HG23	2.13	0.48
17:TB:18:ASP:OD2	17:TB:18:ASP:N	2.47	0.48
18:UB:47:TYR:HA	18:UB:50:ARG:NH2	2.28	0.48
25:BC:4:VAL:HG21	25:BC:11:ARG:NH1	2.28	0.48
35:MC:47:THR:O	35:MC:51:LEU:N	2.43	0.48
39:QC:7:ASN:HB2	39:QC:89:MET:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:VC:33:THR:HA	44:VC:39:PRO:HA	1.95	0.48
1:A:162:A:C5	1:A:163:C:H1'	2.48	0.48
1:A:952:U:H2'	1:A:953:G:H8	1.78	0.48
2:B:715:G:H2'	2:B:716:A:H8	1.78	0.48
2:B:769:G:H5'	2:B:1379:A:N6	2.28	0.48
2:B:1177:A:H2'	2:B:1178:C:O4'	2.14	0.48
4:D:43:A:H2'	4:D:44:A:C8	2.47	0.48
18:R:89:GLU:HB2	19:S:50:PRO:HB3	1.96	0.48
27:AA:44:ARG:O	27:AA:48:GLU:HG3	2.14	0.48
35:JA:229:VAL:HB	35:JA:231:GLU:OE2	2.14	0.48
36:KA:65:ALA:HA	36:KA:100:ALA:CB	2.44	0.48
53:BB:23:ARG:HH11	53:BB:24:LEU:HD22	1.77	0.48
1:DB:1478:C:H2'	1:DB:1479:C:H6	1.79	0.48
1:DB:1511:G:C6	1:DB:1512:U:C4	3.01	0.48
2:EB:1326:U:O2'	2:EB:1327:C:H5'	2.14	0.48
2:EB:1550:C:OP1	2:EB:1727:U:O2'	2.28	0.48
2:EB:1651:G:N2	2:EB:2007:C:C2	2.81	0.48
2:EB:1779:U:C6	2:EB:1783:A:N7	2.81	0.48
2:EB:2515:C:O2'	2:EB:2516:G:H5'	2.14	0.48
3:FB:66:A:H61	3:FB:107:U:H2'	1.79	0.48
9:LB:38:SER:OG	9:LB:40:GLU:OE2	2.31	0.48
4:LC:34:C:H2'	4:LC:35:A:C8	2.47	0.48
35:MC:30:ARG:HH21	35:MC:194:PRO:HB2	1.78	0.48
39:QC:22:GLU:OE1	39:QC:82:ARG:NH2	2.46	0.48
46:XC:3:ARG:NH1	46:XC:8:GLU:HA	2.28	0.48
55:GD:331:GLU:HB3	55:GD:336:LYS:HE2	1.94	0.48
1:A:339:C:H2'	1:A:340:U:C6	2.49	0.48
1:A:448:A:P	1:A:485:G:H22	2.36	0.48
1:A:626:U:H2'	1:A:627:G:H8	1.78	0.48
1:A:1228:C:H4'	46:UA:116:THR:HA	1.96	0.48
1:A:1366:C:H2'	1:A:1367:C:H6	1.78	0.48
1:A:1517:G:H1'	2:B:1919:A:O3'	2.14	0.48
2:B:270(K):G:N1	2:B:270(Q):C:N3	2.53	0.48
2:B:1902:C:OP1	5:E:242:ARG:HD2	2.14	0.48
9:I:58:GLU:HG2	9:I:61:HIS:HB2	1.96	0.48
15:O:12:ARG:NH1	15:O:12:ARG:CG	2.77	0.48
20:T:27:LYS:HG3	20:T:31:GLU:OE2	2.14	0.48
21:U:5:TYR:OH	26:Z:30:ARG:HD2	2.13	0.48
36:KA:86:VAL:HA	36:KA:89:GLU:HB2	1.95	0.48
40:OA:115:ARG:O	40:OA:118:VAL:HB	2.13	0.48
42:QA:11:LYS:O	42:QA:13:ALA:N	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:UA:33:ALA:HA	46:UA:59:TYR:HE2	1.78	0.48
48:WA:55:GLY:O	48:WA:59:MET:HG3	2.12	0.48
1:DB:1228:C:H4'	46:XC:116:THR:HA	1.95	0.48
2:EB:363(F):U:H3'	2:EB:363(G):A:C8	2.48	0.48
2:EB:363(G):A:O2'	2:EB:364:C:OP2	2.30	0.48
2:EB:603:A:N7	2:EB:655:A:C5	2.81	0.48
2:EB:900:A:H2'	2:EB:901:A:C8	2.49	0.48
2:EB:2001:A:H2'	2:EB:2002:G:C8	2.49	0.48
2:EB:2496:C:H5'	14:QB:83:MET:HE3	1.96	0.48
5:HB:132:PRO:HG3	5:HB:190:TYR:CE2	2.48	0.48
7:JB:11:VAL:HG22	7:JB:125:LEU:HB2	1.96	0.48
9:LB:26:VAL:HG12	9:LB:79:VAL:HG21	1.95	0.48
10:MB:67:ARG:HH11	10:MB:68:LEU:CD1	2.27	0.48
36:NC:35:GLU:O	36:NC:39:ILE:HG12	2.14	0.48
50:BD:31:LEU:HD23	50:BD:32:TYR:CZ	2.48	0.48
1:A:1009:G:H2'	1:A:1010:G:H8	1.79	0.48
1:A:1021:G:C2	1:A:1022:G:H1'	2.49	0.48
2:B:270(S):G:O2'	25:Y:79:GLY:HA3	2.14	0.48
2:B:628:G:H2'	2:B:629:G:H8	1.78	0.48
2:B:716:A:C2	2:B:717:G:H1'	2.48	0.48
2:B:947:G:H2'	2:B:948:G:H8	1.79	0.48
17:Q:36:GLU:HG3	17:Q:41:ARG:HE	1.78	0.48
17:Q:108:ARG:HH21	17:Q:112:ARG:HH22	1.62	0.48
23:W:158:PRO:O	23:W:161:VAL:HB	2.14	0.48
40:OA:41:ARG:HG3	40:OA:42:ILE:HD13	1.95	0.48
48:WA:9:GLN:NE2	48:WA:12:ILE:HD12	2.29	0.48
2:EB:263:C:H2'	2:EB:264:C:O4'	2.14	0.48
2:EB:2031:A:H1'	2:EB:2455:G:O2'	2.14	0.48
2:EB:2209:C:O2	2:EB:2216:G:N1	2.47	0.48
15:RB:44:LEU:O	15:RB:48:VAL:HG22	2.13	0.48
35:MC:82:ARG:HB2	35:MC:94:ASN:HD22	1.78	0.48
43:UC:91:PRO:O	43:UC:94:VAL:HG22	2.13	0.48
1:A:237:C:H5''	50:YA:25:ARG:NH1	2.28	0.48
1:A:673:G:H2'	1:A:674:G:C8	2.48	0.48
1:A:736:C:H2'	1:A:737:A:C8	2.48	0.48
1:A:1453:G:H4'	1:A:1454:G:OP2	2.13	0.48
2:B:540:G:H2'	2:B:541:C:C6	2.48	0.48
2:B:604:G:C6	2:B:605:C:C4	3.02	0.48
2:B:1437:C:H2'	2:B:1438:U:C6	2.48	0.48
2:B:1812:A:O2'	5:E:45:ASN:N	2.46	0.48
4:D:22:G:H2'	4:D:23:C:C6	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:23:C:H2'	4:D:24:U:C6	2.49	0.48
7:G:148:LEU:HD11	7:G:193:VAL:HG21	1.96	0.48
8:H:41:GLN:HG2	8:H:154:GLY:O	2.14	0.48
15:O:55:ALA:HA	15:O:80:PHE:CE2	2.49	0.48
20:T:82:LEU:HB3	20:T:84:ARG:NH1	2.28	0.48
23:W:72:ARG:HD3	23:W:72:ARG:HA	1.66	0.48
25:Y:21:ARG:CG	25:Y:21:ARG:NH1	2.75	0.48
27:AA:9:VAL:HG11	27:AA:55:ARG:HH11	1.79	0.48
37:LA:9:CYS:SG	37:LA:31:CYS:SG	3.04	0.48
38:MA:20:GLN:OE1	38:MA:21:ALA:N	2.46	0.48
46:UA:70:LEU:O	46:UA:74:VAL:HG23	2.14	0.48
46:UA:108:ARG:NH2	46:UA:114:ARG:HA	2.29	0.48
1:DB:544:G:H2'	1:DB:545:C:C6	2.49	0.48
1:DB:715:A:H2'	1:DB:716:A:C8	2.49	0.48
2:EB:38:A:H2'	2:EB:39:C:C6	2.49	0.48
2:EB:619:G:H5''	2:EB:620:G:OP2	2.14	0.48
2:EB:2317:C:C2'	2:EB:2318:G:H5'	2.44	0.48
2:EB:2713:A:H3'	2:EB:2714:G:H5''	1.96	0.48
2:EB:2792:G:H1	2:EB:2805:G:H1'	1.78	0.48
9:LB:3:ARG:CZ	9:LB:5:GLY:H	2.27	0.48
18:UB:58:ARG:HA	18:UB:61:TRP:CE3	2.49	0.48
29:FC:40:LYS:HG3	29:FC:41:PRO:O	2.13	0.48
4:LC:76:A:H3'	55:HD:234:GLY:HA3	1.96	0.48
37:OC:12:CYS:HG	37:OC:18:LYS:HZ3	1.50	0.48
37:OC:59:ARG:NH2	37:OC:66:ARG:HH12	2.11	0.48
38:PC:144:THR:HG22	38:PC:147:ASP:CG	2.34	0.48
44:VC:90:GLY:O	44:VC:92:GLU:N	2.47	0.48
2:B:26:G:C6	2:B:27:G:N1	2.82	0.48
2:B:511:U:C5	2:B:512:G:C5	3.02	0.48
2:B:537:C:H2'	2:B:539:G:C8	2.49	0.48
2:B:1796:U:H2'	2:B:1797:C:C6	2.49	0.48
2:B:2711:A:OP2	2:B:2712(A):A:OP2	2.32	0.48
5:E:30:GLU:HB3	5:E:33:LEU:HD12	1.95	0.48
8:H:16:ARG:HB3	8:H:17:PRO:HD3	1.95	0.48
11:K:63:THR:O	11:K:66:LYS:HE3	2.14	0.48
21:U:2:LYS:NZ	21:U:38:GLU:OE2	2.35	0.48
41:PA:5:PRO:HB2	41:PA:32:LYS:NZ	2.28	0.48
1:DB:247:G:OP2	50:BD:100:LYS:N	2.45	0.48
1:DB:1240:U:OP1	40:RC:119:ARG:NH2	2.47	0.48
2:EB:545:G:N2	2:EB:547:A:OP2	2.45	0.48
2:EB:922:U:H2'	2:EB:923:C:C6	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EB:2161:C:H2'	2:EB:2162:G:C8	2.49	0.48
5:HB:11:PRO:O	5:HB:14:ARG:HG2	2.13	0.48
11:NB:9:VAL:HG11	11:NB:48:MET:HB2	1.94	0.48
12:OB:25:LEU:O	12:OB:27:GLY:N	2.46	0.48
53:ED:54:LYS:HG2	53:ED:57:ARG:HH21	1.79	0.48
55:HD:214:LEU:H	55:HD:214:LEU:HD23	1.79	0.48
1:A:1196:U:H6	1:A:1196:U:H5'	1.79	0.47
1:A:1511:G:C6	1:A:1512:U:C4	3.01	0.47
2:B:136:G:H2'	2:B:137(A):C:H6	1.77	0.47
2:B:270(N):U:H4'	2:B:270(O):G:H5'	1.95	0.47
2:B:688:U:OP2	31:EA:2:LYS:NZ	2.42	0.47
2:B:932:G:OP1	27:AA:29:ARG:NH2	2.47	0.47
2:B:1532:C:H42	2:B:1539:G:H1	1.61	0.47
2:B:1550:C:OP1	2:B:1727:U:O2'	2.29	0.47
2:B:2181:G:H2'	2:B:2182:G:C8	2.49	0.47
2:B:2298:A:H2'	2:B:2299:G:O4'	2.13	0.47
2:B:2567:G:H2'	2:B:2568:C:H6	1.76	0.47
2:B:2820:A:OP2	15:O:2:ARG:NH2	2.47	0.47
5:E:75:ILE:H	5:E:75:ILE:HD12	1.78	0.47
10:J:96:ASP:O	10:J:100:ALA:N	2.40	0.47
22:V:89:PHE:O	22:V:91:GLU:N	2.43	0.47
37:LA:191:ARG:HE	37:LA:200:GLU:CD	2.18	0.47
1:DB:1074:G:O4'	35:MC:104:ASN:ND2	2.47	0.47
2:EB:394:A:C6	2:EB:395:U:C4	3.02	0.47
2:EB:571:A:C8	2:EB:2030:A:N6	2.82	0.47
2:EB:817:C:H4'	2:EB:932:G:C5	2.49	0.47
2:EB:1717:G:H1	2:EB:1742:C:H42	1.62	0.47
2:EB:2141:G:N1	2:EB:2142:C:O2	2.47	0.47
35:MC:58:ILE:HA	35:MC:61:LEU:HB3	1.95	0.47
39:QC:100:ASN:HA	51:CD:23:LYS:HZ1	1.78	0.47
41:SC:103:VAL:HB	41:SC:108:GLY:O	2.13	0.47
48:ZC:26:GLU:HG2	48:ZC:81:LEU:HD22	1.96	0.47
2:B:94:G:H2'	2:B:95:G:O4'	2.15	0.47
2:B:2472:G:H2'	2:B:2475:C:H42	1.78	0.47
3:C:3:C:H2'	3:C:4:C:C6	2.49	0.47
5:E:43:ARG:HA	5:E:48:ARG:O	2.14	0.47
5:E:67:PHE:CE1	5:E:106:ILE:HD11	2.49	0.47
17:Q:16:ARG:NH1	17:Q:83:ILE:HB	2.29	0.47
40:OA:150:ALA:HB2	44:SA:50:TYR:CZ	2.49	0.47
48:WA:88:ARG:NH2	48:WA:88:ARG:HB3	2.29	0.47
1:DB:736:C:H2'	1:DB:737:A:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DB:1105:A:H2'	1:DB:1106:G:C8	2.49	0.47
1:DB:1298:C:C4	40:RC:114:ARG:HD2	2.49	0.47
1:DB:1301:U:H2'	1:DB:1303:C:C5	2.48	0.47
2:EB:185:U:H2'	2:EB:186:G:C8	2.49	0.47
2:EB:511:U:C5	2:EB:512:G:C5	3.02	0.47
2:EB:1019:U:HO2'	2:EB:1021:A:H2	1.58	0.47
2:EB:1786:A:H1'	2:EB:1938:A:N6	2.28	0.47
2:EB:2330:G:H2'	2:EB:2331:G:O4'	2.14	0.47
2:EB:2607:G:H2'	2:EB:2608:G:O4'	2.14	0.47
2:EB:2850:A:H2	15:RB:61:HIS:CG	2.31	0.47
3:FB:84:C:H42	3:FB:92:G:H1	1.62	0.47
4:GB:52:G:H1'	4:GB:63:G:N2	2.29	0.47
24:AC:12:ASN:HA	24:AC:14:ARG:NH2	2.29	0.47
37:OC:155:LEU:HD22	37:OC:156:GLU:H	1.79	0.47
45:WC:69:TYR:HD2	45:WC:99:HIS:CD2	2.33	0.47
1:A:110:C:O2'	49:XA:25:ARG:O	2.33	0.47
1:A:537:G:H5''	45:TA:113:ARG:NH1	2.29	0.47
1:A:892:A:O2'	1:A:1415:G:H4'	2.14	0.47
1:A:1417:G:O2'	1:A:1483:A:N6	2.47	0.47
2:B:1043:C:H5	2:B:1112:G:H22	1.62	0.47
5:E:20:ASP:O	5:E:21:PHE:HB2	2.14	0.47
5:E:231:HIS:ND1	5:E:232:PRO:HD2	2.29	0.47
8:H:79:ASN:N	8:H:79:ASN:OD1	2.47	0.47
14:N:21:THR:HA	14:N:98:LYS:HB2	1.96	0.47
19:S:2:PHE:CE2	19:S:41:GLY:HA3	2.50	0.47
35:JA:43:ASP:OD2	35:JA:46:LYS:HB2	2.13	0.47
39:NA:33:TYR:HE2	39:NA:78:GLU:HG3	1.80	0.47
52:AB:3:ARG:NH1	52:AB:8:GLY:O	2.47	0.47
1:DB:1347:G:N7	42:TC:10:ARG:NH2	2.62	0.47
2:EB:521:G:H2'	2:EB:522:G:C8	2.50	0.47
2:EB:953:A:O2'	2:EB:954:G:H5'	2.14	0.47
2:EB:1156:A:OP1	18:UB:55:ARG:NH1	2.47	0.47
2:EB:1339:G:H5''	21:XB:16:LYS:HD3	1.96	0.47
2:EB:1415:U:O2'	2:EB:1417:C:OP1	2.26	0.47
2:EB:2418:A:H2'	2:EB:2419:U:O4'	2.14	0.47
5:HB:148:GLU:HB2	5:HB:151:LYS:HD2	1.97	0.47
8:KB:41:GLN:HE21	8:KB:43:LEU:HD21	1.79	0.47
14:QB:21:THR:HA	14:QB:98:LYS:HB2	1.96	0.47
22:YB:89:PHE:O	22:YB:91:GLU:N	2.47	0.47
25:BC:83:GLU:OE2	25:BC:83:GLU:N	2.47	0.47
37:OC:155:LEU:O	37:OC:159:ARG:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:QC:26:ILE:O	39:QC:30:LEU:HG	2.14	0.47
48:ZC:35:ARG:NH1	48:ZC:35:ARG:CG	2.74	0.47
1:A:38:G:C2	1:A:397:A:C2	3.02	0.47
1:A:1004:A:H5''	1:A:1024:G:H22	1.80	0.47
1:A:1301:U:H2'	1:A:1303:C:C5	2.49	0.47
2:B:619:G:H5''	2:B:620:G:OP2	2.15	0.47
2:B:1675:C:H2'	2:B:1676:A:O4'	2.15	0.47
2:B:1789:A:OP2	5:E:222:ARG:NH1	2.48	0.47
8:H:41:GLN:HE21	8:H:43:LEU:HD21	1.79	0.47
11:K:138:LEU:HD23	11:K:139:GLU:N	2.29	0.47
20:T:88:ARG:HG3	20:T:94:ASP:OD2	2.14	0.47
39:NA:15:ASP:O	39:NA:19:LEU:HB2	2.14	0.47
39:NA:22:GLU:OE1	39:NA:82:ARG:NH2	2.46	0.47
42:QA:27:THR:HG23	42:QA:62:TYR:HA	1.96	0.47
49:XA:12:LYS:HG2	49:XA:13:HIS:CD2	2.50	0.47
1:DB:38:G:C2	1:DB:397:A:C2	3.02	0.47
1:DB:296:U:H2'	1:DB:297:G:C8	2.49	0.47
1:DB:976:G:O5'	1:DB:1358:U:O2'	2.32	0.47
2:EB:1766:U:H2'	2:EB:1767:C:H6	1.79	0.47
7:JB:13:SER:HB3	7:JB:16:GLY:O	2.14	0.47
13:PB:138:LEU:HD23	13:PB:145:PRO:HB3	1.96	0.47
20:WB:11:ARG:NH1	20:WB:99:ARG:O	2.46	0.47
30:GC:8:LYS:HB2	30:GC:54:ILE:HG12	1.97	0.47
30:GC:19:ARG:HG3	30:GC:19:ARG:NH1	2.28	0.47
36:NC:55:VAL:HG22	36:NC:68:VAL:HG13	1.96	0.47
37:OC:127:THR:HG23	37:OC:147:ALA:HB3	1.97	0.47
37:OC:196:LEU:HB3	37:OC:198:VAL:HG12	1.97	0.47
39:QC:18:GLN:HG3	39:QC:21:LEU:HD23	1.96	0.47
39:QC:30:LEU:HD23	39:QC:75:LEU:HD11	1.95	0.47
40:RC:70:LYS:HA	40:RC:71:PRO:HD3	1.68	0.47
46:XC:11:ARG:HH12	46:XC:46:LYS:HD2	1.78	0.47
55:GD:138:TYR:HE1	55:GD:338:ASP:OD2	1.97	0.47
55:HD:134:MET:HG3	55:HD:337:LEU:HD21	1.96	0.47
1:A:67:C:H2'	1:A:68:G:C8	2.49	0.47
1:A:262:A:H2'	1:A:263:A:C8	2.49	0.47
1:A:1427:U:H2'	1:A:1428:A:H8	1.76	0.47
2:B:1009:A:OP2	2:B:1010:A:OP2	2.32	0.47
2:B:1791:A:H3'	2:B:1792:G:H8	1.79	0.47
2:B:2529:G:OP2	2:B:2530:A:H8	1.97	0.47
14:N:27:VAL:HA	14:N:105:GLU:OE2	2.14	0.47
19:S:85:LYS:NZ	19:S:85:LYS:CB	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:90:LEU:HB2	22:V:96:ILE:HG23	1.96	0.47
36:KA:131:ARG:NH1	36:KA:135:LYS:HE3	2.23	0.47
40:OA:78:ARG:HG2	40:OA:79:ARG:HG2	1.96	0.47
1:DB:299:G:H2'	1:DB:300:A:C8	2.49	0.47
1:DB:850:U:H2'	1:DB:851:G:C8	2.49	0.47
2:EB:1025:G:C4	2:EB:1135:C:H1'	2.49	0.47
7:JB:158:THR:O	7:JB:164:ARG:HD2	2.15	0.47
9:LB:25:LYS:HG2	9:LB:34:GLU:HG3	1.95	0.47
10:MB:60:GLU:HG3	10:MB:61:ARG:NH1	2.04	0.47
31:HC:26:GLY:O	31:HC:30:VAL:HG23	2.14	0.47
37:OC:108:LEU:HD22	37:OC:176:LEU:HD13	1.96	0.47
38:PC:9:LYS:HB2	38:PC:112:LEU:HD11	1.97	0.47
46:XC:39:ILE:HD12	46:XC:56:LEU:HD22	1.97	0.47
1:A:983:A:OP1	47:VA:6:LEU:HD21	2.14	0.47
1:A:1309:G:N7	46:UA:99:ARG:NH2	2.63	0.47
2:B:223:A:HO2'	2:B:420:C:HO2'	1.52	0.47
2:B:2689:U:P	2:B:2719:G:H22	2.37	0.47
14:N:65:PHE:HB2	14:N:105:GLU:HB2	1.96	0.47
30:DA:13:CYS:HB2	30:DA:16:CYS:HB3	1.95	0.47
39:NA:67:MET:HG3	39:NA:68:PRO:HD2	1.96	0.47
39:NA:100:ASN:HA	51:ZA:23:LYS:HZ1	1.79	0.47
44:SA:43:SER:HB2	44:SA:68:ALA:HB2	1.97	0.47
46:UA:3:ARG:HH11	46:UA:8:GLU:HG3	1.80	0.47
1:DB:1087:G:N1	1:DB:1088:G:O6	2.47	0.47
2:EB:197:A:N6	2:EB:2430:A:H2'	2.30	0.47
2:EB:455:C:N3	2:EB:472:A:H2'	2.29	0.47
2:EB:578:A:OP1	2:EB:1255:U:O2'	2.27	0.47
2:EB:1585:C:H4'	2:EB:1586:A:OP2	2.14	0.47
2:EB:1863:G:H1	2:EB:1879:C:H42	1.61	0.47
2:EB:2319:G:H22	16:SB:3:ARG:CZ	2.27	0.47
2:EB:2529:G:OP2	2:EB:2530:A:H8	1.97	0.47
2:EB:2697:G:C2	2:EB:2711:A:C2	3.03	0.47
5:HB:75:ILE:O	5:HB:118:VAL:HG23	2.14	0.47
18:UB:83:LEU:CD1	18:UB:113:ALA:HB2	2.44	0.47
31:HC:9:ARG:NH2	31:HC:47:ARG:HD3	2.29	0.47
42:TC:23:ASN:ND2	42:TC:25:LYS:HE2	2.27	0.47
55:GD:109:ARG:HH12	55:GD:210:PRO:HG3	1.80	0.47
55:GD:130:ASP:HB3	55:GD:333:MET:HE1	1.95	0.47
55:GD:139:ALA:HA	55:GD:144:TRP:HE3	1.78	0.47
1:A:87:A:H5''	1:A:88:C:C6	2.50	0.47
1:A:444:C:H2'	1:A:445:G:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:U:H5''	49:XA:38:TYR:CD2	2.50	0.47
1:A:860:A:H2'	1:A:861:G:O4'	2.15	0.47
1:A:978:A:O2'	1:A:1322:C:N3	2.46	0.47
1:A:1097:C:H2'	1:A:1098:C:C6	2.49	0.47
1:A:1240:U:OP1	40:OA:119:ARG:NH2	2.47	0.47
2:B:320:A:H4'	2:B:322:A:C8	2.50	0.47
2:B:1270:C:O2'	2:B:1648:C:OP2	2.29	0.47
2:B:1553:A:HO2'	2:B:1554:A:H8	1.62	0.47
2:B:2336:A:H3'	2:B:2337:G:H8	1.79	0.47
2:B:2478:A:H2'	2:B:2479:G:O4'	2.15	0.47
2:B:2713:A:H3'	2:B:2714:G:H5''	1.97	0.47
2:B:2836:U:C4	2:B:2883:A:N6	2.83	0.47
4:D:10:G:H2'	4:D:11:A:H8	1.79	0.47
4:D:67:C:H2'	4:D:68:C:C6	2.50	0.47
9:I:3:ARG:HH21	9:I:5:GLY:H	1.63	0.47
11:K:35:ARG:HG2	11:K:35:ARG:NH1	2.30	0.47
16:P:76:LYS:O	16:P:80:LEU:HD13	2.15	0.47
22:V:2:ARG:H	22:V:2:ARG:HD3	1.79	0.47
28:BA:13:ARG:HH11	28:BA:21:VAL:HG11	1.80	0.47
28:BA:59:PHE:HA	52:AB:67:VAL:HG21	1.97	0.47
34:HA:22:A:H62	55:GD:196:ILE:HG22	1.80	0.47
38:MA:144:THR:HG23	38:MA:147:ASP:H	1.80	0.47
40:OA:20:ASP:HB3	40:OA:23:VAL:HG23	1.97	0.47
41:PA:23:SER:HA	41:PA:63:LEU:HD23	1.97	0.47
42:QA:5:TYR:CE1	42:QA:16:ARG:HB2	2.50	0.47
43:RA:91:PRO:O	43:RA:94:VAL:HG22	2.14	0.47
47:VA:53:LEU:HD23	47:VA:54:PRO:HD2	1.97	0.47
52:AB:29:ARG:NH1	52:AB:29:ARG:HA	2.30	0.47
1:DB:87:A:H5''	1:DB:88:C:C6	2.50	0.47
1:DB:537:G:H5''	45:WC:113:ARG:NH1	2.30	0.47
1:DB:626:U:H5''	49:AD:38:TYR:CD2	2.50	0.47
1:DB:1297:C:OP1	46:XC:13:LYS:HE3	2.15	0.47
1:DB:1309:G:N7	46:XC:99:ARG:NH2	2.63	0.47
1:DB:1475:G:H4'	2:EB:1689:A:H4'	1.96	0.47
1:DB:1530:G:H2'	1:DB:1531:A:H5''	1.97	0.47
2:EB:251:A:OP1	13:PB:50:ARG:NH2	2.48	0.47
2:EB:478:A:C6	2:EB:480:A:C6	3.03	0.47
2:EB:657:U:H2'	2:EB:658:C:C6	2.50	0.47
2:EB:911:A:H2'	14:QB:9:TYR:OH	2.15	0.47
2:EB:1288:U:C2	2:EB:1327:C:O2	2.67	0.47
2:EB:2498:C:O2'	2:EB:2499:C:H5'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:KB:182:LYS:HE2	8:KB:182:LYS:HB2	1.67	0.47
9:LB:9:ILE:HG12	9:LB:69:ARG:CZ	2.44	0.47
18:UB:82:GLY:HA3	18:UB:113:ALA:HB1	1.97	0.47
20:WB:88:ARG:HG3	20:WB:94:ASP:OD2	2.15	0.47
22:YB:45:VAL:O	22:YB:62:GLU:HA	2.15	0.47
22:YB:76:CYS:SG	22:YB:78:ALA:HB3	2.54	0.47
22:YB:99:CYS:SG	22:YB:100:ALA:N	2.87	0.47
25:BC:21:ARG:CG	25:BC:21:ARG:NH1	2.76	0.47
26:CC:32:LEU:HB2	26:CC:53:LEU:HD12	1.96	0.47
28:EC:13:ARG:HH11	28:EC:21:VAL:HG11	1.78	0.47
35:MC:84:GLU:O	35:MC:219:VAL:HG21	2.15	0.47
35:MC:145:LEU:HD23	35:MC:149:LEU:HD13	1.96	0.47
38:PC:12:LEU:HB3	38:PC:31:LEU:HB2	1.95	0.47
41:SC:78:GLN:HG3	41:SC:80:ILE:H	1.79	0.47
42:TC:48:GLU:OE2	42:TC:51:ARG:HD2	2.13	0.47
44:VC:23:ALA:HB1	44:VC:88:GLY:HA3	1.97	0.47
46:XC:24:GLY:HA2	46:XC:70:LEU:HD12	1.97	0.47
1:A:42:G:H1	1:A:400:C:H42	1.63	0.47
1:A:359:U:H2'	1:A:360:A:H8	1.80	0.47
1:A:370:C:C2	1:A:392:G:C2	3.03	0.47
1:A:1402:4OC:H2'	1:A:1403:C:O4'	2.15	0.47
2:B:108:U:H2'	2:B:109:G:C8	2.50	0.47
2:B:579:G:H2'	2:B:580:C:C6	2.50	0.47
2:B:751:A:C6	2:B:789:A:C5	3.03	0.47
2:B:1818:U:H2'	5:E:157:ARG:HG3	1.97	0.47
8:H:32:PRO:HA	8:H:162:THR:OG1	2.15	0.47
16:P:54:LEU:O	16:P:57:LYS:NZ	2.33	0.47
18:R:82:GLY:HA3	18:R:113:ALA:HB1	1.97	0.47
20:T:57:ASN:HA	20:T:61:ASN:HD22	1.80	0.47
23:W:11:GLU:HB3	23:W:12:GLY:H	1.43	0.47
23:W:124:ILE:HG23	23:W:126:VAL:HG23	1.97	0.47
28:BA:61:ARG:NH1	28:BA:62:ARG:HH22	2.12	0.47
33:GA:2:LYS:NZ	33:GA:4:ARG:HE	2.12	0.47
37:LA:59:ARG:NH2	37:LA:66:ARG:NH1	2.63	0.47
48:WA:33:THR:HG23	48:WA:63:ARG:NH1	2.30	0.47
1:DB:523:A:N1	45:WC:92:0TD:H6	2.30	0.47
1:DB:555:C:H2'	1:DB:556:C:C6	2.50	0.47
1:DB:1147:C:HO2'	42:TC:5:TYR:HH	1.62	0.47
2:EB:445:C:O2'	2:EB:446:G:H5'	2.15	0.47
2:EB:705:A:H1'	5:HB:9:TYR:CE2	2.50	0.47
2:EB:1029:A:H5''	2:EB:1030:G:OP2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EB:1187:G:H5''	19:VB:81:TYR:CE1	2.49	0.47
2:EB:1971:A:N3	5:HB:241:PRO:HD3	2.30	0.47
2:EB:2565:A:H5''	2:EB:2566:A:OP2	2.14	0.47
2:EB:2627:G:O2'	2:EB:2781:A:N1	2.43	0.47
3:FB:112:G:H2'	3:FB:113:C:H6	1.78	0.47
18:UB:34:LYS:HD2	18:UB:34:LYS:HA	1.50	0.47
35:MC:15:VAL:HG21	35:MC:213:LEU:HG	1.95	0.47
47:YC:53:LEU:HD23	47:YC:54:PRO:HD2	1.95	0.47
2:B:247:G:H4'	2:B:386:G:C5	2.50	0.47
2:B:1210:A:C8	2:B:1212:G:C2	3.02	0.47
2:B:2784:C:H2'	2:B:2785:C:H6	1.80	0.47
5:E:223:GLY:HA2	5:E:226:MET:HG3	1.96	0.47
8:H:50:ALA:C	8:H:52:ILE:H	2.18	0.47
8:H:171:ALA:O	8:H:175:LEU:HG	2.14	0.47
9:I:38:SER:OG	9:I:40:GLU:OE2	2.32	0.47
35:JA:155:LEU:HA	35:JA:157:ARG:HH21	1.80	0.47
1:DB:67:C:H2'	1:DB:68:G:C8	2.50	0.47
1:DB:524:G:H2'	1:DB:525:C:C6	2.50	0.47
1:DB:920:U:H2'	1:DB:921:U:C6	2.50	0.47
1:DB:1009:G:H2'	1:DB:1010:G:H8	1.80	0.47
1:DB:1531:A:H5'	1:DB:1532:U:O2	2.14	0.47
2:EB:729:G:H2'	2:EB:1775:U:H1'	1.96	0.47
2:EB:1537:C:H3'	2:EB:1538:G:C8	2.46	0.47
21:XB:5:TYR:HE1	26:CC:30:ARG:NH1	2.11	0.47
30:GC:13:CYS:HB2	30:GC:16:CYS:HB3	1.96	0.47
38:PC:144:THR:HG23	38:PC:147:ASP:H	1.79	0.47
47:YC:40:CYS:SG	47:YC:43:CYS:SG	3.12	0.47
55:HD:195:ARG:HH21	55:HD:197:HIS:HE1	1.61	0.47
1:A:255:G:H2'	1:A:256:U:C6	2.50	0.47
1:A:1329:A:P	46:UA:28:ALA:HB3	2.54	0.47
2:B:185:U:H2'	2:B:186:G:C8	2.50	0.47
2:B:839:U:H3	2:B:939:G:H1	1.63	0.47
2:B:2376:A:N6	16:P:89:ARG:HD3	2.29	0.47
2:B:2880:C:O2'	15:O:90:ARG:HD3	2.14	0.47
3:C:85:G:H1	3:C:91:C:N4	2.13	0.47
3:C:112:G:H2'	3:C:113:C:H6	1.80	0.47
6:F:11:MET:HG2	6:F:24:THR:HA	1.96	0.47
10:J:57:ARG:O	10:J:61:ARG:NH2	2.48	0.47
11:K:66:LYS:O	11:K:70:LYS:HB3	2.15	0.47
35:JA:160:ASP:OD1	35:JA:160:ASP:N	2.47	0.47
39:NA:35:ALA:HB1	39:NA:65:VAL:CG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DB:404:U:H2'	1:DB:405:U:C6	2.50	0.47
2:EB:300:A:OP2	22:YB:86:ARG:NH2	2.48	0.47
2:EB:448:U:O4	2:EB:583:G:H1'	2.15	0.47
2:EB:1592:C:H2'	2:EB:1593:G:H8	1.80	0.47
2:EB:2021:C:OP1	29:FC:12:SER:OG	2.24	0.47
2:EB:2494:G:O2'	14:QB:80:GLU:HA	2.15	0.47
2:EB:2637:U:OP1	6:IB:82:ARG:NH1	2.48	0.47
23:ZB:163:LEU:HD12	23:ZB:163:LEU:H	1.80	0.47
37:OC:191:ARG:HH21	37:OC:200:GLU:CG	2.25	0.47
38:PC:70:PRO:HB2	38:PC:77:PRO:HG3	1.96	0.47
39:QC:6:VAL:HG22	39:QC:90:VAL:HG22	1.97	0.47
39:QC:62:TRP:CH2	39:QC:64:GLN:HB2	2.50	0.47
1:A:60:A:H4'	1:A:61:G:H5'	1.96	0.46
1:A:93:U:H2'	1:A:95:G:C8	2.50	0.46
1:A:404:U:H2'	1:A:405:U:H6	1.80	0.46
1:A:1095:U:H5''	1:A:1109:C:O2	2.15	0.46
2:B:444:C:H4'	7:G:49:ALA:HB2	1.98	0.46
2:B:827:U:H2'	2:B:2068:U:C2	2.50	0.46
2:B:921:G:H2'	2:B:922:U:O4'	2.15	0.46
2:B:1204:A:H61	2:B:1240:U:H2'	1.80	0.46
2:B:1784:A:H4'	2:B:1785:A:H5''	1.97	0.46
2:B:1815:A:OP2	5:E:54:ARG:NH2	2.49	0.46
2:B:2023:G:H4'	2:B:2617:C:O3'	2.14	0.46
2:B:2113:U:H2'	2:B:2114:A:C8	2.50	0.46
3:C:12:C:OP2	3:C:12:C:H6	1.98	0.46
5:E:85:ASP:OD1	5:E:86:PRO:HD2	2.16	0.46
5:E:132:PRO:HG3	5:E:190:TYR:CE2	2.50	0.46
7:G:107:LYS:HD3	7:G:107:LYS:HA	1.73	0.46
20:T:68:ARG:NH1	20:T:111:HIS:HA	2.30	0.46
25:Y:15:ALA:O	25:Y:40:ARG:HG3	2.14	0.46
39:NA:6:VAL:HG22	39:NA:90:VAL:HG22	1.97	0.46
48:WA:26:GLU:HG2	48:WA:81:LEU:HD22	1.95	0.46
1:DB:42:G:H1	1:DB:400:C:H42	1.64	0.46
1:DB:424:G:OP2	1:DB:424:G:H8	1.99	0.46
1:DB:584:G:H2'	1:DB:585:G:C8	2.50	0.46
1:DB:781:A:H4'	1:DB:1522:U:O2'	2.15	0.46
1:DB:1327:C:OP1	54:FD:20:LYS:HB3	2.16	0.46
2:EB:938:G:H2'	2:EB:939:G:H8	1.79	0.46
2:EB:2023:G:H4'	2:EB:2617:C:O3'	2.15	0.46
3:FB:1:U:OP2	3:FB:1:U:H6	1.98	0.46
6:IB:111:ARG:HD3	6:IB:160:TYR:HD2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:JB:170:LEU:HB2	7:JB:173:VAL:HB	1.97	0.46
12:OB:17:ARG:HD2	12:OB:45:GLU:OE1	2.15	0.46
13:PB:19:VAL:HB	13:PB:31:ALA:HB1	1.97	0.46
14:QB:75:THR:HA	14:QB:89:ASN:O	2.16	0.46
17:TB:36:GLU:HG3	17:TB:41:ARG:HE	1.80	0.46
27:DC:3:ARG:NH1	27:DC:60:GLU:HG3	2.30	0.46
37:OC:70:ILE:HD11	37:OC:100:ARG:NH1	2.30	0.46
41:SC:103:VAL:HG21	41:SC:109:ILE:C	2.36	0.46
50:BD:69:LYS:O	50:BD:70:ARG:HD2	2.15	0.46
51:CD:53:ARG:HH21	51:CD:60:ALA:N	2.12	0.46
53:ED:63:ILE:HD12	53:ED:81:LYS:HG2	1.96	0.46
1:A:424:G:H8	1:A:424:G:OP2	1.98	0.46
1:A:737:A:H2'	1:A:738:C:C6	2.50	0.46
1:A:1297:C:OP1	46:UA:13:LYS:HE3	2.14	0.46
2:B:253:C:H2'	2:B:254:G:O4'	2.14	0.46
2:B:1155:A:O3'	18:R:55:ARG:NH1	2.49	0.46
2:B:2141:G:N1	2:B:2142:C:O2	2.48	0.46
2:B:2498:C:O2'	2:B:2499:C:H5'	2.15	0.46
2:B:2591:C:H2'	2:B:2592:G:C8	2.51	0.46
10:J:87:LYS:HE2	10:J:89:TYR:CD1	2.50	0.46
13:M:59:LEU:HD11	32:FA:10:ALA:HA	1.97	0.46
18:R:83:LEU:CD1	18:R:113:ALA:HB2	2.45	0.46
22:V:46:LYS:HG2	22:V:60:PHE:CD1	2.51	0.46
28:BA:61:ARG:NH1	28:BA:62:ARG:NH2	2.63	0.46
37:LA:98:GLU:HG3	37:LA:194:LEU:HD22	1.97	0.46
1:DB:999:U:H1'	1:DB:1042:G:N2	2.29	0.46
1:DB:1245:A:H2'	1:DB:1246:C:C6	2.50	0.46
1:DB:1415:G:H2'	1:DB:1416:G:C8	2.50	0.46
1:DB:1512:U:H2'	1:DB:1513:A:C8	2.50	0.46
2:EB:747:U:O2	2:EB:2014:A:H1'	2.15	0.46
2:EB:848:G:O6	2:EB:929:G:H2'	2.15	0.46
2:EB:1047:G:H2'	2:EB:1110:G:H1	1.80	0.46
2:EB:1359:A:H2	2:EB:1372:U:O4	1.98	0.46
2:EB:1943:U:OP1	55:HD:277:ARG:NH2	2.41	0.46
2:EB:2085:C:O3'	5:HB:262:ARG:NH1	2.48	0.46
2:EB:2094:G:P	10:MB:22:LYS:NZ	2.88	0.46
2:EB:2591:C:H2'	2:EB:2592:G:C8	2.50	0.46
2:EB:2648:C:H2'	2:EB:2649:U:H6	1.80	0.46
2:EB:2818:G:O2'	2:EB:2819:G:H5'	2.15	0.46
11:NB:66:LYS:O	11:NB:70:LYS:HB3	2.15	0.46
27:DC:9:VAL:HG11	27:DC:55:ARG:HH11	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:JC:4:ARG:NH1	33:JC:8:LYS:NZ	2.63	0.46
35:MC:7:VAL:HG21	35:MC:221:LEU:HD21	1.98	0.46
36:NC:6:HIS:HD2	36:NC:8:ILE:H	1.62	0.46
39:QC:15:ASP:OD2	39:QC:18:GLN:HB3	2.15	0.46
55:GD:299:GLY:H	55:GD:306:ARG:HH22	1.64	0.46
1:A:677:U:H1'	44:SA:119:CYS:SG	2.56	0.46
1:A:1095:U:OP1	1:A:1108:G:N2	2.36	0.46
1:A:1105:A:H2'	1:A:1106:G:H8	1.80	0.46
1:A:1152:A:H2'	1:A:1153:C:C6	2.51	0.46
1:A:1226:C:H4'	52:AB:80:TYR:CZ	2.51	0.46
2:B:263:C:H2'	2:B:264:C:O4'	2.15	0.46
6:F:111:ARG:N	6:F:111:ARG:HD2	2.30	0.46
10:J:61:ARG:HA	10:J:61:ARG:HH11	1.81	0.46
10:J:62:LYS:O	10:J:66:GLU:HB2	2.15	0.46
31:EA:9:ARG:NH2	31:EA:47:ARG:HD3	2.30	0.46
31:EA:26:GLY:O	31:EA:30:VAL:HG23	2.16	0.46
39:NA:30:LEU:HD23	39:NA:75:LEU:HD11	1.96	0.46
40:OA:150:ALA:HA	44:SA:59:TYR:HB3	1.98	0.46
41:PA:101:PRO:HG2	41:PA:133:LEU:HD11	1.96	0.46
1:DB:96:G:C6	1:DB:97:U:C4	3.03	0.46
1:DB:428:G:O4'	1:DB:430:A:C8	2.69	0.46
1:DB:673:G:H2'	1:DB:674:G:C8	2.49	0.46
2:EB:639:U:H2'	2:EB:640:C:C6	2.50	0.46
2:EB:880:G:H1	2:EB:897:C:H42	1.63	0.46
2:EB:929:G:H8	2:EB:929:G:O5'	1.99	0.46
2:EB:1093:G:H1	2:EB:1097:U:H5	1.63	0.46
2:EB:1914:C:O3'	55:HD:116:ARG:NH1	2.48	0.46
2:EB:2071:A:H2'	2:EB:2072:G:C8	2.50	0.46
15:RB:13:HIS:CE1	15:RB:16:HIS:HB2	2.50	0.46
23:ZB:102:LEU:HD21	23:ZB:124:ILE:HG22	1.98	0.46
23:ZB:124:ILE:HG23	23:ZB:126:VAL:HG23	1.98	0.46
25:BC:40:ARG:HH22	25:BC:42:GLN:HG2	1.78	0.46
35:MC:118:LEU:HD21	35:MC:138:LEU:HD22	1.96	0.46
35:MC:219:VAL:O	35:MC:222:ILE:HB	2.16	0.46
37:OC:10:ARG:HG3	37:OC:11:LEU:HD12	1.97	0.46
38:PC:75:THR:OG1	38:PC:76:ILE:N	2.48	0.46
44:VC:121:PRO:HG2	44:VC:126:ARG:HB2	1.97	0.46
55:HD:299:GLY:H	55:HD:306:ARG:HH22	1.63	0.46
1:A:1500:A:H5''	1:A:1508:G:H5''	1.98	0.46
2:B:547:A:H5''	2:B:548:A:OP2	2.16	0.46
2:B:603:A:N7	2:B:655:A:C5	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:628:G:H2'	2:B:629:G:C8	2.50	0.46
2:B:848:G:O6	2:B:929:G:H2'	2.16	0.46
2:B:1477:A:H2'	2:B:1478:G:O4'	2.15	0.46
3:C:8:U:O3'	16:P:25:ARG:NH2	2.37	0.46
5:E:176:ARG:HG3	5:E:182:LEU:HD12	1.98	0.46
5:E:257:LEU:HD12	5:E:258:LYS:N	2.31	0.46
6:F:54:GLN:OE1	6:F:55:ASN:N	2.43	0.46
9:I:3:ARG:HG2	9:I:6:ARG:NH1	2.31	0.46
17:Q:36:GLU:CG	17:Q:41:ARG:HE	2.28	0.46
22:V:79:CYS:SG	22:V:81:LYS:HB2	2.55	0.46
36:KA:33:LEU:HA	36:KA:36:ASP:HB3	1.96	0.46
37:LA:25:ARG:C	37:LA:27:TYR:H	2.16	0.46
39:NA:12:PRO:HG2	39:NA:13:ASN:HD22	1.80	0.46
41:PA:91:ARG:HB2	45:TA:7:ILE:HG12	1.97	0.46
1:DB:60:A:H4'	1:DB:61:G:H5'	1.98	0.46
1:DB:748:C:H1'	1:DB:749:C:OP2	2.16	0.46
1:DB:926:G:N2	34:KC:15:A:H5''	2.30	0.46
1:DB:1004:A:H5''	1:DB:1024:G:N2	2.30	0.46
1:DB:1130:A:H2'	1:DB:1131:G:H8	1.81	0.46
2:EB:17:G:H4'	18:UB:25:TRP:HE1	1.79	0.46
2:EB:2336:A:H3'	2:EB:2337:G:H8	1.81	0.46
2:EB:2846:G:H2'	2:EB:2847:U:O4'	2.16	0.46
3:FB:6:C:H2'	3:FB:7:G:C8	2.50	0.46
7:JB:192:LEU:HD22	7:JB:194:MET:HG3	1.96	0.46
7:JB:195:ASP:HB3	7:JB:198:ALA:HB3	1.97	0.46
8:KB:50:ALA:C	8:KB:52:ILE:H	2.19	0.46
9:LB:58:GLU:HG2	9:LB:61:HIS:HB2	1.97	0.46
9:LB:72:ILE:O	9:LB:76:VAL:HG23	2.15	0.46
51:CD:22:VAL:HG23	51:CD:55:ARG:O	2.16	0.46
1:A:753:A:H5'	1:A:754:C:C5	2.50	0.46
1:A:1004:A:H5''	1:A:1024:G:N2	2.31	0.46
1:A:1043:C:H2'	1:A:1044:A:O4'	2.16	0.46
2:B:38:A:H2'	2:B:39:C:C6	2.50	0.46
2:B:1583:A:H5'	2:B:1585:C:H5''	1.97	0.46
2:B:2319:G:H22	16:P:3:ARG:CZ	2.29	0.46
2:B:2401:U:H2'	2:B:2402:C:O4'	2.16	0.46
2:B:2582:G:N2	2:B:2583:G:H1'	2.30	0.46
2:B:2607:G:H2'	2:B:2608:G:O4'	2.16	0.46
5:E:75:ILE:O	5:E:118:VAL:HG23	2.15	0.46
5:E:80:ALA:HB3	5:E:94:LEU:HB3	1.98	0.46
8:H:77:ILE:HG22	8:H:80:PHE:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:125:VAL:HG22	9:I:131:VAL:HG22	1.98	0.46
22:V:43:ASN:HD22	22:V:65:ALA:HB3	1.81	0.46
23:W:102:LEU:HD21	23:W:124:ILE:HG22	1.98	0.46
25:Y:98:LEU:HD23	25:Y:98:LEU:OXT	2.14	0.46
32:FA:52:LYS:HB3	32:FA:53:PRO:HD3	1.97	0.46
35:JA:10:LEU:HA	35:JA:12:GLU:OE1	2.15	0.46
37:LA:134:ASP:C	37:LA:135:LEU:HD13	2.36	0.46
53:BB:63:ILE:HD12	53:BB:81:LYS:HG2	1.98	0.46
1:DB:105:G:C5	1:DB:106:C:C4	3.04	0.46
1:DB:622:A:C8	1:DB:623:C:C6	3.03	0.46
1:DB:1468:A:H2'	1:DB:1469:G:O4'	2.15	0.46
2:EB:361:G:C2	2:EB:362:U:C5	3.03	0.46
2:EB:784:A:C6	5:HB:229:VAL:HG21	2.51	0.46
2:EB:1367:A:N7	2:EB:1368:G:H1'	2.31	0.46
4:GB:22:G:H2'	4:GB:23:C:C6	2.51	0.46
13:PB:122:PRO:HB3	13:PB:141:ALA:O	2.15	0.46
15:RB:55:ALA:HA	15:RB:80:PHE:CE2	2.51	0.46
55:GD:137:ARG:NH1	55:GD:334:GLU:HG3	2.31	0.46
55:GD:139:ALA:HA	55:GD:144:TRP:CE3	2.50	0.46
55:GD:181:GLY:O	55:GD:307:ASN:HB2	2.16	0.46
1:A:1298:C:C4	40:OA:114:ARG:HD2	2.51	0.46
2:B:347:A:H2'	2:B:348:G:C8	2.50	0.46
2:B:587:C:C6	2:B:671:C:H1'	2.51	0.46
5:E:5:LYS:HD2	5:E:5:LYS:HA	1.59	0.46
5:E:155:LEU:HD22	5:E:155:LEU:H	1.81	0.46
5:E:206:LEU:HD23	5:E:206:LEU:HA	1.52	0.46
8:H:114:ILE:HD11	8:H:117:PHE:CG	2.51	0.46
9:I:13:LYS:HA	9:I:14:GLY:HA2	1.60	0.46
13:M:97:PRO:HA	13:M:100:LEU:HD12	1.98	0.46
14:N:58:PHE:HB3	14:N:113:GLN:NE2	2.31	0.46
19:S:29:PRO:HA	19:S:61:VAL:HG22	1.97	0.46
35:JA:84:GLU:O	35:JA:219:VAL:HG21	2.15	0.46
36:KA:88:ARG:HD3	36:KA:101:LEU:HB3	1.98	0.46
38:MA:75:THR:OG1	38:MA:76:ILE:N	2.49	0.46
38:MA:137:GLU:OE2	38:MA:137:GLU:HA	2.16	0.46
43:RA:9:ARG:HA	43:RA:68:HIS:O	2.15	0.46
44:SA:79:SER:HA	44:SA:104:GLN:HB3	1.96	0.46
45:TA:125:PRO:HB2	45:TA:126:LYS:H	1.60	0.46
50:YA:48:GLU:OE2	50:YA:48:GLU:N	2.38	0.46
51:ZA:22:VAL:HG23	51:ZA:55:ARG:O	2.16	0.46
1:DB:1043:C:H2'	1:DB:1044:A:O4'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DB:1107:C:OP1	36:NC:172:ARG:HB2	2.15	0.46
2:EB:363(G):A:OP2	2:EB:363(G):A:H8	1.99	0.46
2:EB:811:U:C2	2:EB:1251:C:C5	3.03	0.46
2:EB:1027:A:C2	2:EB:2488:A:H5'	2.51	0.46
2:EB:1385:G:O2'	2:EB:1396:U:O2	2.29	0.46
2:EB:1590:U:H2'	2:EB:1591:G:C8	2.50	0.46
2:EB:1674:G:N2	2:EB:1677:A:N1	2.59	0.46
2:EB:2059:A:H2'	2:EB:2503:2MA:HM23	1.98	0.46
2:EB:2113:U:H2'	2:EB:2114:A:C8	2.50	0.46
10:MB:110:ASP:HA	10:MB:111:PRO:HD2	1.76	0.46
13:PB:84:ASN:OD1	13:PB:117:GLU:HB2	2.15	0.46
16:SB:15:ARG:NH1	16:SB:15:ARG:HG2	2.30	0.46
25:BC:82:LEU:O	25:BC:85:LEU:HD13	2.16	0.46
26:CC:48:HIS:CE1	26:CC:49:LYS:HG3	2.51	0.46
36:NC:3:ASN:N	36:NC:3:ASN:OD1	2.49	0.46
38:PC:48:ALA:O	38:PC:50:GLU:N	2.49	0.46
41:SC:91:ARG:HB2	45:WC:7:ILE:HG12	1.96	0.46
41:SC:102:ARG:H	41:SC:102:ARG:HD2	1.80	0.46
1:A:419:C:H5''	1:A:513:C:O4'	2.16	0.46
1:A:841:U:H3'	1:A:842:C:H5''	1.98	0.46
2:B:1043:C:C5	2:B:1044:G:C8	3.03	0.46
3:C:31:C:H4'	8:H:29:TRP:CH2	2.51	0.46
6:F:21:VAL:HG22	6:F:23:VAL:HG23	1.97	0.46
6:F:37:ARG:HD3	6:F:42:ASP:CG	2.36	0.46
9:I:25:LYS:HB3	9:I:27:LYS:HZ2	1.79	0.46
10:J:110:ASP:HA	10:J:111:PRO:HD2	1.76	0.46
14:N:75:THR:HG21	14:N:87:LYS:HZ3	1.79	0.46
30:DA:8:LYS:HB2	30:DA:54:ILE:HG12	1.96	0.46
1:DB:924:C:H5'	1:DB:1399:C:OP2	2.16	0.46
1:DB:1021:G:C2	1:DB:1022:G:H1'	2.50	0.46
2:EB:733:G:O6	2:EB:761:A:C8	2.69	0.46
2:EB:1798:U:H5'	5:HB:259:THR:OG1	2.15	0.46
2:EB:2301:C:H2'	2:EB:2302:G:C8	2.50	0.46
2:EB:2592:G:C6	2:EB:2593:U:N3	2.83	0.46
4:GB:28:C:H2'	4:GB:29:G:C8	2.51	0.46
5:HB:71:ASP:OD2	5:HB:72:LYS:N	2.43	0.46
8:KB:39:ILE:HD12	8:KB:157:ILE:HG12	1.98	0.46
8:KB:114:ILE:HD11	8:KB:117:PHE:CG	2.50	0.46
11:NB:35:ARG:HG2	11:NB:35:ARG:NH1	2.30	0.46
13:PB:84:ASN:HB3	13:PB:117:GLU:O	2.16	0.46
22:YB:90:LEU:HB2	22:YB:96:ILE:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:PC:7:GLU:O	38:PC:34:VAL:HA	2.16	0.46
41:SC:81:HIS:HB2	41:SC:138:TRP:HD1	1.81	0.46
46:XC:6:GLY:HA3	46:XC:67:GLU:HG3	1.97	0.46
54:FD:6:ARG:O	54:FD:12:LYS:HE3	2.15	0.46
1:A:96:G:C6	1:A:97:U:C4	3.03	0.46
2:B:27:G:N2	2:B:512:G:H1'	2.31	0.46
2:B:706:A:H2'	2:B:707:G:O4'	2.16	0.46
2:B:1299:G:H22	2:B:1640:C:H5''	1.81	0.46
2:B:1406:U:H2'	2:B:1407:C:C6	2.51	0.46
2:B:2096:U:H2'	2:B:2097:C:C6	2.51	0.46
2:B:2526:G:H1	2:B:2537:U:H3	1.64	0.46
2:B:2852:G:H2'	2:B:2853:C:C6	2.50	0.46
4:D:68:C:H2'	4:D:69:C:C6	2.51	0.46
10:J:68:LEU:O	10:J:71:ILE:HG13	2.16	0.46
26:Z:46:GLN:HB3	26:Z:48:HIS:CE1	2.50	0.46
27:AA:5:LYS:HD3	27:AA:34:GLU:OE2	2.16	0.46
36:KA:35:GLU:O	36:KA:39:ILE:HG12	2.15	0.46
38:MA:76:ILE:HG13	38:MA:93:PRO:HG3	1.97	0.46
42:QA:13:ALA:HB2	42:QA:68:GLY:HA3	1.97	0.46
44:SA:33:THR:HA	44:SA:39:PRO:HA	1.97	0.46
1:DB:110:C:O2'	49:AD:25:ARG:O	2.34	0.46
1:DB:339:C:H2'	1:DB:340:U:C6	2.51	0.46
1:DB:359:U:H2'	1:DB:360:A:H8	1.80	0.46
1:DB:1119:C:H2'	1:DB:1120:G:H8	1.81	0.46
2:EB:38:A:H2'	2:EB:39:C:H6	1.80	0.46
2:EB:90:U:H1'	2:EB:91:A:C8	2.50	0.46
2:EB:165:U:H2'	2:EB:171:G:O4'	2.16	0.46
2:EB:687:C:H5''	31:HC:2:LYS:HE2	1.96	0.46
2:EB:1335:U:H2'	2:EB:1336:A:C8	2.51	0.46
2:EB:1946:U:H2'	2:EB:1947:C:C6	2.51	0.46
14:QB:109:VAL:HG13	14:QB:113:GLN:HB3	1.98	0.46
26:CC:51:ARG:O	26:CC:55:ARG:HG2	2.16	0.46
40:RC:69:VAL:HG21	40:RC:104:LEU:HD21	1.98	0.46
41:SC:92:ARG:HB3	41:SC:94:TYR:CE2	2.50	0.46
44:VC:120:ARG:NH1	44:VC:126:ARG:NH1	2.60	0.46
51:CD:46:GLU:OE2	51:CD:85:LEU:HD12	2.15	0.46
55:GD:130:ASP:N	55:GD:130:ASP:OD1	2.46	0.46
1:A:1346:A:H5''	42:QA:120:ARG:NH1	2.30	0.46
1:A:1435:G:H2'	1:A:1436:U:C6	2.51	0.46
2:B:96:G:H4'	26:Z:48:HIS:CD2	2.50	0.46
2:B:922:U:H2'	2:B:923:C:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2495:G:OP1	14:N:82:ARG:HD2	2.15	0.46
2:B:2531:A:H61	2:B:2662:A:H61	1.64	0.46
5:E:263:ARG:HH11	5:E:263:ARG:HG2	1.81	0.46
7:G:195:ASP:HB3	7:G:198:ALA:HB3	1.98	0.46
8:H:135:LEU:HD13	8:H:135:LEU:HA	1.66	0.46
23:W:31:ARG:H	23:W:31:ARG:HG2	1.59	0.46
35:JA:7:VAL:HG21	35:JA:221:LEU:HD21	1.98	0.46
53:BB:47:GLY:HA2	53:BB:48:LYS:C	2.36	0.46
1:DB:177:C:H2'	1:DB:178:C:H6	1.80	0.46
1:DB:811:C:H4'	1:DB:900:A:N6	2.31	0.46
2:EB:150:C:H2'	2:EB:151:C:C6	2.51	0.46
2:EB:921:G:H2'	2:EB:922:U:O4'	2.15	0.46
2:EB:1153:C:OP1	18:UB:92:ARG:NH2	2.47	0.46
2:EB:1625:C:H2'	2:EB:1626:G:O4'	2.15	0.46
6:IB:11:MET:HG2	6:IB:24:THR:HA	1.96	0.46
10:MB:96:ASP:O	10:MB:100:ALA:N	2.43	0.46
23:ZB:95:PRO:CA	23:ZB:130:PRO:HD3	2.45	0.46
25:BC:46:LEU:HD23	25:BC:46:LEU:HA	1.73	0.46
35:MC:142:LEU:O	35:MC:146:GLN:HG3	2.16	0.46
35:MC:231:GLU:H	35:MC:232:PRO:HD2	1.81	0.46
36:NC:6:HIS:ND1	47:YC:49:HIS:HB3	2.30	0.46
45:WC:69:TYR:HB3	45:WC:99:HIS:HD2	1.81	0.46
51:CD:52:PRO:O	51:CD:56:THR:HG23	2.15	0.46
1:A:859:A:H2'	1:A:860:A:O4'	2.16	0.46
1:A:973:G:H1'	43:RA:54:PHE:CD1	2.51	0.46
2:B:16:G:H2'	2:B:17:G:H8	1.81	0.46
2:B:86:C:H4'	2:B:104:U:H1'	1.97	0.46
2:B:478:A:C6	2:B:480:A:C6	3.04	0.46
2:B:817:C:H4'	2:B:932:G:C5	2.51	0.46
2:B:1025:G:C4	2:B:1135:C:H1'	2.51	0.46
2:B:1047:G:H2'	2:B:1110:G:H22	1.80	0.46
2:B:1057:A:N6	2:B:1059:G:N7	2.64	0.46
2:B:1625:C:H2'	2:B:1626:G:O4'	2.15	0.46
2:B:1754:C:P	17:Q:96:ARG:HH12	2.38	0.46
2:B:1790:C:O2'	5:E:209:ALA:HB2	2.16	0.46
9:I:43:VAL:HA	9:I:52:VAL:HG12	1.98	0.46
15:O:13:HIS:CE1	15:O:16:HIS:HB2	2.51	0.46
15:O:26:LYS:O	15:O:30:THR:HG23	2.15	0.46
26:Z:51:ARG:O	26:Z:55:ARG:HG2	2.15	0.46
1:DB:56:U:H2'	1:DB:57:G:H8	1.81	0.46
1:DB:125:U:H2'	1:DB:126:G:H8	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DB:198:G:C2	1:DB:199:G:C4	3.04	0.46
1:DB:714:G:H2'	1:DB:715:A:C8	2.51	0.46
1:DB:1378:C:C5	1:DB:1379:G:C8	3.04	0.46
2:EB:26:G:C6	2:EB:27:G:N1	2.84	0.46
2:EB:751:A:C6	2:EB:789:A:C5	3.04	0.46
2:EB:1924:C:H4'	4:LC:13:C:H4'	1.98	0.46
2:EB:2557:G:H2'	2:EB:2558:C:H6	1.80	0.46
4:GB:68:C:H2'	4:GB:69:C:C6	2.51	0.46
8:KB:171:ALA:O	8:KB:175:LEU:HG	2.16	0.46
12:OB:15:GLY:O	12:OB:47:ILE:HG13	2.15	0.46
31:HC:31:LEU:HD13	31:HC:31:LEU:HA	1.56	0.46
37:OC:173:TRP:CD1	37:OC:173:TRP:N	2.83	0.46
46:XC:3:ARG:HH11	46:XC:8:GLU:HG3	1.81	0.46
50:BD:27:PHE:CE1	50:BD:36:ILE:HD11	2.51	0.46
53:ED:13:LEU:HB2	53:ED:17:ARG:NH1	2.31	0.46
55:GD:109:ARG:HG3	55:GD:208:GLU:HB2	1.98	0.46
55:HD:188:PRO:HD3	55:HD:197:HIS:HB2	1.98	0.46
1:A:544:G:H2'	1:A:545:C:C6	2.52	0.45
1:A:950:U:H2'	1:A:951:G:H8	1.82	0.45
1:A:1346:A:H5''	42:QA:120:ARG:HH12	1.81	0.45
2:B:150:C:H2'	2:B:151:C:C6	2.51	0.45
2:B:2292:C:OP1	16:P:17:ARG:NH2	2.48	0.45
11:K:25:ARG:H	11:K:25:ARG:HG2	1.59	0.45
11:K:96:GLU:H	11:K:96:GLU:CD	2.19	0.45
17:Q:18:ASP:OD2	17:Q:18:ASP:N	2.47	0.45
25:Y:19:GLN:OE1	25:Y:19:GLN:HA	2.17	0.45
31:EA:8:ASN:C	31:EA:8:ASN:OD1	2.55	0.45
31:EA:31:LEU:HA	31:EA:31:LEU:HD13	1.58	0.45
36:KA:6:HIS:ND1	47:VA:49:HIS:HB3	2.31	0.45
38:MA:12:LEU:HB3	38:MA:31:LEU:HB2	1.98	0.45
50:YA:31:LEU:HD23	50:YA:32:TYR:CZ	2.51	0.45
1:DB:41:G:C2	1:DB:402:G:C2	3.04	0.45
1:DB:806:C:H2'	1:DB:807:A:C8	2.50	0.45
1:DB:949:A:H1'	1:DB:1364:U:C2	2.51	0.45
1:DB:1129:C:H1'	1:DB:1130:A:N7	2.31	0.45
1:DB:1152:A:H5''	43:UC:13:HIS:CG	2.51	0.45
2:EB:731:C:H2'	2:EB:732:C:H6	1.81	0.45
2:EB:1354:A:H2'	2:EB:1355:G:O4'	2.16	0.45
2:EB:2267:A:H5''	2:EB:2268:A:H5'	1.97	0.45
2:EB:2678:C:H2'	2:EB:2679:A:O4'	2.16	0.45
6:IB:111:ARG:N	6:IB:111:ARG:HD2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:IC:54:GLU:O	32:IC:58:ILE:HG13	2.16	0.45
42:TC:10:ARG:NH1	42:TC:75:ASP:OD1	2.48	0.45
42:TC:13:ALA:HB2	42:TC:68:GLY:HA3	1.97	0.45
1:A:56:U:H2'	1:A:57:G:H8	1.80	0.45
1:A:781:A:H4'	1:A:1522:U:O2'	2.15	0.45
2:B:301:G:H1'	2:B:302:C:C6	2.51	0.45
2:B:511:U:H5	2:B:512:G:C5	2.34	0.45
2:B:844:C:C5	2:B:845:G:C6	3.04	0.45
2:B:2404:C:H2'	2:B:2405:G:O4'	2.16	0.45
7:G:46:ARG:NH1	7:G:46:ARG:CG	2.79	0.45
9:I:98:LEU:HD11	9:I:125:VAL:H	1.82	0.45
20:T:8:ARG:O	20:T:9:TYR:HB2	2.16	0.45
21:U:28:PHE:CE1	21:U:47:PHE:HE2	2.34	0.45
25:Y:60:PHE:HE1	25:Y:95:LEU:HD11	1.80	0.45
41:PA:86:ILE:HG21	41:PA:133:LEU:HD13	1.98	0.45
46:UA:3:ARG:HD3	46:UA:8:GLU:OE1	2.16	0.45
48:WA:79:ARG:HD2	48:WA:79:ARG:HA	1.78	0.45
1:DB:626:U:H2'	1:DB:627:G:H8	1.82	0.45
1:DB:923:A:H2'	1:DB:924:C:C6	2.51	0.45
1:DB:974:A:H8	1:DB:974:A:OP1	1.99	0.45
1:DB:1398:A:H5''	1:DB:1399:C:OP1	2.17	0.45
2:EB:1260:G:C6	2:EB:1261:C:C4	3.04	0.45
2:EB:1583:A:H5'	2:EB:1585:C:H5''	1.96	0.45
2:EB:2313:C:P	8:KB:74:LYS:HZ3	2.38	0.45
2:EB:2649:U:H2'	2:EB:2650:U:C6	2.52	0.45
3:FB:3:C:H2'	3:FB:4:C:C6	2.51	0.45
10:MB:133:HIS:CD2	10:MB:135:GLU:HB3	2.51	0.45
16:SB:50:SER:O	16:SB:76:LYS:NZ	2.38	0.45
23:ZB:31:ARG:H	23:ZB:31:ARG:HG2	1.56	0.45
33:JC:2:LYS:NZ	33:JC:4:ARG:HE	2.14	0.45
33:JC:12:ASP:OD1	33:JC:12:ASP:N	2.48	0.45
41:SC:100:ILE:HA	41:SC:101:PRO:HD3	1.74	0.45
45:WC:125:PRO:HB2	45:WC:126:LYS:H	1.62	0.45
46:XC:3:ARG:HD3	46:XC:8:GLU:OE1	2.15	0.45
53:ED:53:LEU:HD12	53:ED:103:GLY:HA3	1.99	0.45
1:A:428:G:O4'	1:A:430:A:C8	2.69	0.45
1:A:693:G:H2'	1:A:694:A:C8	2.51	0.45
1:A:923:A:H2'	1:A:924:C:C6	2.52	0.45
2:B:394:A:C6	2:B:395:U:C4	3.04	0.45
2:B:805:G:O4'	13:M:38:GLN:NE2	2.47	0.45
2:B:1344:G:H4'	2:B:1384:A:C5	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1353:A:H2'	2:B:1354:A:C8	2.52	0.45
2:B:2443:C:OP1	7:G:68:LYS:HD3	2.16	0.45
7:G:110:LEU:HD11	7:G:181:LEU:HG	1.98	0.45
7:G:158:THR:O	7:G:164:ARG:HD2	2.16	0.45
9:I:20:ALA:HB1	9:I:21:PRO:HD2	1.98	0.45
35:JA:197:VAL:HB	35:JA:200:ILE:HG12	1.98	0.45
37:LA:173:TRP:CD1	37:LA:173:TRP:N	2.85	0.45
41:PA:81:HIS:HB2	41:PA:138:TRP:CD1	2.51	0.45
45:TA:105:TYR:C	45:TA:107:ALA:H	2.18	0.45
1:DB:370:C:C2	1:DB:392:G:C2	3.04	0.45
1:DB:857:C:H2'	1:DB:858:G:O4'	2.15	0.45
2:EB:18:C:H4'	18:UB:23:GLY:O	2.16	0.45
2:EB:226:G:C2	2:EB:227:A:C6	3.04	0.45
2:EB:706:A:H2'	2:EB:707:G:O4'	2.16	0.45
2:EB:748:G:H2'	2:EB:750:A:N7	2.31	0.45
2:EB:768:G:O2'	2:EB:1379:A:N1	2.41	0.45
2:EB:892:G:H2'	2:EB:893:C:H4'	1.99	0.45
2:EB:1364:G:P	25:BC:3:LYS:HG3	2.56	0.45
2:EB:1657:C:H2'	2:EB:1658:C:C6	2.49	0.45
2:EB:2141:G:H2'	2:EB:2142:C:H4'	1.98	0.45
2:EB:2376:A:N6	16:SB:89:ARG:HD3	2.31	0.45
2:EB:2773:C:OP1	6:IB:164:ARG:NE	2.46	0.45
7:JB:53:THR:HG22	7:JB:56:GLU:OE2	2.16	0.45
51:CD:53:ARG:H	51:CD:54:ARG:HH21	1.65	0.45
53:ED:43:LEU:HD23	53:ED:43:LEU:HA	1.81	0.45
1:A:1062:U:H2'	1:A:1063:C:C6	2.52	0.45
2:B:947:G:H2'	2:B:948:G:C8	2.51	0.45
5:E:260:ARG:NH2	5:E:266:SER:OG	2.48	0.45
6:F:52:LEU:O	6:F:76:ARG:N	2.39	0.45
9:I:9:ILE:HG12	9:I:69:ARG:CZ	2.47	0.45
15:O:100:LEU:HA	15:O:100:LEU:HD13	1.59	0.45
37:LA:158:ILE:HG13	37:LA:159:ARG:N	2.32	0.45
39:NA:11:ASN:OD1	39:NA:12:PRO:HD2	2.16	0.45
48:WA:85:LEU:HD23	48:WA:85:LEU:HA	1.77	0.45
53:BB:54:LYS:HG2	53:BB:57:ARG:HH21	1.82	0.45
1:DB:153:C:H42	1:DB:168:G:H1	1.64	0.45
1:DB:255:G:H2'	1:DB:256:U:C6	2.51	0.45
1:DB:973:G:H1'	43:UC:54:PHE:CD1	2.51	0.45
1:DB:991:U:C4	1:DB:1212:U:H1'	2.50	0.45
2:EB:71:A:H5''	2:EB:73:A:C8	2.52	0.45
2:EB:553:U:O2'	2:EB:554:U:H5'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EB:573:G:O2'	2:EB:574:C:H3'	2.16	0.45
2:EB:2526:G:H1	2:EB:2537:U:H3	1.63	0.45
3:FB:82:G:H1	3:FB:94:C:N4	1.99	0.45
10:MB:136:VAL:HA	10:MB:137:PRO:HD3	1.81	0.45
18:UB:74:LEU:HB2	18:UB:75:ASN:H	1.64	0.45
36:NC:183:ASP:OD1	36:NC:184:TYR:N	2.49	0.45
43:UC:16:LEU:O	43:UC:19:SER:OG	2.29	0.45
55:HD:139:ALA:HA	55:HD:144:TRP:HE3	1.81	0.45
1:A:922:G:C2	1:A:923:A:C4	3.04	0.45
1:A:1022:G:C6	1:A:1023:G:H1'	2.52	0.45
1:A:1129:C:H1'	1:A:1130:A:N7	2.31	0.45
2:B:38:A:H2'	2:B:39:C:H6	1.82	0.45
2:B:571:A:C8	2:B:2030:A:N6	2.84	0.45
2:B:1287:A:C5	2:B:1288:U:C4	3.03	0.45
2:B:1705:G:C6	2:B:1706:U:C4	3.05	0.45
2:B:2330:G:H2'	2:B:2331:G:O4'	2.17	0.45
2:B:2818:G:O2'	2:B:2819:G:H5'	2.16	0.45
5:E:121:PRO:HA	5:E:132:PRO:HD2	1.99	0.45
6:F:151:TYR:CZ	6:F:154:LYS:HD3	2.52	0.45
8:H:11:TYR:OH	8:H:16:ARG:NH1	2.50	0.45
14:N:75:THR:HG21	14:N:87:LYS:HZ1	1.78	0.45
17:Q:100:TYR:CD1	17:Q:103:ARG:NH1	2.83	0.45
18:R:39:LEU:HA	18:R:39:LEU:HD13	1.76	0.45
35:JA:121:LEU:HD23	35:JA:125:PRO:HG2	1.99	0.45
35:JA:126:GLU:CD	35:JA:130:ARG:HB2	2.36	0.45
41:PA:64:LYS:HG2	41:PA:79:VAL:HG11	1.98	0.45
43:RA:38:ILE:HB	43:RA:71:LEU:HB3	1.97	0.45
1:DB:162:A:C5	1:DB:163:C:H1'	2.51	0.45
1:DB:1373:G:H5''	40:RC:36:LYS:HB2	1.97	0.45
2:EB:547:A:H5''	2:EB:548:A:OP2	2.17	0.45
2:EB:550:G:O2'	2:EB:1220:A:N3	2.42	0.45
2:EB:796:C:H2'	2:EB:797:C:H6	1.80	0.45
2:EB:836:G:C5	2:EB:837:C:C4	3.05	0.45
2:EB:1657:C:OP1	6:IB:136:ARG:N	2.48	0.45
2:EB:2096:U:H2'	2:EB:2097:C:C6	2.52	0.45
2:EB:2345:G:OP2	30:GC:38:LYS:HG2	2.15	0.45
18:UB:32:PHE:CZ	18:UB:36:ARG:NH1	2.84	0.45
24:AC:23:VAL:HG13	24:AC:38:VAL:HG22	1.98	0.45
36:NC:86:VAL:HA	36:NC:89:GLU:HB2	1.98	0.45
37:OC:62:GLN:HE21	37:OC:62:GLN:HA	1.82	0.45
37:OC:127:THR:HA	37:OC:132:ARG:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:PC:39:GLY:O	38:PC:69:VAL:HG12	2.17	0.45
38:PC:45:PHE:CE2	38:PC:47:LYS:HE3	2.51	0.45
41:SC:23:SER:HA	41:SC:63:LEU:HD23	1.97	0.45
55:HD:139:ALA:HA	55:HD:144:TRP:CE3	2.51	0.45
55:HD:181:GLY:O	55:HD:307:ASN:HB2	2.16	0.45
1:A:1105:A:H2'	1:A:1106:G:C8	2.52	0.45
1:A:1245:A:H2'	1:A:1246:C:C6	2.51	0.45
1:A:1295:G:HO2'	46:UA:14:ARG:NH1	2.13	0.45
1:A:1465:C:H2'	1:A:1466:C:O4'	2.17	0.45
2:B:312:G:H5'	2:B:331:A:O2'	2.17	0.45
2:B:1093:G:H1	2:B:1097:U:H5	1.64	0.45
2:B:1156:A:H4'	2:B:1157:G:OP2	2.17	0.45
2:B:1441:G:C2	2:B:1551:C:N3	2.85	0.45
2:B:2168:G:H2'	2:B:2169:A:H3'	1.99	0.45
2:B:2494:G:O2'	14:N:80:GLU:HA	2.17	0.45
8:H:56:ALA:HB2	8:H:153:ARG:NH1	2.21	0.45
10:J:10:GLU:C	10:J:12:LEU:H	2.20	0.45
14:N:64:ILE:HG13	23:W:178:GLU:HG3	1.99	0.45
14:N:109:VAL:HG13	14:N:113:GLN:HB3	1.98	0.45
31:EA:19:ARG:NH1	31:EA:19:ARG:HG2	2.31	0.45
45:TA:124:LYS:HD2	45:TA:125:PRO:HD2	1.99	0.45
53:BB:13:LEU:O	53:BB:17:ARG:HG3	2.16	0.45
1:DB:93:U:H2'	1:DB:95:G:C8	2.52	0.45
1:DB:1329:A:P	46:XC:28:ALA:HB3	2.57	0.45
2:EB:2575:C:OP1	6:IB:144:ARG:HD2	2.16	0.45
2:EB:2593:U:H2'	2:EB:2594:C:H6	1.81	0.45
2:EB:2811:G:H1	2:EB:2889:C:H42	1.64	0.45
20:WB:90:ARG:HG2	20:WB:90:ARG:HH11	1.82	0.45
23:ZB:61:LEU:HD23	23:ZB:67:LEU:HD23	1.97	0.45
32:IC:52:LYS:HB3	32:IC:53:PRO:HD3	1.99	0.45
35:MC:155:LEU:HA	35:MC:157:ARG:NH2	2.32	0.45
48:ZC:33:THR:HG23	48:ZC:63:ARG:NH1	2.31	0.45
49:AD:53:VAL:O	49:AD:57:ARG:HG3	2.17	0.45
52:DD:29:ARG:NH1	52:DD:29:ARG:HA	2.30	0.45
53:ED:9:ASN:C	53:ED:10:LEU:HD22	2.37	0.45
1:A:6:G:O2'	1:A:7:G:H5''	2.17	0.45
1:A:198:G:C2	1:A:199:G:C4	3.04	0.45
1:A:999:U:H1'	1:A:1042:G:N2	2.31	0.45
2:B:27:G:C4	2:B:512:G:N2	2.85	0.45
2:B:90:U:H1'	2:B:91:A:C8	2.52	0.45
2:B:938:G:H2'	2:B:939:G:H8	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:978:G:C2	2:B:986:C:C2	3.05	0.45
2:B:1786:A:H1'	2:B:1938:A:N6	2.32	0.45
2:B:2071:A:H2'	2:B:2072:G:C8	2.52	0.45
2:B:2577:A:H5'	29:CA:3:LYS:NZ	2.31	0.45
10:J:133:HIS:HA	10:J:134:PRO:HD3	1.78	0.45
14:N:75:THR:HA	14:N:89:ASN:O	2.17	0.45
22:V:86:ARG:NH1	22:V:100:ALA:O	2.50	0.45
27:AA:31:LEU:HA	27:AA:31:LEU:HD23	1.76	0.45
31:EA:47:ARG:O	31:EA:48:LYS:HG3	2.16	0.45
37:LA:43:HIS:C	37:LA:45:GLN:H	2.19	0.45
38:MA:39:GLY:O	38:MA:69:VAL:HG12	2.17	0.45
51:ZA:53:ARG:H	51:ZA:54:ARG:HH21	1.63	0.45
2:EB:30:G:H2'	2:EB:31:C:C6	2.52	0.45
2:EB:71:A:H3'	2:EB:71:A:OP2	2.16	0.45
2:EB:587:C:C6	2:EB:671:C:H1'	2.52	0.45
2:EB:733:G:H8	2:EB:733:G:O5'	1.99	0.45
2:EB:827:U:H2'	2:EB:2068:U:C2	2.52	0.45
2:EB:890:A:H2'	2:EB:892:G:C8	2.52	0.45
2:EB:1011:G:C2	2:EB:1013:C:C2	3.04	0.45
2:EB:1301:A:H2	2:EB:1626:G:N3	2.14	0.45
2:EB:2784:C:H2'	2:EB:2785:C:C6	2.52	0.45
2:EB:2821:A:H2'	2:EB:2822:G:O4'	2.17	0.45
4:GB:67:C:H2'	4:GB:68:C:C6	2.52	0.45
6:IB:37:ARG:HD3	6:IB:42:ASP:CG	2.37	0.45
7:JB:46:ARG:NH1	7:JB:46:ARG:CG	2.78	0.45
7:JB:110:LEU:HD11	7:JB:181:LEU:HG	1.99	0.45
10:MB:61:ARG:HA	10:MB:61:ARG:HH11	1.82	0.45
21:XB:35:THR:O	21:XB:39:ILE:HG13	2.17	0.45
35:MC:223:ILE:HA	35:MC:226:ARG:HB3	1.99	0.45
36:NC:19:GLU:HG2	36:NC:54:ARG:NH1	2.32	0.45
38:PC:98:THR:HB	38:PC:117:ASP:HB3	1.98	0.45
38:PC:145:LYS:HB3	38:PC:145:LYS:HZ3	1.81	0.45
42:TC:11:LYS:C	42:TC:13:ALA:H	2.19	0.45
49:AD:58:TYR:O	49:AD:61:SER:OG	2.29	0.45
50:BD:84:LEU:O	50:BD:87:LYS:HG3	2.17	0.45
1:A:338:A:C6	1:A:339:C:C4	3.05	0.45
1:A:909:A:N3	1:A:1413:A:O2'	2.42	0.45
1:A:975:A:O2'	47:VA:32:SER:OG	2.32	0.45
1:A:1049:U:OP1	47:VA:3:ARG:HB2	2.17	0.45
1:A:1163:C:H2'	1:A:1164:G:C8	2.52	0.45
1:A:1422:G:O3'	12:L:49:ARG:NH1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:U:H2'	2:B:171:G:O4'	2.17	0.45
2:B:573:G:O2'	2:B:574:C:H3'	2.17	0.45
2:B:733:G:O5'	2:B:733:G:H8	1.99	0.45
2:B:1029:A:H5''	2:B:1030:G:OP2	2.17	0.45
2:B:1935:G:H1'	2:B:1964:G:N2	2.32	0.45
2:B:2141:G:H2'	2:B:2142:C:H4'	1.98	0.45
2:B:2401:U:H3	2:B:2415:G:H1	1.63	0.45
2:B:2784:C:H2'	2:B:2785:C:C6	2.51	0.45
5:E:61:LEU:HD12	5:E:61:LEU:HA	1.75	0.45
11:K:48:MET:HE2	11:K:48:MET:HB2	1.81	0.45
16:P:10:ARG:HH21	16:P:91:PRO:HB2	1.80	0.45
24:X:50:ASN:HB2	24:X:81:VAL:HB	1.99	0.45
38:MA:121:LYS:HD3	38:MA:122:GLU:N	2.31	0.45
50:YA:29:HIS:HA	50:YA:30:PRO:HD3	1.79	0.45
1:DB:598:U:H2'	1:DB:599:C:H6	1.82	0.45
1:DB:606:G:H21	1:DB:631:G:H2'	1.81	0.45
1:DB:1449:C:H2'	1:DB:1450:U:O4'	2.17	0.45
2:EB:537:C:H2'	2:EB:539:G:H8	1.82	0.45
2:EB:978:G:C2	2:EB:986:C:C2	3.05	0.45
2:EB:2701:C:H2'	2:EB:2702:U:H2'	1.98	0.45
5:HB:263:ARG:HG2	5:HB:263:ARG:HH11	1.82	0.45
9:LB:25:LYS:HB3	9:LB:27:LYS:HZ2	1.82	0.45
15:RB:42:LYS:O	15:RB:45:ARG:HG2	2.17	0.45
20:WB:8:ARG:HA	20:WB:102:HIS:HA	1.99	0.45
24:AC:48:GLY:HA3	24:AC:80:HIS:ND1	2.32	0.45
29:FC:41:PRO:HA	29:FC:42:PRO:HD3	1.84	0.45
39:QC:16:GLN:H	39:QC:16:GLN:HG3	1.39	0.45
41:SC:20:TYR:HA	41:SC:65:TYR:CZ	2.52	0.45
42:TC:81:ILE:O	42:TC:85:LEU:HG	2.16	0.45
46:XC:27:LYS:HB2	46:XC:27:LYS:NZ	2.32	0.45
1:A:991:U:C4	1:A:1212:U:H1'	2.51	0.45
2:B:58:G:C6	2:B:59:U:C4	3.05	0.45
2:B:270(J):G:H4'	25:Y:81:ARG:NE	2.32	0.45
2:B:270(R):C:O3'	10:J:42:SER:HB2	2.17	0.45
2:B:489:G:H2'	2:B:491:G:O4'	2.17	0.45
2:B:675:A:C4	2:B:804:A:C2	3.05	0.45
2:B:929:G:H8	2:B:929:G:O5'	2.00	0.45
2:B:1051:G:H4'	2:B:2752:C:H4'	1.99	0.45
2:B:1604:C:H2'	2:B:1605:C:H6	1.82	0.45
2:B:1799:G:C8	5:E:181:GLU:OE2	2.70	0.45
2:B:2503:2MA:H4'	2:B:2504:U:OP1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2581:G:C6	2:B:2610:C:N3	2.85	0.45
5:E:72:LYS:NZ	5:E:101:GLU:HB3	2.31	0.45
11:K:13:TRP:CE2	11:K:133:GLN:HG2	2.52	0.45
15:O:37:THR:OG1	15:O:40:LYS:HB2	2.16	0.45
23:W:5:LEU:HD13	23:W:47:VAL:HG21	1.99	0.45
23:W:162:GLU:O	23:W:164:ALA:N	2.50	0.45
37:LA:21:LEU:H	37:LA:21:LEU:HG	1.57	0.45
38:MA:9:LYS:HB2	38:MA:112:LEU:HD11	1.99	0.45
48:WA:51:HIS:O	48:WA:54:ARG:HB3	2.16	0.45
50:YA:69:LYS:O	50:YA:70:ARG:HD2	2.16	0.45
1:DB:926:G:N2	34:KC:15:A:OP2	2.46	0.45
2:EB:1526:G:C6	2:EB:1527:G:C2	3.05	0.45
2:EB:1902:C:H5'	5:HB:246:PRO:HD3	1.99	0.45
2:EB:2712(A):A:H5'	2:EB:2713:A:OP2	2.17	0.45
8:KB:106:LEU:HD12	8:KB:110:ALA:HB3	1.99	0.45
9:LB:13:LYS:HA	9:LB:14:GLY:HA2	1.59	0.45
10:MB:75:LEU:HD13	10:MB:105:HIS:NE2	2.32	0.45
10:MB:87:LYS:HE2	10:MB:89:TYR:CD1	2.51	0.45
31:HC:19:ARG:NH1	31:HC:19:ARG:HG2	2.31	0.45
44:VC:79:SER:HA	44:VC:104:GLN:HB3	1.98	0.45
53:ED:50:GLU:H	53:ED:99:LEU:HD12	1.82	0.45
1:A:296:U:H2'	1:A:297:G:C8	2.52	0.45
1:A:542:G:P	37:LA:10:ARG:HH22	2.37	0.45
1:A:559:A:H4'	1:A:560:U:H5''	1.99	0.45
1:A:660:G:H1	1:A:745:C:H42	1.65	0.45
1:A:790:A:C6	1:A:791:G:C6	3.05	0.45
2:B:910:A:C6	2:B:911:A:C6	3.04	0.45
2:B:1093:G:H3'	2:B:1094:U:H5''	1.98	0.45
2:B:2678:C:H2'	2:B:2679:A:O4'	2.17	0.45
4:D:39:C:H4'	44:SA:54:ARG:HH22	1.82	0.45
7:G:140:LEU:HD11	7:G:170:LEU:HD11	1.99	0.45
10:J:4:ILE:HA	10:J:17:GLN:O	2.17	0.45
22:V:43:ASN:CG	22:V:67:LEU:HD21	2.38	0.45
4:IA:65:C:H2'	4:IA:66:C:H6	1.81	0.45
36:KA:6:HIS:HD2	36:KA:8:ILE:H	1.64	0.45
36:KA:19:GLU:HG2	36:KA:54:ARG:NH1	2.32	0.45
37:LA:120:LEU:HD23	37:LA:120:LEU:HA	1.75	0.45
39:NA:100:ASN:HA	51:ZA:23:LYS:NZ	2.32	0.45
42:QA:70:LYS:O	42:QA:74:ILE:HG13	2.17	0.45
46:UA:6:GLY:HA3	46:UA:67:GLU:HG3	1.97	0.45
2:EB:1344:G:H4'	2:EB:1384:A:C5	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EB:1640:C:H5'	2:EB:1641:A:OP2	2.17	0.45
2:EB:1675:C:H2'	2:EB:1676:A:O4'	2.17	0.45
2:EB:1939:5MU:H3'	2:EB:1940:U:H5'	1.99	0.45
5:HB:223:GLY:HA2	5:HB:226:MET:HG3	1.98	0.45
7:JB:167:ALA:HB1	7:JB:173:VAL:HG11	1.99	0.45
8:KB:113:ARG:NH1	28:EC:34:GLU:HG2	2.30	0.45
8:KB:138:GLN:HB3	8:KB:153:ARG:O	2.17	0.45
14:QB:25:ASP:OD1	14:QB:25:ASP:N	2.48	0.45
14:QB:112:GLU:HA	14:QB:115:MET:HB2	1.98	0.45
16:SB:91:PRO:HG2	16:SB:92:TYR:CE1	2.52	0.45
35:MC:212:GLN:NE2	35:MC:235:SER:HB3	2.32	0.45
39:QC:15:ASP:O	39:QC:19:LEU:HB2	2.16	0.45
48:ZC:9:GLN:NE2	48:ZC:12:ILE:HD12	2.32	0.45
55:HD:154:GLY:O	55:HD:156:HIS:N	2.50	0.45
1:A:1412:C:H2'	1:A:1413:A:H8	1.82	0.44
2:B:321:G:O3'	7:G:168:ARG:NH2	2.46	0.44
2:B:1582:C:H2'	2:B:1583:A:C8	2.52	0.44
5:E:72:LYS:HZ2	5:E:101:GLU:HB3	1.81	0.44
5:E:148:GLU:HB2	5:E:151:LYS:HD2	1.99	0.44
6:F:7:VAL:HG23	6:F:51:PHE:CE2	2.52	0.44
14:N:43:THR:HG23	14:N:46:GLN:CD	2.37	0.44
16:P:57:LYS:HD3	16:P:57:LYS:HA	1.75	0.44
24:X:48:GLY:HA3	24:X:80:HIS:ND1	2.32	0.44
35:JA:155:LEU:HA	35:JA:157:ARG:NH2	2.31	0.44
35:JA:219:VAL:O	35:JA:222:ILE:HB	2.17	0.44
37:LA:21:LEU:O	37:LA:26:CYS:SG	2.76	0.44
44:SA:90:GLY:O	44:SA:92:GLU:N	2.50	0.44
50:YA:31:LEU:HD23	50:YA:32:TYR:CE2	2.52	0.44
50:YA:66:SER:OG	50:YA:67:LYS:N	2.50	0.44
53:BB:9:ASN:C	53:BB:10:LEU:HD22	2.38	0.44
2:EB:70:G:H5''	2:EB:112:U:O2	2.18	0.44
2:EB:664:C:H4'	2:EB:941:A:OP1	2.17	0.44
2:EB:1043:C:C5	2:EB:1044:G:C8	3.05	0.44
2:EB:1510:A:C8	2:EB:1511:A:C8	3.05	0.44
2:EB:2478:A:H2'	2:EB:2479:G:O4'	2.17	0.44
2:EB:2784:C:H2'	2:EB:2785:C:H6	1.82	0.44
7:JB:14:PRO:HD2	7:JB:127:GLU:OE2	2.17	0.44
7:JB:107:LYS:HD3	7:JB:107:LYS:HA	1.71	0.44
10:MB:10:GLU:C	10:MB:12:LEU:H	2.20	0.44
35:MC:19:HIS:HB2	35:MC:204:ASN:HB3	1.99	0.44
36:NC:91:LEU:O	36:NC:95:THR:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:ZC:6:GLU:CD	48:ZC:6:GLU:H	2.20	0.44
55:GD:188:PRO:HD3	55:GD:197:HIS:HB2	1.99	0.44
1:A:599:C:H2'	1:A:600:C:C6	2.52	0.44
1:A:689:C:H2'	1:A:690:G:O4'	2.16	0.44
1:A:811:C:H4'	1:A:900:A:N6	2.31	0.44
2:B:18:C:H2'	2:B:19:C:C6	2.52	0.44
2:B:330:A:HO2'	2:B:331:A:H8	1.64	0.44
2:B:1520:U:H2'	2:B:1521:G:O4'	2.17	0.44
2:B:1702:G:C6	2:B:1703:G:C5	3.05	0.44
2:B:1779:U:C6	2:B:1783:A:N7	2.85	0.44
2:B:2846:G:H2'	2:B:2847:U:O4'	2.17	0.44
3:C:1:U:OP2	3:C:1:U:H6	2.00	0.44
10:J:79:ILE:O	10:J:144:VAL:HA	2.18	0.44
15:O:30:THR:HG22	15:O:75:LEU:HD13	1.98	0.44
18:R:104:GLN:NE2	18:R:105:VAL:HG23	2.32	0.44
28:BA:59:PHE:CD1	28:BA:60:GLN:HG3	2.52	0.44
36:KA:3:ASN:N	36:KA:3:ASN:OD1	2.49	0.44
37:LA:70:ILE:HD11	37:LA:100:ARG:NH1	2.33	0.44
37:LA:196:LEU:HB3	37:LA:198:VAL:HG12	1.99	0.44
46:UA:3:ARG:NH1	46:UA:8:GLU:HA	2.33	0.44
53:BB:50:GLU:H	53:BB:99:LEU:HD12	1.82	0.44
53:BB:84:LEU:O	53:BB:88:VAL:HG23	2.16	0.44
1:DB:1004:A:H5''	1:DB:1024:G:H22	1.81	0.44
1:DB:1022:G:C6	1:DB:1023:G:H1'	2.51	0.44
1:DB:1062:U:H2'	1:DB:1063:C:C6	2.51	0.44
2:EB:59:U:H3	2:EB:68:G:H1	1.65	0.44
2:EB:1057:A:N6	2:EB:1059:G:N7	2.64	0.44
2:EB:1417:C:H42	2:EB:1581:G:H1	1.65	0.44
2:EB:2108:C:O2	2:EB:2182:G:N2	2.50	0.44
3:FB:39:A:H2'	3:FB:40:U:C6	2.51	0.44
4:GB:10:G:H2'	4:GB:11:A:H8	1.80	0.44
5:HB:182:LEU:HB3	5:HB:271:ILE:HB	1.98	0.44
7:JB:148:LEU:HD11	7:JB:193:VAL:HG21	1.99	0.44
8:KB:135:LEU:HD13	8:KB:135:LEU:HA	1.63	0.44
10:MB:56:LYS:O	10:MB:60:GLU:HB2	2.17	0.44
14:QB:81:VAL:HG12	24:AC:5:LYS:HZ3	1.80	0.44
16:SB:49:VAL:HG22	16:SB:50:SER:H	1.81	0.44
52:DD:3:ARG:HH22	52:DD:7:LYS:HE2	1.80	0.44
1:A:272:C:H2'	1:A:273:A:C8	2.52	0.44
1:A:889:A:H5'	1:A:891:U:H1'	1.98	0.44
1:A:1119:C:H2'	1:A:1120:G:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1256:A:H2	1:A:1277:C:C2	2.34	0.44
2:B:17:G:H2'	2:B:18:C:H6	1.82	0.44
2:B:270(R):C:OP1	10:J:45:LYS:NZ	2.50	0.44
2:B:361:G:C2	2:B:362:U:C5	3.05	0.44
2:B:363(G):A:O2'	2:B:364:C:OP2	2.34	0.44
2:B:1202:C:H42	2:B:1243:G:H1	1.65	0.44
2:B:1510:A:C8	2:B:1511:A:C8	3.05	0.44
4:D:52:G:H1'	4:D:63:G:H22	1.82	0.44
5:E:71:ASP:N	5:E:71:ASP:OD2	2.50	0.44
8:H:6:ALA:N	8:H:104:GLU:OE2	2.50	0.44
11:K:108:PRO:O	11:K:113:GLY:HA3	2.17	0.44
12:L:15:GLY:O	12:L:47:ILE:HG13	2.16	0.44
13:M:90:ARG:NH1	13:M:90:ARG:HB3	2.33	0.44
15:O:13:HIS:CE1	15:O:15:SER:HB2	2.52	0.44
15:O:67:LEU:HD23	15:O:76:VAL:HG21	1.99	0.44
24:X:5:LYS:HB3	55:GD:265:LYS:HZ2	1.81	0.44
30:DA:19:ARG:HG3	30:DA:19:ARG:NH1	2.31	0.44
36:KA:91:LEU:O	36:KA:95:THR:HG23	2.17	0.44
37:LA:4:TYR:HD2	37:LA:4:TYR:HA	1.64	0.44
37:LA:127:THR:HA	37:LA:132:ARG:HA	1.99	0.44
41:PA:92:ARG:HB3	41:PA:94:TYR:CE2	2.52	0.44
43:RA:79:ARG:O	43:RA:83:GLU:HG3	2.18	0.44
1:DB:1004:A:N6	1:DB:1026:G:O5'	2.50	0.44
2:EB:511:U:H5	2:EB:512:G:C5	2.35	0.44
2:EB:715:G:H2'	2:EB:716:A:C8	2.52	0.44
2:EB:1161:C:O2'	19:VB:8:GLY:HA2	2.17	0.44
2:EB:2123:G:H1	2:EB:2175:C:H42	1.66	0.44
2:EB:2130:U:H2'	2:EB:2131:G:H21	1.82	0.44
6:IB:40:GLU:H	6:IB:40:GLU:HG3	1.47	0.44
22:YB:8:LYS:HG2	22:YB:11:ASP:OD2	2.17	0.44
41:SC:114:THR:O	41:SC:117:GLY:N	2.43	0.44
45:WC:28:LYS:HB2	45:WC:33:ARG:HH21	1.83	0.44
1:A:58:C:O2'	1:A:388:G:N7	2.42	0.44
1:A:457:C:H42	1:A:475:G:H1	1.66	0.44
1:A:995:C:O2'	47:VA:4:LYS:HE2	2.17	0.44
2:B:30:G:H2'	2:B:31:C:C6	2.53	0.44
2:B:43:G:N2	2:B:438:G:C4	2.86	0.44
2:B:59:U:H3	2:B:68:G:H1	1.66	0.44
2:B:953:A:O2'	2:B:954:G:H5'	2.17	0.44
2:B:2108:C:O2	2:B:2182:G:N2	2.51	0.44
2:B:2316:C:H1'	8:H:128:ARG:CZ	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2773:C:OP1	6:F:164:ARG:NE	2.41	0.44
6:F:47:VAL:HG11	6:F:86:PRO:CD	2.47	0.44
14:N:83:MET:HE2	14:N:83:MET:HB2	1.65	0.44
20:T:31:GLU:O	20:T:34:ASN:N	2.51	0.44
35:JA:103:THR:HA	35:JA:180:LEU:HD11	2.00	0.44
1:DB:345:C:H5'	1:DB:346:G:C5	2.52	0.44
1:DB:1201:A:H1'	1:DB:1202:G:OP2	2.17	0.44
1:DB:1226:C:H4'	52:DD:80:TYR:CZ	2.53	0.44
2:EB:270(A):A:H1'	2:EB:370:G:C2	2.53	0.44
2:EB:321:G:C4	2:EB:341:G:H4'	2.53	0.44
2:EB:603:A:C8	2:EB:655:A:C6	3.05	0.44
2:EB:1409:C:H2'	2:EB:1410:G:C8	2.52	0.44
2:EB:1450:C:N4	2:EB:1451:C:H41	2.16	0.44
2:EB:2852:G:H2'	2:EB:2853:C:C6	2.52	0.44
3:FB:12:C:OP2	3:FB:12:C:C6	2.70	0.44
7:JB:50:SER:HA	7:JB:92:PRO:O	2.17	0.44
14:QB:61:GLY:HA2	23:ZB:177:PRO:HB2	2.00	0.44
18:UB:104:GLN:NE2	18:UB:105:VAL:HG23	2.32	0.44
19:VB:19:LYS:H	19:VB:19:LYS:HG2	1.54	0.44
36:NC:36:ASP:OD2	36:NC:57:ILE:HG21	2.17	0.44
36:NC:91:LEU:HD23	36:NC:99:VAL:HA	1.99	0.44
36:NC:92:ALA:HA	36:NC:95:THR:OG1	2.17	0.44
38:PC:95:ALA:O	38:PC:98:THR:OG1	2.20	0.44
41:SC:127:LEU:HD13	41:SC:127:LEU:HA	1.88	0.44
55:GD:134:MET:HG3	55:GD:337:LEU:HD21	1.99	0.44
55:HD:115:VAL:HA	55:HD:203:VAL:HA	2.00	0.44
1:A:224:C:H2'	1:A:225:C:H6	1.83	0.44
1:A:346:G:OP2	17:Q:43:GLN:NE2	2.48	0.44
1:A:542:G:H5'	37:LA:41:GLY:HA3	1.99	0.44
1:A:756:C:H2'	1:A:757:U:O4'	2.18	0.44
1:A:1004:A:N6	1:A:1026:G:O5'	2.51	0.44
1:A:1347:G:N7	42:QA:10:ARG:NH2	2.65	0.44
2:B:312:G:C6	2:B:313:C:C4	3.05	0.44
2:B:458:G:O2'	31:EA:39:ARG:HD3	2.17	0.44
2:B:636:G:OP1	13:M:132:LYS:HE2	2.17	0.44
2:B:692:C:N3	2:B:771:G:C2	2.86	0.44
2:B:1641:A:H2'	2:B:1642:G:O4'	2.18	0.44
6:F:152:LYS:HE3	6:F:152:LYS:HB3	1.87	0.44
8:H:106:LEU:HD12	8:H:110:ALA:HB3	1.98	0.44
9:I:72:ILE:O	9:I:76:VAL:HG23	2.17	0.44
9:I:102:ALA:HA	9:I:117:PRO:HD3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:144:LEU:HD21	23:W:150:LEU:HG	2.00	0.44
27:AA:7:LYS:HB2	27:AA:34:GLU:HG2	1.98	0.44
36:KA:43:LEU:HD23	36:KA:43:LEU:HA	1.82	0.44
38:MA:98:THR:HB	38:MA:117:ASP:HB3	1.98	0.44
39:NA:62:TRP:CH2	39:NA:64:GLN:HB2	2.52	0.44
51:ZA:46:GLU:OE2	51:ZA:85:LEU:HD12	2.18	0.44
1:DB:447:G:O6	1:DB:485:G:O2'	2.23	0.44
1:DB:1309:G:O2'	46:XC:77:ASN:ND2	2.51	0.44
2:EB:6:A:C2	2:EB:7:G:C8	3.06	0.44
2:EB:506:G:H5''	2:EB:509:C:O2'	2.17	0.44
2:EB:637:A:OP1	13:PB:133:SER:OG	2.24	0.44
2:EB:1204:A:H61	2:EB:1240:U:H2'	1.83	0.44
2:EB:2298:A:H2'	2:EB:2299:G:O4'	2.16	0.44
2:EB:2300:G:H2'	2:EB:2301:C:C6	2.52	0.44
2:EB:2516:G:C6	2:EB:2517:C:N4	2.85	0.44
2:EB:2603:G:C6	2:EB:2604:U:C4	3.06	0.44
2:EB:2704:C:H2'	2:EB:2705:A:O4'	2.18	0.44
4:GB:52:G:H1'	4:GB:63:G:H22	1.83	0.44
5:HB:218:ARG:NH1	5:HB:218:ARG:CG	2.78	0.44
7:JB:54:ARG:HA	7:JB:87:GLY:HA3	1.99	0.44
38:PC:137:GLU:OE2	38:PC:137:GLU:HA	2.17	0.44
42:TC:108:VAL:HG12	42:TC:109:VAL:H	1.83	0.44
1:A:35:G:C2	1:A:550:G:C2	3.06	0.44
1:A:539:A:H2'	1:A:540:G:C8	2.53	0.44
1:A:949:A:H1'	1:A:1364:U:C2	2.53	0.44
1:A:962:C:H42	1:A:973:G:H1	1.64	0.44
2:B:176:G:O2'	2:B:177:G:H5'	2.18	0.44
2:B:836:G:C5	2:B:837:C:C4	3.06	0.44
2:B:1301:A:H2	2:B:1626:G:N3	2.16	0.44
2:B:1342:A:OP2	2:B:1602:U:O4	2.35	0.44
2:B:1590:U:H2'	2:B:1591:G:C8	2.53	0.44
2:B:2135:A:H2'	2:B:2136:C:H5'	1.99	0.44
2:B:2425:A:H4'	2:B:2426:A:H5''	1.99	0.44
7:G:167:ALA:HB1	7:G:173:VAL:HG11	1.99	0.44
8:H:33:ARG:O	8:H:162:THR:HG23	2.17	0.44
15:O:38:VAL:HB	15:O:39:PRO:HD3	1.98	0.44
29:CA:25:LEU:HD12	29:CA:25:LEU:H	1.81	0.44
43:RA:16:LEU:O	43:RA:19:SER:OG	2.27	0.44
1:DB:767:A:H2'	1:DB:768:A:O4'	2.18	0.44
1:DB:1075:C:H5''	35:MC:179:LYS:NZ	2.33	0.44
1:DB:1163:C:H2'	1:DB:1164:G:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DB:1442:G:H2'	1:DB:1442:G:N3	2.32	0.44
1:DB:1465:C:H2'	1:DB:1466:C:O4'	2.17	0.44
2:EB:46:C:H42	2:EB:179:G:H1	1.64	0.44
2:EB:1511:A:C8	2:EB:1512:G:C8	3.05	0.44
2:EB:2508:G:P	55:HD:228:ARG:HH22	2.40	0.44
8:KB:6:ALA:N	8:KB:104:GLU:OE2	2.49	0.44
8:KB:43:LEU:C	8:KB:45:GLU:H	2.21	0.44
8:KB:76:SER:HB2	8:KB:84:LYS:HB3	1.99	0.44
9:LB:101:ARG:HH11	9:LB:122:THR:HG22	1.83	0.44
19:VB:71:LEU:HD13	19:VB:71:LEU:HA	1.76	0.44
25:BC:15:ALA:O	25:BC:40:ARG:HG3	2.18	0.44
25:BC:98:LEU:HD23	25:BC:98:LEU:OXT	2.18	0.44
40:RC:104:LEU:HD13	40:RC:104:LEU:HA	1.84	0.44
41:SC:5:PRO:HB2	41:SC:32:LYS:NZ	2.32	0.44
44:VC:43:SER:HB2	44:VC:68:ALA:HB2	2.00	0.44
53:ED:84:LEU:O	53:ED:88:VAL:HG23	2.17	0.44
1:A:106:C:H2'	1:A:107:G:H8	1.83	0.44
1:A:262:A:N6	1:A:263:A:N6	2.66	0.44
1:A:837:G:H2'	1:A:838:G:H8	1.81	0.44
2:B:1288:U:C2	2:B:1327:C:O2	2.71	0.44
2:B:1319:G:O2'	2:B:1320:C:H5'	2.18	0.44
2:B:1742:C:H5'	2:B:1743:G:OP2	2.18	0.44
7:G:65:TRP:HD1	7:G:70:THR:HG21	1.83	0.44
7:G:195:ASP:HB3	7:G:198:ALA:CB	2.47	0.44
8:H:107:LEU:HD22	8:H:177:GLY:O	2.18	0.44
20:T:8:ARG:HA	20:T:102:HIS:HA	1.98	0.44
20:T:19:LEU:HB3	29:CA:25:LEU:HD11	2.00	0.44
21:U:5:TYR:CZ	26:Z:30:ARG:HD2	2.53	0.44
23:W:69:THR:HG22	23:W:90:VAL:HA	2.00	0.44
37:LA:108:LEU:HD23	37:LA:108:LEU:HA	1.75	0.44
47:VA:53:LEU:HD23	47:VA:53:LEU:HA	1.82	0.44
1:DB:262:A:H2'	1:DB:263:A:C8	2.53	0.44
1:DB:837:G:H2'	1:DB:838:G:H8	1.83	0.44
2:EB:347:A:H2'	2:EB:348:G:C8	2.52	0.44
2:EB:1406:U:H2'	2:EB:1407:C:C6	2.53	0.44
2:EB:2135:A:H2'	2:EB:2136:C:H5'	2.00	0.44
2:EB:2788:C:O2'	2:EB:2809:A:N3	2.50	0.44
3:FB:64:C:H5''	3:FB:65:C:OP2	2.18	0.44
8:KB:84:LYS:HE3	8:KB:84:LYS:HB2	1.81	0.44
8:KB:114:ILE:HD11	8:KB:117:PHE:CD1	2.53	0.44
24:AC:23:VAL:HB	24:AC:26:TYR:HE1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BC:72:GLU:O	25:BC:75:GLU:HB3	2.18	0.44
35:MC:83:MET:SD	35:MC:234:PRO:HB2	2.58	0.44
38:PC:31:LEU:HA	38:PC:31:LEU:HD23	1.69	0.44
41:SC:101:PRO:HG2	41:SC:133:LEU:HD11	1.99	0.44
42:TC:5:TYR:CE1	42:TC:16:ARG:HB2	2.49	0.44
43:UC:49:VAL:O	43:UC:60:ARG:HB3	2.18	0.44
44:VC:98:LEU:O	44:VC:101:SER:OG	2.23	0.44
55:GD:137:ARG:HD3	55:GD:334:GLU:O	2.18	0.44
55:HD:138:TYR:HE1	55:HD:338:ASP:OD2	2.01	0.44
1:A:714:G:H2'	1:A:715:A:C8	2.53	0.44
1:A:1064:G:H4'	1:A:1065:U:OP1	2.18	0.44
1:A:1366:C:H2'	1:A:1367:C:C6	2.52	0.44
1:A:1418:A:C2	1:A:1483:A:C2	3.05	0.44
1:A:1442:G:N3	1:A:1442:G:H2'	2.33	0.44
2:B:664:C:H4'	2:B:941:A:OP1	2.18	0.44
7:G:181:LEU:HD11	7:G:186:ILE:HD11	1.98	0.44
25:Y:46:LEU:HD23	25:Y:46:LEU:HA	1.79	0.44
1:DB:368:U:H6	1:DB:368:U:H2'	1.53	0.44
1:DB:645:C:H2'	1:DB:646:U:O4'	2.18	0.44
1:DB:1256:A:H2	1:DB:1277:C:C2	2.35	0.44
2:EB:894:C:O2'	2:EB:895:U:OP2	2.30	0.44
2:EB:1125:G:H3'	2:EB:1126:A:H5''	1.98	0.44
2:EB:2401:U:H2'	2:EB:2402:C:O4'	2.18	0.44
7:JB:150:GLY:HA2	7:JB:172:TRP:CE3	2.53	0.44
23:ZB:69:THR:HG22	23:ZB:90:VAL:HA	1.99	0.44
23:ZB:166:SER:O	23:ZB:169:GLU:HB2	2.18	0.44
28:EC:61:ARG:NH1	28:EC:62:ARG:NH2	2.66	0.44
35:MC:121:LEU:HD23	35:MC:125:PRO:HG2	2.00	0.44
36:NC:33:LEU:HA	36:NC:36:ASP:HB3	1.99	0.44
38:PC:48:ALA:C	38:PC:50:GLU:H	2.20	0.44
38:PC:144:THR:O	38:PC:148:VAL:HG23	2.17	0.44
39:QC:11:ASN:OD1	39:QC:12:PRO:HD2	2.18	0.44
43:UC:38:ILE:HB	43:UC:71:LEU:HB3	1.99	0.44
1:A:540:G:C6	1:A:541:G:C5	3.06	0.44
1:A:1531:A:H5'	1:A:1532:U:O2	2.18	0.44
2:B:565:C:H2'	2:B:566:U:O4'	2.18	0.44
2:B:733:G:O6	2:B:761:A:C8	2.71	0.44
2:B:1152:C:OP1	18:R:84:LYS:HD2	2.18	0.44
2:B:1568:G:H5''	5:E:61:LEU:HD22	2.00	0.44
2:B:2626:C:H2'	2:B:2627:G:C8	2.53	0.44
2:B:2729:G:H4'	6:F:186:GLY:HA2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2780:G:H4'	2:B:2781:A:OP2	2.17	0.44
7:G:156:LEU:HD22	7:G:156:LEU:HA	1.72	0.44
9:I:38:SER:HA	9:I:39:PRO:HD3	1.86	0.44
24:X:5:LYS:HB3	55:GD:265:LYS:HZ1	1.81	0.44
24:X:23:VAL:HB	24:X:26:TYR:HE1	1.82	0.44
35:JA:115:LEU:HB2	35:JA:145:LEU:HD22	2.00	0.44
35:JA:157:ARG:HE	35:JA:157:ARG:N	2.16	0.44
37:LA:155:LEU:HD22	37:LA:156:GLU:H	1.82	0.44
37:LA:155:LEU:O	37:LA:159:ARG:HG3	2.18	0.44
39:NA:12:PRO:HG2	39:NA:13:ASN:ND2	2.33	0.44
39:NA:15:ASP:OD2	39:NA:18:GLN:HB3	2.18	0.44
45:TA:28:LYS:HB2	45:TA:33:ARG:HH21	1.83	0.44
46:UA:39:ILE:HD12	46:UA:56:LEU:HD22	1.99	0.44
1:DB:756:C:O4'	41:SC:1:MET:HG2	2.18	0.44
1:DB:952:U:H2'	1:DB:953:G:H8	1.81	0.44
1:DB:1087:G:H1	1:DB:1098:C:H42	1.66	0.44
1:DB:1391:U:H2'	1:DB:1392:G:C8	2.53	0.44
1:DB:1516:G:N1	1:DB:1519:MA6:OP2	2.51	0.44
2:EB:270(W):G:H2'	2:EB:270(X):G:C8	2.53	0.44
2:EB:1254:A:N1	7:JB:82:ILE:HD11	2.32	0.44
2:EB:1791:A:H3'	2:EB:1792:G:H8	1.82	0.44
2:EB:2674:G:H4'	12:OB:30:ALA:HB2	2.00	0.44
2:EB:2870:C:H2'	2:EB:2871:C:O4'	2.18	0.44
3:FB:31:C:H4'	8:KB:29:TRP:CH2	2.52	0.44
10:MB:93:THR:HG23	10:MB:95:LYS:H	1.83	0.44
14:QB:58:PHE:HB3	14:QB:113:GLN:NE2	2.33	0.44
14:QB:65:PHE:HB2	14:QB:105:GLU:HB2	1.99	0.44
20:WB:19:LEU:HB3	29:FC:25:LEU:HD11	2.00	0.44
30:GC:26:ASN:HB3	30:GC:29:ASN:HB2	2.00	0.44
35:MC:40:HIS:CG	35:MC:190:THR:HG21	2.52	0.44
35:MC:114:ARG:HE	35:MC:118:LEU:HG	1.81	0.44
46:XC:16:ASP:HB3	46:XC:34:LEU:HD11	2.00	0.44
55:HD:308:ARG:HA	55:HD:319:ASP:HA	2.00	0.44
1:A:41:G:H2'	1:A:42:G:C8	2.53	0.43
1:A:142:G:H2'	1:A:143:A:C8	2.53	0.43
1:A:299:G:H2'	1:A:300:A:C8	2.53	0.43
1:A:1449:C:H2'	1:A:1450:U:O4'	2.17	0.43
2:B:545:G:C2	2:B:547:A:OP2	2.71	0.43
2:B:880:G:H1	2:B:897:C:H42	1.65	0.43
2:B:2123:G:H1	2:B:2175:C:H42	1.64	0.43
2:B:2674:G:H4'	12:L:30:ALA:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2704:C:H2'	2:B:2705:A:O4'	2.17	0.43
2:B:2822:G:OP2	6:F:110:GLY:O	2.36	0.43
3:C:6:C:H2'	3:C:7:G:C8	2.53	0.43
6:F:132:HIS:CE1	6:F:133:LYS:HE2	2.53	0.43
7:G:64:ILE:HD11	7:G:75:HIS:CB	2.48	0.43
10:J:56:LYS:O	10:J:60:GLU:HB2	2.18	0.43
13:M:6:LEU:HA	13:M:6:LEU:HD23	1.71	0.43
45:TA:13:LYS:HE3	45:TA:13:LYS:HB3	1.72	0.43
1:DB:339:C:OP2	12:OB:97:ARG:NH1	2.51	0.43
1:DB:922:G:C2	1:DB:923:A:C4	3.06	0.43
1:DB:1435:G:H2'	1:DB:1436:U:C6	2.53	0.43
2:EB:297:C:H2'	2:EB:298:G:O4'	2.18	0.43
2:EB:634:C:H2'	2:EB:635:C:C6	2.53	0.43
2:EB:1353:A:H2'	2:EB:1354:A:C8	2.53	0.43
2:EB:2472:G:H2'	2:EB:2475:C:H42	1.82	0.43
4:GB:21:A:HO2'	4:GB:46:G:H1	1.65	0.43
10:MB:68:LEU:O	10:MB:71:ILE:HG13	2.17	0.43
18:UB:39:LEU:HA	18:UB:39:LEU:HD13	1.72	0.43
19:VB:37:VAL:HG12	19:VB:39:LEU:H	1.83	0.43
28:EC:61:ARG:NH1	28:EC:62:ARG:HH22	2.15	0.43
31:HC:13:ALA:O	31:HC:17:GLY:HA3	2.18	0.43
35:MC:7:VAL:HG23	35:MC:8:LYS:NZ	2.33	0.43
35:MC:23:ARG:HB2	35:MC:23:ARG:NH1	2.33	0.43
38:PC:20:GLN:OE1	38:PC:21:ALA:N	2.51	0.43
50:BD:43:LEU:HD23	50:BD:43:LEU:HA	1.77	0.43
50:BD:66:SER:OG	50:BD:67:LYS:N	2.50	0.43
55:GD:334:GLU:HA	55:GD:334:GLU:OE2	2.17	0.43
1:A:1099:G:OP2	35:JA:148:TYR:OH	2.36	0.43
1:A:1120:G:H2'	1:A:1121:U:C6	2.54	0.43
1:A:1152:A:H5''	43:RA:13:HIS:CG	2.52	0.43
2:B:1161:C:O2'	19:S:8:GLY:HA2	2.18	0.43
2:B:1335:U:H2'	2:B:1336:A:C8	2.54	0.43
2:B:1367:A:N7	2:B:1368:G:H1'	2.33	0.43
2:B:1405:U:H2'	2:B:1406:U:C6	2.53	0.43
2:B:1651:G:N2	2:B:2007:C:C2	2.86	0.43
2:B:1839:G:C8	2:B:1927:A:H1'	2.54	0.43
2:B:2515:C:O2'	2:B:2516:G:H5'	2.18	0.43
2:B:2758:A:C4	9:I:67:LEU:HD21	2.53	0.43
3:C:39:A:H2'	3:C:40:U:C6	2.53	0.43
7:G:13:SER:HB3	7:G:16:GLY:O	2.18	0.43
9:I:26:VAL:HG12	9:I:79:VAL:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:24:GLY:O	11:K:28:THR:HG23	2.18	0.43
13:M:17:LYS:HD2	13:M:27:HIS:CE1	2.53	0.43
25:Y:82:LEU:O	25:Y:85:LEU:HD13	2.19	0.43
33:GA:4:ARG:NH1	33:GA:8:LYS:NZ	2.66	0.43
39:NA:82:ARG:HB2	39:NA:85:VAL:HG23	2.00	0.43
49:XA:25:ARG:NH1	49:XA:25:ARG:HG3	2.34	0.43
1:DB:1203:C:OP1	47:YC:3:ARG:NE	2.51	0.43
2:EB:270(S):G:O2'	25:BC:79:GLY:HA3	2.17	0.43
2:EB:2711:A:OP1	2:EB:2712(A):A:OP1	2.36	0.43
4:GB:43:A:H2'	4:GB:44:A:C8	2.53	0.43
5:HB:245:PRO:HA	5:HB:246:PRO:HD3	1.88	0.43
11:NB:96:GLU:CD	11:NB:96:GLU:H	2.21	0.43
14:QB:81:VAL:HB	24:AC:7:LEU:HD23	2.00	0.43
14:QB:83:MET:HB2	14:QB:83:MET:HE2	1.58	0.43
15:RB:67:LEU:HD23	15:RB:76:VAL:HG21	1.99	0.43
16:SB:49:VAL:HG13	16:SB:73:LEU:HD11	2.00	0.43
31:HC:10:ARG:NH1	31:HC:14:LYS:CE	2.80	0.43
32:IC:10:ALA:O	32:IC:14:VAL:HG22	2.19	0.43
36:NC:40:ARG:HG3	36:NC:55:VAL:HB	1.99	0.43
1:A:8:A:C5	37:LA:209:ARG:HB2	2.54	0.43
2:B:603:A:C8	2:B:655:A:C6	3.06	0.43
2:B:1339:G:H5''	21:U:16:LYS:HD3	2.00	0.43
2:B:1657:C:OP1	6:F:136:ARG:N	2.48	0.43
2:B:2164:C:H42	2:B:2166:G:N2	2.17	0.43
6:F:2:LYS:NZ	6:F:95:ILE:O	2.30	0.43
7:G:149:ASP:OD2	7:G:151:SER:HB3	2.18	0.43
8:H:182:LYS:HB2	8:H:182:LYS:HE2	1.58	0.43
11:K:72:TYR:CE2	11:K:87:LEU:HD23	2.53	0.43
16:P:49:VAL:HG13	16:P:73:LEU:HD11	2.00	0.43
18:R:32:PHE:HZ	18:R:36:ARG:NH1	2.16	0.43
23:W:69:THR:HG22	23:W:90:VAL:HG22	2.00	0.43
25:Y:3:LYS:HB2	25:Y:61:ARG:HH12	1.82	0.43
33:GA:12:ASP:OD1	33:GA:12:ASP:N	2.45	0.43
47:VA:3:ARG:CZ	47:VA:3:ARG:HA	2.48	0.43
1:DB:237:C:H5''	50:BD:25:ARG:CZ	2.48	0.43
1:DB:622:A:C8	1:DB:623:C:C5	3.06	0.43
1:DB:737:A:H2'	1:DB:738:C:C6	2.53	0.43
1:DB:756:C:H2'	1:DB:757:U:O4'	2.18	0.43
1:DB:931:C:N4	1:DB:1386:G:H1	2.10	0.43
2:EB:108:U:H2'	2:EB:109:G:C8	2.54	0.43
2:EB:499:U:H5'	22:YB:46:LYS:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EB:890:A:H2'	2:EB:892:G:H8	1.83	0.43
2:EB:971:C:H2'	2:EB:972:G:O4'	2.18	0.43
2:EB:1011:G:H5''	18:UB:77:SER:OG	2.19	0.43
2:EB:1260:G:H2'	2:EB:1261:C:O4'	2.17	0.43
2:EB:2093:G:C6	2:EB:2225:A:C8	3.06	0.43
6:IB:60:ASN:OD1	6:IB:60:ASN:N	2.49	0.43
7:JB:24:LEU:HD12	7:JB:24:LEU:HA	1.80	0.43
7:JB:195:ASP:HB3	7:JB:198:ALA:CB	2.49	0.43
37:OC:134:ASP:C	37:OC:135:LEU:HD13	2.39	0.43
38:PC:145:LYS:HE2	38:PC:149:GLU:OE1	2.18	0.43
39:QC:35:ALA:HB1	39:QC:65:VAL:CG2	2.48	0.43
55:HD:186:ARG:HB3	55:HD:312:PHE:HB2	2.01	0.43
1:A:177:C:H2'	1:A:178:C:H6	1.82	0.43
1:A:564:C:HO2'	41:PA:91:ARG:HH22	1.57	0.43
1:A:1118:C:H2'	1:A:1119:C:C6	2.53	0.43
1:A:1512:U:H2'	1:A:1513:A:C8	2.53	0.43
2:B:280:C:N3	2:B:361:G:N2	2.67	0.43
2:B:455:C:N3	2:B:472:A:H2'	2.33	0.43
2:B:876:C:H2'	2:B:877:U:O4'	2.19	0.43
2:B:1818:U:O2'	5:E:154:LYS:O	2.30	0.43
2:B:2684:U:OP1	17:Q:53:ARG:HD3	2.19	0.43
2:B:2747:G:C2	2:B:2756:U:C5	3.06	0.43
4:D:28:C:H2'	4:D:29:G:C8	2.53	0.43
6:F:40:GLU:H	6:F:40:GLU:HG3	1.44	0.43
7:G:24:LEU:HA	7:G:24:LEU:HD12	1.71	0.43
9:I:27:LYS:HA	9:I:32:GLU:HB3	2.01	0.43
11:K:39:ARG:HE	11:K:48:MET:CE	2.31	0.43
22:V:9:LYS:HA	22:V:10:GLY:HA2	1.63	0.43
30:DA:44:ARG:HG2	30:DA:44:ARG:HH11	1.83	0.43
38:MA:118:ILE:HG12	38:MA:119:LEU:N	2.33	0.43
39:NA:99:ALA:HB1	51:ZA:23:LYS:HE2	2.00	0.43
42:QA:11:LYS:C	42:QA:13:ALA:H	2.18	0.43
52:AB:41:VAL:HG22	52:AB:44:MET:SD	2.58	0.43
1:DB:272:C:H2'	1:DB:273:A:C8	2.53	0.43
1:DB:475:G:H2'	1:DB:476:G:H8	1.82	0.43
1:DB:598:U:H2'	1:DB:599:C:C6	2.52	0.43
1:DB:1240:U:C6	40:RC:32:ARG:NH1	2.86	0.43
2:EB:548:A:H4'	19:VB:19:LYS:NZ	2.33	0.43
2:EB:2316:C:H1'	8:KB:128:ARG:NH1	2.34	0.43
2:EB:2729:G:H4'	6:IB:186:GLY:HA2	1.99	0.43
7:JB:65:TRP:CD1	7:JB:70:THR:HG21	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:TB:78:LEU:HD23	17:TB:79:HIS:NE2	2.32	0.43
18:UB:94:ASN:O	18:UB:98:LEU:HG	2.17	0.43
20:WB:57:ASN:HA	20:WB:61:ASN:HD22	1.83	0.43
21:XB:60:ARG:CZ	31:HC:47:ARG:HH22	2.31	0.43
23:ZB:11:GLU:HB3	23:ZB:12:GLY:H	1.46	0.43
32:IC:29:LYS:HG3	32:IC:44:LYS:HB2	2.00	0.43
35:MC:103:THR:HA	35:MC:180:LEU:HD11	2.00	0.43
37:OC:59:ARG:HH21	37:OC:66:ARG:NH1	2.15	0.43
37:OC:133:VAL:HG13	37:OC:135:LEU:HD22	1.98	0.43
38:PC:121:LYS:HD3	38:PC:122:GLU:N	2.33	0.43
55:GD:154:GLY:O	55:GD:156:HIS:N	2.51	0.43
1:A:397:A:N6	1:A:548:G:C5	2.86	0.43
2:B:911:A:H2'	14:N:9:TYR:OH	2.18	0.43
2:B:1049:C:O2	2:B:1113:U:H4'	2.19	0.43
2:B:1104:C:H2'	2:B:1105:U:C6	2.53	0.43
2:B:1205:U:H4'	2:B:1206:G:OP2	2.18	0.43
2:B:2001:A:H2'	2:B:2002:G:C8	2.53	0.43
2:B:2575:C:OP1	6:F:144:ARG:HD2	2.19	0.43
2:B:2722:G:H2'	2:B:2723:C:C6	2.54	0.43
7:G:65:TRP:CD1	7:G:70:THR:HG21	2.53	0.43
20:T:12:ILE:HD13	20:T:17:VAL:HG22	2.00	0.43
26:Z:48:HIS:CE1	26:Z:49:LYS:HG3	2.53	0.43
35:JA:142:LEU:O	35:JA:146:GLN:HG3	2.18	0.43
37:LA:170:VAL:HB	37:LA:174:LEU:HB2	2.00	0.43
48:WA:6:GLU:H	48:WA:6:GLU:CD	2.22	0.43
48:WA:17:ARG:HD3	48:WA:26:GLU:OE2	2.19	0.43
51:ZA:65:ILE:HD12	51:ZA:65:ILE:HA	1.92	0.43
1:DB:137:C:H2'	1:DB:138:G:C8	2.51	0.43
1:DB:838:G:HO2'	1:DB:841:U:H6	1.66	0.43
1:DB:1346:A:H5''	42:TC:120:ARG:NH1	2.34	0.43
1:DB:1402:4OC:H2'	1:DB:1403:C:O4'	2.18	0.43
2:EB:401:A:C2	2:EB:402:A:C4	3.07	0.43
2:EB:1002:G:O5'	2:EB:1002:G:H8	2.01	0.43
2:EB:1820:U:H4'	2:EB:1821:A:OP2	2.18	0.43
3:FB:45:A:C4	3:FB:46:A:C8	3.06	0.43
23:ZB:103:ARG:CZ	23:ZB:103:ARG:HA	2.48	0.43
31:HC:21:ARG:HG2	31:HC:21:ARG:HH11	1.84	0.43
33:JC:6:SER:O	33:JC:6:SER:OG	2.31	0.43
39:QC:33:TYR:HE2	39:QC:78:GLU:HG3	1.83	0.43
55:GD:314:GLN:HB3	55:GD:316:ARG:HD2	2.00	0.43
1:A:8:A:C6	37:LA:209:ARG:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:C:O3'	50:YA:25:ARG:NH1	2.39	0.43
1:A:1478:C:H2'	1:A:1479:C:H6	1.83	0.43
2:B:777:A:C2	2:B:778:G:C4	3.07	0.43
2:B:807:U:OP2	13:M:41:ARG:NH2	2.51	0.43
2:B:892:G:H2'	2:B:893:C:H4'	1.99	0.43
2:B:1047:G:H2'	2:B:1110:G:H1	1.84	0.43
18:R:54:LYS:HE2	18:R:54:LYS:HB2	1.83	0.43
23:W:166:SER:O	23:W:169:GLU:HB2	2.18	0.43
24:X:47:PRO:HB3	24:X:59:LEU:HD22	2.01	0.43
27:AA:6:VAL:HB	27:AA:54:VAL:HG21	2.01	0.43
28:BA:57:GLU:HA	28:BA:58:ARG:HA	1.63	0.43
31:EA:19:ARG:HG2	31:EA:19:ARG:HH11	1.84	0.43
35:JA:157:ARG:HE	35:JA:157:ARG:H	1.67	0.43
36:KA:92:ALA:HA	36:KA:95:THR:OG1	2.19	0.43
37:LA:10:ARG:HG3	37:LA:11:LEU:HD12	2.00	0.43
37:LA:12:CYS:SG	37:LA:26:CYS:SG	3.17	0.43
41:PA:63:LEU:HD13	41:PA:63:LEU:HA	1.78	0.43
1:DB:80:G:C2	1:DB:90:C:C2	3.06	0.43
1:DB:338:A:C6	1:DB:339:C:C4	3.06	0.43
1:DB:693:G:H2'	1:DB:694:A:C8	2.53	0.43
1:DB:1152:A:H2'	1:DB:1153:C:C6	2.53	0.43
2:EB:34:C:O2'	2:EB:35:G:C8	2.72	0.43
2:EB:270(J):G:H4'	25:BC:81:ARG:NE	2.33	0.43
2:EB:1742:C:H5'	2:EB:1743:G:OP2	2.18	0.43
2:EB:1971:A:N3	5:HB:240:ALA:HA	2.33	0.43
2:EB:2181:G:H2'	2:EB:2182:G:C8	2.53	0.43
2:EB:2495:G:OP1	14:QB:82:ARG:HD2	2.18	0.43
6:IB:93:VAL:HG11	6:IB:181:LEU:O	2.18	0.43
6:IB:188:VAL:HG13	6:IB:189:PRO:HD2	1.99	0.43
17:TB:36:GLU:CG	17:TB:41:ARG:HE	2.31	0.43
20:WB:23:LEU:HD22	29:FC:25:LEU:HD13	1.99	0.43
28:EC:57:GLU:HA	28:EC:58:ARG:HA	1.64	0.43
34:KC:19:U:C4	34:KC:20:A:C6	3.06	0.43
35:MC:10:LEU:HA	35:MC:12:GLU:OE1	2.17	0.43
35:MC:61:LEU:HD23	35:MC:68:ILE:HD11	2.01	0.43
37:OC:21:LEU:O	37:OC:26:CYS:SG	2.75	0.43
39:QC:100:ASN:HA	51:CD:23:LYS:NZ	2.34	0.43
42:TC:70:LYS:O	42:TC:74:ILE:HG13	2.18	0.43
46:XC:4:ILE:HD12	46:XC:57:ARG:HA	2.01	0.43
49:AD:4:ILE:HA	49:AD:20:VAL:O	2.19	0.43
1:A:601:C:H42	1:A:637:G:H1	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1064:G:H21	1:A:1190:G:H1'	1.82	0.43
2:B:524:U:H2'	2:B:525:U:C6	2.54	0.43
2:B:1186:G:H2'	2:B:1187:G:O4'	2.18	0.43
2:B:1326:U:O2'	2:B:1327:C:H5'	2.18	0.43
2:B:1560:G:H2'	2:B:1561:G:H8	1.84	0.43
2:B:1788:C:H2'	2:B:1789:A:O4'	2.19	0.43
2:B:1920:4OC:H1'	2:B:1920:4OC:HM23	1.47	0.43
2:B:1946:U:H2'	2:B:1947:C:C6	2.54	0.43
2:B:2301:C:H2'	2:B:2302:G:C8	2.53	0.43
3:C:12:C:OP2	3:C:12:C:C6	2.72	0.43
7:G:62:ARG:HG2	7:G:63:LYS:O	2.18	0.43
9:I:64:LEU:HA	9:I:64:LEU:HD23	1.76	0.43
13:M:90:ARG:HB3	13:M:90:ARG:HH11	1.83	0.43
17:Q:26:ASP:OD1	17:Q:120:ARG:NH2	2.41	0.43
17:Q:78:LEU:HD23	17:Q:79:HIS:NE2	2.34	0.43
20:T:86:LEU:HD12	20:T:87:PRO:HD2	2.01	0.43
26:Z:53:LEU:HD22	26:Z:53:LEU:HA	1.79	0.43
37:LA:163:GLU:HA	37:LA:166:LYS:HE2	1.99	0.43
52:AB:3:ARG:HH22	52:AB:7:LYS:HE2	1.82	0.43
1:DB:474:G:H5'	49:AD:81:ARG:HG3	2.01	0.43
2:EB:319:C:H2'	2:EB:320:A:O4'	2.19	0.43
2:EB:817:C:H2'	2:EB:818:G:O4'	2.19	0.43
2:EB:1268:A:H2'	2:EB:1269:A:O4'	2.19	0.43
2:EB:2498:C:OP2	2:EB:2499:C:OP2	2.36	0.43
2:EB:2611:U:H2'	29:FC:2:ALA:O	2.18	0.43
2:EB:2667:C:H1'	9:LB:109:PHE:CD1	2.52	0.43
2:EB:2698:U:H2'	2:EB:2699:C:H6	1.83	0.43
7:JB:57:VAL:HG13	7:JB:59:TYR:H	1.84	0.43
7:JB:183:VAL:O	7:JB:187:VAL:HG12	2.18	0.43
8:KB:138:GLN:HE21	8:KB:149:VAL:HG22	1.83	0.43
9:LB:25:LYS:HB3	9:LB:27:LYS:HZ3	1.83	0.43
11:NB:72:TYR:CE2	11:NB:87:LEU:HD23	2.53	0.43
13:PB:6:LEU:HD23	13:PB:6:LEU:HA	1.71	0.43
35:MC:22:LYS:HA	35:MC:22:LYS:HZ2	1.84	0.43
37:OC:25:ARG:C	37:OC:27:TYR:H	2.17	0.43
39:QC:12:PRO:HG2	39:QC:13:ASN:HD22	1.84	0.43
1:A:93:U:H2'	1:A:95:G:H8	1.83	0.43
1:A:368:U:H6	1:A:368:U:H2'	1.56	0.43
1:A:1118:C:H2'	1:A:1119:C:H6	1.84	0.43
1:A:1152:A:H2'	1:A:1153:C:H6	1.84	0.43
1:A:1201:A:H1'	1:A:1202:G:OP2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1439:C:OP1	53:BB:38:LYS:NZ	2.31	0.43
2:B:657:U:H2'	2:B:658:C:C6	2.54	0.43
2:B:1511:A:C8	2:B:1512:G:C8	3.07	0.43
2:B:2207:C:C2	2:B:2218:G:C2	3.06	0.43
3:C:84:C:H42	3:C:92:G:H1	1.66	0.43
5:E:182:LEU:HB3	5:E:271:ILE:HB	2.01	0.43
7:G:51:THR:HB	7:G:88:VAL:HG21	2.01	0.43
8:H:39:ILE:HD12	8:H:157:ILE:HG12	2.01	0.43
12:L:91:LEU:HD23	12:L:91:LEU:HA	1.79	0.43
16:P:49:VAL:HG22	16:P:50:SER:H	1.83	0.43
24:X:7:LEU:H	4:IA:2:G:C5'	2.31	0.43
4:IA:67:C:H2'	4:IA:68:C:H6	1.84	0.43
36:KA:73:PRO:HA	36:KA:76:VAL:HG23	2.00	0.43
38:MA:144:THR:O	38:MA:148:VAL:HG23	2.18	0.43
45:TA:27:LEU:HD13	45:TA:98:TYR:CE1	2.53	0.43
53:BB:60:GLU:HG3	53:BB:81:LYS:HD2	2.01	0.43
1:DB:790:A:C6	1:DB:791:G:C6	3.06	0.43
1:DB:1058:G:H2'	1:DB:1059:C:O4'	2.19	0.43
1:DB:1325:C:H5''	54:FD:15:ARG:HD3	2.00	0.43
1:DB:1326:C:OP1	54:FD:12:LYS:HE2	2.19	0.43
2:EB:270(G):U:H2'	2:EB:270(H):C:C6	2.53	0.43
2:EB:301:G:H1'	2:EB:302:C:C6	2.54	0.43
2:EB:1060:U:O2'	2:EB:1061:U:OP2	2.25	0.43
2:EB:1205:U:C4	7:JB:171:PRO:HA	2.53	0.43
2:EB:2503:2MA:H4'	2:EB:2504:U:OP1	2.17	0.43
5:HB:206:LEU:HD23	5:HB:206:LEU:HA	1.47	0.43
5:HB:257:LEU:HD12	5:HB:258:LYS:N	2.33	0.43
8:KB:181:ARG:HB2	8:KB:181:ARG:NH1	2.31	0.43
11:NB:4:TYR:CD2	18:UB:100:VAL:HG11	2.53	0.43
14:QB:34:LEU:HD12	14:QB:34:LEU:HA	1.82	0.43
15:RB:38:VAL:HB	15:RB:39:PRO:HD3	2.01	0.43
15:RB:80:PHE:O	15:RB:85:PRO:HD3	2.18	0.43
36:NC:88:ARG:HD3	36:NC:101:LEU:HB3	2.00	0.43
38:PC:77:PRO:HB2	38:PC:78:HIS:CD2	2.54	0.43
41:SC:4:ASP:HB2	41:SC:89:PRO:HG3	2.01	0.43
49:AD:6:LEU:HD22	49:AD:70:ALA:HB2	2.01	0.43
55:HD:314:GLN:HB3	55:HD:316:ARG:HD2	2.01	0.43
1:A:406:G:H1'	1:A:495:A:C6	2.54	0.43
1:A:474:G:H5'	49:XA:81:ARG:HG3	2.01	0.43
1:A:735:C:OP1	51:ZA:68:LYS:HE3	2.19	0.43
2:B:79:G:H2'	2:B:80:G:H8	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:297:C:H2'	2:B:298:G:O4'	2.18	0.43
2:B:774:A:H2'	2:B:774:A:N3	2.34	0.43
2:B:1002:G:H8	2:B:1002:G:O5'	2.01	0.43
2:B:1042:G:H2'	2:B:1043:C:O2	2.19	0.43
2:B:1188:U:O2'	2:B:1189:A:H5'	2.19	0.43
2:B:1364:G:P	25:Y:3:LYS:HG3	2.58	0.43
2:B:2055:C:H5'	2:B:2056:G:O5'	2.18	0.43
2:B:2056:G:O2'	29:CA:8:LYS:NZ	2.48	0.43
2:B:2437:U:H2'	2:B:2438:U:C6	2.53	0.43
2:B:2731:G:C6	2:B:2732:G:C6	3.06	0.43
2:B:2821:A:OP2	15:O:3:HIS:NE2	2.52	0.43
6:F:94:GLU:OE1	6:F:177:PRO:HB3	2.19	0.43
6:F:101:ARG:HD3	6:F:171:GLU:HA	2.00	0.43
8:H:50:ALA:HB3	8:H:52:ILE:HG13	2.00	0.43
21:U:30:VAL:HG21	21:U:39:ILE:HD11	2.01	0.43
26:Z:63:VAL:HA	26:Z:66:GLU:HG2	2.01	0.43
27:AA:53:LEU:HD23	27:AA:53:LEU:HA	1.69	0.43
36:KA:127:ARG:NH2	36:KA:192:THR:OG1	2.52	0.43
38:MA:48:ALA:C	38:MA:50:GLU:H	2.22	0.43
41:PA:4:ASP:HB2	41:PA:89:PRO:HG3	2.01	0.43
1:DB:236:G:H5''	50:BD:42:TYR:OH	2.19	0.43
1:DB:657:G:C2	1:DB:658:G:C8	3.07	0.43
1:DB:926:G:C6	1:DB:1505:G:C6	3.07	0.43
1:DB:975:A:O2'	47:YC:32:SER:OG	2.26	0.43
1:DB:1103:C:H2'	1:DB:1104:G:O4'	2.19	0.43
1:DB:1499:A:OP2	1:DB:1500:A:OP2	2.36	0.43
1:DB:1521:G:H2'	1:DB:1522:U:O4'	2.19	0.43
2:EB:79:G:H2'	2:EB:80:G:H8	1.84	0.43
2:EB:94:G:H2'	2:EB:95:G:O4'	2.17	0.43
2:EB:710:G:H2'	2:EB:711:G:C8	2.53	0.43
2:EB:876:C:H2'	2:EB:877:U:O4'	2.18	0.43
2:EB:1818:U:H2'	5:HB:157:ARG:HG3	2.00	0.43
5:HB:77:ALA:HB2	5:HB:97:TYR:CD1	2.54	0.43
9:LB:64:LEU:HD23	9:LB:64:LEU:HA	1.83	0.43
22:YB:43:ASN:CG	22:YB:67:LEU:HD21	2.39	0.43
24:AC:7:LEU:H	4:LC:2:G:C5'	2.31	0.43
37:OC:113:SER:OG	37:OC:114:ARG:N	2.52	0.43
38:PC:40:ARG:CZ	38:PC:68:GLU:HB3	2.49	0.43
47:YC:27:CYS:HB3	47:YC:43:CYS:SG	2.59	0.43
55:GD:169:ASP:OD1	55:GD:169:ASP:N	2.52	0.43
55:HD:112:PHE:CE2	55:HD:165:LYS:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:A:H5''	1:A:88:C:C5	2.54	0.43
1:A:237:C:H5''	50:YA:25:ARG:CZ	2.48	0.43
1:A:404:U:H2'	1:A:405:U:C6	2.53	0.43
1:A:645:C:H2'	1:A:646:U:O4'	2.18	0.43
2:B:91:A:H2'	2:B:92:G:H8	1.84	0.43
2:B:674:G:O2'	7:G:74:ARG:HD3	2.19	0.43
2:B:1899:G:H2'	2:B:1899:G:N3	2.34	0.43
2:B:1939:5MU:O2	2:B:1967:C:H4'	2.19	0.43
2:B:2376:A:N3	16:P:106:ARG:NH2	2.67	0.43
2:B:2884:U:H2'	2:B:2885:C:O4'	2.19	0.43
3:C:68:C:H2'	3:C:69:G:O4'	2.19	0.43
8:H:114:ILE:HD11	8:H:117:PHE:CD1	2.54	0.43
8:H:122:PRO:HD2	8:H:181:ARG:HH11	1.83	0.43
13:M:19:VAL:HB	13:M:31:ALA:HB1	2.00	0.43
13:M:81:GLN:OE1	13:M:107:LYS:N	2.51	0.43
15:O:65:LEU:HD12	15:O:65:LEU:HA	1.80	0.43
23:W:23:LYS:HG2	23:W:38:TYR:HE1	1.84	0.43
36:KA:20:SER:HG	36:KA:40:ARG:HH22	1.64	0.43
46:UA:16:ASP:HB3	46:UA:34:LEU:HD11	2.00	0.43
47:VA:27:CYS:HB3	47:VA:43:CYS:SG	2.59	0.43
53:BB:87:LYS:O	53:BB:91:LEU:HB2	2.19	0.43
1:DB:540:G:C6	1:DB:541:G:C5	3.06	0.43
2:EB:270(F):G:H1	2:EB:270(V):C:H42	1.67	0.43
2:EB:522:G:C6	2:EB:523:C:C4	3.07	0.43
2:EB:1093:G:H3'	2:EB:1094:U:H5''	2.00	0.43
2:EB:1155:A:O3'	18:UB:55:ARG:NH1	2.52	0.43
2:EB:2319:G:H3'	2:EB:2319:G:OP1	2.18	0.43
2:EB:2514:U:H2'	2:EB:2515:C:H6	1.82	0.43
2:EB:2707:G:H2'	2:EB:2708:G:H8	1.84	0.43
5:HB:72:LYS:NZ	5:HB:101:GLU:HB3	2.33	0.43
9:LB:125:VAL:HG22	9:LB:131:VAL:HG22	2.00	0.43
12:OB:122:LEU:HD23	12:OB:122:LEU:HA	1.89	0.43
25:BC:60:PHE:HE1	25:BC:95:LEU:HD11	1.84	0.43
32:IC:34:TRP:CG	32:IC:35:GLN:N	2.87	0.43
42:TC:33:PHE:HD2	42:TC:33:PHE:HA	1.65	0.43
45:WC:105:TYR:C	45:WC:107:ALA:H	2.23	0.43
55:GD:145:ARG:HB3	55:GD:167:SER:HB2	2.01	0.43
55:HD:109:ARG:HH12	55:HD:210:PRO:HG3	1.84	0.43
1:A:41:G:H2'	1:A:42:G:H8	1.84	0.42
1:A:541:G:H2'	1:A:542:G:H8	1.83	0.42
1:A:1058:G:H2'	1:A:1059:C:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:250:G:H2'	2:B:251:A:C8	2.53	0.42
2:B:960:A:H8	2:B:960:A:O5'	2.02	0.42
2:B:1021:A:C8	2:B:1021:A:H3'	2.54	0.42
2:B:1268:A:H2'	2:B:1269:A:O4'	2.20	0.42
2:B:2508:G:OP1	55:GD:228:ARG:NH2	2.46	0.42
2:B:2711:A:OP1	2:B:2712(A):A:OP1	2.37	0.42
6:F:11:MET:HG2	6:F:24:THR:CB	2.49	0.42
6:F:181:LEU:HD12	6:F:181:LEU:HA	1.81	0.42
12:L:28:SER:O	12:L:29:ASN:HB3	2.19	0.42
19:S:35:LEU:HA	19:S:36:PRO:HD3	1.81	0.42
24:X:53:MET:HA	24:X:58:THR:O	2.19	0.42
36:KA:23:TYR:CG	36:KA:24:ALA:N	2.87	0.42
36:KA:40:ARG:HG3	36:KA:55:VAL:HB	2.00	0.42
36:KA:91:LEU:HD23	36:KA:99:VAL:HA	2.00	0.42
38:MA:7:GLU:O	38:MA:34:VAL:HA	2.19	0.42
39:NA:70:ASP:OD2	39:NA:70:ASP:N	2.48	0.42
42:QA:108:VAL:HG12	42:QA:109:VAL:H	1.85	0.42
1:DB:18:C:H2'	1:DB:19:C:O4'	2.19	0.42
1:DB:599:C:H2'	1:DB:600:C:C6	2.54	0.42
1:DB:1415:G:H1	1:DB:1485:U:H3	1.67	0.42
2:EB:191:A:H2'	2:EB:192:C:C6	2.54	0.42
2:EB:280:C:C2	2:EB:361:G:N2	2.87	0.42
2:EB:1027:A:N6	2:EB:1126:A:C4	2.87	0.42
2:EB:1520:U:H2'	2:EB:1521:G:O4'	2.19	0.42
2:EB:1825:A:C2	2:EB:1826:G:C4	3.07	0.42
2:EB:2808:U:O2'	2:EB:2809:A:H5'	2.19	0.42
6:IB:110:GLY:O	15:RB:3:HIS:CE1	2.72	0.42
14:QB:72:LYS:HA	14:QB:73:PRO:HD2	1.83	0.42
29:FC:17:ASP:N	29:FC:17:ASP:OD2	2.52	0.42
38:PC:79:GLU:H	38:PC:79:GLU:HG2	1.57	0.42
42:TC:89:ASN:HB3	42:TC:92:TYR:CE2	2.54	0.42
44:VC:99:GLN:HE21	44:VC:99:GLN:HB2	1.55	0.42
46:XC:65:LYS:HB3	46:XC:70:LEU:HA	2.01	0.42
55:HD:109:ARG:HG3	55:HD:208:GLU:HB2	2.01	0.42
2:B:322:A:P	7:G:168:ARG:HH21	2.42	0.42
2:B:521:G:H2'	2:B:522:G:C8	2.54	0.42
2:B:862:G:P	14:N:18:LYS:HZ3	2.41	0.42
2:B:1359:A:H2	2:B:1372:U:O4	2.01	0.42
2:B:1441:G:N2	2:B:1551:C:C2	2.88	0.42
2:B:2183:C:H2'	2:B:2184:G:H8	1.84	0.42
4:D:21:A:HO2'	4:D:46:G:H1	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:145:VAL:HB	5:E:155:LEU:HB2	1.99	0.42
5:E:214:TRP:CD1	5:E:214:TRP:N	2.85	0.42
8:H:176:LEU:HA	8:H:176:LEU:HD23	1.72	0.42
10:J:136:VAL:HA	10:J:137:PRO:HD3	1.80	0.42
16:P:71:ARG:NE	16:P:107:GLU:OE1	2.45	0.42
16:P:93:LYS:O	16:P:95:HIS:N	2.53	0.42
17:Q:107:ASP:O	17:Q:111:ARG:HB2	2.19	0.42
19:S:71:LEU:HA	19:S:71:LEU:HD13	1.67	0.42
20:T:82:LEU:HD23	20:T:84:ARG:NH2	2.35	0.42
25:Y:60:PHE:HA	25:Y:91:LYS:HZ1	1.83	0.42
28:BA:58:ARG:HA	28:BA:58:ARG:HD2	1.88	0.42
35:JA:19:HIS:HB2	35:JA:204:ASN:HB3	2.01	0.42
35:JA:97:TRP:HH2	35:JA:176:GLU:CD	2.23	0.42
38:MA:31:LEU:HD11	38:MA:129:ILE:HA	2.00	0.42
42:QA:89:ASN:HB3	42:QA:92:TYR:CE2	2.54	0.42
50:YA:27:PHE:CE1	50:YA:36:ILE:HD11	2.53	0.42
1:DB:978:A:C4	1:DB:1319:A:C2	3.08	0.42
1:DB:1528:U:C2	1:DB:1530:G:C8	3.06	0.42
2:EB:34:C:O2'	2:EB:35:G:H8	2.01	0.42
2:EB:58:G:C6	2:EB:59:U:C4	3.06	0.42
2:EB:274:G:OP2	2:EB:274:G:H8	2.02	0.42
2:EB:301:G:C4	2:EB:302:C:C5	3.06	0.42
2:EB:774:A:H2'	2:EB:774:A:N3	2.34	0.42
2:EB:1547:C:H2'	2:EB:1548:C:C6	2.54	0.42
2:EB:2516:G:C6	2:EB:2517:C:C4	3.08	0.42
6:IB:111:ARG:HD3	6:IB:160:TYR:CD2	2.55	0.42
8:KB:122:PRO:HD2	8:KB:181:ARG:NH1	2.34	0.42
13:PB:112:LEU:HD12	13:PB:127:ALA:HB2	2.00	0.42
23:ZB:54:HIS:CG	23:ZB:101:PRO:HD3	2.54	0.42
26:CC:30:ARG:O	26:CC:34:GLU:HG2	2.19	0.42
28:EC:59:PHE:CD1	28:EC:60:GLN:HG3	2.53	0.42
29:FC:19:ARG:C	29:FC:21:SER:H	2.20	0.42
35:MC:115:LEU:HB2	35:MC:145:LEU:HD22	2.01	0.42
36:NC:73:PRO:HA	36:NC:76:VAL:HG23	2.01	0.42
37:OC:108:LEU:HD23	37:OC:170:VAL:HG11	2.00	0.42
37:OC:149:ALA:HB3	37:OC:152:SER:HB2	2.00	0.42
39:QC:82:ARG:HB2	39:QC:85:VAL:HG23	2.00	0.42
55:HD:110:ASN:HB2	55:HD:208:GLU:HG3	2.01	0.42
1:A:109:A:C6	1:A:326:G:C6	3.07	0.42
1:A:540:G:C5	1:A:541:G:C5	3.07	0.42
1:A:659:U:OP1	48:WA:8:LYS:HD3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:803:G:H2'	1:A:804:U:O4'	2.19	0.42
1:A:926:G:C6	1:A:1505:G:C6	3.07	0.42
2:B:301:G:C4	2:B:302:C:C5	3.06	0.42
2:B:335:C:OP2	22:V:84:ARG:HD3	2.19	0.42
2:B:755:C:H2'	2:B:756:C:C6	2.54	0.42
2:B:894:C:O2'	2:B:895:U:OP2	2.31	0.42
2:B:2300:G:H2'	2:B:2301:C:C6	2.54	0.42
5:E:33:LEU:HD23	5:E:33:LEU:HA	1.88	0.42
6:F:38:THR:H	6:F:42:ASP:HB2	1.85	0.42
7:G:34:TRP:CE2	13:M:8:PRO:HD3	2.54	0.42
26:Z:52:ASP:O	26:Z:56:GLN:HG3	2.19	0.42
36:KA:52:LEU:HD13	36:KA:55:VAL:HG23	2.00	0.42
36:KA:68:VAL:HB	36:KA:103:VAL:HG13	2.01	0.42
38:MA:144:THR:HG22	38:MA:147:ASP:OD2	2.19	0.42
44:SA:67:ASP:HA	44:SA:70:LYS:HD3	2.02	0.42
1:DB:58:C:O2'	1:DB:388:G:N7	2.46	0.42
1:DB:109:A:C6	1:DB:326:G:C6	3.07	0.42
1:DB:161:A:H2'	1:DB:162:A:C8	2.53	0.42
1:DB:539:A:H2'	1:DB:540:G:C8	2.55	0.42
1:DB:962:C:H42	1:DB:973:G:H1	1.65	0.42
2:EB:751:A:H5'	20:WB:90:ARG:HA	2.00	0.42
4:GB:70:G:C2	4:GB:71:C:C6	3.07	0.42
9:LB:98:LEU:HD11	9:LB:125:VAL:H	1.84	0.42
10:MB:87:LYS:HE2	10:MB:89:TYR:HD1	1.84	0.42
26:CC:46:GLN:HB3	26:CC:48:HIS:CE1	2.54	0.42
36:NC:65:ALA:HA	36:NC:100:ALA:HB2	2.01	0.42
41:SC:114:THR:HG22	41:SC:131:GLY:HA3	1.99	0.42
55:GD:308:ARG:HA	55:GD:319:ASP:HA	2.01	0.42
1:A:606:G:H21	1:A:631:G:H2'	1.85	0.42
1:A:1486:G:C6	1:A:1487:G:C6	3.08	0.42
2:B:686:G:H21	2:B:788:A:H61	1.67	0.42
2:B:2603:G:C6	2:B:2604:U:C4	3.08	0.42
3:C:66:A:H61	3:C:107:U:H2'	1.85	0.42
6:F:37:ARG:HD2	6:F:44:TYR:CZ	2.55	0.42
7:G:183:VAL:O	7:G:187:VAL:HG12	2.19	0.42
11:K:91:LEU:HD13	11:K:98:VAL:HG21	2.01	0.42
12:L:14:THR:HG21	12:L:86:ILE:HB	2.00	0.42
13:M:50:ARG:O	13:M:52:GLU:HG3	2.19	0.42
22:V:14:LEU:HD23	22:V:82:PRO:HB3	2.02	0.42
35:JA:215:LEU:HD23	35:JA:215:LEU:HA	1.85	0.42
1:DB:738:C:H5''	39:QC:69:GLU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DB:1306:A:H1'	1:DB:1332:A:C2	2.55	0.42
1:DB:1480:G:H2'	1:DB:1481:U:O4'	2.20	0.42
2:EB:27:G:C4	2:EB:512:G:N2	2.87	0.42
2:EB:176:G:O2'	2:EB:177:G:H5'	2.19	0.42
2:EB:813:U:H2'	2:EB:814:C:C6	2.54	0.42
2:EB:913:U:H4'	2:EB:914:C:OP1	2.19	0.42
2:EB:1021:A:C8	2:EB:1021:A:H3'	2.54	0.42
2:EB:1047:G:H2'	2:EB:1110:G:H22	1.84	0.42
2:EB:1226:A:OP1	19:VB:84:LYS:NZ	2.41	0.42
2:EB:1467:C:N4	2:EB:1525:G:H1	2.10	0.42
2:EB:1799:G:C8	5:HB:181:GLU:OE2	2.70	0.42
2:EB:2425:A:H4'	2:EB:2426:A:H5''	2.01	0.42
2:EB:2536:G:C6	2:EB:2537:U:C4	3.07	0.42
2:EB:2836:U:C4	2:EB:2883:A:N6	2.87	0.42
3:FB:111:U:H2'	3:FB:112:G:H8	1.84	0.42
7:JB:64:ILE:HD11	7:JB:75:HIS:CB	2.49	0.42
8:KB:29:TRP:O	8:KB:33:ARG:NH1	2.52	0.42
10:MB:77:LEU:HB3	10:MB:142:VAL:HG13	2.01	0.42
13:PB:113:LYS:HA	13:PB:129:ALA:O	2.19	0.42
15:RB:13:HIS:ND1	15:RB:15:SER:HB2	2.34	0.42
23:ZB:40:ASP:OD2	23:ZB:41:LEU:N	2.52	0.42
35:MC:126:GLU:CD	35:MC:130:ARG:HB2	2.39	0.42
35:MC:197:VAL:HB	35:MC:200:ILE:HG12	2.01	0.42
40:RC:80:VAL:HB	40:RC:83:ALA:O	2.20	0.42
47:YC:3:ARG:CZ	47:YC:3:ARG:HA	2.49	0.42
48:ZC:48:LYS:O	48:ZC:50:HIS:N	2.50	0.42
1:A:235:C:H2'	1:A:236:G:C8	2.54	0.42
2:B:1125:G:H3'	2:B:1126:A:H5''	2.00	0.42
2:B:1179:C:H2'	2:B:1180:C:C6	2.55	0.42
2:B:1385:G:O2'	2:B:1396:U:O2	2.31	0.42
2:B:1582:C:H2'	2:B:1583:A:H8	1.85	0.42
2:B:1673:U:H5'	2:B:1674:G:OP2	2.19	0.42
2:B:1827:C:C2'	2:B:1828:G:H5'	2.50	0.42
2:B:1952:A:C6	2:B:1953:A:N1	2.87	0.42
5:E:275:LYS:HG2	5:E:276:LYS:H	1.84	0.42
13:M:112:LEU:HD12	13:M:127:ALA:HB2	2.01	0.42
18:R:95:LEU:HD12	18:R:95:LEU:HA	1.87	0.42
35:JA:223:ILE:HA	35:JA:226:ARG:HB3	2.01	0.42
41:PA:100:ILE:HA	41:PA:101:PRO:HD3	1.76	0.42
41:PA:114:THR:O	41:PA:117:GLY:N	2.50	0.42
44:SA:38:ASN:HA	44:SA:39:PRO:HD3	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:ZA:76:LEU:HD13	51:ZA:76:LEU:HA	1.87	0.42
1:DB:87:A:H5''	1:DB:88:C:C5	2.55	0.42
1:DB:457:C:H42	1:DB:475:G:H1	1.67	0.42
1:DB:660:G:H1	1:DB:745:C:H42	1.68	0.42
1:DB:978:A:OP1	1:DB:1361:G:N1	2.43	0.42
1:DB:1034:G:H2'	1:DB:1035:A:C8	2.55	0.42
1:DB:1261:A:N1	1:DB:1275:A:H1'	2.35	0.42
2:EB:250:G:H2'	2:EB:251:A:C8	2.55	0.42
2:EB:1952:A:C6	2:EB:1953:A:N1	2.87	0.42
2:EB:2060:A:OP1	7:JB:69:HIS:N	2.45	0.42
2:EB:2758:A:C4	9:LB:67:LEU:HD21	2.54	0.42
5:HB:155:LEU:H	5:HB:155:LEU:HD22	1.84	0.42
11:NB:4:TYR:OH	11:NB:6:PRO:HA	2.19	0.42
23:ZB:69:THR:HG22	23:ZB:90:VAL:HG22	2.01	0.42
30:GC:44:ARG:HG2	30:GC:44:ARG:HH11	1.85	0.42
36:NC:193:TYR:HE1	36:NC:196:LEU:HD11	1.85	0.42
37:OC:18:LYS:HE3	37:OC:20:TYR:N	2.34	0.42
48:ZC:79:ARG:HA	48:ZC:79:ARG:HD2	1.82	0.42
55:HD:130:ASP:OD1	55:HD:130:ASP:N	2.53	0.42
1:A:1216:G:H5''	47:VA:5:ALA:HB1	2.02	0.42
2:B:27:G:C2	2:B:512:G:N3	2.87	0.42
2:B:108:U:H2'	2:B:109:G:H8	1.84	0.42
2:B:270(W):G:H2'	2:B:270(X):G:C8	2.55	0.42
2:B:631:A:H1'	13:M:66:GLY:HA2	2.02	0.42
2:B:1820:U:H4'	2:B:1821:A:OP2	2.20	0.42
2:B:2695:C:H2'	2:B:2696:U:C6	2.55	0.42
2:B:2761:G:O2'	9:I:143:GLN:NE2	2.53	0.42
8:H:138:GLN:HB3	8:H:153:ARG:O	2.19	0.42
9:I:54:ARG:CZ	9:I:62:LYS:HG2	2.50	0.42
10:J:8:PRO:HG3	10:J:15:VAL:HG12	2.01	0.42
32:FA:8:LYS:O	32:FA:12:LYS:HG3	2.20	0.42
36:KA:75:VAL:HG12	36:KA:83:ARG:NH1	2.34	0.42
40:OA:80:VAL:HB	40:OA:83:ALA:O	2.20	0.42
45:TA:27:LEU:HD13	45:TA:98:TYR:HE1	1.84	0.42
50:YA:59:ILE:HG22	50:YA:73:VAL:HA	2.02	0.42
53:BB:92:LEU:O	53:BB:96:GLY:N	2.52	0.42
1:DB:778:G:H2'	1:DB:779:C:O4'	2.19	0.42
1:DB:1522:U:H2'	1:DB:1523:G:C8	2.55	0.42
2:EB:96:G:OP1	26:CC:46:GLN:NE2	2.45	0.42
2:EB:489:G:H2'	2:EB:491:G:O4'	2.20	0.42
2:EB:1186:G:H2'	2:EB:1187:G:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EB:1425:G:N1	2:EB:1426:G:C2	2.88	0.42
2:EB:2050:C:N4	2:EB:2051:A:C6	2.88	0.42
2:EB:2731:G:C6	2:EB:2732:G:C6	3.08	0.42
2:EB:2821:A:OP2	15:RB:3:HIS:NE2	2.52	0.42
5:HB:71:ASP:OD2	5:HB:71:ASP:N	2.50	0.42
6:IB:38:THR:O	6:IB:42:ASP:N	2.52	0.42
8:KB:11:TYR:OH	8:KB:16:ARG:NH1	2.52	0.42
9:LB:20:ALA:HB1	9:LB:21:PRO:HD2	2.02	0.42
15:RB:65:LEU:HA	15:RB:65:LEU:HD12	1.82	0.42
21:XB:10:ALA:HA	26:CC:37:PHE:CE1	2.54	0.42
23:ZB:137:ILE:HD11	23:ZB:158:PRO:HD3	2.02	0.42
37:OC:109:GLY:HA3	37:OC:165:MET:SD	2.59	0.42
43:UC:9:ARG:HA	43:UC:68:HIS:O	2.20	0.42
44:VC:67:ASP:HA	44:VC:70:LYS:HD3	2.00	0.42
49:AD:25:ARG:NH1	49:AD:25:ARG:HG3	2.34	0.42
1:A:35:G:O2'	45:TA:118:SER:O	2.28	0.42
1:A:601:C:H2'	1:A:602:A:C8	2.54	0.42
1:A:741:G:H2'	1:A:742:G:O4'	2.19	0.42
1:A:1277:C:H1'	1:A:1282:C:H1'	2.01	0.42
1:A:1378:C:C5	1:A:1379:G:C8	3.07	0.42
1:A:1406:U:H2'	1:A:1407:5MC:O4'	2.19	0.42
1:A:1530:G:H2'	1:A:1531:A:H5''	2.00	0.42
2:B:191:A:H2'	2:B:192:C:C6	2.55	0.42
2:B:2335:A:C8	2:B:2337:G:C5	3.07	0.42
2:B:2846:G:C5	2:B:2847:U:C5	3.08	0.42
3:C:45:A:H2'	3:C:46:A:O4'	2.20	0.42
9:I:101:ARG:HH11	9:I:122:THR:HG22	1.83	0.42
10:J:61:ARG:NH1	10:J:61:ARG:N	2.67	0.42
10:J:69:LYS:HD2	10:J:136:VAL:HG13	2.01	0.42
12:L:25:LEU:HA	12:L:25:LEU:HD23	1.58	0.42
18:R:24:TYR:HB2	18:R:29:SER:HB3	2.01	0.42
37:LA:4:TYR:CE1	37:LA:66:ARG:HG2	2.54	0.42
39:NA:35:ALA:HB1	39:NA:65:VAL:HG21	2.02	0.42
53:BB:53:LEU:HD12	53:BB:103:GLY:HA3	2.01	0.42
1:DB:222:U:H2'	1:DB:223:U:H6	1.84	0.42
1:DB:325:A:H2'	1:DB:326:G:O4'	2.20	0.42
1:DB:719:C:O2'	51:CD:49:LYS:HB3	2.19	0.42
1:DB:753:A:H5'	1:DB:754:C:C6	2.55	0.42
1:DB:927:G:C2	1:DB:1391:U:O2	2.72	0.42
1:DB:1064:G:H21	1:DB:1190:G:H1'	1.85	0.42
1:DB:1347:G:H22	1:DB:1374:A:P	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EB:910:A:C5	14:QB:13:GLN:HG3	2.54	0.42
2:EB:1098:A:H3'	2:EB:1099:G:C8	2.54	0.42
2:EB:1266:G:OP2	29:FC:20:ARG:NE	2.52	0.42
2:EB:2404:C:H2'	2:EB:2405:G:O4'	2.20	0.42
2:EB:2625:G:H2'	2:EB:2626:C:O4'	2.20	0.42
2:EB:2839:G:H4'	15:RB:49:ASP:HB3	2.02	0.42
10:MB:72:LEU:HD21	10:MB:107:ILE:HD13	2.02	0.42
14:QB:27:VAL:HA	14:QB:105:GLU:OE2	2.19	0.42
37:OC:85:LYS:HE2	37:OC:85:LYS:HB2	1.88	0.42
43:UC:65:LEU:HD12	43:UC:66:ARG:H	1.85	0.42
47:YC:53:LEU:HD23	47:YC:53:LEU:HA	1.82	0.42
48:ZC:70:LEU:HD22	48:ZC:70:LEU:HA	1.84	0.42
53:ED:9:ASN:O	53:ED:10:LEU:HD22	2.20	0.42
55:HD:253:ILE:HD11	55:HD:278:ILE:HG13	2.01	0.42
1:A:137:C:H2'	1:A:138:G:C8	2.54	0.42
1:A:598:U:H2'	1:A:599:C:C6	2.54	0.42
1:A:1309:G:O2'	46:UA:77:ASN:ND2	2.52	0.42
2:B:78:A:H2'	2:B:79:G:C8	2.54	0.42
2:B:322:A:OP2	7:G:169:ASN:HB2	2.19	0.42
2:B:811:U:C2	2:B:1251:C:C5	3.07	0.42
2:B:1260:G:C6	2:B:1261:C:C4	3.08	0.42
2:B:2115:G:H2'	2:B:2117:A:N7	2.35	0.42
2:B:2331:G:C6	2:B:2332:U:C4	3.08	0.42
5:E:260:ARG:NH2	5:E:264:LYS:HD3	2.35	0.42
6:F:110:GLY:O	15:O:3:HIS:CE1	2.72	0.42
10:J:87:LYS:HE2	10:J:89:TYR:HD1	1.85	0.42
11:K:94:HIS:HB3	11:K:97:ARG:HG3	2.01	0.42
20:T:30:GLU:OE2	20:T:30:GLU:HA	2.17	0.42
35:JA:61:LEU:HD23	35:JA:68:ILE:HD11	2.00	0.42
46:UA:81:LEU:HD22	46:UA:86:CYS:SG	2.60	0.42
1:DB:147:G:C2	1:DB:148:G:H1'	2.54	0.42
1:DB:431:A:H2'	1:DB:432:A:O4'	2.19	0.42
1:DB:601:C:H42	1:DB:637:G:H1	1.68	0.42
1:DB:926:G:C6	1:DB:1505:G:C5	3.08	0.42
1:DB:971:G:H22	1:DB:1363:A:P	2.43	0.42
1:DB:993:G:H4'	1:DB:994:A:OP2	2.20	0.42
2:EB:755:C:H2'	2:EB:756:C:C6	2.55	0.42
2:EB:1043:C:H5	2:EB:1112:G:H22	1.66	0.42
2:EB:1104:C:H2'	2:EB:1105:U:C6	2.54	0.42
2:EB:1656:C:H2'	2:EB:1657:C:C6	2.55	0.42
2:EB:1692:U:H2'	2:EB:1694:C:C5	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EB:2884:U:H2'	2:EB:2885:C:O4'	2.20	0.42
4:GB:63:G:H2'	4:GB:64:G:C8	2.55	0.42
6:IB:47:VAL:HG11	6:IB:86:PRO:CD	2.49	0.42
11:NB:39:ARG:HA	11:NB:40:PRO:HD3	1.88	0.42
15:RB:57:ARG:HB3	15:RB:59:ASP:OD1	2.20	0.42
16:SB:106:ARG:NE	16:SB:112:PHE:O	2.52	0.42
18:UB:47:TYR:O	18:UB:51:LYS:HG3	2.20	0.42
19:VB:85:LYS:HB3	19:VB:85:LYS:HZ3	1.83	0.42
21:XB:64:LYS:HD3	21:XB:64:LYS:HA	1.81	0.42
22:YB:90:LEU:O	22:YB:92:ASN:N	2.53	0.42
23:ZB:133:ILE:HA	23:ZB:134:PRO:HD2	1.95	0.42
25:BC:19:GLN:OE1	25:BC:19:GLN:HA	2.18	0.42
36:NC:119:ARG:O	36:NC:123:GLN:HG3	2.20	0.42
39:QC:10:LEU:HA	39:QC:10:LEU:HD23	1.80	0.42
45:WC:93:LEU:HA	45:WC:94:PRO:HD3	1.76	0.42
51:CD:65:ILE:HD12	51:CD:65:ILE:HA	1.90	0.42
55:GD:314:GLN:HB2	55:GD:316:ARG:HG2	2.02	0.42
1:A:80:G:C2	1:A:90:C:C2	3.08	0.42
1:A:345:C:H5'	1:A:346:G:C5	2.55	0.42
1:A:577:G:H1'	1:A:816:A:C4	2.55	0.42
1:A:939:G:P	40:OA:95:ARG:HH22	2.42	0.42
1:A:981:U:H5'	47:VA:21:TYR:CZ	2.55	0.42
1:A:1054:C:N3	34:HA:22:A:C6	2.88	0.42
1:A:1103:C:OP1	35:JA:96:ARG:NH2	2.52	0.42
1:A:1122:U:O4	1:A:1123:A:N6	2.53	0.42
1:A:1468:A:H2'	1:A:1469:G:O4'	2.20	0.42
2:B:277:C:O2'	2:B:278:A:H8	2.03	0.42
2:B:510:C:OP1	2:B:511:U:OP2	2.38	0.42
2:B:795:C:H2'	2:B:796:C:C6	2.55	0.42
2:B:1188:U:H4'	19:S:79:VAL:HG22	2.01	0.42
2:B:1897:G:H2'	2:B:1898:U:O4'	2.20	0.42
2:B:2138:C:H2'	2:B:2139:C:C6	2.55	0.42
2:B:2139:C:H3'	2:B:2140:C:C6	2.51	0.42
2:B:2287:A:HO2'	2:B:2288:A:P	2.42	0.42
2:B:2351:G:O6	32:FA:39:LYS:HG3	2.20	0.42
2:B:2516:G:C6	2:B:2517:C:N4	2.88	0.42
2:B:2869:G:H2'	2:B:2870:C:O4'	2.20	0.42
18:R:15:LYS:HD2	18:R:15:LYS:HA	1.93	0.42
29:CA:33:CYS:HA	29:CA:34:PRO:HD2	1.90	0.42
36:KA:95:THR:O	36:KA:97:LYS:HG3	2.20	0.42
37:LA:31:CYS:O	37:LA:34:GLU:N	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:LA:62:GLN:HE21	37:LA:62:GLN:HA	1.84	0.42
1:DB:419:C:H5''	1:DB:513:C:O4'	2.20	0.42
2:EB:273(B):G:C2	2:EB:364:C:C2	3.08	0.42
2:EB:383:U:H2'	2:EB:385:C:H5	1.84	0.42
2:EB:2444:G:OP2	7:JB:68:LYS:HD2	2.20	0.42
2:EB:2626:C:H2'	2:EB:2627:G:C8	2.55	0.42
11:NB:24:GLY:O	11:NB:28:THR:HG23	2.19	0.42
17:TB:107:ASP:O	17:TB:111:ARG:HB2	2.20	0.42
4:LC:9:G:O2'	4:LC:10:G:N7	2.52	0.42
35:MC:126:GLU:CD	35:MC:127:ILE:H	2.23	0.42
37:OC:187:ARG:NH2	37:OC:193:ASP:OD2	2.45	0.42
40:RC:80:VAL:HG21	40:RC:85:TYR:HB2	2.01	0.42
46:XC:66:LEU:O	46:XC:69:GLU:HB3	2.20	0.42
52:DD:41:VAL:HG22	52:DD:44:MET:SD	2.59	0.42
55:GD:155:GLU:HG3	55:GD:156:HIS:CE1	2.55	0.42
55:HD:217:ILE:H	55:HD:217:ILE:HG13	1.53	0.42
1:A:272:C:H2'	1:A:273:A:H8	1.84	0.42
1:A:437:U:H5'	37:LA:155:LEU:HD11	2.02	0.42
1:A:622:A:C8	1:A:623:C:C6	3.08	0.42
1:A:806:C:H2'	1:A:807:A:C8	2.55	0.42
1:A:974:A:H8	1:A:974:A:OP1	2.02	0.42
1:A:1254:C:OP1	43:RA:45:ARG:HB3	2.20	0.42
1:A:1258:G:H2'	1:A:1259:C:C6	2.55	0.42
2:B:89:G:C6	2:B:90:U:C4	3.08	0.42
2:B:270(A):A:H1'	2:B:370:G:C2	2.55	0.42
2:B:305:U:H2'	2:B:306:U:C6	2.55	0.42
2:B:2667:C:H1'	9:I:109:PHE:CD1	2.53	0.42
8:H:77:ILE:HD13	8:H:77:ILE:HA	1.90	0.42
12:L:3:GLN:HG3	12:L:4:PRO:O	2.20	0.42
14:N:61:GLY:HA2	23:W:177:PRO:HB2	2.02	0.42
15:O:80:PHE:O	15:O:85:PRO:HD3	2.19	0.42
36:KA:183:ASP:OD1	36:KA:184:TYR:N	2.53	0.42
37:LA:101:LEU:HB2	37:LA:138:TYR:HB3	2.01	0.42
39:NA:45:LEU:H	39:NA:45:LEU:HG	1.58	0.42
41:PA:127:LEU:HD13	41:PA:127:LEU:HA	1.87	0.42
50:YA:43:LEU:HD23	50:YA:43:LEU:HA	1.75	0.42
1:DB:435:C:H2'	1:DB:436:C:C6	2.55	0.42
1:DB:540:G:C5	1:DB:541:G:C5	3.07	0.42
1:DB:579:G:H2'	1:DB:580:U:C6	2.55	0.42
1:DB:1060:C:N4	36:NC:2:GLY:HA3	2.35	0.42
2:EB:16:G:H2'	2:EB:17:G:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EB:43:G:N2	2:EB:438:G:C4	2.88	0.42
2:EB:323:G:C6	2:EB:333:G:C5	3.08	0.42
2:EB:715:G:H2'	2:EB:716:A:H8	1.84	0.42
2:EB:911:A:H2'	14:QB:9:TYR:CZ	2.55	0.42
2:EB:1431:U:H2'	2:EB:1432:C:C6	2.54	0.42
2:EB:1439:A:H2'	2:EB:1440:G:O4'	2.19	0.42
2:EB:1541:U:H2'	2:EB:1542:G:O4'	2.20	0.42
2:EB:1701:A:H5''	2:EB:1702:G:OP2	2.20	0.42
2:EB:2404:C:H1'	13:PB:67:MET:HE1	2.01	0.42
6:IB:54:GLN:OE1	6:IB:55:ASN:N	2.48	0.42
6:IB:63:LEU:HA	6:IB:63:LEU:HD23	1.75	0.42
6:IB:170:LEU:HD12	6:IB:170:LEU:HA	1.70	0.42
9:LB:28:GLY:HA3	9:LB:79:VAL:HB	2.02	0.42
9:LB:54:ARG:CZ	9:LB:62:LYS:HG2	2.49	0.42
13:PB:17:LYS:HD2	13:PB:27:HIS:CE1	2.55	0.42
14:QB:64:ILE:HG13	23:ZB:178:GLU:HG3	2.01	0.42
19:VB:15:GLU:HB3	19:VB:16:PRO:HD2	2.01	0.42
20:WB:82:LEU:HD23	20:WB:84:ARG:NH1	2.35	0.42
26:CC:66:GLU:HA	26:CC:69:ARG:HH21	1.85	0.42
27:DC:5:LYS:HD3	27:DC:34:GLU:OE2	2.20	0.42
35:MC:116:GLU:HG2	35:MC:153:ARG:HH22	1.85	0.42
35:MC:179:LYS:HE3	35:MC:179:LYS:HB2	1.87	0.42
39:QC:22:GLU:O	39:QC:26:ILE:HG23	2.20	0.42
40:RC:46:ALA:O	40:RC:50:ILE:HG13	2.20	0.42
41:SC:56:LYS:HA	41:SC:57:PRO:HD3	1.81	0.42
46:XC:45:VAL:O	46:XC:48:LEU:HB2	2.20	0.42
50:BD:31:LEU:HD23	50:BD:32:TYR:CE2	2.55	0.42
1:A:756:C:O4'	41:PA:1:MET:HG2	2.19	0.41
1:A:854:G:H3'	1:A:871:U:O4	2.20	0.41
1:A:976:G:O5'	1:A:1358:U:O2'	2.37	0.41
2:B:6:A:C2	2:B:7:G:C8	3.08	0.41
2:B:1187:G:H8	2:B:1187:G:O5'	2.03	0.41
2:B:1260:G:H2'	2:B:1261:C:O4'	2.19	0.41
2:B:1464:C:H2'	2:B:1465:G:H8	1.82	0.41
2:B:1526:G:C6	2:B:1527:G:C2	3.07	0.41
2:B:1598:C:H2'	2:B:1599:C:H6	1.85	0.41
2:B:1692:U:H2'	2:B:1694:C:C5	2.55	0.41
3:C:111:U:H2'	3:C:112:G:H8	1.85	0.41
5:E:95:LEU:HD23	5:E:95:LEU:HA	1.83	0.41
9:I:95:ARG:HG3	9:I:106:THR:HB	2.02	0.41
13:M:88:LEU:HD23	13:M:88:LEU:HA	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:67:ARG:NH1	14:N:105:GLU:OE2	2.53	0.41
16:P:15:ARG:NH1	16:P:15:ARG:HG2	2.34	0.41
20:T:86:LEU:HG	20:T:88:ARG:HD3	2.02	0.41
23:W:4:ARG:NH2	23:W:60:GLU:HG2	2.35	0.41
23:W:133:ILE:HA	23:W:134:PRO:HD2	1.94	0.41
35:JA:167:PRO:HG2	35:JA:188:ALA:HB2	2.02	0.41
37:LA:149:ALA:HB3	37:LA:152:SER:HB2	2.02	0.41
41:PA:31:PHE:O	41:PA:35:ILE:HG13	2.20	0.41
41:PA:86:ILE:O	41:PA:88:LYS:HD2	2.20	0.41
42:QA:127:LYS:HB2	42:QA:127:LYS:HE3	1.79	0.41
45:TA:69:TYR:HD2	45:TA:99:HIS:CD2	2.38	0.41
1:DB:93:U:H2'	1:DB:95:G:H8	1.84	0.41
1:DB:601:C:H2'	1:DB:602:A:C8	2.55	0.41
1:DB:1120:G:H2'	1:DB:1121:U:C6	2.55	0.41
1:DB:1277:C:H1'	1:DB:1282:C:H1'	2.02	0.41
1:DB:1346:A:OP1	42:TC:120:ARG:NH1	2.44	0.41
2:EB:524:U:H2'	2:EB:525:U:C6	2.55	0.41
2:EB:528:A:HO2'	2:EB:529:A:P	2.42	0.41
2:EB:579:G:H2'	2:EB:580:C:C6	2.54	0.41
2:EB:674:G:O2'	7:JB:74:ARG:HD3	2.20	0.41
2:EB:1042:G:H2'	2:EB:1043:C:O2	2.19	0.41
2:EB:1322:A:C5	2:EB:1323:U:C5	3.08	0.41
2:EB:1477:A:H2'	2:EB:1478:G:O4'	2.19	0.41
2:EB:1759:A:C8	2:EB:2696:U:H1'	2.55	0.41
2:EB:2168:G:H2'	2:EB:2169:A:H3'	2.01	0.41
2:EB:2676:C:O2	2:EB:2732:G:N2	2.51	0.41
2:EB:2709:G:O2'	2:EB:2710:C:H5'	2.19	0.41
10:MB:9:LEU:HD12	10:MB:10:GLU:OE2	2.20	0.41
10:MB:42:SER:OG	10:MB:43:ASN:N	2.53	0.41
14:QB:75:THR:HG21	14:QB:87:LYS:HZ3	1.80	0.41
15:RB:67:LEU:HD22	15:RB:67:LEU:HA	1.90	0.41
23:ZB:24:LEU:HA	23:ZB:25:PRO:HD2	1.91	0.41
23:ZB:162:GLU:O	23:ZB:164:ALA:N	2.53	0.41
46:XC:97:PRO:HG3	46:XC:107:ALA:HB1	2.02	0.41
55:GD:110:ASN:OD1	55:GD:110:ASN:N	2.52	0.41
55:GD:149:MET:HB2	55:GD:150:SER:H	1.56	0.41
55:HD:137:ARG:HD3	55:HD:334:GLU:O	2.19	0.41
55:HD:169:ASP:OD1	55:HD:169:ASP:N	2.53	0.41
1:A:25:C:H2'	1:A:26:A:C8	2.55	0.41
1:A:67:C:H2'	1:A:68:G:H8	1.84	0.41
2:B:319:C:H2'	2:B:320:A:O4'	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:507:A:O2'	2:B:508:G:OP2	2.32	0.41
2:B:813:U:H2'	2:B:814:C:C6	2.55	0.41
2:B:836:G:H2'	2:B:837:C:C6	2.55	0.41
2:B:952:G:C6	2:B:953:A:N7	2.88	0.41
2:B:1002:G:C6	2:B:1003:G:C5	3.09	0.41
2:B:1019:U:OP1	2:B:1035:U:O2'	2.26	0.41
2:B:1425:G:N1	2:B:1426:G:C2	2.88	0.41
2:B:2038:G:H2'	2:B:2039:C:O4'	2.19	0.41
2:B:2209:C:O2	2:B:2216:G:N1	2.53	0.41
2:B:2246:G:H1'	2:B:2426:A:C2	2.55	0.41
2:B:2406:U:H5''	2:B:2408:U:OP2	2.19	0.41
2:B:2637:U:OP1	6:F:82:ARG:NH1	2.53	0.41
3:C:45:A:C4	3:C:46:A:C8	3.08	0.41
8:H:43:LEU:C	8:H:45:GLU:H	2.23	0.41
18:R:34:LYS:HD2	18:R:34:LYS:HA	1.48	0.41
35:JA:22:LYS:HZ2	35:JA:22:LYS:HA	1.85	0.41
35:JA:126:GLU:CD	35:JA:127:ILE:H	2.24	0.41
35:JA:163:PHE:HD1	35:JA:163:PHE:HA	1.71	0.41
37:LA:30:LYS:HG3	37:LA:35:ARG:NH1	2.36	0.41
37:LA:194:LEU:HD12	37:LA:194:LEU:O	2.20	0.41
38:MA:9:LYS:HZ3	38:MA:10:MET:H	1.69	0.41
48:WA:28:GLN:O	48:WA:32:LEU:HD23	2.20	0.41
50:YA:84:LEU:HD12	50:YA:87:LYS:HE2	2.02	0.41
1:DB:67:C:H2'	1:DB:68:G:H8	1.85	0.41
1:DB:403:C:O2'	37:OC:122:ARG:NH2	2.36	0.41
1:DB:1346:A:H5''	42:TC:120:ARG:HH12	1.86	0.41
1:DB:1366:C:H2'	1:DB:1367:C:H6	1.84	0.41
2:EB:1448:G:O2'	2:EB:1529:A:N1	2.43	0.41
2:EB:2292:C:OP1	16:SB:17:ARG:NH2	2.50	0.41
2:EB:2403:C:N3	2:EB:2415:G:C2	2.88	0.41
6:IB:7:VAL:HG23	6:IB:51:PHE:CE2	2.53	0.41
6:IB:181:LEU:HD12	6:IB:181:LEU:HA	1.84	0.41
7:JB:156:LEU:HD22	7:JB:156:LEU:HA	1.77	0.41
10:MB:109:ILE:HB	10:MB:130:TYR:CZ	2.55	0.41
11:NB:120:LEU:HG	11:NB:122:VAL:HG23	2.02	0.41
15:RB:54:LEU:O	15:RB:57:ARG:HB2	2.19	0.41
18:UB:15:LYS:HD2	18:UB:15:LYS:HA	1.94	0.41
33:JC:1:MET:SD	33:JC:35:ARG:HB2	2.60	0.41
36:NC:61:ALA:C	36:NC:63:ASN:H	2.23	0.41
38:PC:53:LEU:O	38:PC:57:LYS:N	2.51	0.41
43:UC:79:ARG:O	43:UC:83:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:HD:149:MET:HB2	55:HD:150:SER:H	1.56	0.41
1:A:540:G:H2'	1:A:541:G:O4'	2.20	0.41
1:A:598:U:H2'	1:A:599:C:H6	1.86	0.41
1:A:1034:G:H2'	1:A:1035:A:C8	2.55	0.41
1:A:1060:C:N4	36:KA:2:GLY:HA3	2.35	0.41
1:A:1221:G:OP1	52:AB:36:ARG:HD2	2.21	0.41
1:A:1347:G:HO2'	1:A:1373:G:H1	1.65	0.41
2:B:46:C:H42	2:B:179:G:H1	1.68	0.41
2:B:195:A:H5''	2:B:196:A:OP2	2.21	0.41
2:B:270(G):U:H2'	2:B:270(H):C:C6	2.55	0.41
2:B:528:A:OP2	11:K:114:ARG:NH2	2.53	0.41
2:B:545:G:N2	2:B:548:A:H62	2.18	0.41
2:B:1098:A:H3'	2:B:1099:G:C8	2.55	0.41
2:B:2130:U:H2'	2:B:2131:G:H21	1.85	0.41
2:B:2209:C:H1'	2:B:2216:G:N2	2.34	0.41
2:B:2271:G:H2'	2:B:2272:U:C6	2.55	0.41
2:B:2505:G:O6	2:B:2576:G:H2'	2.20	0.41
2:B:2821:A:H2'	2:B:2822:G:O4'	2.20	0.41
7:G:101:LEU:HG	7:G:102:PRO:HD2	2.02	0.41
27:AA:50:VAL:O	27:AA:54:VAL:HG12	2.20	0.41
28:BA:62:ARG:HA	28:BA:62:ARG:CZ	2.49	0.41
29:CA:19:ARG:C	29:CA:21:SER:H	2.23	0.41
38:MA:145:LYS:HB3	38:MA:145:LYS:HZ2	1.81	0.41
40:OA:46:ALA:O	40:OA:50:ILE:HG13	2.20	0.41
40:OA:69:VAL:HG21	40:OA:104:LEU:HD21	2.02	0.41
41:PA:56:LYS:HA	41:PA:57:PRO:HD3	1.80	0.41
41:PA:81:HIS:HB2	41:PA:138:TRP:HD1	1.84	0.41
49:XA:19:ILE:H	49:XA:19:ILE:HG13	1.75	0.41
1:DB:59:A:N3	1:DB:59:A:H2'	2.34	0.41
1:DB:1366:C:O3'	43:UC:60:ARG:NH2	2.53	0.41
2:EB:760:G:H2'	2:EB:761:A:O4'	2.19	0.41
2:EB:1310:G:H1	2:EB:1604:C:N4	2.13	0.41
2:EB:1641:A:H2'	2:EB:1642:G:O4'	2.20	0.41
2:EB:2053:G:H1	2:EB:2616:C:H42	1.69	0.41
3:FB:86:G:H1	3:FB:90:C:H42	1.67	0.41
5:HB:95:LEU:HA	5:HB:95:LEU:HD23	1.83	0.41
5:HB:231:HIS:ND1	5:HB:232:PRO:HD2	2.35	0.41
11:NB:38:HIS:O	18:UB:67:ALA:HB1	2.21	0.41
12:OB:113:LYS:O	12:OB:117:LEU:HG	2.20	0.41
13:PB:81:GLN:OE1	13:PB:107:LYS:N	2.50	0.41
16:SB:93:LYS:O	16:SB:95:HIS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:UB:24:TYR:HB2	18:UB:29:SER:HB3	2.03	0.41
23:ZB:53:ILE:HD11	23:ZB:99:TYR:HB2	2.03	0.41
27:DC:6:VAL:HB	27:DC:54:VAL:HG21	2.02	0.41
35:MC:167:PRO:HG2	35:MC:188:ALA:HB2	2.01	0.41
42:TC:127:LYS:HE3	42:TC:127:LYS:HB2	1.82	0.41
55:GD:110:ASN:HB2	55:GD:208:GLU:HG3	2.01	0.41
55:HD:110:ASN:OD1	55:HD:110:ASN:N	2.53	0.41
55:HD:156:HIS:HA	55:HD:157:GLY:HA2	1.75	0.41
1:A:222:U:H2'	1:A:223:U:H6	1.85	0.41
1:A:300:A:H1'	1:A:565:U:O2	2.20	0.41
1:A:1129:C:O2	1:A:1130:A:N6	2.38	0.41
1:A:1301:U:H2'	1:A:1303:C:H5	1.84	0.41
1:A:1397:C:N3	1:A:1402:4OC:OP1	2.54	0.41
2:B:705:A:H1'	5:E:9:TYR:CE2	2.55	0.41
2:B:710:G:H2'	2:B:711:G:C8	2.55	0.41
2:B:729:G:H5'	2:B:730:C:H5''	2.01	0.41
2:B:1031:G:O6	2:B:1032:A:N6	2.53	0.41
2:B:1394:U:O2	21:U:16:LYS:NZ	2.52	0.41
2:B:1593:G:C6	2:B:1594:G:C6	3.08	0.41
2:B:1766:U:H2'	2:B:1767:C:H6	1.85	0.41
2:B:2536:G:C6	2:B:2537:U:C4	3.08	0.41
3:C:16:G:N2	3:C:69:G:H1'	2.35	0.41
3:C:29:A:H2'	3:C:30:C:O4'	2.20	0.41
7:G:40:GLN:HE22	7:G:182:ASN:HB2	1.85	0.41
9:I:55:PRO:HD2	9:I:61:HIS:CD2	2.55	0.41
10:J:133:HIS:CD2	10:J:135:GLU:HB3	2.55	0.41
11:K:99:LEU:O	11:K:103:VAL:HG23	2.20	0.41
17:Q:113:LYS:O	17:Q:115:ARG:NH1	2.53	0.41
20:T:110:LYS:HA	20:T:110:LYS:HD2	1.86	0.41
23:W:17:ALA:HA	23:W:20:ARG:NH1	2.36	0.41
23:W:103:ARG:CZ	23:W:103:ARG:HA	2.50	0.41
28:BA:13:ARG:HH11	28:BA:21:VAL:CG1	2.34	0.41
31:EA:10:ARG:HH11	31:EA:14:LYS:HE3	1.85	0.41
35:JA:40:HIS:CG	35:JA:190:THR:HG21	2.55	0.41
37:LA:4:TYR:HE1	37:LA:66:ARG:HA	1.84	0.41
37:LA:113:SER:OG	37:LA:114:ARG:N	2.53	0.41
38:MA:40:ARG:CZ	38:MA:68:GLU:HB3	2.50	0.41
39:NA:76:ALA:O	39:NA:80:ARG:HG3	2.20	0.41
1:DB:41:G:H2'	1:DB:42:G:C8	2.55	0.41
1:DB:406:G:H1'	1:DB:495:A:C6	2.56	0.41
1:DB:540:G:H2'	1:DB:541:G:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DB:542:G:H5'	37:OC:41:GLY:HA3	2.01	0.41
1:DB:841:U:H3'	1:DB:842:C:H5''	2.01	0.41
1:DB:1079:G:O3'	38:PC:14:ARG:NH2	2.53	0.41
1:DB:1122:U:O4	1:DB:1123:A:N6	2.54	0.41
1:DB:1138:G:H2'	1:DB:1140:C:C5	2.55	0.41
1:DB:1258:G:H2'	1:DB:1259:C:C6	2.55	0.41
1:DB:1288:A:O3'	54:FD:10:ARG:NH2	2.53	0.41
2:EB:536:A:H2'	2:EB:537:C:C6	2.56	0.41
2:EB:1674:G:N3	2:EB:1676:A:N6	2.69	0.41
2:EB:2531:A:H61	2:EB:2662:A:H61	1.69	0.41
2:EB:2582:G:H21	2:EB:2583:G:H1'	1.84	0.41
2:EB:2717:G:C6	2:EB:2718:G:N7	2.89	0.41
9:LB:27:LYS:HA	9:LB:32:GLU:HB3	2.01	0.41
23:ZB:33:LEU:HG	23:ZB:34:ASN:N	2.36	0.41
23:ZB:125:LEU:HB3	23:ZB:165:VAL:HG13	2.02	0.41
26:CC:53:LEU:HD22	26:CC:53:LEU:HA	1.77	0.41
36:NC:67:THR:HG22	36:NC:102:ASN:HB3	2.02	0.41
37:OC:4:TYR:CE1	37:OC:66:ARG:HG2	2.55	0.41
38:PC:9:LYS:HZ3	38:PC:10:MET:H	1.67	0.41
39:QC:25:ILE:HD11	39:QC:82:ARG:HG3	2.03	0.41
39:QC:45:LEU:H	39:QC:45:LEU:HG	1.55	0.41
40:RC:45:ASP:O	40:RC:49:ILE:HG12	2.20	0.41
40:RC:56:GLN:N	40:RC:56:GLN:OE1	2.53	0.41
41:SC:63:LEU:HD13	41:SC:63:LEU:HA	1.77	0.41
1:A:452:A:O2'	1:A:453:A:OP2	2.25	0.41
1:A:564:C:H5'	50:YA:32:TYR:HE1	1.86	0.41
1:A:743:U:H2'	1:A:744:C:C6	2.55	0.41
1:A:1528:U:C2	1:A:1530:G:C8	3.09	0.41
2:B:197:A:N6	2:B:2430:A:H2'	2.35	0.41
2:B:323:G:C6	2:B:333:G:C5	3.08	0.41
2:B:784:A:H5'	2:B:785:G:OP1	2.20	0.41
2:B:858:U:O2	2:B:2268:A:H2'	2.19	0.41
2:B:1310:G:H1	2:B:1604:C:N4	2.15	0.41
2:B:1696:G:H3'	2:B:1697:G:H8	1.85	0.41
3:C:104:A:O4'	23:W:29:TYR:HE1	2.04	0.41
6:F:111:ARG:HD3	6:F:160:TYR:CD2	2.55	0.41
10:J:60:GLU:O	10:J:64:GLU:N	2.43	0.41
13:M:84:ASN:OD1	13:M:117:GLU:HB2	2.20	0.41
15:O:33:ARG:HH12	29:CA:58:LEU:HA	1.86	0.41
22:V:52:SER:HB2	22:V:53:PRO:HD2	2.03	0.41
22:V:90:LEU:O	22:V:92:ASN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:NA:97:PHE:CB	51:ZA:32:ARG:HH11	2.34	0.41
42:QA:23:ASN:ND2	42:QA:25:LYS:HE2	2.24	0.41
42:QA:34:ASN:O	42:QA:38:GLN:NE2	2.52	0.41
45:TA:93:LEU:HD23	45:TA:93:LEU:HA	1.80	0.41
46:UA:20:THR:C	46:UA:22:ILE:H	2.24	0.41
53:BB:43:LEU:HD23	53:BB:43:LEU:HA	1.84	0.41
1:DB:41:G:H2'	1:DB:42:G:H8	1.85	0.41
1:DB:287:U:H2'	1:DB:288:A:C8	2.54	0.41
2:EB:84:A:N1	2:EB:98:G:O2'	2.49	0.41
2:EB:186:G:H2'	2:EB:187:G:C8	2.54	0.41
2:EB:608:A:H2'	2:EB:609(A):A:C8	2.56	0.41
2:EB:1043:C:H2'	2:EB:1044:G:H5'	2.03	0.41
2:EB:1604:C:H2'	2:EB:1605:C:H6	1.84	0.41
2:EB:1784:A:H4'	2:EB:1785:A:C5'	2.50	0.41
2:EB:1935:G:H1'	2:EB:1964:G:N2	2.35	0.41
2:EB:2577:A:H5'	29:FC:3:LYS:NZ	2.35	0.41
2:EB:2846:G:C5	2:EB:2847:U:C5	3.08	0.41
4:GB:42:G:H5'	40:RC:143:ARG:NH1	2.35	0.41
5:HB:20:ASP:O	5:HB:21:PHE:HB2	2.21	0.41
15:RB:30:THR:HG22	15:RB:75:LEU:HD13	2.02	0.41
27:DC:31:LEU:C	27:DC:33:GLN:H	2.24	0.41
35:MC:21:ARG:HH11	35:MC:23:ARG:HD3	1.79	0.41
36:NC:123:GLN:HB3	36:NC:128:PHE:HD2	1.85	0.41
49:AD:73:LEU:HA	49:AD:73:LEU:HD23	1.84	0.41
50:BD:81:ARG:HD2	50:BD:81:ARG:HA	1.89	0.41
51:CD:27:GLY:O	51:CD:29:PHE:HD2	2.03	0.41
55:GD:253:ILE:HD11	55:GD:278:ILE:HG13	2.02	0.41
1:A:127:G:C2	1:A:128:G:C8	3.09	0.41
1:A:324:G:O2'	1:A:326:G:N7	2.40	0.41
1:A:866:C:C4	1:A:867:G:H1'	2.56	0.41
1:A:1191:A:H5''	36:KA:4:LYS:HZ2	1.86	0.41
1:A:1370:G:H2'	1:A:1371:G:H8	1.86	0.41
2:B:226:G:C2	2:B:227:A:C6	3.08	0.41
2:B:492:A:H2'	2:B:493:G:O4'	2.20	0.41
2:B:913:U:H4'	2:B:914:C:OP1	2.20	0.41
2:B:1064:C:O2'	2:B:1074:G:N2	2.53	0.41
2:B:1142(B):A:C5	2:B:1144:G:C5	3.08	0.41
2:B:1488:G:H1	2:B:1501:C:H42	1.68	0.41
2:B:1774:C:O5'	2:B:1774:C:H6	2.03	0.41
2:B:2183:C:H2'	2:B:2184:G:C8	2.56	0.41
2:B:2208:U:H4'	5:E:151:LYS:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:63:G:H2'	4:D:64:G:C8	2.55	0.41
7:G:170:LEU:HB2	7:G:173:VAL:HB	2.02	0.41
8:H:29:TRP:O	8:H:33:ARG:NH1	2.54	0.41
9:I:7:LEU:HA	9:I:8:PRO:HD3	1.77	0.41
10:J:72:LEU:HD21	10:J:107:ILE:HD13	2.03	0.41
12:L:56:ASP:N	12:L:56:ASP:OD1	2.52	0.41
12:L:113:LYS:O	12:L:117:LEU:HG	2.21	0.41
19:S:58:VAL:HG21	19:S:100:ARG:NH1	2.34	0.41
23:W:163:LEU:H	23:W:163:LEU:HD12	1.85	0.41
25:Y:2:SER:HB3	25:Y:46:LEU:HD12	2.01	0.41
29:CA:36:CYS:SG	29:CA:38:ALA:HB2	2.61	0.41
37:LA:26:CYS:SG	37:LA:31:CYS:SG	3.03	0.41
37:LA:98:GLU:OE2	37:LA:103:ASN:ND2	2.43	0.41
38:MA:45:PHE:CE2	38:MA:47:LYS:HE3	2.55	0.41
41:PA:4:ASP:HA	41:PA:5:PRO:HD2	1.90	0.41
42:QA:118:LYS:HB3	42:QA:119:ALA:H	1.67	0.41
45:TA:104:VAL:O	45:TA:107:ALA:HB3	2.21	0.41
49:XA:53:VAL:O	49:XA:57:ARG:HG3	2.21	0.41
1:DB:448:A:P	1:DB:485:G:H22	2.41	0.41
1:DB:1118:C:H2'	1:DB:1119:C:C6	2.56	0.41
1:DB:1254:C:OP1	43:UC:45:ARG:HB3	2.20	0.41
1:DB:1370:G:H2'	1:DB:1371:G:H8	1.86	0.41
2:EB:1693:U:O2'	5:HB:14:ARG:NH2	2.54	0.41
2:EB:1774:C:O5'	2:EB:1774:C:H6	2.04	0.41
2:EB:2307:G:N2	2:EB:2311:A:O2'	2.54	0.41
2:EB:2505:G:O6	2:EB:2576:G:H2'	2.21	0.41
3:FB:81:G:C6	3:FB:82:G:C5	3.09	0.41
5:HB:26:LYS:HE2	5:HB:94:LEU:HD12	2.03	0.41
8:KB:176:LEU:HD23	8:KB:176:LEU:HA	1.76	0.41
9:LB:43:VAL:HA	9:LB:52:VAL:HG12	2.01	0.41
16:SB:57:LYS:HA	16:SB:57:LYS:HD3	1.75	0.41
16:SB:71:ARG:NE	16:SB:107:GLU:OE1	2.47	0.41
23:ZB:40:ASP:HB3	23:ZB:43:GLU:CB	2.50	0.41
31:HC:3:ARG:HD3	31:HC:3:ARG:HA	1.85	0.41
35:MC:69:LEU:O	35:MC:163:PHE:N	2.52	0.41
35:MC:112:VAL:HG22	35:MC:149:LEU:HD23	2.02	0.41
35:MC:215:LEU:HD23	35:MC:215:LEU:HA	1.80	0.41
37:OC:23:GLY:HA3	37:OC:112:VAL:CG1	2.50	0.41
43:UC:49:VAL:HB	47:YC:41:ARG:HB2	2.02	0.41
45:WC:11:VAL:HG13	50:BD:29:HIS:HD2	1.85	0.41
45:WC:56:ALA:O	45:WC:58:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:ED:92:LEU:O	53:ED:96:GLY:N	2.53	0.41
55:GD:319:ASP:OD2	55:GD:344:ILE:HD11	2.21	0.41
1:A:18:C:H2'	1:A:19:C:O4'	2.20	0.41
1:A:96:G:H2'	1:A:97:U:C6	2.56	0.41
1:A:997:U:H3	1:A:1044:A:H61	1.68	0.41
1:A:1366:C:O3'	43:RA:60:ARG:NH2	2.52	0.41
1:A:1372:U:H2'	1:A:1373:G:O4'	2.21	0.41
2:B:22:C:H2'	2:B:23:G:O4'	2.21	0.41
2:B:321:G:C4	2:B:341:G:H4'	2.56	0.41
2:B:394:A:O2'	2:B:395:U:H5'	2.21	0.41
2:B:2316:C:H1'	8:H:128:ARG:NH1	2.35	0.41
2:B:2707:G:H2'	2:B:2708:G:H8	1.85	0.41
5:E:68:LYS:HD2	5:E:70:TRP:CZ2	2.55	0.41
5:E:166:GLN:HE21	5:E:166:GLN:HB3	1.66	0.41
7:G:150:GLY:HA2	7:G:172:TRP:CE3	2.56	0.41
8:H:135:LEU:HB2	8:H:155:MET:HG2	2.02	0.41
10:J:75:LEU:HD13	10:J:105:HIS:NE2	2.36	0.41
15:O:29:LEU:HD12	15:O:29:LEU:HA	1.89	0.41
16:P:17:ARG:NH1	16:P:17:ARG:HG2	2.35	0.41
16:P:68:GLN:OE1	16:P:71:ARG:NH1	2.54	0.41
21:U:53:LYS:HD3	21:U:55:ASN:HD21	1.85	0.41
25:Y:40:ARG:HE	25:Y:40:ARG:HB2	1.77	0.41
27:AA:26:LEU:HD23	27:AA:26:LEU:HA	1.90	0.41
31:EA:29:LYS:O	31:EA:33:ARG:HG3	2.20	0.41
37:LA:148:VAL:HG21	37:LA:158:ILE:HD13	2.02	0.41
38:MA:95:ALA:O	38:MA:98:THR:OG1	2.22	0.41
39:NA:10:LEU:HD23	39:NA:10:LEU:HA	1.77	0.41
41:PA:86:ILE:HD13	41:PA:86:ILE:HA	1.88	0.41
42:QA:111:ARG:HD2	47:VA:61:TRP:NE1	2.36	0.41
1:DB:272:C:H2'	1:DB:273:A:H8	1.86	0.41
1:DB:743:U:H2'	1:DB:744:C:C6	2.56	0.41
1:DB:803:G:H2'	1:DB:804:U:O4'	2.21	0.41
1:DB:1315:U:H2'	1:DB:1316:G:O4'	2.21	0.41
2:EB:479:A:H1'	2:EB:480:A:H5''	2.02	0.41
2:EB:768:G:H2'	2:EB:769:G:H8	1.85	0.41
2:EB:1105:U:H2'	2:EB:1106:G:H8	1.86	0.41
2:EB:1188:U:O2'	2:EB:1189:A:H5'	2.21	0.41
2:EB:2056:G:O2'	29:FC:8:LYS:NZ	2.49	0.41
2:EB:2115:G:H2'	2:EB:2117:A:N7	2.36	0.41
2:EB:2488:A:C6	2:EB:2489:G:C6	3.07	0.41
2:EB:2707:G:H2'	2:EB:2708:G:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:FB:45:A:O4'	8:KB:95:ARG:NH1	2.54	0.41
3:FB:83:G:H1	3:FB:93:C:H42	1.69	0.41
11:NB:5:VAL:HA	11:NB:6:PRO:HD3	1.86	0.41
11:NB:97:ARG:HA	11:NB:100:GLU:HB2	2.03	0.41
14:QB:17:LEU:HD23	14:QB:17:LEU:H	1.85	0.41
16:SB:15:ARG:HG2	16:SB:88:ASP:OD2	2.20	0.41
23:ZB:127:LYS:N	23:ZB:164:ALA:HB2	2.35	0.41
28:EC:13:ARG:HH11	28:EC:21:VAL:CG1	2.34	0.41
37:OC:4:TYR:HD2	37:OC:4:TYR:HA	1.65	0.41
44:VC:27:ASN:OD1	44:VC:28:THR:N	2.46	0.41
52:DD:18:LYS:HE3	52:DD:31:ILE:HG23	2.02	0.41
55:HD:178:GLU:OE2	55:HD:308:ARG:NH1	2.53	0.41
2:B:155:C:H6	2:B:155:C:H2'	1.70	0.41
2:B:238:C:H2'	2:B:239:U:O4'	2.21	0.41
2:B:627:A:C4	2:B:636:G:N2	2.88	0.41
2:B:1354:A:H2'	2:B:1355:G:O4'	2.20	0.41
2:B:1493:C:H4'	2:B:1494:A:OP2	2.21	0.41
2:B:1541:U:H2'	2:B:1542:G:O4'	2.19	0.41
2:B:1863:G:H1	2:B:1879:C:H42	1.67	0.41
4:D:41:C:H2'	4:D:42:G:H8	1.86	0.41
6:F:38:THR:O	6:F:42:ASP:N	2.53	0.41
9:I:101:ARG:HH11	9:I:122:THR:CG2	2.34	0.41
4:IA:51:C:C4	4:IA:52:G:N7	2.89	0.41
35:JA:47:THR:O	35:JA:51:LEU:N	2.47	0.41
45:TA:69:TYR:HB3	45:TA:99:HIS:HD2	1.85	0.41
48:WA:39:LEU:O	48:WA:43:LEU:HG	2.21	0.41
48:WA:66:LEU:HA	48:WA:66:LEU:HD12	1.82	0.41
49:XA:60:LEU:HA	49:XA:60:LEU:HD13	1.80	0.41
51:ZA:54:ARG:H	51:ZA:54:ARG:NE	2.08	0.41
1:DB:238:G:P	50:BD:25:ARG:HH22	2.43	0.41
1:DB:324:G:O2'	1:DB:326:G:N7	2.38	0.41
1:DB:836:G:C6	1:DB:851:G:C6	3.09	0.41
2:EB:710:G:H2'	2:EB:711:G:H8	1.85	0.41
2:EB:1151:G:O3'	18:UB:81:HIS:HB2	2.21	0.41
2:EB:1153:C:H2'	2:EB:1154:G:O4'	2.21	0.41
2:EB:1156:A:H4'	2:EB:1157:G:OP2	2.21	0.41
2:EB:1359:A:H2'	2:EB:1360:A:H5'	2.03	0.41
2:EB:2406:U:H5''	2:EB:2408:U:OP2	2.21	0.41
5:HB:5:LYS:HD2	5:HB:5:LYS:HA	1.63	0.41
5:HB:75:ILE:HD12	5:HB:75:ILE:H	1.85	0.41
5:HB:118:VAL:N	5:HB:129:ASN:OD1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:LB:164:TYR:HB2	9:LB:167:GLU:HB2	2.03	0.41
11:NB:128:HIS:HA	11:NB:129:PRO:HD3	1.91	0.41
19:VB:28:GLU:HA	19:VB:29:PRO:HD2	1.87	0.41
20:WB:82:LEU:HB3	20:WB:84:ARG:NH1	2.36	0.41
21:XB:5:TYR:OH	26:CC:30:ARG:HD2	2.21	0.41
23:ZB:4:ARG:HG2	23:ZB:58:VAL:HB	2.02	0.41
24:AC:5:LYS:HB3	55:HD:265:LYS:NZ	2.36	0.41
24:AC:50:ASN:HB2	24:AC:81:VAL:HB	2.03	0.41
28:EC:62:ARG:HA	28:EC:62:ARG:CZ	2.50	0.41
35:MC:157:ARG:HE	35:MC:157:ARG:N	2.18	0.41
36:NC:150:LYS:HG3	36:NC:169:ALA:HB2	2.01	0.41
37:OC:108:LEU:HD23	37:OC:108:LEU:HA	1.77	0.41
37:OC:163:GLU:HA	37:OC:166:LYS:HE2	2.01	0.41
41:SC:86:ILE:HG13	41:SC:133:LEU:HD22	2.03	0.41
45:WC:27:LEU:HD13	45:WC:98:TYR:CE1	2.56	0.41
48:ZC:34:LEU:HD12	48:ZC:34:LEU:HA	1.91	0.41
51:CD:41:LYS:HB3	51:CD:41:LYS:HE3	1.83	0.41
55:GD:138:TYR:OH	55:GD:341:ILE:HD11	2.21	0.41
55:GD:247:THR:HG23	55:GD:254:VAL:HG12	2.02	0.41
1:A:427:U:C4	1:A:428:G:C6	3.09	0.41
1:A:431:A:H2'	1:A:432:A:O4'	2.21	0.41
1:A:450:G:H4'	49:XA:41:PRO:O	2.21	0.41
1:A:524:G:H2'	1:A:525:C:C6	2.55	0.41
1:A:577:G:C8	1:A:816:A:C6	3.08	0.41
1:A:719:C:O2'	51:ZA:49:LYS:HB3	2.20	0.41
1:A:738:C:H5''	39:NA:69:GLU:HB2	2.02	0.41
1:A:836:G:C6	1:A:851:G:C6	3.08	0.41
1:A:952:U:H2'	1:A:953:G:C8	2.55	0.41
1:A:978:A:C4	1:A:1319:A:C2	3.09	0.41
1:A:1005:A:N1	1:A:1024:G:H1'	2.36	0.41
1:A:1123:A:H2	1:A:1150:U:H3	1.69	0.41
1:A:1167:A:H2'	1:A:1169:A:O4'	2.21	0.41
1:A:1473:A:H2'	1:A:1474:G:C8	2.56	0.41
2:B:185:U:H2'	2:B:186:G:H8	1.86	0.41
2:B:243:U:OP2	32:FA:8:LYS:NZ	2.53	0.41
2:B:656:G:C6	2:B:657:U:C4	3.09	0.41
2:B:724:U:H2'	2:B:725:G:O4'	2.21	0.41
2:B:744:G:H2'	2:B:745:G:O4'	2.21	0.41
2:B:1020:A:H4'	2:B:1021:A:O5'	2.20	0.41
2:B:1105:U:H2'	2:B:1106:G:H8	1.86	0.41
2:B:1798:U:H5'	5:E:259:THR:OG1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1907:G:H2'	2:B:1908:C:C6	2.56	0.41
2:B:1939:5MU:H3'	2:B:1940:U:H5'	2.02	0.41
2:B:2056:G:OP2	2:B:2057:A:OP2	2.39	0.41
2:B:2119:A:H2	2:B:2170:A:H2'	1.84	0.41
2:B:2168:G:O2'	2:B:2170:A:N7	2.54	0.41
2:B:2466:C:C2	2:B:2485:G:C2	3.09	0.41
2:B:2712(A):A:H5'	2:B:2713:A:OP2	2.19	0.41
2:B:2810:A:H2'	2:B:2811:G:O4'	2.21	0.41
5:E:52:ARG:HB2	5:E:53:PHE:CE2	2.56	0.41
5:E:75:ILE:HG22	5:E:76:PRO:O	2.21	0.41
6:F:63:LEU:HD23	6:F:63:LEU:HA	1.79	0.41
8:H:62:LEU:HD22	8:H:62:LEU:HA	1.86	0.41
8:H:123:ASN:C	8:H:125:PHE:H	2.24	0.41
10:J:5:LEU:H	10:J:5:LEU:HD12	1.85	0.41
12:L:102:VAL:HB	12:L:106:LEU:HD12	2.03	0.41
15:O:54:LEU:O	15:O:57:ARG:HB2	2.20	0.41
19:S:74:LYS:HA	19:S:74:LYS:HD2	1.90	0.41
23:W:33:LEU:HG	23:W:34:ASN:N	2.36	0.41
23:W:68:PRO:O	23:W:91:LEU:N	2.48	0.41
25:Y:72:GLU:O	25:Y:75:GLU:HB3	2.21	0.41
35:JA:7:VAL:HG23	35:JA:8:LYS:NZ	2.35	0.41
35:JA:76:GLN:H	35:JA:76:GLN:HG3	1.65	0.41
35:JA:82:ARG:HB2	35:JA:94:ASN:ND2	2.36	0.41
36:KA:131:ARG:HH11	36:KA:135:LYS:CE	2.25	0.41
38:MA:48:ALA:O	38:MA:50:GLU:N	2.54	0.41
38:MA:50:GLU:OE2	38:MA:51:VAL:N	2.44	0.41
38:MA:69:VAL:HA	38:MA:70:PRO:HD3	1.79	0.41
39:NA:14:LEU:HD23	39:NA:14:LEU:HA	1.80	0.41
39:NA:75:LEU:O	39:NA:79:LEU:HG	2.21	0.41
41:PA:28:ALA:HA	41:PA:59:LEU:HG	2.02	0.41
42:QA:55:ALA:HA	42:QA:58:ARG:HB2	2.03	0.41
43:RA:7:LYS:HZ1	43:RA:40:LEU:HD23	1.86	0.41
43:RA:96:ILE:HD12	43:RA:96:ILE:O	2.21	0.41
44:SA:23:ALA:HB1	44:SA:88:GLY:HA3	2.01	0.41
47:VA:24:CYS:HB3	47:VA:28:GLY:H	1.85	0.41
48:WA:34:LEU:HD12	48:WA:34:LEU:HA	1.95	0.41
1:DB:6:G:O2'	1:DB:7:G:H5''	2.20	0.41
1:DB:127:G:C2	1:DB:128:G:C8	3.09	0.41
1:DB:142:G:H2'	1:DB:143:A:C8	2.56	0.41
1:DB:303:A:H2'	1:DB:304:U:O4'	2.21	0.41
1:DB:377:G:H2'	1:DB:378:G:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DB:442:C:H2'	1:DB:443:C:C6	2.56	0.41
1:DB:740:U:OP2	48:ZC:2:PRO:HB3	2.21	0.41
1:DB:769:G:H4'	1:DB:1513:A:H4'	2.02	0.41
1:DB:1240:U:C5	40:RC:32:ARG:NH1	2.89	0.41
1:DB:1328:C:H2'	1:DB:1329:A:C8	2.55	0.41
1:DB:1406:U:H2'	1:DB:1407:5MC:O4'	2.21	0.41
2:EB:1493:C:N3	2:EB:2210:G:C4	2.88	0.41
2:EB:1667:G:O2'	2:EB:1991:U:O4	2.31	0.41
2:EB:1786:A:C2	2:EB:1938:A:C5	3.08	0.41
2:EB:1812:A:O2'	5:HB:45:ASN:N	2.54	0.41
2:EB:1897:G:H2'	2:EB:1898:U:O4'	2.21	0.41
2:EB:1899:G:N3	2:EB:1899:G:H2'	2.36	0.41
2:EB:1916:A:H2'	2:EB:1917:PSU:O4'	2.21	0.41
2:EB:1999:C:H4'	2:EB:2723:C:O2	2.21	0.41
2:EB:2119:A:H2	2:EB:2170:A:H2'	1.85	0.41
2:EB:2164:C:H42	2:EB:2166:G:N2	2.19	0.41
2:EB:2207:C:C2	2:EB:2218:G:C2	3.09	0.41
2:EB:2319:G:N2	16:SB:3:ARG:HA	2.36	0.41
2:EB:2533:A:H4'	2:EB:2664:G:H4'	2.03	0.41
2:EB:2633:G:H2'	2:EB:2634:G:O4'	2.21	0.41
2:EB:2695:C:O2'	2:EB:2696:U:H5'	2.21	0.41
2:EB:2869:G:H2'	2:EB:2870:C:O4'	2.21	0.41
4:GB:28:C:H2'	4:GB:29:G:H8	1.86	0.41
4:GB:38:A:H2'	4:GB:39:C:O4'	2.20	0.41
4:GB:40:C:H2'	4:GB:41:C:C6	2.56	0.41
5:HB:61:LEU:HD12	5:HB:61:LEU:HA	1.83	0.41
6:IB:11:MET:HG2	6:IB:24:THR:CB	2.50	0.41
6:IB:101:ARG:HD3	6:IB:171:GLU:HA	2.03	0.41
8:KB:33:ARG:O	8:KB:162:THR:HG23	2.21	0.41
8:KB:62:LEU:HA	8:KB:62:LEU:HD22	1.83	0.41
9:LB:154:PRO:HA	9:LB:161:GLY:HA3	2.02	0.41
11:NB:41:ASP:OD1	11:NB:48:MET:HE1	2.21	0.41
12:OB:101:PRO:HD2	17:TB:70:VAL:HB	2.03	0.41
13:PB:49:ARG:HB3	32:IC:61:LEU:CD2	2.51	0.41
13:PB:75:ILE:H	13:PB:75:ILE:HG12	1.77	0.41
13:PB:90:ARG:HB3	13:PB:90:ARG:NH1	2.36	0.41
20:WB:7:ALA:HB3	20:WB:50:VAL:HG22	2.02	0.41
22:YB:2:ARG:H	22:YB:2:ARG:HD3	1.84	0.41
22:YB:20:TYR:CZ	22:YB:43:ASN:HA	2.56	0.41
22:YB:66:PRO:O	22:YB:67:LEU:HD23	2.20	0.41
34:KC:13:A:H2'	34:KC:14:A:H4'	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:NC:6:HIS:HA	36:NC:7:PRO:HD2	1.95	0.41
37:OC:12:CYS:SG	37:OC:31:CYS:SG	3.18	0.41
37:OC:170:VAL:HB	37:OC:174:LEU:HB2	2.03	0.41
37:OC:190:ASP:O	37:OC:193:ASP:HB2	2.21	0.41
38:PC:118:ILE:HG12	38:PC:119:LEU:H	1.85	0.41
46:XC:20:THR:C	46:XC:22:ILE:H	2.24	0.41
50:BD:59:ILE:HG22	50:BD:73:VAL:HA	2.02	0.41
54:FD:12:LYS:HB3	54:FD:17:THR:O	2.20	0.41
55:GD:221:ASP:HB2	55:GD:250:PRO:HD3	2.03	0.41
55:GD:306:ARG:HE	55:GD:306:ARG:HB2	1.69	0.41
1:A:81:G:N2	1:A:89:U:O2	2.54	0.41
1:A:745:C:H1'	1:A:836:G:O2'	2.21	0.41
1:A:978:A:OP1	1:A:1361:G:N1	2.41	0.41
1:A:1261:A:N1	1:A:1275:A:H1'	2.36	0.41
1:A:1423:G:P	12:L:49:ARG:HH12	2.44	0.41
2:B:262:A:H2'	2:B:263:C:O4'	2.20	0.41
2:B:307:G:H22	2:B:310:A:P	2.44	0.41
2:B:706:A:C2	2:B:707:G:H1'	2.56	0.41
2:B:911:A:H2'	14:N:9:TYR:CZ	2.56	0.41
2:B:1392:A:C6	2:B:1393:A:C6	3.09	0.41
2:B:2303:G:H1	2:B:2313:C:H42	1.69	0.41
2:B:2777:G:C8	2:B:2777:G:H3'	2.56	0.41
2:B:2864:G:OP1	17:Q:119:LYS:HE3	2.22	0.41
5:E:142:VAL:HA	5:E:194:GLY:H	1.85	0.41
9:I:55:PRO:HB2	9:I:56:SER:H	1.72	0.41
9:I:164:TYR:HB2	9:I:167:GLU:HB2	2.01	0.41
12:L:4:PRO:O	12:L:5:GLN:HB2	2.21	0.41
14:N:79:LEU:O	14:N:80:GLU:HB3	2.21	0.41
29:CA:51:TYR:CE2	29:CA:56:LYS:HD3	2.55	0.41
31:EA:10:ARG:NH1	31:EA:14:LYS:CE	2.83	0.41
33:GA:2:LYS:NZ	33:GA:4:ARG:NE	2.69	0.41
34:HA:19:U:C4	34:HA:20:A:C6	3.09	0.41
36:KA:65:ALA:HA	36:KA:100:ALA:HB2	2.02	0.41
40:OA:70:LYS:HA	40:OA:71:PRO:HD3	1.68	0.41
42:QA:107:ARG:H	42:QA:107:ARG:HG2	1.65	0.41
46:UA:65:LYS:HB3	46:UA:70:LEU:HA	2.02	0.41
46:UA:66:LEU:O	46:UA:69:GLU:HB3	2.21	0.41
49:XA:14:ASN:N	49:XA:15:PRO:HD3	2.35	0.41
52:AB:29:ARG:HA	52:AB:29:ARG:HH11	1.86	0.41
1:DB:77:C:H2'	1:DB:78:G:C8	2.56	0.41
1:DB:78:G:H2'	1:DB:79:G:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DB:465:A:O2'	1:DB:466:G:H5'	2.21	0.41
1:DB:859:A:H2'	1:DB:860:A:O4'	2.21	0.41
1:DB:866:C:C4	1:DB:867:G:H1'	2.56	0.41
1:DB:950:U:H2'	1:DB:951:G:H8	1.85	0.41
1:DB:1366:C:H2'	1:DB:1367:C:C6	2.56	0.41
2:EB:305:U:H2'	2:EB:306:U:C6	2.56	0.41
2:EB:545:G:C2	2:EB:547:A:OP2	2.74	0.41
2:EB:675:A:C4	2:EB:804:A:C2	3.09	0.41
2:EB:1051:G:H4'	2:EB:2752:C:H4'	2.02	0.41
2:EB:1493:C:H42	2:EB:2210:G:H1'	1.86	0.41
2:EB:1592:C:H2'	2:EB:1593:G:C8	2.56	0.41
2:EB:1823:G:OP1	5:HB:54:ARG:NH1	2.50	0.41
2:EB:1882:C:H2'	2:EB:1883:G:O4'	2.20	0.41
2:EB:1927:A:C6	2:EB:1928:A:C6	3.08	0.41
2:EB:2316:C:H1'	8:KB:128:ARG:CZ	2.50	0.41
21:XB:53:LYS:HD3	21:XB:55:ASN:HD21	1.85	0.41
23:ZB:123:ASP:OD2	23:ZB:123:ASP:N	2.54	0.41
38:PC:31:LEU:HD11	38:PC:129:ILE:HA	2.03	0.41
46:XC:59:TYR:CD2	46:XC:60:VAL:HG13	2.56	0.41
50:BD:29:HIS:HA	50:BD:30:PRO:HD3	1.75	0.41
1:A:49:U:C2	1:A:361:G:N2	2.89	0.40
1:A:59:A:H2'	1:A:59:A:N3	2.36	0.40
1:A:125:U:C2	1:A:126:G:N7	2.89	0.40
1:A:145:G:N2	1:A:146:G:H1'	2.36	0.40
1:A:767:A:H2'	1:A:768:A:O4'	2.21	0.40
1:A:1048:G:OP1	47:VA:3:ARG:HB3	2.21	0.40
1:A:1240:U:C2	40:OA:32:ARG:HD2	2.56	0.40
1:A:1500:A:OP2	1:A:1505:G:OP2	2.39	0.40
2:B:284:U:H2'	2:B:285:C:C6	2.56	0.40
2:B:362:U:O2'	2:B:363(A):G:H5''	2.21	0.40
2:B:484:C:H2'	2:B:485:C:C6	2.56	0.40
2:B:900:A:C4	2:B:901:A:C8	3.09	0.40
2:B:1011:G:C2	2:B:1013:C:C2	3.09	0.40
2:B:1469:A:H2'	2:B:1470:G:O4'	2.21	0.40
2:B:1778:U:O2'	2:B:1779:U:H5'	2.21	0.40
2:B:2071:A:H2'	2:B:2072:G:H8	1.86	0.40
2:B:2353:G:O2'	24:X:33:ALA:O	2.29	0.40
2:B:2572:A:C8	6:F:144:ARG:HD3	2.56	0.40
2:B:2811:G:H1	2:B:2889:C:H42	1.67	0.40
8:H:115:ARG:NH2	46:UA:7:VAL:HG13	2.36	0.40
9:I:28:GLY:HA3	9:I:79:VAL:HB	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:67:LEU:O	9:I:71:LEU:HB2	2.21	0.40
13:M:122:PRO:O	13:M:123:LEU:HD23	2.21	0.40
15:O:48:VAL:HA	15:O:51:LEU:HD12	2.03	0.40
23:W:4:ARG:HG2	23:W:58:VAL:HB	2.03	0.40
23:W:95:PRO:CA	23:W:130:PRO:HD3	2.48	0.40
23:W:137:ILE:HD11	23:W:158:PRO:HD3	2.03	0.40
40:OA:22:LEU:HA	40:OA:25:ALA:HB3	2.03	0.40
42:QA:48:GLU:N	42:QA:49:PRO:HD2	2.36	0.40
43:RA:65:LEU:HD12	43:RA:66:ARG:H	1.86	0.40
46:UA:4:ILE:HA	46:UA:5:ALA:HA	1.73	0.40
1:DB:540:G:H2'	1:DB:541:G:C8	2.56	0.40
1:DB:659:U:OP1	48:ZC:8:LYS:HD3	2.21	0.40
1:DB:671:G:H2'	1:DB:672:U:O4'	2.21	0.40
1:DB:741:G:H2'	1:DB:742:G:O4'	2.21	0.40
1:DB:1152:A:H2'	1:DB:1153:C:H6	1.87	0.40
1:DB:1269:A:H5'	54:FD:19:GLY:HA2	2.02	0.40
1:DB:1338:G:C6	1:DB:1339:A:C6	3.09	0.40
1:DB:1403:C:H1'	1:DB:1500:A:N1	2.36	0.40
2:EB:687:C:H2'	2:EB:688:U:O4'	2.22	0.40
2:EB:828:U:C5	2:EB:2247:A:H4'	2.56	0.40
2:EB:1457:A:C2	2:EB:2703:C:N3	2.89	0.40
2:EB:1751:C:H2'	2:EB:1752:C:C6	2.56	0.40
2:EB:2305:A:C6	2:EB:2306:C:C4	3.10	0.40
8:KB:7:LEU:HD22	8:KB:7:LEU:HA	1.92	0.40
14:QB:79:LEU:O	14:QB:80:GLU:HB3	2.20	0.40
14:QB:109:VAL:HG12	14:QB:114:ALA:HB2	2.03	0.40
35:MC:163:PHE:HD1	35:MC:163:PHE:HA	1.72	0.40
36:NC:23:TYR:CG	36:NC:24:ALA:N	2.89	0.40
37:OC:205:GLU:OE2	38:PC:100:VAL:HG23	2.21	0.40
40:RC:146:GLU:HA	40:RC:146:GLU:OE2	2.20	0.40
46:XC:4:ILE:HA	46:XC:5:ALA:HA	1.72	0.40
53:ED:45:GLN:HB3	53:ED:46:GLU:OE2	2.21	0.40
1:A:153:C:H42	1:A:168:G:H1	1.69	0.40
1:A:227:G:H2'	1:A:228:A:C8	2.56	0.40
1:A:287:U:H2'	1:A:288:A:C8	2.54	0.40
1:A:584:G:H2'	1:A:585:G:C8	2.57	0.40
1:A:685:G:C2	1:A:686:U:C4	3.09	0.40
1:A:904:C:H2'	1:A:905:U:O4'	2.22	0.40
1:A:993:G:H4'	1:A:994:A:OP2	2.21	0.40
1:A:1150:U:O4	1:A:1151:A:N6	2.51	0.40
1:A:1240:U:C6	40:OA:32:ARG:NH1	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:401:A:C2	2:B:402:A:C4	3.09	0.40
2:B:1409:C:H2'	2:B:1410:G:C8	2.56	0.40
2:B:1449:G:H2'	2:B:1450:C:C6	2.56	0.40
2:B:1882:C:H2'	2:B:1883:G:O4'	2.21	0.40
2:B:2367:G:O2'	2:B:2368:C:H5'	2.21	0.40
2:B:2788:C:O2'	2:B:2809:A:N3	2.49	0.40
3:C:75:G:H1'	23:W:27:VAL:HG11	2.03	0.40
5:E:51:VAL:HG11	5:E:54:ARG:NH1	2.36	0.40
26:Z:17:SER:O	26:Z:20:GLU:N	2.46	0.40
36:KA:142:MET:HG3	36:KA:170:GLN:HB2	2.04	0.40
53:BB:101:GLY:O	53:BB:103:GLY:N	2.54	0.40
1:DB:977:A:O2'	1:DB:979:C:OP2	2.31	0.40
1:DB:1240:U:C2	40:RC:32:ARG:HD2	2.56	0.40
1:DB:1347:G:N2	1:DB:1374:A:O5'	2.47	0.40
1:DB:1474:G:H4'	2:EB:1701:A:N3	2.36	0.40
2:EB:778:G:C6	2:EB:779:U:N3	2.89	0.40
2:EB:1056:G:N2	2:EB:1102:C:OP2	2.52	0.40
2:EB:2138:C:H2'	2:EB:2139:C:C6	2.55	0.40
6:IB:195:LEU:HA	6:IB:195:LEU:HD22	1.78	0.40
9:LB:55:PRO:HD2	9:LB:61:HIS:CD2	2.55	0.40
14:QB:34:LEU:HD12	14:QB:130:LYS:O	2.21	0.40
19:VB:1:MET:HA	19:VB:42:GLY:HA3	2.03	0.40
24:AC:6:GLY:O	4:LC:1:C:O2'	2.35	0.40
30:GC:19:ARG:HG3	30:GC:19:ARG:HH11	1.85	0.40
36:NC:139:GLN:HB3	36:NC:140:ARG:CZ	2.52	0.40
39:QC:14:LEU:HA	39:QC:14:LEU:HD23	1.81	0.40
47:YC:24:CYS:HB3	47:YC:28:GLY:H	1.86	0.40
49:AD:38:TYR:CZ	49:AD:50:LYS:HB2	2.56	0.40
55:GD:314:GLN:CB	55:GD:316:ARG:HG2	2.51	0.40
1:A:303:A:H2'	1:A:304:U:O4'	2.20	0.40
1:A:321:A:C2	1:A:333:G:C2	3.10	0.40
1:A:523:A:N1	45:TA:92:0TD:H6	2.37	0.40
1:A:1327:C:OP1	54:CB:20:LYS:HB3	2.21	0.40
2:B:971:C:H2'	2:B:972:G:O4'	2.22	0.40
2:B:1971:A:N3	5:E:240:ALA:HA	2.36	0.40
2:B:2011:U:H2'	2:B:2012:G:O4'	2.21	0.40
2:B:2514:U:H2'	2:B:2515:C:H6	1.84	0.40
2:B:2540:C:H2'	2:B:2541:A:O4'	2.22	0.40
2:B:2633:G:H2'	2:B:2634:G:O4'	2.21	0.40
2:B:2808:U:O2'	2:B:2809:A:H5'	2.22	0.40
4:D:71:C:H2'	4:D:72:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:60:ASN:OD1	6:F:60:ASN:N	2.51	0.40
8:H:31:VAL:HA	8:H:32:PRO:HD3	1.91	0.40
11:K:97:ARG:HA	11:K:100:GLU:HB2	2.03	0.40
11:K:128:HIS:HA	11:K:129:PRO:HD3	1.93	0.40
30:DA:27:LYS:HD2	30:DA:27:LYS:HA	1.91	0.40
32:FA:23:VAL:HG12	32:FA:49:VAL:HA	2.02	0.40
35:JA:23:ARG:NH1	35:JA:23:ARG:HB2	2.36	0.40
37:LA:108:LEU:HD23	37:LA:170:VAL:HG11	2.02	0.40
38:MA:43:LEU:HD12	38:MA:44:GLY:H	1.86	0.40
41:PA:69:ARG:O	41:PA:74:PRO:HA	2.22	0.40
49:XA:38:TYR:CZ	49:XA:50:LYS:HB2	2.56	0.40
1:DB:251:G:H4'	1:DB:252:U:O5'	2.21	0.40
1:DB:574:A:H5''	1:DB:575:G:OP2	2.21	0.40
1:DB:1507:A:C2	1:DB:1508:G:C4	3.09	0.40
2:EB:22:C:H2'	2:EB:23:G:O4'	2.21	0.40
2:EB:41:C:H2'	2:EB:43:G:O4'	2.21	0.40
2:EB:265:A:H1'	2:EB:266:G:O4'	2.22	0.40
2:EB:634:C:H2'	2:EB:635:C:H6	1.87	0.40
2:EB:956:G:OP2	14:QB:14:ARG:NH1	2.52	0.40
2:EB:2041:U:H2'	2:EB:2042:A:C8	2.57	0.40
2:EB:2592:G:C6	2:EB:2593:U:C2	3.09	0.40
10:MB:82:ARG:HB3	10:MB:83:ALA:H	1.78	0.40
12:OB:3:GLN:HG3	12:OB:4:PRO:O	2.22	0.40
15:RB:33:ARG:HH12	29:FC:58:LEU:HA	1.86	0.40
31:HC:27:GLY:O	31:HC:30:VAL:HB	2.22	0.40
32:IC:53:PRO:O	32:IC:57:ARG:HG3	2.22	0.40
34:KC:21:A:H2'	55:HD:197:HIS:CD2	2.57	0.40
35:MC:21:ARG:HB3	35:MC:22:LYS:H	1.62	0.40
35:MC:105:PHE:HA	35:MC:108:ILE:HG22	2.04	0.40
36:NC:28:GLN:HA	36:NC:31:HIS:CE1	2.56	0.40
43:UC:96:ILE:O	43:UC:96:ILE:HD12	2.21	0.40
45:WC:89:ARG:HH12	45:WC:95:GLY:H	1.69	0.40
55:GD:217:ILE:H	55:GD:217:ILE:HG13	1.53	0.40
55:HD:314:GLN:CB	55:HD:316:ARG:HG2	2.52	0.40
55:HD:334:GLU:HA	55:HD:334:GLU:OE2	2.20	0.40
1:A:147:G:C2	1:A:148:G:H1'	2.55	0.40
1:A:161:A:H2'	1:A:162:A:C8	2.57	0.40
1:A:908:A:H2'	1:A:909:A:C8	2.56	0.40
1:A:1103:C:H2'	1:A:1104:G:O4'	2.22	0.40
1:A:1480:G:H2'	1:A:1481:U:O4'	2.21	0.40
1:A:1522:U:H2'	1:A:1523:G:C8	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:528:A:P	11:K:114:ARG:HH22	2.44	0.40
2:B:634:C:H2'	2:B:635:C:C6	2.56	0.40
2:B:690:G:H2'	2:B:691:C:C6	2.56	0.40
2:B:1635:G:C2	2:B:1636:C:C2	3.09	0.40
2:B:1751:C:H2'	2:B:1752:C:C6	2.57	0.40
2:B:2364:C:H2'	2:B:2365:G:O4'	2.21	0.40
2:B:2582:G:H21	2:B:2583:G:H1'	1.87	0.40
2:B:2595:G:N2	2:B:2599:G:C5	2.90	0.40
3:C:48:A:P	16:P:30:ARG:HH22	2.44	0.40
3:C:86:G:H1	3:C:90:C:H42	1.68	0.40
7:G:184:TYR:O	7:G:188:ARG:HB2	2.21	0.40
8:H:138:GLN:HE21	8:H:149:VAL:HG22	1.86	0.40
10:J:53:ALA:HB1	10:J:57:ARG:NH1	2.37	0.40
10:J:128:LEU:HD12	10:J:128:LEU:H	1.86	0.40
17:Q:129:ARG:HD2	17:Q:129:ARG:O	2.21	0.40
35:JA:149:LEU:O	35:JA:151:GLY:N	2.55	0.40
36:KA:35:GLU:HG3	36:KA:59:ARG:HH22	1.87	0.40
36:KA:85:ARG:HG2	36:KA:88:ARG:NH2	2.36	0.40
37:LA:202:LEU:HD12	37:LA:202:LEU:HA	1.76	0.40
38:MA:20:GLN:HE21	38:MA:25:ARG:NH2	2.19	0.40
1:DB:262:A:N6	1:DB:263:A:N6	2.69	0.40
1:DB:344:A:H4'	1:DB:345:C:OP2	2.21	0.40
1:DB:952:U:H2'	1:DB:953:G:C8	2.57	0.40
1:DB:986:A:C6	1:DB:987:G:C6	3.09	0.40
1:DB:1099:G:OP2	35:MC:148:TYR:OH	2.40	0.40
1:DB:1301:U:H2'	1:DB:1303:C:H5	1.85	0.40
2:EB:492:A:H2'	2:EB:493:G:O4'	2.21	0.40
2:EB:777:A:C2	2:EB:778:G:C4	3.10	0.40
2:EB:926:A:H2'	2:EB:928:G:H8	1.87	0.40
2:EB:1670:C:C4	2:EB:1671:U:C2	3.09	0.40
2:EB:2307:G:H5'	2:EB:2308:G:C2	2.56	0.40
3:FB:11:C:H3'	3:FB:12:C:C6	2.56	0.40
3:FB:45:A:H2'	3:FB:46:A:O4'	2.21	0.40
7:JB:117:ARG:NH1	7:JB:117:ARG:HG2	2.36	0.40
12:OB:102:VAL:HB	12:OB:106:LEU:HD12	2.02	0.40
24:AC:17:GLN:N	24:AC:17:GLN:HE21	2.20	0.40
25:BC:3:LYS:HB3	25:BC:4:VAL:H	1.59	0.40
4:LC:2:G:H2'	4:LC:3:C:C6	2.57	0.40
36:NC:75:VAL:HG12	36:NC:83:ARG:NH1	2.36	0.40
37:OC:70:ILE:HG23	37:OC:75:PHE:HB2	2.04	0.40
40:RC:80:VAL:HG11	40:RC:85:TYR:CD2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:SC:64:LYS:HG2	41:SC:79:VAL:HG11	2.03	0.40
42:TC:48:GLU:N	42:TC:49:PRO:HD2	2.36	0.40
42:TC:111:ARG:HD2	47:YC:61:TRP:CE2	2.56	0.40
45:WC:124:LYS:HA	45:WC:125:PRO:HD2	1.93	0.40
53:ED:51:GLU:O	53:ED:55:ILE:HG12	2.21	0.40
1:A:78:G:H2'	1:A:79:G:O4'	2.22	0.40
1:A:1306:A:H1'	1:A:1332:A:C2	2.57	0.40
1:A:1521:G:H2'	1:A:1522:U:O4'	2.22	0.40
2:B:331:A:C4	2:B:1209:G:C6	3.09	0.40
2:B:500:G:N2	2:B:503:A:C8	2.90	0.40
2:B:957:A:N1	2:B:2458:G:H4'	2.37	0.40
2:B:2041:U:H2'	2:B:2042:A:C8	2.55	0.40
2:B:2557:G:H2'	2:B:2558:C:H6	1.83	0.40
2:B:2625:G:H2'	2:B:2626:C:O4'	2.22	0.40
2:B:2637:U:H1'	2:B:2782:G:N2	2.37	0.40
2:B:2717:G:C6	2:B:2718:G:N7	2.90	0.40
22:V:99:CYS:SG	22:V:100:ALA:N	2.95	0.40
23:W:136:PHE:HD1	23:W:136:PHE:HA	1.77	0.40
36:KA:122:GLU:O	36:KA:126:ARG:HG2	2.22	0.40
40:OA:56:GLN:OE1	40:OA:56:GLN:N	2.55	0.40
44:SA:27:ASN:ND2	44:SA:55:LYS:HD3	2.37	0.40
1:DB:96:G:H2'	1:DB:97:U:C6	2.56	0.40
1:DB:157:G:C2	1:DB:165:C:C2	3.10	0.40
1:DB:451:A:C2	1:DB:480:U:C4	3.09	0.40
1:DB:1221:G:OP1	52:DD:36:ARG:HD2	2.22	0.40
1:DB:1293:G:H2'	1:DB:1294:G:H8	1.86	0.40
1:DB:1347:G:HO2'	1:DB:1373:G:H1	1.68	0.40
2:EB:748:G:H5'	2:EB:749:C:OP2	2.22	0.40
2:EB:836:G:H2'	2:EB:837:C:C6	2.57	0.40
2:EB:932:G:P	27:DC:24:LYS:HZ1	2.45	0.40
2:EB:963:U:H2'	2:EB:964:C:C6	2.57	0.40
2:EB:1142(B):A:C5	2:EB:1144:G:C5	3.10	0.40
2:EB:1791:A:N6	2:EB:1828:G:O2'	2.55	0.40
2:EB:1878:G:C6	2:EB:1879:C:C4	3.10	0.40
2:EB:2183:C:H2'	2:EB:2184:G:H8	1.86	0.40
2:EB:2271:G:H2'	2:EB:2272:U:C6	2.57	0.40
2:EB:2301:C:H2'	2:EB:2302:G:H8	1.86	0.40
2:EB:2839:G:H5'	15:RB:46:GLY:HA2	2.04	0.40
2:EB:2843:G:H1	2:EB:2874:C:H42	1.69	0.40
2:EB:2864:G:OP1	17:TB:119:LYS:HE3	2.22	0.40
3:FB:68:C:H2'	3:FB:69:G:O4'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:MB:4:ILE:HA	10:MB:17:GLN:O	2.21	0.40
11:NB:91:LEU:HD13	11:NB:98:VAL:HG21	2.04	0.40
14:QB:63:LYS:NZ	23:ZB:175:VAL:HG21	2.37	0.40
15:RB:50:HIS:O	15:RB:54:LEU:HB2	2.22	0.40
25:BC:7:ILE:HG23	25:BC:98:LEU:HD11	2.03	0.40
27:DC:31:LEU:HA	27:DC:31:LEU:HD23	1.77	0.40
29:FC:33:CYS:HA	29:FC:34:PRO:HD2	1.89	0.40
33:JC:2:LYS:NZ	33:JC:4:ARG:NE	2.70	0.40
38:PC:77:PRO:HB2	38:PC:78:HIS:HD2	1.87	0.40
42:TC:65:VAL:HG21	42:TC:73:GLN:HB3	2.03	0.40
43:UC:7:LYS:HZ1	43:UC:40:LEU:HD23	1.86	0.40
46:XC:3:ARG:HH11	46:XC:8:GLU:CG	2.34	0.40
49:AD:67:THR:O	49:AD:71:ARG:N	2.50	0.40
50:BD:13:ASP:O	50:BD:49:GLU:OE2	2.40	0.40
53:ED:20:LEU:HD23	53:ED:20:LEU:HA	1.92	0.40
55:HD:195:ARG:HH21	55:HD:197:HIS:CE1	2.38	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	273/275 (99%)	243 (89%)	25 (9%)	5 (2%)	7	36
5	HB	273/275 (99%)	243 (89%)	25 (9%)	5 (2%)	7	36
6	F	202/206 (98%)	180 (89%)	20 (10%)	2 (1%)	13	47
6	IB	202/206 (98%)	181 (90%)	19 (9%)	2 (1%)	13	47
7	G	200/205 (98%)	187 (94%)	9 (4%)	4 (2%)	6	34
7	JB	200/205 (98%)	186 (93%)	10 (5%)	4 (2%)	6	34
8	H	179/182 (98%)	152 (85%)	20 (11%)	7 (4%)	2	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	KB	179/182 (98%)	151 (84%)	22 (12%)	6 (3%)	3	25
9	I	172/180 (96%)	155 (90%)	14 (8%)	3 (2%)	7	37
9	LB	172/180 (96%)	154 (90%)	15 (9%)	3 (2%)	7	37
10	J	144/148 (97%)	118 (82%)	17 (12%)	9 (6%)	1	13
10	MB	144/148 (97%)	118 (82%)	16 (11%)	10 (7%)	1	11
11	K	138/140 (99%)	125 (91%)	12 (9%)	1 (1%)	19	53
11	NB	138/140 (99%)	126 (91%)	11 (8%)	1 (1%)	19	53
12	L	120/122 (98%)	106 (88%)	12 (10%)	2 (2%)	7	37
12	OB	120/122 (98%)	106 (88%)	12 (10%)	2 (2%)	7	37
13	M	148/150 (99%)	132 (89%)	11 (7%)	5 (3%)	3	25
13	PB	148/150 (99%)	131 (88%)	12 (8%)	5 (3%)	3	25
14	N	139/141 (99%)	126 (91%)	11 (8%)	2 (1%)	9	40
14	QB	139/141 (99%)	125 (90%)	12 (9%)	2 (1%)	9	40
15	O	116/118 (98%)	109 (94%)	5 (4%)	2 (2%)	7	37
15	RB	116/118 (98%)	107 (92%)	7 (6%)	2 (2%)	7	37
16	P	108/112 (96%)	99 (92%)	7 (6%)	2 (2%)	6	35
16	SB	108/112 (96%)	100 (93%)	6 (6%)	2 (2%)	6	35
17	Q	135/146 (92%)	118 (87%)	12 (9%)	5 (4%)	2	22
17	TB	135/146 (92%)	118 (87%)	13 (10%)	4 (3%)	3	26
18	R	115/118 (98%)	106 (92%)	8 (7%)	1 (1%)	14	49
18	UB	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	14	49
19	S	99/101 (98%)	91 (92%)	6 (6%)	2 (2%)	6	34
19	VB	99/101 (98%)	89 (90%)	8 (8%)	2 (2%)	6	34
20	T	110/113 (97%)	104 (94%)	4 (4%)	2 (2%)	7	36
20	WB	110/113 (97%)	103 (94%)	5 (4%)	2 (2%)	7	36
21	U	93/96 (97%)	84 (90%)	8 (9%)	1 (1%)	12	45
21	XB	93/96 (97%)	84 (90%)	8 (9%)	1 (1%)	12	45
22	V	105/110 (96%)	89 (85%)	11 (10%)	5 (5%)	2	17
22	YB	105/110 (96%)	91 (87%)	9 (9%)	5 (5%)	2	17
23	W	187/206 (91%)	165 (88%)	21 (11%)	1 (0%)	25	59
23	ZB	187/206 (91%)	165 (88%)	21 (11%)	1 (0%)	25	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	AC	82/85 (96%)	70 (85%)	10 (12%)	2 (2%)	5	30
24	X	82/85 (96%)	69 (84%)	11 (13%)	2 (2%)	5	30
25	BC	95/98 (97%)	84 (88%)	10 (10%)	1 (1%)	12	45
25	Y	95/98 (97%)	86 (90%)	8 (8%)	1 (1%)	12	45
26	CC	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
26	Z	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
27	AA	58/60 (97%)	53 (91%)	4 (7%)	1 (2%)	7	37
27	DC	58/60 (97%)	53 (91%)	4 (7%)	1 (2%)	7	37
28	BA	67/71 (94%)	47 (70%)	19 (28%)	1 (2%)	8	39
28	EC	67/71 (94%)	47 (70%)	20 (30%)	0	100	100
29	CA	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	7	36
29	FC	57/60 (95%)	51 (90%)	5 (9%)	1 (2%)	7	36
30	DA	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
30	GC	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
31	EA	46/49 (94%)	46 (100%)	0	0	100	100
31	HC	46/49 (94%)	46 (100%)	0	0	100	100
32	FA	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
32	IC	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
33	GA	35/37 (95%)	27 (77%)	8 (23%)	0	100	100
33	JC	35/37 (95%)	27 (77%)	8 (23%)	0	100	100
35	JA	232/256 (91%)	189 (82%)	29 (12%)	14 (6%)	1	13
35	MC	232/256 (91%)	188 (81%)	30 (13%)	14 (6%)	1	13
36	KA	204/239 (85%)	172 (84%)	24 (12%)	8 (4%)	2	21
36	NC	204/239 (85%)	172 (84%)	24 (12%)	8 (4%)	2	21
37	LA	206/209 (99%)	179 (87%)	20 (10%)	7 (3%)	3	25
37	OC	206/209 (99%)	182 (88%)	16 (8%)	8 (4%)	2	21
38	MA	149/162 (92%)	132 (89%)	11 (7%)	6 (4%)	2	21
38	PC	149/162 (92%)	132 (89%)	10 (7%)	7 (5%)	2	18
39	NA	99/101 (98%)	88 (89%)	9 (9%)	2 (2%)	6	34
39	QC	99/101 (98%)	89 (90%)	8 (8%)	2 (2%)	6	34
40	OA	153/156 (98%)	133 (87%)	13 (8%)	7 (5%)	2	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	RC	153/156 (98%)	133 (87%)	13 (8%)	7 (5%)	2	18
41	PA	136/138 (99%)	125 (92%)	9 (7%)	2 (2%)	8	39
41	SC	136/138 (99%)	126 (93%)	9 (7%)	1 (1%)	19	53
42	QA	125/128 (98%)	105 (84%)	17 (14%)	3 (2%)	5	30
42	TC	125/128 (98%)	105 (84%)	16 (13%)	4 (3%)	3	25
43	RA	96/105 (91%)	81 (84%)	12 (12%)	3 (3%)	3	26
43	UC	96/105 (91%)	81 (84%)	12 (12%)	3 (3%)	3	26
44	SA	114/129 (88%)	101 (89%)	10 (9%)	3 (3%)	4	28
44	VC	114/129 (88%)	101 (89%)	9 (8%)	4 (4%)	3	24
45	TA	119/132 (90%)	104 (87%)	11 (9%)	4 (3%)	3	25
45	WC	119/132 (90%)	104 (87%)	11 (9%)	4 (3%)	3	25
46	UA	115/126 (91%)	102 (89%)	12 (10%)	1 (1%)	14	49
46	XC	115/126 (91%)	102 (89%)	11 (10%)	2 (2%)	7	37
47	VA	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
47	YC	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
48	WA	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	5	31
48	ZC	86/89 (97%)	81 (94%)	3 (4%)	2 (2%)	5	31
49	AD	81/88 (92%)	73 (90%)	7 (9%)	1 (1%)	11	43
49	XA	81/88 (92%)	73 (90%)	7 (9%)	1 (1%)	11	43
50	BD	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
50	YA	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
51	CD	68/88 (77%)	62 (91%)	5 (7%)	1 (2%)	8	39
51	ZA	68/88 (77%)	61 (90%)	6 (9%)	1 (2%)	8	39
52	AB	81/93 (87%)	63 (78%)	14 (17%)	4 (5%)	2	17
52	DD	81/93 (87%)	63 (78%)	14 (17%)	4 (5%)	2	17
53	BB	97/106 (92%)	90 (93%)	3 (3%)	4 (4%)	2	20
53	ED	97/106 (92%)	90 (93%)	3 (3%)	4 (4%)	2	20
54	CB	22/27 (82%)	18 (82%)	4 (18%)	0	100	100
54	FD	22/27 (82%)	18 (82%)	4 (18%)	0	100	100
55	GD	253/365 (69%)	207 (82%)	35 (14%)	11 (4%)	2	19
55	HD	253/365 (69%)	206 (81%)	37 (15%)	10 (4%)	2	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	11990/12846 (93%)	10568 (88%)	1121 (9%)	301 (2%)	4 29

All (301) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	31	LYS
6	F	192	ASN
7	G	21	ALA
7	G	130	ALA
8	H	74	LYS
8	H	126	ASP
9	I	126	PRO
10	J	89	TYR
11	K	111	PRO
12	L	26	LYS
12	L	29	ASN
13	M	149	GLU
16	P	94	TYR
19	S	53	GLU
22	V	92	ASN
23	W	163	LEU
24	X	3	HIS
24	X	10	THR
35	JA	17	PHE
37	LA	26	CYS
38	MA	11	ILE
40	OA	4	ARG
5	HB	31	LYS
6	IB	192	ASN
7	JB	21	ALA
7	JB	130	ALA
8	KB	74	LYS
8	KB	126	ASP
9	LB	126	PRO
10	MB	89	TYR
11	NB	111	PRO
12	OB	26	LYS
12	OB	29	ASN
13	PB	149	GLU
16	SB	94	TYR
19	VB	53	GLU
22	YB	92	ASN

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Mol	Chain	Res	Type
23	ZB	163	LEU
24	AC	3	HIS
24	AC	10	THR
35	MC	17	PHE
37	OC	26	CYS
38	PC	11	ILE
40	RC	4	ARG
5	E	122	ASP
5	E	234	GLY
5	E	236	GLY
7	G	86	GLY
8	H	47	LYS
9	I	55	PRO
9	I	173	PRO
10	J	92	VAL
13	M	143	GLY
15	O	2	ARG
18	R	115	ALA
20	T	68	ARG
22	V	78	ALA
22	V	91	GLU
25	Y	3	LYS
27	AA	2	PRO
35	JA	128	GLU
36	KA	61	ALA
37	LA	3	ARG
38	MA	66	MET
38	MA	85	GLY
39	NA	34	GLY
40	OA	6	ARG
40	OA	51	GLN
40	OA	54	THR
42	QA	51	ARG
42	QA	96	LEU
42	QA	127	LYS
43	RA	77	PRO
44	SA	91	ARG
45	TA	12	ARG
45	TA	62	SER
45	TA	125	PRO
49	XA	82	GLN
52	AB	45	VAL

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Mol	Chain	Res	Type
52	AB	67	VAL
53	BB	102	GLY
5	HB	122	ASP
5	HB	234	GLY
5	HB	236	GLY
7	JB	86	GLY
8	KB	47	LYS
9	LB	55	PRO
9	LB	173	PRO
13	PB	143	GLY
15	RB	2	ARG
18	UB	115	ALA
19	VB	79	VAL
20	WB	68	ARG
22	YB	78	ALA
22	YB	91	GLU
25	BC	3	LYS
27	DC	2	PRO
35	MC	128	GLU
36	NC	61	ALA
37	OC	3	ARG
37	OC	4	TYR
38	PC	85	GLY
39	QC	34	GLY
40	RC	51	GLN
40	RC	54	THR
40	RC	79	ARG
42	TC	51	ARG
42	TC	96	LEU
42	TC	127	LYS
43	UC	77	PRO
44	VC	91	ARG
45	WC	12	ARG
45	WC	62	SER
45	WC	125	PRO
49	AD	82	GLN
52	DD	45	VAL
52	DD	67	VAL
53	ED	102	GLY
55	GD	144	TRP
55	HD	144	TRP
7	G	22	ALA

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Mol	Chain	Res	Type
8	H	24	GLY
8	H	43	LEU
8	H	124	SER
10	J	85	GLU
10	J	88	ILE
13	M	29	LYS
13	M	36	LYS
13	M	122	PRO
15	O	107	ASP
21	U	22	ALA
22	V	103	GLY
35	JA	36	ARG
35	JA	43	ASP
35	JA	124	SER
35	JA	150	SER
36	KA	26	LYS
36	KA	107	GLN
37	LA	4	TYR
37	LA	180	GLY
40	OA	79	ARG
43	RA	78	ASN
52	AB	27	GLU
8	KB	43	LEU
8	KB	124	SER
10	MB	84	GLY
10	MB	85	GLU
10	MB	88	ILE
13	PB	29	LYS
13	PB	36	LYS
13	PB	122	PRO
20	WB	63	ASP
21	XB	22	ALA
22	YB	103	GLY
35	MC	36	ARG
35	MC	43	ASP
35	MC	124	SER
35	MC	150	SER
36	NC	26	LYS
36	NC	102	ASN
36	NC	107	GLN
37	OC	180	GLY
38	PC	66	MET

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Mol	Chain	Res	Type
40	RC	6	ARG
40	RC	82	GLY
43	UC	78	ASN
52	DD	27	GLU
52	DD	43	GLU
55	GD	102	PRO
55	GD	340	LEU
55	HD	102	PRO
55	HD	340	LEU
5	E	29	PRO
6	F	52	LEU
10	J	84	GLY
10	J	106	GLY
10	J	117	GLU
17	Q	55	ASN
19	S	79	VAL
20	T	63	ASP
35	JA	20	GLU
35	JA	78	GLN
35	JA	158	LEU
35	JA	204	ASN
36	KA	3	ASN
36	KA	102	ASN
36	KA	156	ARG
37	LA	30	LYS
39	NA	100	ASN
51	ZA	87	ARG
52	AB	43	GLU
53	BB	97	ALA
5	HB	29	PRO
6	IB	52	LEU
7	JB	22	ALA
8	KB	24	GLY
10	MB	106	GLY
10	MB	117	GLU
10	MB	145	VAL
16	SB	61	ASN
17	TB	55	ASN
35	MC	20	GLU
35	MC	78	GLN
35	MC	158	LEU
37	OC	22	LYS

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Mol	Chain	Res	Type
37	OC	27	TYR
37	OC	30	LYS
39	QC	100	ASN
48	ZC	49	ASP
51	CD	87	ARG
53	ED	71	THR
53	ED	97	ALA
55	GD	217	ILE
55	GD	300	SER
55	HD	217	ILE
10	J	137	PRO
10	J	145	VAL
16	P	61	ASN
17	Q	2	ASN
35	JA	21	ARG
35	JA	126	GLU
37	LA	22	LYS
37	LA	27	TYR
38	MA	49	PRO
40	OA	82	GLY
41	PA	2	LEU
44	SA	78	GLN
48	WA	49	ASP
48	WA	88	ARG
53	BB	47	GLY
53	BB	71	THR
10	MB	82	ARG
10	MB	137	PRO
14	QB	57	HIS
17	TB	58	ASN
17	TB	95	ARG
35	MC	21	ARG
35	MC	126	GLU
35	MC	204	ASN
36	NC	3	ASN
36	NC	156	ARG
38	PC	49	PRO
38	PC	65	ASN
42	TC	52	ALA
44	VC	78	GLN
44	VC	117	ASN
48	ZC	88	ARG

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Mol	Chain	Res	Type
55	GD	143	ARG
55	GD	155	GLU
55	GD	259	ASP
55	HD	143	ARG
55	HD	215	PRO
55	HD	300	SER
55	HD	355	ALA
14	N	57	HIS
17	Q	94	ALA
17	Q	95	ARG
17	Q	128	GLU
22	V	51	VAL
43	RA	93	GLY
45	TA	88	GLY
46	UA	10	PRO
15	RB	107	ASP
17	TB	128	GLU
29	FC	57	VAL
41	SC	2	LEU
43	UC	93	GLY
55	GD	215	PRO
55	GD	355	ALA
55	HD	155	GLU
29	CA	57	VAL
38	MA	154	GLY
14	QB	15	GLY
22	YB	51	VAL
45	WC	88	GLY
46	XC	10	PRO
55	GD	233	GLY
36	KA	51	GLY
38	MA	74	GLY
44	SA	118	GLY
10	MB	92	VAL
38	PC	74	GLY
44	VC	118	GLY
53	ED	47	GLY
55	HD	233	GLY
8	H	177	GLY
14	N	15	GLY
35	JA	72	GLY
36	KA	81	GLY

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Mol	Chain	Res	Type
35	MC	72	GLY
36	NC	81	GLY
37	OC	5	ILE
38	PC	154	GLY
46	XC	100	GLY
28	BA	54	GLY
35	JA	223	ILE
40	OA	17	VAL
41	PA	90	GLY
35	MC	223	ILE
36	NC	51	GLY
40	RC	17	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	
5	E	217/217 (100%)	197 (91%)	20 (9%)	7	31
5	HB	217/217 (100%)	197 (91%)	20 (9%)	7	31
6	F	165/166 (99%)	145 (88%)	20 (12%)	4	21
6	IB	165/166 (99%)	145 (88%)	20 (12%)	4	21
7	G	161/162 (99%)	142 (88%)	19 (12%)	4	22
7	JB	161/162 (99%)	142 (88%)	19 (12%)	4	22
8	H	154/156 (99%)	134 (87%)	20 (13%)	3	19
8	KB	154/156 (99%)	136 (88%)	18 (12%)	4	22
9	I	144/148 (97%)	130 (90%)	14 (10%)	6	28
9	LB	144/148 (97%)	130 (90%)	14 (10%)	6	28
10	J	122/124 (98%)	105 (86%)	17 (14%)	3	17
10	MB	122/124 (98%)	106 (87%)	16 (13%)	3	18
11	K	119/119 (100%)	107 (90%)	12 (10%)	6	27
11	NB	119/119 (100%)	108 (91%)	11 (9%)	7	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	100/100 (100%)	91 (91%)	9 (9%)	8	31
12	OB	100/100 (100%)	90 (90%)	10 (10%)	6	28
13	M	116/116 (100%)	103 (89%)	13 (11%)	5	24
13	PB	116/116 (100%)	101 (87%)	15 (13%)	3	19
14	N	111/111 (100%)	99 (89%)	12 (11%)	5	25
14	QB	111/111 (100%)	98 (88%)	13 (12%)	4	22
15	O	101/101 (100%)	89 (88%)	12 (12%)	4	22
15	RB	101/101 (100%)	89 (88%)	12 (12%)	4	22
16	P	87/88 (99%)	83 (95%)	4 (5%)	23	52
16	SB	87/88 (99%)	83 (95%)	4 (5%)	23	52
17	Q	121/128 (94%)	112 (93%)	9 (7%)	11	37
17	TB	121/128 (94%)	113 (93%)	8 (7%)	14	42
18	R	93/94 (99%)	83 (89%)	10 (11%)	5	25
18	UB	93/94 (99%)	84 (90%)	9 (10%)	6	28
19	S	82/82 (100%)	70 (85%)	12 (15%)	2	15
19	VB	82/82 (100%)	72 (88%)	10 (12%)	4	20
20	T	91/92 (99%)	81 (89%)	10 (11%)	5	25
20	WB	91/92 (99%)	81 (89%)	10 (11%)	5	25
21	U	77/78 (99%)	73 (95%)	4 (5%)	19	49
21	XB	77/78 (99%)	73 (95%)	4 (5%)	19	49
22	V	87/91 (96%)	81 (93%)	6 (7%)	13	40
22	YB	87/91 (96%)	81 (93%)	6 (7%)	13	40
23	W	163/179 (91%)	142 (87%)	21 (13%)	3	19
23	ZB	163/179 (91%)	143 (88%)	20 (12%)	4	20
24	AC	66/67 (98%)	57 (86%)	9 (14%)	3	17
24	X	66/67 (98%)	57 (86%)	9 (14%)	3	17
25	BC	81/83 (98%)	70 (86%)	11 (14%)	3	17
25	Y	81/83 (98%)	70 (86%)	11 (14%)	3	17
26	CC	66/67 (98%)	62 (94%)	4 (6%)	15	44
26	Z	66/67 (98%)	62 (94%)	4 (6%)	15	44
27	AA	52/52 (100%)	48 (92%)	4 (8%)	10	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	DC	52/52 (100%)	49 (94%)	3 (6%)	17	45
28	BA	59/63 (94%)	51 (86%)	8 (14%)	3	17
28	EC	59/63 (94%)	51 (86%)	8 (14%)	3	17
29	CA	51/52 (98%)	46 (90%)	5 (10%)	6	28
29	FC	51/52 (98%)	46 (90%)	5 (10%)	6	28
30	DA	51/52 (98%)	47 (92%)	4 (8%)	10	35
30	GC	51/52 (98%)	46 (90%)	5 (10%)	6	28
31	EA	41/42 (98%)	35 (85%)	6 (15%)	2	15
31	HC	41/42 (98%)	35 (85%)	6 (15%)	2	15
32	FA	54/55 (98%)	47 (87%)	7 (13%)	3	19
32	IC	54/55 (98%)	48 (89%)	6 (11%)	5	24
33	GA	34/34 (100%)	30 (88%)	4 (12%)	4	22
33	JC	34/34 (100%)	30 (88%)	4 (12%)	4	22
35	JA	202/220 (92%)	177 (88%)	25 (12%)	4	20
35	MC	202/220 (92%)	177 (88%)	25 (12%)	4	20
36	KA	160/188 (85%)	146 (91%)	14 (9%)	8	32
36	NC	160/188 (85%)	145 (91%)	15 (9%)	7	30
37	LA	180/181 (99%)	159 (88%)	21 (12%)	4	22
37	OC	180/181 (99%)	157 (87%)	23 (13%)	3	19
38	MA	116/123 (94%)	100 (86%)	16 (14%)	3	17
38	PC	116/123 (94%)	99 (85%)	17 (15%)	2	15
39	NA	90/90 (100%)	80 (89%)	10 (11%)	5	24
39	QC	90/90 (100%)	79 (88%)	11 (12%)	4	20
40	OA	126/127 (99%)	120 (95%)	6 (5%)	21	51
40	RC	126/127 (99%)	120 (95%)	6 (5%)	21	51
41	PA	119/119 (100%)	107 (90%)	12 (10%)	6	27
41	SC	119/119 (100%)	108 (91%)	11 (9%)	7	31
42	QA	98/99 (99%)	86 (88%)	12 (12%)	4	20
42	TC	98/99 (99%)	86 (88%)	12 (12%)	4	20
43	RA	88/92 (96%)	81 (92%)	7 (8%)	10	35
43	UC	88/92 (96%)	81 (92%)	7 (8%)	10	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	SA	88/99 (89%)	85 (97%)	3 (3%)	32	60
44	VC	88/99 (89%)	85 (97%)	3 (3%)	32	60
45	TA	102/108 (94%)	95 (93%)	7 (7%)	13	40
45	WC	102/108 (94%)	95 (93%)	7 (7%)	13	40
46	UA	94/101 (93%)	82 (87%)	12 (13%)	3	19
46	XC	94/101 (93%)	83 (88%)	11 (12%)	4	22
47	VA	49/50 (98%)	47 (96%)	2 (4%)	26	55
47	YC	49/50 (98%)	47 (96%)	2 (4%)	26	55
48	WA	79/80 (99%)	72 (91%)	7 (9%)	8	32
48	ZC	79/80 (99%)	72 (91%)	7 (9%)	8	32
49	AD	72/74 (97%)	66 (92%)	6 (8%)	9	33
49	XA	72/74 (97%)	66 (92%)	6 (8%)	9	33
50	BD	94/97 (97%)	86 (92%)	8 (8%)	8	33
50	YA	94/97 (97%)	86 (92%)	8 (8%)	8	33
51	CD	61/77 (79%)	56 (92%)	5 (8%)	9	34
51	ZA	61/77 (79%)	56 (92%)	5 (8%)	9	34
52	AB	72/80 (90%)	65 (90%)	7 (10%)	6	28
52	DD	72/80 (90%)	65 (90%)	7 (10%)	6	28
53	BB	76/82 (93%)	70 (92%)	6 (8%)	10	35
53	ED	76/82 (93%)	70 (92%)	6 (8%)	10	35
54	CB	19/22 (86%)	18 (95%)	1 (5%)	19	48
54	FD	19/22 (86%)	18 (95%)	1 (5%)	19	48
55	GD	206/305 (68%)	179 (87%)	27 (13%)	3	18
55	HD	206/305 (68%)	179 (87%)	27 (13%)	3	18
All	All	10114/10666 (95%)	9077 (90%)	1037 (10%)	6	27

All (1037) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	3	VAL
5	E	20	ASP
5	E	61	LEU
5	E	88	ARG
5	E	94	LEU

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Mol	Chain	Res	Type
5	E	98	VAL
5	E	99	ASP
5	E	101	GLU
5	E	131	LEU
5	E	155	LEU
5	E	182	LEU
5	E	200	ASP
5	E	211	ARG
5	E	218	ARG
5	E	221	VAL
5	E	222	ARG
5	E	242	ARG
5	E	262	ARG
5	E	263	ARG
5	E	266	SER
6	F	9	VAL
6	F	13	ARG
6	F	21	VAL
6	F	40	GLU
6	F	73	GLU
6	F	75	VAL
6	F	92	THR
6	F	93	VAL
6	F	102	VAL
6	F	107	THR
6	F	116	VAL
6	F	117	MET
6	F	119	ARG
6	F	128	SER
6	F	146	THR
6	F	165	VAL
6	F	170	LEU
6	F	178	GLU
6	F	181	LEU
6	F	195	LEU
7	G	6	MET
7	G	19	GLU
7	G	24	LEU
7	G	50	SER
7	G	51	THR
7	G	54	ARG
7	G	57	VAL

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Mol	Chain	Res	Type
7	G	64	ILE
7	G	74	ARG
7	G	82	ILE
7	G	95	ARG
7	G	98	SER
7	G	156	LEU
7	G	158	THR
7	G	176	LEU
7	G	183	VAL
7	G	191	ARG
7	G	192	LEU
7	G	196	LEU
8	H	7	LEU
8	H	8	LYS
8	H	22	ARG
8	H	33	ARG
8	H	35	GLU
8	H	53	LEU
8	H	60	LEU
8	H	62	LEU
8	H	70	VAL
8	H	79	ASN
8	H	83	ARG
8	H	91	ARG
8	H	115	ARG
8	H	117	PHE
8	H	136	ARG
8	H	139	LEU
8	H	150	ASP
8	H	161	THR
8	H	170	ARG
8	H	182	LYS
9	I	3	ARG
9	I	17	VAL
9	I	24	VAL
9	I	32	GLU
9	I	33	LEU
9	I	41	MET
9	I	51	ARG
9	I	52	VAL
9	I	71	LEU
9	I	104	GLU

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Mol	Chain	Res	Type
9	I	107	VAL
9	I	114	VAL
9	I	127	GLU
9	I	140	LYS
10	J	2	LYS
10	J	5	LEU
10	J	19	VAL
10	J	31	LEU
10	J	54	GLN
10	J	61	ARG
10	J	76	THR
10	J	77	LEU
10	J	88	ILE
10	J	89	TYR
10	J	92	VAL
10	J	107	ILE
10	J	108	THR
10	J	112	LYS
10	J	118	LYS
10	J	128	LEU
10	J	145	VAL
11	K	1	MET
11	K	34	LEU
11	K	55	VAL
11	K	68	GLU
11	K	69	GLN
11	K	70	LYS
11	K	75	TYR
11	K	83	LYS
11	K	90	MET
11	K	99	LEU
11	K	131	GLN
11	K	140	VAL
12	L	24	VAL
12	L	32	TYR
12	L	38	VAL
12	L	61	VAL
12	L	69	VAL
12	L	70	LYS
12	L	98	VAL
12	L	99	PHE
12	L	121	VAL

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Mol	Chain	Res	Type
13	M	4	SER
13	M	15	ARG
13	M	42	SER
13	M	45	LEU
13	M	57	THR
13	M	68	GLN
13	M	71	VAL
13	M	75	ILE
13	M	83	VAL
13	M	88	LEU
13	M	90	ARG
13	M	96	THR
13	M	112	LEU
14	N	7	MET
14	N	17	LEU
14	N	18	LYS
14	N	43	THR
14	N	56	ARG
14	N	58	PHE
14	N	75	THR
14	N	82	ARG
14	N	83	MET
14	N	103	MET
14	N	109	VAL
14	N	110	THR
15	O	1	MET
15	O	6	SER
15	O	24	GLN
15	O	28	LEU
15	O	29	LEU
15	O	48	VAL
15	O	65	LEU
15	O	67	LEU
15	O	102	GLU
15	O	103	ARG
15	O	105	ARG
15	O	113	LEU
16	P	3	ARG
16	P	4	LEU
16	P	58	LEU
16	P	98	VAL
17	Q	23	ARG

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Mol	Chain	Res	Type
17	Q	53	ARG
17	Q	57	PHE
17	Q	66	VAL
17	Q	80	SER
17	Q	108	ARG
17	Q	112	ARG
17	Q	115	ARG
17	Q	128	GLU
18	R	18	LEU
18	R	30	LYS
18	R	31	SER
18	R	34	LYS
18	R	36	ARG
18	R	39	LEU
18	R	54	LYS
18	R	70	ARG
18	R	89	GLU
18	R	95	LEU
19	S	1	MET
19	S	7	THR
19	S	13	ARG
19	S	19	LYS
19	S	22	VAL
19	S	34	GLU
19	S	39	LEU
19	S	43	GLU
19	S	61	VAL
19	S	62	LEU
19	S	68	LYS
19	S	79	VAL
20	T	1	MET
20	T	2	GLU
20	T	11	ARG
20	T	15	ARG
20	T	18	ARG
20	T	30	GLU
20	T	37	ARG
20	T	59	VAL
20	T	67	ASP
20	T	107	LEU
21	U	2	LYS
21	U	13	LEU

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Mol	Chain	Res	Type
21	U	27	THR
21	U	68	ARG
22	V	2	ARG
22	V	9	LYS
22	V	81	LYS
22	V	90	LEU
22	V	97	ARG
22	V	99	CYS
23	W	18	LEU
23	W	31	ARG
23	W	35	ARG
23	W	67	LEU
23	W	72	ARG
23	W	74	VAL
23	W	91	LEU
23	W	103	ARG
23	W	121	HIS
23	W	131	ARG
23	W	132	ASN
23	W	133	ILE
23	W	136	PHE
23	W	137	ILE
23	W	150	LEU
23	W	154	ASP
23	W	163	LEU
23	W	165	VAL
23	W	168	GLU
23	W	169	GLU
23	W	182	LYS
24	X	5	LYS
24	X	7	LEU
24	X	11	ARG
24	X	17	GLN
24	X	30	VAL
24	X	31	VAL
24	X	63	VAL
24	X	64	ASP
24	X	84	LEU
25	Y	14	VAL
25	Y	21	ARG
25	Y	27	GLU
25	Y	40	ARG

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Mol	Chain	Res	Type
25	Y	41	ARG
25	Y	52	ARG
25	Y	59	THR
25	Y	73	LEU
25	Y	82	LEU
25	Y	88	LYS
25	Y	94	LEU
26	Z	3	LEU
26	Z	41	ILE
26	Z	44	LEU
26	Z	53	LEU
27	AA	9	VAL
27	AA	23	LEU
27	AA	35	ARG
27	AA	54	VAL
28	BA	39	CYS
28	BA	43	TYR
28	BA	47	GLN
28	BA	49	PHE
28	BA	61	ARG
28	BA	62	ARG
28	BA	67	TYR
28	BA	69	LYS
29	CA	6	VAL
29	CA	8	LYS
29	CA	25	LEU
29	CA	55	ARG
29	CA	57	VAL
30	DA	18	ARG
30	DA	30	THR
30	DA	34	LEU
30	DA	43	CYS
31	EA	1	MET
31	EA	4	THR
31	EA	24	THR
31	EA	31	LEU
31	EA	43	THR
31	EA	46	VAL
32	FA	6	THR
32	FA	29	LYS
32	FA	31	HIS
32	FA	32	LEU

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Mol	Chain	Res	Type
32	FA	34	TRP
32	FA	49	VAL
32	FA	59	LYS
33	GA	7	VAL
33	GA	22	ARG
33	GA	26	ILE
33	GA	33	LYS
35	JA	8	LYS
35	JA	10	LEU
35	JA	16	HIS
35	JA	19	HIS
35	JA	21	ARG
35	JA	22	LYS
35	JA	24	TRP
35	JA	44	LEU
35	JA	45	GLN
35	JA	60	ASP
35	JA	76	GLN
35	JA	97	TRP
35	JA	111	ARG
35	JA	126	GLU
35	JA	129	GLU
35	JA	141	GLU
35	JA	145	LEU
35	JA	157	ARG
35	JA	158	LEU
35	JA	160	ASP
35	JA	163	PHE
35	JA	185	ILE
35	JA	187	LEU
35	JA	190	THR
35	JA	193	ASP
36	KA	16	ARG
36	KA	30	ARG
36	KA	31	HIS
36	KA	37	GLN
36	KA	70	VAL
36	KA	76	VAL
36	KA	101	LEU
36	KA	108	ASN
36	KA	115	LEU
36	KA	131	ARG

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Mol	Chain	Res	Type
36	KA	140	ARG
36	KA	191	THR
36	KA	193	TYR
36	KA	195	VAL
37	LA	4	TYR
37	LA	5	ILE
37	LA	21	LEU
37	LA	26	CYS
37	LA	27	TYR
37	LA	57	ARG
37	LA	62	GLN
37	LA	76	ARG
37	LA	77	ASN
37	LA	78	LEU
37	LA	127	THR
37	LA	135	LEU
37	LA	141	ARG
37	LA	158	ILE
37	LA	170	VAL
37	LA	173	TRP
37	LA	182	LYS
37	LA	184	LYS
37	LA	194	LEU
37	LA	202	LEU
37	LA	209	ARG
38	MA	10	MET
38	MA	20	GLN
38	MA	24	ARG
38	MA	41	VAL
38	MA	50	GLU
38	MA	60	TYR
38	MA	68	GLU
38	MA	72	GLN
38	MA	75	THR
38	MA	79	GLU
38	MA	91	LEU
38	MA	100	VAL
38	MA	136	MET
38	MA	142	LEU
38	MA	145	LYS
38	MA	155	GLU
39	NA	16	GLN

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Mol	Chain	Res	Type
39	NA	36	ARG
39	NA	37	VAL
39	NA	43	LEU
39	NA	45	LEU
39	NA	64	GLN
39	NA	69	GLU
39	NA	74	ASP
39	NA	83	ASP
39	NA	89	MET
40	OA	5	ARG
40	OA	8	GLU
40	OA	10	ARG
40	OA	24	THR
40	OA	104	LEU
40	OA	115	ARG
41	PA	1	MET
41	PA	29	SER
41	PA	50	ARG
41	PA	52	ASP
41	PA	88	LYS
41	PA	91	ARG
41	PA	102	ARG
41	PA	113	SER
41	PA	120	THR
41	PA	133	LEU
41	PA	135	CYS
41	PA	136	GLU
42	QA	2	GLU
42	QA	4	TYR
42	QA	16	ARG
42	QA	27	THR
42	QA	33	PHE
42	QA	36	TYR
42	QA	38	GLN
42	QA	65	VAL
42	QA	75	ASP
42	QA	108	VAL
42	QA	121	ARG
42	QA	127	LYS
43	RA	44	VAL
43	RA	74	ILE
43	RA	76	ASN

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Mol	Chain	Res	Type
43	RA	86	MET
43	RA	88	LEU
43	RA	89	ASP
43	RA	95	GLU
44	SA	34	ASP
44	SA	80	VAL
44	SA	99	GLN
45	TA	6	THR
45	TA	20	LYS
45	TA	44	THR
45	TA	52	LEU
45	TA	60	LEU
45	TA	83	VAL
45	TA	86	ARG
46	UA	3	ARG
46	UA	4	ILE
46	UA	11	ARG
46	UA	19	LEU
46	UA	27	LYS
46	UA	32	GLU
46	UA	37	THR
46	UA	58	GLU
46	UA	65	LYS
46	UA	70	LEU
46	UA	90	LEU
46	UA	101	GLN
47	VA	6	LEU
47	VA	7	ILE
48	WA	4	THR
48	WA	35	ARG
48	WA	38	ARG
48	WA	39	LEU
48	WA	66	LEU
48	WA	70	LEU
48	WA	83	GLU
49	XA	11	SER
49	XA	20	VAL
49	XA	60	LEU
49	XA	67	THR
49	XA	72	ARG
49	XA	82	GLN
50	YA	35	VAL

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Mol	Chain	Res	Type
50	YA	37	LYS
50	YA	63	ARG
50	YA	75	ARG
50	YA	87	LYS
50	YA	93	GLN
50	YA	96	GLN
50	YA	100	LYS
51	ZA	19	LYS
51	ZA	26	LEU
51	ZA	32	ARG
51	ZA	46	GLU
51	ZA	54	ARG
52	AB	3	ARG
52	AB	11	VAL
52	AB	12	ASP
52	AB	15	LEU
52	AB	64	GLU
52	AB	77	THR
52	AB	83	HIS
53	BB	15	ARG
53	BB	31	SER
53	BB	53	LEU
53	BB	62	LEU
53	BB	72	LEU
53	BB	91	LEU
54	CB	10	ARG
5	HB	3	VAL
5	HB	20	ASP
5	HB	61	LEU
5	HB	88	ARG
5	HB	94	LEU
5	HB	98	VAL
5	HB	99	ASP
5	HB	101	GLU
5	HB	131	LEU
5	HB	134	ARG
5	HB	182	LEU
5	HB	193	VAL
5	HB	200	ASP
5	HB	211	ARG
5	HB	218	ARG
5	HB	221	VAL

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Mol	Chain	Res	Type
5	HB	222	ARG
5	HB	242	ARG
5	HB	263	ARG
5	HB	266	SER
6	IB	9	VAL
6	IB	13	ARG
6	IB	21	VAL
6	IB	40	GLU
6	IB	66	HIS
6	IB	73	GLU
6	IB	75	VAL
6	IB	92	THR
6	IB	93	VAL
6	IB	102	VAL
6	IB	107	THR
6	IB	116	VAL
6	IB	119	ARG
6	IB	128	SER
6	IB	146	THR
6	IB	165	VAL
6	IB	170	LEU
6	IB	178	GLU
6	IB	181	LEU
6	IB	195	LEU
7	JB	6	MET
7	JB	24	LEU
7	JB	50	SER
7	JB	51	THR
7	JB	54	ARG
7	JB	57	VAL
7	JB	64	ILE
7	JB	74	ARG
7	JB	82	ILE
7	JB	95	ARG
7	JB	98	SER
7	JB	156	LEU
7	JB	158	THR
7	JB	174	VAL
7	JB	176	LEU
7	JB	183	VAL
7	JB	191	ARG
7	JB	192	LEU

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Mol	Chain	Res	Type
7	JB	196	LEU
8	KB	7	LEU
8	KB	22	ARG
8	KB	33	ARG
8	KB	35	GLU
8	KB	53	LEU
8	KB	60	LEU
8	KB	62	LEU
8	KB	70	VAL
8	KB	79	ASN
8	KB	83	ARG
8	KB	115	ARG
8	KB	117	PHE
8	KB	136	ARG
8	KB	139	LEU
8	KB	150	ASP
8	KB	161	THR
8	KB	170	ARG
8	KB	182	LYS
9	LB	3	ARG
9	LB	17	VAL
9	LB	24	VAL
9	LB	32	GLU
9	LB	33	LEU
9	LB	41	MET
9	LB	51	ARG
9	LB	52	VAL
9	LB	71	LEU
9	LB	104	GLU
9	LB	107	VAL
9	LB	114	VAL
9	LB	127	GLU
9	LB	140	LYS
10	MB	2	LYS
10	MB	5	LEU
10	MB	19	VAL
10	MB	31	LEU
10	MB	54	GLN
10	MB	61	ARG
10	MB	76	THR
10	MB	77	LEU
10	MB	88	ILE

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Mol	Chain	Res	Type
10	MB	89	TYR
10	MB	107	ILE
10	MB	108	THR
10	MB	112	LYS
10	MB	118	LYS
10	MB	128	LEU
10	MB	145	VAL
11	NB	1	MET
11	NB	34	LEU
11	NB	55	VAL
11	NB	69	GLN
11	NB	70	LYS
11	NB	75	TYR
11	NB	83	LYS
11	NB	90	MET
11	NB	99	LEU
11	NB	131	GLN
11	NB	140	VAL
12	OB	21	CYS
12	OB	24	VAL
12	OB	32	TYR
12	OB	38	VAL
12	OB	61	VAL
12	OB	69	VAL
12	OB	70	LYS
12	OB	98	VAL
12	OB	99	PHE
12	OB	121	VAL
13	PB	4	SER
13	PB	15	ARG
13	PB	40	SER
13	PB	42	SER
13	PB	45	LEU
13	PB	57	THR
13	PB	68	GLN
13	PB	71	VAL
13	PB	75	ILE
13	PB	83	VAL
13	PB	88	LEU
13	PB	90	ARG
13	PB	96	THR
13	PB	112	LEU

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Mol	Chain	Res	Type
13	PB	125	VAL
14	QB	7	MET
14	QB	17	LEU
14	QB	18	LYS
14	QB	56	ARG
14	QB	58	PHE
14	QB	75	THR
14	QB	79	LEU
14	QB	82	ARG
14	QB	83	MET
14	QB	103	MET
14	QB	109	VAL
14	QB	110	THR
14	QB	141	GLN
15	RB	1	MET
15	RB	6	SER
15	RB	24	GLN
15	RB	28	LEU
15	RB	29	LEU
15	RB	48	VAL
15	RB	65	LEU
15	RB	67	LEU
15	RB	102	GLU
15	RB	103	ARG
15	RB	105	ARG
15	RB	113	LEU
16	SB	3	ARG
16	SB	4	LEU
16	SB	58	LEU
16	SB	98	VAL
17	TB	23	ARG
17	TB	53	ARG
17	TB	66	VAL
17	TB	80	SER
17	TB	108	ARG
17	TB	112	ARG
17	TB	115	ARG
17	TB	128	GLU
18	UB	18	LEU
18	UB	30	LYS
18	UB	34	LYS
18	UB	36	ARG

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Mol	Chain	Res	Type
18	UB	39	LEU
18	UB	54	LYS
18	UB	70	ARG
18	UB	72	HIS
18	UB	89	GLU
19	VB	1	MET
19	VB	7	THR
19	VB	13	ARG
19	VB	19	LYS
19	VB	22	VAL
19	VB	34	GLU
19	VB	43	GLU
19	VB	61	VAL
19	VB	62	LEU
19	VB	79	VAL
20	WB	1	MET
20	WB	2	GLU
20	WB	11	ARG
20	WB	15	ARG
20	WB	18	ARG
20	WB	30	GLU
20	WB	37	ARG
20	WB	59	VAL
20	WB	67	ASP
20	WB	107	LEU
21	XB	2	LYS
21	XB	13	LEU
21	XB	27	THR
21	XB	68	ARG
22	YB	2	ARG
22	YB	9	LYS
22	YB	81	LYS
22	YB	90	LEU
22	YB	97	ARG
22	YB	99	CYS
23	ZB	18	LEU
23	ZB	31	ARG
23	ZB	35	ARG
23	ZB	72	ARG
23	ZB	74	VAL
23	ZB	91	LEU
23	ZB	103	ARG

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Mol	Chain	Res	Type
23	ZB	121	HIS
23	ZB	131	ARG
23	ZB	132	ASN
23	ZB	133	ILE
23	ZB	136	PHE
23	ZB	137	ILE
23	ZB	150	LEU
23	ZB	154	ASP
23	ZB	163	LEU
23	ZB	165	VAL
23	ZB	168	GLU
23	ZB	169	GLU
23	ZB	182	LYS
24	AC	5	LYS
24	AC	7	LEU
24	AC	11	ARG
24	AC	17	GLN
24	AC	30	VAL
24	AC	31	VAL
24	AC	63	VAL
24	AC	64	ASP
24	AC	84	LEU
25	BC	5	CYS
25	BC	14	VAL
25	BC	21	ARG
25	BC	27	GLU
25	BC	40	ARG
25	BC	41	ARG
25	BC	52	ARG
25	BC	59	THR
25	BC	82	LEU
25	BC	88	LYS
25	BC	94	LEU
26	CC	3	LEU
26	CC	41	ILE
26	CC	44	LEU
26	CC	53	LEU
27	DC	9	VAL
27	DC	23	LEU
27	DC	54	VAL
28	EC	39	CYS
28	EC	43	TYR

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Mol	Chain	Res	Type
28	EC	47	GLN
28	EC	49	PHE
28	EC	61	ARG
28	EC	62	ARG
28	EC	67	TYR
28	EC	69	LYS
29	FC	6	VAL
29	FC	8	LYS
29	FC	25	LEU
29	FC	55	ARG
29	FC	57	VAL
30	GC	18	ARG
30	GC	30	THR
30	GC	34	LEU
30	GC	43	CYS
30	GC	48	VAL
31	HC	1	MET
31	HC	4	THR
31	HC	24	THR
31	HC	31	LEU
31	HC	43	THR
31	HC	46	VAL
32	IC	6	THR
32	IC	29	LYS
32	IC	31	HIS
32	IC	32	LEU
32	IC	34	TRP
32	IC	49	VAL
33	JC	7	VAL
33	JC	22	ARG
33	JC	26	ILE
33	JC	33	LYS
35	MC	8	LYS
35	MC	10	LEU
35	MC	16	HIS
35	MC	19	HIS
35	MC	21	ARG
35	MC	22	LYS
35	MC	24	TRP
35	MC	44	LEU
35	MC	45	GLN
35	MC	60	ASP

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Mol	Chain	Res	Type
35	MC	76	GLN
35	MC	97	TRP
35	MC	111	ARG
35	MC	126	GLU
35	MC	129	GLU
35	MC	141	GLU
35	MC	145	LEU
35	MC	157	ARG
35	MC	158	LEU
35	MC	160	ASP
35	MC	163	PHE
35	MC	185	ILE
35	MC	187	LEU
35	MC	190	THR
35	MC	193	ASP
36	NC	15	THR
36	NC	16	ARG
36	NC	30	ARG
36	NC	31	HIS
36	NC	37	GLN
36	NC	70	VAL
36	NC	76	VAL
36	NC	101	LEU
36	NC	108	ASN
36	NC	115	LEU
36	NC	131	ARG
36	NC	140	ARG
36	NC	191	THR
36	NC	193	TYR
36	NC	195	VAL
37	OC	4	TYR
37	OC	5	ILE
37	OC	21	LEU
37	OC	26	CYS
37	OC	27	TYR
37	OC	57	ARG
37	OC	62	GLN
37	OC	76	ARG
37	OC	77	ASN
37	OC	78	LEU
37	OC	127	THR
37	OC	135	LEU

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Mol	Chain	Res	Type
37	OC	141	ARG
37	OC	148	VAL
37	OC	158	ILE
37	OC	170	VAL
37	OC	173	TRP
37	OC	182	LYS
37	OC	184	LYS
37	OC	194	LEU
37	OC	196	LEU
37	OC	202	LEU
37	OC	209	ARG
38	PC	10	MET
38	PC	20	GLN
38	PC	24	ARG
38	PC	41	VAL
38	PC	50	GLU
38	PC	60	TYR
38	PC	68	GLU
38	PC	72	GLN
38	PC	75	THR
38	PC	79	GLU
38	PC	91	LEU
38	PC	100	VAL
38	PC	107	ARG
38	PC	136	MET
38	PC	142	LEU
38	PC	145	LYS
38	PC	155	GLU
39	QC	14	LEU
39	QC	16	GLN
39	QC	36	ARG
39	QC	37	VAL
39	QC	43	LEU
39	QC	45	LEU
39	QC	64	GLN
39	QC	69	GLU
39	QC	74	ASP
39	QC	83	ASP
39	QC	89	MET
40	RC	5	ARG
40	RC	8	GLU
40	RC	10	ARG

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Mol	Chain	Res	Type
40	RC	24	THR
40	RC	104	LEU
40	RC	115	ARG
41	SC	29	SER
41	SC	50	ARG
41	SC	52	ASP
41	SC	88	LYS
41	SC	91	ARG
41	SC	102	ARG
41	SC	113	SER
41	SC	120	THR
41	SC	133	LEU
41	SC	135	CYS
41	SC	136	GLU
42	TC	2	GLU
42	TC	4	TYR
42	TC	16	ARG
42	TC	27	THR
42	TC	33	PHE
42	TC	36	TYR
42	TC	38	GLN
42	TC	65	VAL
42	TC	75	ASP
42	TC	108	VAL
42	TC	121	ARG
42	TC	127	LYS
43	UC	44	VAL
43	UC	74	ILE
43	UC	76	ASN
43	UC	86	MET
43	UC	88	LEU
43	UC	89	ASP
43	UC	95	GLU
44	VC	34	ASP
44	VC	80	VAL
44	VC	99	GLN
45	WC	6	THR
45	WC	20	LYS
45	WC	44	THR
45	WC	52	LEU
45	WC	60	LEU
45	WC	83	VAL

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Mol	Chain	Res	Type
45	WC	86	ARG
46	XC	3	ARG
46	XC	4	ILE
46	XC	11	ARG
46	XC	27	LYS
46	XC	32	GLU
46	XC	37	THR
46	XC	58	GLU
46	XC	65	LYS
46	XC	70	LEU
46	XC	90	LEU
46	XC	101	GLN
47	YC	6	LEU
47	YC	7	ILE
48	ZC	4	THR
48	ZC	35	ARG
48	ZC	38	ARG
48	ZC	39	LEU
48	ZC	66	LEU
48	ZC	70	LEU
48	ZC	83	GLU
49	AD	11	SER
49	AD	20	VAL
49	AD	60	LEU
49	AD	67	THR
49	AD	72	ARG
49	AD	82	GLN
50	BD	35	VAL
50	BD	37	LYS
50	BD	63	ARG
50	BD	75	ARG
50	BD	87	LYS
50	BD	93	GLN
50	BD	96	GLN
50	BD	100	LYS
51	CD	19	LYS
51	CD	26	LEU
51	CD	32	ARG
51	CD	46	GLU
51	CD	54	ARG
52	DD	3	ARG
52	DD	11	VAL

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Mol	Chain	Res	Type
52	DD	12	ASP
52	DD	15	LEU
52	DD	64	GLU
52	DD	77	THR
52	DD	83	HIS
53	ED	15	ARG
53	ED	31	SER
53	ED	53	LEU
53	ED	62	LEU
53	ED	72	LEU
53	ED	91	LEU
54	FD	10	ARG
55	GD	107	ASP
55	GD	110	ASN
55	GD	115	VAL
55	GD	130	ASP
55	GD	146	VAL
55	GD	149	MET
55	GD	156	HIS
55	GD	184	VAL
55	GD	193	GLN
55	GD	203	VAL
55	GD	208	GLU
55	GD	209	LEU
55	GD	211	ASP
55	GD	214	LEU
55	GD	229	SER
55	GD	237	VAL
55	GD	260	GLU
55	GD	274	LEU
55	GD	277	ARG
55	GD	300	SER
55	GD	306	ARG
55	GD	316	ARG
55	GD	318	THR
55	GD	325	THR
55	GD	326	LEU
55	GD	327	TYR
55	GD	345	ILE
55	HD	107	ASP
55	HD	110	ASN
55	HD	115	VAL

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Mol	Chain	Res	Type
55	HD	123	GLU
55	HD	130	ASP
55	HD	146	VAL
55	HD	149	MET
55	HD	156	HIS
55	HD	184	VAL
55	HD	193	GLN
55	HD	203	VAL
55	HD	208	GLU
55	HD	209	LEU
55	HD	211	ASP
55	HD	214	LEU
55	HD	229	SER
55	HD	237	VAL
55	HD	274	LEU
55	HD	277	ARG
55	HD	300	SER
55	HD	306	ARG
55	HD	316	ARG
55	HD	318	THR
55	HD	325	THR
55	HD	326	LEU
55	HD	327	TYR
55	HD	345	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (113) such sidechains are listed below:

Mol	Chain	Res	Type
5	E	112	GLN
6	F	132	HIS
7	G	8	GLN
8	H	41	GLN
9	I	61	HIS
9	I	143	GLN
10	J	54	GLN
11	K	69	GLN
13	M	27	HIS
14	N	123	HIS
15	O	24	GLN
15	O	50	HIS
15	O	71	GLN
16	P	61	ASN

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Mol	Chain	Res	Type
16	P	84	GLN
17	Q	58	ASN
17	Q	136	GLN
21	U	55	ASN
21	U	82	GLN
22	V	43	ASN
23	W	50	GLN
24	X	17	GLN
28	BA	47	GLN
33	GA	34	GLN
35	JA	25	ASN
36	KA	104	GLN
36	KA	108	ASN
36	KA	123	GLN
36	KA	136	GLN
36	KA	139	GLN
36	KA	170	GLN
37	LA	62	GLN
37	LA	119	GLN
37	LA	160	GLN
39	NA	13	ASN
39	NA	64	GLN
39	NA	94	GLN
40	OA	96	GLN
40	OA	97	GLN
42	QA	23	ASN
43	RA	33	GLN
44	SA	99	GLN
46	UA	77	ASN
46	UA	101	GLN
48	WA	9	GLN
48	WA	13	GLN
49	XA	65	GLN
50	YA	26	GLN
50	YA	96	GLN
52	AB	23	ASN
5	HB	112	GLN
5	HB	166	GLN
6	IB	132	HIS
7	JB	8	GLN
8	KB	41	GLN
9	LB	61	HIS

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Mol	Chain	Res	Type
9	LB	143	GLN
10	MB	54	GLN
11	NB	69	GLN
12	OB	3	GLN
13	PB	27	HIS
15	RB	50	HIS
15	RB	71	GLN
16	SB	61	ASN
16	SB	84	GLN
17	TB	58	ASN
17	TB	136	GLN
21	XB	82	GLN
22	YB	43	ASN
23	ZB	50	GLN
23	ZB	73	GLN
23	ZB	75	ASN
24	AC	17	GLN
33	JC	34	GLN
35	MC	25	ASN
36	NC	104	GLN
36	NC	108	ASN
36	NC	123	GLN
36	NC	136	GLN
36	NC	139	GLN
36	NC	170	GLN
37	OC	62	GLN
37	OC	119	GLN
37	OC	160	GLN
39	QC	13	ASN
39	QC	64	GLN
39	QC	94	GLN
40	RC	86	GLN
40	RC	96	GLN
40	RC	97	GLN
42	TC	23	ASN
43	UC	33	GLN
44	VC	38	ASN
44	VC	99	GLN
46	XC	77	ASN
46	XC	101	GLN
48	ZC	9	GLN
48	ZC	13	GLN

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Mol	Chain	Res	Type
49	AD	65	GLN
50	BD	26	GLN
50	BD	96	GLN
52	DD	23	ASN
55	GD	185	GLN
55	GD	197	HIS
55	GD	236	HIS
55	GD	264	HIS
55	GD	287	GLN
55	GD	320	HIS
55	GD	352	GLN
55	HD	197	HIS
55	HD	236	HIS
55	HD	320	HIS
55	HD	352	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1502/1507 (99%)	228 (15%)	10 (0%)
1	DB	1502/1507 (99%)	223 (14%)	10 (0%)
2	B	2876/2880 (99%)	498 (17%)	15 (0%)
2	EB	2876/2880 (99%)	496 (17%)	15 (0%)
3	C	119/120 (99%)	18 (15%)	0
3	FB	119/120 (99%)	17 (14%)	0
34	HA	9/27 (33%)	4 (44%)	1 (11%)
34	KC	9/27 (33%)	4 (44%)	1 (11%)
4	D	76/77 (98%)	13 (17%)	0
4	GB	76/77 (98%)	13 (17%)	0
4	IA	76/77 (98%)	7 (9%)	0
4	LC	76/77 (98%)	7 (9%)	0
All	All	9316/9376 (99%)	1528 (16%)	52 (0%)

All (1528) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	6	G
1	A	8	A
1	A	9	G
1	A	32	A

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Mol	Chain	Res	Type
1	A	33	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	52	G
1	A	59	A
1	A	61	G
1	A	79	G
1	A	82	U
1	A	85	U
1	A	86	U
1	A	87	A
1	A	88	C
1	A	90	C
1	A	101	A
1	A	116	A
1	A	121	C
1	A	129(B)	G
1	A	131	C
1	A	144	G
1	A	149	A
1	A	163	C
1	A	174	C
1	A	182	U
1	A	188	U
1	A	189	U
1	A	195	A
1	A	197	A
1	A	201	C
1	A	208	U
1	A	209	U
1	A	210	U
1	A	240	C
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	289	G
1	A	321	A
1	A	328	C

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Mol	Chain	Res	Type
1	A	332	G
1	A	346	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	368	U
1	A	372	C
1	A	373	A
1	A	397	A
1	A	398	C
1	A	406	G
1	A	412	A
1	A	413	G
1	A	414	A
1	A	424	G
1	A	429	U
1	A	439	A
1	A	452	A
1	A	465	A
1	A	482	A
1	A	484	G
1	A	485	G
1	A	496	A
1	A	497	U
1	A	500	G
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	521	G
1	A	531	U
1	A	532	A
1	A	545	C
1	A	547	A
1	A	548	G
1	A	549	C
1	A	559	A
1	A	560	U
1	A	561	U
1	A	562	C
1	A	564	C

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Mol	Chain	Res	Type
1	A	567	G
1	A	573	A
1	A	575	G
1	A	576	G
1	A	577	G
1	A	630	G
1	A	631	G
1	A	653	A
1	A	665	A
1	A	688	G
1	A	703	G
1	A	723	U
1	A	724	G
1	A	731	G
1	A	749	C
1	A	755	G
1	A	774	G
1	A	777	A
1	A	793	U
1	A	794	A
1	A	816	A
1	A	817	C
1	A	818	G
1	A	819	A
1	A	828	A
1	A	842	C
1	A	843	U
1	A	848	C
1	A	851	G
1	A	859	A
1	A	872	A
1	A	902	G
1	A	914	A
1	A	920	U
1	A	926	G
1	A	927	G
1	A	931	C
1	A	934	C
1	A	935	A
1	A	960	U
1	A	969	A
1	A	971	G

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Mol	Chain	Res	Type
1	A	972	C
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	989	C
1	A	992	U
1	A	993	G
1	A	998(A)	G
1	A	1001	G
1	A	1002	G
1	A	1004	A
1	A	1007	C
1	A	1009	G
1	A	1012	U
1	A	1022	G
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1028(B)	C
1	A	1028(C)	C
1	A	1029	G
1	A	1030	C
1	A	1033	G
1	A	1034	G
1	A	1044	A
1	A	1053	G
1	A	1065	U
1	A	1081	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1126	U
1	A	1137	C
1	A	1138	G
1	A	1146	A
1	A	1152	A
1	A	1154	G
1	A	1157	A
1	A	1159	U
1	A	1171	G
1	A	1174	G

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Mol	Chain	Res	Type
1	A	1183	A
1	A	1184	G
1	A	1196	U
1	A	1197	G
1	A	1199	U
1	A	1201	A
1	A	1202	G
1	A	1212	U
1	A	1213	A
1	A	1225	A
1	A	1227	A
1	A	1236	A
1	A	1238	A
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1263	C
1	A	1270	C
1	A	1279	A
1	A	1280	A
1	A	1286	A
1	A	1287	A
1	A	1289	A
1	A	1299	A
1	A	1302	U
1	A	1305	G
1	A	1315	U
1	A	1336	C
1	A	1340	A
1	A	1347	G
1	A	1353	G
1	A	1362(B)	C
1	A	1363	A
1	A	1397	C
1	A	1398	A
1	A	1419	G
1	A	1429	C
1	A	1442	G
1	A	1451	A
1	A	1452	C
1	A	1453	G

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Mol	Chain	Res	Type
1	A	1492	A
1	A	1493	A
1	A	1494	G
1	A	1503	A
1	A	1504	G
1	A	1506	U
1	A	1507	A
1	A	1517	G
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1532	U
2	B	10	G
2	B	14	A
2	B	34	C
2	B	35	G
2	B	46	C
2	B	51	G
2	B	58	G
2	B	61	G
2	B	71	A
2	B	74	A
2	B	75	G
2	B	91	A
2	B	95	G
2	B	118	A
2	B	120	U
2	B	125	G
2	B	128	C
2	B	129	C
2	B	149	A
2	B	154(A)	C
2	B	155	C
2	B	181	A
2	B	182	A
2	B	196	A
2	B	199	A
2	B	200	U
2	B	205	G
2	B	212	G
2	B	214	G

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Mol	Chain	Res	Type
2	B	215	G
2	B	216	A
2	B	221	A
2	B	222	A
2	B	225	A
2	B	228	A
2	B	229	A
2	B	245	G
2	B	248	G
2	B	249	C
2	B	250	G
2	B	265	A
2	B	270(L)	C
2	B	270(M)	U
2	B	270(N)	U
2	B	270(O)	G
2	B	270(P)	U
2	B	270(Q)	C
2	B	271	G
2	B	278	A
2	B	302	C
2	B	311	A
2	B	317	G
2	B	323	G
2	B	324	A
2	B	329	G
2	B	330	A
2	B	331	A
2	B	332	A
2	B	352	G
2	B	353	G
2	B	363(A)	G
2	B	363(G)	A
2	B	386	G
2	B	405	U
2	B	406	G
2	B	411	G
2	B	412	A
2	B	418	G
2	B	421	U
2	B	444	C
2	B	456	C

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Mol	Chain	Res	Type
2	B	457	A
2	B	458	G
2	B	467	G
2	B	473	G
2	B	481	G
2	B	491	G
2	B	494	G
2	B	504	U
2	B	505	A
2	B	508	G
2	B	509	C
2	B	527	C
2	B	528	A
2	B	529	A
2	B	531	C
2	B	532	A
2	B	533	G
2	B	546	C
2	B	547	A
2	B	563	G
2	B	571	A
2	B	573	G
2	B	575	A
2	B	603	A
2	B	604	G
2	B	607	U
2	B	615	G
2	B	616	A
2	B	617	G
2	B	627	A
2	B	637	A
2	B	645	C
2	B	646	A
2	B	654	U
2	B	668	G
2	B	677	A
2	B	682	G
2	B	686	G
2	B	717	G
2	B	730	C
2	B	740	U
2	B	748	G

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Mol	Chain	Res	Type
2	B	749	C
2	B	765	G
2	B	775	G
2	B	776	G
2	B	782	A
2	B	784	A
2	B	785	G
2	B	792	G
2	B	793	A
2	B	800	A
2	B	805	G
2	B	812	C
2	B	819	A
2	B	827	U
2	B	828	U
2	B	846	C
2	B	859	G
2	B	866	A
2	B	878	A
2	B	879	G
2	B	886	C
2	B	887	A
2	B	888	C
2	B	889	C
2	B	890	A
2	B	893	C
2	B	894	C
2	B	895	U
2	B	896	A
2	B	907	U
2	B	910	A
2	B	917	A
2	B	932	G
2	B	941	A
2	B	944	G
2	B	945	A
2	B	946	G
2	B	959	A
2	B	961	C
2	B	973	A
2	B	974(A)	G
2	B	974(B)	C

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Mol	Chain	Res	Type
2	B	983	A
2	B	989	G
2	B	996	A
2	B	1005	C
2	B	1012	U
2	B	1013	C
2	B	1022	G
2	B	1023	U
2	B	1025	G
2	B	1026	U
2	B	1027	A
2	B	1033	U
2	B	1045	A
2	B	1046	A
2	B	1047	G
2	B	1049	C
2	B	1057	A
2	B	1060	U
2	B	1061	U
2	B	1062	G
2	B	1063	G
2	B	1064	C
2	B	1066	U
2	B	1068	G
2	B	1069	A
2	B	1070	A
2	B	1071	G
2	B	1072	C
2	B	1073	A
2	B	1074	G
2	B	1075	C
2	B	1076	C
2	B	1077	A
2	B	1078	U
2	B	1079	C
2	B	1083	U
2	B	1086	A
2	B	1087	G
2	B	1088	A
2	B	1089	G
2	B	1092	C
2	B	1093	G

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Mol	Chain	Res	Type
2	B	1094	U
2	B	1095	A
2	B	1096	A
2	B	1097	U
2	B	1098	A
2	B	1101	U
2	B	1107	G
2	B	1111	A
2	B	1112	G
2	B	1126	A
2	B	1129	A
2	B	1130	U
2	B	1135	C
2	B	1136	G
2	B	1139	G
2	B	1142(B)	A
2	B	1143	A
2	B	1174	A
2	B	1175	U
2	B	1177	A
2	B	1205	U
2	B	1210	A
2	B	1211	U
2	B	1218	C
2	B	1220	A
2	B	1252	G
2	B	1253	A
2	B	1256	G
2	B	1271	G
2	B	1272	A
2	B	1273	U
2	B	1300	U
2	B	1301	A
2	B	1302	A
2	B	1320	C
2	B	1340	U
2	B	1345	C
2	B	1352	U
2	B	1359	A
2	B	1360	A
2	B	1365	A
2	B	1380	G

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Mol	Chain	Res	Type
2	B	1385	G
2	B	1395	A
2	B	1416	G
2	B	1417	C
2	B	1419	A
2	B	1420	U
2	B	1421	G
2	B	1427	A
2	B	1428	C
2	B	1437	C
2	B	1444(B)	A
2	B	1449(B)	A
2	B	1454	U
2	B	1455	G
2	B	1460	A
2	B	1461	G
2	B	1467	C
2	B	1471	A
2	B	1478	G
2	B	1483	G
2	B	1493	C
2	B	1497	U
2	B	1510	A
2	B	1511	A
2	B	1512	G
2	B	1532	C
2	B	1534	G
2	B	1535	U
2	B	1537	C
2	B	1538	G
2	B	1544	C
2	B	1554	A
2	B	1558	A
2	B	1569	A
2	B	1578	U
2	B	1585	C
2	B	1586	A
2	B	1608	A
2	B	1609	A
2	B	1610	A
2	B	1618	A
2	B	1630(B)	C

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Mol	Chain	Res	Type
2	B	1631	A
2	B	1647	G
2	B	1648	C
2	B	1651	G
2	B	1654	A
2	B	1669	A
2	B	1672	C
2	B	1674	G
2	B	1675	C
2	B	1694	C
2	B	1700	A
2	B	1701	A
2	B	1703	G
2	B	1728	G
2	B	1729	A
2	B	1730	U
2	B	1731	G
2	B	1743	G
2	B	1750	G
2	B	1756	G
2	B	1761	C
2	B	1762	A
2	B	1763	G
2	B	1764	G
2	B	1773	A
2	B	1776	G
2	B	1779	U
2	B	1780	A
2	B	1782	C
2	B	1791	A
2	B	1800	C
2	B	1801	G
2	B	1811	G
2	B	1816	G
2	B	1847	A
2	B	1858	G
2	B	1859	A
2	B	1878	G
2	B	1900	A
2	B	1903	G
2	B	1906	G
2	B	1929	G

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Mol	Chain	Res	Type
2	B	1930	G
2	B	1934	C
2	B	1936	A
2	B	1937	A
2	B	1938	A
2	B	1939	5MU
2	B	1940	U
2	B	1955	U
2	B	1963	U
2	B	1967	C
2	B	1970	A
2	B	1971	A
2	B	1972	A
2	B	1984	G
2	B	1992	G
2	B	1993	U
2	B	1997	G
2	B	2020	A
2	B	2022	U
2	B	2023	G
2	B	2030	A
2	B	2031	A
2	B	2032	G
2	B	2033	A
2	B	2043	C
2	B	2049	G
2	B	2055	C
2	B	2056	G
2	B	2060	A
2	B	2061	G
2	B	2062	A
2	B	2069	G
2	B	2080	G
2	B	2100	G
2	B	2107	C
2	B	2110	G
2	B	2124	G
2	B	2125	G
2	B	2127	G
2	B	2129	C
2	B	2130	U
2	B	2131	G

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Mol	Chain	Res	Type
2	B	2132	U
2	B	2133	G
2	B	2138	C
2	B	2139	C
2	B	2142	C
2	B	2144	U
2	B	2147	G
2	B	2149	G
2	B	2156	G
2	B	2157	G
2	B	2158	A
2	B	2160	G
2	B	2162	G
2	B	2167	U
2	B	2168	G
2	B	2169	A
2	B	2171	A
2	B	2172	U
2	B	2173	A
2	B	2176	A
2	B	2189	U
2	B	2190	G
2	B	2198	A
2	B	2210	G
2	B	2211	G
2	B	2212	A
2	B	2213	U
2	B	2215	G
2	B	2225	A
2	B	2238	G
2	B	2239	G
2	B	2243	U
2	B	2252	G
2	B	2269	A
2	B	2273	A
2	B	2275	C
2	B	2278	A
2	B	2280	G
2	B	2283	C
2	B	2287	A
2	B	2305	A
2	B	2308	G

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Mol	Chain	Res	Type
2	B	2309	A
2	B	2311	A
2	B	2312	U
2	B	2319	G
2	B	2320	A
2	B	2321	G
2	B	2325	G
2	B	2334	G
2	B	2336	A
2	B	2345	G
2	B	2347	C
2	B	2350	C
2	B	2383	G
2	B	2384	G
2	B	2385	C
2	B	2402	C
2	B	2422	A
2	B	2423	U
2	B	2425	A
2	B	2429	G
2	B	2430	A
2	B	2434	A
2	B	2439	A
2	B	2441	C
2	B	2448	A
2	B	2468	G
2	B	2469	A
2	B	2476	A
2	B	2500	U
2	B	2502	G
2	B	2504	U
2	B	2505	G
2	B	2506	U
2	B	2518	A
2	B	2520	C
2	B	2525	G
2	B	2529	G
2	B	2534	A
2	B	2554	U
2	B	2562	U
2	B	2566	A
2	B	2567	G

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Mol	Chain	Res	Type
2	B	2573	C
2	B	2574	G
2	B	2578	G
2	B	2586	C
2	B	2596	U
2	B	2602	A
2	B	2609	U
2	B	2611	U
2	B	2612	C
2	B	2615	U
2	B	2630	G
2	B	2689	U
2	B	2702	U
2	B	2703	C
2	B	2712(A)	A
2	B	2713	A
2	B	2714	G
2	B	2726	U
2	B	2733	A
2	B	2751	G
2	B	2757	A
2	B	2764	A
2	B	2765	A
2	B	2766	G
2	B	2777	G
2	B	2778	A
2	B	2790	A
2	B	2791	C
2	B	2792	G
2	B	2793	G
2	B	2797	U
2	B	2798	C
2	B	2799	A
2	B	2801	A
2	B	2802	G
2	B	2807	G
2	B	2810	A
2	B	2820	A
2	B	2821	A
2	B	2823	A
2	B	2833	G
2	B	2834	G

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Mol	Chain	Res	Type
2	B	2835	A
2	B	2872	G
2	B	2876	G
2	B	2880	C
2	B	2892	A
2	B	2896	C
2	B	2897	U
3	C	9	G
3	C	12	C
3	C	13	A
3	C	30	C
3	C	41	U
3	C	42	C
3	C	44	G
3	C	45	A
3	C	56	G
3	C	63	G
3	C	65	C
3	C	66	A
3	C	67	G
3	C	73	A
3	C	88	C
3	C	90	C
3	C	109	G
3	C	119	A
4	D	6	G
4	D	9	G
4	D	13	C
4	D	16	C
4	D	17(A)	U
4	D	18	G
4	D	19	G
4	D	20	U
4	D	27	U
4	D	35	A
4	D	47	U
4	D	48	C
4	D	61	C
34	HA	14	A
34	HA	15	A
34	HA	16	A
34	HA	21	A

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Mol	Chain	Res	Type
4	IA	2	G
4	IA	18	G
4	IA	20	U
4	IA	47	U
4	IA	48	C
4	IA	52	G
4	IA	76	A
1	DB	5	U
1	DB	6	G
1	DB	8	A
1	DB	9	G
1	DB	32	A
1	DB	39	G
1	DB	47	C
1	DB	48	C
1	DB	51	A
1	DB	52	G
1	DB	59	A
1	DB	61	G
1	DB	79	G
1	DB	82	U
1	DB	85	U
1	DB	86	U
1	DB	87	A
1	DB	88	C
1	DB	101	A
1	DB	116	A
1	DB	121	C
1	DB	129(B)	G
1	DB	131	C
1	DB	144	G
1	DB	149	A
1	DB	163	C
1	DB	174	C
1	DB	182	U
1	DB	188	U
1	DB	189	U
1	DB	195	A
1	DB	197	A
1	DB	201	C
1	DB	208	U
1	DB	209	U

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Mol	Chain	Res	Type
1	DB	210	U
1	DB	240	C
1	DB	245	C
1	DB	247	G
1	DB	251	G
1	DB	266	G
1	DB	267	C
1	DB	289	G
1	DB	321	A
1	DB	328	C
1	DB	332	G
1	DB	346	G
1	DB	352	C
1	DB	353	A
1	DB	354	G
1	DB	367	U
1	DB	372	C
1	DB	373	A
1	DB	397	A
1	DB	398	C
1	DB	406	G
1	DB	412	A
1	DB	413	G
1	DB	414	A
1	DB	424	G
1	DB	429	U
1	DB	439	A
1	DB	452	A
1	DB	465	A
1	DB	482	A
1	DB	484	G
1	DB	485	G
1	DB	496	A
1	DB	497	U
1	DB	500	G
1	DB	509	A
1	DB	510	A
1	DB	511	C
1	DB	518	C
1	DB	531	U
1	DB	532	A
1	DB	545	C

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Mol	Chain	Res	Type
1	DB	547	A
1	DB	548	G
1	DB	549	C
1	DB	559	A
1	DB	560	U
1	DB	561	U
1	DB	562	C
1	DB	564	C
1	DB	567	G
1	DB	573	A
1	DB	575	G
1	DB	576	G
1	DB	577	G
1	DB	630	G
1	DB	631	G
1	DB	653	A
1	DB	665	A
1	DB	688	G
1	DB	703	G
1	DB	723	U
1	DB	724	G
1	DB	731	G
1	DB	749	C
1	DB	755	G
1	DB	774	G
1	DB	777	A
1	DB	793	U
1	DB	794	A
1	DB	816	A
1	DB	817	C
1	DB	818	G
1	DB	819	A
1	DB	828	A
1	DB	842	C
1	DB	843	U
1	DB	848	C
1	DB	851	G
1	DB	859	A
1	DB	872	A
1	DB	902	G
1	DB	914	A
1	DB	920	U

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Mol	Chain	Res	Type
1	DB	926	G
1	DB	927	G
1	DB	931	C
1	DB	934	C
1	DB	935	A
1	DB	960	U
1	DB	969	A
1	DB	971	G
1	DB	972	C
1	DB	974	A
1	DB	975	A
1	DB	976	G
1	DB	977	A
1	DB	989	C
1	DB	992	U
1	DB	993	G
1	DB	998(A)	G
1	DB	1001	G
1	DB	1002	G
1	DB	1004	A
1	DB	1007	C
1	DB	1009	G
1	DB	1012	U
1	DB	1022	G
1	DB	1025	U
1	DB	1026	G
1	DB	1027	C
1	DB	1028(B)	C
1	DB	1028(C)	C
1	DB	1029	G
1	DB	1030	C
1	DB	1033	G
1	DB	1034	G
1	DB	1044	A
1	DB	1053	G
1	DB	1065	U
1	DB	1081	G
1	DB	1094	G
1	DB	1095	U
1	DB	1101	A
1	DB	1126	U
1	DB	1137	C

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Mol	Chain	Res	Type
1	DB	1138	G
1	DB	1146	A
1	DB	1152	A
1	DB	1154	G
1	DB	1157	A
1	DB	1159	U
1	DB	1171	G
1	DB	1183	A
1	DB	1184	G
1	DB	1196	U
1	DB	1197	G
1	DB	1199	U
1	DB	1201	A
1	DB	1202	G
1	DB	1212	U
1	DB	1213	A
1	DB	1225	A
1	DB	1227	A
1	DB	1236	A
1	DB	1238	A
1	DB	1256	A
1	DB	1257	U
1	DB	1258	G
1	DB	1260	C
1	DB	1263	C
1	DB	1270	C
1	DB	1279	A
1	DB	1280	A
1	DB	1286	A
1	DB	1287	A
1	DB	1289	A
1	DB	1299	A
1	DB	1301	U
1	DB	1302	U
1	DB	1305	G
1	DB	1315	U
1	DB	1320	C
1	DB	1336	C
1	DB	1340	A
1	DB	1347	G
1	DB	1353	G
1	DB	1362(B)	C

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Mol	Chain	Res	Type
1	DB	1397	C
1	DB	1398	A
1	DB	1419	G
1	DB	1442	G
1	DB	1451	A
1	DB	1452	C
1	DB	1453	G
1	DB	1492	A
1	DB	1493	A
1	DB	1494	G
1	DB	1503	A
1	DB	1504	G
1	DB	1506	U
1	DB	1507	A
1	DB	1517	G
1	DB	1520	G
1	DB	1529	G
1	DB	1530	G
1	DB	1531	A
1	DB	1532	U
2	EB	10	G
2	EB	14	A
2	EB	34	C
2	EB	35	G
2	EB	46	C
2	EB	51	G
2	EB	58	G
2	EB	61	G
2	EB	71	A
2	EB	74	A
2	EB	75	G
2	EB	91	A
2	EB	95	G
2	EB	118	A
2	EB	120	U
2	EB	125	G
2	EB	128	C
2	EB	129	C
2	EB	154(A)	C
2	EB	155	C
2	EB	181	A
2	EB	182	A

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Mol	Chain	Res	Type
2	EB	196	A
2	EB	199	A
2	EB	200	U
2	EB	205	G
2	EB	212	G
2	EB	214	G
2	EB	215	G
2	EB	216	A
2	EB	221	A
2	EB	222	A
2	EB	225	A
2	EB	228	A
2	EB	229	A
2	EB	245	G
2	EB	248	G
2	EB	249	C
2	EB	265	A
2	EB	270(L)	C
2	EB	270(M)	U
2	EB	270(N)	U
2	EB	270(O)	G
2	EB	270(P)	U
2	EB	270(Q)	C
2	EB	271	G
2	EB	278	A
2	EB	302	C
2	EB	311	A
2	EB	317	G
2	EB	324	A
2	EB	329	G
2	EB	330	A
2	EB	332	A
2	EB	352	G
2	EB	353	G
2	EB	363(A)	G
2	EB	363(G)	A
2	EB	386	G
2	EB	405	U
2	EB	406	G
2	EB	411	G
2	EB	412	A
2	EB	418	G

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Mol	Chain	Res	Type
2	EB	421	U
2	EB	444	C
2	EB	456	C
2	EB	457	A
2	EB	458	G
2	EB	467	G
2	EB	473	G
2	EB	481	G
2	EB	491	G
2	EB	494	G
2	EB	504	U
2	EB	505	A
2	EB	508	G
2	EB	509	C
2	EB	527	C
2	EB	528	A
2	EB	529	A
2	EB	531	C
2	EB	532	A
2	EB	533	G
2	EB	546	C
2	EB	547	A
2	EB	563	G
2	EB	571	A
2	EB	573	G
2	EB	575	A
2	EB	593	G
2	EB	603	A
2	EB	604	G
2	EB	607	U
2	EB	609(B)	G
2	EB	615	G
2	EB	616	A
2	EB	617	G
2	EB	627	A
2	EB	637	A
2	EB	645	C
2	EB	646	A
2	EB	654	U
2	EB	668	G
2	EB	677	A
2	EB	682	G

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Mol	Chain	Res	Type
2	EB	686	G
2	EB	717	G
2	EB	730	C
2	EB	740	U
2	EB	748	G
2	EB	749	C
2	EB	765	G
2	EB	775	G
2	EB	776	G
2	EB	782	A
2	EB	784	A
2	EB	785	G
2	EB	792	G
2	EB	793	A
2	EB	805	G
2	EB	812	C
2	EB	819	A
2	EB	827	U
2	EB	828	U
2	EB	846	C
2	EB	856	C
2	EB	859	G
2	EB	866	A
2	EB	878	A
2	EB	879	G
2	EB	886	C
2	EB	887	A
2	EB	888	C
2	EB	889	C
2	EB	890	A
2	EB	893	C
2	EB	894	C
2	EB	895	U
2	EB	896	A
2	EB	907	U
2	EB	910	A
2	EB	917	A
2	EB	932	G
2	EB	941	A
2	EB	944	G
2	EB	945	A
2	EB	946	G

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Mol	Chain	Res	Type
2	EB	959	A
2	EB	961	C
2	EB	973	A
2	EB	974(A)	G
2	EB	974(B)	C
2	EB	983	A
2	EB	989	G
2	EB	996	A
2	EB	1005	C
2	EB	1012	U
2	EB	1013	C
2	EB	1022	G
2	EB	1023	U
2	EB	1025	G
2	EB	1026	U
2	EB	1027	A
2	EB	1033	U
2	EB	1045	A
2	EB	1046	A
2	EB	1047	G
2	EB	1049	C
2	EB	1057	A
2	EB	1060	U
2	EB	1061	U
2	EB	1062	G
2	EB	1063	G
2	EB	1064	C
2	EB	1066	U
2	EB	1068	G
2	EB	1069	A
2	EB	1070	A
2	EB	1071	G
2	EB	1072	C
2	EB	1073	A
2	EB	1074	G
2	EB	1075	C
2	EB	1076	C
2	EB	1077	A
2	EB	1078	U
2	EB	1079	C
2	EB	1083	U
2	EB	1086	A

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Mol	Chain	Res	Type
2	EB	1087	G
2	EB	1088	A
2	EB	1089	G
2	EB	1092	C
2	EB	1093	G
2	EB	1094	U
2	EB	1095	A
2	EB	1096	A
2	EB	1097	U
2	EB	1098	A
2	EB	1101	U
2	EB	1107	G
2	EB	1111	A
2	EB	1112	G
2	EB	1126	A
2	EB	1129	A
2	EB	1130	U
2	EB	1135	C
2	EB	1136	G
2	EB	1139	G
2	EB	1142(B)	A
2	EB	1143	A
2	EB	1174	A
2	EB	1175	U
2	EB	1177	A
2	EB	1205	U
2	EB	1210	A
2	EB	1211	U
2	EB	1220	A
2	EB	1252	G
2	EB	1253	A
2	EB	1256	G
2	EB	1269	A
2	EB	1271	G
2	EB	1272	A
2	EB	1273	U
2	EB	1300	U
2	EB	1301	A
2	EB	1302	A
2	EB	1313	U
2	EB	1320	C
2	EB	1340	U

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Mol	Chain	Res	Type
2	EB	1345	C
2	EB	1352	U
2	EB	1359	A
2	EB	1360	A
2	EB	1365	A
2	EB	1380	G
2	EB	1385	G
2	EB	1395	A
2	EB	1416	G
2	EB	1417	C
2	EB	1419	A
2	EB	1420	U
2	EB	1421	G
2	EB	1427	A
2	EB	1428	C
2	EB	1437	C
2	EB	1444(B)	A
2	EB	1449(B)	A
2	EB	1454	U
2	EB	1455	G
2	EB	1460	A
2	EB	1461	G
2	EB	1467	C
2	EB	1471	A
2	EB	1478	G
2	EB	1483	G
2	EB	1493	C
2	EB	1497	U
2	EB	1510	A
2	EB	1511	A
2	EB	1512	G
2	EB	1532	C
2	EB	1534	G
2	EB	1535	U
2	EB	1537	C
2	EB	1538	G
2	EB	1544	C
2	EB	1554	A
2	EB	1558	A
2	EB	1566	A
2	EB	1569	A
2	EB	1578	U

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Mol	Chain	Res	Type
2	EB	1585	C
2	EB	1586	A
2	EB	1608	A
2	EB	1609	A
2	EB	1610	A
2	EB	1618	A
2	EB	1630(B)	C
2	EB	1631	A
2	EB	1647	G
2	EB	1648	C
2	EB	1651	G
2	EB	1654	A
2	EB	1669	A
2	EB	1672	C
2	EB	1674	G
2	EB	1675	C
2	EB	1700	A
2	EB	1701	A
2	EB	1703	G
2	EB	1728	G
2	EB	1729	A
2	EB	1730	U
2	EB	1731	G
2	EB	1743	G
2	EB	1750	G
2	EB	1756	G
2	EB	1761	C
2	EB	1762	A
2	EB	1763	G
2	EB	1764	G
2	EB	1773	A
2	EB	1776	G
2	EB	1779	U
2	EB	1780	A
2	EB	1782	C
2	EB	1791	A
2	EB	1800	C
2	EB	1801	G
2	EB	1811	G
2	EB	1816	G
2	EB	1847	A
2	EB	1858	G

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Mol	Chain	Res	Type
2	EB	1859	A
2	EB	1878	G
2	EB	1900	A
2	EB	1903	G
2	EB	1906	G
2	EB	1929	G
2	EB	1930	G
2	EB	1936	A
2	EB	1937	A
2	EB	1938	A
2	EB	1939	5MU
2	EB	1940	U
2	EB	1955	U
2	EB	1963	U
2	EB	1967	C
2	EB	1970	A
2	EB	1971	A
2	EB	1972	A
2	EB	1984	G
2	EB	1992	G
2	EB	1993	U
2	EB	1997	G
2	EB	2020	A
2	EB	2022	U
2	EB	2023	G
2	EB	2030	A
2	EB	2031	A
2	EB	2032	G
2	EB	2033	A
2	EB	2043	C
2	EB	2049	G
2	EB	2055	C
2	EB	2056	G
2	EB	2060	A
2	EB	2061	G
2	EB	2062	A
2	EB	2069	G
2	EB	2080	G
2	EB	2100	G
2	EB	2107	C
2	EB	2110	G
2	EB	2124	G

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Mol	Chain	Res	Type
2	EB	2125	G
2	EB	2127	G
2	EB	2129	C
2	EB	2130	U
2	EB	2131	G
2	EB	2132	U
2	EB	2133	G
2	EB	2138	C
2	EB	2139	C
2	EB	2142	C
2	EB	2144	U
2	EB	2147	G
2	EB	2149	G
2	EB	2156	G
2	EB	2157	G
2	EB	2158	A
2	EB	2160	G
2	EB	2162	G
2	EB	2167	U
2	EB	2168	G
2	EB	2169	A
2	EB	2171	A
2	EB	2172	U
2	EB	2173	A
2	EB	2176	A
2	EB	2189	U
2	EB	2190	G
2	EB	2198	A
2	EB	2210	G
2	EB	2211	G
2	EB	2212	A
2	EB	2213	U
2	EB	2215	G
2	EB	2225	A
2	EB	2238	G
2	EB	2239	G
2	EB	2243	U
2	EB	2252	G
2	EB	2269	A
2	EB	2273	A
2	EB	2275	C
2	EB	2278	A

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Mol	Chain	Res	Type
2	EB	2280	G
2	EB	2283	C
2	EB	2287	A
2	EB	2305	A
2	EB	2308	G
2	EB	2309	A
2	EB	2311	A
2	EB	2312	U
2	EB	2319	G
2	EB	2320	A
2	EB	2321	G
2	EB	2325	G
2	EB	2334	G
2	EB	2336	A
2	EB	2347	C
2	EB	2350	C
2	EB	2383	G
2	EB	2384	G
2	EB	2385	C
2	EB	2402	C
2	EB	2422	A
2	EB	2423	U
2	EB	2425	A
2	EB	2429	G
2	EB	2430	A
2	EB	2434	A
2	EB	2439	A
2	EB	2441	C
2	EB	2448	A
2	EB	2468	G
2	EB	2469	A
2	EB	2476	A
2	EB	2500	U
2	EB	2502	G
2	EB	2504	U
2	EB	2505	G
2	EB	2506	U
2	EB	2518	A
2	EB	2520	C
2	EB	2525	G
2	EB	2529	G
2	EB	2534	A

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Mol	Chain	Res	Type
2	EB	2554	U
2	EB	2562	U
2	EB	2566	A
2	EB	2567	G
2	EB	2573	C
2	EB	2574	G
2	EB	2578	G
2	EB	2585	U
2	EB	2586	C
2	EB	2596	U
2	EB	2602	A
2	EB	2609	U
2	EB	2611	U
2	EB	2612	C
2	EB	2615	U
2	EB	2630	G
2	EB	2689	U
2	EB	2702	U
2	EB	2703	C
2	EB	2712(A)	A
2	EB	2713	A
2	EB	2714	G
2	EB	2726	U
2	EB	2733	A
2	EB	2751	G
2	EB	2757	A
2	EB	2764	A
2	EB	2765	A
2	EB	2766	G
2	EB	2777	G
2	EB	2778	A
2	EB	2790	A
2	EB	2791	C
2	EB	2792	G
2	EB	2793	G
2	EB	2797	U
2	EB	2798	C
2	EB	2799	A
2	EB	2801	A
2	EB	2802	G
2	EB	2807	G
2	EB	2810	A

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Mol	Chain	Res	Type
2	EB	2820	A
2	EB	2821	A
2	EB	2823	A
2	EB	2833	G
2	EB	2834	G
2	EB	2835	A
2	EB	2872	G
2	EB	2876	G
2	EB	2880	C
2	EB	2892	A
2	EB	2896	C
2	EB	2897	U
3	FB	9	G
3	FB	12	C
3	FB	13	A
3	FB	30	C
3	FB	41	U
3	FB	42	C
3	FB	44	G
3	FB	45	A
3	FB	56	G
3	FB	63	G
3	FB	65	C
3	FB	66	A
3	FB	67	G
3	FB	73	A
3	FB	88	C
3	FB	90	C
3	FB	109	G
4	GB	6	G
4	GB	9	G
4	GB	13	C
4	GB	16	C
4	GB	17(A)	U
4	GB	18	G
4	GB	19	G
4	GB	20	U
4	GB	27	U
4	GB	35	A
4	GB	47	U
4	GB	48	C
4	GB	61	C

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Mol	Chain	Res	Type
34	KC	14	A
34	KC	15	A
34	KC	16	A
34	KC	21	A
4	LC	2	G
4	LC	18	G
4	LC	20	U
4	LC	47	U
4	LC	48	C
4	LC	52	G
4	LC	76	A

All (52) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	115	G
1	A	509	A
1	A	560	U
1	A	563	A
1	A	572	A
1	A	687	A
1	A	723	U
1	A	748	C
1	A	913	A
1	A	1201	A
2	B	34	C
2	B	196	A
2	B	507	A
2	B	528	A
2	B	784	A
2	B	974(A)	G
2	B	1060	U
2	B	1088	A
2	B	1210	A
2	B	1379	A
2	B	1608	A
2	B	1992	G
2	B	2032	G
2	B	2422	A
2	B	2833	G
34	HA	22	A
1	DB	115	G

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Mol	Chain	Res	Type
1	DB	509	A
1	DB	560	U
1	DB	563	A
1	DB	572	A
1	DB	687	A
1	DB	723	U
1	DB	748	C
1	DB	913	A
1	DB	1201	A
2	EB	34	C
2	EB	196	A
2	EB	507	A
2	EB	528	A
2	EB	784	A
2	EB	974(A)	G
2	EB	1060	U
2	EB	1210	A
2	EB	1301	A
2	EB	1379	A
2	EB	1608	A
2	EB	1992	G
2	EB	2032	G
2	EB	2422	A
2	EB	2833	G
34	KC	22	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	PSU	DB	516	1	18,21,22	1.82	3 (16%)	21,30,33	1.34	3 (14%)
2	OMG	EB	2251	4,2	19,26,27	2.04	5 (26%)	21,38,41	1.39	4 (19%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5MC	A	1400	1	19,22,23	2.34	4 (21%)	26,32,35	1.21	4 (15%)
2	PSU	B	1911	2	18,21,22	1.52	2 (11%)	21,30,33	1.71	5 (23%)
4	5MU	IA	54	4,56	19,22,23	2.14	3 (15%)	27,32,35	2.22	10 (37%)
2	5MU	EB	1939	2	19,22,23	2.22	5 (26%)	27,32,35	2.60	8 (29%)
1	5MC	DB	1407	1	19,22,23	3.12	4 (21%)	26,32,35	1.17	2 (7%)
1	MA6	A	1518	1	19,26,27	1.98	5 (26%)	18,38,41	1.78	3 (16%)
4	5MC	IA	32	4	19,22,23	2.61	4 (21%)	26,32,35	1.30	3 (11%)
4	4SU	D	8	4	18,21,22	4.82	7 (38%)	25,30,33	5.36	10 (40%)
1	5MC	A	967	1	19,22,23	2.52	5 (26%)	26,32,35	1.31	3 (11%)
2	5MC	B	1962	2	19,22,23	2.65	4 (21%)	26,32,35	1.29	2 (7%)
1	M2G	DB	966	1	20,27,28	2.28	5 (25%)	19,40,43	1.31	3 (15%)
1	4OC	DB	1402	1	20,23,24	1.07	2 (10%)	25,32,35	1.59	7 (28%)
1	2MG	A	1207	1	18,26,27	2.17	3 (16%)	16,38,41	1.68	4 (25%)
4	5MU	GB	54	4	19,22,23	2.07	3 (15%)	27,32,35	2.12	8 (29%)
1	2MG	DB	1207	1	18,26,27	2.19	3 (16%)	16,38,41	1.72	4 (25%)
2	PSU	EB	2605	2	18,21,22	1.48	2 (11%)	21,30,33	1.66	5 (23%)
4	4SU	IA	8	4	18,21,22	4.77	7 (38%)	25,30,33	5.16	11 (44%)
4	5MC	GB	32	4	19,22,23	2.65	4 (21%)	26,32,35	1.13	3 (11%)
2	PSU	EB	1917	2	18,21,22	1.71	2 (11%)	21,30,33	1.82	6 (28%)
1	MA6	DB	1519	1	19,26,27	2.02	5 (26%)	18,38,41	1.76	3 (16%)
45	0TD	WC	92	45	8,9,10	3.17	2 (25%)	6,11,13	3.11	3 (50%)
2	4OC	B	1920	2	19,22,24	1.14	1 (5%)	25,31,35	0.85	1 (4%)
1	MA6	A	1519	1	19,26,27	2.04	5 (26%)	18,38,41	1.82	3 (16%)
1	UR3	DB	1498	1	19,22,23	1.92	1 (5%)	26,32,35	1.42	3 (11%)
2	2MU	B	2552	2	19,22,24	2.72	5 (26%)	25,31,36	2.18	6 (24%)
2	PSU	B	1917	2	18,21,22	1.77	3 (16%)	21,30,33	1.84	5 (23%)
1	5MC	DB	967	1	19,22,23	2.39	5 (26%)	26,32,35	1.32	3 (11%)
2	PSU	EB	1911	2	18,21,22	1.58	2 (11%)	21,30,33	2.09	6 (28%)
4	PSU	LC	55	4	18,21,22	1.90	3 (16%)	21,30,33	1.71	5 (23%)
1	PSU	A	516	1	18,21,22	1.93	3 (16%)	21,30,33	1.47	5 (23%)
2	5MC	B	1942	2	19,22,23	2.99	4 (21%)	26,32,35	1.38	4 (15%)
2	2MA	B	2503	2	17,25,26	1.46	2 (11%)	16,37,40	1.53	3 (18%)
4	5MU	D	54	4	19,22,23	2.10	3 (15%)	27,32,35	1.99	8 (29%)
4	PSU	GB	55	4	18,21,22	1.65	3 (16%)	21,30,33	1.58	3 (14%)
4	PSU	IA	55	4	18,21,22	1.91	2 (11%)	21,30,33	1.87	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	M2G	A	966	1	20,27,28	2.33	4 (20%)	19,40,43	1.37	3 (15%)
1	UR3	A	1498	1	19,22,23	1.79	2 (10%)	26,32,35	1.55	4 (15%)
2	PSU	B	2605	2	18,21,22	1.59	3 (16%)	21,30,33	1.69	4 (19%)
4	4SU	GB	8	4	18,21,22	4.63	7 (38%)	25,30,33	6.22	9 (36%)
4	5MC	D	32	4	19,22,23	2.65	4 (21%)	26,32,35	0.97	2 (7%)
2	5MU	B	1915	2	19,22,23	1.95	3 (15%)	27,32,35	2.45	6 (22%)
45	0TD	TA	92	45	8,9,10	2.60	2 (25%)	6,11,13	3.29	3 (50%)
1	5MC	DB	1400	1	19,22,23	2.45	4 (21%)	26,32,35	1.26	4 (15%)
1	7MG	DB	527	1	23,26,27	2.94	7 (30%)	27,39,42	2.28	9 (33%)
2	2MU	EB	2552	56,2	19,22,24	2.56	3 (15%)	25,31,36	2.26	5 (20%)
4	PSU	D	55	4	18,21,22	1.76	2 (11%)	21,30,33	1.48	2 (9%)
4	4SU	LC	8	4	18,21,22	4.70	7 (38%)	25,30,33	6.03	11 (44%)
2	5MC	EB	1942	2	19,22,23	2.95	4 (21%)	26,32,35	1.44	4 (15%)
2	4OC	EB	1920	2	19,22,24	1.03	1 (5%)	25,31,35	0.84	0
2	5MC	EB	1962	56,2	19,22,23	2.61	5 (26%)	26,32,35	1.24	2 (7%)
2	2MA	EB	2503	2	17,25,26	1.45	2 (11%)	16,37,40	1.73	3 (18%)
2	OMG	B	2251	4,2	19,26,27	2.05	3 (15%)	21,38,41	1.22	4 (19%)
1	5MC	A	1407	1	19,22,23	2.87	4 (21%)	26,32,35	1.24	1 (3%)
1	5MC	DB	1404	1	19,22,23	2.61	4 (21%)	26,32,35	1.28	3 (11%)
1	MA6	DB	1518	1	19,26,27	2.01	5 (26%)	18,38,41	2.03	3 (16%)
4	5MC	LC	32	4	19,22,23	2.33	4 (21%)	26,32,35	1.32	3 (11%)
1	4OC	A	1402	1	20,23,24	1.11	2 (10%)	25,32,35	1.30	5 (20%)
1	5MC	A	1404	1	19,22,23	2.78	4 (21%)	26,32,35	1.21	1 (3%)
2	5MU	B	1939	2	19,22,23	2.28	3 (15%)	27,32,35	2.47	8 (29%)
4	5MU	LC	54	4	19,22,23	2.22	3 (15%)	27,32,35	1.83	7 (25%)
2	5MU	EB	1915	2	19,22,23	2.02	3 (15%)	27,32,35	2.31	5 (18%)
1	7MG	A	527	1	23,26,27	2.98	7 (30%)	27,39,42	2.09	8 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	DB	516	1	-	0/7/25/26	0/2/2/2
2	OMG	EB	2251	4,2	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	A	1400	1	-	1/7/25/26	0/2/2/2
2	PSU	B	1911	2	-	0/7/25/26	0/2/2/2
4	5MU	IA	54	4,56	-	0/7/25/26	0/2/2/2
2	5MU	EB	1939	2	-	0/7/25/26	0/2/2/2
1	5MC	DB	1407	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1518	1	-	1/7/29/30	0/3/3/3
4	5MC	IA	32	4	-	0/7/25/26	0/2/2/2
4	4SU	D	8	4	-	2/7/25/26	0/2/2/2
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
2	5MC	B	1962	2	-	0/7/25/26	0/2/2/2
1	M2G	DB	966	1	-	0/7/29/30	0/3/3/3
1	4OC	DB	1402	1	-	2/9/29/30	0/2/2/2
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
4	5MU	GB	54	4	-	0/7/25/26	0/2/2/2
1	2MG	DB	1207	1	-	0/5/27/28	0/3/3/3
2	PSU	EB	2605	2	-	0/7/25/26	0/2/2/2
4	4SU	IA	8	4	-	0/7/25/26	0/2/2/2
4	5MC	GB	32	4	-	0/7/25/26	0/2/2/2
2	PSU	EB	1917	2	-	0/7/25/26	0/2/2/2
1	MA6	DB	1519	1	-	3/7/29/30	0/3/3/3
45	0TD	WC	92	45	-	5/7/12/14	-
2	4OC	B	1920	2	-	4/9/27/30	0/2/2/2
1	MA6	A	1519	1	-	3/7/29/30	0/3/3/3
1	UR3	DB	1498	1	-	0/7/25/26	0/2/2/2
2	2MU	B	2552	2	-	0/9/27/28	0/2/2/2
2	PSU	B	1917	2	-	0/7/25/26	0/2/2/2
1	5MC	DB	967	1	-	0/7/25/26	0/2/2/2
2	PSU	EB	1911	2	-	0/7/25/26	0/2/2/2
4	PSU	LC	55	4	-	0/7/25/26	0/2/2/2
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
2	5MC	B	1942	2	-	0/7/25/26	0/2/2/2
2	2MA	B	2503	2	-	1/3/25/26	0/3/3/3
4	5MU	D	54	4	-	0/7/25/26	0/2/2/2
4	PSU	GB	55	4	-	0/7/25/26	0/2/2/2
4	PSU	IA	55	4	-	0/7/25/26	0/2/2/2
1	M2G	A	966	1	-	0/7/29/30	0/3/3/3
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
2	PSU	B	2605	2	-	0/7/25/26	0/2/2/2
4	4SU	GB	8	4	-	2/7/25/26	0/2/2/2
4	5MC	D	32	4	-	0/7/25/26	0/2/2/2
2	5MU	B	1915	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	0TD	TA	92	45	-	4/7/12/14	-
1	5MC	DB	1400	1	-	2/7/25/26	0/2/2/2
1	7MG	DB	527	1	-	2/7/37/38	0/3/3/3
2	2MU	EB	2552	56,2	-	0/9/27/28	0/2/2/2
4	PSU	D	55	4	-	0/7/25/26	0/2/2/2
4	4SU	LC	8	4	-	0/7/25/26	0/2/2/2
2	5MC	EB	1942	2	-	0/7/25/26	0/2/2/2
2	4OC	EB	1920	2	-	3/9/27/30	0/2/2/2
2	5MC	EB	1962	56,2	-	0/7/25/26	0/2/2/2
2	2MA	EB	2503	2	-	1/3/25/26	0/3/3/3
2	OMG	B	2251	4,2	-	1/5/27/28	0/3/3/3
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	5MC	DB	1404	1	-	0/7/25/26	0/2/2/2
1	MA6	DB	1518	1	-	1/7/29/30	0/3/3/3
4	5MC	LC	32	4	-	0/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
2	5MU	B	1939	2	-	0/7/25/26	0/2/2/2
4	5MU	LC	54	4	-	0/7/25/26	0/2/2/2
2	5MU	EB	1915	2	-	0/7/25/26	0/2/2/2
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3

All (233) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	8	4SU	C4-N3	12.89	1.50	1.37
4	LC	8	4SU	C4-N3	12.62	1.50	1.37
4	IA	8	4SU	C4-N3	12.22	1.50	1.37
4	GB	8	4SU	C4-N3	12.11	1.50	1.37
4	IA	8	4SU	O2-C2	11.93	1.44	1.23
4	D	8	4SU	O2-C2	11.72	1.43	1.23
1	DB	1407	5MC	C5-C4	-11.71	1.35	1.44
2	B	1942	5MC	C5-C4	-11.38	1.35	1.44
4	GB	8	4SU	O2-C2	11.26	1.43	1.23
4	LC	8	4SU	O2-C2	11.23	1.42	1.23
2	EB	1942	5MC	C5-C4	-10.94	1.35	1.44
1	A	1407	5MC	C5-C4	-10.52	1.36	1.44
1	A	527	7MG	O6-C6	9.92	1.42	1.23
1	A	1404	5MC	C5-C4	-9.70	1.36	1.44
1	DB	527	7MG	O6-C6	9.48	1.41	1.23
4	GB	32	5MC	C5-C4	-9.20	1.37	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1962	5MC	C5-C4	-9.18	1.37	1.44
4	D	32	5MC	C5-C4	-9.04	1.37	1.44
2	EB	1962	5MC	C5-C4	-8.89	1.37	1.44
1	DB	1404	5MC	C5-C4	-8.59	1.37	1.44
2	B	2552	2MU	O4-C4	8.49	1.41	1.24
2	EB	2552	2MU	O4-C4	8.46	1.41	1.24
4	IA	32	5MC	C5-C4	-8.39	1.37	1.44
1	A	967	5MC	C5-C4	-8.31	1.37	1.44
1	DB	1400	5MC	C5-C4	-7.99	1.38	1.44
1	DB	1498	UR3	O4-C4	7.73	1.40	1.23
45	WC	92	0TD	CB-CA	-7.67	1.52	1.54
1	DB	527	7MG	C5-N7	7.46	1.45	1.35
1	A	1207	2MG	O6-C6	7.40	1.40	1.23
1	DB	967	5MC	C5-C4	-7.31	1.38	1.44
1	DB	1207	2MG	O6-C6	7.30	1.40	1.23
1	DB	966	M2G	O6-C6	7.21	1.40	1.23
1	A	966	M2G	O6-C6	7.18	1.40	1.23
4	LC	54	5MU	O4-C4	7.10	1.37	1.23
1	A	527	7MG	C5-N7	7.09	1.44	1.35
1	A	1400	5MC	C5-C4	-7.02	1.38	1.44
4	LC	32	5MC	C5-C4	-6.76	1.39	1.44
1	A	1498	UR3	O4-C4	6.72	1.37	1.23
2	B	2251	OMG	O6-C6	6.64	1.38	1.23
4	IA	54	5MU	O4-C4	6.48	1.35	1.23
2	EB	1939	5MU	O4-C4	6.42	1.35	1.23
2	B	1939	5MU	O4-C4	6.42	1.35	1.23
4	D	54	5MU	O4-C4	6.31	1.35	1.23
2	EB	2251	OMG	O6-C6	6.25	1.37	1.23
4	D	8	4SU	C6-C5	6.19	1.49	1.35
4	IA	55	PSU	C6-C5	6.17	1.42	1.35
4	GB	8	4SU	C6-C5	6.17	1.49	1.35
4	GB	54	5MU	O4-C4	6.13	1.35	1.23
45	TA	92	0TD	CB-CA	-6.10	1.52	1.54
2	EB	1915	5MU	O4-C4	6.05	1.35	1.23
4	IA	8	4SU	C2-N1	5.97	1.47	1.38
4	D	8	4SU	C4-S4	5.96	1.79	1.68
4	LC	8	4SU	C2-N1	5.95	1.47	1.38
4	IA	8	4SU	C6-C5	5.84	1.48	1.35
4	LC	8	4SU	C6-C5	5.83	1.48	1.35
4	LC	55	PSU	C6-C5	5.81	1.41	1.35
4	GB	8	4SU	C4-S4	5.75	1.79	1.68
2	B	1939	5MU	C4-C5	-5.69	1.35	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	516	PSU	C6-C5	5.68	1.41	1.35
2	B	1915	5MU	O4-C4	5.60	1.34	1.23
4	IA	54	5MU	C4-C5	-5.57	1.35	1.44
2	B	1917	PSU	C6-C5	5.55	1.41	1.35
4	D	55	PSU	C6-C5	5.55	1.41	1.35
4	LC	8	4SU	C4-S4	5.53	1.78	1.68
2	B	2552	2MU	C3'-C2'	-5.53	1.40	1.53
4	IA	8	4SU	C4-S4	5.51	1.78	1.68
4	D	54	5MU	C4-C5	-5.49	1.35	1.44
4	GB	54	5MU	C4-C5	-5.48	1.35	1.44
2	EB	1917	PSU	C6-C5	5.41	1.41	1.35
4	GB	55	PSU	C6-C5	5.36	1.41	1.35
2	EB	1939	5MU	C4-C5	-5.30	1.36	1.44
4	LC	54	5MU	C4-C5	-5.30	1.36	1.44
4	GB	8	4SU	C2-N1	5.27	1.46	1.38
2	EB	1911	PSU	C6-C5	5.15	1.41	1.35
2	EB	1915	5MU	C4-C5	-5.14	1.36	1.44
1	DB	516	PSU	C6-C5	5.11	1.40	1.35
1	DB	1519	MA6	C6-N6	4.95	1.48	1.37
4	D	8	4SU	C2-N1	4.95	1.46	1.38
1	A	966	M2G	C2-N2	4.91	1.44	1.35
4	IA	32	5MC	C6-C5	4.87	1.42	1.34
2	B	1915	5MU	C4-C5	-4.86	1.36	1.44
1	DB	966	M2G	C2-N2	4.81	1.44	1.35
4	LC	32	5MC	C6-C5	4.78	1.42	1.34
2	EB	2552	2MU	C3'-C2'	-4.75	1.42	1.53
2	B	1911	PSU	C6-C5	4.74	1.40	1.35
1	DB	1518	MA6	C6-N6	4.71	1.48	1.37
2	EB	2605	PSU	C6-C5	4.69	1.40	1.35
2	B	2503	2MA	C8-N7	4.51	1.41	1.34
1	A	1400	5MC	C6-C5	4.46	1.41	1.34
1	A	1519	MA6	C4-N3	4.43	1.41	1.35
1	DB	967	5MC	C4-N4	4.43	1.45	1.34
4	LC	32	5MC	C4-N4	4.42	1.45	1.34
1	DB	1518	MA6	C6-N1	4.38	1.38	1.32
2	EB	2503	2MA	C8-N7	4.36	1.41	1.34
1	A	1518	MA6	C6-N1	4.34	1.38	1.32
1	A	1518	MA6	C6-N6	4.31	1.47	1.37
1	A	1519	MA6	C6-N6	4.28	1.47	1.37
2	B	2605	PSU	C6-C5	4.26	1.40	1.35
1	A	1519	MA6	C6-N1	4.24	1.38	1.32
1	A	966	M2G	C2-N3	4.23	1.36	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	IA	32	5MC	C4-N4	4.23	1.44	1.34
1	A	967	5MC	C4-N4	4.20	1.44	1.34
2	B	1962	5MC	C4-N4	4.19	1.44	1.34
1	A	1518	MA6	C4-N3	4.17	1.41	1.35
4	D	32	5MC	C6-C5	4.16	1.41	1.34
1	DB	1404	5MC	C4-N4	4.14	1.44	1.34
1	DB	1400	5MC	C4-N4	4.11	1.44	1.34
1	A	1404	5MC	C6-C5	4.10	1.41	1.34
4	D	32	5MC	C4-N4	4.09	1.44	1.34
1	DB	1400	5MC	C6-C5	4.08	1.41	1.34
1	A	1400	5MC	C4-N4	4.07	1.44	1.34
2	EB	1962	5MC	C4-N4	4.07	1.44	1.34
2	B	1962	5MC	C6-N1	-4.06	1.31	1.38
4	GB	32	5MC	C4-N4	4.06	1.44	1.34
1	DB	1519	MA6	C6-N1	4.03	1.38	1.32
4	GB	32	5MC	C6-C5	4.00	1.41	1.34
1	DB	1518	MA6	C4-N3	3.99	1.41	1.35
1	DB	1404	5MC	C6-C5	3.89	1.40	1.34
1	DB	1407	5MC	C6-N1	-3.87	1.31	1.38
1	A	1207	2MG	C2-N2	3.87	1.41	1.33
1	DB	1404	5MC	C6-N1	-3.86	1.31	1.38
1	DB	1407	5MC	C4-N4	3.85	1.43	1.34
1	A	1407	5MC	C4-N4	3.82	1.43	1.34
2	EB	2251	OMG	C2-N2	3.81	1.43	1.34
1	A	1404	5MC	C4-N4	3.79	1.43	1.34
1	DB	1519	MA6	C4-N3	3.79	1.40	1.35
2	EB	1942	5MC	C4-N4	3.78	1.43	1.34
1	A	527	7MG	C8-N9	-3.78	1.43	1.45
1	A	1407	5MC	C6-N1	-3.73	1.31	1.38
1	DB	1207	2MG	C2-N2	3.70	1.41	1.33
1	A	967	5MC	C6-N1	-3.69	1.31	1.38
1	DB	967	5MC	C6-C5	3.69	1.40	1.34
1	DB	966	M2G	C2-N3	3.65	1.35	1.30
1	DB	527	7MG	C4-N9	3.60	1.42	1.37
2	B	1920	4OC	C4-N4	3.57	1.42	1.33
2	EB	1942	5MC	C6-N1	-3.57	1.31	1.38
2	EB	1962	5MC	C6-N1	-3.56	1.31	1.38
1	A	516	PSU	C6-N1	3.54	1.42	1.36
1	A	1407	5MC	C6-C5	3.52	1.40	1.34
1	DB	967	5MC	C6-N1	-3.51	1.32	1.38
1	A	967	5MC	C6-C5	3.49	1.40	1.34
1	DB	1407	5MC	C6-C5	3.49	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	EB	1962	5MC	C6-C5	3.47	1.40	1.34
45	WC	92	0TD	CB-SB	-3.47	1.78	1.82
2	B	1942	5MC	C6-N1	-3.47	1.32	1.38
2	B	1942	5MC	C4-N4	3.44	1.42	1.34
2	B	2605	PSU	C6-N1	3.43	1.41	1.36
2	B	2251	OMG	C2-N2	3.42	1.42	1.34
4	LC	55	PSU	C6-N1	3.39	1.41	1.36
1	DB	516	PSU	C6-N1	3.38	1.41	1.36
1	A	527	7MG	C2-N2	3.36	1.42	1.34
1	A	527	7MG	C4-N9	3.36	1.42	1.37
1	DB	527	7MG	C2-N2	3.32	1.42	1.34
4	IA	8	4SU	C5-C4	3.28	1.46	1.42
2	B	1939	5MU	C6-C5	3.27	1.39	1.34
2	EB	1942	5MC	C6-C5	3.25	1.39	1.34
2	EB	1920	4OC	C4-N4	3.24	1.41	1.33
2	B	1942	5MC	C6-C5	3.23	1.39	1.34
4	GB	32	5MC	C6-N1	-3.21	1.32	1.38
1	A	1519	MA6	C2-N1	3.20	1.39	1.33
1	DB	1519	MA6	C2-N1	3.20	1.39	1.33
2	EB	2503	2MA	C6-N6	3.19	1.40	1.27
1	DB	527	7MG	C6-N1	-3.17	1.32	1.38
4	IA	55	PSU	C6-N1	3.16	1.41	1.36
4	D	55	PSU	C6-N1	3.15	1.41	1.36
1	DB	1518	MA6	C6-C5	-3.15	1.40	1.44
4	LC	54	5MU	C6-C5	3.03	1.39	1.34
1	A	1402	4OC	C4-N4	3.02	1.42	1.36
2	B	2503	2MA	C6-N6	3.00	1.39	1.27
1	DB	1400	5MC	C6-N1	-2.99	1.32	1.38
4	D	32	5MC	C6-N1	-2.97	1.32	1.38
1	A	1404	5MC	C6-N1	-2.97	1.33	1.38
4	D	8	4SU	C5-C4	2.96	1.46	1.42
2	EB	1939	5MU	C6-C5	2.92	1.39	1.34
1	DB	527	7MG	C8-N9	-2.91	1.44	1.45
1	A	527	7MG	C6-N1	-2.91	1.33	1.38
2	B	1962	5MC	C6-C5	2.87	1.39	1.34
4	GB	55	PSU	C6-N1	2.87	1.41	1.36
4	GB	54	5MU	C6-C5	2.84	1.39	1.34
4	IA	54	5MU	C6-C5	2.84	1.39	1.34
1	DB	1402	4OC	C4-N4	2.84	1.42	1.36
2	B	1917	PSU	C6-N1	2.82	1.40	1.36
1	A	1402	4OC	C4-N3	2.81	1.37	1.32
1	A	1400	5MC	C6-N1	-2.78	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	DB	1402	4OC	C4-N3	2.78	1.37	1.32
1	A	1518	MA6	C2-N1	2.78	1.38	1.33
2	EB	1917	PSU	C6-N1	2.78	1.40	1.36
45	TA	92	0TD	CB-SB	-2.77	1.79	1.82
1	DB	1207	2MG	C5-C6	-2.76	1.42	1.47
1	A	1519	MA6	C6-C5	-2.74	1.40	1.44
1	A	516	PSU	C1'-C5	2.72	1.56	1.50
1	DB	516	PSU	C1'-C5	2.71	1.56	1.50
4	D	54	5MU	C6-C5	2.70	1.39	1.34
2	B	2552	2MU	C3'-C4'	-2.69	1.46	1.53
2	EB	2251	OMG	C6-N1	-2.69	1.33	1.37
2	EB	2605	PSU	C6-N1	2.69	1.40	1.36
2	EB	1911	PSU	C6-N1	2.66	1.40	1.36
2	B	1915	5MU	C6-C5	2.63	1.38	1.34
1	DB	527	7MG	C2-N3	2.61	1.39	1.33
1	A	1518	MA6	C6-C5	-2.61	1.40	1.44
2	EB	1915	5MU	C6-C5	2.60	1.38	1.34
4	LC	32	5MC	C6-N1	-2.60	1.33	1.38
4	GB	8	4SU	C2-N3	-2.58	1.33	1.38
2	B	2605	PSU	O4'-C1'	-2.56	1.40	1.43
1	DB	1519	MA6	C6-C5	-2.56	1.40	1.44
2	B	1911	PSU	C6-N1	2.56	1.40	1.36
2	EB	2552	2MU	C3'-C4'	-2.55	1.46	1.53
1	A	1207	2MG	C5-C6	-2.55	1.42	1.47
1	A	527	7MG	C2-N3	2.53	1.39	1.33
4	GB	8	4SU	C5-C4	2.52	1.45	1.42
2	B	2251	OMG	C6-N1	-2.44	1.34	1.37
4	LC	8	4SU	C2-N3	-2.42	1.33	1.38
2	B	2552	2MU	O3'-C3'	-2.42	1.37	1.43
1	DB	967	5MC	C4-N3	2.42	1.38	1.34
4	IA	32	5MC	C6-N1	-2.41	1.33	1.38
4	LC	55	PSU	C2-N1	2.38	1.39	1.36
4	GB	55	PSU	C1'-C5	2.37	1.55	1.50
4	D	8	4SU	C2-N3	-2.37	1.33	1.38
2	EB	1962	5MC	C4-N3	2.31	1.37	1.34
1	DB	1518	MA6	C2-N1	2.29	1.38	1.33
1	A	1498	UR3	C4-N3	-2.28	1.36	1.40
1	DB	966	M2G	C5-C4	-2.25	1.37	1.43
1	A	966	M2G	C5-C4	-2.24	1.37	1.43
4	IA	8	4SU	C2-N3	-2.23	1.34	1.38
4	LC	8	4SU	C5-C4	2.21	1.45	1.42
2	EB	2251	OMG	C5-C4	-2.17	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	EB	2251	OMG	C5-C6	-2.17	1.43	1.47
2	EB	1939	5MU	C2-N1	-2.15	1.35	1.38
1	DB	966	M2G	C6-N1	-2.15	1.34	1.37
1	A	967	5MC	C4-N3	2.10	1.37	1.34
2	B	1917	PSU	O4'-C1'	-2.08	1.41	1.43
2	B	2552	2MU	C4-N3	-2.04	1.35	1.38
2	EB	1939	5MU	O2-C2	-2.04	1.19	1.23

All (294) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	GB	8	4SU	C4-N3-C2	-19.85	108.28	127.31
4	LC	8	4SU	C4-N3-C2	-16.98	111.03	127.31
4	LC	8	4SU	C1'-N1-C2	13.91	142.57	117.59
4	GB	8	4SU	C1'-N1-C2	11.38	138.02	117.59
4	D	8	4SU	C1'-N1-C2	11.26	137.82	117.59
4	IA	8	4SU	C1'-N1-C2	11.04	137.42	117.59
4	D	8	4SU	O2-C2-N1	-11.03	108.44	122.80
4	GB	8	4SU	O2-C2-N1	-10.99	108.49	122.80
4	IA	8	4SU	S4-C4-N3	-10.56	109.15	120.20
4	IA	8	4SU	C4-N3-C2	-10.50	117.25	127.31
4	IA	8	4SU	C1'-N1-C6	-10.45	98.45	120.78
4	GB	8	4SU	C1'-N1-C6	-10.30	98.77	120.78
4	LC	8	4SU	C1'-N1-C6	-10.24	98.89	120.78
4	LC	8	4SU	C6-C5-C4	-10.22	111.10	119.95
4	D	8	4SU	C1'-N1-C6	-10.13	99.12	120.78
4	LC	8	4SU	C5-C4-S4	-9.81	113.10	124.31
4	D	8	4SU	C4-N3-C2	-9.11	118.58	127.31
4	IA	8	4SU	C5-C4-S4	-9.04	113.98	124.31
4	D	8	4SU	S4-C4-N3	-8.12	111.70	120.20
4	GB	8	4SU	C5-C4-S4	-8.00	115.17	124.31
4	D	8	4SU	O2-C2-N3	-7.89	106.95	121.49
4	D	8	4SU	C6-C5-C4	-7.84	113.16	119.95
2	B	1915	5MU	C5-C4-N3	7.69	122.01	115.32
4	D	8	4SU	C5-C4-S4	-7.62	115.61	124.31
4	GB	8	4SU	C6-C5-C4	-7.37	113.57	119.95
4	GB	8	4SU	O2-C2-N3	-7.07	108.46	121.49
45	TA	92	0TD	CSB-SB-CB	6.96	114.87	102.36
2	EB	1939	5MU	N3-C2-N1	6.69	123.60	114.89
2	EB	1915	5MU	C5-C4-N3	6.60	121.06	115.32
2	B	1939	5MU	N3-C2-N1	6.44	123.28	114.89
45	WC	92	0TD	CSB-SB-CB	6.37	113.82	102.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1915	5MU	C4-N3-C2	-5.89	119.62	127.34
2	EB	2552	2MU	C4-N3-C2	-5.83	119.37	126.61
1	DB	1518	MA6	N3-C2-N1	-5.80	120.80	128.67
1	DB	527	7MG	C5-C6-N1	5.62	120.83	110.94
2	EB	1939	5MU	C4-N3-C2	-5.60	120.00	127.34
4	GB	8	4SU	S4-C4-N3	-5.51	114.44	120.20
2	B	2552	2MU	N3-C2-N1	5.51	122.06	114.89
2	B	2552	2MU	C4-N3-C2	-5.47	119.82	126.61
2	EB	1915	5MU	C4-N3-C2	-5.42	120.23	127.34
4	IA	8	4SU	C5-C4-N3	5.42	119.79	114.75
1	A	1498	UR3	C4-N3-C2	-5.39	120.25	124.58
2	EB	1915	5MU	O4-C4-C5	-5.33	118.82	124.92
2	EB	1911	PSU	C4-N3-C2	-5.31	119.06	126.37
1	DB	1498	UR3	C4-N3-C2	-5.28	120.33	124.58
4	LC	8	4SU	S4-C4-N3	-5.24	114.72	120.20
2	EB	2503	2MA	C4-N3-C2	-5.20	119.31	123.30
4	IA	8	4SU	O2-C2-N1	-5.19	116.05	122.80
2	B	1939	5MU	C4-N3-C2	-5.16	120.57	127.34
2	EB	2552	2MU	O2-C2-N1	-5.14	116.10	122.80
4	IA	8	4SU	O2-C2-N3	-5.12	112.04	121.49
2	EB	2552	2MU	N3-C2-N1	5.11	121.54	114.89
1	A	1518	MA6	N3-C2-N1	-5.10	121.75	128.67
4	LC	8	4SU	C5-C6-N1	-5.06	113.61	121.84
2	EB	1939	5MU	C6-C5-C4	5.01	122.15	118.02
1	DB	1518	MA6	C2-N1-C6	5.00	121.74	116.84
2	EB	1911	PSU	N1-C2-N3	4.96	120.40	115.17
4	GB	54	5MU	C4-N3-C2	-4.96	120.84	127.34
4	GB	54	5MU	C5-C4-N3	4.92	119.60	115.32
4	IA	54	5MU	N3-C2-N1	4.91	121.29	114.89
1	A	1519	MA6	C2-N1-C6	4.88	121.62	116.84
1	DB	527	7MG	C2-N3-C4	4.83	120.62	112.30
4	IA	8	4SU	N3-C2-N1	4.81	121.15	114.89
1	A	527	7MG	C5-C6-N1	4.80	119.38	110.94
1	DB	1519	MA6	C2-N1-C6	4.78	121.53	116.84
4	D	8	4SU	C5-C6-N1	-4.78	114.06	121.84
2	B	2605	PSU	C4-N3-C2	-4.68	119.92	126.37
4	D	54	5MU	C4-N3-C2	-4.64	121.25	127.34
4	IA	54	5MU	C4-N3-C2	-4.60	121.31	127.34
4	LC	8	4SU	N3-C2-N1	4.59	120.86	114.89
1	A	527	7MG	C2-N3-C4	4.57	120.18	112.30
4	IA	55	PSU	N1-C2-N3	4.55	119.97	115.17
4	D	54	5MU	C5-C4-N3	4.51	119.24	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1939	5MU	C6-C5-C4	4.49	121.72	118.02
2	B	2552	2MU	O2-C2-N1	-4.46	116.99	122.80
1	A	1519	MA6	N3-C2-N1	-4.46	122.62	128.67
4	GB	54	5MU	N3-C2-N1	4.39	120.60	114.89
2	EB	2605	PSU	C4-N3-C2	-4.33	120.41	126.37
2	EB	1917	PSU	C4-N3-C2	-4.28	120.47	126.37
2	B	1917	PSU	N1-C2-N3	4.28	119.68	115.17
2	EB	1917	PSU	N1-C2-N3	4.26	119.66	115.17
1	A	967	5MC	C5-C6-N1	-4.24	118.71	123.31
1	DB	967	5MC	C5-C6-N1	-4.20	118.75	123.31
2	EB	1942	5MC	C5-C6-N1	-4.20	118.75	123.31
4	LC	8	4SU	O2-C2-N1	-4.19	117.34	122.80
4	IA	55	PSU	C4-N3-C2	-4.19	120.60	126.37
2	B	1915	5MU	N3-C2-N1	4.19	120.34	114.89
2	B	1915	5MU	O4-C4-C5	-4.14	120.18	124.92
1	A	1518	MA6	C2-N1-C6	4.11	120.87	116.84
4	LC	55	PSU	C4-N3-C2	-4.11	120.71	126.37
2	B	1917	PSU	C4-N3-C2	-4.09	120.74	126.37
1	DB	1519	MA6	N3-C2-N1	-4.09	123.13	128.67
2	B	1911	PSU	C4-N3-C2	-4.08	120.76	126.37
2	EB	1939	5MU	C5-C6-N1	-4.05	118.91	123.31
1	A	1407	5MC	C5-C6-N1	-4.03	118.93	123.31
1	A	1404	5MC	C5-C6-N1	-4.03	118.94	123.31
2	B	1939	5MU	C6-N1-C2	-4.02	117.30	121.30
1	DB	527	7MG	N9-C4-N3	4.00	131.33	125.46
4	D	54	5MU	N3-C2-N1	4.00	120.09	114.89
4	LC	8	4SU	O2-C2-N3	-4.00	114.12	121.49
2	B	1962	5MC	C5-C6-N1	-3.99	118.98	123.31
4	IA	54	5MU	C6-N1-C2	-3.98	117.34	121.30
2	EB	1962	5MC	C5-C6-N1	-3.98	118.99	123.31
4	GB	55	PSU	C4-N3-C2	-3.97	120.90	126.37
1	DB	527	7MG	C5-C4-N3	-3.96	120.69	128.13
1	DB	1404	5MC	C5-C6-N1	-3.95	119.02	123.31
4	LC	54	5MU	C4-N3-C2	-3.93	122.19	127.34
2	EB	1939	5MU	O2-C2-N1	-3.88	117.75	122.80
2	B	1911	PSU	N1-C2-N3	3.85	119.23	115.17
4	IA	54	5MU	O4-C4-C5	-3.85	120.51	124.92
4	GB	54	5MU	O4-C4-C5	-3.84	120.53	124.92
2	B	1942	5MC	C5-C6-N1	-3.83	119.15	123.31
4	LC	54	5MU	N3-C2-N1	3.81	119.85	114.89
1	A	527	7MG	N9-C4-N3	3.78	131.00	125.46
4	IA	54	5MU	C6-C5-C4	3.75	121.11	118.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2503	2MA	C4-N3-C2	-3.73	120.44	123.30
4	GB	55	PSU	N1-C2-N3	3.70	119.08	115.17
1	A	527	7MG	C5-C4-N3	-3.70	121.19	128.13
4	D	55	PSU	C4-N3-C2	-3.69	121.29	126.37
2	EB	1939	5MU	C6-N1-C2	-3.67	117.65	121.30
1	A	1207	2MG	N1-C2-N2	3.66	120.30	116.56
1	DB	1400	5MC	C5-C6-N1	-3.64	119.36	123.31
1	DB	1207	2MG	N1-C2-N2	3.64	120.27	116.56
2	B	1939	5MU	O2-C2-N1	-3.62	118.09	122.80
2	B	1939	5MU	C5-C6-N1	-3.61	119.39	123.31
2	EB	1915	5MU	N3-C2-N1	3.60	119.58	114.89
4	D	54	5MU	O4-C4-C5	-3.59	120.81	124.92
1	DB	1207	2MG	C8-N7-C5	3.59	108.66	102.55
1	DB	527	7MG	O6-C6-C5	-3.58	118.83	127.62
2	EB	2605	PSU	N1-C2-N3	3.56	118.93	115.17
2	EB	2552	2MU	O4-C4-C5	-3.51	119.11	125.16
4	GB	32	5MC	C5-C6-N1	-3.51	119.50	123.31
4	LC	54	5MU	O4-C4-C5	-3.50	120.91	124.92
4	LC	32	5MC	C5-C6-N1	-3.49	119.53	123.31
4	IA	32	5MC	C5-C6-N1	-3.48	119.53	123.31
1	DB	1407	5MC	C5-C6-N1	-3.47	119.54	123.31
4	LC	55	PSU	N1-C2-N3	3.47	118.83	115.17
4	IA	54	5MU	C5-C4-N3	3.47	118.34	115.32
4	D	55	PSU	N1-C2-N3	3.45	118.81	115.17
2	EB	2503	2MA	C8-N7-C5	3.45	108.42	102.55
1	A	516	PSU	C4-N3-C2	-3.43	121.64	126.37
2	EB	2552	2MU	C5-C4-N3	3.43	119.60	114.80
1	A	1207	2MG	C8-N7-C5	3.41	108.35	102.55
4	LC	54	5MU	C6-C5-C4	3.35	120.78	118.02
4	IA	8	4SU	C5-C6-N1	-3.34	116.41	121.84
1	A	966	M2G	C8-N7-C5	3.33	108.22	102.55
4	GB	8	4SU	C5-C6-N1	-3.29	116.50	121.84
2	EB	1939	5MU	C5M-C5-C6	-3.26	118.44	122.85
2	B	1917	PSU	O2-C2-N1	-3.22	119.47	122.79
1	A	527	7MG	O6-C6-C5	-3.21	119.73	127.62
2	EB	1915	5MU	C5-C6-N1	-3.20	119.84	123.31
1	DB	966	M2G	C8-N7-C5	3.18	107.96	102.55
1	DB	527	7MG	C6-C5-C4	-3.17	116.82	122.40
2	B	2251	OMG	C8-N7-C5	3.16	107.93	102.55
2	B	2503	2MA	C5-C6-N1	3.13	119.96	114.12
45	TA	92	0TD	OD2-CG-OD1	-3.12	117.00	124.08
1	DB	516	PSU	C4-N3-C2	-3.12	122.07	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DB	1402	4OC	CM4-N4-C4	-3.12	116.36	122.45
2	B	2503	2MA	C8-N7-C5	3.11	107.84	102.55
4	LC	32	5MC	O2-C2-N3	-3.10	117.44	122.33
1	A	1400	5MC	C5-C6-N1	-3.05	120.00	123.31
4	LC	54	5MU	C5-C4-N3	3.04	117.97	115.32
1	DB	1402	4OC	C6-C5-C4	3.04	120.67	117.00
4	D	32	5MC	C5-C6-N1	-3.03	120.02	123.31
1	A	1402	4OC	CM4-N4-C4	-3.01	116.57	122.45
45	WC	92	0TD	OD2-CG-OD1	-2.97	117.34	124.08
2	EB	2251	OMG	C8-N7-C5	2.97	107.60	102.55
2	B	2552	2MU	O4-C4-C5	-2.95	120.08	125.16
2	EB	2251	OMG	CM2-O2'-C2'	2.93	121.99	114.47
1	DB	516	PSU	C6-C5-C4	-2.91	116.21	118.17
4	D	54	5MU	C5-C6-N1	-2.90	120.16	123.31
2	B	1962	5MC	CM5-C5-C6	-2.89	118.94	122.85
2	B	2605	PSU	C5-C6-N1	-2.89	118.13	122.14
1	A	527	7MG	C6-C5-C4	-2.87	117.36	122.40
2	EB	1911	PSU	O2-C2-N1	-2.85	119.85	122.79
2	B	2605	PSU	N1-C2-N3	2.84	118.16	115.17
2	B	1915	5MU	C5-C6-N1	-2.83	120.24	123.31
2	EB	1911	PSU	C5-C6-N1	-2.83	118.22	122.14
1	DB	1402	4OC	C1'-N1-C6	-2.82	114.75	120.78
4	IA	32	5MC	O2-C2-N3	-2.81	117.90	122.33
2	B	2552	2MU	C5-C4-N3	2.78	118.69	114.80
4	GB	54	5MU	C6-N1-C2	-2.78	118.54	121.30
2	B	1939	5MU	C5-C4-N3	2.76	117.72	115.32
1	A	966	M2G	C5-C6-N1	2.75	119.32	114.07
2	EB	1942	5MC	C1'-N1-C6	-2.75	116.63	121.15
2	B	1942	5MC	C5-C4-N4	-2.75	117.53	121.39
1	A	1400	5MC	CM5-C5-C6	-2.74	119.14	122.85
2	B	2605	PSU	C5-C4-N3	2.73	122.55	116.55
1	A	516	PSU	C6-C5-C4	-2.71	116.34	118.17
2	EB	1939	5MU	C5-C4-N3	2.71	117.68	115.32
1	A	527	7MG	N2-C2-N1	2.71	122.48	116.76
4	GB	54	5MU	C5-C6-N1	-2.70	120.38	123.31
4	LC	54	5MU	C5-C6-N1	-2.70	120.39	123.31
1	DB	966	M2G	C5-C6-N1	2.70	119.21	114.07
1	A	1400	5MC	O2-C2-N3	-2.70	118.08	122.33
1	DB	1400	5MC	CM5-C5-C6	-2.68	119.22	122.85
2	EB	1942	5MC	C5-C4-N4	-2.67	117.63	121.39
4	LC	32	5MC	C5-C4-N3	-2.67	119.01	121.75
4	IA	54	5MU	C1'-N1-C2	2.67	122.39	117.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	EB	2251	OMG	C5-C6-N1	2.67	119.16	114.07
2	B	1917	PSU	C6-C5-C4	2.65	119.96	118.17
1	DB	1404	5MC	C5-C4-N3	-2.64	119.05	121.75
4	LC	55	PSU	C5-C6-N1	-2.63	118.49	122.14
1	DB	527	7MG	N2-C2-N1	2.62	122.30	116.76
2	EB	1917	PSU	C6-C5-C4	2.61	119.94	118.17
1	DB	967	5MC	C1'-N1-C6	-2.61	116.86	121.15
2	B	1939	5MU	C5M-C5-C6	-2.59	119.34	122.85
1	A	1207	2MG	N2-C2-N3	-2.59	117.22	120.51
4	IA	54	5MU	C5M-C5-C6	-2.58	119.36	122.85
1	DB	1207	2MG	C5-C6-N1	2.57	118.97	114.07
1	A	966	M2G	C2-N1-C6	-2.55	118.73	123.99
4	IA	32	5MC	C5-C4-N3	-2.54	119.15	121.75
1	DB	527	7MG	C2-N1-C6	-2.51	120.55	125.11
1	DB	1404	5MC	CM5-C5-C6	-2.51	119.46	122.85
4	IA	8	4SU	C6-N1-C2	2.50	124.04	121.00
2	EB	1917	PSU	O2-C2-N1	-2.50	120.21	122.79
4	D	54	5MU	C6-C5-C4	2.50	120.08	118.02
1	DB	1207	2MG	N2-C2-N3	-2.50	117.33	120.51
1	DB	967	5MC	CM5-C5-C6	-2.49	119.48	122.85
4	LC	54	5MU	C6-N1-C2	-2.49	118.83	121.30
4	IA	54	5MU	C5-C6-N1	-2.48	120.62	123.31
1	DB	1402	4OC	C5-C4-N4	-2.48	116.96	122.40
1	DB	1400	5MC	C5-C4-N3	-2.46	119.23	121.75
1	A	1402	4OC	C6-C5-C4	2.46	119.97	117.00
2	B	1942	5MC	O2-C2-N3	-2.44	118.48	122.33
4	GB	54	5MU	C6-C5-C4	2.44	120.03	118.02
1	DB	1402	4OC	CM2-O2'-C2'	2.44	120.73	114.47
1	A	967	5MC	C1'-N1-C6	-2.44	117.14	121.15
1	A	1498	UR3	C6-N1-C2	-2.43	119.81	121.80
1	DB	1519	MA6	C4-C5-N7	-2.42	106.78	109.34
4	LC	8	4SU	C6-N1-C2	-2.41	118.06	121.00
1	DB	1400	5MC	O2-C2-N3	-2.41	118.53	122.33
4	IA	55	PSU	C6-C5-C4	2.41	119.80	118.17
1	DB	1402	4OC	C1'-N1-C2	2.40	123.73	118.44
2	EB	1962	5MC	CM5-C5-C6	-2.40	119.61	122.85
2	EB	1917	PSU	C5-C6-N1	-2.39	118.82	122.14
2	B	2552	2MU	C6-N1-C2	-2.39	118.09	121.00
2	EB	2605	PSU	C5-C4-N3	2.38	121.80	116.55
2	B	1915	5MU	C5M-C5-C4	2.38	121.32	118.78
4	IA	55	PSU	C5-C6-N1	-2.36	118.86	122.14
1	DB	1498	UR3	O2-C2-N1	-2.36	117.52	122.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	PSU	C5-C4-N3	2.36	121.74	116.55
4	GB	32	5MC	C5-C4-N3	-2.35	119.34	121.75
45	WC	92	0TD	OD2-CG-CB	2.35	118.24	113.15
4	GB	55	PSU	O2-C2-N1	-2.35	120.36	122.79
4	D	8	4SU	C5-C4-N3	2.34	116.93	114.75
1	A	1498	UR3	C5-C4-N3	2.33	118.11	115.04
1	DB	516	PSU	C5-C4-N3	2.33	121.69	116.55
2	B	1911	PSU	C5-C6-N1	-2.33	118.91	122.14
2	B	1917	PSU	C5-C6-N1	-2.33	118.91	122.14
2	B	1911	PSU	C6-C5-C4	2.32	119.74	118.17
1	A	967	5MC	CM5-C5-C6	-2.32	119.71	122.85
2	B	2251	OMG	C5-C6-N1	2.31	118.47	114.07
2	B	1942	5MC	C1'-N1-C6	-2.31	117.35	121.15
1	DB	966	M2G	C2-N1-C6	-2.29	119.26	123.99
1	DB	1498	UR3	C3U-N3-C2	2.28	121.31	117.33
45	TA	92	0TD	OD2-CG-CB	2.28	118.08	113.15
2	EB	2605	PSU	O4-C4-C5	-2.28	118.35	124.01
2	EB	2503	2MA	C5-C6-N1	2.27	118.36	114.12
1	A	516	PSU	O2-C2-N1	-2.27	120.45	122.79
4	D	54	5MU	C5M-C5-C6	-2.27	119.78	122.85
1	DB	527	7MG	C6-C5-N7	2.27	135.44	131.93
4	IA	54	5MU	O2-C2-N3	-2.26	117.31	121.49
2	EB	1911	PSU	C5-C4-N3	2.25	121.51	116.55
4	LC	55	PSU	C6-C5-C4	2.25	119.69	118.17
4	D	32	5MC	C5-C4-N3	-2.24	119.46	121.75
2	EB	2251	OMG	C2-N1-C6	-2.23	121.02	125.11
1	A	1519	MA6	C4-C5-N7	-2.23	106.98	109.34
1	A	1207	2MG	C5-C6-N1	2.23	118.32	114.07
1	DB	1402	4OC	O2-C2-N3	-2.20	118.86	122.33
1	A	1518	MA6	C4-C5-N7	-2.20	107.02	109.34
4	GB	54	5MU	C5M-C5-C6	-2.19	119.89	122.85
1	A	1498	UR3	O2-C2-N1	-2.19	117.90	122.78
1	A	1402	4OC	C1'-N1-C2	2.17	123.23	118.44
4	LC	55	PSU	O4-C4-C5	-2.16	118.65	124.01
4	D	54	5MU	C6-N1-C2	-2.14	119.17	121.30
1	A	1402	4OC	C5-C4-N4	-2.13	117.72	122.40
1	DB	1518	MA6	N1-C6-N6	2.12	119.28	116.83
2	EB	1942	5MC	O2-C2-N3	-2.12	118.99	122.33
1	A	1402	4OC	C1'-N1-C6	-2.11	116.26	120.78
2	EB	1911	PSU	O4-C4-C5	-2.10	118.79	124.01
1	DB	1407	5MC	C5-C4-N4	-2.09	118.45	121.39
1	A	1400	5MC	C5-C4-N3	-2.08	119.62	121.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	IA	55	PSU	O2-C2-N3	-2.07	118.18	121.86
2	B	2251	OMG	CM2-O2'-C2'	2.06	119.77	114.47
4	IA	55	PSU	C6-N1-C2	-2.05	120.79	122.69
2	B	1920	4OC	C2'-C1'-N1	-2.04	110.36	114.24
1	A	527	7MG	C6-C5-N7	2.04	135.09	131.93
4	GB	32	5MC	CM5-C5-C6	-2.04	120.10	122.85
2	EB	2605	PSU	C5-C6-N1	-2.03	119.32	122.14
1	A	516	PSU	N1-C2-N3	2.02	117.30	115.17
2	B	1911	PSU	O4'-C1'-C2'	2.02	107.94	105.15
2	B	2251	OMG	C2-N1-C6	-2.01	121.44	125.11
2	EB	1917	PSU	O4'-C1'-C2'	2.00	107.92	105.15

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1519	MA6	O4'-C4'-C5'-O5'
2	B	1920	4OC	C1'-C2'-O2'-CM2
2	B	2251	OMG	C1'-C2'-O2'-CM2
45	TA	92	0TD	CA-CB-SB-CSB
45	TA	92	0TD	SB-CB-CG-OD2
45	TA	92	0TD	SB-CB-CG-OD1
1	DB	1519	MA6	O4'-C4'-C5'-O5'
2	EB	1920	4OC	C1'-C2'-O2'-CM2
2	EB	2251	OMG	C1'-C2'-O2'-CM2
45	WC	92	0TD	O-C-CA-CB
45	WC	92	0TD	SB-CB-CG-OD2
45	WC	92	0TD	SB-CB-CG-OD1
1	A	1519	MA6	C3'-C4'-C5'-O5'
1	DB	1519	MA6	C3'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
2	B	1920	4OC	O4'-C4'-C5'-O5'
2	B	1920	4OC	C3'-C4'-C5'-O5'
1	DB	1402	4OC	O4'-C4'-C5'-O5'
2	EB	1920	4OC	O4'-C4'-C5'-O5'
2	EB	1920	4OC	C3'-C4'-C5'-O5'
4	D	8	4SU	C2'-C1'-N1-C2
4	GB	8	4SU	C2'-C1'-N1-C2
1	A	527	7MG	C3'-C4'-C5'-O5'
1	DB	1400	5MC	O4'-C4'-C5'-O5'
1	DB	527	7MG	C3'-C4'-C5'-O5'
4	GB	8	4SU	C2'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
1	A	1402	4OC	C3'-C4'-C5'-O5'
4	D	8	4SU	C2'-C1'-N1-C6
1	DB	1402	4OC	C3'-C4'-C5'-O5'
1	A	1519	MA6	C4'-C5'-O5'-P
1	DB	1519	MA6	C4'-C5'-O5'-P
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1518	MA6	C5-C6-N6-C10
1	DB	1518	MA6	C5-C6-N6-C10
1	DB	1400	5MC	C3'-C4'-C5'-O5'
2	EB	2503	2MA	C4'-C5'-O5'-P
2	B	2503	2MA	C4'-C5'-O5'-P
1	A	527	7MG	O4'-C4'-C5'-O5'
45	WC	92	0TD	CA-CB-SB-CSB
45	TA	92	0TD	CG-CB-SB-CSB
45	WC	92	0TD	CG-CB-SB-CSB
1	DB	527	7MG	O4'-C4'-C5'-O5'
2	B	1920	4OC	C2'-C1'-N1-C2

There are no ring outliers.

31 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	EB	1939	5MU	1	0
1	DB	1407	5MC	1	0
1	A	1518	MA6	1	0
1	A	967	5MC	1	0
1	DB	966	M2G	1	0
1	DB	1402	4OC	1	0
4	GB	54	5MU	1	0
2	EB	1917	PSU	1	0
1	DB	1519	MA6	1	0
45	WC	92	0TD	3	0
2	B	1920	4OC	1	0
1	DB	1498	UR3	1	0
2	B	2552	2MU	2	0
1	DB	967	5MC	1	0
2	B	2503	2MA	3	0
4	D	54	5MU	1	0
4	GB	55	PSU	1	0
1	A	966	M2G	1	0
1	A	1498	UR3	1	0
4	GB	8	4SU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1915	5MU	1	0
45	TA	92	0TD	3	0
2	EB	2552	2MU	2	0
4	D	55	PSU	1	0
2	EB	1942	5MC	1	0
2	EB	2503	2MA	4	0
1	A	1407	5MC	1	0
1	DB	1518	MA6	1	0
1	A	1402	4OC	2	0
2	B	1939	5MU	2	0
2	EB	1915	5MU	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 1528 ligands modelled in this entry, 1528 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

**Warning:** The R factor obtained from EDS is 0.2204, which does not match the depositor's R factor of 0.0. Please interpret the results in this section carefully.

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	A	1495/1507 (99%)	-0.07	32 (2%) 63 41	94, 141, 205, 274	0
1	DB	1495/1507 (99%)	0.03	28 (1%) 66 44	100, 130, 190, 262	0
2	B	2869/2880 (99%)	-0.17	40 (1%) 73 51	77, 97, 192, 252	0
2	EB	2869/2880 (99%)	-0.02	52 (1%) 67 45	88, 112, 211, 267	0
3	C	120/120 (100%)	-0.24	0 100 100	108, 129, 142, 160	0
3	FB	120/120 (100%)	0.11	1 (0%) 82 64	119, 157, 177, 190	0
4	D	73/77 (94%)	0.17	5 (6%) 25 17	112, 214, 233, 236	0
4	GB	73/77 (94%)	0.19	2 (2%) 56 35	131, 210, 227, 231	0
4	IA	73/77 (94%)	0.16	6 (8%) 19 13	90, 125, 134, 141	0
4	LC	73/77 (94%)	-0.07	2 (2%) 56 35	108, 132, 144, 148	0
5	E	275/275 (100%)	-0.06	9 (3%) 49 30	79, 88, 98, 107	0
5	HB	275/275 (100%)	-0.05	10 (3%) 46 29	86, 102, 112, 122	0
6	F	204/206 (99%)	-0.09	1 (0%) 87 72	78, 102, 123, 133	0
6	IB	204/206 (99%)	-0.14	2 (0%) 79 59	90, 116, 136, 147	0
7	G	202/205 (98%)	-0.31	0 100 100	71, 100, 121, 131	0
7	JB	202/205 (98%)	-0.12	6 (2%) 52 33	84, 115, 132, 137	0
8	H	181/182 (99%)	-0.01	8 (4%) 39 25	132, 140, 158, 161	0
8	KB	181/182 (99%)	0.08	5 (2%) 55 34	146, 166, 178, 180	0
9	I	174/180 (96%)	-0.14	5 (2%) 54 34	112, 121, 128, 139	0
9	LB	174/180 (96%)	0.55	17 (9%) 14 10	158, 192, 207, 212	0
10	J	146/148 (98%)	0.10	6 (4%) 42 26	102, 140, 148, 150	0
10	MB	146/148 (98%)	0.40	11 (7%) 22 15	123, 153, 164, 166	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
11	K	140/140 (100%)	-0.18	1 (0%) 84 66	84, 100, 119, 128	0
11	NB	140/140 (100%)	0.08	9 (6%) 27 18	100, 122, 137, 142	0
12	L	122/122 (100%)	-0.13	4 (3%) 49 30	87, 100, 110, 114	0
12	OB	122/122 (100%)	-0.11	3 (2%) 58 37	97, 107, 115, 118	0
13	M	150/150 (100%)	0.03	6 (4%) 43 26	76, 106, 131, 135	0
13	PB	150/150 (100%)	0.09	6 (4%) 43 26	93, 118, 148, 150	0
14	N	141/141 (100%)	-0.09	4 (2%) 55 34	94, 105, 118, 126	0
14	QB	141/141 (100%)	-0.02	1 (0%) 84 66	106, 126, 140, 148	0
15	O	118/118 (100%)	-0.25	0 100 100	87, 101, 114, 120	0
15	RB	118/118 (100%)	-0.20	0 100 100	97, 111, 121, 125	0
16	P	110/112 (98%)	-0.19	2 (1%) 67 45	116, 127, 132, 134	0
16	SB	110/112 (98%)	0.07	1 (0%) 81 61	139, 155, 162, 165	0
17	Q	137/146 (93%)	-0.11	5 (3%) 46 29	99, 111, 155, 184	0
17	TB	137/146 (93%)	-0.02	3 (2%) 62 40	108, 117, 147, 158	0
18	R	117/118 (99%)	-0.28	0 100 100	78, 95, 108, 111	0
18	UB	117/118 (99%)	0.10	5 (4%) 40 25	92, 116, 131, 137	0
19	S	101/101 (100%)	-0.42	0 100 100	80, 105, 116, 121	0
19	VB	101/101 (100%)	-0.18	1 (0%) 79 59	96, 127, 136, 141	0
20	T	112/113 (99%)	-0.42	0 100 100	77, 90, 113, 123	0
20	WB	112/113 (99%)	-0.26	1 (0%) 81 61	89, 102, 121, 133	0
21	U	95/96 (98%)	-0.24	1 (1%) 77 56	87, 93, 104, 111	0
21	XB	95/96 (98%)	0.07	3 (3%) 50 31	107, 121, 129, 131	0
22	V	107/110 (97%)	-0.05	2 (1%) 66 44	97, 106, 122, 125	0
22	YB	107/110 (97%)	0.32	5 (4%) 37 24	114, 124, 143, 146	0
23	W	189/206 (91%)	-0.18	2 (1%) 77 56	111, 129, 139, 142	0
23	ZB	189/206 (91%)	-0.13	1 (0%) 87 72	132, 151, 162, 167	0
24	AC	84/85 (98%)	0.48	9 (10%) 12 9	116, 122, 137, 141	0
24	X	84/85 (98%)	0.35	10 (11%) 10 8	100, 105, 124, 130	0
25	BC	97/98 (98%)	0.34	6 (6%) 28 18	92, 116, 142, 154	0
25	Y	97/98 (98%)	0.26	7 (7%) 23 16	82, 99, 125, 135	0
26	CC	70/72 (97%)	0.23	3 (4%) 40 25	126, 133, 136, 139	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
26	Z	70/72 (97%)	-0.04	6 (8%)	18 12	95, 101, 106, 112	0
27	AA	60/60 (100%)	-0.41	0	100 100	92, 104, 123, 130	0
27	DC	60/60 (100%)	-0.17	0	100 100	108, 120, 133, 138	0
28	BA	69/71 (97%)	-0.10	0	100 100	162, 179, 201, 205	0
28	EC	69/71 (97%)	-0.04	0	100 100	189, 197, 207, 209	0
29	CA	59/60 (98%)	-0.05	1 (1%)	69 47	79, 106, 122, 126	0
29	FC	59/60 (98%)	-0.11	1 (1%)	69 47	88, 116, 131, 133	0
30	DA	53/54 (98%)	0.38	3 (5%)	30 19	161, 165, 168, 169	0
30	GC	53/54 (98%)	0.66	6 (11%)	11 8	188, 192, 195, 195	0
31	EA	48/49 (97%)	0.32	5 (10%)	13 9	72, 77, 87, 89	0
31	HC	48/49 (97%)	0.54	2 (4%)	41 25	89, 92, 102, 107	0
32	FA	64/65 (98%)	0.07	2 (3%)	51 32	83, 94, 110, 118	0
32	IC	64/65 (98%)	0.02	3 (4%)	37 24	98, 109, 127, 132	0
33	GA	37/37 (100%)	0.87	7 (18%)	4 4	154, 154, 155, 155	0
33	JC	37/37 (100%)	1.14	9 (24%)	2 2	167, 167, 167, 167	0
34	HA	11/27 (40%)	0.61	1 (9%)	16 11	120, 128, 144, 147	0
34	KC	11/27 (40%)	0.33	1 (9%)	16 11	124, 129, 145, 145	0
35	JA	234/256 (91%)	-0.02	7 (2%)	52 33	148, 164, 183, 190	0
35	MC	234/256 (91%)	-0.01	6 (2%)	57 36	139, 159, 176, 188	0
36	KA	206/239 (86%)	-0.14	5 (2%)	59 38	143, 156, 173, 176	0
36	NC	206/239 (86%)	-0.09	2 (0%)	79 59	142, 155, 172, 176	0
37	LA	208/209 (99%)	0.58	18 (8%)	17 12	132, 148, 157, 161	0
37	OC	208/209 (99%)	0.35	18 (8%)	17 12	117, 128, 135, 139	0
38	MA	151/162 (93%)	0.08	6 (3%)	43 26	125, 138, 145, 157	0
38	PC	151/162 (93%)	-0.05	9 (5%)	29 19	114, 125, 133, 144	0
39	NA	101/101 (100%)	-0.24	1 (0%)	79 59	119, 129, 134, 144	0
39	QC	101/101 (100%)	-0.28	2 (1%)	64 43	125, 134, 141, 147	0
40	OA	155/156 (99%)	0.13	8 (5%)	34 21	141, 155, 164, 165	0
40	RC	155/156 (99%)	0.12	9 (5%)	30 19	142, 153, 160, 163	0
41	PA	138/138 (100%)	0.03	7 (5%)	34 22	124, 141, 147, 152	0
41	SC	138/138 (100%)	-0.21	1 (0%)	84 66	116, 129, 137, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
42	QA	127/128 (99%)	0.21	11 (8%) 17 12	134, 179, 187, 189	0
42	TC	127/128 (99%)	0.22	9 (7%) 23 16	145, 173, 181, 183	0
43	RA	98/105 (93%)	0.22	2 (2%) 64 43	144, 182, 195, 196	0
43	UC	98/105 (93%)	0.17	2 (2%) 64 43	148, 176, 181, 183	0
44	SA	116/129 (89%)	0.02	4 (3%) 48 30	108, 126, 133, 142	0
44	VC	116/129 (89%)	0.03	7 (6%) 29 19	109, 130, 137, 143	0
45	TA	121/132 (91%)	0.06	3 (2%) 58 37	115, 121, 128, 132	0
45	WC	121/132 (91%)	-0.18	3 (2%) 58 37	108, 114, 123, 128	0
46	UA	117/126 (92%)	0.28	11 (9%) 15 11	132, 167, 173, 174	0
46	XC	117/126 (92%)	0.25	9 (7%) 21 14	147, 178, 186, 187	0
47	VA	60/61 (98%)	0.25	2 (3%) 49 30	151, 158, 167, 168	0
47	YC	60/61 (98%)	0.32	3 (5%) 35 22	152, 160, 176, 177	0
48	WA	88/89 (98%)	-0.16	2 (2%) 61 39	108, 126, 138, 140	0
48	ZC	88/89 (98%)	-0.34	2 (2%) 61 39	110, 127, 133, 135	0
49	AD	83/88 (94%)	0.07	5 (6%) 29 19	118, 123, 137, 154	0
49	XA	83/88 (94%)	0.54	8 (9%) 15 11	137, 156, 170, 187	0
50	BD	99/105 (94%)	0.13	8 (8%) 19 13	111, 120, 124, 126	0
50	YA	99/105 (94%)	0.18	5 (5%) 34 22	109, 128, 135, 138	0
51	CD	70/88 (79%)	-0.11	1 (1%) 73 51	125, 134, 141, 144	0
51	ZA	70/88 (79%)	-0.12	3 (4%) 40 25	120, 130, 138, 141	0
52	AB	83/93 (89%)	0.01	0 100 100	143, 170, 175, 177	0
52	DD	83/93 (89%)	0.13	2 (2%) 59 38	158, 183, 188, 189	0
53	BB	99/106 (93%)	0.40	11 (11%) 12 9	141, 154, 170, 172	0
53	ED	99/106 (93%)	0.15	7 (7%) 23 16	119, 140, 155, 156	0
54	CB	24/27 (88%)	1.15	4 (16%) 5 5	155, 165, 170, 174	0
54	FD	24/27 (88%)	1.35	7 (29%) 1 2	160, 168, 173, 175	0
55	GD	255/365 (69%)	-0.09	8 (3%) 51 32	94, 137, 163, 184	0
55	HD	255/365 (69%)	-0.06	8 (3%) 51 32	117, 143, 169, 180	0
All	All	21472/22222 (96%)	-0.01	642 (2%) 52 33	71, 124, 185, 274	0

All (642) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	BC	2	SER	11.3
25	Y	2	SER	9.9
24	AC	3	HIS	8.4
24	X	3	HIS	8.0
9	LB	71	LEU	6.9
37	OC	42	GLN	6.4
2	EB	270(C)	A	6.4
33	JC	5	ALA	6.3
2	EB	1058	G	6.2
42	TC	119	ALA	6.2
38	MA	122	GLU	6.1
17	Q	54	ARG	6.0
50	BD	45	HIS	5.9
10	MB	80	PRO	5.5
2	EB	270(D)	C	5.5
33	JC	23	VAL	5.5
37	LA	42	GLN	5.4
11	NB	80	GLY	5.4
55	GD	156	HIS	5.3
9	LB	67	LEU	5.2
35	JA	240	GLN	5.2
43	RA	53	PRO	5.2
31	HC	2	LYS	5.2
10	J	79	ILE	5.2
25	BC	47	GLN	5.2
13	PB	35	HIS	5.1
37	LA	2	GLY	5.1
46	XC	116	THR	5.1
24	X	2	ALA	5.1
38	PC	20	GLN	4.9
42	TC	121	ARG	4.9
37	LA	9	CYS	4.9
2	EB	546	C	4.8
11	NB	109	LYS	4.8
11	NB	111	PRO	4.8
25	Y	48	LYS	4.8
41	PA	1	MET	4.8
49	XA	42	ARG	4.8
38	PC	21	ALA	4.8
24	AC	2	ALA	4.8
38	MA	126	ARG	4.8
37	LA	6	GLY	4.7
38	PC	124	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
18	UB	3	ARG	4.7
46	UA	27	LYS	4.7
9	LB	143	GLN	4.7
46	UA	116	THR	4.6
8	KB	73	ALA	4.6
37	LA	7	PRO	4.6
1	A	1491	G	4.6
8	KB	84	LYS	4.6
2	EB	2799	A	4.6
37	OC	9	CYS	4.6
2	EB	1094	U	4.5
44	SA	42	TRP	4.5
37	LA	156	GLU	4.5
37	LA	154	ASN	4.5
46	UA	114	ARG	4.5
2	B	2894	G	4.5
37	LA	31	CYS	4.5
2	B	270(B)	A	4.4
17	TB	53	ARG	4.4
24	X	4	LYS	4.3
35	JA	27	LYS	4.3
37	LA	5	ILE	4.3
37	OC	26	CYS	4.3
13	PB	34	GLY	4.3
42	TC	123	PRO	4.3
31	EA	6	GLN	4.3
22	YB	60	PHE	4.3
31	EA	2	LYS	4.3
44	VC	42	TRP	4.2
48	WA	69	TYR	4.2
30	DA	22	ALA	4.2
1	DB	619	U	4.1
54	CB	25	LYS	4.1
50	YA	17	LYS	4.1
2	B	1762	A	4.1
21	XB	63	LYS	4.1
25	BC	48	LYS	4.1
37	LA	26	CYS	4.1
12	OB	22	ILE	4.1
1	DB	84	U	4.1
23	W	104	PHE	4.1
1	A	1531	A	4.0

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Mol	Chain	Res	Type	RSRZ
9	LB	144	VAL	4.0
33	GA	23	VAL	4.0
41	PA	129	VAL	4.0
9	LB	139	GLN	4.0
49	AD	13	HIS	4.0
24	X	5	LYS	4.0
37	OC	5	ILE	3.9
34	KC	13	A	3.9
33	JC	4	ARG	3.9
2	B	270(C)	A	3.9
2	EB	270(B)	A	3.9
42	QA	121	ARG	3.9
1	A	1202	G	3.9
33	GA	18	ARG	3.9
13	M	142	GLY	3.9
49	XA	41	PRO	3.9
55	GD	154	GLY	3.9
12	OB	41	ALA	3.9
55	GD	155	GLU	3.8
10	MB	78	THR	3.8
46	XC	102	ARG	3.8
9	LB	138	LYS	3.8
35	JA	196	LEU	3.8
53	BB	84	LEU	3.8
43	UC	58	ASP	3.8
2	B	2758	A	3.8
54	CB	7	ARG	3.8
2	EB	412	A	3.8
25	BC	44	PRO	3.8
2	B	270(M)	U	3.8
37	OC	31	CYS	3.7
46	XC	27	LYS	3.7
37	OC	2	GLY	3.7
5	E	51	VAL	3.7
49	XA	39	TYR	3.7
51	ZA	54	ARG	3.7
46	XC	19	LEU	3.7
1	A	84	U	3.6
36	KA	62	ASP	3.6
1	A	88	C	3.6
38	MA	128	PRO	3.6
33	GA	3	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
38	MA	20	GLN	3.6
12	L	22	ILE	3.6
5	HB	265	PRO	3.6
2	B	654	U	3.6
8	H	134	GLY	3.6
9	LB	141	VAL	3.6
18	UB	89	GLU	3.6
8	H	133	LEU	3.6
37	LA	45	GLN	3.5
11	NB	114	ARG	3.5
24	AC	19	LYS	3.5
2	B	1760	A	3.5
42	TC	122	ALA	3.5
29	FC	8	LYS	3.5
37	LA	12	CYS	3.5
53	BB	59	ALA	3.5
9	I	71	LEU	3.5
13	M	35	HIS	3.4
1	A	768	A	3.4
45	WC	119	LYS	3.4
11	NB	110	GLY	3.4
40	RC	33	ASP	3.4
42	QA	110	GLU	3.4
54	FD	18	TYR	3.4
2	EB	567	A	3.4
55	GD	153	GLU	3.4
25	BC	46	LEU	3.4
25	Y	47	GLN	3.4
44	VC	41	THR	3.4
33	JC	17	ILE	3.4
1	A	60	A	3.4
46	UA	87	TYR	3.4
30	DA	23	THR	3.3
30	GC	39	TYR	3.3
30	GC	23	THR	3.3
44	SA	31	THR	3.3
42	TC	115	GLY	3.3
33	JC	18	ARG	3.3
26	Z	52	ASP	3.3
9	LB	174	GLY	3.3
31	HC	23	ARG	3.3
41	SC	1	MET	3.3

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Mol	Chain	Res	Type	RSRZ
45	WC	73	GLU	3.3
2	B	524	U	3.3
37	OC	38	TYR	3.3
11	NB	112	LEU	3.3
2	B	352	G	3.3
25	Y	42	GLN	3.3
42	TC	9	ARG	3.3
35	JA	239	VAL	3.2
37	OC	37	PRO	3.2
12	L	5	GLN	3.2
37	OC	36	ARG	3.2
4	IA	15	G	3.2
54	FD	2	GLY	3.2
2	EB	1496	A	3.2
46	UA	17	VAL	3.2
40	OA	77	SER	3.2
42	QA	127	LYS	3.2
42	QA	124	GLN	3.2
45	TA	109	GLY	3.2
1	A	707	C	3.2
5	E	9	TYR	3.2
8	H	156	ASP	3.2
38	PC	123	LEU	3.2
53	BB	64	ASP	3.1
1	A	990	C	3.1
8	H	157	ILE	3.1
35	JA	197	VAL	3.1
46	UA	98	VAL	3.1
41	PA	116	LYS	3.1
46	UA	102	ARG	3.1
46	XC	118	ALA	3.1
13	PB	29	LYS	3.1
55	HD	230	SER	3.1
9	LB	74	ASN	3.1
17	Q	53	ARG	3.1
23	ZB	28	MET	3.1
7	JB	171	PRO	3.1
2	B	1637	A	3.1
1	DB	27	G	3.0
26	Z	51	ARG	3.0
5	HB	253	GLN	3.0
39	QC	16	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
54	FD	16	GLY	3.0
16	SB	6	ALA	3.0
2	EB	1083	U	3.0
38	MA	124	GLY	3.0
40	RC	85	TYR	3.0
35	MC	71	VAL	3.0
44	VC	39	PRO	3.0
8	KB	74	LYS	3.0
26	Z	3	LEU	3.0
24	X	11	ARG	3.0
38	PC	18	ARG	3.0
4	D	49	G	3.0
42	TC	118	LYS	3.0
2	EB	528	A	3.0
47	VA	29	ARG	3.0
18	UB	2	PRO	3.0
2	EB	2894	G	2.9
26	CC	1	MET	3.0
24	AC	4	LYS	2.9
46	XC	117	VAL	2.9
55	GD	327	TYR	2.9
8	KB	89	GLY	2.9
9	LB	147	ASN	2.9
44	VC	31	THR	2.9
1	A	294	U	2.9
5	E	54	ARG	2.9
49	AD	42	ARG	2.9
33	JC	6	SER	2.9
47	VA	2	ALA	2.9
44	VC	26	ASN	2.9
10	MB	72	LEU	2.9
14	N	80	GLU	2.9
1	DB	1414	U	2.9
11	NB	113	GLY	2.9
22	YB	59	GLY	2.9
24	X	8	GLY	2.9
53	BB	63	ILE	2.9
31	EA	5	TRP	2.9
35	MC	165	VAL	2.9
36	NC	5	ILE	2.9
1	DB	10	A	2.9
55	HD	327	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	1058	G	2.9
2	EB	2160	G	2.9
42	QA	119	ALA	2.8
1	A	427	U	2.8
1	DB	766	A	2.8
1	DB	974	A	2.8
4	IA	59	A	2.8
22	YB	46	LYS	2.8
51	CD	68	LYS	2.8
5	E	243	GLY	2.8
8	KB	85	GLY	2.8
40	RC	80	VAL	2.8
49	XA	13	HIS	2.8
8	H	41	GLN	2.8
18	UB	84	LYS	2.8
1	A	706	A	2.8
2	B	1759	A	2.8
2	EB	505	A	2.8
2	EB	1762	A	2.8
24	X	55	ARG	2.8
4	IA	16	C	2.8
46	XC	87	TYR	2.8
26	Z	1	MET	2.8
5	E	11	PRO	2.8
47	YC	2	ALA	2.8
17	Q	52	ILE	2.8
25	BC	45	ASN	2.8
1	DB	1260	C	2.8
1	A	971	G	2.8
49	XA	29	ASP	2.8
26	Z	61	LEU	2.8
21	U	16	LYS	2.8
2	B	155	C	2.7
2	B	2885	C	2.7
40	RC	83	ALA	2.7
1	DB	1258	G	2.7
4	GB	47	U	2.7
8	H	39	ILE	2.7
33	JC	1	MET	2.7
47	YC	36	PHE	2.7
5	E	237	GLU	2.7
22	YB	62	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
35	JA	193	ASP	2.7
2	B	154(A)	C	2.7
2	EB	365	C	2.7
33	GA	21	GLY	2.7
5	HB	156	ALA	2.7
40	OA	7	ALA	2.7
9	I	2	SER	2.7
25	Y	45	ASN	2.7
6	F	168	MET	2.7
2	EB	366	C	2.7
24	AC	11	ARG	2.7
45	TA	16	GLU	2.7
52	DD	2	PRO	2.7
44	SA	29	ILE	2.7
2	B	2759	G	2.7
2	B	1892	C	2.7
2	EB	687	C	2.7
10	MB	90	GLY	2.7
40	RC	81	GLY	2.7
38	PC	121	LYS	2.7
1	A	1364	U	2.7
30	GC	22	ALA	2.6
4	IA	21	A	2.6
10	J	54	GLN	2.6
36	NC	87	LEU	2.6
2	B	2509	G	2.6
55	HD	155	GLU	2.6
37	LA	10	ARG	2.6
5	HB	9	TYR	2.6
1	DB	1320	C	2.6
9	I	139	GLN	2.6
32	FA	35	GLN	2.6
32	IC	46	ARG	2.6
44	VC	122	LYS	2.6
9	LB	137	ASP	2.6
9	I	67	LEU	2.6
53	ED	12	ALA	2.6
1	DB	983	A	2.6
16	P	29	PHE	2.6
24	X	57	PHE	2.6
54	CB	21	TYR	2.6
53	ED	11	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	82	U	2.6
2	EB	547	A	2.6
34	HA	13	A	2.6
38	PC	19	MET	2.6
50	YA	68	ARG	2.6
40	OA	82	GLY	2.6
55	GD	194	GLY	2.6
1	DB	1259	C	2.5
2	EB	2760	C	2.5
55	HD	153	GLU	2.5
25	Y	43	TYR	2.5
1	DB	971	G	2.5
2	EB	1973	G	2.5
4	LC	59	A	2.5
49	XA	14	ASN	2.5
37	OC	12	CYS	2.5
50	BD	100	LYS	2.5
1	A	89	U	2.5
1	DB	1364	U	2.5
2	B	1326	U	2.5
9	LB	72	ILE	2.5
33	GA	17	ILE	2.5
53	ED	8	ARG	2.5
1	DB	1224	G	2.5
2	B	2854	G	2.5
1	DB	60	A	2.5
2	EB	477	A	2.5
2	EB	2135	A	2.5
20	WB	97	LYS	2.5
30	GC	10	LEU	2.5
36	KA	87	LEU	2.5
50	BD	35	VAL	2.5
24	AC	8	GLY	2.5
40	RC	109	ASN	2.5
2	EB	279	C	2.5
2	EB	413	C	2.5
10	MB	45	LYS	2.5
24	AC	18	ALA	2.5
1	A	769	G	2.5
2	EB	2412	A	2.5
9	LB	140	LYS	2.5
22	V	94	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
37	OC	40	PRO	2.5
43	UC	83	GLU	2.5
39	QC	89	MET	2.5
1	DB	982	U	2.5
7	JB	100	THR	2.5
31	EA	43	THR	2.5
1	A	63	C	2.5
1	A	1228	C	2.5
2	EB	2827	C	2.5
7	JB	87	GLY	2.5
14	N	18	LYS	2.5
37	OC	157	LEU	2.5
10	MB	145	VAL	2.5
1	A	353	A	2.5
26	CC	66	GLU	2.5
50	YA	45	HIS	2.5
2	B	1772	G	2.4
4	D	7	G	2.4
13	M	70	GLN	2.5
50	BD	44	ALA	2.4
14	N	85	LYS	2.4
5	HB	147	LEU	2.4
10	J	41	GLU	2.4
10	MB	41	GLU	2.4
1	A	1170	A	2.4
1	A	1229	A	2.4
10	MB	58	LEU	2.4
54	FD	9	ARG	2.4
2	B	615	G	2.4
2	EB	1358	G	2.4
2	EB	2805	G	2.4
30	GC	38	LYS	2.4
50	BD	68	ARG	2.4
55	HD	154	GLY	2.4
16	P	36	TYR	2.4
22	YB	61	ILE	2.4
9	I	137	ASP	2.4
9	LB	145	ALA	2.4
4	D	50	U	2.4
42	QA	9	ARG	2.4
13	M	58	THR	2.4
31	EA	1	MET	2.4

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Mol	Chain	Res	Type	RSRZ
40	OA	81	GLY	2.4
52	DD	41	VAL	2.4
10	J	89	TYR	2.4
49	XA	15	PRO	2.4
4	IA	13	C	2.4
4	LC	48	C	2.4
21	XB	2	LYS	2.4
37	LA	8	VAL	2.4
37	OC	86	LYS	2.4
5	HB	247	ALA	2.4
42	QA	106	ALA	2.4
1	A	112	G	2.4
1	DB	769	G	2.4
14	QB	75	THR	2.3
41	PA	118	VAL	2.3
48	ZC	3	ILE	2.3
5	E	276	LYS	2.3
1	A	10	A	2.3
1	DB	1428	A	2.3
5	E	13	ARG	2.3
49	AD	60	LEU	2.3
54	FD	4	GLY	2.3
2	B	1828	G	2.3
10	J	111	PRO	2.3
53	BB	8	ARG	2.3
2	B	2551	C	2.3
50	BD	43	LEU	2.3
40	RC	74	GLU	2.3
2	B	2892	A	2.3
33	GA	16	VAL	2.3
44	SA	30	VAL	2.3
50	YA	18	THR	2.3
13	PB	33	ARG	2.3
55	HD	277	ARG	2.3
13	M	140	ALA	2.3
51	ZA	52	PRO	2.3
1	A	1192	C	2.3
1	DB	972	C	2.3
36	KA	186	PHE	2.3
46	UA	16	ASP	2.3
7	JB	59	TYR	2.3
2	EB	422	A	2.3

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Mol	Chain	Res	Type	RSRZ
53	BB	80	ARG	2.3
51	ZA	51	LEU	2.3
32	IC	65	GLU	2.3
9	LB	133	VAL	2.3
37	OC	45	GLN	2.3
45	TA	32	PHE	2.3
46	UA	101	GLN	2.3
46	XC	88	ARG	2.3
55	GD	231	GLY	2.3
9	LB	64	LEU	2.3
23	W	28	MET	2.3
1	A	1361	G	2.3
1	DB	978	A	2.3
2	B	1048	A	2.3
2	EB	1578	U	2.3
33	GA	4	ARG	2.3
37	OC	13	ARG	2.3
49	AD	30	GLY	2.3
53	ED	10	LEU	2.3
5	HB	153	ALA	2.3
17	TB	36	GLU	2.2
2	EB	1049	C	2.2
2	EB	1185	C	2.2
4	D	1	C	2.2
19	VB	38	LEU	2.2
37	LA	124	GLY	2.2
2	B	2388	A	2.2
53	BB	11	SER	2.2
1	DB	1143	G	2.2
49	XA	43	LYS	2.2
42	QA	66	ARG	2.2
48	WA	73	GLU	2.2
11	NB	107	LEU	2.2
11	K	77	GLY	2.2
41	PA	131	GLY	2.2
45	WC	115	LYS	2.2
55	HD	160	LYS	2.2
9	LB	68	THR	2.2
7	JB	78	ILE	2.2
2	B	270(D)	C	2.2
2	EB	280	C	2.2
41	PA	119	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	DB	426	G	2.2
2	EB	273(B)	G	2.2
53	BB	14	LYS	2.2
24	AC	41	ARG	2.2
33	JC	3	VAL	2.2
30	DA	10	LEU	2.2
17	Q	98	LYS	2.2
32	IC	44	LYS	2.2
42	TC	117	HIS	2.2
46	UA	26	GLY	2.2
55	GD	157	GLY	2.2
1	A	87	A	2.2
2	B	1057	A	2.2
2	B	2269	A	2.2
2	EB	2518	A	2.2
54	FD	24	ARG	2.2
12	L	4	PRO	2.2
24	X	9	SER	2.2
49	AD	29	ASP	2.2
1	A	1053	G	2.2
2	B	2550	G	2.2
53	ED	30	LYS	2.2
12	OB	5	GLN	2.2
37	OC	4	TYR	2.2
42	QA	120	ARG	2.2
1	DB	82	U	2.2
4	D	47	U	2.2
2	B	528	A	2.2
53	BB	10	LEU	2.2
10	MB	143	SER	2.2
6	IB	127	ASP	2.2
10	J	112	LYS	2.1
53	ED	29	LYS	2.1
54	CB	2	GLY	2.1
33	JC	36	GLN	2.1
35	MC	214	ILE	2.1
50	BD	65	ILE	2.1
40	RC	79	ARG	2.1
47	YC	29	ARG	2.1
1	A	428	G	2.1
7	JB	140	LEU	2.1
55	HD	231	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	DB	1093	A	2.1
2	EB	1579	A	2.1
2	EB	2386	C	2.1
11	NB	115	ARG	2.1
37	LA	139	ARG	2.1
40	OA	2	ALA	2.1
13	M	39	LYS	2.1
32	FA	52	LYS	2.1
35	JA	194	PRO	2.1
26	CC	52	ASP	2.1
21	XB	71	GLY	2.1
36	KA	39	ILE	2.1
2	B	728	G	2.1
53	BB	12	ALA	2.1
10	MB	54	GLN	2.1
18	UB	5	LYS	2.1
1	DB	632	A	2.1
2	EB	331	A	2.1
2	EB	2269	A	2.1
2	B	790	C	2.1
2	EB	2313	C	2.1
5	HB	243	GLY	2.1
8	H	40	ASN	2.1
42	TC	12	GLU	2.1
54	FD	13	ILE	2.1
35	MC	163	PHE	2.1
8	H	135	LEU	2.1
37	OC	112	VAL	2.1
17	TB	60	THR	2.1
1	A	1017	G	2.1
2	EB	352	G	2.1
3	FB	100	G	2.1
2	B	2062	A	2.1
25	Y	46	LEU	2.1
2	B	409	C	2.1
30	GC	8	LYS	2.1
42	QA	109	VAL	2.1
48	ZC	2	PRO	2.1
50	YA	47	PRO	2.1
5	E	244	ARG	2.1
5	HB	161	THR	2.1
46	UA	20	THR	2.1

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Mol	Chain	Res	Type	RSRZ
12	L	99	PHE	2.1
14	N	24	GLY	2.1
40	OA	74	GLU	2.1
24	X	19	LYS	2.1
29	CA	10	LYS	2.1
38	MA	88	LYS	2.1
41	PA	133	LEU	2.1
10	MB	92	VAL	2.1
44	VC	24	SER	2.1
2	EB	195	A	2.0
2	EB	278	A	2.0
2	EB	476	G	2.0
2	EB	615	G	2.0
2	EB	2802	G	2.0
4	GB	45	G	2.0
1	A	1259	C	2.0
1	A	1490	C	2.0
40	OA	156	TRP	2.0
13	PB	30	THR	2.0
35	MC	152	PHE	2.0
39	NA	92	LYS	2.0
17	Q	55	ASN	2.0
40	RC	77	SER	2.0
5	HB	171	ASP	2.0
50	BD	46	ASP	2.0
24	AC	55	ARG	2.0
2	B	2585	U	2.0
4	IA	20	U	2.0
22	V	14	LEU	2.0
35	MC	215	LEU	2.0
46	XC	20	THR	2.0
53	BB	104	LEU	2.0
2	B	567	A	2.0
2	EB	1057	A	2.0
2	EB	1095	A	2.0
38	PC	22	GLY	2.0
40	OA	80	VAL	2.0
1	DB	1058	G	2.0
2	EB	1954	G	2.0
1	DB	307	C	2.0
2	B	1648	C	2.0
2	EB	192	C	2.0

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Mol	Chain	Res	Type	RSRZ
6	IB	129	HIS	2.0
26	Z	55	ARG	2.0
37	OC	43	HIS	2.0
36	KA	152	ILE	2.0
37	LA	151	LYS	2.0
38	PC	88	LYS	2.0
42	QA	123	PRO	2.0
13	PB	3	LEU	2.0
37	LA	21	LEU	2.0
43	RA	54	PHE	2.0
53	ED	24	LEU	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
4	PSU	D	55	20/21	0.58	0.11	232,233,236,237	0
4	5MU	D	54	21/22	0.63	0.10	229,231,233,234	0
4	4SU	GB	8	20/21	0.68	0.11	215,218,219,219	0
4	PSU	GB	55	20/21	0.71	0.08	226,228,230,231	0
4	5MU	GB	54	21/22	0.72	0.08	225,227,229,229	0
4	4SU	D	8	20/21	0.75	0.10	218,221,222,223	0
4	PSU	IA	55	20/21	0.85	0.10	135,137,138,138	0
45	0TD	TA	92	10/11	0.85	0.26	123,123,124,124	0
4	5MC	D	32	21/22	0.88	0.09	177,177,177,177	0
2	5MU	B	1915	21/22	0.88	0.09	119,120,123,123	0
1	PSU	DB	516	20/21	0.88	0.09	125,126,129,129	0
4	5MU	LC	54	21/22	0.89	0.09	140,141,144,144	0
4	5MC	GB	32	21/22	0.89	0.09	178,178,178,179	0
4	PSU	LC	55	20/21	0.89	0.07	141,142,144,144	0
45	0TD	WC	92	10/11	0.90	0.16	119,120,120,120	0
2	PSU	B	1911	20/21	0.90	0.09	104,107,109,109	0
1	5MC	A	1400	21/22	0.90	0.13	121,123,125,126	0
2	5MU	EB	1939	21/22	0.90	0.17	93,94,95,95	0
4	4SU	IA	8	20/21	0.91	0.20	122,124,125,126	0
2	4OC	EB	1920	21/23	0.91	0.09	112,114,115,116	0
1	2MG	DB	1207	24/25	0.91	0.10	156,157,160,162	0
1	4OC	DB	1402	22/23	0.91	0.10	115,116,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	5MC	LC	32	21/22	0.91	0.11	128,128,129,129	0
2	PSU	EB	1917	20/21	0.91	0.08	117,119,121,122	0
2	OMG	B	2251	24/25	0.92	0.10	83,84,85,86	0
4	5MU	IA	54	21/22	0.92	0.08	134,134,137,138	0
2	5MU	EB	1915	21/22	0.92	0.06	129,131,132,133	0
1	2MG	A	1207	24/25	0.92	0.08	148,150,153,154	0
1	5MC	A	967	21/22	0.92	0.09	130,131,133,134	0
4	5MC	IA	32	21/22	0.92	0.11	126,126,126,127	0
1	7MG	DB	527	24/25	0.92	0.11	117,118,119,120	0
2	5MU	B	1939	21/22	0.92	0.13	84,85,86,86	0
1	PSU	A	516	20/21	0.93	0.07	132,134,137,137	0
2	5MC	EB	1942	21/22	0.93	0.08	101,103,104,104	0
2	5MC	EB	1962	21/22	0.93	0.11	98,99,101,102	0
1	5MC	DB	1400	21/22	0.93	0.11	119,121,123,124	0
2	5MC	B	1942	21/22	0.93	0.09	90,92,93,94	0
1	UR3	DB	1498	21/22	0.93	0.14	111,111,112,112	0
2	4OC	B	1920	21/23	0.93	0.10	102,104,106,107	0
4	4SU	LC	8	20/21	0.93	0.13	130,133,134,134	0
1	M2G	DB	966	25/26	0.93	0.10	130,132,134,134	0
1	5MC	DB	967	21/22	0.93	0.08	131,133,135,136	0
2	2MA	EB	2503	23/24	0.94	0.10	88,89,90,90	0
1	4OC	A	1402	22/23	0.94	0.11	115,116,117,117	0
2	PSU	B	1917	20/21	0.94	0.07	107,108,111,112	0
1	5MC	A	1407	21/22	0.94	0.08	104,105,107,108	0
1	MA6	DB	1518	24/25	0.94	0.17	102,104,105,106	0
1	7MG	A	527	24/25	0.94	0.11	122,124,125,126	0
2	2MU	EB	2552	21/23	0.95	0.14	96,97,98,98	0
1	M2G	A	966	25/26	0.95	0.10	129,130,132,132	0
2	5MC	B	1962	21/22	0.95	0.07	92,93,95,97	0
2	PSU	EB	1911	20/21	0.95	0.07	113,116,117,118	0
1	5MC	A	1404	21/22	0.95	0.09	106,107,108,109	0
2	PSU	B	2605	20/21	0.95	0.10	79,81,81,81	0
1	MA6	A	1518	24/25	0.96	0.11	99,102,104,104	0
1	MA6	DB	1519	24/25	0.96	0.13	103,105,106,106	0
2	2MA	B	2503	23/24	0.96	0.08	78,78,79,79	0
1	5MC	DB	1407	21/22	0.96	0.09	107,109,110,110	0
2	OMG	EB	2251	24/25	0.96	0.11	95,96,98,98	0
1	UR3	A	1498	21/22	0.96	0.11	107,108,109,109	0
2	2MU	B	2552	21/23	0.97	0.13	84,86,86,86	0
1	MA6	A	1519	24/25	0.97	0.10	100,102,104,104	0
2	PSU	EB	2605	20/21	0.97	0.08	89,90,91,91	0
1	5MC	DB	1404	21/22	0.97	0.09	107,108,109,109	0



## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
56	MG	EB	3285	1/1	-0.40	0.20	220,220,220,220	0
56	MG	EB	3189	1/1	-0.39	0.12	241,241,241,241	0
56	MG	B	3188	1/1	-0.38	0.35	217,217,217,217	0
56	MG	B	3142	1/1	-0.33	0.19	214,214,214,214	0
56	MG	D	105	1/1	-0.29	0.20	208,208,208,208	0
56	MG	EB	3170	1/1	-0.29	0.15	187,187,187,187	0
56	MG	LB	204	1/1	-0.28	0.23	197,197,197,197	0
56	MG	A	1746	1/1	-0.22	0.35	173,173,173,173	0
56	MG	A	1688	1/1	-0.22	0.20	167,167,167,167	0
56	MG	DB	1736	1/1	-0.16	0.25	212,212,212,212	0
56	MG	RC	201	1/1	-0.10	0.39	142,142,142,142	0
56	MG	B	3391	1/1	-0.08	0.15	240,240,240,240	0
56	MG	DB	1729	1/1	-0.08	0.18	159,159,159,159	0
56	MG	EB	3026	1/1	-0.07	0.14	175,175,175,175	0
56	MG	EB	3016	1/1	-0.05	0.35	243,243,243,243	0
56	MG	EB	3195	1/1	-0.01	0.22	152,152,152,152	0
56	MG	A	1711	1/1	-0.01	0.37	130,130,130,130	0
56	MG	A	1728	1/1	0.00	0.20	160,160,160,160	0
56	MG	GB	103	1/1	-0.00	0.23	211,211,211,211	0
56	MG	A	1680	1/1	0.00	0.37	176,176,176,176	0
56	MG	B	3352	1/1	0.00	0.20	183,183,183,183	0
56	MG	DB	1681	1/1	0.01	0.33	149,149,149,149	0
56	MG	B	3288	1/1	0.03	0.22	208,208,208,208	0
56	MG	VA	101	1/1	0.03	0.44	140,140,140,140	0
56	MG	A	1640	1/1	0.05	0.39	134,134,134,134	0
56	MG	DB	1690	1/1	0.06	0.31	139,139,139,139	0
56	MG	RA	201	1/1	0.08	0.18	165,165,165,165	0
56	MG	B	3392	1/1	0.08	0.18	192,192,192,192	0
56	MG	A	1755	1/1	0.08	0.19	176,176,176,176	0
56	MG	EB	2945	1/1	0.09	0.52	139,139,139,139	0
56	MG	B	3025	1/1	0.10	0.35	234,234,234,234	0
56	MG	EB	3014	1/1	0.11	0.21	136,136,136,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	A	1729	1/1	0.11	0.40	152,152,152,152	0
56	MG	B	3304	1/1	0.12	0.28	237,237,237,237	0
56	MG	KB	201	1/1	0.12	0.19	173,173,173,173	0
56	MG	KA	301	1/1	0.13	0.34	157,157,157,157	0
56	MG	B	3175	1/1	0.13	0.45	154,154,154,154	0
56	MG	W	302	1/1	0.13	0.38	129,129,129,129	0
56	MG	GB	102	1/1	0.13	0.13	204,204,204,204	0
56	MG	W	310	1/1	0.14	0.13	134,134,134,134	0
56	MG	B	2960	1/1	0.16	0.57	223,223,223,223	0
56	MG	GD	404	1/1	0.17	0.27	135,135,135,135	0
56	MG	B	3315	1/1	0.20	0.13	203,203,203,203	0
56	MG	A	1707	1/1	0.20	0.20	163,163,163,163	0
56	MG	EB	3177	1/1	0.20	0.21	122,122,122,122	0
56	MG	B	3384	1/1	0.20	0.25	161,161,161,161	0
56	MG	EB	3251	1/1	0.22	0.09	158,158,158,158	0
56	MG	DB	1742	1/1	0.22	0.26	142,142,142,142	0
56	MG	B	2966	1/1	0.22	0.43	106,106,106,106	0
56	MG	A	1742	1/1	0.22	0.23	179,179,179,179	0
56	MG	Q	202	1/1	0.23	0.22	148,148,148,148	0
56	MG	EB	2936	1/1	0.23	0.48	128,128,128,128	0
56	MG	FB	216	1/1	0.23	0.36	141,141,141,141	0
56	MG	DB	1761	1/1	0.25	0.19	152,152,152,152	0
56	MG	GB	101	1/1	0.25	0.21	202,202,202,202	0
56	MG	A	1627	1/1	0.25	0.26	127,127,127,127	0
56	MG	EB	2944	1/1	0.25	0.26	102,102,102,102	0
56	MG	A	1745	1/1	0.25	0.19	219,219,219,219	0
56	MG	EB	2982	1/1	0.25	0.40	133,133,133,133	0
56	MG	DB	1617	1/1	0.25	0.44	136,136,136,136	0
56	MG	TC	201	1/1	0.25	0.27	177,177,177,177	0
56	MG	B	3274	1/1	0.25	0.32	118,118,118,118	0
56	MG	EB	3132	1/1	0.26	0.33	140,140,140,140	0
56	MG	XC	201	1/1	0.26	0.14	171,171,171,171	0
56	MG	EB	3050	1/1	0.26	0.36	160,160,160,160	0
56	MG	EB	3067	1/1	0.27	0.17	131,131,131,131	0
56	MG	GB	105	1/1	0.27	0.24	172,172,172,172	0
56	MG	LB	202	1/1	0.28	0.32	181,181,181,181	0
56	MG	EB	3102	1/1	0.28	0.21	126,126,126,126	0
56	MG	D	102	1/1	0.28	0.15	210,210,210,210	0
56	MG	DB	1601	1/1	0.29	0.40	122,122,122,122	0
56	MG	B	3124	1/1	0.29	0.22	155,155,155,155	0
56	MG	EB	3120	1/1	0.29	0.39	143,143,143,143	0
56	MG	JC	102	1/1	0.29	0.17	146,146,146,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	EB	3019	1/1	0.30	0.30	113,113,113,113	0
56	MG	DB	1685	1/1	0.30	0.19	177,177,177,177	0
56	MG	A	1618	1/1	0.31	0.34	126,126,126,126	0
56	MG	A	1634	1/1	0.31	0.50	134,134,134,134	0
56	MG	EB	3103	1/1	0.31	0.41	103,103,103,103	0
56	MG	EB	2971	1/1	0.31	0.40	112,112,112,112	0
56	MG	DB	1602	1/1	0.32	0.54	97,97,97,97	0
56	MG	DB	1703	1/1	0.32	0.44	163,163,163,163	0
56	MG	DB	1714	1/1	0.32	0.38	99,99,99,99	0
56	MG	B	3262	1/1	0.32	0.45	143,143,143,143	0
56	MG	LB	205	1/1	0.32	0.10	197,197,197,197	0
56	MG	B	2908	1/1	0.33	0.33	95,95,95,95	0
56	MG	A	1675	1/1	0.33	0.30	118,118,118,118	0
56	MG	FB	208	1/1	0.34	0.15	171,171,171,171	0
56	MG	DB	1623	1/1	0.34	0.28	121,121,121,121	0
56	MG	DB	1686	1/1	0.34	0.35	124,124,124,124	0
56	MG	VA	102	1/1	0.35	0.11	159,159,159,159	0
56	MG	EB	3259	1/1	0.35	0.24	141,141,141,141	0
56	MG	B	3176	1/1	0.35	0.22	144,144,144,144	0
56	MG	DB	1648	1/1	0.36	0.17	143,143,143,143	0
56	MG	A	1659	1/1	0.36	0.16	153,153,153,153	0
56	MG	B	3134	1/1	0.36	0.36	129,129,129,129	0
56	MG	FB	212	1/1	0.36	0.33	160,160,160,160	0
56	MG	A	1635	1/1	0.36	0.25	138,138,138,138	0
56	MG	B	3287	1/1	0.36	0.25	151,151,151,151	0
56	MG	B	3022	1/1	0.36	0.28	118,118,118,118	0
56	MG	DB	1712	1/1	0.36	0.17	199,199,199,199	0
56	MG	A	1705	1/1	0.36	0.38	143,143,143,143	0
56	MG	JA	303	1/1	0.37	0.11	161,161,161,161	0
56	MG	A	1752	1/1	0.37	0.33	160,160,160,160	0
56	MG	IB	302	1/1	0.37	0.34	95,95,95,95	0
56	MG	EB	2966	1/1	0.38	0.40	99,99,99,99	0
56	MG	A	1662	1/1	0.38	0.26	154,154,154,154	0
56	MG	LA	301	1/1	0.38	0.19	139,139,139,139	0
56	MG	GD	402	1/1	0.38	0.20	124,124,124,124	0
56	MG	MC	301	1/1	0.38	0.23	149,149,149,149	0
56	MG	FB	205	1/1	0.39	0.41	143,143,143,143	0
56	MG	EB	3201	1/1	0.39	0.24	133,133,133,133	0
56	MG	JA	301	1/1	0.39	0.22	143,143,143,143	0
56	MG	DB	1615	1/1	0.39	0.68	122,122,122,122	0
56	MG	A	1656	1/1	0.39	0.18	229,229,229,229	0
56	MG	A	1622	1/1	0.40	0.37	147,147,147,147	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	LC	102	1/1	0.40	0.24	124,124,124,124	0
56	MG	A	1633	1/1	0.40	0.20	140,140,140,140	0
56	MG	DB	1654	1/1	0.40	0.21	165,165,165,165	0
56	MG	TB	203	1/1	0.41	0.19	152,152,152,152	0
56	MG	A	1726	1/1	0.41	0.22	167,167,167,167	0
56	MG	DB	1645	1/1	0.41	0.28	139,139,139,139	0
56	MG	DB	1733	1/1	0.42	0.38	127,127,127,127	0
56	MG	A	1657	1/1	0.42	0.34	164,164,164,164	0
56	MG	A	1699	1/1	0.43	0.28	143,143,143,143	0
56	MG	B	3282	1/1	0.43	0.23	147,147,147,147	0
56	MG	FB	203	1/1	0.43	0.37	125,125,125,125	0
56	MG	B	3119	1/1	0.43	0.46	100,100,100,100	0
56	MG	A	1649	1/1	0.43	0.47	125,125,125,125	0
56	MG	SB	201	1/1	0.44	0.09	149,149,149,149	0
56	MG	EB	2969	1/1	0.44	0.29	127,127,127,127	0
56	MG	D	103	1/1	0.44	0.09	175,175,175,175	0
56	MG	EB	2925	1/1	0.44	0.55	88,88,88,88	0
56	MG	EB	2995	1/1	0.44	0.30	152,152,152,152	0
56	MG	GD	405	1/1	0.44	0.28	117,117,117,117	0
56	MG	LC	105	1/1	0.45	0.15	136,136,136,136	0
56	MG	EB	2989	1/1	0.45	0.30	179,179,179,179	0
56	MG	A	1647	1/1	0.45	0.40	149,149,149,149	0
56	MG	DB	1725	1/1	0.45	0.34	166,166,166,166	0
56	MG	A	1623	1/1	0.45	0.54	132,132,132,132	0
56	MG	FB	206	1/1	0.45	0.38	124,124,124,124	0
56	MG	B	3086	1/1	0.45	0.14	151,151,151,151	0
56	MG	P	201	1/1	0.45	0.13	129,129,129,129	0
56	MG	DB	1610	1/1	0.46	0.85	109,109,109,109	0
56	MG	A	1661	1/1	0.46	0.37	145,145,145,145	0
56	MG	EB	3191	1/1	0.46	0.19	151,151,151,151	0
56	MG	A	1758	1/1	0.46	0.19	188,188,188,188	0
56	MG	DB	1758	1/1	0.46	0.28	207,207,207,207	0
56	MG	A	1615	1/1	0.46	0.30	118,118,118,118	0
56	MG	EB	3066	1/1	0.46	0.19	172,172,172,172	0
56	MG	C	206	1/1	0.47	0.30	130,130,130,130	0
56	MG	EB	3266	1/1	0.47	0.23	138,138,138,138	0
56	MG	B	3154	1/1	0.47	0.28	136,136,136,136	0
56	MG	FB	201	1/1	0.47	0.42	117,117,117,117	0
56	MG	LC	106	1/1	0.47	0.12	124,124,124,124	0
56	MG	C	202	1/1	0.47	0.20	106,106,106,106	0
56	MG	B	3180	1/1	0.48	0.22	179,179,179,179	0
56	MG	DB	1756	1/1	0.48	0.33	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	C	213	1/1	0.48	0.20	139,139,139,139	0
56	MG	EB	3181	1/1	0.48	0.38	155,155,155,155	0
56	MG	LC	108	1/1	0.48	0.11	125,125,125,125	0
56	MG	A	1636	1/1	0.48	0.25	140,140,140,140	0
56	MG	DB	1640	1/1	0.49	0.31	121,121,121,121	0
56	MG	B	2936	1/1	0.49	0.62	94,94,94,94	0
56	MG	DB	1627	1/1	0.49	0.31	104,104,104,104	0
56	MG	AC	102	1/1	0.49	0.48	98,98,98,98	0
56	MG	UC	201	1/1	0.49	0.34	164,164,164,164	0
56	MG	DB	1722	1/1	0.49	0.17	117,117,117,117	0
56	MG	ZC	101	1/1	0.49	0.10	126,126,126,126	0
56	MG	DB	1628	1/1	0.49	0.23	115,115,115,115	0
56	MG	FB	217	1/1	0.49	0.18	139,139,139,139	0
56	MG	EB	3250	1/1	0.49	0.23	134,134,134,134	0
56	MG	DB	1684	1/1	0.50	0.27	133,133,133,133	0
56	MG	EB	3022	1/1	0.50	0.39	114,114,114,114	0
56	MG	B	3123	1/1	0.50	0.33	103,103,103,103	0
56	MG	A	1611	1/1	0.50	0.26	149,149,149,149	0
56	MG	K	202	1/1	0.50	0.33	105,105,105,105	0
56	MG	B	3010	1/1	0.50	0.30	116,116,116,116	0
56	MG	WA	102	1/1	0.50	0.14	124,124,124,124	0
56	MG	A	1691	1/1	0.50	0.20	113,113,113,113	0
56	MG	EB	2951	1/1	0.51	0.26	95,95,95,95	0
56	MG	EB	3142	1/1	0.51	0.38	136,136,136,136	0
56	MG	EB	2992	1/1	0.51	0.39	91,91,91,91	0
56	MG	DB	1709	1/1	0.51	0.13	107,107,107,107	0
56	MG	A	1717	1/1	0.51	0.74	144,144,144,144	0
56	MG	YA	201	1/1	0.51	0.28	106,106,106,106	0
56	MG	EB	2979	1/1	0.51	0.49	111,111,111,111	0
56	MG	DB	1668	1/1	0.51	0.26	99,99,99,99	0
56	MG	EB	2978	1/1	0.52	0.32	103,103,103,103	0
56	MG	B	2944	1/1	0.52	0.31	115,115,115,115	0
56	MG	A	1735	1/1	0.52	0.15	131,131,131,131	0
56	MG	DB	1621	1/1	0.52	0.32	110,110,110,110	0
56	MG	JB	302	1/1	0.52	0.12	116,116,116,116	0
56	MG	EB	2939	1/1	0.52	0.41	99,99,99,99	0
56	MG	B	3026	1/1	0.52	0.18	116,116,116,116	0
56	MG	LB	203	1/1	0.52	0.21	168,168,168,168	0
56	MG	EB	3059	1/1	0.52	0.22	122,122,122,122	0
56	MG	B	3246	1/1	0.53	0.14	125,125,125,125	0
56	MG	EB	2984	1/1	0.53	0.30	127,127,127,127	0
56	MG	EB	3186	1/1	0.53	0.22	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DB	1660	1/1	0.53	0.20	131,131,131,131	0
56	MG	B	3218	1/1	0.53	0.11	109,109,109,109	0
56	MG	DB	1718	1/1	0.53	0.28	145,145,145,145	0
56	MG	DB	1717	1/1	0.54	0.21	124,124,124,124	0
56	MG	A	1701	1/1	0.54	0.45	141,141,141,141	0
56	MG	EB	2942	1/1	0.54	0.23	138,138,138,138	0
56	MG	IA	102	1/1	0.54	0.28	124,124,124,124	0
56	MG	B	3131	1/1	0.54	0.23	112,112,112,112	0
56	MG	A	1703	1/1	0.54	0.16	136,136,136,136	0
56	MG	B	2903	1/1	0.54	0.44	107,107,107,107	0
56	MG	CD	102	1/1	0.54	0.12	122,122,122,122	0
56	MG	EB	3128	1/1	0.54	0.30	161,161,161,161	0
56	MG	EB	3049	1/1	0.54	0.27	106,106,106,106	0
56	MG	EB	3134	1/1	0.54	0.26	154,154,154,154	0
56	MG	EB	3260	1/1	0.55	0.28	220,220,220,220	0
56	MG	EB	3149	1/1	0.55	0.27	113,113,113,113	0
56	MG	HB	304	1/1	0.55	0.29	100,100,100,100	0
56	MG	DB	1657	1/1	0.55	0.17	102,102,102,102	0
56	MG	A	1704	1/1	0.55	0.30	137,137,137,137	0
56	MG	EA	101	1/1	0.55	0.17	91,91,91,91	0
56	MG	A	1613	1/1	0.55	0.47	116,116,116,116	0
56	MG	EB	2950	1/1	0.55	0.41	124,124,124,124	0
56	MG	DB	1614	1/1	0.55	0.42	94,94,94,94	0
56	MG	B	3404	1/1	0.55	0.23	121,121,121,121	0
56	MG	DB	1721	1/1	0.55	0.41	134,134,134,134	0
56	MG	EB	2911	1/1	0.55	0.55	111,111,111,111	0
56	MG	J	202	1/1	0.55	0.26	138,138,138,138	0
56	MG	W	304	1/1	0.55	0.26	119,119,119,119	0
56	MG	A	1696	1/1	0.56	0.32	152,152,152,152	0
56	MG	B	3145	1/1	0.56	0.38	123,123,123,123	0
56	MG	YB	202	1/1	0.56	0.23	116,116,116,116	0
56	MG	ZB	302	1/1	0.56	0.14	154,154,154,154	0
56	MG	DB	1697	1/1	0.56	0.31	105,105,105,105	0
56	MG	A	1738	1/1	0.56	0.40	144,144,144,144	0
56	MG	EB	3203	1/1	0.56	0.19	130,130,130,130	0
56	MG	EB	3205	1/1	0.56	0.21	138,138,138,138	0
56	MG	A	1678	1/1	0.56	0.29	145,145,145,145	0
56	MG	A	1644	1/1	0.56	0.41	114,114,114,114	0
56	MG	A	1718	1/1	0.57	0.15	171,171,171,171	0
56	MG	C	212	1/1	0.57	0.23	128,128,128,128	0
56	MG	DB	1641	1/1	0.57	0.29	146,146,146,146	0
56	MG	DB	1603	1/1	0.57	0.44	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	A	1630	1/1	0.57	0.49	116,116,116,116	0
56	MG	B	3046	1/1	0.57	0.25	126,126,126,126	0
56	MG	EB	3138	1/1	0.57	0.09	116,116,116,116	0
56	MG	B	3251	1/1	0.57	0.15	154,154,154,154	0
56	MG	B	3261	1/1	0.57	0.10	187,187,187,187	0
56	MG	LB	201	1/1	0.57	0.23	159,159,159,159	0
56	MG	EB	3047	1/1	0.57	0.47	98,98,98,98	0
56	MG	EB	2974	1/1	0.57	0.21	114,114,114,114	0
56	MG	W	311	1/1	0.57	0.11	134,134,134,134	0
56	MG	DB	1680	1/1	0.57	0.34	137,137,137,137	0
56	MG	D	106	1/1	0.57	0.18	227,227,227,227	0
56	MG	B	3063	1/1	0.57	0.30	100,100,100,100	0
56	MG	EB	3087	1/1	0.57	0.17	156,156,156,156	0
56	MG	HD	402	1/1	0.57	0.20	128,128,128,128	0
56	MG	DB	1775	1/1	0.58	0.19	143,143,143,143	0
56	MG	B	2916	1/1	0.58	0.36	93,93,93,93	0
56	MG	BB	201	1/1	0.58	0.25	131,131,131,131	0
56	MG	C	223	1/1	0.58	0.22	132,132,132,132	0
56	MG	B	2933	1/1	0.58	0.40	89,89,89,89	0
56	MG	B	3137	1/1	0.58	0.26	132,132,132,132	0
56	MG	EB	3153	1/1	0.58	0.27	103,103,103,103	0
56	MG	W	303	1/1	0.58	0.20	125,125,125,125	0
56	MG	PA	202	1/1	0.58	0.19	142,142,142,142	0
56	MG	A	1651	1/1	0.58	0.38	107,107,107,107	0
56	MG	A	1601	1/1	0.58	0.37	94,94,94,94	0
56	MG	J	201	1/1	0.58	0.28	134,134,134,134	0
56	MG	B	3150	1/1	0.58	0.23	113,113,113,113	0
56	MG	DB	1612	1/1	0.59	0.21	112,112,112,112	0
56	MG	V	502	1/1	0.59	0.28	100,100,100,100	0
56	MG	A	1721	1/1	0.59	0.21	95,95,95,95	0
56	MG	NA	202	1/1	0.59	0.11	126,126,126,126	0
56	MG	EB	2988	1/1	0.59	0.41	104,104,104,104	0
56	MG	DB	1620	1/1	0.59	0.38	126,126,126,126	0
56	MG	DB	1704	1/1	0.59	0.20	127,127,127,127	0
56	MG	DB	1707	1/1	0.59	0.17	108,108,108,108	0
56	MG	EB	3002	1/1	0.59	0.35	116,116,116,116	0
56	MG	OA	202	1/1	0.59	0.10	135,135,135,135	0
56	MG	A	1709	1/1	0.59	0.35	164,164,164,164	0
56	MG	FB	213	1/1	0.59	0.29	137,137,137,137	0
56	MG	B	2947	1/1	0.59	0.49	108,108,108,108	0
56	MG	TA	202	1/1	0.59	0.32	114,114,114,114	0
56	MG	EB	3237	1/1	0.59	0.29	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	B	3308	1/1	0.59	0.28	109,109,109,109	0
56	MG	A	1628	1/1	0.60	0.65	116,116,116,116	0
56	MG	OA	201	1/1	0.60	0.23	142,142,142,142	0
56	MG	EB	3232	1/1	0.60	0.22	145,145,145,145	0
56	MG	DB	1606	1/1	0.60	0.23	90,90,90,90	0
56	MG	DB	1607	1/1	0.60	0.74	110,110,110,110	0
56	MG	A	1681	1/1	0.60	0.25	169,169,169,169	0
56	MG	DB	1705	1/1	0.60	0.27	130,130,130,130	0
56	MG	DB	1611	1/1	0.60	0.38	101,101,101,101	0
56	MG	XC	202	1/1	0.60	0.24	157,157,157,157	0
56	MG	YC	101	1/1	0.60	0.20	158,158,158,158	0
56	MG	A	1679	1/1	0.60	0.58	116,116,116,116	0
56	MG	B	2967	1/1	0.60	0.41	125,125,125,125	0
56	MG	AC	101	1/1	0.60	0.21	115,115,115,115	0
56	MG	DB	1751	1/1	0.60	0.32	130,130,130,130	0
56	MG	EB	3200	1/1	0.60	0.31	111,111,111,111	0
56	MG	MA	202	1/1	0.60	0.13	129,129,129,129	0
56	MG	EB	3284	1/1	0.61	0.23	103,103,103,103	0
56	MG	B	2942	1/1	0.61	0.43	116,116,116,116	0
56	MG	B	3159	1/1	0.61	0.26	90,90,90,90	0
56	MG	CD	101	1/1	0.61	0.12	124,124,124,124	0
56	MG	B	3347	1/1	0.61	0.12	124,124,124,124	0
56	MG	A	1692	1/1	0.61	0.77	145,145,145,145	0
56	MG	B	3037	1/1	0.61	0.38	102,102,102,102	0
56	MG	TA	201	1/1	0.61	0.16	118,118,118,118	0
56	MG	EB	3275	1/1	0.61	0.40	135,135,135,135	0
56	MG	B	3089	1/1	0.62	0.39	86,86,86,86	0
56	MG	B	3006	1/1	0.62	0.45	97,97,97,97	0
56	MG	B	3302	1/1	0.62	0.20	105,105,105,105	0
56	MG	HB	302	1/1	0.62	0.14	120,120,120,120	0
56	MG	DB	1770	1/1	0.62	0.27	137,137,137,137	0
56	MG	DB	1773	1/1	0.62	0.35	109,109,109,109	0
56	MG	EB	3283	1/1	0.62	0.12	166,166,166,166	0
56	MG	A	1602	1/1	0.62	0.44	98,98,98,98	0
56	MG	DB	1699	1/1	0.62	0.59	106,106,106,106	0
56	MG	EB	2913	1/1	0.62	0.36	89,89,89,89	0
56	MG	B	3075	1/1	0.62	0.38	76,76,76,76	0
56	MG	DB	1667	1/1	0.62	0.20	115,115,115,115	0
56	MG	WA	101	1/1	0.62	0.12	126,126,126,126	0
56	MG	B	3126	1/1	0.62	0.17	99,99,99,99	0
56	MG	DB	1740	1/1	0.62	0.11	130,130,130,130	0
56	MG	DB	1741	1/1	0.62	0.31	135,135,135,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	IA	104	1/1	0.62	0.25	123,123,123,123	0
56	MG	B	2968	1/1	0.62	0.33	97,97,97,97	0
56	MG	EB	3139	1/1	0.62	0.35	103,103,103,103	0
56	MG	B	2940	1/1	0.63	0.27	88,88,88,88	0
56	MG	B	3213	1/1	0.63	0.13	92,92,92,92	0
56	MG	A	1645	1/1	0.63	0.35	137,137,137,137	0
56	MG	B	3219	1/1	0.63	0.34	131,131,131,131	0
56	MG	EB	3135	1/1	0.63	0.13	111,111,111,111	0
56	MG	B	2963	1/1	0.63	0.35	86,86,86,86	0
56	MG	DB	1677	1/1	0.63	0.28	158,158,158,158	0
56	MG	A	1694	1/1	0.63	0.12	168,168,168,168	0
56	MG	EB	3084	1/1	0.63	0.32	87,87,87,87	0
56	MG	C	216	1/1	0.63	0.24	123,123,123,123	0
56	MG	DC	101	1/1	0.63	0.20	112,112,112,112	0
56	MG	JB	301	1/1	0.63	0.50	89,89,89,89	0
56	MG	DB	1760	1/1	0.63	0.30	102,102,102,102	0
56	MG	B	3257	1/1	0.63	0.19	96,96,96,96	0
56	MG	EB	3180	1/1	0.63	0.16	114,114,114,114	0
56	MG	EB	3107	1/1	0.64	0.33	108,108,108,108	0
56	MG	W	307	1/1	0.64	0.14	125,125,125,125	0
56	MG	DB	1670	1/1	0.64	0.35	167,167,167,167	0
56	MG	B	3291	1/1	0.64	0.17	142,142,142,142	0
56	MG	EB	2909	1/1	0.64	0.60	88,88,88,88	0
56	MG	LC	101	1/1	0.64	0.15	132,132,132,132	0
56	MG	DB	1678	1/1	0.64	0.23	106,106,106,106	0
56	MG	EB	3246	1/1	0.64	0.46	105,105,105,105	0
56	MG	B	3003	1/1	0.64	0.23	84,84,84,84	0
56	MG	B	3362	1/1	0.64	0.11	118,118,118,118	0
56	MG	A	1612	1/1	0.64	0.26	118,118,118,118	0
56	MG	A	1663	1/1	0.64	0.46	113,113,113,113	0
56	MG	EB	3060	1/1	0.64	0.21	95,95,95,95	0
56	MG	EB	3271	1/1	0.64	0.09	127,127,127,127	0
56	MG	EB	3163	1/1	0.64	0.16	144,144,144,144	0
56	MG	B	3170	1/1	0.64	0.14	117,117,117,117	0
56	MG	DB	1663	1/1	0.64	0.26	96,96,96,96	0
56	MG	EB	3082	1/1	0.64	0.38	112,112,112,112	0
56	MG	DB	1691	1/1	0.64	0.19	109,109,109,109	0
56	MG	EB	3086	1/1	0.64	0.24	104,104,104,104	0
56	MG	EB	2946	1/1	0.64	0.20	124,124,124,124	0
56	MG	C	220	1/1	0.64	0.23	122,122,122,122	0
56	MG	WB	202	1/1	0.64	0.18	96,96,96,96	0
56	MG	EB	3011	1/1	0.64	0.14	163,163,163,163	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	EB	3244	1/1	0.65	0.20	96,96,96,96	0
56	MG	B	3065	1/1	0.65	0.34	98,98,98,98	0
56	MG	B	3343	1/1	0.65	0.09	106,106,106,106	0
56	MG	C	208	1/1	0.65	0.32	99,99,99,99	0
56	MG	B	3249	1/1	0.65	0.28	149,149,149,149	0
56	MG	AB	3301	1/1	0.65	0.12	136,136,136,136	0
56	MG	PC	201	1/1	0.65	0.40	106,106,106,106	0
56	MG	EB	3216	1/1	0.65	0.36	129,129,129,129	0
56	MG	H	201	1/1	0.65	0.11	129,129,129,129	0
56	MG	W	308	1/1	0.65	0.14	132,132,132,132	0
56	MG	B	3195	1/1	0.66	0.26	115,115,115,115	0
56	MG	B	2951	1/1	0.66	0.34	111,111,111,111	0
56	MG	DB	1682	1/1	0.66	0.12	128,128,128,128	0
56	MG	EB	3176	1/1	0.66	0.09	106,106,106,106	0
56	MG	EB	3018	1/1	0.66	0.15	110,110,110,110	0
56	MG	EB	3179	1/1	0.66	0.39	121,121,121,121	0
56	MG	B	2953	1/1	0.66	0.42	107,107,107,107	0
56	MG	B	2984	1/1	0.66	0.36	96,96,96,96	0
56	MG	DB	1604	1/1	0.66	0.42	103,103,103,103	0
56	MG	EB	3110	1/1	0.66	0.26	120,120,120,120	0
56	MG	EB	3112	1/1	0.66	0.21	124,124,124,124	0
56	MG	EB	3035	1/1	0.66	0.60	116,116,116,116	0
56	MG	EB	3122	1/1	0.66	0.16	174,174,174,174	0
56	MG	B	3031	1/1	0.66	0.30	87,87,87,87	0
56	MG	A	1629	1/1	0.66	0.32	123,123,123,123	0
56	MG	A	1610	1/1	0.66	0.32	108,108,108,108	0
56	MG	DB	1636	1/1	0.66	0.25	137,137,137,137	0
56	MG	GD	401	1/1	0.66	0.41	95,95,95,95	0
56	MG	A	1631	1/1	0.66	0.29	131,131,131,131	0
56	MG	IA	108	1/1	0.66	0.20	130,130,130,130	0
56	MG	EB	2960	1/1	0.66	0.50	95,95,95,95	0
56	MG	EB	3076	1/1	0.66	0.34	116,116,116,116	0
56	MG	EB	2904	1/1	0.67	0.65	79,79,79,79	0
56	MG	SA	201	1/1	0.67	0.16	106,106,106,106	0
56	MG	FA	101	1/1	0.67	0.52	111,111,111,111	0
56	MG	QB	203	1/1	0.67	0.10	103,103,103,103	0
56	MG	EB	3262	1/1	0.67	0.10	112,112,112,112	0
56	MG	HA	101	1/1	0.67	0.13	123,123,123,123	0
56	MG	VB	201	1/1	0.67	0.16	114,114,114,114	0
56	MG	A	1607	1/1	0.67	0.53	92,92,92,92	0
56	MG	A	1617	1/1	0.67	0.17	100,100,100,100	0
56	MG	Q	203	1/1	0.67	0.15	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	EB	3029	1/1	0.67	0.13	90,90,90,90	0
56	MG	EB	2941	1/1	0.67	0.37	103,103,103,103	0
56	MG	EB	3290	1/1	0.67	0.08	131,131,131,131	0
56	MG	DB	1720	1/1	0.67	0.19	143,143,143,143	0
56	MG	DB	1674	1/1	0.67	0.12	130,130,130,130	0
56	MG	B	3056	1/1	0.67	0.33	117,117,117,117	0
56	MG	B	2924	1/1	0.67	0.42	87,87,87,87	0
56	MG	DB	1726	1/1	0.67	0.21	135,135,135,135	0
56	MG	ZA	101	1/1	0.67	0.22	124,124,124,124	0
56	MG	DB	1626	1/1	0.67	0.22	111,111,111,111	0
56	MG	FB	214	1/1	0.67	0.34	128,128,128,128	0
56	MG	A	1734	1/1	0.67	0.30	110,110,110,110	0
56	MG	EB	3190	1/1	0.67	0.09	111,111,111,111	0
56	MG	C	211	1/1	0.67	0.23	119,119,119,119	0
56	MG	W	305	1/1	0.67	0.27	129,129,129,129	0
56	MG	DB	1638	1/1	0.67	0.21	103,103,103,103	0
56	MG	B	3380	1/1	0.67	0.21	97,97,97,97	0
56	MG	B	3074	1/1	0.67	0.32	94,94,94,94	0
56	MG	DB	1644	1/1	0.67	0.25	105,105,105,105	0
56	MG	DB	1698	1/1	0.67	0.34	112,112,112,112	0
56	MG	B	3225	1/1	0.67	0.21	116,116,116,116	0
56	MG	DB	1764	1/1	0.67	0.29	110,110,110,110	0
56	MG	DB	1646	1/1	0.67	0.24	101,101,101,101	0
56	MG	J	204	1/1	0.67	0.11	138,138,138,138	0
56	MG	C	217	1/1	0.67	0.16	113,113,113,113	0
56	MG	EB	2986	1/1	0.68	0.24	95,95,95,95	0
56	MG	B	2956	1/1	0.68	0.35	99,99,99,99	0
56	MG	EB	3123	1/1	0.68	0.42	103,103,103,103	0
56	MG	EB	3057	1/1	0.68	0.56	95,95,95,95	0
56	MG	B	3181	1/1	0.68	0.24	106,106,106,106	0
56	MG	DB	1766	1/1	0.68	0.31	122,122,122,122	0
56	MG	EB	3199	1/1	0.68	0.28	117,117,117,117	0
56	MG	A	1706	1/1	0.68	0.21	135,135,135,135	0
56	MG	A	1670	1/1	0.68	0.14	139,139,139,139	0
56	MG	B	3018	1/1	0.68	0.44	88,88,88,88	0
56	MG	EB	2902	1/1	0.68	0.45	89,89,89,89	0
56	MG	FB	204	1/1	0.68	0.22	130,130,130,130	0
56	MG	DB	1622	1/1	0.68	0.47	103,103,103,103	0
56	MG	QB	201	1/1	0.68	0.16	99,99,99,99	0
56	MG	B	2921	1/1	0.68	0.35	88,88,88,88	0
56	MG	EB	3235	1/1	0.68	0.14	122,122,122,122	0
56	MG	MA	201	1/1	0.68	0.38	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	A	1604	1/1	0.68	0.54	105,105,105,105	0
56	MG	EB	3245	1/1	0.68	0.12	128,128,128,128	0
56	MG	A	1605	1/1	0.68	0.29	103,103,103,103	0
56	MG	DB	1664	1/1	0.68	0.13	137,137,137,137	0
56	MG	A	1660	1/1	0.68	0.35	125,125,125,125	0
56	MG	HD	401	1/1	0.68	0.49	97,97,97,97	0
56	MG	B	3370	1/1	0.68	0.63	214,214,214,214	0
56	MG	B	3186	1/1	0.69	0.12	109,109,109,109	0
56	MG	EB	2993	1/1	0.69	0.19	88,88,88,88	0
56	MG	DB	1750	1/1	0.69	0.28	116,116,116,116	0
56	MG	DB	1671	1/1	0.69	0.39	112,112,112,112	0
56	MG	IA	103	1/1	0.69	0.31	124,124,124,124	0
56	MG	LC	103	1/1	0.69	0.48	126,126,126,126	0
56	MG	DB	1639	1/1	0.69	0.68	140,140,140,140	0
56	MG	B	3152	1/1	0.69	0.21	107,107,107,107	0
56	MG	EB	2947	1/1	0.69	0.44	106,106,106,106	0
56	MG	B	3309	1/1	0.69	0.19	111,111,111,111	0
56	MG	B	3133	1/1	0.69	0.12	169,169,169,169	0
56	MG	QC	201	1/1	0.69	0.36	120,120,120,120	0
56	MG	C	205	1/1	0.69	0.21	114,114,114,114	0
56	MG	A	1616	1/1	0.69	0.33	99,99,99,99	0
56	MG	B	2915	1/1	0.69	0.37	85,85,85,85	0
56	MG	I	201	1/1	0.69	0.15	130,130,130,130	0
56	MG	MB	201	1/1	0.69	0.16	153,153,153,153	0
56	MG	B	3051	1/1	0.69	0.34	106,106,106,106	0
56	MG	A	1730	1/1	0.69	0.29	119,119,119,119	0
56	MG	DB	1693	1/1	0.69	0.21	111,111,111,111	0
56	MG	B	3236	1/1	0.69	0.09	122,122,122,122	0
56	MG	TB	205	1/1	0.69	0.05	121,121,121,121	0
56	MG	J	205	1/1	0.69	0.14	134,134,134,134	0
56	MG	A	1698	1/1	0.69	0.20	160,160,160,160	0
56	MG	EB	2935	1/1	0.69	0.46	98,98,98,98	0
56	MG	EB	3072	1/1	0.69	0.37	98,98,98,98	0
56	MG	B	3151	1/1	0.69	0.22	105,105,105,105	0
56	MG	DB	1700	1/1	0.70	0.20	145,145,145,145	0
56	MG	DB	1616	1/1	0.70	0.28	100,100,100,100	0
56	MG	A	1710	1/1	0.70	0.27	126,126,126,126	0
56	MG	A	1732	1/1	0.70	0.33	149,149,149,149	0
56	MG	B	3085	1/1	0.70	0.20	106,106,106,106	0
56	MG	EB	2976	1/1	0.70	0.27	113,113,113,113	0
56	MG	EB	3119	1/1	0.70	0.20	134,134,134,134	0
56	MG	B	2928	1/1	0.70	0.24	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	EB	3038	1/1	0.70	0.20	97,97,97,97	0
56	MG	EB	2927	1/1	0.70	0.32	90,90,90,90	0
56	MG	B	3127	1/1	0.70	0.28	96,96,96,96	0
56	MG	A	1632	1/1	0.70	0.20	124,124,124,124	0
56	MG	B	3103	1/1	0.70	0.23	90,90,90,90	0
56	MG	DB	1609	1/1	0.70	0.28	116,116,116,116	0
56	MG	EB	3230	1/1	0.70	0.10	100,100,100,100	0
56	MG	TB	201	1/1	0.70	0.19	112,112,112,112	0
56	MG	B	3110	1/1	0.70	0.38	94,94,94,94	0
56	MG	B	3205	1/1	0.70	0.33	82,82,82,82	0
56	MG	DB	1694	1/1	0.70	0.28	125,125,125,125	0
56	MG	B	3314	1/1	0.70	0.15	99,99,99,99	0
56	MG	EB	3000	1/1	0.70	0.26	114,114,114,114	0
56	MG	EB	3079	1/1	0.70	0.29	139,139,139,139	0
56	MG	B	3160	1/1	0.70	0.19	92,92,92,92	0
56	MG	DB	1774	1/1	0.70	0.24	128,128,128,128	0
56	MG	B	3316	1/1	0.70	0.13	151,151,151,151	0
56	MG	A	1713	1/1	0.71	0.15	116,116,116,116	0
56	MG	B	3178	1/1	0.71	0.13	140,140,140,140	0
56	MG	DB	1752	1/1	0.71	0.08	156,156,156,156	0
56	MG	B	2904	1/1	0.71	0.45	74,74,74,74	0
56	MG	EB	3053	1/1	0.71	0.22	113,113,113,113	0
56	MG	B	3093	1/1	0.71	0.23	120,120,120,120	0
56	MG	B	3356	1/1	0.71	0.13	92,92,92,92	0
56	MG	A	1684	1/1	0.71	0.36	113,113,113,113	0
56	MG	DB	1633	1/1	0.71	0.51	106,106,106,106	0
56	MG	DB	1635	1/1	0.71	0.25	120,120,120,120	0
56	MG	B	3367	1/1	0.71	0.22	102,102,102,102	0
56	MG	EB	3141	1/1	0.71	0.31	96,96,96,96	0
56	MG	FB	209	1/1	0.71	0.26	132,132,132,132	0
56	MG	MA	203	1/1	0.71	0.13	143,143,143,143	0
56	MG	B	3053	1/1	0.71	0.37	101,101,101,101	0
56	MG	S	203	1/1	0.71	0.07	112,112,112,112	0
56	MG	F	301	1/1	0.71	0.27	106,106,106,106	0
56	MG	DB	1738	1/1	0.71	0.43	108,108,108,108	0
56	MG	DB	1643	1/1	0.71	0.38	109,109,109,109	0
56	MG	EB	2910	1/1	0.71	0.38	87,87,87,87	0
56	MG	B	3244	1/1	0.71	0.12	82,82,82,82	0
56	MG	EB	3106	1/1	0.71	0.14	120,120,120,120	0
56	MG	B	2911	1/1	0.71	0.18	61,61,61,61	0
56	MG	EB	2924	1/1	0.71	0.34	89,89,89,89	0
56	MG	EB	3257	1/1	0.72	0.18	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	OB	202	1/1	0.72	0.14	100,100,100,100	0
56	MG	B	2989	1/1	0.72	0.32	109,109,109,109	0
56	MG	EB	2948	1/1	0.72	0.49	123,123,123,123	0
56	MG	B	3390	1/1	0.72	0.20	124,124,124,124	0
56	MG	B	3216	1/1	0.72	0.15	157,157,157,157	0
56	MG	A	1683	1/1	0.72	0.51	106,106,106,106	0
56	MG	B	3036	1/1	0.72	0.37	110,110,110,110	0
56	MG	EB	3001	1/1	0.72	0.25	112,112,112,112	0
56	MG	EB	2933	1/1	0.72	0.29	95,95,95,95	0
56	MG	EB	3225	1/1	0.72	0.17	115,115,115,115	0
56	MG	B	3122	1/1	0.72	0.19	90,90,90,90	0
56	MG	C	204	1/1	0.72	0.19	114,114,114,114	0
56	MG	A	1654	1/1	0.72	0.18	154,154,154,154	0
56	MG	A	1723	1/1	0.72	0.29	180,180,180,180	0
56	MG	A	1643	1/1	0.72	0.39	117,117,117,117	0
56	MG	EB	3182	1/1	0.72	0.21	107,107,107,107	0
56	MG	A	1727	1/1	0.72	0.23	106,106,106,106	0
56	MG	A	1682	1/1	0.72	0.15	191,191,191,191	0
56	MG	B	3099	1/1	0.72	0.27	87,87,87,87	0
56	MG	EB	3278	1/1	0.73	0.22	106,106,106,106	0
56	MG	DB	1618	1/1	0.73	0.57	101,101,101,101	0
56	MG	B	3125	1/1	0.73	0.42	107,107,107,107	0
56	MG	EB	3207	1/1	0.73	0.10	121,121,121,121	0
56	MG	EB	3101	1/1	0.73	0.20	96,96,96,96	0
56	MG	B	3247	1/1	0.73	0.07	146,146,146,146	0
56	MG	B	2959	1/1	0.73	0.18	78,78,78,78	0
56	MG	EB	2996	1/1	0.73	0.46	86,86,86,86	0
56	MG	DB	1673	1/1	0.73	0.26	105,105,105,105	0
56	MG	EB	3109	1/1	0.73	0.13	112,112,112,112	0
56	MG	MB	202	1/1	0.73	0.16	148,148,148,148	0
56	MG	EB	3054	1/1	0.73	0.28	102,102,102,102	0
56	MG	K	201	1/1	0.73	0.14	111,111,111,111	0
56	MG	FB	210	1/1	0.73	0.26	143,143,143,143	0
56	MG	DB	1624	1/1	0.73	0.35	111,111,111,111	0
56	MG	B	3276	1/1	0.73	0.14	83,83,83,83	0
56	MG	OA	203	1/1	0.73	0.14	142,142,142,142	0
56	MG	B	3054	1/1	0.73	0.38	89,89,89,89	0
56	MG	EB	3068	1/1	0.73	0.29	92,92,92,92	0
56	MG	B	3401	1/1	0.73	0.14	111,111,111,111	0
56	MG	B	3283	1/1	0.73	0.42	226,226,226,226	0
56	MG	EB	3263	1/1	0.73	0.11	133,133,133,133	0
56	MG	B	3285	1/1	0.73	0.59	132,132,132,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	B	2923	1/1	0.73	0.40	78,78,78,78	0
56	MG	DB	1665	1/1	0.73	0.24	129,129,129,129	0
56	MG	EB	3121	1/1	0.74	0.22	116,116,116,116	0
56	MG	A	1753	1/1	0.74	0.21	125,125,125,125	0
56	MG	WB	201	1/1	0.74	0.24	102,102,102,102	0
56	MG	A	1743	1/1	0.74	0.12	174,174,174,174	0
56	MG	B	2914	1/1	0.74	0.41	93,93,93,93	0
56	MG	B	2929	1/1	0.74	0.34	90,90,90,90	0
56	MG	EB	3133	1/1	0.74	0.23	91,91,91,91	0
56	MG	A	1603	1/1	0.74	0.35	88,88,88,88	0
56	MG	BC	101	1/1	0.74	0.20	116,116,116,116	0
56	MG	I	202	1/1	0.74	0.09	122,122,122,122	0
56	MG	DB	1649	1/1	0.74	0.33	106,106,106,106	0
56	MG	C	210	1/1	0.74	0.13	123,123,123,123	0
56	MG	A	1671	1/1	0.74	0.18	131,131,131,131	0
56	MG	EB	3074	1/1	0.74	0.21	91,91,91,91	0
56	MG	DB	1772	1/1	0.74	0.09	109,109,109,109	0
56	MG	B	3132	1/1	0.74	0.41	104,104,104,104	0
56	MG	Y	103	1/1	0.74	0.20	115,115,115,115	0
56	MG	EB	3166	1/1	0.74	0.36	113,113,113,113	0
56	MG	MC	302	1/1	0.74	0.12	138,138,138,138	0
56	MG	EB	3012	1/1	0.74	0.33	90,90,90,90	0
56	MG	EB	3085	1/1	0.74	0.26	117,117,117,117	0
56	MG	B	2918	1/1	0.74	0.30	76,76,76,76	0
56	MG	DB	1732	1/1	0.74	0.17	147,147,147,147	0
56	MG	EB	2961	1/1	0.74	0.30	94,94,94,94	0
56	MG	B	3116	1/1	0.74	0.31	122,122,122,122	0
56	MG	B	3266	1/1	0.74	0.10	149,149,149,149	0
56	MG	EB	3105	1/1	0.74	0.20	97,97,97,97	0
56	MG	B	3273	1/1	0.74	0.12	104,104,104,104	0
56	MG	EB	2973	1/1	0.74	0.39	91,91,91,91	0
56	MG	EB	3286	1/1	0.74	0.26	123,123,123,123	0
56	MG	A	1712	1/1	0.74	0.15	125,125,125,125	0
56	MG	B	3077	1/1	0.74	0.42	99,99,99,99	0
56	MG	TA	203	1/1	0.74	0.07	113,113,113,113	0
56	MG	DB	1746	1/1	0.74	0.32	104,104,104,104	0
56	MG	B	3340	1/1	0.74	0.12	89,89,89,89	0
56	MG	TB	204	1/1	0.74	0.15	112,112,112,112	0
56	MG	HD	403	1/1	0.74	0.14	129,129,129,129	0
56	MG	B	3098	1/1	0.75	0.30	86,86,86,86	0
56	MG	EB	2962	1/1	0.75	0.55	114,114,114,114	0
56	MG	N	202	1/1	0.75	0.20	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	B	3268	1/1	0.75	0.08	94,94,94,94	0
56	MG	DB	1749	1/1	0.75	0.17	113,113,113,113	0
56	MG	EB	2914	1/1	0.75	0.35	94,94,94,94	0
56	MG	EB	3094	1/1	0.75	0.19	110,110,110,110	0
56	MG	D	104	1/1	0.75	0.14	131,131,131,131	0
56	MG	B	3190	1/1	0.75	0.28	88,88,88,88	0
56	MG	PC	202	1/1	0.75	0.21	123,123,123,123	0
56	MG	B	3369	1/1	0.75	0.09	89,89,89,89	0
56	MG	RB	204	1/1	0.75	0.16	100,100,100,100	0
56	MG	B	2906	1/1	0.75	0.38	78,78,78,78	0
56	MG	TC	202	1/1	0.75	0.09	156,156,156,156	0
56	MG	IA	105	1/1	0.75	0.43	116,116,116,116	0
56	MG	B	3082	1/1	0.75	0.27	90,90,90,90	0
56	MG	DB	1661	1/1	0.75	0.28	97,97,97,97	0
56	MG	DB	1762	1/1	0.75	0.26	122,122,122,122	0
56	MG	A	1668	1/1	0.75	0.28	126,126,126,126	0
56	MG	BD	202	1/1	0.75	0.08	108,108,108,108	0
56	MG	EB	2991	1/1	0.75	0.28	90,90,90,90	0
56	MG	A	1676	1/1	0.75	0.37	127,127,127,127	0
56	MG	B	2905	1/1	0.75	0.59	80,80,80,80	0
56	MG	DB	1666	1/1	0.75	0.27	108,108,108,108	0
56	MG	B	3258	1/1	0.75	0.22	107,107,107,107	0
56	MG	B	2986	1/1	0.75	0.40	81,81,81,81	0
56	MG	DB	1669	1/1	0.75	0.30	154,154,154,154	0
56	MG	B	3096	1/1	0.75	0.27	111,111,111,111	0
56	MG	C	201	1/1	0.75	0.41	94,94,94,94	0
56	MG	B	3228	1/1	0.76	0.14	119,119,119,119	0
56	MG	A	1697	1/1	0.76	0.38	104,104,104,104	0
56	MG	DB	1631	1/1	0.76	0.26	106,106,106,106	0
56	MG	EB	2972	1/1	0.76	0.18	104,104,104,104	0
56	MG	L	207	1/1	0.76	0.17	101,101,101,101	0
56	MG	EB	3289	1/1	0.76	0.26	109,109,109,109	0
56	MG	E	301	1/1	0.76	0.29	71,71,71,71	0
56	MG	E	302	1/1	0.76	0.16	93,93,93,93	0
56	MG	NA	201	1/1	0.76	0.16	129,129,129,129	0
56	MG	EB	3231	1/1	0.76	0.35	119,119,119,119	0
56	MG	NB	201	1/1	0.76	0.18	115,115,115,115	0
56	MG	A	1748	1/1	0.76	0.09	97,97,97,97	0
56	MG	B	3163	1/1	0.76	0.18	89,89,89,89	0
56	MG	B	3184	1/1	0.76	0.29	116,116,116,116	0
56	MG	RB	203	1/1	0.76	0.38	114,114,114,114	0
56	MG	EB	3240	1/1	0.76	0.08	155,155,155,155	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	DB	1767	1/1	0.76	0.11	106,106,106,106	0
56	MG	FB	211	1/1	0.76	0.16	146,146,146,146	0
56	MG	DB	1731	1/1	0.76	0.22	133,133,133,133	0
56	MG	B	3317	1/1	0.76	0.25	120,120,120,120	0
56	MG	B	3331	1/1	0.76	0.42	105,105,105,105	0
56	MG	B	3078	1/1	0.76	0.28	89,89,89,89	0
56	MG	J	203	1/1	0.76	0.20	104,104,104,104	0
56	MG	B	3100	1/1	0.76	0.34	97,97,97,97	0
56	MG	A	1759	1/1	0.76	0.18	176,176,176,176	0
56	MG	EB	2954	1/1	0.76	0.67	103,103,103,103	0
56	MG	DB	1650	1/1	0.76	0.34	103,103,103,103	0
56	MG	DB	1708	1/1	0.76	0.21	106,106,106,106	0
56	MG	EB	3073	1/1	0.76	0.20	105,105,105,105	0
56	MG	DB	1652	1/1	0.76	0.35	122,122,122,122	0
56	MG	EB	2915	1/1	0.77	0.57	96,96,96,96	0
56	MG	EB	2922	1/1	0.77	0.38	79,79,79,79	0
56	MG	FB	207	1/1	0.77	0.15	138,138,138,138	0
56	MG	EB	3030	1/1	0.77	0.22	110,110,110,110	0
56	MG	XB	102	1/1	0.77	0.15	124,124,124,124	0
56	MG	A	1614	1/1	0.77	0.21	108,108,108,108	0
56	MG	YB	204	1/1	0.77	0.09	118,118,118,118	0
56	MG	B	2964	1/1	0.77	0.57	88,88,88,88	0
56	MG	EB	3043	1/1	0.77	0.17	119,119,119,119	0
56	MG	EB	3044	1/1	0.77	0.14	118,118,118,118	0
56	MG	B	3114	1/1	0.77	0.21	86,86,86,86	0
56	MG	EB	2929	1/1	0.77	0.29	98,98,98,98	0
56	MG	EB	2930	1/1	0.77	0.39	84,84,84,84	0
56	MG	Y	104	1/1	0.77	0.08	101,101,101,101	0
56	MG	Z	103	1/1	0.77	0.05	92,92,92,92	0
56	MG	B	2912	1/1	0.77	0.18	86,86,86,86	0
56	MG	G	302	1/1	0.77	0.42	73,73,73,73	0
56	MG	DB	1692	1/1	0.77	0.11	137,137,137,137	0
56	MG	B	3040	1/1	0.77	0.14	79,79,79,79	0
56	MG	EB	2943	1/1	0.77	0.38	93,93,93,93	0
56	MG	B	3394	1/1	0.77	0.33	107,107,107,107	0
56	MG	B	3024	1/1	0.77	0.30	85,85,85,85	0
56	MG	A	1725	1/1	0.77	0.09	119,119,119,119	0
56	MG	EB	3160	1/1	0.77	0.25	108,108,108,108	0
56	MG	QC	202	1/1	0.77	0.19	124,124,124,124	0
56	MG	EB	2999	1/1	0.77	0.22	101,101,101,101	0
56	MG	B	3238	1/1	0.77	0.40	93,93,93,93	0
56	MG	EB	3077	1/1	0.77	0.20	133,133,133,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DB	1613	1/1	0.77	0.35	97,97,97,97	0
56	MG	B	3165	1/1	0.77	0.17	75,75,75,75	0
56	MG	EB	3004	1/1	0.77	0.45	102,102,102,102	0
56	MG	EB	3281	1/1	0.77	0.17	95,95,95,95	0
56	MG	EB	2903	1/1	0.77	0.46	100,100,100,100	0
56	MG	AD	101	1/1	0.77	0.34	108,108,108,108	0
56	MG	B	2952	1/1	0.77	0.29	78,78,78,78	0
56	MG	OB	203	1/1	0.77	0.07	95,95,95,95	0
56	MG	JA	302	1/1	0.77	0.20	146,146,146,146	0
56	MG	W	306	1/1	0.77	0.18	122,122,122,122	0
56	MG	EB	3287	1/1	0.77	0.33	110,110,110,110	0
56	MG	B	3275	1/1	0.77	0.13	116,116,116,116	0
56	MG	B	3029	1/1	0.77	0.45	85,85,85,85	0
56	MG	EB	3021	1/1	0.77	0.18	111,111,111,111	0
56	MG	W	309	1/1	0.77	0.19	121,121,121,121	0
56	MG	EB	3025	1/1	0.77	0.89	103,103,103,103	0
56	MG	B	3138	1/1	0.78	0.35	106,106,106,106	0
56	MG	B	3193	1/1	0.78	0.25	81,81,81,81	0
56	MG	B	2976	1/1	0.78	0.44	96,96,96,96	0
56	MG	DB	1765	1/1	0.78	0.14	122,122,122,122	0
56	MG	EB	3223	1/1	0.78	0.11	97,97,97,97	0
56	MG	ZB	301	1/1	0.78	0.21	137,137,137,137	0
56	MG	A	1693	1/1	0.78	0.23	107,107,107,107	0
56	MG	B	3248	1/1	0.78	0.33	103,103,103,103	0
56	MG	B	3207	1/1	0.78	0.48	98,98,98,98	0
56	MG	B	3208	1/1	0.78	0.11	118,118,118,118	0
56	MG	A	1646	1/1	0.78	0.22	117,117,117,117	0
56	MG	EB	2998	1/1	0.78	0.23	86,86,86,86	0
56	MG	IA	107	1/1	0.78	0.41	108,108,108,108	0
56	MG	EB	3070	1/1	0.78	0.17	104,104,104,104	0
56	MG	EB	3071	1/1	0.78	0.35	100,100,100,100	0
56	MG	HB	301	1/1	0.78	0.24	103,103,103,103	0
56	MG	B	3305	1/1	0.78	0.08	120,120,120,120	0
56	MG	LC	107	1/1	0.78	0.10	110,110,110,110	0
56	MG	A	1669	1/1	0.78	0.27	93,93,93,93	0
56	MG	HB	307	1/1	0.78	0.14	102,102,102,102	0
56	MG	B	3002	1/1	0.78	0.52	85,85,85,85	0
56	MG	EB	3159	1/1	0.78	0.10	104,104,104,104	0
56	MG	A	1652	1/1	0.78	0.34	123,123,123,123	0
56	MG	EB	3009	1/1	0.78	0.18	93,93,93,93	0
56	MG	EB	3164	1/1	0.78	0.08	114,114,114,114	0
56	MG	A	1667	1/1	0.78	0.23	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	EB	3168	1/1	0.78	0.33	88,88,88,88	0
56	MG	EB	2957	1/1	0.78	0.42	91,91,91,91	0
56	MG	EB	3174	1/1	0.78	0.33	98,98,98,98	0
56	MG	WC	201	1/1	0.78	0.11	96,96,96,96	0
56	MG	WC	202	1/1	0.78	0.15	121,121,121,121	0
56	MG	B	3267	1/1	0.78	0.13	112,112,112,112	0
56	MG	EB	3279	1/1	0.78	0.42	95,95,95,95	0
56	MG	DB	1629	1/1	0.78	0.24	100,100,100,100	0
56	MG	DB	1743	1/1	0.78	0.14	104,104,104,104	0
56	MG	A	1722	1/1	0.78	0.12	96,96,96,96	0
56	MG	EB	2968	1/1	0.78	0.22	112,112,112,112	0
56	MG	B	3231	1/1	0.78	0.28	91,91,91,91	0
56	MG	B	3335	1/1	0.78	0.10	128,128,128,128	0
56	MG	EB	2923	1/1	0.78	0.38	97,97,97,97	0
56	MG	B	3232	1/1	0.78	0.20	83,83,83,83	0
56	MG	C	207	1/1	0.78	0.37	127,127,127,127	0
56	MG	B	3233	1/1	0.78	0.34	95,95,95,95	0
56	MG	EB	2928	1/1	0.78	0.33	95,95,95,95	0
56	MG	B	2971	1/1	0.78	0.16	82,82,82,82	0
56	MG	B	3277	1/1	0.78	0.18	106,106,106,106	0
56	MG	B	3346	1/1	0.79	0.11	85,85,85,85	0
56	MG	A	1666	1/1	0.79	0.29	105,105,105,105	0
56	MG	EB	3156	1/1	0.79	0.61	109,109,109,109	0
56	MG	EB	3078	1/1	0.79	0.24	110,110,110,110	0
56	MG	DB	1724	1/1	0.79	0.34	107,107,107,107	0
56	MG	B	3139	1/1	0.79	0.19	97,97,97,97	0
56	MG	KC	101	1/1	0.79	0.20	113,113,113,113	0
56	MG	EB	3256	1/1	0.79	0.08	106,106,106,106	0
56	MG	B	3076	1/1	0.79	0.17	88,88,88,88	0
56	MG	DB	1769	1/1	0.79	0.14	92,92,92,92	0
56	MG	B	3357	1/1	0.79	0.14	88,88,88,88	0
56	MG	IB	303	1/1	0.79	0.10	112,112,112,112	0
56	MG	EB	2983	1/1	0.79	0.32	88,88,88,88	0
56	MG	EB	3088	1/1	0.79	0.36	97,97,97,97	0
56	MG	B	3027	1/1	0.79	0.22	95,95,95,95	0
56	MG	EB	2985	1/1	0.79	0.23	91,91,91,91	0
56	MG	EB	3036	1/1	0.79	0.31	102,102,102,102	0
56	MG	EB	3037	1/1	0.79	0.22	95,95,95,95	0
56	MG	A	1625	1/1	0.79	0.13	137,137,137,137	0
56	MG	A	1624	1/1	0.79	0.30	111,111,111,111	0
56	MG	EB	3183	1/1	0.79	0.34	119,119,119,119	0
56	MG	RC	202	1/1	0.79	0.22	152,152,152,152	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	B	3032	1/1	0.79	0.24	87,87,87,87	0
56	MG	EB	3187	1/1	0.79	0.18	134,134,134,134	0
56	MG	B	3111	1/1	0.79	0.20	84,84,84,84	0
56	MG	B	2945	1/1	0.79	0.34	82,82,82,82	0
56	MG	DB	1605	1/1	0.79	0.25	106,106,106,106	0
56	MG	EB	3113	1/1	0.79	0.43	114,114,114,114	0
56	MG	EB	3052	1/1	0.79	0.38	106,106,106,106	0
56	MG	EB	2907	1/1	0.79	0.38	97,97,97,97	0
56	MG	A	1747	1/1	0.79	0.92	150,150,150,150	0
56	MG	B	3326	1/1	0.79	0.07	94,94,94,94	0
56	MG	B	3330	1/1	0.79	0.10	88,88,88,88	0
56	MG	B	3284	1/1	0.79	0.26	79,79,79,79	0
56	MG	B	3118	1/1	0.79	0.23	96,96,96,96	0
56	MG	RA	202	1/1	0.79	0.18	152,152,152,152	0
56	MG	B	2950	1/1	0.79	0.41	92,92,92,92	0
56	MG	B	3407	1/1	0.79	0.08	78,78,78,78	0
56	MG	EB	3010	1/1	0.79	0.20	84,84,84,84	0
56	MG	B	3408	1/1	0.79	0.19	119,119,119,119	0
56	MG	U	102	1/1	0.79	0.05	102,102,102,102	0
56	MG	B	3263	1/1	0.79	0.17	99,99,99,99	0
56	MG	IC	102	1/1	0.80	0.12	105,105,105,105	0
56	MG	A	1731	1/1	0.80	0.26	102,102,102,102	0
56	MG	DB	1715	1/1	0.80	0.43	107,107,107,107	0
56	MG	B	3239	1/1	0.80	0.13	78,78,78,78	0
56	MG	B	2930	1/1	0.80	0.33	78,78,78,78	0
56	MG	B	3001	1/1	0.80	0.29	88,88,88,88	0
56	MG	A	1642	1/1	0.80	0.19	106,106,106,106	0
56	MG	A	1689	1/1	0.80	0.30	105,105,105,105	0
56	MG	EB	2975	1/1	0.80	0.36	105,105,105,105	0
56	MG	DB	1689	1/1	0.80	0.22	111,111,111,111	0
56	MG	B	3318	1/1	0.80	0.15	95,95,95,95	0
56	MG	B	3280	1/1	0.80	0.22	94,94,94,94	0
56	MG	DB	1728	1/1	0.80	0.10	99,99,99,99	0
56	MG	B	3083	1/1	0.80	0.34	100,100,100,100	0
56	MG	B	3250	1/1	0.80	0.10	96,96,96,96	0
56	MG	B	2910	1/1	0.80	0.43	83,83,83,83	0
56	MG	EB	3083	1/1	0.80	0.28	106,106,106,106	0
56	MG	EB	3219	1/1	0.80	0.32	105,105,105,105	0
56	MG	SC	201	1/1	0.80	0.18	124,124,124,124	0
56	MG	EB	3221	1/1	0.80	0.39	103,103,103,103	0
56	MG	D	101	1/1	0.80	0.10	123,123,123,123	0
56	MG	L	201	1/1	0.80	0.21	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	B	3220	1/1	0.80	0.08	88,88,88,88	0
56	MG	DB	1739	1/1	0.80	0.25	113,113,113,113	0
56	MG	B	3155	1/1	0.80	0.19	101,101,101,101	0
56	MG	EB	3092	1/1	0.80	0.25	108,108,108,108	0
56	MG	EB	3236	1/1	0.80	0.15	103,103,103,103	0
56	MG	B	3187	1/1	0.80	0.18	84,84,84,84	0
56	MG	EB	3239	1/1	0.80	0.20	123,123,123,123	0
56	MG	EB	3098	1/1	0.80	0.38	102,102,102,102	0
56	MG	B	3061	1/1	0.80	0.33	109,109,109,109	0
56	MG	A	1650	1/1	0.80	0.39	108,108,108,108	0
56	MG	EB	3169	1/1	0.80	0.32	87,87,87,87	0
56	MG	R	202	1/1	0.80	0.21	101,101,101,101	0
56	MG	EB	3104	1/1	0.80	0.30	103,103,103,103	0
56	MG	A	1702	1/1	0.80	0.22	115,115,115,115	0
56	MG	T	201	1/1	0.80	0.16	94,94,94,94	0
56	MG	A	1665	1/1	0.80	0.18	115,115,115,115	0
56	MG	EB	2917	1/1	0.80	0.34	89,89,89,89	0
56	MG	WA	103	1/1	0.81	0.17	126,126,126,126	0
56	MG	B	3128	1/1	0.81	0.28	94,94,94,94	0
56	MG	EB	3254	1/1	0.81	0.16	123,123,123,123	0
56	MG	IC	101	1/1	0.81	0.22	108,108,108,108	0
56	MG	EB	3108	1/1	0.81	0.34	127,127,127,127	0
56	MG	B	3224	1/1	0.81	0.08	93,93,93,93	0
56	MG	HB	306	1/1	0.81	0.15	108,108,108,108	0
56	MG	B	3325	1/1	0.81	0.25	113,113,113,113	0
56	MG	HB	308	1/1	0.81	0.14	108,108,108,108	0
56	MG	B	3147	1/1	0.81	0.21	94,94,94,94	0
56	MG	B	3226	1/1	0.81	0.17	90,90,90,90	0
56	MG	EB	3116	1/1	0.81	0.31	93,93,93,93	0
56	MG	B	3171	1/1	0.81	0.42	81,81,81,81	0
56	MG	EB	3188	1/1	0.81	0.17	89,89,89,89	0
56	MG	EB	2931	1/1	0.81	0.23	80,80,80,80	0
56	MG	A	1672	1/1	0.81	0.22	137,137,137,137	0
56	MG	B	3197	1/1	0.81	0.07	116,116,116,116	0
56	MG	B	2962	1/1	0.81	0.26	83,83,83,83	0
56	MG	EB	3197	1/1	0.81	0.38	94,94,94,94	0
56	MG	EB	2981	1/1	0.81	0.21	97,97,97,97	0
56	MG	B	3015	1/1	0.81	0.29	71,71,71,71	0
56	MG	B	2993	1/1	0.81	0.24	86,86,86,86	0
56	MG	DB	1701	1/1	0.81	0.10	119,119,119,119	0
56	MG	DB	1608	1/1	0.81	0.41	94,94,94,94	0
56	MG	PB	202	1/1	0.81	0.44	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	A	1626	1/1	0.81	0.27	122,122,122,122	0
56	MG	EB	3213	1/1	0.81	0.31	103,103,103,103	0
56	MG	B	3269	1/1	0.81	0.41	110,110,110,110	0
56	MG	B	3272	1/1	0.81	0.30	104,104,104,104	0
56	MG	EB	2990	1/1	0.81	0.26	75,75,75,75	0
56	MG	EB	2908	1/1	0.81	0.27	88,88,88,88	0
56	MG	EB	3089	1/1	0.81	0.25	109,109,109,109	0
56	MG	EB	3090	1/1	0.81	0.23	86,86,86,86	0
56	MG	B	3214	1/1	0.81	0.13	79,79,79,79	0
56	MG	B	3363	1/1	0.81	0.54	229,229,229,229	0
56	MG	EB	3097	1/1	0.81	0.14	87,87,87,87	0
56	MG	DB	1710	1/1	0.81	0.21	136,136,136,136	0
56	MG	W	301	1/1	0.81	0.10	107,107,107,107	0
56	MG	A	1658	1/1	0.81	0.39	109,109,109,109	0
56	MG	A	1749	1/1	0.81	0.15	95,95,95,95	0
56	MG	B	3097	1/1	0.81	0.46	99,99,99,99	0
56	MG	EB	3173	1/1	0.81	0.19	103,103,103,103	0
56	MG	B	3373	1/1	0.81	0.08	109,109,109,109	0
57	ZN	BA	101	1/1	0.81	0.17	180,180,180,180	0
56	MG	A	1695	1/1	0.82	0.17	105,105,105,105	0
56	MG	B	2917	1/1	0.82	0.42	79,79,79,79	0
56	MG	B	3320	1/1	0.82	0.14	85,85,85,85	0
56	MG	IA	101	1/1	0.82	0.17	119,119,119,119	0
56	MG	EB	3081	1/1	0.82	0.25	81,81,81,81	0
56	MG	B	3177	1/1	0.82	0.12	92,92,92,92	0
56	MG	EB	3023	1/1	0.82	0.26	101,101,101,101	0
56	MG	A	1608	1/1	0.82	0.25	82,82,82,82	0
56	MG	A	1736	1/1	0.82	0.14	148,148,148,148	0
56	MG	B	3130	1/1	0.82	0.23	82,82,82,82	0
56	MG	EB	2934	1/1	0.82	0.64	86,86,86,86	0
56	MG	EB	3143	1/1	0.82	0.34	89,89,89,89	0
56	MG	EB	3146	1/1	0.82	0.18	99,99,99,99	0
56	MG	DB	1656	1/1	0.82	0.21	105,105,105,105	0
56	MG	T	202	1/1	0.82	0.26	98,98,98,98	0
56	MG	DB	1771	1/1	0.82	0.10	106,106,106,106	0
56	MG	EB	3226	1/1	0.82	0.38	102,102,102,102	0
56	MG	EB	3091	1/1	0.82	0.11	97,97,97,97	0
56	MG	B	3055	1/1	0.82	0.28	82,82,82,82	0
56	MG	B	2978	1/1	0.82	0.38	78,78,78,78	0
56	MG	B	2948	1/1	0.82	0.35	93,93,93,93	0
56	MG	DB	1734	1/1	0.82	0.13	121,121,121,121	0
56	MG	EB	2901	1/1	0.82	0.37	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	B	3062	1/1	0.82	0.26	86,86,86,86	0
56	MG	DB	1737	1/1	0.82	0.32	110,110,110,110	0
56	MG	B	2934	1/1	0.82	0.34	82,82,82,82	0
56	MG	B	3227	1/1	0.82	0.36	83,83,83,83	0
56	MG	B	3192	1/1	0.82	0.20	123,123,123,123	0
56	MG	A	1685	1/1	0.82	0.36	149,149,149,149	0
56	MG	B	3038	1/1	0.82	0.19	80,80,80,80	0
56	MG	B	2902	1/1	0.82	0.55	61,61,61,61	0
56	MG	B	3234	1/1	0.82	0.14	87,87,87,87	0
56	MG	B	3313	1/1	0.82	0.18	133,133,133,133	0
56	MG	EB	2965	1/1	0.82	0.30	84,84,84,84	0
56	MG	B	3271	1/1	0.82	0.10	100,100,100,100	0
56	MG	B	3199	1/1	0.82	0.40	98,98,98,98	0
56	MG	HC	101	1/1	0.82	0.14	102,102,102,102	0
56	MG	B	3378	1/1	0.82	0.27	101,101,101,101	0
56	MG	B	3172	1/1	0.82	0.39	97,97,97,97	0
57	ZN	EC	101	1/1	0.82	0.11	199,199,199,199	0
56	MG	EB	3148	1/1	0.83	0.15	134,134,134,134	0
56	MG	B	3395	1/1	0.83	0.20	99,99,99,99	0
56	MG	EB	3152	1/1	0.83	0.25	106,106,106,106	0
56	MG	B	3286	1/1	0.83	0.11	95,95,95,95	0
56	MG	B	2922	1/1	0.83	0.32	74,74,74,74	0
56	MG	DB	1757	1/1	0.83	0.34	106,106,106,106	0
56	MG	EB	3032	1/1	0.83	0.25	95,95,95,95	0
56	MG	B	3017	1/1	0.83	0.53	84,84,84,84	0
56	MG	DB	1630	1/1	0.83	0.21	105,105,105,105	0
56	MG	B	3167	1/1	0.83	0.29	100,100,100,100	0
56	MG	B	3298	1/1	0.83	0.16	96,96,96,96	0
56	MG	GB	104	1/1	0.83	0.14	152,152,152,152	0
56	MG	A	1641	1/1	0.83	0.36	107,107,107,107	0
56	MG	B	3019	1/1	0.83	0.19	83,83,83,83	0
56	MG	EB	3249	1/1	0.83	0.33	137,137,137,137	0
56	MG	B	3200	1/1	0.83	0.14	111,111,111,111	0
56	MG	DB	1679	1/1	0.83	0.20	134,134,134,134	0
56	MG	EB	3253	1/1	0.83	0.30	120,120,120,120	0
56	MG	B	3058	1/1	0.83	0.61	89,89,89,89	0
56	MG	IB	301	1/1	0.83	0.18	88,88,88,88	0
56	MG	I	203	1/1	0.83	0.08	111,111,111,111	0
56	MG	B	3140	1/1	0.83	0.18	84,84,84,84	0
56	MG	DB	1683	1/1	0.83	0.31	109,109,109,109	0
56	MG	B	3033	1/1	0.83	0.23	101,101,101,101	0
56	MG	B	3243	1/1	0.83	0.15	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DB	1730	1/1	0.83	0.08	108,108,108,108	0
56	MG	B	3020	1/1	0.83	0.45	91,91,91,91	0
56	MG	EB	3114	1/1	0.83	0.11	135,135,135,135	0
56	MG	EB	3273	1/1	0.83	0.13	88,88,88,88	0
56	MG	B	3094	1/1	0.83	0.18	87,87,87,87	0
56	MG	B	3021	1/1	0.83	0.47	93,93,93,93	0
56	MG	C	214	1/1	0.83	0.17	97,97,97,97	0
56	MG	EB	3280	1/1	0.83	0.12	105,105,105,105	0
56	MG	A	1653	1/1	0.83	0.26	114,114,114,114	0
56	MG	EB	2958	1/1	0.83	0.31	78,78,78,78	0
56	MG	EB	3008	1/1	0.83	0.18	92,92,92,92	0
56	MG	EB	2959	1/1	0.83	0.25	99,99,99,99	0
56	MG	QB	202	1/1	0.83	0.11	103,103,103,103	0
56	MG	B	3383	1/1	0.83	0.20	114,114,114,114	0
56	MG	BD	201	1/1	0.83	0.07	122,122,122,122	0
56	MG	M	201	1/1	0.83	0.19	77,77,77,77	0
56	MG	B	3069	1/1	0.83	0.14	79,79,79,79	0
56	MG	DB	1619	1/1	0.83	0.36	86,86,86,86	0
56	MG	EB	3291	1/1	0.83	0.23	90,90,90,90	0
56	MG	TB	202	1/1	0.83	0.07	111,111,111,111	0
56	MG	O	201	1/1	0.83	0.30	93,93,93,93	0
56	MG	EB	3209	1/1	0.83	0.32	97,97,97,97	0
56	MG	B	3005	1/1	0.83	0.14	72,72,72,72	0
56	MG	DB	1662	1/1	0.83	0.36	108,108,108,108	0
56	MG	B	3043	1/1	0.83	0.42	85,85,85,85	0
56	MG	B	2920	1/1	0.83	0.19	82,82,82,82	0
56	MG	A	1637	1/1	0.83	0.39	92,92,92,92	0
56	MG	B	3106	1/1	0.84	0.19	103,103,103,103	0
56	MG	B	3303	1/1	0.84	0.26	91,91,91,91	0
56	MG	DB	1748	1/1	0.84	0.17	121,121,121,121	0
56	MG	B	3364	1/1	0.84	0.21	95,95,95,95	0
56	MG	B	3156	1/1	0.84	0.17	92,92,92,92	0
56	MG	P	202	1/1	0.84	0.14	126,126,126,126	0
56	MG	EB	3125	1/1	0.84	0.20	96,96,96,96	0
56	MG	EB	2932	1/1	0.84	0.46	80,80,80,80	0
56	MG	B	3107	1/1	0.84	0.24	96,96,96,96	0
56	MG	EB	3222	1/1	0.84	0.27	92,92,92,92	0
56	MG	C	218	1/1	0.84	0.21	123,123,123,123	0
56	MG	C	219	1/1	0.84	0.23	131,131,131,131	0
56	MG	B	3229	1/1	0.84	0.17	112,112,112,112	0
56	MG	EB	2994	1/1	0.84	0.37	87,87,87,87	0
56	MG	B	3191	1/1	0.84	0.14	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	A	1715	1/1	0.84	0.14	137,137,137,137	0
56	MG	B	3008	1/1	0.84	0.38	96,96,96,96	0
56	MG	B	3113	1/1	0.84	0.26	96,96,96,96	0
56	MG	B	3166	1/1	0.84	0.14	105,105,105,105	0
56	MG	B	3386	1/1	0.84	0.13	108,108,108,108	0
56	MG	B	2949	1/1	0.84	0.40	82,82,82,82	0
56	MG	PA	201	1/1	0.84	0.10	129,129,129,129	0
56	MG	EB	3005	1/1	0.84	0.28	99,99,99,99	0
56	MG	EB	3006	1/1	0.84	0.56	103,103,103,103	0
56	MG	EB	3247	1/1	0.84	0.26	156,156,156,156	0
56	MG	EB	3158	1/1	0.84	0.14	105,105,105,105	0
56	MG	A	1751	1/1	0.84	0.07	116,116,116,116	0
56	MG	B	3242	1/1	0.84	0.38	89,89,89,89	0
56	MG	B	3049	1/1	0.84	0.15	73,73,73,73	0
56	MG	DB	1672	1/1	0.84	0.29	104,104,104,104	0
56	MG	B	3071	1/1	0.84	0.19	90,90,90,90	0
56	MG	B	3327	1/1	0.84	0.22	92,92,92,92	0
56	MG	B	2926	1/1	0.84	0.34	74,74,74,74	0
56	MG	A	1638	1/1	0.84	0.25	102,102,102,102	0
56	MG	EB	3172	1/1	0.84	0.49	120,120,120,120	0
56	MG	B	3334	1/1	0.84	0.32	87,87,87,87	0
56	MG	A	1655	1/1	0.84	0.36	96,96,96,96	0
56	MG	B	3338	1/1	0.84	0.23	119,119,119,119	0
56	MG	B	3148	1/1	0.84	0.40	103,103,103,103	0
56	MG	CA	102	1/1	0.84	0.23	81,81,81,81	0
56	MG	EB	3099	1/1	0.84	0.32	103,103,103,103	0
56	MG	B	3179	1/1	0.84	0.10	106,106,106,106	0
56	MG	DB	1735	1/1	0.84	0.18	101,101,101,101	0
56	MG	YA	202	1/1	0.84	0.15	128,128,128,128	0
56	MG	A	1720	1/1	0.84	0.20	110,110,110,110	0
56	MG	ED	201	1/1	0.84	0.31	122,122,122,122	0
56	MG	EB	3034	1/1	0.84	0.35	106,106,106,106	0
56	MG	B	2957	1/1	0.84	0.22	81,81,81,81	0
56	MG	A	1621	1/1	0.84	0.20	115,115,115,115	0
56	MG	EB	2921	1/1	0.84	0.29	77,77,77,77	0
56	MG	EB	2977	1/1	0.84	0.20	120,120,120,120	0
56	MG	EB	3042	1/1	0.84	0.27	113,113,113,113	0
56	MG	B	3297	1/1	0.84	0.15	100,100,100,100	0
56	MG	L	203	1/1	0.84	0.21	104,104,104,104	0
56	MG	B	3105	1/1	0.84	0.20	83,83,83,83	0
56	MG	B	3115	1/1	0.85	0.27	114,114,114,114	0
56	MG	EB	2940	1/1	0.85	0.31	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	B	3348	1/1	0.85	0.13	98,98,98,98	0
56	MG	G	301	1/1	0.85	0.32	89,89,89,89	0
56	MG	B	2938	1/1	0.85	0.17	86,86,86,86	0
56	MG	EB	3238	1/1	0.85	0.31	100,100,100,100	0
56	MG	FC	102	1/1	0.85	0.12	101,101,101,101	0
56	MG	DB	1776	1/1	0.85	0.12	94,94,94,94	0
56	MG	B	3217	1/1	0.85	0.23	93,93,93,93	0
56	MG	EB	3241	1/1	0.85	0.21	102,102,102,102	0
56	MG	B	3004	1/1	0.85	0.38	80,80,80,80	0
56	MG	B	3361	1/1	0.85	0.15	95,95,95,95	0
56	MG	A	1724	1/1	0.85	0.18	122,122,122,122	0
56	MG	EB	3051	1/1	0.85	0.26	95,95,95,95	0
56	MG	B	3311	1/1	0.85	0.17	87,87,87,87	0
56	MG	A	1639	1/1	0.85	0.27	95,95,95,95	0
56	MG	DB	1745	1/1	0.85	0.25	102,102,102,102	0
56	MG	B	3007	1/1	0.85	0.29	88,88,88,88	0
56	MG	B	3101	1/1	0.85	0.33	95,95,95,95	0
56	MG	B	2988	1/1	0.85	0.33	87,87,87,87	0
56	MG	EB	3065	1/1	0.85	0.12	92,92,92,92	0
56	MG	A	1760	1/1	0.85	0.34	101,101,101,101	0
56	MG	B	3045	1/1	0.85	0.28	84,84,84,84	0
56	MG	EB	3115	1/1	0.85	0.24	106,106,106,106	0
56	MG	Y	102	1/1	0.85	0.09	79,79,79,79	0
56	MG	EB	3117	1/1	0.85	0.24	92,92,92,92	0
56	MG	EB	2963	1/1	0.85	0.18	85,85,85,85	0
56	MG	EB	2918	1/1	0.85	0.35	92,92,92,92	0
56	MG	B	2927	1/1	0.85	0.36	87,87,87,87	0
56	MG	B	3230	1/1	0.85	0.10	93,93,93,93	0
56	MG	B	3068	1/1	0.85	0.22	82,82,82,82	0
56	MG	EB	3196	1/1	0.85	0.17	100,100,100,100	0
56	MG	EB	3075	1/1	0.85	0.17	95,95,95,95	0
56	MG	B	3091	1/1	0.85	0.25	86,86,86,86	0
56	MG	EB	3130	1/1	0.85	0.29	97,97,97,97	0
56	MG	B	3289	1/1	0.85	0.18	93,93,93,93	0
56	MG	A	1677	1/1	0.85	0.17	115,115,115,115	0
56	MG	DB	1763	1/1	0.85	0.05	120,120,120,120	0
56	MG	EB	3080	1/1	0.85	0.29	92,92,92,92	0
56	MG	B	3292	1/1	0.85	0.10	107,107,107,107	0
56	MG	B	3295	1/1	0.85	0.10	90,90,90,90	0
56	MG	EB	3295	1/1	0.85	0.10	109,109,109,109	0
56	MG	EB	3215	1/1	0.85	0.98	119,119,119,119	0
56	MG	FB	202	1/1	0.85	0.15	135,135,135,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	B	3296	1/1	0.85	0.16	101,101,101,101	0
56	MG	B	2977	1/1	0.85	0.27	83,83,83,83	0
56	MG	DB	1768	1/1	0.85	0.24	104,104,104,104	0
56	MG	B	3209	1/1	0.85	0.26	97,97,97,97	0
56	MG	B	3158	1/1	0.85	0.13	92,92,92,92	0
56	MG	DB	1696	1/1	0.85	0.27	105,105,105,105	0
56	MG	EB	3151	1/1	0.85	0.09	119,119,119,119	0
57	ZN	YB	201	1/1	0.85	0.25	147,147,147,147	0
56	MG	EB	2937	1/1	0.85	0.44	95,95,95,95	0
56	MG	Z	102	1/1	0.86	0.05	95,95,95,95	0
56	MG	B	3332	1/1	0.86	0.12	102,102,102,102	0
56	MG	C	209	1/1	0.86	0.14	96,96,96,96	0
56	MG	EB	3136	1/1	0.86	0.10	96,96,96,96	0
56	MG	A	1687	1/1	0.86	0.06	167,167,167,167	0
56	MG	G	304	1/1	0.86	0.13	80,80,80,80	0
56	MG	EB	3198	1/1	0.86	0.38	92,92,92,92	0
56	MG	B	2958	1/1	0.86	0.32	80,80,80,80	0
56	MG	EB	3093	1/1	0.86	0.13	115,115,115,115	0
56	MG	EB	2970	1/1	0.86	0.21	90,90,90,90	0
56	MG	EB	3144	1/1	0.86	0.15	106,106,106,106	0
56	MG	A	1733	1/1	0.86	0.17	91,91,91,91	0
56	MG	A	1744	1/1	0.86	0.14	118,118,118,118	0
56	MG	A	1620	1/1	0.86	0.33	98,98,98,98	0
56	MG	EB	3100	1/1	0.86	0.28	92,92,92,92	0
56	MG	A	1664	1/1	0.86	0.43	105,105,105,105	0
56	MG	V	503	1/1	0.86	0.07	99,99,99,99	0
56	MG	EB	3217	1/1	0.86	0.18	93,93,93,93	0
56	MG	EB	3062	1/1	0.86	0.12	89,89,89,89	0
56	MG	EB	3064	1/1	0.86	0.24	91,91,91,91	0
56	MG	A	1690	1/1	0.86	0.06	111,111,111,111	0
56	MG	B	3034	1/1	0.86	0.29	109,109,109,109	0
56	MG	EB	3015	1/1	0.86	0.14	94,94,94,94	0
56	MG	A	1606	1/1	0.86	0.48	99,99,99,99	0
56	MG	EB	3227	1/1	0.86	0.34	109,109,109,109	0
56	MG	EB	3229	1/1	0.86	0.11	111,111,111,111	0
56	MG	EB	3165	1/1	0.86	0.15	88,88,88,88	0
56	MG	DB	1754	1/1	0.86	0.25	129,129,129,129	0
56	MG	B	2994	1/1	0.86	0.28	75,75,75,75	0
56	MG	EB	3234	1/1	0.86	0.12	168,168,168,168	0
56	MG	EB	3020	1/1	0.86	0.20	90,90,90,90	0
56	MG	B	3153	1/1	0.86	0.07	165,165,165,165	0
56	MG	B	3108	1/1	0.86	0.13	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	A	1739	1/1	0.86	0.06	151,151,151,151	0
56	MG	A	1740	1/1	0.86	0.36	129,129,129,129	0
56	MG	EB	2916	1/1	0.86	0.42	78,78,78,78	0
56	MG	EB	2949	1/1	0.86	0.36	93,93,93,93	0
56	MG	EB	3242	1/1	0.86	0.32	103,103,103,103	0
56	MG	B	2943	1/1	0.86	0.20	77,77,77,77	0
56	MG	B	2972	1/1	0.86	0.25	72,72,72,72	0
56	MG	EB	2919	1/1	0.86	0.55	80,80,80,80	0
56	MG	B	3136	1/1	0.86	0.10	91,91,91,91	0
56	MG	W	312	1/1	0.86	0.07	126,126,126,126	0
56	MG	N	203	1/1	0.86	0.12	113,113,113,113	0
56	MG	B	3095	1/1	0.86	0.32	99,99,99,99	0
56	MG	B	3300	1/1	0.86	0.12	117,117,117,117	0
56	MG	B	3161	1/1	0.87	0.20	81,81,81,81	0
56	MG	EB	3243	1/1	0.87	0.12	106,106,106,106	0
56	MG	B	2995	1/1	0.87	0.43	84,84,84,84	0
56	MG	EB	3124	1/1	0.87	0.34	115,115,115,115	0
56	MG	B	2979	1/1	0.87	0.47	86,86,86,86	0
56	MG	R	201	1/1	0.87	0.27	100,100,100,100	0
56	MG	EB	2905	1/1	0.87	0.35	78,78,78,78	0
56	MG	B	3255	1/1	0.87	0.09	89,89,89,89	0
56	MG	B	3374	1/1	0.87	0.40	102,102,102,102	0
56	MG	B	3376	1/1	0.87	0.56	92,92,92,92	0
56	MG	DB	1676	1/1	0.87	0.18	120,120,120,120	0
56	MG	DB	1642	1/1	0.87	0.22	92,92,92,92	0
56	MG	EB	3039	1/1	0.87	0.36	102,102,102,102	0
56	MG	DB	1713	1/1	0.87	0.28	143,143,143,143	0
56	MG	EB	3140	1/1	0.87	0.20	124,124,124,124	0
56	MG	EB	3261	1/1	0.87	0.05	115,115,115,115	0
56	MG	B	2981	1/1	0.87	0.28	82,82,82,82	0
56	MG	B	2969	1/1	0.87	0.23	83,83,83,83	0
56	MG	EB	2956	1/1	0.87	0.39	92,92,92,92	0
56	MG	EB	3269	1/1	0.87	0.12	103,103,103,103	0
56	MG	MC	303	1/1	0.87	0.07	140,140,140,140	0
56	MG	B	2985	1/1	0.87	0.25	89,89,89,89	0
56	MG	EB	3272	1/1	0.87	0.35	128,128,128,128	0
56	MG	EB	3145	1/1	0.87	0.10	95,95,95,95	0
56	MG	B	3057	1/1	0.87	0.44	76,76,76,76	0
56	MG	DB	1719	1/1	0.87	0.09	113,113,113,113	0
56	MG	EB	3214	1/1	0.87	0.07	128,128,128,128	0
56	MG	DB	1647	1/1	0.87	0.15	123,123,123,123	0
56	MG	B	2925	1/1	0.87	0.28	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	B	3264	1/1	0.87	0.19	97,97,97,97	0
56	MG	OB	201	1/1	0.87	0.19	96,96,96,96	0
56	MG	EB	3218	1/1	0.87	0.23	92,92,92,92	0
56	MG	DB	1723	1/1	0.87	0.13	102,102,102,102	0
56	MG	B	3265	1/1	0.87	0.16	85,85,85,85	0
56	MG	B	3023	1/1	0.87	0.25	79,79,79,79	0
56	MG	EB	3061	1/1	0.87	0.28	86,86,86,86	0
56	MG	EB	2926	1/1	0.87	0.52	101,101,101,101	0
56	MG	B	2907	1/1	0.87	0.15	79,79,79,79	0
56	MG	EB	3293	1/1	0.87	0.15	85,85,85,85	0
56	MG	B	3354	1/1	0.87	0.13	103,103,103,103	0
56	MG	A	1609	1/1	0.87	0.20	74,74,74,74	0
56	MG	EB	3013	1/1	0.87	0.28	81,81,81,81	0
56	MG	B	2992	1/1	0.87	0.43	80,80,80,80	0
56	MG	EB	3069	1/1	0.87	0.21	86,86,86,86	0
56	MG	B	3406	1/1	0.87	0.29	86,86,86,86	0
56	MG	A	1756	1/1	0.87	0.07	170,170,170,170	0
56	MG	DB	1695	1/1	0.87	0.15	109,109,109,109	0
56	MG	B	3322	1/1	0.87	0.12	90,90,90,90	0
56	MG	B	3410	1/1	0.87	0.14	127,127,127,127	0
56	MG	B	3203	1/1	0.87	0.19	82,82,82,82	0
56	MG	YB	203	1/1	0.87	0.17	130,130,130,130	0
56	MG	B	2935	1/1	0.87	0.40	79,79,79,79	0
56	MG	DB	1632	1/1	0.87	0.72	110,110,110,110	0
56	MG	EB	3157	1/1	0.88	0.34	88,88,88,88	0
56	MG	B	3306	1/1	0.88	0.14	82,82,82,82	0
56	MG	EB	3048	1/1	0.88	0.15	88,88,88,88	0
56	MG	L	202	1/1	0.88	0.41	91,91,91,91	0
56	MG	EB	3162	1/1	0.88	0.10	87,87,87,87	0
56	MG	EB	2997	1/1	0.88	0.29	85,85,85,85	0
56	MG	EB	2952	1/1	0.88	0.21	94,94,94,94	0
56	MG	B	2987	1/1	0.88	0.46	82,82,82,82	0
56	MG	B	3341	1/1	0.88	0.08	94,94,94,94	0
56	MG	Z	101	1/1	0.88	0.23	97,97,97,97	0
56	MG	B	3121	1/1	0.88	0.18	95,95,95,95	0
56	MG	EB	3003	1/1	0.88	0.40	86,86,86,86	0
56	MG	B	2946	1/1	0.88	0.27	84,84,84,84	0
56	MG	B	3312	1/1	0.88	0.18	80,80,80,80	0
56	MG	B	3135	1/1	0.88	0.12	66,66,66,66	0
56	MG	EB	3063	1/1	0.88	0.23	109,109,109,109	0
56	MG	B	3398	1/1	0.88	0.19	89,89,89,89	0
56	MG	B	3052	1/1	0.88	0.25	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	B	2939	1/1	0.88	0.16	76,76,76,76	0
56	MG	B	2999	1/1	0.88	0.29	68,68,68,68	0
56	MG	HB	303	1/1	0.88	0.37	94,94,94,94	0
56	MG	DB	1675	1/1	0.88	0.20	110,110,110,110	0
56	MG	B	3042	1/1	0.88	0.44	87,87,87,87	0
56	MG	B	3358	1/1	0.88	0.26	83,83,83,83	0
56	MG	DB	1637	1/1	0.88	0.41	106,106,106,106	0
56	MG	R	203	1/1	0.88	0.47	84,84,84,84	0
56	MG	B	2991	1/1	0.88	0.30	84,84,84,84	0
56	MG	E	303	1/1	0.88	0.09	104,104,104,104	0
56	MG	B	3411	1/1	0.88	0.11	83,83,83,83	0
56	MG	B	3412	1/1	0.88	0.16	91,91,91,91	0
56	MG	B	3294	1/1	0.88	0.12	92,92,92,92	0
56	MG	B	3072	1/1	0.88	0.30	88,88,88,88	0
56	MG	V	505	1/1	0.88	0.15	113,113,113,113	0
56	MG	B	3323	1/1	0.88	0.14	83,83,83,83	0
56	MG	EB	3270	1/1	0.88	0.24	89,89,89,89	0
56	MG	EB	2938	1/1	0.88	0.34	90,90,90,90	0
56	MG	B	3366	1/1	0.88	0.19	108,108,108,108	0
56	MG	EB	3031	1/1	0.88	0.20	95,95,95,95	0
56	MG	B	3144	1/1	0.88	0.12	100,100,100,100	0
56	MG	EB	3206	1/1	0.88	0.17	93,93,93,93	0
56	MG	B	3182	1/1	0.88	0.28	98,98,98,98	0
56	MG	EB	3208	1/1	0.88	0.45	99,99,99,99	0
56	MG	B	3129	1/1	0.88	0.09	106,106,106,106	0
56	MG	B	3328	1/1	0.88	0.16	93,93,93,93	0
56	MG	DB	1653	1/1	0.88	0.17	95,95,95,95	0
56	MG	A	1648	1/1	0.88	0.13	139,139,139,139	0
56	MG	RB	202	1/1	0.88	0.11	98,98,98,98	0
56	MG	B	3256	1/1	0.88	0.47	94,94,94,94	0
56	MG	EB	3041	1/1	0.88	0.19	90,90,90,90	0
56	MG	B	3212	1/1	0.88	0.18	95,95,95,95	0
56	MG	B	3035	1/1	0.88	0.19	78,78,78,78	0
56	MG	B	3259	1/1	0.88	0.28	85,85,85,85	0
56	MG	EB	3292	1/1	0.88	0.10	91,91,91,91	0
56	MG	EB	3095	1/1	0.88	0.29	110,110,110,110	0
56	MG	EB	3096	1/1	0.88	0.26	96,96,96,96	0
56	MG	EB	3224	1/1	0.88	0.22	93,93,93,93	0
56	MG	EB	3154	1/1	0.88	0.07	114,114,114,114	0
56	MG	EB	3046	1/1	0.88	0.30	104,104,104,104	0
56	MG	A	1750	1/1	0.89	0.18	130,130,130,130	0
56	MG	B	3349	1/1	0.89	0.30	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	EB	3233	1/1	0.89	0.21	83,83,83,83	0
56	MG	EB	3184	1/1	0.89	0.10	120,120,120,120	0
56	MG	EB	3288	1/1	0.89	0.12	111,111,111,111	0
56	MG	B	3092	1/1	0.89	0.22	86,86,86,86	0
56	MG	B	3073	1/1	0.89	0.17	87,87,87,87	0
56	MG	B	3194	1/1	0.89	0.06	110,110,110,110	0
56	MG	B	3385	1/1	0.89	0.11	83,83,83,83	0
56	MG	B	3210	1/1	0.89	0.20	87,87,87,87	0
56	MG	EB	3033	1/1	0.89	0.39	103,103,103,103	0
56	MG	EB	3193	1/1	0.89	0.19	106,106,106,106	0
56	MG	B	3389	1/1	0.89	0.10	98,98,98,98	0
56	MG	PB	201	1/1	0.89	0.22	99,99,99,99	0
56	MG	L	204	1/1	0.89	0.12	104,104,104,104	0
56	MG	B	3237	1/1	0.89	0.27	73,73,73,73	0
56	MG	IA	106	1/1	0.89	0.06	112,112,112,112	0
56	MG	B	3011	1/1	0.89	0.09	91,91,91,91	0
56	MG	EB	3111	1/1	0.89	0.16	127,127,127,127	0
56	MG	M	204	1/1	0.89	0.32	88,88,88,88	0
56	MG	N	201	1/1	0.89	0.08	111,111,111,111	0
56	MG	DB	1651	1/1	0.89	0.23	107,107,107,107	0
56	MG	B	3299	1/1	0.89	0.13	103,103,103,103	0
56	MG	B	3336	1/1	0.89	0.15	86,86,86,86	0
56	MG	EB	3255	1/1	0.89	0.19	108,108,108,108	0
56	MG	EB	3161	1/1	0.89	0.10	78,78,78,78	0
56	MG	EB	3045	1/1	0.89	0.31	84,84,84,84	0
56	MG	EB	3210	1/1	0.89	0.36	103,103,103,103	0
56	MG	DB	1625	1/1	0.89	0.18	87,87,87,87	0
56	MG	B	3013	1/1	0.89	0.24	84,84,84,84	0
56	MG	DB	1688	1/1	0.89	0.12	113,113,113,113	0
56	MG	B	3365	1/1	0.89	0.17	82,82,82,82	0
56	MG	B	3339	1/1	0.89	0.24	98,98,98,98	0
56	MG	B	3240	1/1	0.89	0.16	100,100,100,100	0
56	MG	DB	1759	1/1	0.89	0.12	102,102,102,102	0
56	MG	Y	101	1/1	0.89	0.34	88,88,88,88	0
56	MG	B	2996	1/1	0.89	0.35	75,75,75,75	0
56	MG	EB	3017	1/1	0.89	0.18	93,93,93,93	0
56	MG	EB	3175	1/1	0.89	0.07	106,106,106,106	0
56	MG	B	2998	1/1	0.89	0.18	66,66,66,66	0
56	MG	B	3090	1/1	0.89	0.20	85,85,85,85	0
56	MG	B	3290	1/1	0.89	0.09	90,90,90,90	0
56	MG	R	204	1/1	0.89	0.34	86,86,86,86	0
56	MG	EB	2953	1/1	0.89	0.31	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	B	3009	1/1	0.90	0.13	81,81,81,81	0
56	MG	EB	3126	1/1	0.90	0.10	82,82,82,82	0
56	MG	Q	201	1/1	0.90	0.13	115,115,115,115	0
56	MG	B	3206	1/1	0.90	0.07	105,105,105,105	0
56	MG	A	1741	1/1	0.90	0.12	86,86,86,86	0
56	MG	EB	3167	1/1	0.90	0.23	103,103,103,103	0
56	MG	B	3396	1/1	0.90	0.15	101,101,101,101	0
56	MG	B	3254	1/1	0.90	0.24	102,102,102,102	0
56	MG	B	2990	1/1	0.90	0.29	72,72,72,72	0
56	MG	EB	2964	1/1	0.90	0.12	98,98,98,98	0
56	MG	B	3012	1/1	0.90	0.33	98,98,98,98	0
56	MG	B	3164	1/1	0.90	0.38	91,91,91,91	0
56	MG	E	304	1/1	0.90	0.08	92,92,92,92	0
56	MG	B	3319	1/1	0.90	0.10	80,80,80,80	0
56	MG	EB	3294	1/1	0.90	0.17	117,117,117,117	0
56	MG	B	2954	1/1	0.90	0.25	67,67,67,67	0
56	MG	B	3059	1/1	0.90	0.11	74,74,74,74	0
56	MG	M	202	1/1	0.90	0.17	87,87,87,87	0
56	MG	EB	3024	1/1	0.90	0.23	100,100,100,100	0
56	MG	B	3120	1/1	0.90	0.26	80,80,80,80	0
56	MG	B	3387	1/1	0.90	0.28	87,87,87,87	0
56	MG	EB	3058	1/1	0.90	0.32	102,102,102,102	0
56	MG	EB	3028	1/1	0.90	0.32	95,95,95,95	0
56	MG	B	3414	1/1	0.90	0.17	93,93,93,93	0
56	MG	B	3109	1/1	0.90	0.41	86,86,86,86	0
56	MG	EB	3118	1/1	0.90	0.09	102,102,102,102	0
56	MG	EB	3155	1/1	0.90	0.17	108,108,108,108	0
56	MG	B	3060	1/1	0.90	0.37	95,95,95,95	0
56	MG	DB	1687	1/1	0.90	0.14	96,96,96,96	0
56	MG	DB	1711	1/1	0.90	0.26	115,115,115,115	0
56	MG	EB	2955	1/1	0.90	0.27	85,85,85,85	0
56	MG	EB	3007	1/1	0.90	0.30	89,89,89,89	0
56	MG	EB	3277	1/1	0.90	0.17	91,91,91,91	0
56	MG	B	3079	1/1	0.90	0.17	86,86,86,86	0
56	MG	B	3388	1/1	0.91	0.15	93,93,93,93	0
56	MG	B	3067	1/1	0.91	0.16	71,71,71,71	0
56	MG	B	3310	1/1	0.91	0.17	93,93,93,93	0
56	MG	B	3201	1/1	0.91	0.11	87,87,87,87	0
56	MG	DB	1753	1/1	0.91	0.24	119,119,119,119	0
56	MG	RB	205	1/1	0.91	0.21	95,95,95,95	0
56	MG	EB	2906	1/1	0.91	0.50	79,79,79,79	0
56	MG	B	3202	1/1	0.91	0.26	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	B	3252	1/1	0.91	0.27	90,90,90,90	0
56	MG	DB	1727	1/1	0.91	0.23	108,108,108,108	0
56	MG	B	3235	1/1	0.91	0.34	82,82,82,82	0
56	MG	A	1757	1/1	0.91	0.07	99,99,99,99	0
56	MG	EB	3127	1/1	0.91	0.14	99,99,99,99	0
56	MG	B	2955	1/1	0.91	0.39	76,76,76,76	0
56	MG	EB	3129	1/1	0.91	0.20	80,80,80,80	0
56	MG	B	3399	1/1	0.91	0.36	89,89,89,89	0
56	MG	C	215	1/1	0.91	0.06	123,123,123,123	0
56	MG	B	3221	1/1	0.91	0.18	89,89,89,89	0
56	MG	B	3047	1/1	0.91	0.38	88,88,88,88	0
56	MG	B	2980	1/1	0.91	0.24	75,75,75,75	0
56	MG	EB	3171	1/1	0.91	0.25	93,93,93,93	0
56	MG	B	2970	1/1	0.91	0.49	72,72,72,72	0
56	MG	EB	2920	1/1	0.91	0.64	87,87,87,87	0
56	MG	EB	2980	1/1	0.91	0.35	82,82,82,82	0
56	MG	B	3087	1/1	0.91	0.17	83,83,83,83	0
56	MG	A	1719	1/1	0.91	0.19	126,126,126,126	0
56	MG	S	202	1/1	0.91	0.08	105,105,105,105	0
56	MG	B	3245	1/1	0.91	0.16	85,85,85,85	0
56	MG	EB	3220	1/1	0.91	0.09	107,107,107,107	0
56	MG	GD	403	1/1	0.91	0.07	95,95,95,95	0
56	MG	B	2941	1/1	0.91	0.31	79,79,79,79	0
56	MG	B	3353	1/1	0.91	0.07	93,93,93,93	0
56	MG	B	2901	1/1	0.91	0.40	60,60,60,60	0
56	MG	B	2919	1/1	0.91	0.18	74,74,74,74	0
56	MG	B	3329	1/1	0.91	0.13	105,105,105,105	0
57	ZN	V	501	1/1	0.91	0.15	130,130,130,130	0
56	MG	LC	104	1/1	0.91	0.14	101,101,101,101	0
56	MG	EB	3185	1/1	0.91	0.20	101,101,101,101	0
56	MG	L	206	1/1	0.91	0.09	97,97,97,97	0
56	MG	B	3368	1/1	0.92	0.17	90,90,90,90	0
56	MG	EB	3056	1/1	0.92	0.25	87,87,87,87	0
56	MG	EB	3211	1/1	0.92	0.21	100,100,100,100	0
56	MG	EB	3212	1/1	0.92	0.15	100,100,100,100	0
56	MG	B	3403	1/1	0.92	0.20	101,101,101,101	0
56	MG	B	3215	1/1	0.92	0.07	156,156,156,156	0
56	MG	V	504	1/1	0.92	0.18	101,101,101,101	0
56	MG	DB	1655	1/1	0.92	0.24	116,116,116,116	0
56	MG	B	3405	1/1	0.92	0.17	120,120,120,120	0
56	MG	B	3198	1/1	0.92	0.07	107,107,107,107	0
56	MG	DB	1658	1/1	0.92	0.19	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	B	3371	1/1	0.92	0.65	80,80,80,80	0
56	MG	FB	215	1/1	0.92	0.09	135,135,135,135	0
56	MG	EB	3265	1/1	0.92	0.10	98,98,98,98	0
56	MG	B	3102	1/1	0.92	0.42	84,84,84,84	0
56	MG	B	3409	1/1	0.92	0.08	89,89,89,89	0
56	MG	B	3041	1/1	0.92	0.38	81,81,81,81	0
56	MG	A	1754	1/1	0.92	0.17	112,112,112,112	0
56	MG	B	3278	1/1	0.92	0.15	83,83,83,83	0
56	MG	B	3413	1/1	0.92	0.09	98,98,98,98	0
56	MG	DB	1634	1/1	0.92	0.20	99,99,99,99	0
56	MG	B	3185	1/1	0.92	0.13	82,82,82,82	0
56	MG	B	3050	1/1	0.92	0.15	87,87,87,87	0
56	MG	B	3222	1/1	0.92	0.12	96,96,96,96	0
56	MG	EB	3150	1/1	0.92	0.23	88,88,88,88	0
56	MG	B	3223	1/1	0.92	0.19	82,82,82,82	0
56	MG	B	3355	1/1	0.92	0.12	81,81,81,81	0
56	MG	EB	3040	1/1	0.92	0.49	115,115,115,115	0
56	MG	B	3066	1/1	0.92	0.30	77,77,77,77	0
56	MG	B	3307	1/1	0.92	0.12	86,86,86,86	0
56	MG	A	1700	1/1	0.92	0.21	96,96,96,96	0
56	MG	B	3359	1/1	0.92	0.10	79,79,79,79	0
56	MG	DB	1744	1/1	0.92	0.11	126,126,126,126	0
56	MG	B	3141	1/1	0.92	0.34	89,89,89,89	0
56	MG	B	3044	1/1	0.92	0.16	69,69,69,69	0
56	MG	B	3143	1/1	0.92	0.27	83,83,83,83	0
56	MG	A	1674	1/1	0.92	0.06	98,98,98,98	0
56	MG	A	1708	1/1	0.92	0.14	89,89,89,89	0
56	MG	DB	1716	1/1	0.92	0.08	119,119,119,119	0
56	MG	B	3146	1/1	0.92	0.43	81,81,81,81	0
56	MG	B	3080	1/1	0.92	0.25	99,99,99,99	0
56	MG	B	3279	1/1	0.93	0.14	79,79,79,79	0
56	MG	B	2973	1/1	0.93	0.48	80,80,80,80	0
56	MG	B	3301	1/1	0.93	0.20	101,101,101,101	0
56	MG	B	3281	1/1	0.93	0.10	88,88,88,88	0
56	MG	WB	203	1/1	0.93	0.20	82,82,82,82	0
56	MG	B	3324	1/1	0.93	0.07	94,94,94,94	0
56	MG	B	2983	1/1	0.93	0.24	71,71,71,71	0
56	MG	DB	1659	1/1	0.93	0.13	106,106,106,106	0
56	MG	EB	3267	1/1	0.93	0.15	82,82,82,82	0
56	MG	B	2974	1/1	0.93	0.53	68,68,68,68	0
56	MG	B	3088	1/1	0.93	0.48	88,88,88,88	0
56	MG	B	3048	1/1	0.93	0.22	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	A	1737	1/1	0.93	0.07	97,97,97,97	0
56	MG	EB	3178	1/1	0.93	0.49	90,90,90,90	0
56	MG	B	2931	1/1	0.93	0.34	74,74,74,74	0
56	MG	EB	3276	1/1	0.93	0.20	121,121,121,121	0
56	MG	B	2965	1/1	0.93	0.39	86,86,86,86	0
56	MG	B	3270	1/1	0.93	0.07	81,81,81,81	0
56	MG	L	205	1/1	0.93	0.06	110,110,110,110	0
56	MG	B	3253	1/1	0.93	0.46	98,98,98,98	0
56	MG	B	3081	1/1	0.93	0.19	76,76,76,76	0
56	MG	B	2913	1/1	0.93	0.51	66,66,66,66	0
56	MG	B	3196	1/1	0.93	0.06	158,158,158,158	0
56	MG	RB	201	1/1	0.93	0.16	105,105,105,105	0
56	MG	M	203	1/1	0.93	0.20	84,84,84,84	0
56	MG	B	3241	1/1	0.93	0.35	92,92,92,92	0
56	MG	B	2937	1/1	0.93	0.41	81,81,81,81	0
56	MG	B	3183	1/1	0.93	0.15	85,85,85,85	0
56	MG	B	3168	1/1	0.93	0.21	79,79,79,79	0
56	MG	B	3400	1/1	0.93	0.42	83,83,83,83	0
56	MG	B	3345	1/1	0.93	0.10	82,82,82,82	0
56	MG	B	3402	1/1	0.93	0.20	109,109,109,109	0
56	MG	EB	3258	1/1	0.93	0.14	90,90,90,90	0
56	MG	B	3039	1/1	0.94	0.12	83,83,83,83	0
56	MG	DB	1747	1/1	0.94	0.12	106,106,106,106	0
56	MG	B	3397	1/1	0.94	0.15	85,85,85,85	0
56	MG	A	1686	1/1	0.94	0.09	116,116,116,116	0
56	MG	B	3377	1/1	0.94	0.13	93,93,93,93	0
56	MG	EB	3027	1/1	0.94	0.13	95,95,95,95	0
56	MG	B	3016	1/1	0.94	0.47	81,81,81,81	0
56	MG	B	3379	1/1	0.94	0.12	104,104,104,104	0
56	MG	EB	3248	1/1	0.94	0.12	100,100,100,100	0
56	MG	EB	3282	1/1	0.94	0.11	95,95,95,95	0
56	MG	DB	1706	1/1	0.94	0.12	111,111,111,111	0
56	MG	B	3070	1/1	0.94	0.10	72,72,72,72	0
56	MG	B	3382	1/1	0.94	0.05	92,92,92,92	0
56	MG	B	3173	1/1	0.94	0.08	74,74,74,74	0
56	MG	B	3174	1/1	0.94	0.20	96,96,96,96	0
56	MG	A	1619	1/1	0.94	0.26	100,100,100,100	0
56	MG	B	3189	1/1	0.94	0.12	96,96,96,96	0
56	MG	B	3204	1/1	0.94	0.14	76,76,76,76	0
56	MG	EB	3228	1/1	0.94	0.11	111,111,111,111	0
56	MG	B	2982	1/1	0.94	0.29	96,96,96,96	0
56	MG	B	2961	1/1	0.94	0.24	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	EB	3202	1/1	0.94	0.08	89,89,89,89	0
56	MG	EB	2912	1/1	0.94	0.30	76,76,76,76	0
56	MG	V	506	1/1	0.94	0.09	119,119,119,119	0
56	MG	B	3351	1/1	0.94	0.06	99,99,99,99	0
56	MG	B	3117	1/1	0.94	0.17	92,92,92,92	0
56	MG	B	3000	1/1	0.94	0.17	76,76,76,76	0
56	MG	C	222	1/1	0.94	0.07	119,119,119,119	0
56	MG	B	3028	1/1	0.94	0.12	72,72,72,72	0
56	MG	A	1673	1/1	0.94	0.12	153,153,153,153	0
56	MG	B	3162	1/1	0.95	0.28	88,88,88,88	0
56	MG	B	3030	1/1	0.95	0.20	76,76,76,76	0
56	MG	A	1716	1/1	0.95	0.14	95,95,95,95	0
56	MG	EB	3131	1/1	0.95	0.12	97,97,97,97	0
56	MG	C	221	1/1	0.95	0.11	121,121,121,121	0
56	MG	S	201	1/1	0.95	0.20	98,98,98,98	0
56	MG	EB	3204	1/1	0.95	0.13	92,92,92,92	0
56	MG	B	3344	1/1	0.95	0.13	93,93,93,93	0
56	MG	EB	3252	1/1	0.95	0.13	99,99,99,99	0
56	MG	B	2932	1/1	0.95	0.23	73,73,73,73	0
56	MG	EB	2987	1/1	0.95	0.22	82,82,82,82	0
56	MG	B	3372	1/1	0.95	0.11	76,76,76,76	0
56	MG	DB	1702	1/1	0.95	0.10	111,111,111,111	0
56	MG	B	3084	1/1	0.95	0.04	89,89,89,89	0
56	MG	U	101	1/1	0.95	0.13	85,85,85,85	0
56	MG	B	3360	1/1	0.95	0.06	78,78,78,78	0
56	MG	XB	101	1/1	0.95	0.12	119,119,119,119	0
56	MG	B	3375	1/1	0.95	0.11	79,79,79,79	0
56	MG	B	2975	1/1	0.95	0.26	72,72,72,72	0
56	MG	B	3393	1/1	0.95	0.09	99,99,99,99	0
56	MG	B	3064	1/1	0.95	0.23	89,89,89,89	0
56	MG	EB	3264	1/1	0.95	0.09	93,93,93,93	0
56	MG	B	3112	1/1	0.95	0.18	84,84,84,84	0
56	MG	B	3211	1/1	0.95	0.11	81,81,81,81	0
56	MG	B	2997	1/1	0.95	0.27	75,75,75,75	0
56	MG	B	3014	1/1	0.95	0.27	78,78,78,78	0
57	ZN	FC	101	1/1	0.95	0.06	142,142,142,142	0
56	MG	EB	3268	1/1	0.96	0.10	94,94,94,94	0
56	MG	B	3350	1/1	0.96	0.11	79,79,79,79	0
56	MG	B	3293	1/1	0.96	0.06	87,87,87,87	0
56	MG	EB	3137	1/1	0.96	0.39	91,91,91,91	0
56	MG	B	3104	1/1	0.96	0.10	76,76,76,76	0
56	MG	B	3342	1/1	0.96	0.19	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	B	3333	1/1	0.96	0.13	91,91,91,91	0
56	MG	A	1714	1/1	0.96	0.56	115,115,115,115	0
56	MG	HB	305	1/1	0.96	0.13	96,96,96,96	0
56	MG	B	3260	1/1	0.96	0.11	98,98,98,98	0
56	MG	EB	3192	1/1	0.96	0.12	88,88,88,88	0
56	MG	B	3321	1/1	0.96	0.19	88,88,88,88	0
56	MG	EB	3194	1/1	0.96	0.16	89,89,89,89	0
56	MG	B	3337	1/1	0.96	0.17	101,101,101,101	0
56	MG	B	2909	1/1	0.96	0.25	74,74,74,74	0
56	MG	B	3169	1/1	0.96	0.29	82,82,82,82	0
57	ZN	GC	101	1/1	0.96	0.09	156,156,156,156	0
56	MG	DB	1755	1/1	0.97	0.05	142,142,142,142	0
56	MG	EB	3274	1/1	0.97	0.20	100,100,100,100	0
56	MG	B	3381	1/1	0.97	0.11	80,80,80,80	0
57	ZN	CA	101	1/1	0.97	0.03	134,134,134,134	0
56	MG	DB	1777	1/1	0.97	0.10	110,110,110,110	0
56	MG	B	3157	1/1	0.97	0.21	77,77,77,77	0
56	MG	C	203	1/1	0.97	0.06	125,125,125,125	0
56	MG	G	303	1/1	0.97	0.08	75,75,75,75	0
56	MG	B	3149	1/1	0.98	0.08	92,92,92,92	0
56	MG	EB	3055	1/1	0.98	0.14	80,80,80,80	0
56	MG	EB	2967	1/1	0.98	0.33	86,86,86,86	0
57	ZN	DA	101	1/1	0.98	0.05	141,141,141,141	0
57	ZN	JC	101	1/1	0.98	0.05	159,159,159,159	0
57	ZN	GA	101	1/1	0.99	0.02	132,132,132,132	0
56	MG	EB	3147	1/1	0.99	0.03	165,165,165,165	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.