



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 6, 2020 – 06:06 am BST

PDB ID : 6OXI
Title : Dimeric E.coli YoeB bound to Thermus thermophilus 70S post-cleavage (UAA)
Authors : Pavelich, I.J.; Hoffer, E.D.; Maehigashi, T.; Dunham, C.M.
Deposited on : 2019-05-13
Resolution : 3.50 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : **FAILED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

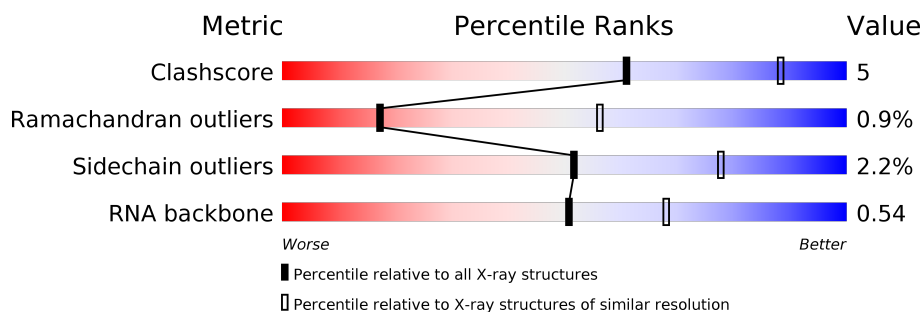
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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))
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RNA backbone	3102	1002 (4.00-3.00)


























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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	QA	1521	61% 31% 7% ..
1	XA	1521	63% 28% 8% .
2	QB	256	70% 19% . . 8%
2	XB	256	76% 15% . 8%
3	QC	239	75% 10% 14%
3	XC	239	72% 13% . 14%
4	QD	209	76% 22% .













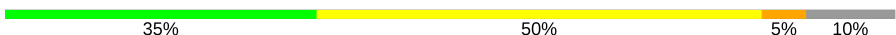












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Mol	Chain	Length	Quality of chain
4	XD	209	 81% 18%
5	QE	162	 80% 13% 7%
5	XE	162	 78% 15% 7%
6	QF	101	 81% 18% .
6	XF	101	 85% 14% .
7	QG	156	 88% 11% .
7	XG	156	 83% 15% ...
8	QH	138	 75% 23% ..
8	XH	138	 86% 13% ..
9	QI	128	 79% 19% ..
9	XI	128	 78% 20% .
10	QJ	105	 76% 15% .. 6%
10	XJ	105	 66% 24% . 9%
11	QK	129	 78% 13% . 8%
11	XK	129	 79% 10% . 10%
12	QL	132	 81% 12% . 5%
12	XL	132	 76% 15% . 8%
13	QM	126	 69% 22% . . 5%
13	XM	126	 75% 17% . 6%
14	QN	61	 82% 16% .
14	XN	61	 75% 23% .
15	QO	89	 92% 7% .
15	XO	89	 91% 7% .
16	QP	88	 78% 17% 5%
16	XP	88	 85% 8% . 5%















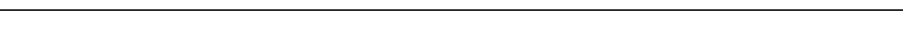




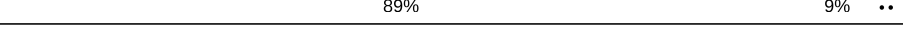





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Mol	Chain	Length	Quality of chain
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QX	20	
23	XX	20	
24	QY	84	
24	QZ	84	
24	XY	84	
24	XZ	84	
25	R0	85	
25	Y0	85	
26	R1	98	
26	Y1	98	
27	R2	72	
27	Y2	72	
28	R3	60	

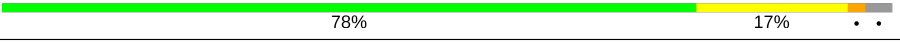















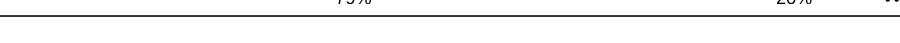
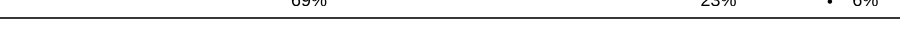
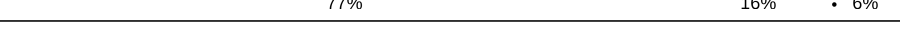

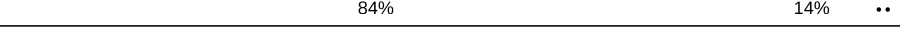
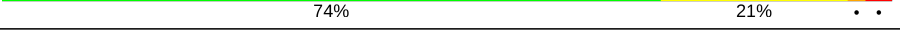



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Mol	Chain	Length	Quality of chain
28	Y3	60	 83% 15% .
29	R4	71	 59% 30% 6% . .
29	Y4	71	 76% 18% . .
30	R5	60	 72% 27% .
30	Y5	60	 85% 13% .
31	R6	54	 72% 22% . .
31	Y6	54	 85% 13% .
32	R7	49	 88% 8% .
32	Y7	49	 84% 14% .
33	R8	65	 74% 17% 6% . .
33	Y8	65	 71% 23% 5% .
34	R9	37	 70% 30%
34	Y9	37	 81% 19%
35	RA	2915	 61% 31% 6% . .
35	YA	2915	 64% 29% 6% . .
36	RB	124	 57% 33% . . .
36	YB	124	 63% 24% 9% . .
37	RD	276	 76% 20% . .
37	YD	276	 89% 9% . .
38	RE	206	 73% 25% . .
38	YE	206	 81% 18% .
39	RF	210	 87% 9% .
39	YF	210	 78% 17% . .
40	RG	182	 80% 18% . . .
40	YG	182	 80% 18% . . .

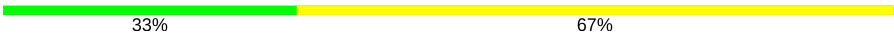
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Mol	Chain	Length	Quality of chain
41	RH	180	
41	YH	180	
42	RI	148	
42	YI	148	
43	RN	140	
43	YN	140	
44	RO	122	
44	YO	122	
45	RP	150	
45	YP	150	
46	RQ	141	
46	YQ	141	
47	RR	118	
47	YR	118	
48	RS	112	
48	YS	112	
49	RT	146	
49	YT	146	
50	RU	118	
50	YU	118	
51	RV	101	
51	YV	101	
52	RW	113	
52	YW	113	
53	RX	96	

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Mol	Chain	Length	Quality of chain
53	YX	96	
54	RY	110	
54	YY	110	
55	RZ	206	
55	YZ	206	
56	ZA	3	
56	ZB	3	

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 295153 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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QA	1510	Total	C	N	O	P	0	0	0
			32452	14444	6009	10489	1510			
1	XA	1507	Total	C	N	O	P	0	0	0
			32389	14416	5999	10467	1507			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	QB	235	Total	C	N	O	S	0	0	0
			1907	1217	342	343	5			
2	XB	236	Total	C	N	O	S	0	0	0
			1915	1223	343	344	5			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	QC	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
3	XC	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	QD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
4	XD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	QE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
5	XE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	QF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	XF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	QG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	XG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	QH	137	Total	C	N	O	S	0	0	0
			1108	700	214	192	2			
8	XH	137	Total	C	N	O	S	0	0	0
			1108	700	214	192	2			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	QI	127	Total	C	N	O		0	0	0
			1010	639	197	174				
9	XI	126	Total	C	N	O		0	0	0
			998	633	193	172				

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	QJ	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	XJ	96	Total	C	N	O	S	0	0	0
			777	487	153	136	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	QK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	XK	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	QL	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			
12	XL	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	QM	120	Total	C	N	O	S	0	0	0
			955	591	197	165	2			
13	XM	119	Total	C	N	O	S	0	0	0
			946	585	195	164	2			

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	QO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	XO	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	QP	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
16	XP	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	QQ	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
17	XQ	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	QR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	XR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QS	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
19	XS	83	Total	C	N	O	S	0	0	0
			656	418	123	113	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	QT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	XT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	QU	25	Total	C	N	O	0	0	0
			217	134	52	31			
21	XU	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 22 is a RNA chain called P-site tRNA-fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	XV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	18	Total	C	N	O	P	0	0	0
			394	176	79	121	18			
23	XX	18	Total	C	N	O	P	0	0	0
			394	176	79	121	18			

- Molecule 24 is a protein called Addiction module toxin, Txe/YoeB family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			
24	QZ	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			
24	XY	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			
24	XZ	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			

- Molecule 25 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	R0	81	Total	C	N	O	S	0	0	0
			643	398	137	107	1			
25	Y0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			

- Molecule 26 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	R1	94	Total	C	N	O	S	0	0	0
			737	463	146	127	1			
26	Y1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

- Molecule 27 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	R2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			
27	Y2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

- Molecule 28 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
28	R3	59	Total	C	N	O	0	0	0
			469	298	90	81			
28	Y3	59	Total	C	N	O	0	0	0
			469	298	90	81			

- Molecule 29 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	R4	69	Total	C	N	O	S	0	0	0
			565	356	103	101	5			
29	Y4	69	Total	C	N	O	S	0	0	0
			565	356	103	101	5			

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	R5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
30	Y5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 31 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	R6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	Y6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			

- Molecule 32 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	R7	47	Total	C	N	O	S	0	0	0
			409	251	102	54	2			
32	Y7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 33 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	R8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
33	Y8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 34 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	R9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
34	Y9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 35 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	RA	2891	Total	C	N	O	P	0	0	0
			62266	27713	11649	20014	2890			
35	YA	2878	Total	C	N	O	P	0	0	0
			61981	27587	11589	19928	2877			

- Molecule 36 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	RB	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			
36	YB	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			

- Molecule 37 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	RD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
37	YD	274	Total	C	N	O	S	0	0	0
			2135	1347	426	359	3			

- Molecule 38 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	RE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
38	YE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 39 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	RF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
39	YF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

- Molecule 40 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	RG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
40	YG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 41 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	RH	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
41	YH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 42 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	RI	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			
42	YI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 43 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	RN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
43	YN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 44 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	RO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
44	YO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 45 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	RP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
45	YP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 46 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	RQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
46	YQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 47 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
47	RR	117	Total	C	N	O	0	0	0
			960	599	202	159			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
47	YR	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 48 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	RS	111	Total	C	N	O	0	0	0
			882	556	176	150			
48	YS	111	Total	C	N	O	0	0	0
			882	556	176	150			

- Molecule 49 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	RT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
49	YT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	RU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
50	YU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 51 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	RV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
51	YV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 52 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	RW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			
52	YW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

- Molecule 53 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	RX	92	Total	C	N	O	0	0	0
			725	471	131	123			
53	YX	92	Total	C	N	O	0	0	0
			725	471	131	123			

- Molecule 54 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	RY	107	Total	C	N	O	S	0	0	0
			818	525	155	132	6			
54	YY	107	Total	C	N	O	S	0	0	0
			818	525	155	132	6			

- Molecule 55 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	RZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			
55	YZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			

- Molecule 56 is a RNA chain called CCPuro.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	ZA	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			
56	ZB	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	93	Total	Mg	0	0
			93	93		
57	YV	1	Total	Mg	0	0
			1	1		
57	RP	1	Total	Mg	0	0
			1	1		
57	YA	335	Total	Mg	0	0
			335	335		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	Y5	1	Total 1	Mg 1	0	0
57	YR	1	Total 1	Mg 1	0	0
57	Y9	1	Total 1	Mg 1	0	0
57	QD	1	Total 1	Mg 1	0	0
57	RN	1	Total 1	Mg 1	0	0
57	XE	1	Total 1	Mg 1	0	0
57	Y1	1	Total 1	Mg 1	0	0
57	YD	4	Total 4	Mg 4	0	0
57	QV	3	Total 3	Mg 3	0	0
57	YO	1	Total 1	Mg 1	0	0
57	XA	99	Total 99	Mg 99	0	0
57	RQ	4	Total 4	Mg 4	0	0
57	R0	2	Total 2	Mg 2	0	0
57	RO	1	Total 1	Mg 1	0	0
57	Y0	2	Total 2	Mg 2	0	0
57	YG	1	Total 1	Mg 1	0	0
57	YQ	5	Total 5	Mg 5	0	0
57	RY	1	Total 1	Mg 1	0	0
57	XF	1	Total 1	Mg 1	0	0
57	RR	1	Total 1	Mg 1	0	0
57	RD	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	RA	302	Total 302	Mg 302	0	0
57	Y3	1	Total 1	Mg 1	0	0
57	YF	1	Total 1	Mg 1	0	0
57	YP	1	Total 1	Mg 1	0	0
57	RE	1	Total 1	Mg 1	0	0
57	XL	1	Total 1	Mg 1	0	0
57	YB	3	Total 3	Mg 3	0	0
57	QY	1	Total 1	Mg 1	0	0
57	XV	4	Total 4	Mg 4	0	0
57	RB	3	Total 3	Mg 3	0	0
57	R3	1	Total 1	Mg 1	0	0
57	QE	1	Total 1	Mg 1	0	0
57	XM	1	Total 1	Mg 1	0	0
57	YE	5	Total 5	Mg 5	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	QD	1	Total	Fe	S	0	0
			8	4	4		
58	XD	1	Total	Fe	S	0	0
			8	4	4		

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

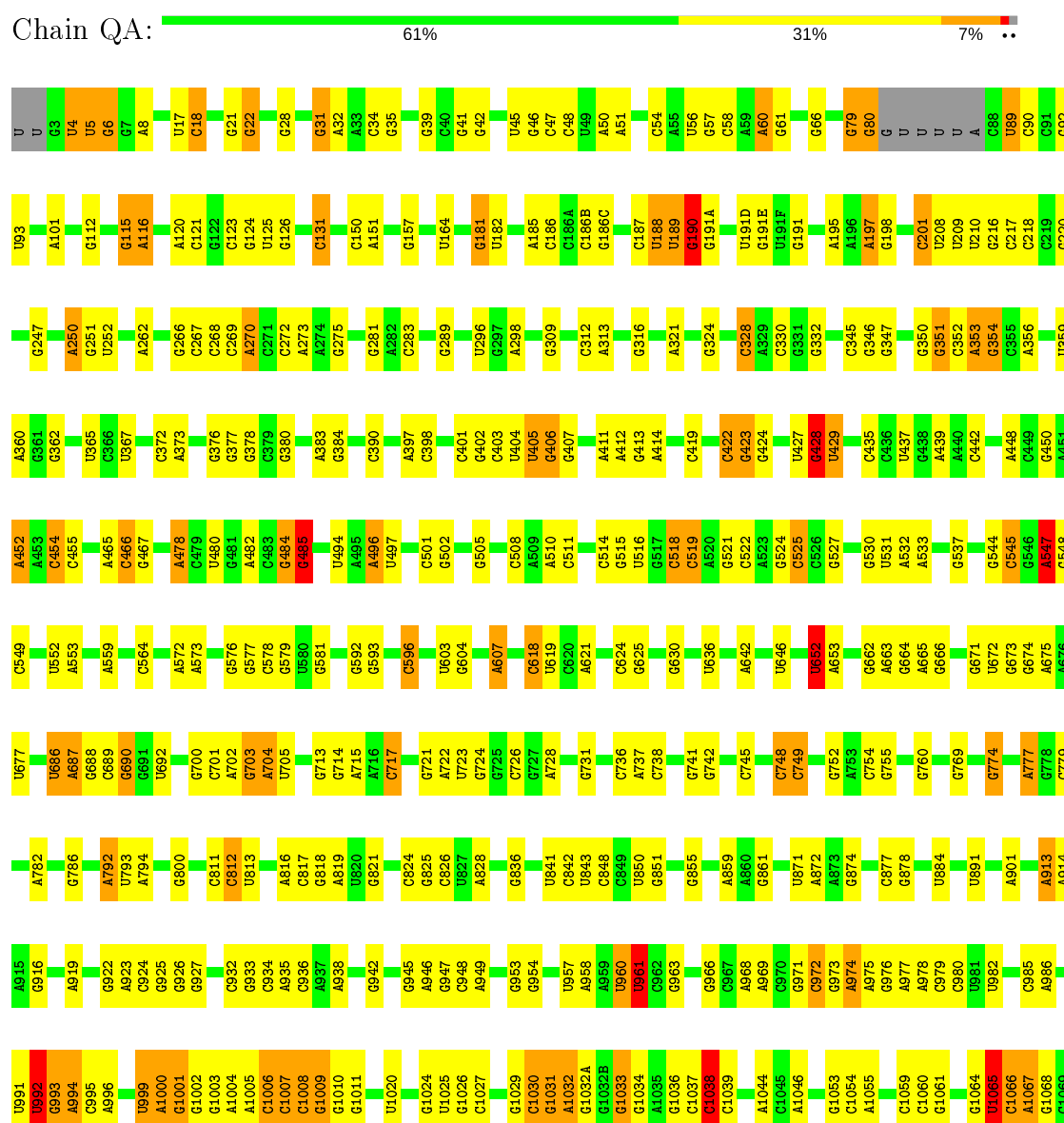
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	Y6	1	Total	Zn	0	0
			1	1		
59	QN	1	Total	Zn	0	0
			1	1		
59	XN	1	Total	Zn	0	0
			1	1		
59	Y4	1	Total	Zn	0	0
			1	1		
59	R6	1	Total	Zn	0	0
			1	1		
59	R5	1	Total	Zn	0	0
			1	1		
59	R4	1	Total	Zn	0	0
			1	1		
59	R9	1	Total	Zn	0	0
			1	1		

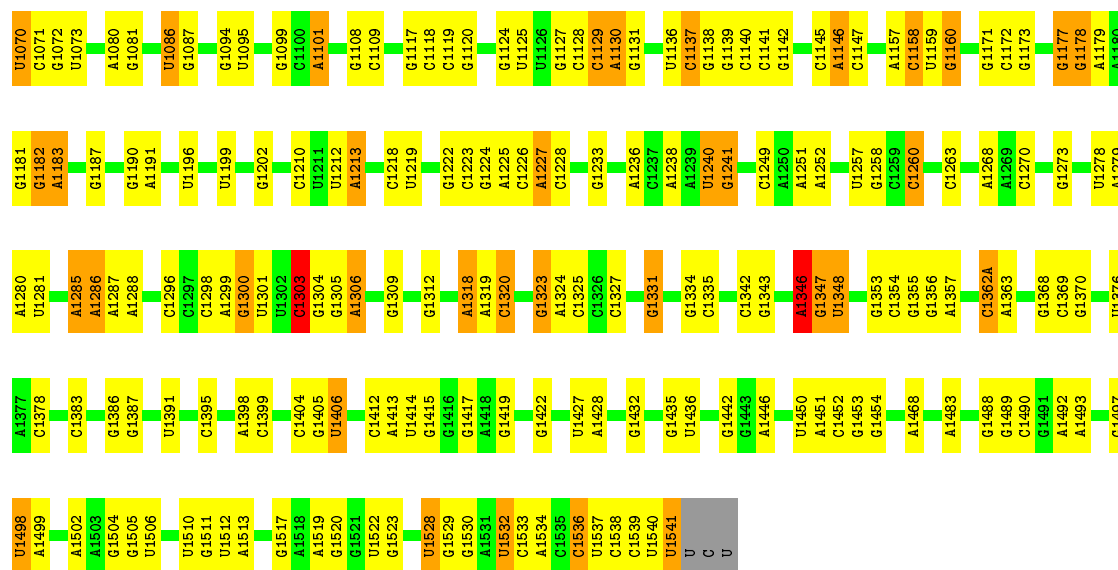
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

Note EDS failed to run properly.

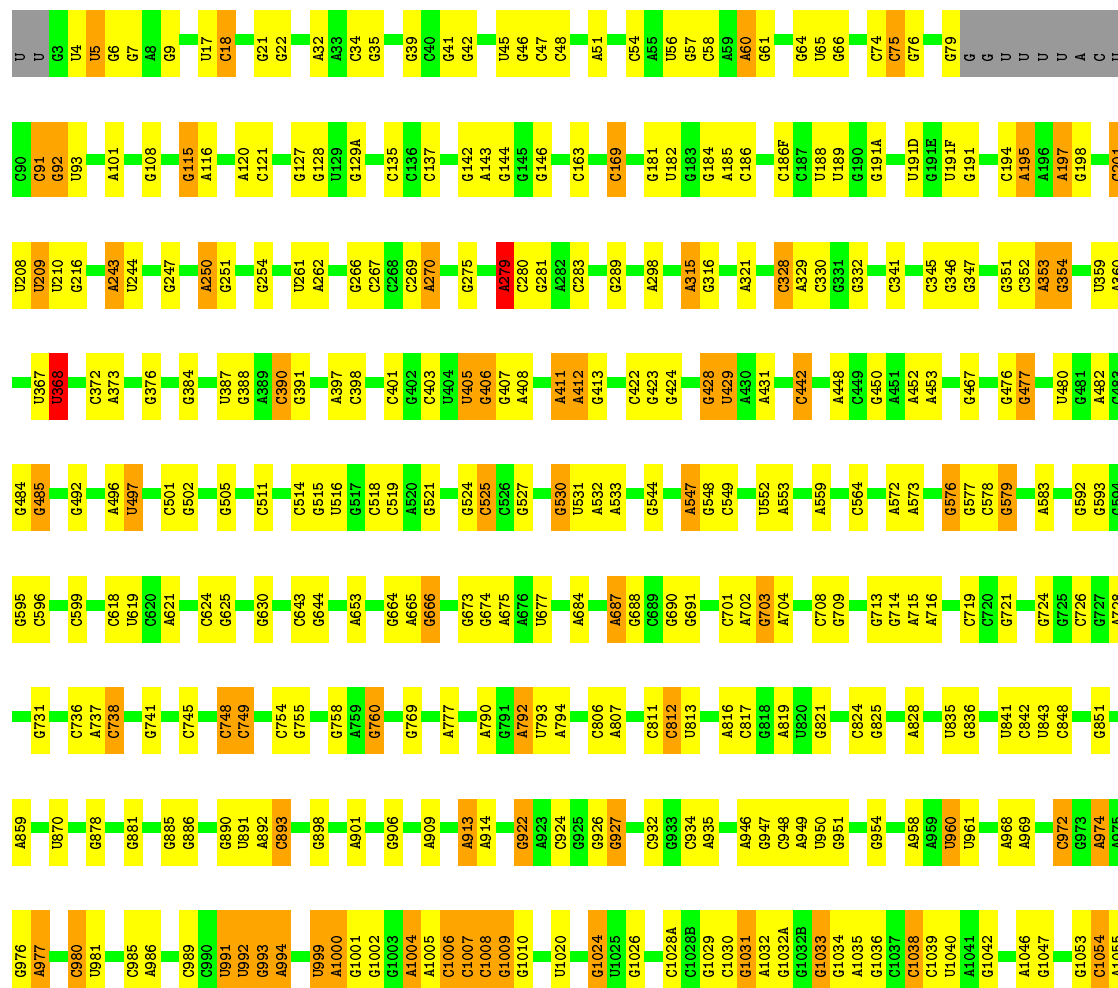
• Molecule 1: 16S rRNA

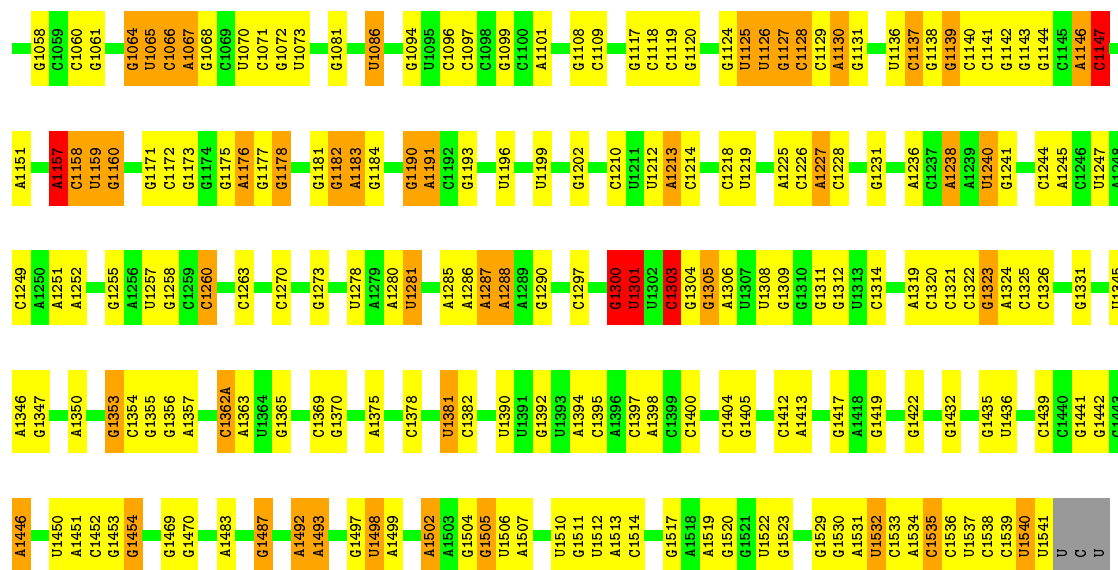




• Molecule 1: 16S rRNA

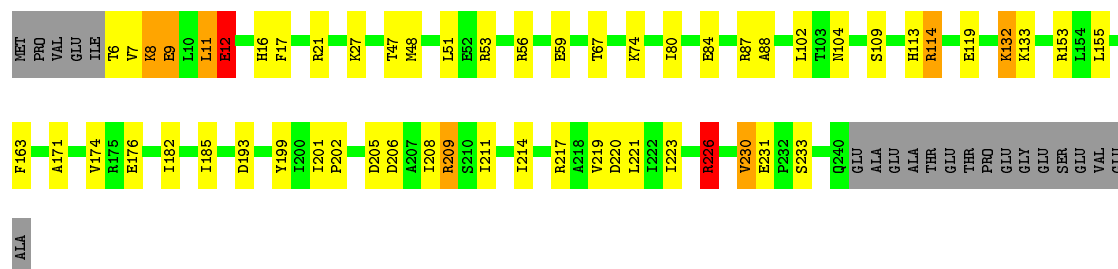
Chain XA: 63% 28% 8%





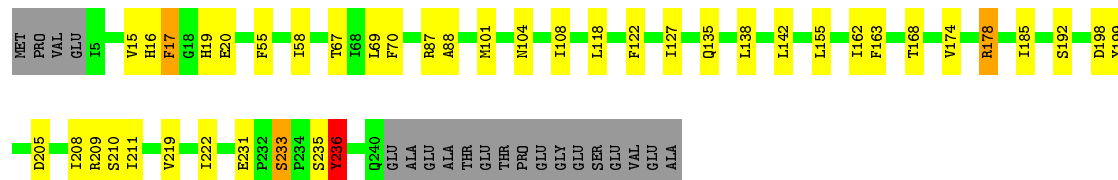
• Molecule 2: 30S ribosomal protein S2

Chain QB: 70% 19% 8%



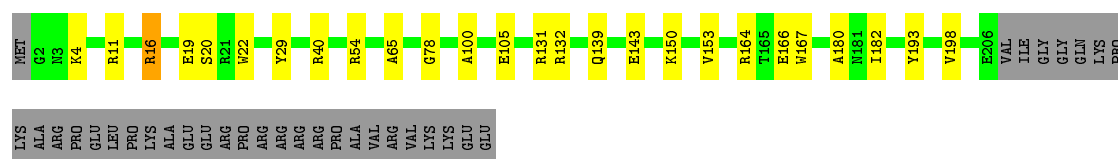
• Molecule 2: 30S ribosomal protein S2

Chain XB: 76% 15% 8%



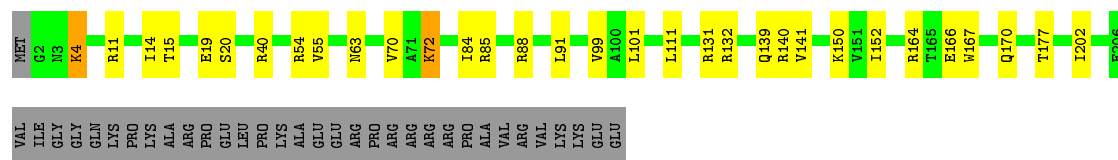
• Molecule 3: 30S ribosomal protein S3

Chain QC: 75% 10% 14%




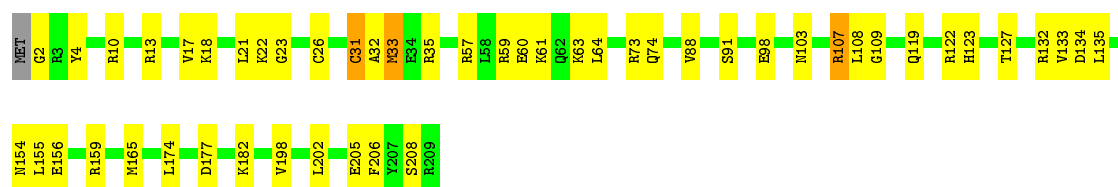
- Molecule 3: 30S ribosomal protein S3

Chain XC: 




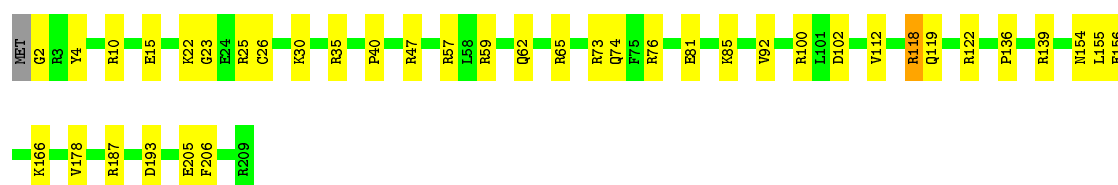
- Molecule 4: 30S ribosomal protein S4

Chain QD: 




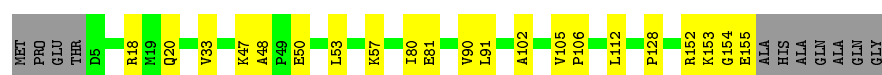
- Molecule 4: 30S ribosomal protein S4

Chain XD: 




- Molecule 5: 30S ribosomal protein S5

Chain QE: 




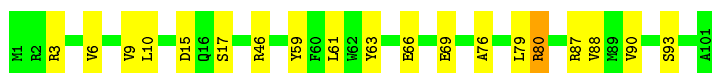
- Molecule 5: 30S ribosomal protein S5

Chain XE: 



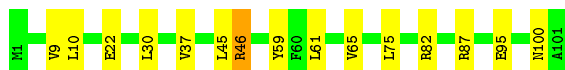
- Molecule 6: 30S ribosomal protein S6

Chain QF: 



- Molecule 6: 30S ribosomal protein S6

Chain XF: 85% 14%



- Molecule 7: 30S ribosomal protein S7

Chain QG: 88% 11%



- Molecule 7: 30S ribosomal protein S7

Chain XG: 83% 15%



- Molecule 8: 30S ribosomal protein S8

Chain QH: 75% 23%



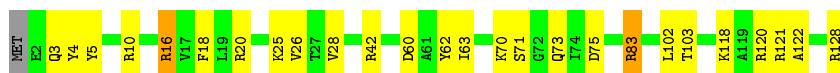
- Molecule 8: 30S ribosomal protein S8

Chain XH: 86% 13%



- Molecule 9: 30S ribosomal protein S9

Chain QI: 79% 19%



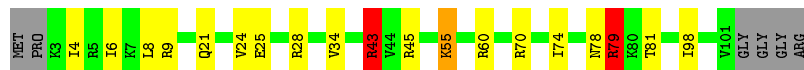
- Molecule 9: 30S ribosomal protein S9

Chain XI: 78% 20%



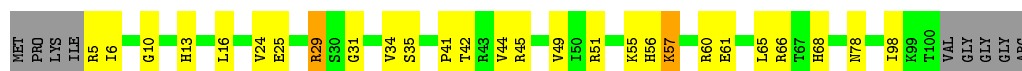
- Molecule 10: 30S ribosomal protein S10

Chain QJ: 76% 15% • • 6%



- Molecule 10: 30S ribosomal protein S10

Chain XJ: 66% 24% • 9%



- Molecule 11: 30S ribosomal protein S11

Chain QK: 78% 13% • 8%



- Molecule 11: 30S ribosomal protein S11

Chain XK: 79% 10% • 10%



- Molecule 12: 30S ribosomal protein S12

Chain QL: 81% 12% • 5%



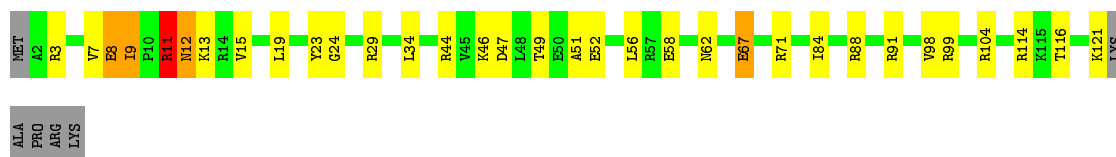
- Molecule 12: 30S ribosomal protein S12

Chain XL: 76% 15% • 8%



- Molecule 13: 30S ribosomal protein S13

Chain QM: 69% 22% • • 5%



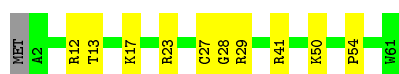
- Molecule 13: 30S ribosomal protein S13

Chain XM: 75% 17% 6%



- Molecule 14: 30S ribosomal protein S14 type Z

Chain QN: 82% 16%



- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN: 75% 23%



- Molecule 15: 30S ribosomal protein S15

Chain QO: 92% 7%



- Molecule 15: 30S ribosomal protein S15

Chain XO: 91% 7%




- Molecule 16: 30S ribosomal protein S16

Chain QP: 78% 17% 5%



- Molecule 16: 30S ribosomal protein S16

Chain XP:  85% 8% 5%




- Molecule 17: 30S ribosomal protein S17

Chain QQ:  84% 10% 5%



- Molecule 17: 30S ribosomal protein S17

Chain XQ:  78% 16% 5%



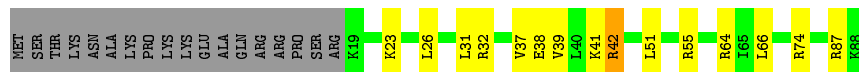
- Molecule 18: 30S ribosomal protein S18

Chain QR:  59% 19% 20%



- Molecule 18: 30S ribosomal protein S18

Chain XR:  63% 16% 20%



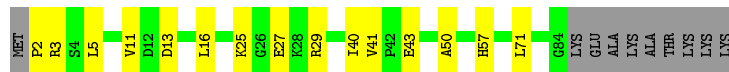
- Molecule 19: 30S ribosomal protein S19

Chain QS:  68% 18% 11%




- Molecule 19: 30S ribosomal protein S19

Chain XS:  73% 16% 11%



- Molecule 20: 30S ribosomal protein S20

Chain QT:  82% 11% 7%



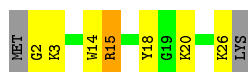
- Molecule 20: 30S ribosomal protein S20

Chain XT:  70% 23% 7%



- Molecule 21: 30S ribosomal protein Thx

Chain QU:  67% 22% 7%




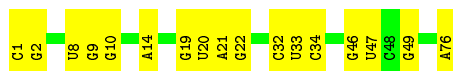
- Molecule 21: 30S ribosomal protein Thx

Chain XU:  70% 22% 7%




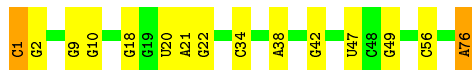
- Molecule 22: P-site tRNA-fMet

Chain QV:  78% 22%




- Molecule 22: P-site tRNA-fMet

Chain XV:  81% 17%



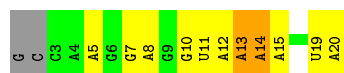
- Molecule 23: mRNA

Chain QX:  35% 50% 5% 10%




- Molecule 23: mRNA

Chain XX:  35% 45% 10% 10%



- Molecule 24: Addiction module toxin, Txe/YoeB family

Chain QY:  77% 23%




- Molecule 24: Addiction module toxin, Txe/YoeB family

Chain QZ:  74% 23% .




- Molecule 24: Addiction module toxin, Txe/YoeB family

Chain XY:  79% 21%



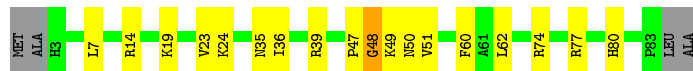
- Molecule 24: Addiction module toxin, Txe/YoeB family

Chain XZ:  81% 18% .



- Molecule 25: 50S ribosomal protein L27

Chain R0:  74% 20% . 5%




- Molecule 25: 50S ribosomal protein L27

Chain Y0:  75% 20% . .




- Molecule 26: 50S ribosomal protein L28

Chain R1:  85% 9% . .



- Molecule 26: 50S ribosomal protein L28

Chain Y1:  77% 22% .




- Molecule 27: 50S ribosomal protein L29

Chain R2:  68% 26% . .




- Molecule 27: 50S ribosomal protein L29

Chain Y2:  85% 11% .




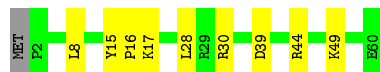
- Molecule 28: 50S ribosomal protein L30

Chain R3:  82% 17% .



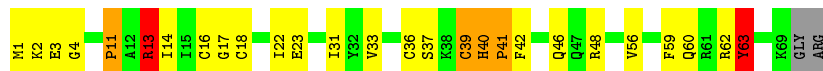
- Molecule 28: 50S ribosomal protein L30

Chain Y3:  83% 15% .




- Molecule 29: 50S ribosomal protein L31

Chain R4:  59% 30% 6% . .



- Molecule 29: 50S ribosomal protein L31

Chain Y4:  76% 18% . .




- Molecule 30: 50S ribosomal protein L32

Chain R5:  72% 27% .



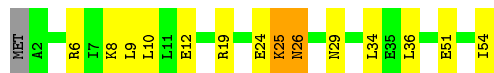
- Molecule 30: 50S ribosomal protein L32

Chain Y5:  85% 13% .




- Molecule 31: 50S ribosomal protein L33

Chain R6:  72% 22% . .




- Molecule 31: 50S ribosomal protein L33

Chain Y6:  85% 13% .




- Molecule 32: 50S ribosomal protein L34

Chain R7:  88% 8% .



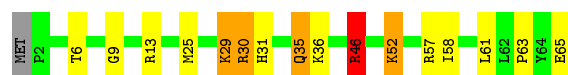
- Molecule 32: 50S ribosomal protein L34

Chain Y7:  84% 14% .



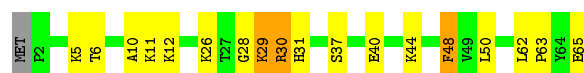
- Molecule 33: 50S ribosomal protein L35

Chain R8: 



- Molecule 33: 50S ribosomal protein L35

Chain Y8: 




- Molecule 34: 50S ribosomal protein L36

Chain R9: 



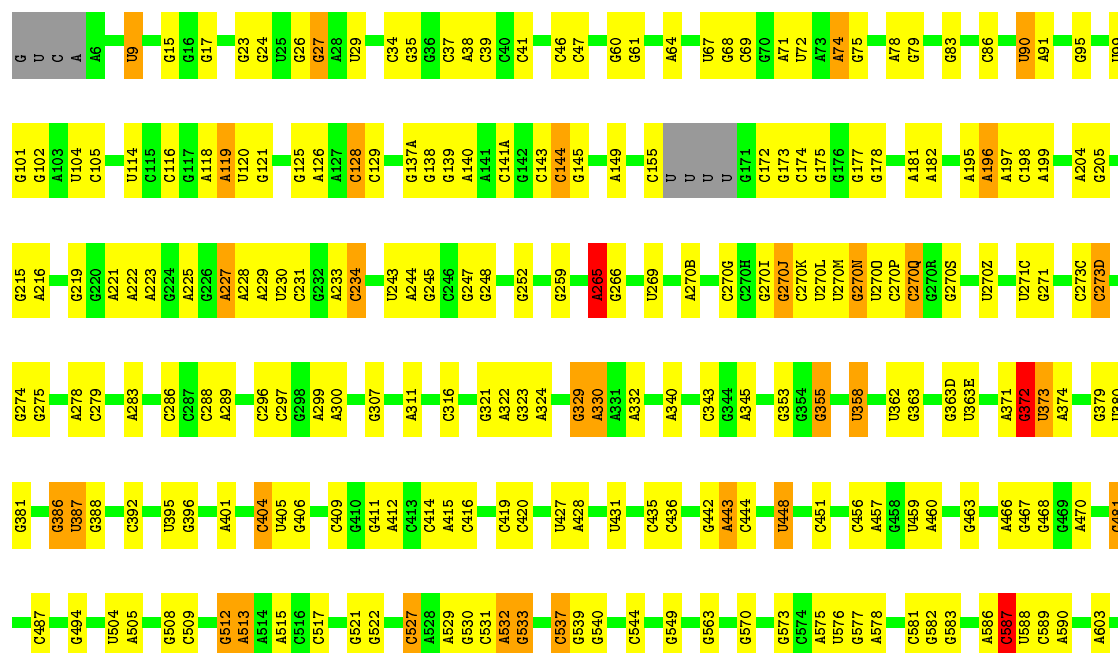
- Molecule 34: 50S ribosomal protein L36

Chain Y9: 



- Molecule 35: 23S rRNA

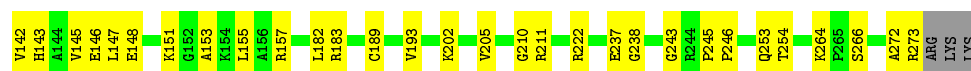
Chain RA: 







A2117	A2020	A1901	G1763	A1632	U1516	G1418	A1301	G1187	A1088	C992	A896	C812	6669	U614
U2118	C2021	C1902	G1764	G1633	U1516	G1419	A1308	U1188	A1089	G993	C897	6613	4670	6615
A2119	U2022	G1903	A1634	G1635	G1522	U1421	G1309	G1191	G1093	C995	C904	C814	6674	4616
G2120	G2023	G1906	G1769	G1636	G1523	G1422	G1310	G1195	A1094	A996	G906	C817	4675	4621
G2123	G2024	A1637	A1773	G1637	G1524	G1423	G1311	C1196	A1095	G997	U907	A819	4676	4622
A2126	C2025	G1640	C1774	G1640	G1525	G1424	U1313	A1204	A1096	C998	A910	A820	6679	6623
C2026	C2026	G1910	U1779	C1644	A1528	A1427	C1314	U1205	G1099	U999	G915	A821	6680	6624
G2027	U2028	U1911	A1780	C1644	U1535	G1428	U1316	U1210	C1102	C1005	G916	G823	6681	4627
C2029	G2028	A1912	C1781	G1648	U1536	G1429	A1317	U1211	A1103	A1009	A917	U827	6686	6628
G2030	A2030	C1914	A1782	G1648	U1537	U1431	U1329	G1212	G1106	A1010	G918	U828	6629	6630
A2031	A2031	U1915	A1783	G1682	G1538	C1432	C1330	A1213	G1110	G1011	G919	U831	4633	4633
G2032	G2032	C1920	A1784	G1683	G1539	U1433	A1342	A1214	A1103	U1012	G918	U832	6634	6634
A2033	A2033	U1923	C1788	A1654	G1540	A1434	A1342	A1220	G1113	C1013	G918	U833	4637	4637
G2034	G2034	A1655	A1791	A1655	A1543	G1437	U1352	A1220	U1113	G1017	G918	U834	6636	6636
C2035	C2035	G1929	G1792	C1657	C1544	A1444A	A1353	C1225	G1122	A1020	G931	U835	6639	6639
G2036	G2036	G1930	G1792	C1657	A1545	C1445	A1354	G1226	A1126	G1021	G932	U836	6640	6640
C2037	G2037	C1934	U1798	G1667	C1547	A1449	A1359	G1227	A1127	G1023	G933	U837	6641	6641
G2038	G2038	G1935	G1799	A1688	A1554	G1449A	A1360	G1228	A1128	G1024	G934	U838	6642	6642
U2041	A2042	A1937	C1800	A1688	A1554	G1449A	A1360	C1233	A1129	G1025	G934	U839	6645	6645
C2043	C2043	A1938	G1801	A1669	A1554	G1449A	A1360	C1233	A1130	G1026	G934	U840	4646	4646
G2052	G2052	G1948	A1802	G1674	A1558	G1455	C1363	C1233	G1136	G1027	G934	U841	6652	6652
C2055	C2055	U1955	A1809	C1675	G1559	G1459	G1368	G1236	G1139	A1044	G934	U842	4653	4653
G2056	G2056	U1956	G1816	C1675	G1560	G1459	G1368	A1237	C1140	A1045	G934	U843	4654	4654
A2059	A2059	G1957	G1816	U1679	A1566	G1460	G1369	G1243	U1141	A1046	G934	U844	4655	4655
A2060	A2060	C1958	U1819	U1680	A1567	G1461	G1370	G1243	U1142	A1047	G934	U845	4656	4656
G2061	G2061	U1963	U1820	U1680	A1568	G1462	G1370	G1243	U1143	A1048	G934	U846	4657	4657
A2062	A2062	G1964	G1824	U1680	A1569	G1463	G1370	G1243	U1144	A1049	G934	U847	4658	4658
C2063	C2063	C1965	G1824	U1680	A1570	G1464	G1370	G1243	U1145	A1050	G934	U848	4659	4659
G2064	G2064	A1966	G1827	U1680	A1571	G1465	G1370	G1243	U1146	A1051	G934	U849	4660	4660
C2065	C2065	C1967	G1828	U1680	A1572	G1466	G1370	G1243	U1147	A1052	G934	U850	4661	4661
G2069	G2069	A1970	G1829	U1680	A1573	G1467	G1370	G1243	U1148	A1053	G934	U851	4662	4662
C2073	C2073	A1971	C1830	U1680	A1574	G1468	G1370	G1243	U1149	A1054	G934	U852	4663	4663
U2074	U2074	A1972	G1831	U1680	A1575	G1469	G1370	G1243	U1150	A1055	G934	U853	4664	4664
U2075	U2075	C1979	G1835	U1680	A1576	G1470	G1370	G1243	U1151	A1056	G934	U854	4665	4665
U2086	U2086	G1980	A1847	U1680	A1577	G1471	G1370	G1243	U1152	A1057	G934	U855	4666	4666
G2093	G2093	A1981	G1858	U1680	A1578	G1472	G1370	G1243	U1153	A1058	G934	U856	4667	4667
C2174	C2174	C1982	A1859	U1680	A1579	G1473	G1370	G1243	U1154	A1059	G934	U857	4668	4668
C2177	C2177	U1992	G1872	U1680	A1580	G1474	G1370	G1243	U1155	A1060	G934	U858	4669	4669
C2178	C2178	U1993	G1873	U1680	A1581	G1475	G1370	G1243	U1156	A1061	G934	U859	4670	4670
G2187	G2187	C1996	C1875	U1680	A1582	G1476	G1370	G1243	U1157	A1062	G934	U860	4671	4671
C2188	C2188	U2001	C1881	U1680	A1583	G1477	G1370	G1243	U1158	A1063	G934	U861	4672	4672
U2189	U2189	G2002	C1882	U1680	A1584	G1478	G1370	G1243	U1159	A1064	G934	U862	4673	4673
G2190	G2190	C2003	G1883	U1680	A1585	G1479	G1370	G1243	U1160	A1065	G934	U863	4674	4674
G2191	G2191	C2004	G1884	U1680	A1586	G1480	G1370	G1243	U1161	A1066	G934	U864	4675	4675
G2192	G2192	C2005	G1885	U1680	A1587	G1481	G1370	G1243	U1162	A1067	G934	U865	4676	4676
A2198	A2198	G2010	A1889	U1680	A1588	G1482	G1370	G1243	U1163	A1068	G934	U866	4677	4677
G2199	G2199	C2011	C1889	U1680	A1589	G1483	G1370	G1243	U1164	A1069	G934	U867	4678	4678
G2205	G2205	G2012	A1900	U1680	A1590	G1484	G1370	G1243	U1165	A1070	G934	U868	4679	4679
					A1511	G1416	G1417	U1300	G1184	A1085	G934	U869	4680	4680
					G1512	G1416	G1417	U1300	G1184	A1086	G934	U870	4681	4681
					G1512	G1416	G1417	U1300	G1184	A1087	G934	U871	4682	4682
					G1512	G1416	G1417	U1300	G1184	A1088	G934	U872	4683	4683
					G1512	G1416	G1417	U1300	G1184	A1089	G934	U873	4684	4684
					G1512	G1416	G1417	U1300	G1184	A1090	G934	U874	4685	4685
					G1512	G1416	G1417	U1300	G1184	A1091	G934	U875	4686	4686
					G1512	G1416	G1417	U1300	G1184	A1092	G934	U876	4687	4687
					G1512	G1416	G1417	U1300	G1184	A1093	G934	U877	4688	4688
					G1512	G1416	G1417	U1300	G1184	A1094	G934	U878	4689	4689
					G1512	G1416	G1417	U1300	G1184	A1095	G934	U879	4690	4690
					G1512	G1416	G1417	U1300	G1184	A1096	G934	U880	4691	4691
					G1512	G1416	G1417	U1300	G1184	A1097	G934	U881	4692	4692
					G1512	G1416	G1417	U1300	G1184	A1098	G934	U882	4693	4693
					G1512	G1416	G1417	U1300	G1184	A1099	G934	U883	4694	4694
					G1512	G1416	G1417	U1300	G1184	A1100	G934	U884	4695	4695
					G1512	G1416	G1417	U1300	G1184	A1101	G934	U885	4696	4696
					G1512	G1416	G1417	U1300	G1184	A1102	G934	U886	4697	4697
					G1512	G1416	G1417	U1300	G1184	A1103	G934	U887	4698	4698
					G1512	G1416	G1417	U1300	G1184	A1104	G934	U888	4699	4699
					G1512	G1416	G1417	U1300	G1184	A1105	G934	U889	4700	4700
					G1512	G1416	G1417	U1300	G1184	A1106	G934	U890	4701	4701
					G1512	G1416	G1417	U1300	G1184	A1107	G934	U891	4702	4702
					G1512	G1416	G1417	U1300	G1184	A1108	G934	U892	4703	4703
					G1512	G1416	G1417	U1300	G1184	A1109	G934	U893	4704	4704
					G1512	G1416	G1417	U1300	G1184	A1110	G934	U894	4705	4705
					G1512	G1416	G1417	U1300	G1184	A1111	G934	U895	4706	4706
					G1512	G1416	G1417	U1300	G1184	A1112	G934	U896	4707	4707
					G1512	G1416	G1417	U1300	G1184	A1113	G934	U897	4708	4708
					G1512	G1416	G1417	U1300	G1184	A1114	G934	U898	4709	4709
					G1512	G1416	G1417	U1300	G1184	A1115	G934	U899	4710	4710
					G1512	G1416	G1417	U1300	G1184	A1116	G934	U900	4711	4711
					G1512	G1416	G1417	U1300	G1184	A1117	G934	U901	4712	4712
					G1512	G1416	G1417	U1300	G1184	A1118	G934	U902	4713	4713
					G1512	G1416	G1417	U1300	G1184	A1119	G934	U903	4714	4714
					G1512	G1416	G1417	U1300	G1184	A1120	G934	U904	4715	4715
					G1512	G1416	G1417	U1300	G1184	A1121	G934	U905	4716	4716
					G1512	G1416	G1417	U1300	G1184	A1122	G934	U906	4717	4717
					G1512	G1416	G1417	U1300	G1184	A1123	G934	U907	4718	4718
					G1512	G1416	G1417	U1300	G1184	A1124	G934	U908	4719	4719
					G1512	G1416	G1417	U1300	G1184	A1125	G934	U909	4720	4720
					G1512	G1416	G1417	U1300	G1184	A1126	G934	U910	4721	4721
					G1512	G1416	G1417	U1300	G1184	A1127	G934	U911	4722	4722
					G1512	G1416	G1417	U1300	G1184	A1128	G934	U912	4723	4723
					G1512	G1416	G1417	U1300	G1184	A1129	G934	U913	4724	4724
					G1512	G1416	G1417	U1300	G1184	A1130	G934	U914	4725	4725
					G1512	G1416	G1417	U1300	G1184	A1131	G934	U915	4726	4726
					G1512	G1416	G1417	U1300	G1184	A1132	G934	U9		



- Molecule 37: 50S ribosomal protein L2

Chain YD: 89% 9% ..



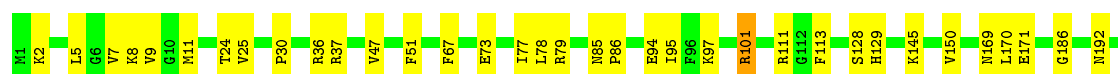
- Molecule 38: 50S ribosomal protein L3

Chain RE: 73% 25% ..



- Molecule 38: 50S ribosomal protein L3

Chain YE: 81% 18% .



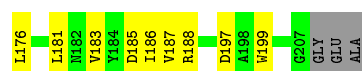
- Molecule 39: 50S ribosomal protein L4

Chain RF: 87% 9% .




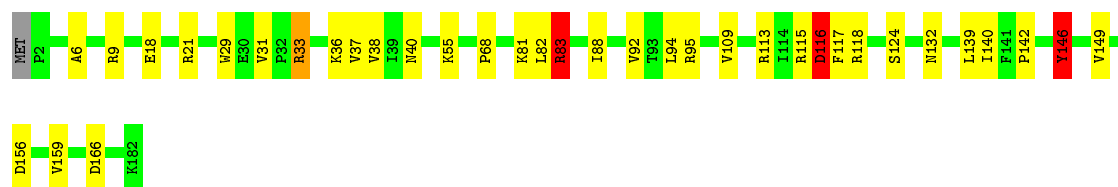
- Molecule 39: 50S ribosomal protein L4

Chain YF: 78% 17% . .




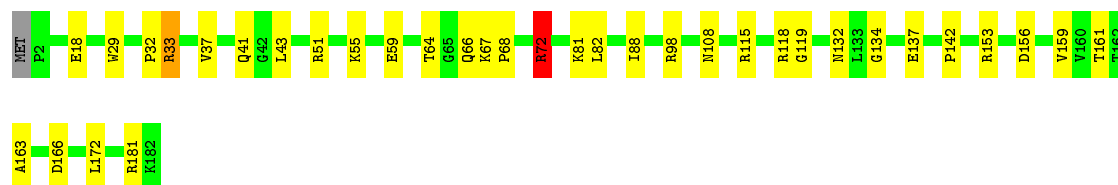
- Molecule 40: 50S ribosomal protein L5

Chain RG:  80% 18% ...




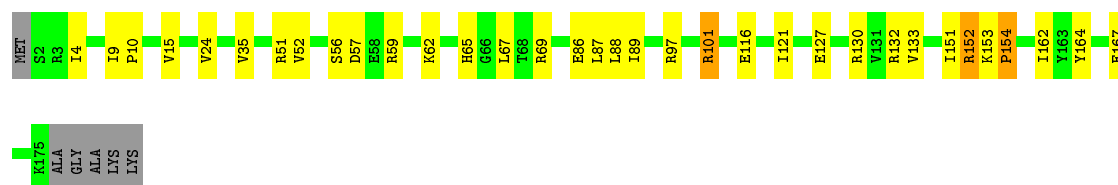
- Molecule 40: 50S ribosomal protein L5

Chain YG:  80% 18% ...




- Molecule 41: 50S ribosomal protein L6

Chain RH:  78% 17% ..




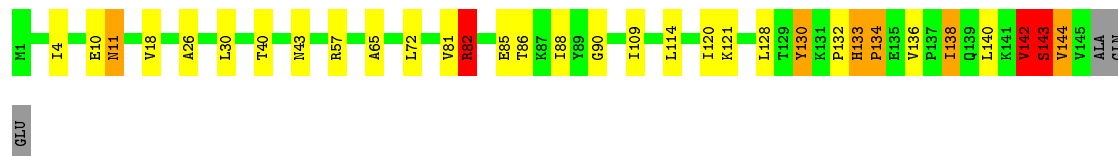
- Molecule 41: 50S ribosomal protein L6

Chain YH:  84% 12% ..




- Molecule 42: 50S ribosomal protein L9

Chain RI:  76% 16% ...



- Molecule 42: 50S ribosomal protein L9

Chain YI:  86% 9% ...



- Molecule 43: 50S ribosomal protein L13

Chain RN: 79% 17% ...



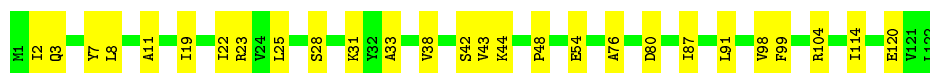
- Molecule 43: 50S ribosomal protein L13

Chain YN: 83% 14% ..



- Molecule 44: 50S ribosomal protein L14

Chain RO: 78% 22%



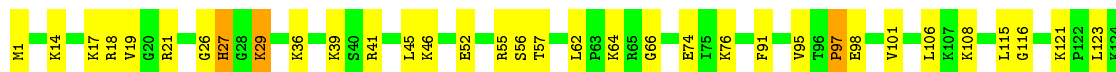
- Molecule 44: 50S ribosomal protein L14

Chain YO: 80% 20%



- Molecule 45: 50S ribosomal protein L15

Chain RP: 75% 23% .



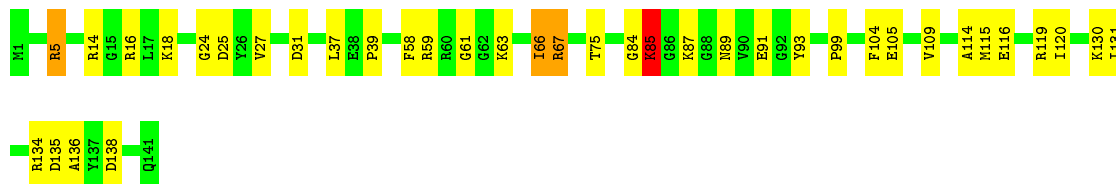
- Molecule 45: 50S ribosomal protein L15

Chain YP: 81% 19% .




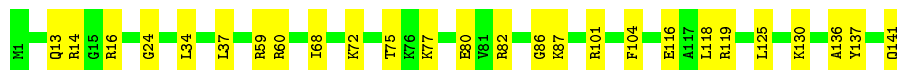
- Molecule 46: 50S ribosomal protein L16

Chain RQ:  73% 24% ..




- Molecule 46: 50S ribosomal protein L16

Chain YQ:  82% 18%




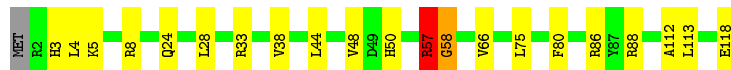
- Molecule 47: 50S ribosomal protein L17

Chain RR:  81% 16% ..




- Molecule 47: 50S ribosomal protein L17

Chain YR:  81% 16% ...




- Molecule 48: 50S ribosomal protein L18

Chain RS:  78% 21% .



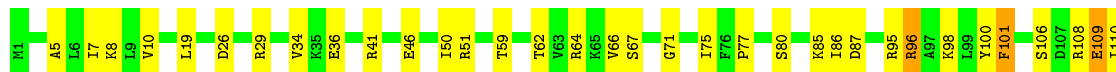
- Molecule 48: 50S ribosomal protein L18

Chain YS:  79% 20% ..



- Molecule 49: 50S ribosomal protein L19

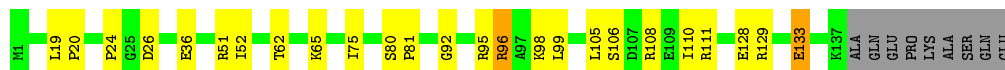
Chain RT:  69% 23% . 6%





- Molecule 49: 50S ribosomal protein L19

Chain YT: 77% 16% 6%



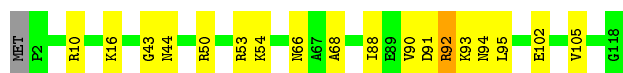
- Molecule 50: 50S ribosomal protein L20

Chain RU: 82% 15% ...



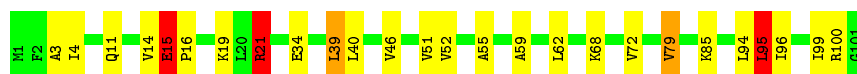
- Molecule 50: 50S ribosomal protein L20

Chain YU: 84% 14% ..



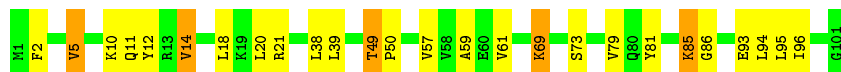
- Molecule 51: 50S ribosomal protein L21

Chain RV: 74% 21% . .



- Molecule 51: 50S ribosomal protein L21

Chain YV: 74% 21% 5%



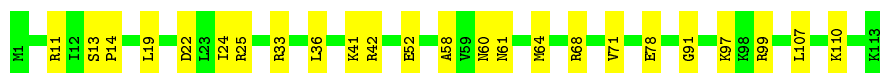
- Molecule 52: 50S ribosomal protein L22

Chain RW: 88% 11% .



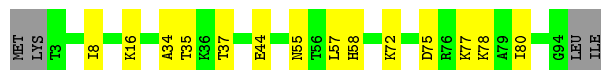
- Molecule 52: 50S ribosomal protein L22

Chain YW: 79% 21%



- Molecule 53: 50S ribosomal protein L23

Chain RX: 81% 15%



- Molecule 53: 50S ribosomal protein L23

Chain YX: 81% 14%



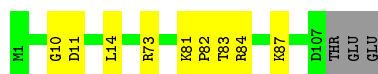
- Molecule 54: 50S ribosomal protein L24

Chain RY: 79% 17%



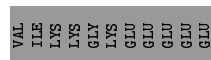
- Molecule 54: 50S ribosomal protein L24

Chain YY: 89% 8%



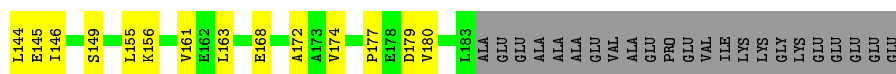
- Molecule 55: 50S ribosomal protein L25

Chain RZ: 76% 12% 11%



- Molecule 55: 50S ribosomal protein L25

Chain YZ: 66% 23% 11%



- Molecule 56: CCPuro

Chain ZA:  33% 67%

 C1 C2 A3

- Molecule 56: CCPuro

Chain ZB:  67% 33%

 C1 C2 A3

4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	214.68Å 453.51Å 609.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	146.72 – 3.50	Depositor
% Data completeness (in resolution range)	98.0 (146.72-3.50)	Depositor
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.216 , 0.246	Depositor
Wilson B-factor (Å ²)	89.9	Xtriage
Anisotropy	0.032	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	295153	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: MG, A3P, ZN, PPU, SF4

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	QA	0.35	1/36324 (0.0%)	1.07	174/56690 (0.3%)
1	XA	1.32	6/36254 (0.0%)	1.08	179/56581 (0.3%)
2	QB	0.57	4/1942 (0.2%)	0.84	4/2619 (0.2%)
2	XB	0.39	0/1950	0.77	4/2630 (0.2%)
3	QC	0.38	0/1629	0.76	1/2195 (0.0%)
3	XC	0.38	0/1629	0.79	4/2195 (0.2%)
4	QD	0.38	0/1733	0.73	2/2318 (0.1%)
4	XD	0.38	0/1733	0.78	4/2318 (0.2%)
5	QE	0.36	0/1171	0.71	0/1576
5	XE	0.33	0/1171	0.67	0/1576
6	QF	0.32	0/856	0.67	0/1154
6	XF	0.33	0/856	0.70	1/1154 (0.1%)
7	QG	0.38	0/1276	0.75	0/1709
7	XG	0.36	0/1276	0.66	1/1709 (0.1%)
8	QH	0.32	0/1128	0.70	0/1517
8	XH	0.31	0/1128	0.72	3/1517 (0.2%)
9	QI	0.47	0/1029	0.87	2/1379 (0.1%)
9	XI	0.37	0/1017	0.79	2/1365 (0.1%)
10	QJ	0.44	1/814 (0.1%)	0.96	7/1095 (0.6%)
10	XJ	0.41	1/790 (0.1%)	0.81	2/1063 (0.2%)
11	QK	0.40	1/900 (0.1%)	0.71	0/1213
11	XK	0.38	0/879	0.73	2/1187 (0.2%)
12	QL	0.34	0/991	0.81	0/1327
12	XL	0.39	0/972	0.82	1/1301 (0.1%)
13	QM	0.42	0/965	0.92	4/1292 (0.3%)
13	XM	0.40	0/956	0.82	2/1281 (0.2%)
14	QN	0.43	0/501	0.82	1/664 (0.2%)
14	XN	0.32	0/501	0.72	1/664 (0.2%)
15	QO	0.34	0/745	0.66	1/992 (0.1%)
15	XO	0.28	0/740	0.55	0/987
16	QP	0.36	0/721	0.80	2/970 (0.2%)
16	XP	0.34	0/721	0.77	1/970 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.37	0/847	0.77	4/1131 (0.4%)
17	XQ	0.33	0/847	0.66	0/1131
18	QR	0.41	1/579 (0.2%)	0.81	0/768
18	XR	0.38	0/579	0.77	1/768 (0.1%)
19	QS	0.45	0/680	0.93	1/915 (0.1%)
19	XS	0.32	0/671	0.78	1/904 (0.1%)
20	QT	0.36	0/765	0.81	0/1007
20	XT	0.35	0/765	0.81	2/1007 (0.2%)
21	QU	0.43	0/221	0.89	1/288 (0.3%)
21	XU	0.31	0/221	0.83	0/288
22	QV	0.33	0/1832	1.01	4/2855 (0.1%)
22	XV	0.33	0/1832	1.02	3/2855 (0.1%)
23	QX	0.33	0/414	0.96	2/645 (0.3%)
23	XX	0.30	0/414	0.92	2/645 (0.3%)
24	QY	0.40	0/743	0.78	1/1002 (0.1%)
24	QZ	0.61	2/743 (0.3%)	0.99	2/1002 (0.2%)
24	XY	0.35	0/743	0.74	1/1002 (0.1%)
24	XZ	0.45	0/743	0.90	2/1002 (0.2%)
25	R0	0.39	0/652	0.87	2/867 (0.2%)
25	Y0	0.35	0/657	0.76	0/874
26	R1	0.43	1/744 (0.1%)	0.78	2/989 (0.2%)
26	Y1	0.36	0/770	0.73	0/1022
27	R2	0.43	0/583	0.90	4/771 (0.5%)
27	Y2	0.31	0/583	0.65	0/771
28	R3	0.31	0/474	0.67	0/635
28	Y3	0.33	0/474	0.73	0/635
29	R4	0.63	0/578	1.13	3/776 (0.4%)
29	Y4	0.40	0/578	0.93	3/776 (0.4%)
30	R5	0.37	0/473	0.72	1/639 (0.2%)
30	Y5	0.46	0/473	0.74	0/639
31	R6	0.38	0/460	0.85	1/613 (0.2%)
31	Y6	0.39	0/460	0.74	0/613
32	R7	0.31	0/417	0.64	0/550
32	Y7	0.33	0/426	0.64	0/561
33	R8	0.48	0/525	0.97	4/691 (0.6%)
33	Y8	0.51	0/525	0.80	0/691
34	R9	0.41	0/310	0.80	0/407
34	Y9	0.38	0/310	0.85	1/407 (0.2%)
35	RA	0.37	0/69739	1.11	428/108870 (0.4%)
35	YA	0.38	0/69419	1.11	379/108369 (0.3%)
36	RB	0.40	0/2881	1.13	17/4494 (0.4%)
36	YB	0.47	1/2881 (0.0%)	1.21	31/4494 (0.7%)
37	RD	0.40	0/2165	0.86	6/2919 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	YD	0.35	0/2185	0.74	4/2944 (0.1%)
38	RE	0.48	0/1601	0.93	4/2160 (0.2%)
38	YE	0.39	0/1592	0.86	4/2149 (0.2%)
39	RF	0.33	0/1620	0.70	2/2194 (0.1%)
39	YF	0.37	1/1620 (0.1%)	0.72	3/2194 (0.1%)
40	RG	0.38	0/1499	0.88	5/2016 (0.2%)
40	YG	0.50	3/1499 (0.2%)	0.82	2/2016 (0.1%)
41	RH	0.47	0/1362	1.04	5/1841 (0.3%)
41	YH	0.39	0/1356	0.77	3/1834 (0.2%)
42	RI	2.84	2/1146 (0.2%)	1.40	9/1551 (0.6%)
42	YI	0.44	0/1151	0.92	4/1558 (0.3%)
43	RN	0.43	0/1131	0.83	3/1525 (0.2%)
43	YN	0.33	0/1131	0.72	3/1525 (0.2%)
44	RO	0.33	0/943	0.70	0/1269
44	YO	0.35	0/943	0.72	0/1269
45	RP	0.45	0/1162	0.96	4/1544 (0.3%)
45	YP	0.36	0/1152	0.86	3/1533 (0.2%)
46	RQ	0.50	2/1143 (0.2%)	0.89	3/1527 (0.2%)
46	YQ	0.34	0/1143	0.73	1/1527 (0.1%)
47	RR	0.32	0/974	0.76	3/1302 (0.2%)
47	YR	0.35	0/974	0.84	4/1302 (0.3%)
48	RS	0.38	0/892	0.83	1/1187 (0.1%)
48	YS	0.43	0/892	0.85	2/1187 (0.2%)
49	RT	0.45	0/1155	0.87	1/1542 (0.1%)
49	YT	0.45	1/1155 (0.1%)	0.83	4/1542 (0.3%)
50	RU	0.38	0/982	0.68	1/1306 (0.1%)
50	YU	0.37	0/982	0.64	0/1306
51	RV	0.72	2/790 (0.3%)	1.15	6/1057 (0.6%)
51	YV	1.42	8/790 (1.0%)	1.02	4/1057 (0.4%)
52	RW	0.33	0/911	0.70	0/1220
52	YW	0.33	0/911	0.69	0/1220
53	RX	0.34	0/739	0.68	0/993
53	YX	0.35	0/739	0.66	0/993
54	RY	0.38	0/831	0.75	1/1108 (0.1%)
54	YY	0.35	0/831	0.76	0/1108
55	RZ	0.39	0/1493	0.84	3/2026 (0.1%)
55	YZ	0.36	0/1493	0.77	0/2026
56	ZA	0.52	0/40	1.41	1/60 (1.7%)
56	ZB	0.58	0/40	1.53	0/60
All	All	0.60	38/319487 (0.0%)	1.03	1407/477274 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	QB	0	1
7	XG	0	1
8	XH	0	1
10	QJ	0	1
11	XK	0	1
24	QZ	0	1
37	RD	0	2
37	YD	0	1
38	RE	0	1
40	RG	0	2
40	YG	0	1
41	RH	0	2
41	YH	0	1
42	RI	0	4
47	RR	0	1
47	YR	0	1
51	RV	0	1
All	All	0	23

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	XA	368	U	C2-N3	131.42	2.29	1.37
1	XA	368	U	N3-C4	105.69	2.33	1.38
42	RI	82	ARG	CZ-NH1	93.68	2.54	1.33
1	XA	368	U	N1-C2	92.50	2.21	1.38
1	XA	368	U	N1-C6	90.74	2.19	1.38
1	XA	368	U	C4-C5	83.89	2.19	1.43
1	XA	368	U	C5-C6	79.02	2.05	1.34
51	YV	85	LYS	CD-CE	23.53	2.10	1.51
51	YV	85	LYS	CE-NZ	15.44	1.87	1.49
51	YV	85	LYS	CB-CG	11.18	1.82	1.52
51	YV	85	LYS	CG-CD	9.90	1.86	1.52
24	QZ	22	ARG	CZ-NH1	8.88	1.44	1.33
2	QB	132	LYS	CD-CE	8.71	1.73	1.51
51	RV	51	VAL	CB-CG2	-8.08	1.35	1.52
40	YG	72	ARG	CG-CD	7.85	1.71	1.51
42	RI	82	ARG	NE-CZ	7.83	1.43	1.33
51	YV	69	LYS	CD-CE	-7.83	1.31	1.51
40	YG	72	ARG	CD-NE	7.36	1.58	1.46
51	RV	51	VAL	CB-CG1	-7.18	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	YV	14	VAL	CB-CG2	-6.71	1.38	1.52
51	YV	5	VAL	CB-CG2	-6.26	1.39	1.52
2	QB	12	GLU	CG-CD	-6.06	1.42	1.51
2	QB	8	LYS	C-N	6.03	1.48	1.34
40	YG	72	ARG	CB-CG	5.85	1.68	1.52
36	YB	116	G	C2'-C1'	-5.80	1.47	1.53
2	QB	8	LYS	N-CA	5.73	1.57	1.46
49	YT	133	GLU	CB-CG	-5.67	1.41	1.52
1	QA	496	A	N9-C4	5.44	1.41	1.37
46	RQ	85	LYS	CD-CE	-5.44	1.37	1.51
24	QZ	22	ARG	CZ-NH2	5.35	1.40	1.33
39	YF	127	GLU	CB-CG	5.33	1.62	1.52
10	XJ	57	LYS	CD-CE	5.21	1.64	1.51
11	QK	92	GLU	CG-CD	5.20	1.59	1.51
18	QR	83	GLU	CB-CG	5.17	1.61	1.52
26	R1	67	ILE	C-N	5.14	1.44	1.34
10	QJ	43	ARG	CG-CD	5.07	1.64	1.51
51	YV	49	THR	CB-CG2	-5.05	1.35	1.52
46	RQ	85	LYS	CE-NZ	-5.03	1.36	1.49

All (1407) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	RI	82	ARG	NE-CZ-NH2	-27.28	106.66	120.30
42	RI	82	ARG	NE-CZ-NH1	20.23	130.42	120.30
42	RI	82	ARG	CD-NE-CZ	15.62	145.47	123.60
51	YV	85	LYS	CD-CE-NZ	15.45	147.22	111.70
51	RV	21	ARG	NE-CZ-NH1	14.43	127.52	120.30
35	YA	289	A	O5'-P-OP1	-14.36	92.78	105.70
1	QA	1301	U	C2-N1-C1'	11.98	132.08	117.70
1	QA	1301	U	N1-C2-O2	11.52	130.87	122.80
24	QZ	50	HIS	C-N-CA	11.24	149.81	121.70
42	RI	11	ASN	C-N-CA	10.97	149.12	121.70
38	RE	79	ARG	NE-CZ-NH1	-10.95	114.82	120.30
37	RD	33	LEU	C-N-CA	10.74	148.54	121.70
1	QA	999	U	C2-N1-C1'	10.58	130.40	117.70
38	YE	101	ARG	CA-CB-CG	10.50	136.50	113.40
35	RA	2128	C	C2-N1-C1'	10.46	130.31	118.80
1	XA	1301	U	C2-N1-C1'	10.31	130.07	117.70
1	XA	754	C	C2-N1-C1'	10.28	130.11	118.80
1	XA	368	U	N3-C2-O2	10.18	129.32	122.20
1	QA	1301	U	N3-C2-O2	-10.18	115.08	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	754	C	C2-N1-C1'	10.13	129.95	118.80
36	YB	31	C	C2-N1-C1'	10.05	129.85	118.80
19	QS	29	ARG	CG-CD-NE	-9.98	90.85	111.80
1	XA	368	U	C2-N3-C4	-9.96	121.02	127.00
47	YR	57	ARG	NE-CZ-NH1	-9.91	115.34	120.30
35	YA	624	C	C6-N1-C2	-9.89	116.34	120.30
35	YA	2063	C	N1-C2-O2	9.85	124.81	118.90
10	QJ	79	ARG	NE-CZ-NH1	9.70	125.15	120.30
35	RA	2666	C	N1-C2-O2	9.68	124.71	118.90
42	RI	143	SER	C-N-CA	9.63	145.76	121.70
1	QA	754	C	N1-C2-O2	9.59	124.65	118.90
35	RA	1774	C	N1-C2-O2	9.44	124.56	118.90
35	RA	856	C	C6-N1-C2	-9.38	116.55	120.30
1	XA	328	C	N1-C2-O2	9.36	124.52	118.90
1	XA	328	C	C2-N1-C1'	9.28	129.01	118.80
35	RA	269	U	N1-C2-O2	9.26	129.28	122.80
40	YG	72	ARG	NE-CZ-NH1	-9.24	115.68	120.30
1	QA	1066	C	N1-C2-O2	9.09	124.36	118.90
35	RA	2128	C	N1-C2-O2	9.08	124.35	118.90
35	YA	1225	C	O4'-C1'-N1	9.00	115.40	108.20
35	RA	1640	C	N1-C2-O2	8.97	124.28	118.90
35	YA	1882	C	C2-N1-C1'	8.97	128.67	118.80
1	XA	1301	U	N1-C2-O2	8.93	129.05	122.80
41	RH	101	ARG	CG-CD-NE	-8.92	93.07	111.80
35	YA	828	U	C2-N1-C1'	8.91	128.40	117.70
35	YA	1313	U	N1-C2-O2	8.91	129.04	122.80
35	RA	1774	C	N3-C2-O2	-8.90	115.67	121.90
35	YA	2063	C	N3-C2-O2	-8.88	115.68	121.90
35	RA	2827	C	C2-N1-C1'	8.87	128.56	118.80
13	QM	114	ARG	CG-CD-NE	-8.86	93.20	111.80
35	YA	363(E)	U	N1-C2-O2	8.85	128.99	122.80
51	RV	21	ARG	NE-CZ-NH2	-8.84	115.88	120.30
35	RA	1313	U	N1-C2-O2	8.78	128.95	122.80
35	YA	2474	C	N1-C2-O2	8.77	124.16	118.90
35	RA	1881	C	C2-N1-C1'	8.74	128.41	118.80
36	YB	31	C	N1-C2-O2	8.74	124.14	118.90
35	RA	2584	U	N3-C2-O2	-8.72	116.09	122.20
1	QA	1158	C	C2-N1-C1'	8.71	128.38	118.80
35	RA	607	U	N3-C2-O2	-8.69	116.12	122.20
35	RA	269	U	C2-N1-C1'	8.67	128.10	117.70
1	QA	1147	C	N1-C2-O2	8.66	124.10	118.90
35	RA	1407	C	C2-N1-C1'	8.60	128.26	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	1313	U	N3-C2-O2	-8.58	116.19	122.20
35	YA	363(E)	U	C2-N1-C1'	8.56	127.97	117.70
35	RA	1313	U	C2-N1-C1'	8.55	127.96	117.70
35	YA	1406	U	C5-C6-N1	8.54	126.97	122.70
4	XD	118	ARG	CG-CD-NE	8.53	129.72	111.80
3	XC	140	ARG	NE-CZ-NH2	-8.47	116.06	120.30
35	RA	856	C	C5-C6-N1	8.47	125.23	121.00
1	QA	1158	C	N1-C2-O2	8.44	123.97	118.90
35	YA	269	U	N1-C2-O2	8.43	128.70	122.80
37	YD	88	ARG	CD-NE-CZ	8.43	135.40	123.60
35	YA	1313	U	C2-N1-C1'	8.42	127.81	117.70
3	XC	140	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	XA	135	C	C6-N1-C2	-8.38	116.95	120.30
35	RA	269	U	N3-C2-O2	-8.34	116.36	122.20
55	RZ	112	ARG	CG-CD-NE	-8.33	94.30	111.80
35	YA	69	C	N1-C2-O2	8.33	123.90	118.90
35	RA	1180	C	C2-N1-C1'	8.29	127.92	118.80
35	YA	624	C	C2-N1-C1'	8.25	127.87	118.80
43	RN	61	ARG	CG-CD-NE	-8.23	94.51	111.80
35	RA	2788	C	N1-C2-O2	8.22	123.83	118.90
38	YE	101	ARG	CG-CD-NE	8.22	129.06	111.80
35	YA	1313	U	N3-C2-O2	-8.19	116.47	122.20
35	YA	2128	C	C2-N1-C1'	8.17	127.79	118.80
35	RA	613	U	C2-N1-C1'	8.14	127.47	117.70
1	XA	1381	U	N1-C2-O2	8.10	128.47	122.80
2	QB	132	LYS	CD-CE-NZ	8.10	130.32	111.70
35	YA	856	C	C6-N1-C2	-8.08	117.07	120.30
38	YE	101	ARG	CD-NE-CZ	-8.05	112.33	123.60
1	XA	368	U	C2-N1-C1'	-8.04	108.05	117.70
1	QA	999	U	N1-C2-O2	8.00	128.40	122.80
1	XA	754	C	N1-C2-O2	8.00	123.70	118.90
35	YA	193	U	C2-N1-C1'	8.00	127.30	117.70
1	XA	135	C	N1-C2-O2	8.00	123.70	118.90
1	XA	1007	C	C2-N1-C1'	7.99	127.58	118.80
35	YA	93	C	C2-N1-C1'	7.98	127.58	118.80
35	YA	624	C	C5-C6-N1	7.97	124.98	121.00
35	YA	193	U	N1-C2-O2	7.96	128.37	122.80
1	QA	252	U	C2-N1-C1'	7.96	127.25	117.70
1	QA	1006	C	C2-N1-C1'	7.95	127.55	118.80
35	RA	607	U	N1-C2-O2	7.94	128.36	122.80
35	RA	2688	U	N3-C2-O2	-7.94	116.64	122.20
35	YA	1406	U	C2-N1-C1'	7.93	127.22	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	2787	C	C2-N1-C1'	7.90	127.49	118.80
35	YA	2712	U	C2-N1-C1'	7.88	127.16	117.70
35	YA	270(U)	C	N1-C2-O2	7.88	123.63	118.90
1	XA	1301	U	N3-C2-O2	-7.87	116.69	122.20
35	RA	1588	C	C2-N1-C1'	7.87	127.45	118.80
1	XA	91	C	N3-C2-O2	-7.87	116.39	121.90
35	RA	1407	C	C6-N1-C2	-7.86	117.16	120.30
1	XA	368	U	C6-N1-C2	7.85	125.71	121.00
35	YA	828	U	N1-C2-O2	7.83	128.28	122.80
36	YB	47	C	N1-C2-O2	7.82	123.59	118.90
1	XA	1260	C	N3-C2-O2	-7.82	116.43	121.90
35	RA	2788	C	N3-C2-O2	-7.81	116.43	121.90
1	XA	330	C	N1-C2-O2	7.81	123.58	118.90
35	YA	2226	C	N1-C2-O2	7.80	123.58	118.90
1	QA	1066	C	C2-N1-C1'	7.79	127.37	118.80
35	RA	2666	C	N3-C2-O2	-7.79	116.45	121.90
35	YA	1774	C	N1-C2-O2	7.78	123.57	118.90
35	YA	1882	C	C6-N1-C2	-7.77	117.19	120.30
1	QA	1301	U	C6-N1-C1'	-7.77	110.32	121.20
1	XA	1260	C	N1-C2-O2	7.76	123.56	118.90
1	XA	1535	C	N1-C2-O2	7.76	123.56	118.90
1	XA	91	C	N1-C2-O2	7.73	123.54	118.90
35	RA	363(E)	U	N1-C2-O2	7.73	128.21	122.80
35	RA	708	C	C2-N1-C1'	7.73	127.30	118.80
35	YA	277	C	N1-C2-O2	7.71	123.52	118.90
1	QA	328	C	C2-N1-C1'	7.69	127.26	118.80
1	XA	328	C	C6-N1-C2	-7.68	117.23	120.30
1	QA	1158	C	N3-C2-O2	-7.67	116.53	121.90
1	QA	1038	C	P-O3'-C3'	7.64	128.87	119.70
35	YA	363(E)	U	N3-C2-O2	-7.64	116.85	122.20
36	YB	31	C	C6-N1-C2	-7.64	117.25	120.30
1	QA	754	C	N3-C2-O2	-7.63	116.56	121.90
35	YA	193	U	N3-C2-O2	-7.62	116.86	122.20
1	QA	1301	U	C5-C6-N1	7.61	126.51	122.70
15	QO	89	GLY	N-CA-C	-7.61	94.06	113.10
41	RH	153	LYS	N-CA-C	7.61	131.54	111.00
35	RA	2063	C	C6-N1-C2	-7.60	117.26	120.30
1	QA	328	C	C6-N1-C2	-7.60	117.26	120.30
35	YA	1881	C	C2-N1-C1'	7.60	127.16	118.80
35	RA	613	U	N3-C2-O2	-7.60	116.88	122.20
36	RB	27	C	N1-C2-O2	7.59	123.46	118.90
35	YA	2791	C	C2-N3-C4	-7.58	116.11	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	2177	C	N1-C2-O2	7.57	123.44	118.90
35	YA	1314	C	C2-N1-C1'	7.55	127.11	118.80
35	RA	749	C	N1-C2-O2	7.55	123.43	118.90
41	YH	3	ARG	CD-NE-CZ	7.55	134.17	123.60
1	XA	197	A	P-O3'-C3'	7.55	128.76	119.70
1	XA	1381	U	N3-C2-O2	-7.54	116.92	122.20
35	RA	2787	C	C6-N1-C2	-7.53	117.29	120.30
35	YA	527	C	C2-N1-C1'	7.52	127.08	118.80
1	QA	197	A	P-O3'-C3'	7.52	128.72	119.70
35	YA	613	U	C2-N1-C1'	7.48	126.67	117.70
35	RA	613	U	N1-C2-O2	7.47	128.03	122.80
35	RA	2335	A	O4'-C1'-N9	7.47	114.18	108.20
35	YA	269	U	C2-N1-C1'	7.46	126.66	117.70
1	XA	328	C	N3-C2-O2	-7.43	116.70	121.90
35	YA	2312	U	C5-C6-N1	7.43	126.42	122.70
1	XA	1086	U	N1-C2-O2	7.43	128.00	122.80
1	QA	999	U	N3-C2-O2	-7.42	117.00	122.20
1	QA	961	U	N3-C2-O2	-7.42	117.01	122.20
35	YA	1774	C	N3-C2-O2	-7.41	116.71	121.90
35	RA	1956	U	N3-C2-O2	-7.40	117.02	122.20
35	YA	2210	G	N3-C4-C5	-7.40	124.90	128.60
35	YA	2394	C	N1-C2-O2	7.39	123.33	118.90
1	QA	328	C	N1-C2-O2	7.38	123.33	118.90
35	RA	2667	C	N1-C2-O2	7.38	123.33	118.90
35	YA	1882	C	C5-C6-N1	7.37	124.69	121.00
35	RA	2128	C	C6-N1-C1'	-7.37	111.96	120.80
35	RA	1314	C	C2-N1-C1'	7.36	126.90	118.80
1	QA	454	C	N1-C2-O2	7.35	123.31	118.90
1	XA	135	C	N3-C2-O2	-7.35	116.75	121.90
35	YA	2312	U	C2-N1-C1'	7.35	126.52	117.70
35	RA	286	C	C2-N1-C1'	7.35	126.88	118.80
35	RA	856	C	C2-N1-C1'	7.35	126.88	118.80
35	RA	2063	C	C2-N1-C1'	7.33	126.87	118.80
1	XA	754	C	C6-N1-C1'	-7.33	112.00	120.80
35	YA	603	A	P-O3'-C3'	7.33	128.49	119.70
35	YA	1920	C	C5-C6-N1	7.32	124.66	121.00
35	YA	2294	C	C6-N1-C2	-7.32	117.37	120.30
35	YA	2063	C	C2-N1-C1'	7.32	126.85	118.80
17	QQ	100	LYS	C-N-CA	7.30	139.96	121.70
1	QA	754	C	C6-N1-C1'	-7.30	112.04	120.80
35	YA	2474	C	C2-N1-C1'	7.29	126.82	118.80
35	YA	1774	C	C6-N1-C2	-7.28	117.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	2226	C	N1-C2-O2	7.28	123.27	118.90
35	RA	2868	A	C8-N9-C4	-7.28	102.89	105.80
36	YB	116	G	C1'-O4'-C4'	-7.27	104.08	109.90
47	RR	3	HIS	C-N-CA	7.23	139.78	121.70
35	YA	372	G	P-O3'-C3'	7.23	128.38	119.70
45	YP	15	ARG	CG-CD-NE	7.23	126.98	111.80
35	RA	1640	C	C2-N1-C1'	7.23	126.75	118.80
35	YA	613	U	N3-C2-O2	-7.22	117.14	122.20
35	YA	613	U	N1-C2-O2	7.22	127.86	122.80
36	YB	27	C	N1-C2-O2	7.22	123.23	118.90
35	YA	856	C	C5-C6-N1	7.21	124.61	121.00
35	RA	2787	C	N1-C2-O2	7.18	123.21	118.90
35	YA	269	U	N3-C2-O2	-7.18	117.17	122.20
35	YA	1558	A	P-O3'-C3'	7.18	128.32	119.70
35	RA	1558	A	P-O3'-C3'	7.17	128.31	119.70
1	XA	1263	C	C2-N1-C1'	7.17	126.68	118.80
35	YA	837	C	N1-C2-O2	7.16	123.20	118.90
35	RA	363(E)	U	C2-N1-C1'	7.16	126.29	117.70
35	YA	1956	U	N3-C2-O2	-7.15	117.20	122.20
35	YA	856	C	C2-N1-C1'	7.14	126.66	118.80
35	RA	974(A)	C	C2-N1-C1'	7.14	126.66	118.80
6	XF	46	ARG	CG-CD-NE	-7.13	96.82	111.80
35	YA	2827	C	C2-N1-C1'	7.13	126.64	118.80
1	QA	1158	C	C6-N1-C2	-7.12	117.45	120.30
45	RP	97	PRO	C-N-CA	7.12	139.49	121.70
35	YA	1881	C	C5-C6-N1	7.11	124.56	121.00
35	YA	974(A)	C	C6-N1-C2	7.11	123.14	120.30
1	QA	1065	U	P-O3'-C3'	7.11	128.23	119.70
36	YB	8	U	N1-C2-O2	7.11	127.78	122.80
1	QA	999	U	C6-N1-C1'	-7.10	111.26	121.20
35	RA	2063	C	N1-C2-O2	7.10	123.16	118.90
35	YA	828	U	N3-C2-O2	-7.10	117.23	122.20
35	RA	2559	C	C2-N1-C1'	7.09	126.60	118.80
35	RA	1774	C	C6-N1-C2	-7.09	117.46	120.30
35	RA	2128	C	N3-C2-O2	-7.09	116.94	121.90
35	YA	2210	G	C4-N9-C1'	7.08	135.71	126.50
1	QA	717	C	N1-C2-O2	7.08	123.15	118.90
36	YB	117	G	N3-C2-N2	7.07	124.85	119.90
35	RA	1502	C	C2-N1-C1'	7.07	126.58	118.80
1	QA	328	C	N3-C2-O2	-7.07	116.95	121.90
41	RH	151	ILE	N-CA-C	-7.07	91.92	111.00
26	R1	21	ARG	CG-CD-NE	7.06	126.62	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	RI	144	VAL	N-CA-C	-7.06	91.95	111.00
35	YA	652	C	N1-C2-O2	7.05	123.13	118.90
35	RA	2712	U	C2-N1-C1'	7.05	126.16	117.70
40	RG	116	ASP	C-N-CA	7.05	139.32	121.70
38	RE	54	GLN	C-N-CA	7.04	139.31	121.70
1	XA	1147	C	N1-C2-O2	7.04	123.12	118.90
35	RA	1300	U	P-O3'-C3'	7.03	128.14	119.70
1	XA	328	C	P-O3'-C3'	7.03	128.13	119.70
35	YA	2474	C	N3-C2-O2	-7.01	116.99	121.90
35	YA	286	C	C2-N1-C1'	7.01	126.51	118.80
35	YA	1920	C	C6-N1-C2	-7.00	117.50	120.30
35	RA	105	C	C2-N1-C1'	6.99	126.49	118.80
4	XD	73	ARG	CA-CB-CG	6.98	128.76	113.40
35	YA	2321	G	N3-C4-C5	-6.98	125.11	128.60
35	RA	2128	C	C6-N1-C2	-6.97	117.51	120.30
35	YA	2178	C	C6-N1-C2	-6.97	117.51	120.30
10	QJ	43	ARG	CD-NE-CZ	-6.97	113.84	123.60
35	RA	2827	C	C5-C6-N1	6.96	124.48	121.00
35	RA	2688	U	N1-C2-O2	6.96	127.67	122.80
35	RA	2591	C	C6-N1-C2	-6.95	117.52	120.30
37	RD	33	LEU	CA-CB-CG	6.95	131.28	115.30
35	RA	837	C	N1-C2-O2	6.95	123.07	118.90
45	RP	56	SER	C-N-CA	6.94	139.05	121.70
35	YA	1180	C	C2-N1-C1'	6.93	126.43	118.80
1	QA	250	A	P-O3'-C3'	6.93	128.02	119.70
35	YA	1437	C	C2-N1-C1'	6.93	126.42	118.80
1	QA	1006	C	N1-C2-O2	6.92	123.06	118.90
37	RD	35	LYS	N-CA-C	-6.92	92.31	111.00
35	YA	2128	C	N1-C2-O2	6.92	123.06	118.90
35	YA	1022	G	P-O3'-C3'	6.91	128.00	119.70
42	RI	82	ARG	CG-CD-NE	6.91	126.31	111.80
35	RA	1179	C	C2-N1-C1'	6.91	126.40	118.80
1	XA	1301	U	C6-N1-C1'	-6.91	111.53	121.20
35	YA	2585	U	C2-N1-C1'	6.91	125.99	117.70
1	QA	1528	U	P-O3'-C3'	6.90	127.98	119.70
2	QB	226	ARG	CG-CD-NE	6.90	126.28	111.80
48	RS	107	GLU	N-CA-C	-6.89	92.38	111.00
35	RA	90	U	P-O3'-C3'	6.89	127.97	119.70
1	XA	1065	U	P-O3'-C3'	6.89	127.97	119.70
1	XA	1038	C	P-O3'-C3'	6.89	127.97	119.70
35	RA	721	C	C2-N1-C1'	6.89	126.38	118.80
35	RA	288	C	C2-N1-C1'	6.88	126.37	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	RD	237	GLU	N-CA-C	-6.88	92.42	111.00
35	YA	1881	C	C6-N1-C2	-6.88	117.55	120.30
35	YA	904	C	C2-N1-C1'	6.87	126.36	118.80
35	YA	2294	C	C2-N1-C1'	6.86	126.34	118.80
35	YA	2394	C	N3-C2-O2	-6.86	117.10	121.90
1	XA	1054	C	P-O3'-C3'	6.85	127.92	119.70
48	YS	110	LEU	CA-CB-CG	6.84	131.04	115.30
47	YR	58	GLY	N-CA-C	6.84	130.21	113.10
35	RA	1022	G	P-O3'-C3'	6.84	127.91	119.70
35	YA	1640	C	N1-C2-O2	6.84	123.00	118.90
1	QA	992	U	P-O3'-C3'	6.84	127.91	119.70
1	XA	1067	A	P-O3'-C3'	6.84	127.91	119.70
1	QA	1066	C	C5-C6-N1	6.83	124.42	121.00
35	RA	1598	C	N1-C2-O2	6.83	123.00	118.90
42	YI	145	VAL	N-CA-C	6.83	129.45	111.00
51	RV	39	LEU	CB-CG-CD2	6.83	122.61	111.00
35	RA	363(E)	U	N3-C2-O2	-6.83	117.42	122.20
10	QJ	79	ARG	CD-NE-CZ	6.83	133.16	123.60
35	YA	273(F)	C	C6-N1-C2	-6.83	117.57	120.30
1	QA	283	C	N1-C2-O2	6.82	123.00	118.90
35	YA	2177	C	N3-C2-O2	-6.82	117.12	121.90
1	XA	1260	C	C6-N1-C2	-6.82	117.57	120.30
1	QA	687	A	P-O3'-C3'	6.81	127.88	119.70
35	YA	2584	U	N3-C2-O2	-6.81	117.43	122.20
1	XA	1086	U	N3-C2-O2	-6.80	117.44	122.20
1	QA	1067	A	P-O3'-C3'	6.80	127.86	119.70
35	RA	1171	G	P-O3'-C3'	6.80	127.86	119.70
1	QA	186	C	C2-N1-C1'	6.80	126.28	118.80
35	YA	1956	U	N1-C2-O2	6.80	127.56	122.80
1	XA	1000	A	P-O3'-C3'	6.79	127.84	119.70
35	RA	2787	C	C5-C6-N1	6.78	124.39	121.00
35	YA	1225	C	N3-C4-C5	-6.78	119.19	121.90
35	YA	1314	C	C5-C6-N1	6.78	124.39	121.00
35	YA	2210	G	N3-C4-N9	6.78	130.07	126.00
29	Y4	67	TYR	CB-CA-C	6.78	123.95	110.40
17	QQ	101	ARG	CA-CB-CG	-6.77	98.50	113.40
39	RF	133	ASN	N-CA-C	-6.77	92.72	111.00
35	YA	2226	C	C6-N1-C2	-6.77	117.59	120.30
11	XK	96	ARG	CD-NE-CZ	6.77	133.07	123.60
1	XA	58	C	C6-N1-C2	-6.76	117.59	120.30
38	YE	101	ARG	N-CA-CB	-6.76	98.43	110.60
1	QA	181	G	P-O3'-C3'	6.76	127.81	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	687	A	P-O3'-C3'	6.75	127.80	119.70
35	YA	607	U	N1-C2-O2	6.75	127.52	122.80
2	XB	178	ARG	CA-CB-CG	6.74	128.23	113.40
35	RA	2394	C	N1-C2-O2	6.73	122.94	118.90
35	RA	2808	U	N3-C2-O2	-6.72	117.49	122.20
1	XA	748	C	P-O3'-C3'	6.72	127.77	119.70
35	YA	1171	G	P-O3'-C3'	6.72	127.77	119.70
35	YA	2584	U	C2-N1-C1'	6.72	125.76	117.70
35	YA	607	U	N3-C2-O2	-6.72	117.50	122.20
35	YA	1979	C	C6-N1-C2	-6.72	117.61	120.30
1	QA	932	C	C2-N1-C1'	6.71	126.19	118.80
36	YB	31	C	C6-N1-C1'	-6.71	112.74	120.80
1	QA	748	C	P-O3'-C3'	6.71	127.75	119.70
35	RA	119	A	P-O3'-C3'	6.71	127.75	119.70
1	QA	186	C	N1-C2-O2	6.71	122.92	118.90
1	QA	1224	G	N3-C4-N9	-6.71	121.97	126.00
35	RA	907	U	N3-C2-O2	-6.70	117.51	122.20
42	RI	142	VAL	C-N-CA	6.70	138.44	121.70
1	XA	992	U	P-O3'-C3'	6.69	127.73	119.70
1	XA	1381	U	C2-N1-C1'	6.68	125.72	117.70
35	RA	2063	C	N3-C2-O2	-6.68	117.23	121.90
35	YA	975	G	N3-C4-N9	6.67	130.00	126.00
1	QA	1147	C	N3-C2-O2	-6.67	117.23	121.90
35	RA	2447	G	P-O3'-C3'	6.67	127.71	119.70
1	QA	1066	C	C6-N1-C2	-6.67	117.63	120.30
35	YA	1005	C	C2-N1-C1'	6.67	126.13	118.80
35	RA	273(C)	C	N1-C2-O2	6.66	122.90	118.90
35	RA	2118	U	C2-N1-C1'	6.66	125.70	117.70
35	YA	288	C	C5-C6-N1	6.66	124.33	121.00
35	RA	404	C	P-O3'-C3'	6.66	127.69	119.70
4	XD	47	ARG	CA-CB-CG	-6.65	98.76	113.40
35	YA	119	A	P-O3'-C3'	6.65	127.68	119.70
1	XA	328	C	C5-C6-N1	6.65	124.32	121.00
1	QA	1066	C	N3-C2-O2	-6.64	117.25	121.90
1	XA	1439	C	C2-N1-C1'	6.64	126.10	118.80
35	RA	2439	A	P-O3'-C3'	6.64	127.66	119.70
35	YA	2212	A	OP1-P-OP2	-6.63	109.65	119.60
22	QV	32	C	N1-C2-O2	6.63	122.88	118.90
13	QM	11	ARG	CB-CA-C	6.63	123.65	110.40
29	R4	63	TYR	CA-CB-CG	6.62	125.98	113.40
1	XA	137	C	C2-N1-C1'	6.62	126.08	118.80
35	RA	2808	U	N1-C2-O2	6.62	127.43	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	1930	G	P-O3'-C3'	6.62	127.64	119.70
18	XR	42	ARG	CG-CD-NE	-6.62	97.90	111.80
27	R2	71	ASN	C-N-CA	6.61	138.22	121.70
35	RA	2827	C	C6-N1-C2	-6.61	117.66	120.30
35	YA	1588	C	C2-N1-C1'	6.61	126.07	118.80
1	XA	442	C	C2-N1-C1'	6.60	126.06	118.80
48	YS	109	GLY	C-N-CA	6.59	138.19	121.70
16	QP	54	GLU	N-CA-CB	-6.59	98.74	110.60
35	RA	1956	U	N1-C2-O2	6.59	127.41	122.80
1	QA	454	C	N3-C2-O2	-6.59	117.29	121.90
35	RA	2584	U	C2-N1-C1'	6.58	125.60	117.70
35	YA	2321	G	C4-N9-C1'	6.58	135.06	126.50
36	RB	47	C	N1-C2-O2	6.58	122.85	118.90
1	XA	5	U	P-O3'-C3'	6.58	127.59	119.70
35	YA	893	C	C2-N1-C1'	6.57	126.02	118.80
36	YB	77	U	N1-C2-O2	6.57	127.39	122.80
1	QA	913	A	P-O3'-C3'	6.56	127.58	119.70
35	RA	1735	C	C2-N1-C1'	6.56	126.02	118.80
47	RR	76	VAL	N-CA-C	-6.56	93.29	111.00
35	YA	1417	C	C5-C6-N1	6.55	124.27	121.00
35	YA	69	C	N3-C2-O2	-6.54	117.32	121.90
35	RA	1294	U	N3-C2-O2	-6.54	117.62	122.20
35	YA	708	C	C2-N1-C1'	6.54	125.99	118.80
35	RA	2868	A	N7-C8-N9	6.54	117.07	113.80
23	QX	11	U	P-O3'-C3'	6.53	127.54	119.70
1	XA	1137	C	P-O3'-C3'	6.53	127.54	119.70
35	YA	2791	C	N1-C2-N3	6.53	123.77	119.20
1	QA	792	A	P-O3'-C3'	6.53	127.53	119.70
46	RQ	85	LYS	CD-CE-NZ	-6.53	96.68	111.70
1	QA	1263	C	C2-N1-C1'	6.53	125.98	118.80
35	RA	2688	U	C2-N1-C1'	6.53	125.53	117.70
35	RA	1882	C	C2-N1-C1'	6.52	125.97	118.80
1	QA	812	C	P-O3'-C3'	6.52	127.53	119.70
35	RA	1699	G	P-O3'-C3'	6.50	127.51	119.70
1	QA	484	G	P-O3'-C3'	6.50	127.50	119.70
35	RA	435	C	N1-C2-O2	6.49	122.79	118.90
35	YA	32	C	C2-N1-C1'	6.49	125.93	118.80
38	RE	64	LYS	CD-CE-NZ	-6.48	96.80	111.70
35	YA	358	U	C2-N1-C1'	6.48	125.47	117.70
1	QA	442	C	C2-N1-C1'	6.47	125.92	118.80
1	QA	547	A	P-O3'-C3'	6.47	127.47	119.70
35	RA	544	C	C2-N1-C1'	6.47	125.92	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	93	C	C6-N1-C2	-6.46	117.71	120.30
27	R2	72	ALA	N-CA-C	6.46	128.44	111.00
35	RA	2559	C	C6-N1-C2	-6.46	117.72	120.30
23	XX	13	A	O5'-P-OP1	6.46	118.45	110.70
35	RA	1437	C	C5-C6-N1	6.46	124.23	121.00
35	YA	867	C	N1-C2-O2	6.46	122.77	118.90
40	RG	146	TYR	CA-CB-CG	6.45	125.66	113.40
1	XA	60	A	P-O3'-C3'	6.45	127.44	119.70
35	YA	358	U	N1-C2-O2	6.45	127.31	122.80
33	R8	46	ARG	CG-CD-NE	-6.45	98.26	111.80
49	YT	133	GLU	CB-CA-C	-6.45	97.51	110.40
35	RA	2065	C	C5-C6-N1	6.44	124.22	121.00
4	QD	208	SER	N-CA-C	-6.44	93.62	111.00
1	XA	754	C	N3-C2-O2	-6.44	117.39	121.90
35	YA	1499	C	C2-N1-C1'	6.44	125.88	118.80
35	RA	1640	C	N3-C2-O2	-6.44	117.39	121.90
21	QU	15	ARG	CG-CD-NE	-6.43	98.29	111.80
35	YA	1314	C	C6-N1-C2	-6.43	117.73	120.30
35	RA	227	A	P-O3'-C3'	6.43	127.42	119.70
35	RA	2666	C	C6-N1-C2	-6.43	117.73	120.30
24	QZ	22	ARG	NE-CZ-NH2	6.43	123.51	120.30
36	YB	31	C	C5-C6-N1	6.42	124.21	121.00
35	RA	2294	C	C6-N1-C2	-6.42	117.73	120.30
1	XA	1535	C	C2-N1-C1'	6.42	125.86	118.80
1	XA	547	A	P-O3'-C3'	6.41	127.39	119.70
1	QA	1346	A	P-O3'-C3'	6.40	127.38	119.70
1	XA	1382	C	N1-C2-O2	6.40	122.74	118.90
1	XA	75	C	C2-N1-C1'	6.40	125.84	118.80
35	YA	234	C	N1-C2-O2	6.40	122.74	118.90
35	YA	270(U)	C	N3-C2-O2	-6.39	117.42	121.90
1	XA	893	C	C5-C6-N1	6.39	124.20	121.00
35	RA	2847	U	N1-C2-O2	6.38	127.27	122.80
35	RA	2092	U	P-O3'-C3'	6.38	127.35	119.70
35	RA	234	C	N1-C2-O2	6.37	122.72	118.90
35	RA	1979	C	C6-N1-C2	-6.37	117.75	120.30
1	QA	1260	C	N3-C2-O2	-6.36	117.45	121.90
35	YA	883	G	N1-C6-O6	-6.36	116.08	119.90
35	YA	1640	C	C6-N1-C2	-6.36	117.76	120.30
1	QA	1325	C	C2-N1-C1'	6.36	125.79	118.80
1	XA	368	U	N1-C2-O2	-6.36	118.35	122.80
35	RA	1314	C	C5-C6-N1	6.35	124.17	121.00
35	YA	2712	U	N1-C2-O2	6.35	127.24	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	RZ	62	PRO	C-N-CA	6.34	137.56	121.70
36	RB	77	U	N1-C2-O2	6.34	127.24	122.80
1	QA	1006	C	C5-C6-N1	6.33	124.17	121.00
1	XA	1158	C	C2-N1-C1'	6.33	125.76	118.80
36	YB	118	G	N1-C6-O6	-6.33	116.10	119.90
35	RA	1653	G	P-O3'-C3'	6.33	127.29	119.70
35	YA	2447	G	P-O3'-C3'	6.33	127.29	119.70
35	RA	387	U	P-O3'-C3'	6.32	127.29	119.70
36	RB	3	C	N1-C2-O2	6.32	122.69	118.90
35	YA	2688	U	N3-C2-O2	-6.32	117.78	122.20
35	RA	1644	C	N1-C2-O2	6.31	122.69	118.90
35	RA	2712	U	O4'-C1'-N1	6.31	113.25	108.20
36	YB	31	C	N3-C2-O2	-6.31	117.48	121.90
35	RA	2752	C	N1-C2-O2	6.31	122.69	118.90
35	RA	372	G	P-O3'-C3'	6.31	127.27	119.70
35	RA	1406	U	C2-N1-C1'	6.31	125.27	117.70
1	QA	428	G	P-O3'-C3'	6.31	127.27	119.70
35	YA	2439	A	P-O3'-C3'	6.31	127.27	119.70
1	XA	1498	U	P-O3'-C3'	6.30	127.26	119.70
35	YA	2874	C	C2-N1-C1'	6.30	125.73	118.80
35	YA	2312	U	N1-C2-O2	6.29	127.20	122.80
35	RA	2666	C	C2-N1-C1'	6.29	125.72	118.80
1	XA	1004	A	P-O3'-C3'	6.29	127.25	119.70
24	XZ	83	HIS	C-N-CA	6.29	137.42	121.70
1	XA	913	A	P-O3'-C3'	6.28	127.24	119.70
1	QA	115	G	P-O3'-C3'	6.28	127.23	119.70
35	RA	2863	C	C2-N1-C1'	6.28	125.70	118.80
1	QA	1347	G	P-O3'-C3'	6.27	127.22	119.70
35	RA	974(A)	C	N1-C2-O2	6.27	122.66	118.90
35	RA	2585	U	C2-N1-C1'	6.27	125.22	117.70
13	QM	8	GLU	C-N-CA	6.26	137.35	121.70
35	RA	2477	C	C2-N1-C1'	6.26	125.69	118.80
50	RU	92	ARG	C-N-CA	6.26	137.35	121.70
1	XA	932	C	C2-N1-C1'	6.26	125.69	118.80
35	YA	1882	C	N1-C2-O2	6.26	122.66	118.90
1	QA	1498	U	P-O3'-C3'	6.25	127.21	119.70
35	RA	1417	C	C5-C6-N1	6.25	124.13	121.00
35	RA	2874	C	C2-N1-C1'	6.25	125.68	118.80
35	RA	1318	C	C2-N1-C1'	6.25	125.67	118.80
1	XA	1190	G	P-O3'-C3'	6.25	127.20	119.70
35	YA	2211	G	P-O3'-C3'	6.25	127.20	119.70
35	YA	2312	U	N3-C2-O2	-6.25	117.83	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	1644	C	N3-C2-O2	-6.24	117.53	121.90
36	YB	77	U	N3-C2-O2	-6.24	117.83	122.20
1	QA	485	G	OP2-P-O3'	6.24	118.92	105.20
35	YA	2559	C	N1-C2-O2	6.24	122.64	118.90
35	YA	343	C	C6-N1-C2	-6.23	117.81	120.30
35	RA	797	C	C5-C6-N1	6.23	124.11	121.00
35	RA	907	U	N1-C2-O2	6.23	127.16	122.80
1	XA	1535	C	N3-C2-O2	-6.23	117.54	121.90
35	RA	1474	C	N1-C2-O2	6.22	122.64	118.90
35	RA	1992	G	P-O3'-C3'	6.22	127.17	119.70
35	YA	140	A	N7-C8-N9	6.22	116.91	113.80
1	XA	792	A	P-O3'-C3'	6.22	127.17	119.70
35	YA	270(Q)	C	N1-C2-O2	6.22	122.63	118.90
35	RA	105	C	N1-C2-O2	6.22	122.63	118.90
47	RR	75	LEU	CA-CB-CG	6.21	129.59	115.30
8	XH	60	ARG	NE-CZ-NH2	-6.21	117.19	120.30
35	RA	1332	G	N7-C8-N9	6.21	116.21	113.10
35	RA	2188	C	N3-C2-O2	-6.21	117.55	121.90
35	YA	2585	U	N1-C2-O2	6.21	127.15	122.80
35	RA	1588	C	C5-C6-N1	6.21	124.10	121.00
1	QA	60	A	P-O3'-C3'	6.21	127.15	119.70
35	RA	1180	C	N1-C2-O2	6.21	122.62	118.90
35	YA	2474	C	C6-N1-C2	-6.21	117.82	120.30
35	YA	93	C	C5-C6-N1	6.20	124.10	121.00
35	YA	2712	U	O4'-C1'-N1	6.20	113.16	108.20
35	RA	837	C	C6-N1-C2	-6.20	117.82	120.30
35	YA	1658	C	C5-C6-N1	6.20	124.10	121.00
1	QA	960	U	N1-C2-O2	6.20	127.14	122.80
35	RA	837	C	N3-C2-O2	-6.20	117.56	121.90
35	RA	286	C	N1-C2-O2	6.19	122.62	118.90
35	YA	2477	C	C2-N1-C1'	6.19	125.61	118.80
35	YA	2226	C	N3-C2-O2	-6.19	117.57	121.90
1	QA	268	C	C2-N1-C1'	6.19	125.61	118.80
35	YA	1225	C	C4'-C3'-C2'	6.19	108.79	102.60
35	YA	153	C	N1-C2-O2	6.19	122.61	118.90
35	YA	270(U)	C	C2-N1-C1'	6.19	125.61	118.80
35	YA	527	C	N1-C2-O2	6.19	122.61	118.90
35	RA	2481	G	P-O3'-C3'	6.18	127.12	119.70
1	XA	428	G	P-O3'-C3'	6.18	127.12	119.70
1	XA	1301	U	C5-C6-N1	6.18	125.79	122.70
35	RA	2559	C	C5-C6-N1	6.18	124.09	121.00
35	YA	1437	C	C5-C6-N1	6.18	124.09	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	1505	C	C5-C6-N1	6.18	124.09	121.00
35	YA	1437	C	C6-N1-C2	-6.18	117.83	120.30
1	XA	1128	C	C6-N1-C2	-6.18	117.83	120.30
37	YD	274	ARG	C-N-CA	6.18	137.14	121.70
1	XA	1007	C	C5-C6-N1	6.17	124.09	121.00
35	YA	2226	C	C5-C6-N1	6.17	124.09	121.00
35	RA	1437	C	C6-N1-C2	-6.17	117.83	120.30
1	QA	1224	G	C4-N9-C1'	-6.16	118.49	126.50
35	YA	2063	C	C6-N1-C2	-6.16	117.83	120.30
35	YA	277	C	N3-C2-O2	-6.16	117.59	121.90
35	RA	1881	C	C6-N1-C2	-6.16	117.84	120.30
35	RA	708	C	N1-C2-O2	6.16	122.59	118.90
2	XB	235	SER	C-N-CA	6.16	137.09	121.70
35	YA	1644	C	N1-C2-O2	6.16	122.59	118.90
9	QI	83	ARG	CA-CB-CG	-6.15	99.86	113.40
35	RA	1180	C	C5-C6-N1	6.15	124.08	121.00
35	RA	1407	C	N1-C2-O2	6.15	122.59	118.90
1	QA	1532	U	P-O3'-C3'	6.15	127.08	119.70
42	YI	14	ASP	CB-CG-OD1	6.14	123.83	118.30
22	QV	34	C	C2-N1-C1'	6.14	125.56	118.80
1	QA	1362(A)	C	N3-C2-O2	-6.14	117.60	121.90
35	RA	9	U	N1-C2-O2	6.14	127.10	122.80
35	YA	2752	C	N1-C2-O2	6.14	122.58	118.90
35	YA	2294	C	C5-C6-N1	6.14	124.07	121.00
35	YA	752	A	P-O3'-C3'	6.14	127.06	119.70
37	RD	122	ASP	C-N-CA	6.13	137.02	121.70
1	QA	31	G	P-O3'-C3'	6.12	127.05	119.70
1	XA	1532	U	P-O3'-C3'	6.12	127.05	119.70
35	YA	1505	C	C2-N1-C1'	6.12	125.53	118.80
35	RA	828	U	N1-C2-O2	6.12	127.08	122.80
35	RA	1204	A	O4'-C1'-N9	6.12	113.10	108.20
35	RA	2584	U	C6-N1-C2	-6.12	117.33	121.00
39	RF	99	TYR	CA-CB-CG	6.12	125.02	113.40
49	YT	99	LEU	CA-CB-CG	6.12	129.37	115.30
35	RA	2128	C	C5-C6-N1	6.11	124.06	121.00
24	XZ	84	TYR	N-CA-C	-6.11	94.50	111.00
35	YA	837	C	N3-C2-O2	-6.11	117.62	121.90
56	ZA	1	C	N1-C2-O2	6.11	122.57	118.90
35	YA	974	G	C4-N9-C1'	-6.11	118.56	126.50
35	YA	1653	G	P-O3'-C3'	6.10	127.03	119.70
35	RA	105	C	C5-C6-N1	6.10	124.05	121.00
33	R8	36	LYS	N-CA-C	-6.10	94.53	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	1407	C	C5-C6-N1	6.10	124.05	121.00
1	QA	435	C	C2-N1-C1'	6.10	125.51	118.80
39	YF	197	ASP	N-CA-C	-6.10	94.53	111.00
1	QA	1406	U	N1-C2-O2	6.10	127.07	122.80
1	QA	353	A	OP2-P-O3'	6.09	118.61	105.20
35	RA	2527	C	C2-N1-C1'	6.09	125.50	118.80
36	YB	8	U	N3-C2-O2	-6.09	117.94	122.20
35	RA	2585	U	N1-C2-O2	6.09	127.06	122.80
1	XA	812	C	P-O3'-C3'	6.09	127.01	119.70
35	YA	1226	G	O5'-P-OP1	-6.09	100.22	105.70
1	XA	960	U	P-O3'-C3'	6.09	127.01	119.70
35	YA	1294	U	C5-C6-N1	6.09	125.74	122.70
35	RA	1300	U	OP2-P-O3'	6.09	118.59	105.20
35	YA	358	U	N3-C2-O2	-6.09	117.94	122.20
35	RA	358	U	N1-C2-O2	6.08	127.06	122.80
35	RA	1640	C	C6-N1-C2	-6.08	117.87	120.30
35	YA	2177	C	C6-N1-C2	-6.08	117.87	120.30
35	RA	288	C	N1-C2-O2	6.07	122.55	118.90
35	YA	930	U	N1-C2-O2	6.07	127.05	122.80
36	YB	47	C	C2-N1-C1'	6.07	125.48	118.80
35	YA	856	C	N1-C2-O2	6.07	122.54	118.90
35	RA	1406	U	N1-C2-O2	6.07	127.05	122.80
35	YA	1559	G	P-O3'-C3'	6.06	126.98	119.70
1	XA	115	G	P-O3'-C3'	6.06	126.98	119.70
1	XA	1325	C	C6-N1-C2	-6.06	117.88	120.30
1	XA	186	C	N1-C2-O2	6.05	122.53	118.90
35	RA	1658	C	C5-C6-N1	6.04	124.02	121.00
1	XA	74	C	C2-N1-C1'	6.04	125.45	118.80
35	RA	1474	C	C2-N1-C1'	6.04	125.45	118.80
35	RA	1588	C	N1-C2-O2	6.04	122.53	118.90
1	XA	690	G	O4'-C1'-N9	6.04	113.03	108.20
1	XA	135	C	C5-C6-N1	6.04	124.02	121.00
1	XA	754	C	C6-N1-C2	-6.04	117.89	120.30
35	YA	435	C	N1-C2-O2	6.04	122.52	118.90
35	RA	2129	C	C5-C6-N1	6.03	124.02	121.00
35	RA	2827	C	N1-C2-O2	6.03	122.52	118.90
1	QA	201	C	P-O3'-C3'	6.03	126.94	119.70
35	RA	708	C	C5-C6-N1	6.03	124.01	121.00
35	RA	2889	C	C2-N1-C1'	6.03	125.43	118.80
35	YA	1644	C	N3-C2-O2	-6.03	117.68	121.90
35	YA	2041	U	N1-C2-O2	6.02	127.02	122.80
1	QA	1224	G	C8-N9-C1'	6.02	134.82	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	828	U	C6-N1-C1'	-6.02	112.77	121.20
35	RA	279	C	C6-N1-C2	-6.01	117.89	120.30
40	YG	72	ARG	NE-CZ-NH2	6.01	123.31	120.30
35	YA	2610	C	P-O3'-C3'	6.01	126.91	119.70
35	YA	1152	C	C2-N1-C1'	6.01	125.41	118.80
35	YA	2312	U	C6-N1-C2	-6.01	117.40	121.00
35	RA	1085	A	P-O3'-C3'	6.00	126.91	119.70
1	QA	1395	C	N1-C2-O2	6.00	122.50	118.90
49	RT	59	THR	N-CA-C	-6.00	94.79	111.00
51	YV	50	PRO	CA-N-CD	-6.00	103.10	111.50
35	RA	2651	C	N1-C2-O2	6.00	122.50	118.90
36	RB	88	C	N1-C2-O2	6.00	122.50	118.90
1	QA	1033	G	N3-C4-N9	6.00	129.60	126.00
35	YA	1735	C	C2-N1-C1'	6.00	125.40	118.80
2	QB	12	GLU	CG-CD-OE1	-6.00	106.31	118.30
35	RA	1699	G	OP1-P-O3'	6.00	118.39	105.20
1	QA	972	C	C6-N1-C2	-5.99	117.90	120.30
35	RA	894	C	N1-C2-O2	5.99	122.50	118.90
35	YA	817	C	C6-N1-C2	-5.99	117.91	120.30
35	RA	2776	A	P-O3'-C3'	5.99	126.88	119.70
35	YA	2726	U	N3-C2-O2	-5.99	118.01	122.20
35	RA	512	G	O4'-C1'-N9	5.98	112.99	108.20
35	YA	1152	C	C6-N1-C2	-5.98	117.91	120.30
1	QA	201	C	OP1-P-O3'	5.98	118.36	105.20
35	RA	1598	C	C2-N1-C1'	5.98	125.38	118.80
35	RA	1881	C	C5-C6-N1	5.98	123.99	121.00
35	RA	2394	C	C2-N1-C1'	5.98	125.38	118.80
35	YA	9	U	N1-C2-O2	5.98	126.99	122.80
35	RA	1881	C	C6-N1-C1'	-5.98	113.62	120.80
1	XA	186	C	C2-N1-C1'	5.97	125.37	118.80
35	RA	828	U	N3-C2-O2	-5.97	118.02	122.20
35	YA	2776	A	P-O3'-C3'	5.97	126.86	119.70
1	XA	330	C	C6-N1-C2	-5.97	117.91	120.30
35	YA	2827	C	N1-C2-O2	5.96	122.48	118.90
1	XA	250	A	P-O3'-C3'	5.96	126.85	119.70
1	QA	1260	C	N1-C2-O2	5.96	122.48	118.90
1	QA	749	C	C6-N1-C2	-5.96	117.92	120.30
35	YA	2849	U	P-O3'-C3'	5.96	126.85	119.70
35	RA	1332	G	C4-N9-C1'	5.96	134.24	126.50
35	RA	2896	C	N1-C2-O2	5.96	122.47	118.90
1	XA	1007	C	P-O3'-C3'	5.96	126.85	119.70
35	RA	1882	C	C6-N1-C2	-5.95	117.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	114	U	C2-N1-C1'	5.95	124.84	117.70
35	RA	828	U	C2-N1-C1'	5.95	124.84	117.70
35	RA	2477	C	N1-C2-O2	5.95	122.47	118.90
35	RA	2294	C	C2-N1-C1'	5.94	125.34	118.80
35	YA	930	U	N3-C2-O2	-5.94	118.04	122.20
35	YA	1233	C	C2-N1-C1'	5.94	125.34	118.80
1	QA	496	A	C2-N3-C4	5.94	113.57	110.60
35	RA	2873	A	N7-C8-N9	5.94	116.77	113.80
45	RP	26	GLY	N-CA-C	-5.94	98.26	113.10
14	XN	13	THR	N-CA-C	5.94	127.03	111.00
35	RA	2849	U	P-O3'-C3'	5.93	126.82	119.70
35	RA	1180	C	C6-N1-C2	-5.93	117.93	120.30
1	XA	1000	A	OP1-P-O3'	5.93	118.25	105.20
4	QD	33	MET	CG-SD-CE	-5.93	90.72	100.20
35	RA	2827	C	C6-N1-C1'	-5.93	113.69	120.80
42	RI	120	ILE	N-CA-C	5.93	127.00	111.00
35	YA	2226	C	C2-N1-C1'	5.93	125.32	118.80
35	RA	358	U	N3-C2-O2	-5.92	118.05	122.20
1	XA	1502	A	N7-C8-N9	5.92	116.76	113.80
35	RA	1233	C	C6-N1-C2	-5.92	117.93	120.30
1	XA	328	C	C6-N1-C1'	-5.92	113.69	120.80
35	RA	1437	C	C2-N1-C1'	5.92	125.31	118.80
35	RA	2226	C	N3-C2-O2	-5.91	117.76	121.90
29	R4	13	ARG	CG-CD-NE	5.91	124.21	111.80
35	RA	2689	U	P-O3'-C3'	5.91	126.79	119.70
35	RA	69	C	C2-N1-C1'	5.91	125.30	118.80
35	RA	1694	C	P-O3'-C3'	5.91	126.79	119.70
1	QA	999	U	C5-C6-N1	5.90	125.65	122.70
45	YP	71	VAL	N-CA-C	5.90	126.93	111.00
35	RA	279	C	C2-N1-C1'	5.90	125.29	118.80
10	QJ	28	ARG	NE-CZ-NH1	5.90	123.25	120.30
35	RA	1588	C	C6-N1-C2	-5.90	117.94	120.30
35	YA	857	C	C2-N1-C1'	5.90	125.29	118.80
1	QA	1031	G	C4-N9-C1'	5.89	134.16	126.50
35	RA	2652	C	C6-N1-C2	-5.89	117.94	120.30
35	RA	1506	C	C2-N1-C1'	5.89	125.28	118.80
35	RA	9	U	C2-N1-C1'	5.89	124.77	117.70
35	YA	1474	C	C2-N1-C1'	5.89	125.28	118.80
35	RA	2467	C	C6-N1-C1'	5.88	127.86	120.80
1	QA	1383	C	N1-C2-O2	5.88	122.43	118.90
1	XA	1300	G	P-O3'-C3'	5.88	126.75	119.70
35	YA	1675	C	N3-C2-O2	-5.88	117.79	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	1233	C	C2-N1-C1'	5.88	125.26	118.80
1	QA	1007	C	P-O3'-C3'	5.87	126.75	119.70
1	QA	525	C	C5-C6-N1	5.87	123.93	121.00
1	XA	442	C	C6-N1-C2	-5.87	117.95	120.30
1	QA	419	C	C2-N1-C1'	5.87	125.25	118.80
35	RA	2210	G	C4-N9-C1'	5.86	134.12	126.50
10	QJ	43	ARG	NE-CZ-NH1	-5.86	117.37	120.30
35	YA	2688	U	C2-N1-C1'	5.86	124.73	117.70
35	YA	2178	C	C2-N1-C1'	5.86	125.24	118.80
1	QA	1000	A	P-O3'-C3'	5.85	126.72	119.70
35	RA	1909	C	C2-N1-C1'	5.85	125.24	118.80
1	XA	341	C	C2-N1-C1'	5.85	125.24	118.80
35	YA	1267	U	C2-N1-C1'	5.85	124.72	117.70
35	YA	2128	C	C6-N1-C1'	-5.85	113.78	120.80
35	RA	1911	U	N1-C2-O2	5.85	126.89	122.80
35	YA	797	C	C6-N1-C2	-5.85	117.96	120.30
1	XA	315	A	P-O3'-C3'	5.85	126.72	119.70
1	QA	5	U	P-O3'-C3'	5.84	126.71	119.70
35	YA	277	C	C6-N1-C2	-5.84	117.96	120.30
1	XA	92	G	P-O3'-C3'	5.84	126.71	119.70
1	XA	1190	G	OP2-P-O3'	5.84	118.05	105.20
35	YA	286	C	N1-C2-O2	5.84	122.41	118.90
36	YB	37	C	N1-C2-O2	5.83	122.40	118.90
35	RA	2211	G	P-O3'-C3'	5.83	126.70	119.70
35	RA	416	C	C2-N1-C1'	5.83	125.21	118.80
35	YA	1911	U	N1-C2-O2	5.83	126.88	122.80
35	RA	198	C	C5-C6-N1	5.83	123.91	121.00
1	XA	749	C	C6-N1-C2	-5.82	117.97	120.30
1	XA	283	C	N1-C2-O2	5.82	122.39	118.90
16	XP	32	TYR	CA-CB-CG	5.82	124.45	113.40
35	YA	2343	C	C2-N1-C1'	5.82	125.20	118.80
42	YI	144	VAL	C-N-CA	5.82	136.24	121.70
1	QA	283	C	C5-C6-N1	5.81	123.91	121.00
1	XA	1031	G	N3-C4-C5	-5.81	125.69	128.60
35	RA	1559	G	P-O3'-C3'	5.81	126.68	119.70
1	XA	137	C	N1-C2-O2	5.81	122.39	118.90
51	RV	15	GLU	CB-CA-C	5.81	122.02	110.40
51	YV	85	LYS	CG-CD-CE	5.81	129.33	111.90
1	QA	1301	U	C6-N1-C2	-5.81	117.52	121.00
17	QQ	101	ARG	N-CA-C	-5.81	95.32	111.00
2	QB	230	VAL	C-N-CA	5.80	136.20	121.70
35	RA	783	A	C2-N3-C4	5.80	113.50	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	270(Q)	C	C6-N1-C2	-5.80	117.98	120.30
23	QX	11	U	OP1-P-O3'	5.80	117.96	105.20
35	RA	343	C	C6-N1-C2	-5.80	117.98	120.30
35	YA	289	A	N7-C8-N9	5.80	116.70	113.80
36	YB	27	C	N3-C2-O2	-5.80	117.84	121.90
1	XA	1031	G	C4-N9-C1'	5.80	134.03	126.50
35	YA	2701	C	C6-N1-C2	-5.79	117.98	120.30
35	YA	114	U	C2-N1-C1'	5.79	124.65	117.70
35	YA	1313	U	C6-N1-C1'	-5.79	113.09	121.20
35	RA	343	C	N1-C2-O2	5.79	122.37	118.90
35	RA	2527	C	C6-N1-C2	-5.79	117.99	120.30
35	YA	1656	C	C5-C6-N1	5.78	123.89	121.00
35	YA	537	C	C5-C6-N1	5.78	123.89	121.00
1	QA	405	U	N1-C2-O2	5.77	126.84	122.80
35	RA	1502	C	N1-C2-O2	5.77	122.36	118.90
35	RA	1318	C	C5-C6-N1	5.76	123.88	121.00
1	QA	1007	C	C2-N1-C1'	5.76	125.14	118.80
1	QA	1137	C	P-O3'-C3'	5.76	126.61	119.70
35	RA	708	C	C6-N1-C2	-5.76	118.00	120.30
1	XA	442	C	C5-C6-N1	5.76	123.88	121.00
35	RA	2667	C	N3-C2-O2	-5.75	117.87	121.90
43	YN	35	ARG	N-CA-C	-5.75	95.47	111.00
35	YA	1656	C	C6-N1-C2	-5.75	118.00	120.30
35	RA	2108	C	C2-N1-C1'	5.75	125.12	118.80
1	QA	960	U	P-O3'-C3'	5.75	126.60	119.70
35	RA	2575	C	C5-C6-N1	5.74	123.87	121.00
35	YA	1781	C	N1-C2-O2	5.74	122.34	118.90
1	QA	754	C	C6-N1-C2	-5.74	118.00	120.30
1	QA	1536	C	N1-C2-O2	5.74	122.34	118.90
36	YB	66	A	P-O3'-C3'	5.74	126.59	119.70
35	RA	487	C	N1-C2-O2	5.74	122.34	118.90
35	RA	527	C	N1-C2-O2	5.74	122.34	118.90
35	RA	1640	C	C5-C6-N1	5.74	123.87	121.00
43	RN	114	ARG	N-CA-C	-5.74	95.52	111.00
1	XA	243	A	P-O3'-C3'	5.73	126.58	119.70
35	RA	105	C	C6-N1-C2	-5.73	118.01	120.30
35	YA	1675	C	N1-C2-O2	5.73	122.34	118.90
35	RA	2294	C	C5-C6-N1	5.73	123.86	121.00
1	XA	1303	C	N1-C2-O2	5.73	122.34	118.90
1	QA	960	U	N3-C2-O2	-5.73	118.19	122.20
35	RA	752	A	P-O3'-C3'	5.73	126.57	119.70
1	XA	279	A	P-O3'-C3'	5.73	126.57	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	190	G	P-O3'-C3'	5.72	126.57	119.70
35	RA	1188	U	N1-C2-O2	5.72	126.81	122.80
35	YA	1774	C	C2-N1-C1'	5.72	125.10	118.80
1	XA	1109	C	N1-C2-O2	5.72	122.33	118.90
35	RA	2466	C	N1-C2-O2	5.72	122.33	118.90
35	YA	2342	C	C6-N1-C2	-5.72	118.01	120.30
35	YA	1781	C	C2-N1-C1'	5.72	125.09	118.80
35	RA	1499	C	C2-N1-C1'	5.71	125.09	118.80
35	YA	277	C	C2-N1-C1'	5.71	125.08	118.80
35	YA	12	U	N3-C2-O2	-5.71	118.20	122.20
35	RA	806	C	C6-N1-C2	-5.71	118.02	120.30
35	YA	2128	C	C5-C6-N1	5.71	123.86	121.00
35	RA	2467	C	C6-N1-C2	-5.71	118.02	120.30
35	YA	1370	C	C2-N1-C1'	5.70	125.07	118.80
35	RA	2527	C	C5-C6-N1	5.70	123.85	121.00
37	YD	88	ARG	NE-CZ-NH2	-5.70	117.45	120.30
35	YA	965	C	C6-N1-C2	-5.70	118.02	120.30
35	YA	1640	C	C2-N1-C1'	5.70	125.06	118.80
35	YA	1640	C	C5-C6-N1	5.69	123.85	121.00
35	YA	1915	U	N1-C2-O2	5.69	126.78	122.80
1	XA	442	C	N1-C2-O2	5.69	122.31	118.90
35	YA	172	C	C2-N1-C1'	5.69	125.06	118.80
35	RA	1679	U	N3-C2-O2	-5.69	118.22	122.20
35	YA	2307	G	O4'-C1'-N9	5.69	112.75	108.20
1	XA	330	C	N3-C2-O2	-5.69	117.92	121.90
35	YA	2210	G	C8-N9-C1'	-5.69	119.61	127.00
1	QA	1306	A	C2-N3-C4	5.69	113.44	110.60
36	YB	118	G	N3-C4-C5	-5.69	125.76	128.60
35	YA	2559	C	C5-C6-N1	5.68	123.84	121.00
25	R0	51	VAL	N-CA-C	-5.67	95.68	111.00
35	YA	18	C	C6-N1-C2	-5.67	118.03	120.30
35	YA	1915	U	N3-C2-O2	-5.67	118.23	122.20
35	YA	1505	C	C6-N1-C2	-5.67	118.03	120.30
1	QA	442	C	N1-C2-O2	5.67	122.30	118.90
1	QA	485	G	P-O3'-C3'	5.67	126.50	119.70
10	QJ	79	ARG	NE-CZ-NH2	-5.67	117.47	120.30
35	YA	2394	C	C6-N1-C2	-5.67	118.03	120.30
35	RA	2343	C	N1-C2-O2	5.66	122.30	118.90
1	QA	1006	C	C6-N1-C1'	-5.66	114.01	120.80
1	QA	1325	C	C6-N1-C2	-5.66	118.04	120.30
1	QA	1033	G	C4-N9-C1'	5.65	133.85	126.50
1	XA	1006	C	C2-N1-C1'	5.65	125.02	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	363(E)	U	C6-N1-C1'	-5.65	113.29	121.20
35	YA	2712	U	C6-N1-C1'	-5.65	113.29	121.20
35	RA	753	C	C6-N1-C2	-5.65	118.04	120.30
35	RA	1313	U	C6-N1-C1'	-5.64	113.30	121.20
35	YA	2096	U	N1-C2-O2	5.64	126.75	122.80
55	RZ	112	ARG	CB-CA-C	5.64	121.68	110.40
1	QA	442	C	C6-N1-C2	-5.64	118.04	120.30
35	RA	1064	C	N1-C2-O2	5.64	122.28	118.90
35	YA	270(U)	C	C6-N1-C2	-5.64	118.05	120.30
10	QJ	28	ARG	CG-CD-NE	5.64	123.64	111.80
35	RA	1427	A	P-O3'-C3'	5.64	126.46	119.70
1	QA	1536	C	C6-N1-C2	-5.63	118.05	120.30
35	RA	753	C	C5-C6-N1	5.63	123.82	121.00
35	RA	1502	C	C5-C6-N1	5.63	123.82	121.00
35	YA	1267	U	N3-C2-O2	-5.63	118.26	122.20
35	RA	1909	C	C6-N1-C2	-5.63	118.05	120.30
35	YA	1294	U	N1-C2-O2	5.63	126.74	122.80
36	YB	77	U	C2-N1-C1'	5.63	124.46	117.70
35	YA	1427	A	P-O3'-C3'	5.63	126.45	119.70
35	YA	2604	U	N3-C2-O2	-5.63	118.26	122.20
35	RA	1180	C	C6-N1-C1'	-5.63	114.05	120.80
1	XA	54	C	N1-C2-O2	5.63	122.28	118.90
35	RA	279	C	C5-C6-N1	5.62	123.81	121.00
1	XA	1439	C	N1-C2-O2	5.62	122.28	118.90
36	RB	47	C	C2-N1-C1'	5.62	124.98	118.80
1	XA	738	C	C5-C6-N1	5.62	123.81	121.00
35	RA	128	C	C6-N1-C2	-5.62	118.05	120.30
36	RB	27	C	C5-C6-N1	5.62	123.81	121.00
35	YA	1588	C	C5-C6-N1	5.62	123.81	121.00
35	YA	2103	C	C5-C6-N1	5.61	123.81	121.00
35	RA	2584	U	N1-C2-O2	5.61	126.73	122.80
35	RA	904	C	C2-N1-C1'	5.61	124.97	118.80
1	QA	1031	G	N3-C4-C5	-5.61	125.80	128.60
35	RA	1881	C	N1-C2-O2	5.61	122.26	118.90
35	RA	2739	U	N3-C2-O2	-5.61	118.28	122.20
22	XV	1	C	P-O3'-C3'	5.61	126.43	119.70
1	QA	419	C	C6-N1-C2	-5.61	118.06	120.30
35	RA	635	C	C6-N1-C2	-5.61	118.06	120.30
35	RA	1152	C	N1-C2-O2	5.61	122.26	118.90
35	RA	2559	C	N1-C2-O2	5.61	122.26	118.90
1	XA	525	C	C5-C6-N1	5.61	123.80	121.00
35	YA	556	G	C6-C5-N7	-5.61	127.04	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	1157	A	P-O3'-C3'	5.60	126.42	119.70
35	RA	1233	C	C5-C6-N1	5.60	123.80	121.00
1	XA	1007	C	C6-N1-C2	-5.60	118.06	120.30
35	YA	2225	A	P-O3'-C3'	5.60	126.42	119.70
35	RA	1735	C	C5-C6-N1	5.59	123.80	121.00
35	YA	69	C	C2-N1-C1'	5.59	124.95	118.80
35	YA	140	A	C8-N9-C4	-5.59	103.56	105.80
35	YA	975	G	N3-C4-C5	-5.59	125.80	128.60
35	YA	1406	U	N1-C2-O2	5.59	126.72	122.80
43	YN	114	ARG	N-CA-C	-5.59	95.90	111.00
35	RA	1779	U	C2-N1-C1'	5.59	124.41	117.70
35	RA	2118	U	N1-C2-O2	5.59	126.72	122.80
35	YA	1934	C	C2-N1-C1'	5.59	124.95	118.80
35	RA	1394	U	C6-N1-C2	-5.59	117.65	121.00
35	RA	1505	C	C6-N1-C2	-5.59	118.06	120.30
35	YA	1882	C	C6-N1-C1'	-5.59	114.09	120.80
1	QA	1147	C	C2-N1-C1'	5.58	124.94	118.80
35	RA	2604	U	N1-C2-O2	5.58	126.71	122.80
35	RA	436	C	N1-C2-O2	5.58	122.25	118.90
1	QA	999	U	OP1-P-O3'	5.58	117.47	105.20
35	RA	856	C	N1-C2-O2	5.58	122.25	118.90
35	YA	2477	C	N1-C2-O2	5.58	122.25	118.90
35	RA	2243	U	N3-C2-O2	-5.58	118.30	122.20
1	XA	186	C	C6-N1-C2	-5.57	118.07	120.30
35	YA	530	G	C5-C6-O6	-5.57	125.26	128.60
9	XI	102	LEU	CA-CB-CG	5.57	128.12	115.30
36	YB	47	C	C5-C6-N1	5.57	123.79	121.00
35	RA	1314	C	N1-C2-O2	5.57	122.24	118.90
36	RB	37	C	N1-C2-O2	5.57	122.24	118.90
1	XA	186	C	C5-C6-N1	5.57	123.78	121.00
1	XA	330	C	C5-C6-N1	5.57	123.78	121.00
1	XA	1031	G	N3-C4-N9	5.56	129.34	126.00
35	YA	9	U	C2-N1-C1'	5.56	124.38	117.70
35	RA	2043	C	C6-N1-C2	-5.55	118.08	120.30
35	YA	1979	C	N1-C2-O2	5.55	122.23	118.90
1	QA	1158	C	C6-N1-C1'	-5.54	114.15	120.80
40	RG	83	ARG	CG-CD-NE	5.54	123.44	111.80
35	YA	154	G	N3-C4-N9	5.54	129.33	126.00
1	XA	169	C	C6-N1-C2	-5.54	118.08	120.30
1	XA	1007	C	C6-N1-C1'	-5.54	114.15	120.80
8	XH	60	ARG	CD-NE-CZ	5.54	131.36	123.60
1	QA	252	U	C5-C6-N1	5.54	125.47	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	1332	G	C6-C5-N7	-5.54	127.08	130.40
34	Y9	37	GLY	N-CA-C	-5.54	99.25	113.10
1	XA	690	G	C4-N9-C1'	5.54	133.70	126.50
1	QA	1109	C	N1-C2-O2	5.54	122.22	118.90
35	RA	1644	C	C6-N1-C2	-5.54	118.09	120.30
36	RB	27	C	C2-N1-C1'	5.54	124.89	118.80
1	QA	960	U	C2-N1-C1'	5.53	124.34	117.70
1	QA	652	U	N1-C2-O2	5.53	126.67	122.80
35	RA	544	C	N1-C2-O2	5.53	122.22	118.90
35	YA	1188	U	N1-C2-O2	5.53	126.67	122.80
36	RB	87	G	N1-C6-O6	-5.53	116.58	119.90
35	YA	1180	C	N1-C2-O2	5.53	122.22	118.90
36	YB	8	U	C2-N1-C1'	5.53	124.33	117.70
1	QA	58	C	C5-C6-N1	5.53	123.76	121.00
35	RA	269	U	C5-C6-N1	5.53	125.46	122.70
35	RA	2108	C	C6-N1-C2	-5.52	118.09	120.30
1	QA	1033	G	C8-N9-C1'	-5.52	119.82	127.00
35	RA	1318	C	C6-N1-C2	-5.52	118.09	120.30
35	YA	2559	C	C6-N1-C2	-5.52	118.09	120.30
35	RA	2540	C	C6-N1-C2	-5.52	118.09	120.30
1	QA	1031	G	N3-C4-N9	5.52	129.31	126.00
35	RA	2006	C	N1-C2-O2	5.52	122.21	118.90
35	YA	652	C	C6-N1-C2	-5.51	118.09	120.30
35	RA	286	C	C5-C6-N1	5.51	123.76	121.00
35	RA	1950	G	O4'-C1'-N9	5.51	112.61	108.20
35	YA	752	A	OP2-P-O3'	5.51	117.33	105.20
1	QA	652	U	N3-C2-O2	-5.51	118.34	122.20
35	YA	652	C	C2-N1-C1'	5.51	124.86	118.80
35	YA	2471	C	C2-N1-C1'	5.51	124.86	118.80
35	RA	758	C	N3-C2-O2	-5.51	118.05	121.90
25	R0	48	GLY	N-CA-C	5.50	126.86	113.10
35	RA	1505	C	C2-N1-C1'	5.50	124.85	118.80
1	XA	703	G	P-O3'-C3'	5.50	126.30	119.70
35	RA	1406	U	N3-C2-O2	-5.50	118.35	122.20
35	YA	1180	C	C5-C6-N1	5.50	123.75	121.00
35	YA	652	C	N3-C2-O2	-5.50	118.05	121.90
1	QA	454	C	C6-N1-C2	-5.50	118.10	120.30
1	QA	18	C	C5-C6-N1	5.49	123.75	121.00
1	QA	1260	C	C6-N1-C2	-5.49	118.10	120.30
35	RA	2873	A	C8-N9-C4	-5.49	103.60	105.80
1	XA	1381	U	C5-C6-N1	5.49	125.45	122.70
35	YA	904	C	N1-C2-O2	5.49	122.20	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	2210	G	C2-N3-C4	5.49	114.64	111.90
35	RA	265	A	O4'-C1'-N9	5.49	112.59	108.20
36	RB	27	C	N3-C2-O2	-5.49	118.06	121.90
11	XK	96	ARG	CB-CG-CD	-5.49	97.33	111.60
35	YA	273(D)	C	C2-N1-C1'	5.49	124.84	118.80
46	RQ	5	ARG	CG-CD-NE	5.49	123.32	111.80
1	XA	1260	C	C2-N1-C1'	5.48	124.83	118.80
35	RA	41	C	C6-N1-C2	-5.48	118.11	120.30
13	XM	8	GLU	N-CA-C	-5.48	96.20	111.00
1	QA	1008	C	O5'-P-OP1	5.48	117.28	110.70
35	RA	9	U	N3-C2-O2	-5.48	118.36	122.20
35	RA	431	U	C5-C6-N1	5.48	125.44	122.70
35	YA	270(Q)	C	N3-C2-O2	-5.48	118.06	121.90
35	YA	288	C	C2-N1-C1'	5.48	124.83	118.80
1	XA	1040	U	C2-N1-C1'	5.48	124.27	117.70
35	RA	650	C	C6-N1-C2	-5.47	118.11	120.30
22	XV	56	C	N1-C2-O2	5.47	122.19	118.90
35	YA	2585	U	N3-C2-O2	-5.47	118.37	122.20
1	XA	1325	C	C2-N1-C1'	5.47	124.82	118.80
35	YA	193	U	C5-C6-N1	5.47	125.44	122.70
35	RA	930	U	N1-C2-O2	5.47	126.63	122.80
29	Y4	67	TYR	N-CA-C	-5.47	96.23	111.00
35	RA	436	C	N3-C2-O2	-5.47	118.07	121.90
1	XA	1228	C	N1-C2-O2	5.47	122.18	118.90
35	YA	2604	U	N1-C2-O2	5.47	126.63	122.80
29	Y4	67	TYR	CA-CB-CG	5.46	123.78	113.40
1	XA	1263	C	C6-N1-C2	-5.46	118.12	120.30
35	RA	2394	C	N3-C2-O2	-5.46	118.08	121.90
3	XC	140	ARG	CD-NE-CZ	5.46	131.24	123.60
1	QA	1006	C	C6-N1-C2	-5.46	118.12	120.30
1	QA	1406	U	N3-C2-O2	-5.46	118.38	122.20
1	XA	1362(A)	C	N3-C2-O2	-5.46	118.08	121.90
1	QA	932	C	C6-N1-C2	-5.45	118.12	120.30
24	QY	63	GLU	CB-CA-C	-5.45	99.49	110.40
35	RA	1314	C	C6-N1-C2	-5.45	118.12	120.30
35	RA	2712	U	N1-C2-O2	5.45	126.62	122.80
36	RB	77	U	N3-C2-O2	-5.45	118.39	122.20
1	XA	1126	U	C5-C6-N1	5.45	125.42	122.70
35	YA	2702	U	O5'-P-OP1	5.45	117.24	110.70
35	RA	2041	U	N1-C2-O2	5.45	126.61	122.80
35	YA	2527	C	C2-N1-C1'	5.45	124.79	118.80
24	XY	49	LYS	C-N-CA	5.44	135.30	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	2808	U	N1-C2-O2	5.44	126.61	122.80
35	YA	288	C	OP1-P-O3'	5.44	117.17	105.20
1	QA	330	C	N1-C2-O2	5.44	122.16	118.90
1	XA	368	U	N3-C4-C5	5.44	117.86	114.60
35	YA	1528	A	N7-C8-N9	5.44	116.52	113.80
35	RA	1698	A	O4'-C1'-N9	5.43	112.55	108.20
1	XA	137	C	C6-N1-C2	-5.43	118.13	120.30
35	YA	2244	U	N3-C4-O4	5.43	123.20	119.40
35	YA	2712	U	N3-C2-O2	-5.43	118.40	122.20
1	QA	1303	C	C2-N1-C1'	5.43	124.78	118.80
1	XA	169	C	C5-C6-N1	5.43	123.72	121.00
35	YA	894	C	C2-N1-C1'	5.43	124.78	118.80
35	YA	1233	C	C6-N1-C2	-5.43	118.13	120.30
35	RA	2066	C	N1-C2-O2	5.43	122.16	118.90
35	RA	69	C	C6-N1-C2	-5.42	118.13	120.30
35	RA	1963	U	N1-C2-O2	5.42	126.60	122.80
35	RA	143	C	C6-N1-C2	-5.42	118.13	120.30
35	RA	2787	C	N3-C2-O2	-5.42	118.11	121.90
35	RA	2847	U	N3-C2-O2	-5.42	118.41	122.20
37	YD	88	ARG	CB-CA-C	-5.42	99.56	110.40
2	XB	236	TYR	N-CA-CB	-5.42	100.85	110.60
35	YA	286	C	C6-N1-C2	-5.42	118.13	120.30
35	YA	1979	C	N3-C2-O2	-5.42	118.11	121.90
35	RA	1506	C	C6-N1-C2	-5.42	118.13	120.30
51	RV	39	LEU	CA-CB-CG	5.42	127.75	115.30
49	YT	105	LEU	CA-CB-CG	5.42	127.75	115.30
10	XJ	31	GLY	N-CA-C	5.41	126.63	113.10
1	QA	518	C	P-O3'-C3'	5.41	126.19	119.70
35	RA	2889	C	C6-N1-C2	-5.41	118.14	120.30
1	XA	353	A	OP2-P-O3'	5.41	117.10	105.20
1	QA	18	C	C6-N1-C2	-5.41	118.14	120.30
17	QQ	101	ARG	CD-NE-CZ	5.41	131.17	123.60
27	R2	47	ASN	C-N-CA	5.41	135.22	121.70
35	RA	1735	C	C6-N1-C2	-5.41	118.14	120.30
38	RE	116	VAL	C-N-CA	5.41	135.22	121.70
35	YA	1256	G	C4-N9-C1'	5.41	133.53	126.50
35	RA	195	A	P-O3'-C3'	5.41	126.19	119.70
35	YA	9	U	N3-C2-O2	-5.41	118.42	122.20
35	YA	1474	C	N1-C2-O2	5.41	122.14	118.90
39	YF	129	PHE	N-CA-C	5.41	125.60	111.00
1	QA	1225	A	C4-N9-C1'	5.40	136.02	126.30
35	RA	143	C	C5-C6-N1	5.40	123.70	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	1742	C	C6-N1-C2	-5.40	118.14	120.30
35	RA	273(C)	C	C2-N1-C1'	5.39	124.73	118.80
35	RA	530	G	N1-C6-O6	5.39	123.14	119.90
1	QA	442	C	C5-C6-N1	5.39	123.69	121.00
35	RA	47	C	C6-N1-C2	-5.39	118.14	120.30
41	RH	67	LEU	CA-CB-CG	5.39	127.70	115.30
35	RA	269	U	C6-N1-C1'	-5.39	113.65	121.20
35	RA	2571	C	C6-N1-C2	-5.39	118.14	120.30
35	YA	1881	C	N1-C2-O2	5.38	122.13	118.90
35	RA	1920	C	C5-C6-N1	5.38	123.69	121.00
35	YA	2808	U	N3-C2-O2	-5.38	118.43	122.20
1	QA	283	C	C6-N1-C2	-5.38	118.15	120.30
35	RA	1781	C	N1-C2-O2	5.38	122.13	118.90
36	RB	77	U	C2-N1-C1'	5.38	124.16	117.70
35	RA	537	C	C5-C6-N1	5.38	123.69	121.00
1	QA	1008	C	C2-N1-C1'	5.37	124.71	118.80
1	QA	79	G	N3-C4-C5	-5.37	125.92	128.60
1	QA	268	C	C6-N1-C2	-5.37	118.15	120.30
35	RA	2321	G	N3-C4-C5	-5.37	125.92	128.60
1	XA	169	C	N1-C2-O2	5.37	122.12	118.90
14	QN	13	THR	N-CA-C	5.37	125.50	111.00
35	RA	143	C	C2-N1-C1'	5.37	124.70	118.80
35	RA	1992	G	OP2-P-O3'	5.37	117.00	105.20
13	XM	108	ARG	N-CA-C	5.37	125.48	111.00
35	YA	153	C	C2-N1-C1'	5.36	124.69	118.80
35	YA	234	C	N3-C2-O2	-5.36	118.15	121.90
35	YA	2139	C	C2-N1-C1'	5.36	124.69	118.80
35	YA	2144	U	P-O3'-C3'	5.36	126.13	119.70
35	RA	358	U	C5-C6-N1	5.36	125.38	122.70
35	RA	481	G	O4'-C1'-N9	5.36	112.49	108.20
35	RA	1774	C	C2-N1-C1'	5.36	124.69	118.80
35	RA	1911	U	N3-C2-O2	-5.36	118.45	122.20
1	XA	341	C	C6-N1-C2	-5.35	118.16	120.30
35	YA	1934	C	N1-C2-O2	5.35	122.11	118.90
3	QC	78	GLY	N-CA-C	5.35	126.48	113.10
35	YA	1294	U	C2-N1-C1'	5.35	124.12	117.70
29	R4	22	ILE	C-N-CA	5.35	135.07	121.70
1	XA	1535	C	C6-N1-C2	-5.35	118.16	120.30
35	YA	2321	G	N3-C4-N9	5.35	129.21	126.00
39	YF	199	TRP	N-CA-C	-5.35	96.56	111.00
35	RA	1909	C	C5-C6-N1	5.35	123.67	121.00
35	RA	2667	C	C6-N1-C2	-5.35	118.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	137	C	C5-C6-N1	5.35	123.67	121.00
35	RA	1474	C	C5-C6-N1	5.34	123.67	121.00
35	YA	1909	C	C6-N1-C2	-5.34	118.16	120.30
35	YA	2683	C	N1-C2-O2	5.34	122.10	118.90
35	RA	2752	C	C2-N1-C1'	5.34	124.67	118.80
35	YA	1788	C	C6-N1-C2	-5.34	118.17	120.30
35	YA	2096	U	C2-N1-C1'	5.34	124.11	117.70
35	RA	530	G	C5-C6-O6	-5.34	125.40	128.60
7	XG	111	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	QA	717	C	C2-N1-C1'	5.33	124.67	118.80
35	RA	930	U	N3-C2-O2	-5.33	118.47	122.20
1	XA	330	C	C2-N1-C1'	5.33	124.67	118.80
35	YA	2205	C	C6-N1-C2	-5.33	118.17	120.30
35	YA	2604	U	C2-N1-C1'	5.33	124.10	117.70
35	YA	2873	A	N7-C8-N9	5.33	116.47	113.80
35	RA	1417	C	C2-N1-C1'	5.33	124.67	118.80
36	YB	30	C	C6-N1-C2	-5.33	118.17	120.30
1	QA	252	U	N3-C2-O2	-5.33	118.47	122.20
1	QA	749	C	N1-C2-O2	5.33	122.10	118.90
35	RA	1502	C	C6-N1-C2	-5.33	118.17	120.30
35	YA	1675	C	C6-N1-C2	-5.33	118.17	120.30
36	RB	27	C	C6-N1-C2	-5.33	118.17	120.30
40	RG	146	TYR	N-CA-CB	-5.33	101.02	110.60
35	RA	1931	U	C5-C6-N1	5.32	125.36	122.70
2	XB	178	ARG	CG-CD-NE	5.32	122.98	111.80
1	XA	1147	C	C2-N1-C1'	5.32	124.65	118.80
35	YA	930	U	C2-N1-C1'	5.32	124.08	117.70
35	RA	860	U	N1-C2-O2	5.32	126.52	122.80
51	RV	95	LEU	CA-CB-CG	5.31	127.52	115.30
35	RA	934	G	N3-C4-N9	5.31	129.19	126.00
35	RA	1395	A	O4'-C1'-N9	5.31	112.45	108.20
35	RA	587	C	P-O3'-C3'	5.31	126.07	119.70
42	YI	10	GLU	CA-CB-CG	5.31	125.08	113.40
35	RA	2210	G	N3-C4-N9	5.31	129.19	126.00
35	YA	41	C	C2-N1-C1'	5.31	124.64	118.80
35	YA	527	C	C6-N1-C1'	-5.31	114.43	120.80
1	XA	405	U	N1-C2-O2	5.30	126.51	122.80
51	YV	95	LEU	CA-CB-CG	5.30	127.49	115.30
35	RA	1011	G	C4-N9-C1'	-5.30	119.61	126.50
35	RA	721	C	C6-N1-C2	-5.30	118.18	120.30
1	QA	705	U	N3-C2-O2	-5.29	118.49	122.20
1	XA	932	C	C5-C6-N1	5.29	123.65	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	YR	75	LEU	CA-CB-CG	5.29	127.48	115.30
35	RA	104	U	N1-C2-O2	5.29	126.51	122.80
35	RA	1735	C	N1-C2-O2	5.29	122.08	118.90
35	YA	797	C	C5-C6-N1	5.29	123.65	121.00
1	XA	1033	G	P-O3'-C3'	5.29	126.05	119.70
35	RA	1474	C	C6-N1-C2	-5.29	118.19	120.30
35	RA	1934	C	N1-C2-O2	5.29	122.07	118.90
1	XA	75	C	C5-C6-N1	5.29	123.64	121.00
35	RA	2205	C	C6-N1-C2	-5.28	118.19	120.30
35	YA	2096	U	N3-C2-O2	-5.28	118.50	122.20
45	YP	104	GLY	N-CA-C	5.28	126.30	113.10
35	YA	587	C	P-O3'-C3'	5.28	126.03	119.70
22	QV	32	C	N3-C2-O2	-5.27	118.21	121.90
35	RA	1475	G	N3-C4-N9	5.27	129.16	126.00
35	RA	2063	C	C5-C6-N1	5.27	123.64	121.00
35	RA	1930	G	OP2-P-O3'	5.27	116.79	105.20
35	RA	2571	C	C5-C6-N1	5.27	123.63	121.00
1	XA	749	C	N3-C2-O2	-5.27	118.21	121.90
35	YA	372	G	OP2-P-O3'	5.27	116.79	105.20
35	YA	556	G	N7-C8-N9	5.27	115.73	113.10
35	YA	1075	C	C5-C6-N1	5.27	123.63	121.00
1	QA	186	C	C6-N1-C2	-5.26	118.19	120.30
35	RA	273(D)	C	C2-N1-C1'	5.26	124.59	118.80
1	QA	435	C	C5-C6-N1	5.26	123.63	121.00
10	XJ	35	SER	N-CA-C	-5.26	96.79	111.00
35	YA	2343	C	N1-C2-O2	5.26	122.06	118.90
35	RA	2703	C	N1-C2-O2	5.26	122.06	118.90
35	YA	1819	A	P-O3'-C3'	5.26	126.01	119.70
30	R5	51	TYR	CA-CB-CG	5.26	123.39	113.40
35	YA	893	C	N1-C2-O2	5.25	122.05	118.90
35	RA	1462	C	N3-C2-O2	-5.25	118.22	121.90
35	RA	2467	C	N3-C2-O2	-5.25	118.22	121.90
35	RA	358	U	C2-N1-C1'	5.25	124.00	117.70
20	XT	96	GLY	C-N-CA	5.25	134.82	121.70
35	RA	1462	C	N1-C2-O2	5.25	122.05	118.90
35	RA	1786	A	C4-N9-C1'	5.25	135.75	126.30
1	XA	169	C	C2-N1-C1'	5.25	124.57	118.80
35	RA	1005	C	C6-N1-C2	-5.25	118.20	120.30
35	RA	1947	C	N1-C2-O2	5.25	122.05	118.90
35	RA	2394	C	C6-N1-C2	-5.25	118.20	120.30
36	YB	47	C	N3-C2-O2	-5.25	118.23	121.90
35	RA	1407	C	C6-N1-C1'	-5.25	114.51	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	YQ	59	ARG	C-N-CA	5.25	134.81	121.70
43	YN	114	ARG	C-N-CA	5.24	134.81	121.70
35	RA	372	G	OP2-P-O3'	5.24	116.73	105.20
1	XA	1128	C	C5-C6-N1	5.24	123.62	121.00
1	QA	1490	C	C6-N1-C2	-5.24	118.20	120.30
35	YA	2726	U	O4'-C1'-N1	5.24	112.39	108.20
40	RG	9	ARG	CG-CD-NE	5.24	122.80	111.80
9	XI	85	LEU	CA-CB-CG	5.24	127.34	115.30
35	YA	1735	C	C5-C6-N1	5.23	123.62	121.00
1	QA	455	C	C2-N1-C1'	5.23	124.56	118.80
1	QA	932	C	C5-C6-N1	5.23	123.61	121.00
1	XA	1395	C	C2-N1-C1'	5.23	124.55	118.80
35	YA	2584	U	C6-N1-C2	-5.23	117.86	121.00
35	YA	857	C	C5-C6-N1	5.23	123.61	121.00
9	QI	62	TYR	N-CA-C	-5.22	96.90	111.00
1	XA	999	U	OP1-P-O3'	5.22	116.69	105.20
4	XD	154	ASN	C-N-CA	5.22	134.75	121.70
35	RA	104	U	N3-C2-O2	-5.22	118.55	122.20
35	RA	1963	U	N3-C2-O2	-5.22	118.55	122.20
35	RA	2730	C	C6-N1-C2	-5.22	118.21	120.30
35	RA	1588	C	C6-N1-C1'	-5.22	114.54	120.80
35	YA	435	C	N3-C2-O2	-5.22	118.25	121.90
35	YA	708	C	N1-C2-O2	5.22	122.03	118.90
35	RA	41	C	C2-N1-C1'	5.21	124.54	118.80
35	RA	234	C	N3-C2-O2	-5.21	118.25	121.90
35	RA	893	C	N1-C2-O2	5.21	122.03	118.90
35	RA	2585	U	N3-C2-O2	-5.21	118.55	122.20
35	YA	2456	C	C5-C6-N1	5.21	123.61	121.00
35	RA	435	C	N3-C2-O2	-5.21	118.25	121.90
1	XA	209	U	C2-N1-C1'	5.21	123.95	117.70
35	RA	1819	A	P-O3'-C3'	5.21	125.95	119.70
1	XA	1382	C	C6-N1-C2	-5.21	118.22	120.30
49	YT	96	ARG	CA-CB-CG	5.21	124.86	113.40
1	QA	1347	G	OP2-P-O3'	5.21	116.65	105.20
35	RA	288	C	C5-C6-N1	5.21	123.60	121.00
35	RA	1934	C	C2-N1-C1'	5.21	124.53	118.80
35	RA	2540	C	C2-N1-C1'	5.21	124.53	118.80
1	XA	1158	C	N1-C2-O2	5.21	122.02	118.90
35	RA	1430	C	C5-C6-N1	5.20	123.60	121.00
1	QA	1378	C	N1-C2-O2	5.20	122.02	118.90
35	RA	1544	C	C2-N1-C1'	5.20	124.52	118.80
35	YA	2128	C	C6-N1-C2	-5.20	118.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	315	A	OP2-P-O3'	5.20	116.63	105.20
1	XA	1128	C	N1-C2-O2	5.20	122.02	118.90
35	YA	974	G	C8-N9-C1'	5.20	133.75	127.00
35	YA	2342	C	C2-N1-C1'	5.19	124.51	118.80
35	YA	634	C	C6-N1-C2	-5.19	118.22	120.30
1	QA	1263	C	N1-C2-O2	5.19	122.02	118.90
35	RA	1304	C	C6-N1-C2	-5.19	118.22	120.30
1	XA	341	C	C5-C6-N1	5.19	123.60	121.00
1	QA	312	C	C2-N1-C1'	5.19	124.51	118.80
1	XA	58	C	C5-C6-N1	5.19	123.59	121.00
1	XA	1007	C	OP1-P-O3'	5.18	116.61	105.20
35	RA	1385	G	O4'-C1'-N9	5.18	112.35	108.20
36	YB	117	G	OP1-P-O3'	5.18	116.60	105.20
35	RA	2604	U	N3-C2-O2	-5.18	118.58	122.20
35	RA	2739	U	N1-C2-O2	5.18	126.43	122.80
3	XC	63	ASN	N-CA-C	-5.18	97.02	111.00
35	YA	114	U	N1-C2-O2	5.18	126.43	122.80
47	YR	57	ARG	CB-CA-C	5.18	120.76	110.40
1	XA	1502	A	C4-N9-C1'	5.18	135.62	126.30
1	QA	1000	A	OP1-P-O3'	5.18	116.59	105.20
35	RA	1911	U	C2-N1-C1'	5.18	123.91	117.70
1	XA	1263	C	N1-C2-O2	5.18	122.01	118.90
35	YA	1993	U	N1-C2-O2	5.18	126.42	122.80
36	YB	27	C	C6-N1-C2	-5.18	118.23	120.30
1	XA	1128	C	N3-C2-O2	-5.17	118.28	121.90
1	QA	405	U	N3-C2-O2	-5.17	118.58	122.20
35	RA	2666	C	C5-C6-N1	5.17	123.58	121.00
36	RB	8	U	N1-C2-O2	5.17	126.42	122.80
35	YA	527	C	N3-C2-O2	-5.17	118.28	121.90
35	YA	2461	C	C2-N1-C1'	5.17	124.48	118.80
35	RA	243	U	N1-C2-O2	5.16	126.42	122.80
35	RA	1475	G	C4-N9-C1'	5.16	133.21	126.50
35	RA	708	C	C6-N1-C1'	-5.16	114.61	120.80
1	XA	1382	C	N3-C2-O2	-5.16	118.29	121.90
35	YA	31	C	C5-C6-N1	5.16	123.58	121.00
35	YA	93	C	C6-N1-C1'	-5.16	114.61	120.80
33	R8	46	ARG	N-CA-CB	-5.16	101.31	110.60
35	RA	128	C	P-O3'-C3'	5.16	125.89	119.70
35	RA	2210	G	N3-C4-C5	-5.16	126.02	128.60
1	XA	1086	U	C5-C6-N1	5.16	125.28	122.70
35	YA	157	U	N1-C2-O2	5.16	126.41	122.80
35	RA	273(C)	C	N3-C2-O2	-5.16	118.29	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	510	C	N1-C2-O2	5.15	121.99	118.90
35	RA	2292	C	C5-C6-N1	5.15	123.58	121.00
35	RA	2294	C	N1-C2-O2	5.15	121.99	118.90
1	QA	961	U	N1-C2-O2	5.15	126.41	122.80
35	YA	273(D)	C	N1-C2-O2	5.15	121.99	118.90
35	YA	1294	U	N3-C2-O2	-5.15	118.59	122.20
35	YA	1754	C	N1-C2-O2	5.15	121.99	118.90
1	QA	328	C	C5-C6-N1	5.15	123.58	121.00
1	QA	1027	C	N1-C2-O2	5.15	121.99	118.90
20	XT	8	ARG	CG-CD-NE	5.15	122.61	111.80
45	RP	116	GLY	N-CA-C	5.15	125.97	113.10
35	RA	1678	G	C4-N9-C1'	5.15	133.19	126.50
1	QA	749	C	C5-C6-N1	5.14	123.57	121.00
31	R6	26	ASN	N-CA-C	-5.14	97.12	111.00
35	RA	1950	G	C4-N9-C1'	5.14	133.18	126.50
37	RD	131	LEU	CA-CB-CG	5.13	127.11	115.30
33	R8	35	GLN	N-CA-CB	5.13	119.84	110.60
35	RA	1920	C	C6-N1-C2	-5.13	118.25	120.30
35	YA	9	U	C5-C6-N1	5.13	125.27	122.70
35	YA	1911	U	N3-C2-O2	-5.13	118.61	122.20
35	RA	273(D)	C	C6-N1-C2	-5.13	118.25	120.30
1	XA	368	U	C5-C4-O4	-5.13	122.82	125.90
27	R2	46	GLN	C-N-CA	5.13	134.52	121.70
35	RA	1079	C	N1-C2-O2	5.13	121.98	118.90
1	QA	1059	C	C6-N1-C2	-5.12	118.25	120.30
35	RA	2108	C	C5-C6-N1	5.12	123.56	121.00
35	YA	2648	C	C2-N1-C1'	5.12	124.43	118.80
35	RA	613	U	C6-N1-C1'	-5.12	114.03	121.20
13	QM	11	ARG	N-CA-C	-5.12	97.18	111.00
1	XA	497	U	N1-C2-O2	5.12	126.38	122.80
1	QA	1008	C	P-O3'-C3'	5.12	125.84	119.70
26	R1	85	LEU	C-N-CA	5.12	134.49	121.70
35	YA	2874	C	C6-N1-C2	-5.12	118.25	120.30
8	XH	60	ARG	CG-CD-NE	5.12	122.54	111.80
36	RB	15	A	OP1-P-O3'	5.11	116.45	105.20
35	RA	1882	C	C5-C6-N1	5.11	123.56	121.00
35	YA	1430	C	C5-C6-N1	5.11	123.56	121.00
35	RA	9	U	C5-C6-N1	5.11	125.25	122.70
41	RH	151	ILE	C-N-CA	5.11	134.48	121.70
1	XA	932	C	C6-N1-C2	-5.11	118.26	120.30
35	YA	289	A	C8-N9-C4	-5.11	103.76	105.80
35	YA	413	C	C5-C6-N1	5.11	123.56	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	1394	U	C5-C6-N1	5.11	125.25	122.70
54	RY	56	PRO	C-N-CA	5.11	134.47	121.70
1	XA	1439	C	C6-N1-C2	-5.11	118.26	120.30
41	YH	3	ARG	NE-CZ-NH1	-5.11	117.75	120.30
12	XL	104	VAL	C-N-CA	5.11	134.46	121.70
1	QA	54	C	N1-C2-O2	5.10	121.96	118.90
43	RN	35	ARG	N-CA-C	-5.10	97.22	111.00
1	XA	75	C	C6-N1-C2	-5.10	118.26	120.30
16	QP	23	ASP	N-CA-C	-5.10	97.23	111.00
1	QA	496	A	N3-C4-N9	5.10	131.48	127.40
35	RA	2726	U	C2-N1-C1'	5.10	123.82	117.70
35	YA	1835	G	N3-C4-C5	-5.10	126.05	128.60
35	YA	2166	G	P-O3'-C3'	5.10	125.82	119.70
35	RA	749	C	N3-C2-O2	-5.10	118.33	121.90
35	RA	1931	U	N1-C2-O2	5.10	126.37	122.80
35	YA	93	C	N1-C2-O2	5.10	121.96	118.90
35	RA	1788	C	C6-N1-C2	-5.10	118.26	120.30
35	RA	1499	C	N1-C2-O2	5.09	121.96	118.90
35	YA	2205	C	C5-C6-N1	5.09	123.55	121.00
23	XX	13	A	OP1-P-OP2	-5.09	111.96	119.60
35	RA	141(A)	C	C6-N1-C2	-5.09	118.26	120.30
1	XA	1009	G	O5'-P-OP1	5.09	116.81	110.70
35	YA	343	C	C5-C6-N1	5.09	123.55	121.00
35	YA	1774	C	C5-C6-N1	5.09	123.55	121.00
35	YA	2827	C	C5-C6-N1	5.09	123.55	121.00
36	YB	27	C	C2-N1-C1'	5.09	124.39	118.80
1	QA	596	C	C6-N1-C2	-5.08	118.27	120.30
35	RA	1079	C	C2-N1-C1'	5.08	124.39	118.80
35	YA	273(D)	C	C6-N1-C2	-5.08	118.27	120.30
35	YA	692	C	C6-N1-C2	-5.08	118.27	120.30
35	RA	2712	U	C6-N1-C1'	-5.08	114.08	121.20
35	YA	12	U	C2-N1-C1'	5.08	123.80	117.70
35	YA	69	C	C6-N1-C2	-5.08	118.27	120.30
19	XS	25	LYS	N-CA-C	-5.08	97.28	111.00
35	RA	2041	U	N3-C2-O2	-5.08	118.64	122.20
1	XA	749	C	N1-C2-O2	5.08	121.95	118.90
35	YA	613	U	C5-C6-N1	5.08	125.24	122.70
35	RA	1528	A	N7-C8-N9	5.08	116.34	113.80
35	RA	527	C	C2-N1-C1'	5.08	124.38	118.80
35	RA	2540	C	C5-C6-N1	5.08	123.54	121.00
35	RA	527	C	N3-C2-O2	-5.07	118.35	121.90
35	YA	2073	C	C6-N1-C2	-5.07	118.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	2467	C	C5-C4-N4	5.07	123.75	120.20
1	XA	1008	C	P-O3'-C3'	5.07	125.78	119.70
35	YA	104	U	N1-C2-O2	5.07	126.35	122.80
36	YB	118	G	C5-C6-O6	5.07	131.64	128.60
1	XA	1007	C	N1-C2-O2	5.07	121.94	118.90
36	YB	22	U	N1-C2-O2	5.07	126.35	122.80
41	YH	3	ARG	CB-CA-C	-5.07	100.27	110.40
1	QA	754	C	C5-C6-N1	5.06	123.53	121.00
35	RA	2726	U	N3-C2-O2	-5.06	118.66	122.20
1	QA	936	C	N1-C2-O2	5.06	121.94	118.90
35	RA	845	G	P-O3'-C3'	5.06	125.77	119.70
35	RA	2723	C	C6-N1-C2	-5.06	118.28	120.30
1	QA	812	C	OP2-P-O3'	5.06	116.33	105.20
1	QA	891	U	N1-C2-O2	5.06	126.34	122.80
1	QA	1395	C	N3-C2-O2	-5.06	118.36	121.90
35	RA	2089	U	C5-C6-N1	5.06	125.23	122.70
46	RQ	84	GLY	C-N-CA	5.06	134.34	121.70
1	XA	431	A	N1-C6-N6	-5.06	115.57	118.60
1	XA	1086	U	C2-N1-C1'	5.06	123.77	117.70
35	YA	343	C	N1-C2-O2	5.06	121.93	118.90
35	YA	2791	C	C6-N1-C1'	5.06	126.87	120.80
1	QA	1325	C	C5-C6-N1	5.05	123.53	121.00
35	YA	104	U	N3-C2-O2	-5.05	118.66	122.20
35	RA	2859	G	P-O3'-C3'	5.05	125.76	119.70
35	RA	286	C	C6-N1-C1'	-5.05	114.74	120.80
35	YA	373	U	N3-C2-O2	-5.05	118.66	122.20
35	YA	2602	A	C4-N9-C1'	5.05	135.39	126.30
35	RA	1024	G	N3-C4-N9	5.05	129.03	126.00
1	XA	1305	G	P-O3'-C3'	5.05	125.76	119.70
35	YA	2689	U	P-O3'-C3'	5.05	125.76	119.70
1	XA	354	G	C4-N9-C1'	5.05	133.06	126.50
35	YA	669	G	N3-C4-N9	5.05	129.03	126.00
36	YB	117	G	N1-C2-N2	-5.05	111.66	116.20
1	QA	1160	G	N3-C4-N9	5.04	129.03	126.00
35	YA	1588	C	C6-N1-C2	-5.04	118.28	120.30
1	QA	690	G	O4'-C1'-N9	5.04	112.23	108.20
22	QV	32	C	C2-N1-C1'	5.04	124.35	118.80
35	RA	1011	G	C8-N9-C1'	5.04	133.55	127.00
35	RA	2210	G	C8-N9-C1'	-5.04	120.45	127.00
35	RA	86	C	C2-N1-C1'	5.04	124.34	118.80
35	RA	544	C	C6-N1-C2	-5.04	118.28	120.30
35	RA	355	G	C6-C5-N7	-5.04	127.38	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	1882	C	N1-C2-O2	5.04	121.92	118.90
35	YA	867	C	N3-C2-O2	-5.04	118.37	121.90
35	YA	971	C	C6-N1-C2	-5.04	118.28	120.30
35	YA	2859	G	P-O3'-C3'	5.04	125.75	119.70
35	RA	2321	G	C4-N9-C1'	5.04	133.05	126.50
1	XA	18	C	C5-C6-N1	5.04	123.52	121.00
1	XA	1024	G	N3-C4-C5	-5.04	126.08	128.60
35	YA	1658	C	C6-N1-C2	-5.04	118.29	120.30
35	RA	2896	C	N3-C2-O2	-5.03	118.38	121.90
1	XA	201	C	P-O3'-C3'	5.03	125.74	119.70
35	YA	2752	C	N3-C2-O2	-5.03	118.38	121.90
35	RA	2730	C	C2-N1-C1'	5.03	124.33	118.80
22	XV	34	C	C2-N1-C1'	5.03	124.33	118.80
35	YA	1385	G	O4'-C1'-N9	5.03	112.22	108.20
36	RB	77	U	C5-C6-N1	5.03	125.21	122.70
35	YA	1433	U	N1-C2-O2	5.03	126.32	122.80
35	YA	154	G	C4-N9-C1'	5.03	133.03	126.50
35	YA	1679	U	N3-C2-O2	-5.03	118.68	122.20
35	YA	2065	C	C5-C6-N1	5.03	123.51	121.00
35	YA	834	C	C6-N1-C2	-5.02	118.29	120.30
35	YA	1406	U	C6-N1-C2	-5.02	117.98	121.00
35	YA	2880	C	C6-N1-C2	-5.02	118.29	120.30
35	YA	817	C	C5-C6-N1	5.02	123.51	121.00
35	YA	527	C	O4'-C1'-N1	5.02	112.21	108.20
35	YA	806	C	C6-N1-C2	-5.01	118.30	120.30
35	RA	837	C	C5-C6-N1	5.01	123.51	121.00
35	RA	1306	C	C6-N1-C2	-5.01	118.30	120.30
1	XA	1065	U	OP2-P-O3'	5.01	116.23	105.20
35	YA	76	C	C6-N1-C2	-5.01	118.30	120.30
1	XA	1024	G	N3-C4-N9	5.01	129.01	126.00
35	RA	758	C	N1-C2-O2	5.01	121.91	118.90
35	RA	1979	C	N1-C2-O2	5.01	121.91	118.90
35	YA	12	U	N1-C2-O2	5.01	126.31	122.80
1	QA	283	C	C2-N3-C4	5.01	122.40	119.90
35	YA	837	C	C6-N1-C2	-5.01	118.30	120.30
35	YA	1640	C	N3-C2-O2	-5.01	118.39	121.90
35	YA	1742	C	C6-N1-C2	-5.01	118.30	120.30
35	RA	279	C	N1-C2-O2	5.00	121.90	118.90
1	XA	1024	G	C4-N9-C1'	5.00	133.01	126.50
35	YA	1993	U	N3-C2-O2	-5.00	118.70	122.20
35	RA	907	U	C2-N1-C1'	5.00	123.70	117.70
35	YA	2177	C	C2-N1-C1'	5.00	124.30	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	2889	C	N1-C2-O2	5.00	121.90	118.90
35	YA	363(E)	U	C5-C6-N1	5.00	125.20	122.70

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	QB	12	GLU	Sidechain
10	QJ	79	ARG	Sidechain
24	QZ	50	HIS	Peptide
37	RD	33	LEU	Peptide
37	RD	35	LYS	Peptide
38	RE	79	ARG	Sidechain
40	RG	116	ASP	Peptide
40	RG	83	ARG	Sidechain
41	RH	116	GLU	Sidechain
41	RH	9	ILE	Peptide
42	RI	11	ASN	Peptide
42	RI	142	VAL	Peptide
42	RI	143	SER	Peptide
42	RI	82	ARG	Sidechain
47	RR	3	HIS	Peptide
51	RV	15	GLU	Sidechain
7	XG	111	ARG	Sidechain
8	XH	60	ARG	Sidechain
11	XK	96	ARG	Sidechain
37	YD	88	ARG	Sidechain
40	YG	72	ARG	Sidechain
41	YH	3	ARG	Sidechain
47	YR	57	ARG	Sidechain

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	QA	32452	0	16383	236	0
1	XA	32389	0	16350	215	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	QB	1907	0	1958	31	0
2	XB	1915	0	1969	26	0
3	QC	1605	0	1668	13	0
3	XC	1605	0	1668	16	0
4	QD	1703	0	1767	31	0
4	XD	1703	0	1767	23	0
5	QE	1155	0	1213	12	0
5	XE	1155	0	1213	13	0
6	QF	843	0	857	13	0
6	XF	843	0	857	10	0
7	QG	1257	0	1296	7	0
7	XG	1257	0	1296	17	0
8	QH	1108	0	1165	23	0
8	XH	1108	0	1165	13	0
9	QI	1010	0	1037	16	0
9	XI	998	0	1024	18	0
10	QJ	801	0	849	11	0
10	XJ	777	0	816	18	0
11	QK	885	0	904	12	0
11	XK	864	0	881	9	0
12	QL	975	0	1062	11	0
12	XL	956	0	1046	13	0
13	QM	955	0	1021	26	0
13	XM	946	0	1008	15	0
14	QN	492	0	529	5	0
14	XN	492	0	529	11	0
15	QO	734	0	771	4	0
15	XO	729	0	768	3	0
16	QP	705	0	725	12	0
16	XP	705	0	725	6	0
17	QQ	834	0	904	7	0
17	XQ	834	0	904	11	0
18	QR	574	0	644	9	0
18	XR	574	0	644	12	0
19	QS	665	0	686	15	0
19	XS	656	0	666	9	0
20	QT	763	0	861	8	0
20	XT	763	0	861	15	0
21	QU	217	0	234	5	0
21	XU	217	0	234	6	0
22	QV	1640	0	837	4	0
22	XV	1640	0	837	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	QX	394	0	196	2	0
23	XX	394	0	196	4	0
24	QY	723	0	713	10	0
24	QZ	723	0	712	11	0
24	XY	723	0	713	9	0
24	XZ	723	0	713	7	0
25	R0	643	0	667	13	0
25	Y0	648	0	672	15	0
26	R1	737	0	813	6	0
26	Y1	763	0	848	18	0
27	R2	581	0	629	9	0
27	Y2	581	0	629	3	0
28	R3	469	0	518	5	0
28	Y3	469	0	518	5	0
29	R4	565	0	561	24	0
29	Y4	565	0	559	10	0
30	R5	459	0	476	12	0
30	Y5	459	0	480	6	0
31	R6	453	0	474	10	0
31	Y6	453	0	474	4	0
32	R7	409	0	454	3	0
32	Y7	418	0	467	6	0
33	R8	517	0	582	10	0
33	Y8	517	0	582	12	0
34	R9	307	0	337	9	0
34	Y9	307	0	336	4	0
35	RA	62266	0	31392	344	0
35	YA	61981	0	31243	331	0
36	RB	2576	0	1303	27	0
36	YB	2576	0	1305	19	0
37	RD	2115	0	2194	39	0
37	YD	2135	0	2221	20	0
38	RE	1568	0	1634	40	0
38	YE	1559	0	1617	23	0
39	RF	1585	0	1632	14	0
39	YF	1585	0	1632	26	0
40	RG	1474	0	1535	23	0
40	YG	1474	0	1535	20	0
41	RH	1336	0	1418	12	0
41	YH	1330	0	1407	18	0
42	RI	1131	0	1216	16	0
42	YI	1136	0	1223	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	RN	1104	0	1180	16	0
43	YN	1104	0	1180	14	0
44	RO	933	0	996	17	0
44	YO	933	0	996	16	0
45	RP	1145	0	1228	28	0
45	YP	1135	0	1212	16	0
46	RQ	1122	0	1179	26	0
46	YQ	1122	0	1179	20	0
47	RR	960	0	1021	12	0
47	YR	960	0	1021	11	0
48	RS	882	0	943	14	0
48	YS	882	0	943	15	0
49	RT	1141	0	1202	21	0
49	YT	1141	0	1202	13	0
50	RU	964	0	1022	19	0
50	YU	964	0	1022	22	0
51	RV	779	0	852	16	0
51	YV	779	0	852	25	0
52	RW	900	0	964	8	0
52	YW	900	0	964	16	0
53	RX	725	0	778	11	0
53	YX	725	0	778	8	0
54	RY	818	0	913	12	0
54	YY	818	0	913	5	0
55	RZ	1461	0	1493	17	0
55	YZ	1461	0	1493	28	0
56	ZA	74	0	51	2	0
56	ZB	74	0	51	7	0
57	QA	93	0	0	0	0
57	QD	1	0	0	0	0
57	QE	1	0	0	0	0
57	QV	3	0	0	0	0
57	QY	1	0	0	0	0
57	R0	2	0	0	0	0
57	R3	1	0	0	0	0
57	RA	302	0	0	0	0
57	RB	3	0	0	0	0
57	RD	2	0	0	0	0
57	RE	1	0	0	0	0
57	RN	1	0	0	0	0
57	RO	1	0	0	0	0
57	RP	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	RQ	4	0	0	0	0
57	RR	1	0	0	0	0
57	RY	1	0	0	0	0
57	XA	99	0	0	0	0
57	XE	1	0	0	0	0
57	XF	1	0	0	0	0
57	XL	1	0	0	0	0
57	XM	1	0	0	0	0
57	XV	4	0	0	0	0
57	Y0	2	0	0	0	0
57	Y1	1	0	0	0	0
57	Y3	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y9	1	0	0	0	0
57	YA	335	0	0	0	0
57	YB	3	0	0	0	0
57	YD	4	0	0	0	0
57	YE	5	0	0	0	0
57	YF	1	0	0	0	0
57	YG	1	0	0	0	0
57	YO	1	0	0	0	0
57	YP	1	0	0	0	0
57	YQ	5	0	0	0	0
57	YR	1	0	0	0	0
57	YV	1	0	0	0	0
58	QD	8	0	0	0	0
58	XD	8	0	0	0	0
59	QN	1	0	0	0	0
59	R4	1	0	0	0	0
59	R5	1	0	0	0	0
59	R6	1	0	0	0	0
59	R9	1	0	0	0	0
59	XN	1	0	0	0	0
59	Y4	1	0	0	0	0
59	Y6	1	0	0	0	0
All	All	295153	0	201053	2175	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 5.

All (2175) 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)
51:YV:85:LYS:CG	51:YV:85:LYS:CD	1.86	1.53
51:YV:85:LYS:CG	51:YV:85:LYS:CB	1.82	1.50
1:XA:368:U:C5	1:XA:368:U:C6	2.05	1.45
51:YV:85:LYS:CE	51:YV:85:LYS:NZ	1.87	1.36
51:YV:85:LYS:CE	51:YV:85:LYS:CD	2.10	1.30
1:XA:368:U:C5	1:XA:368:U:C4	2.19	1.29
23:QX:20:A3P:C1'	23:QX:20:A3P:O4'	1.67	1.27
29:R4:39:CYS:C	29:R4:41:PRO:HD3	1.58	1.22
23:XX:20:A3P:O4'	23:XX:20:A3P:C1'	1.66	1.15
1:XA:368:U:C6	1:XA:368:U:N1	2.19	1.10
1:XA:368:U:N1	1:XA:368:U:C2	2.21	1.08
29:R4:39:CYS:O	29:R4:41:PRO:HD3	1.54	1.04
35:RA:1311:G:N2	35:RA:1603:A:H62	1.57	1.03
1:XA:368:U:C2	1:XA:368:U:N3	2.29	1.00
35:RA:1311:G:H21	35:RA:1603:A:N6	1.61	0.98
1:XA:368:U:C4	1:XA:368:U:N3	2.33	0.95
29:R4:18:CYS:HB3	29:R4:39:CYS:SG	2.07	0.94
29:R4:39:CYS:SG	29:R4:39:CYS:O	2.28	0.91
29:R4:39:CYS:O	29:R4:41:PRO:CD	2.18	0.90
35:YA:2141:G:H1	35:YA:2150:U:H3	1.20	0.87
35:RA:1311:G:H21	35:RA:1603:A:H62	0.87	0.84
35:YA:2808:U:H3	35:YA:2892:A:H62	1.22	0.83
6:XF:46:ARG:HH22	18:XR:37:VAL:HG11	1.43	0.83
29:R4:36:CYS:HB3	29:R4:39:CYS:HB3	1.63	0.80
29:R4:18:CYS:CB	29:R4:39:CYS:SG	2.71	0.78
51:RV:16:PRO:HD3	51:RV:99:ILE:HD11	1.64	0.78
35:RA:676:A:H8	35:RA:2069:G:H21	1.31	0.77
29:R4:39:CYS:C	29:R4:41:PRO:CD	2.50	0.76
33:Y8:26:LYS:HG2	33:Y8:48:PHE:HD2	1.52	0.74
51:RV:40:LEU:HB2	51:RV:46:VAL:HG12	1.70	0.73
35:YA:676:A:H8	35:YA:2069:G:H21	1.35	0.73
1:QA:663:A:H61	1:QA:742:G:H1	1.37	0.73
35:RA:2141:G:H1	35:RA:2150:U:H3	1.35	0.73
51:RV:15:GLU:HG3	51:RV:16:PRO:HD2	1.72	0.70
35:RA:2584:U:H5'	56:ZA:3:PPU:H103	1.73	0.70
24:QY:7:GLU:N	24:QY:7:GLU:OE1	2.18	0.70
35:RA:1857:G:H21	35:RA:1885:A:H62	1.39	0.70
13:XM:94:ARG:HH12	35:YA:887:A:H5'	1.57	0.69
42:RI:82:ARG:NH1	42:RI:82:ARG:CZ	2.54	0.69
1:XA:1357:A:H61	1:XA:1365:G:H1	1.38	0.69
56:ZA:3:PPU:H93	56:ZA:3:PPU:N7	2.06	0.69
29:R4:36:CYS:HB3	29:R4:39:CYS:CB	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Y7:11:LYS:HE2	35:YA:686:G:H5''	1.73	0.69
56:ZB:3:PPU:H93	56:ZB:3:PPU:N7	2.07	0.69
46:RQ:24:GLY:HA2	46:RQ:67:ARG:HH21	1.58	0.69
29:Y4:16:CYS:SG	29:Y4:17:GLY:N	2.66	0.68
46:RQ:75:THR:HA	46:RQ:89:ASN:HA	1.75	0.68
33:R8:25:MET:HG3	45:RP:64:LYS:HB3	1.75	0.68
1:XA:1086:U:H3	1:XA:1099:G:H22	1.39	0.68
38:RE:9:VAL:HB	38:RE:25:VAL:HG23	1.75	0.68
35:YA:67:U:H3	35:YA:74:A:H2	1.42	0.68
46:RQ:66:ILE:HA	46:RQ:104:PHE:HA	1.74	0.68
36:RB:118:G:HO2'	36:RB:119:A:C4'	2.07	0.68
49:RT:36:GLU:HG3	49:RT:41:ARG:HE	1.58	0.68
3:QC:150:LYS:HE3	3:QC:167:TRP:HE1	1.57	0.67
4:QD:154:ASN:HA	4:QD:159:ARG:HH21	1.59	0.67
1:XA:452:A:H62	1:XA:480:U:H3	1.42	0.67
9:QI:25:LYS:N	9:QI:60:ASP:OD1	2.28	0.67
36:RB:3:C:N4	36:RB:118:G:H1	1.93	0.67
35:YA:1053:C:H42	35:YA:1106:G:H1	1.40	0.67
35:RA:259:G:H21	35:RA:621:A:H8	1.41	0.67
38:RE:11:MET:HG2	38:RE:24:THR:HG22	1.76	0.67
1:XA:677:U:H3	1:XA:713:G:H22	1.42	0.67
13:XM:99:ARG:HB2	13:XM:101:GLN:HE22	1.60	0.67
36:YB:22:U:H3	36:YB:61:G:H1	1.42	0.66
3:XC:70:VAL:HG12	3:XC:72:LYS:H	1.61	0.66
6:XF:9:VAL:HB	6:XF:87:ARG:HB2	1.78	0.66
33:Y8:6:THR:HG22	33:Y8:63:PRO:HD2	1.77	0.66
4:QD:18:LYS:NZ	4:QD:31:CYS:SG	2.60	0.65
45:YP:126:VAL:HG12	45:YP:146:VAL:HB	1.75	0.65
35:YA:845:G:H21	35:YA:933:A:H61	1.43	0.65
38:YE:9:VAL:HB	38:YE:25:VAL:HG23	1.78	0.65
35:RA:68:G:H21	35:RA:74:A:H5'	1.62	0.65
38:RE:25:VAL:HG12	38:RE:183:LEU:HD22	1.77	0.65
43:RN:22:THR:OG1	43:RN:23:LEU:N	2.30	0.65
35:YA:994:C:O2	51:YV:10:LYS:NZ	2.30	0.65
35:RA:845:G:H21	35:RA:933:A:H61	1.44	0.65
8:XH:10:LEU:HD22	8:XH:83:ILE:HD11	1.79	0.65
2:QB:9:GLU:HA	2:QB:12:GLU:HG2	1.79	0.65
1:XA:1157:A:C2	1:XA:1178:G:N2	2.64	0.65
41:YH:4:ILE:HG22	41:YH:69:ARG:HD2	1.78	0.65
41:YH:54:ARG:HH21	41:YH:57:ASP:HA	1.62	0.64
1:XA:1030:C:N4	1:XA:1032:A:N7	2.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:XD:62:GLN:HE22	4:XD:65:ARG:HH21	1.45	0.64
14:QN:23:ARG:NH1	14:QN:28:GLY:O	2.30	0.64
34:R9:13:LYS:HE3	34:R9:28:GLU:HG2	1.79	0.64
55:YZ:91:LEU:HD23	55:YZ:130:PRO:HB3	1.78	0.64
24:QY:7:GLU:H	24:QY:7:GLU:CD	2.01	0.64
1:XA:1238:A:H62	1:XA:1301:U:H3	1.46	0.64
1:XA:991:U:H3	1:XA:1213:A:H62	1.45	0.64
45:YP:86:LYS:HB3	45:YP:118:GLY:HA3	1.77	0.64
35:RA:2777:G:H5''	35:RA:2778:A:H5'	1.80	0.64
5:QE:81:GLU:HG3	5:QE:90:VAL:HG12	1.80	0.64
35:YA:1464:C:HO2'	35:YA:1528:A:H8	1.46	0.64
35:YA:1899:G:H21	35:YA:1902:C:H41	1.46	0.64
35:RA:2303:G:N3	40:RG:132:ASN:ND2	2.46	0.64
50:YU:92:ARG:HD2	51:YV:11:GLN:HB2	1.79	0.64
1:QA:782:A:H62	1:QA:800:G:H21	1.46	0.64
38:RE:16:ARG:NH2	38:RE:171:GLU:OE2	2.31	0.64
1:QA:1422:G:H5''	44:RO:48:PRO:HB3	1.80	0.63
36:RB:3:C:C4	36:RB:118:G:N1	2.57	0.63
2:QB:84:GLU:HB3	2:QB:219:VAL:HG21	1.80	0.63
38:RE:24:THR:HG23	38:RE:186:GLY:HA2	1.79	0.63
44:YO:104:ARG:NH1	49:YT:36:GLU:OE1	2.32	0.63
35:RA:2245:U:H5'	35:RA:2246:G:H5'	1.79	0.63
35:YA:1009:A:OP2	43:YN:37:LYS:NZ	2.30	0.63
35:YA:974:G:O2'	35:YA:975:G:N7	2.29	0.63
38:YE:201:THR:HG22	38:YE:203:LYS:H	1.64	0.63
33:Y8:30:ARG:HH21	45:YP:63:PRO:HB2	1.64	0.63
50:YU:92:ARG:NH1	51:YV:11:GLN:O	2.32	0.63
41:RH:101:ARG:NH2	41:RH:121:ILE:O	2.30	0.63
13:QM:23:TYR:HB3	13:QM:67:GLU:HG2	1.81	0.63
2:XB:87:ARG:HH21	2:XB:219:VAL:HB	1.63	0.62
4:XD:166:LYS:HB2	4:XD:178:VAL:HG11	1.81	0.62
1:QA:4:U:O2	8:QH:105:ARG:NH1	2.31	0.62
35:RA:993:G:OP1	50:RU:50:ARG:NH2	2.32	0.62
24:QY:5:TRP:HB2	24:QZ:3:LEU:HB2	1.81	0.62
36:RB:118:G:O2'	36:RB:119:A:O4'	2.18	0.62
36:RB:30:C:H1'	36:RB:57:A:H61	1.64	0.62
46:YQ:136:ALA:HB1	55:YZ:52:SER:HB3	1.80	0.62
1:QA:692:U:OP2	11:QK:26:ASN:ND2	2.33	0.62
17:QQ:66:SER:O	17:QQ:70:ARG:NH1	2.32	0.62
20:QT:30:LYS:HZ3	20:QT:72:LEU:HD21	1.64	0.62
26:R1:49:VAL:HG11	26:R1:70:VAL:HG11	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:RV:62:LEU:HD11	51:RV:95:LEU:HB2	1.82	0.62
2:XB:231:GLU:HG3	2:XB:233:SER:H	1.65	0.62
35:RA:17:G:H4'	50:RU:25:TRP:HE1	1.65	0.62
29:Y4:1:MET:SD	40:YG:98:ARG:NH1	2.72	0.62
39:RF:153:SER:HB2	39:RF:190:GLU:H	1.65	0.62
49:RT:51:ARG:HG2	49:RT:98:LYS:HD2	1.81	0.62
35:YA:345:A:O2'	35:YA:346:A:N7	2.33	0.62
26:R1:21:ARG:NH2	35:RA:2079:U:OP1	2.33	0.62
55:RZ:52:SER:O	55:RZ:54:HIS:N	2.31	0.62
7:XG:79:ARG:HE	7:XG:84:ASN:HB2	1.64	0.62
35:YA:727:A:OP1	35:YA:1431:U:O2'	2.18	0.62
12:QL:114:LYS:O	12:QL:117:ARG:NH1	2.33	0.61
1:QA:1306:A:N6	1:QA:1331:G:O2'	2.33	0.61
42:RI:88:ILE:HG22	42:RI:90:GLY:H	1.64	0.61
1:XA:674:G:H2'	1:XA:675:A:H8	1.65	0.61
35:RA:67:U:H3	35:RA:74:A:H2	1.47	0.61
31:R6:25:LYS:NZ	31:R6:51:GLU:OE2	2.34	0.61
35:RA:956:G:OP2	46:RQ:14:ARG:NH2	2.33	0.61
19:XS:41:VAL:HG12	19:XS:43:GLU:H	1.66	0.61
35:YA:2304:G:H22	35:YA:2312:U:H3	1.47	0.61
2:QB:16:HIS:HE1	2:QB:209:ARG:HG2	1.65	0.61
35:RA:2618:G:H21	38:RE:150:VAL:HG21	1.65	0.61
54:RY:102:CYS:SG	54:RY:103:GLY:N	2.74	0.61
47:YR:38:VAL:HG12	47:YR:112:ALA:HB2	1.83	0.61
35:YA:2010:G:H5''	52:YW:42:ARG:HB2	1.83	0.61
25:Y0:55:ARG:NH1	35:YA:2364:C:OP1	2.34	0.61
38:YE:2:LYS:HB2	38:YE:95:ILE:HD12	1.83	0.61
13:XM:6:GLY:O	40:YG:115:ARG:NH1	2.34	0.61
1:QA:1130:A:O2'	9:QI:3:GLN:NE2	2.34	0.60
44:RO:104:ARG:HH21	49:RT:34:VAL:HG11	1.66	0.60
50:RU:92:ARG:HD2	51:RV:11:GLN:HB2	1.82	0.60
12:XL:117:ARG:HB2	12:XL:122:THR:HB	1.82	0.60
11:QK:124:LYS:O	11:QK:127:LYS:NZ	2.34	0.60
55:RZ:135:GLU:HG2	55:RZ:136:PHE:HD1	1.66	0.60
4:XD:187:ARG:NH2	4:XD:193:ASP:OD2	2.35	0.60
40:YG:37:VAL:HG22	40:YG:159:VAL:HG12	1.84	0.60
55:YZ:119:GLU:O	55:YZ:122:ARG:NH1	2.34	0.60
18:QR:31:LEU:HD12	18:QR:66:LEU:HB2	1.82	0.60
29:R4:59:PHE:HA	29:R4:62:ARG:HG2	1.82	0.60
35:RA:1451:C:O2'	35:RA:1457:A:N6	2.34	0.60
9:QI:28:VAL:HB	9:QI:63:ILE:HG13	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:XJ:10:GLY:HA3	10:XJ:16:LEU:HD21	1.84	0.60
1:QA:217:C:O2'	1:QA:466:C:N4	2.34	0.60
35:RA:1139:G:O2'	35:RA:1143:A:N6	2.32	0.60
33:Y8:11:LYS:NZ	33:Y8:65:GLU:OE2	2.33	0.60
35:YA:1992:G:N2	35:YA:1996:C:O2'	2.35	0.60
41:RH:164:TYR:HB2	41:RH:167:GLU:HB2	1.82	0.60
1:QA:1252:A:H61	1:QA:1285:A:H61	1.48	0.60
6:QF:10:LEU:HB2	6:QF:59:TYR:HB3	1.84	0.60
40:RG:29:TRP:O	40:RG:33:ARG:NH1	2.35	0.60
39:YF:120:GLU:OE2	45:YP:1:MET:N	2.34	0.60
35:RA:2393:A:H4'	45:RP:62:LEU:H	1.67	0.60
35:RA:265:A:N6	35:RA:427:U:O2'	2.34	0.60
49:RT:19:LEU:HD22	49:RT:86:ILE:HG22	1.84	0.60
3:XC:84:ILE:HG12	3:XC:88:ARG:HE	1.67	0.60
9:XI:48:GLU:OE1	9:XI:51:ARG:NH2	2.35	0.60
1:QA:674:G:H2'	1:QA:675:A:H8	1.67	0.60
30:R5:19:ARG:NH2	35:RA:1264:G:OP1	2.35	0.60
36:RB:118:G:H2'	36:RB:119:A:O4'	2.02	0.60
35:YA:1482:U:H3	35:YA:1512:G:H1	1.48	0.60
35:YA:2135:A:H62	35:YA:2156:G:H21	1.50	0.60
37:YD:17:THR:HB	37:YD:205:VAL:H	1.66	0.60
35:RA:959:A:N3	35:RA:2457:U:O2'	2.33	0.59
22:XV:76:A:O3'	35:YA:2602:A:N6	2.35	0.59
35:RA:1265:A:H61	35:RA:2013:A:H5''	1.67	0.59
35:RA:587:C:OP2	45:RP:21:ARG:NH1	2.32	0.59
50:RU:95:LEU:HD13	51:RV:4:ILE:HD13	1.82	0.59
24:XY:16:TRP:NE1	24:XY:80:CYS:O	2.34	0.59
35:RA:1900:A:H1'	35:RA:1970:A:H2'	1.83	0.59
12:XL:39:VAL:HB	12:XL:57:LYS:HB3	1.83	0.59
35:YA:2305:A:H5''	40:YG:134:GLY:HA3	1.84	0.59
1:QA:1086:U:H3	1:QA:1099:G:H22	1.51	0.59
3:QC:153:VAL:HG22	3:QC:198:VAL:HG12	1.85	0.59
35:RA:2010:G:H5''	52:RW:42:ARG:HB2	1.84	0.59
37:RD:25:THR:HG21	37:RD:81:ALA:HA	1.84	0.59
54:RY:83:THR:OG1	54:RY:84:ARG:N	2.35	0.59
7:XG:111:ARG:NH2	7:XG:126:ASP:OD2	2.36	0.59
15:XO:16:ALA:HB1	15:XO:21:ASP:HB3	1.83	0.59
48:YS:106:ARG:NH1	48:YS:107:GLU:OE2	2.35	0.59
36:RB:118:G:O2'	36:RB:119:A:C4'	2.51	0.59
1:QA:422:C:O2'	1:QA:423:G:N2	2.35	0.59
1:QA:664:G:H22	1:QA:741:G:H1	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:768:G:O2'	35:RA:1379:A:N6	2.33	0.59
1:XA:452:A:OP1	16:XP:43:LYS:NZ	2.36	0.59
19:XS:50:ALA:HB1	19:XS:57:HIS:HB3	1.85	0.59
35:YA:2789:C:O2'	35:YA:2893:G:N2	2.33	0.59
31:R6:26:ASN:ND2	31:R6:29:ASN:OD1	2.34	0.59
38:RE:14:ILE:HG21	38:RE:173:VAL:HG11	1.84	0.59
46:RQ:75:THR:HG22	46:RQ:89:ASN:HB2	1.83	0.59
43:YN:73:THR:HB	43:YN:82:LEU:HD11	1.84	0.59
50:YU:92:ARG:HD3	50:YU:94:ASN:HB3	1.85	0.59
5:QE:80:ILE:HG22	5:QE:91:LEU:HB2	1.85	0.58
1:XA:413:G:N2	1:XA:429:U:OP2	2.35	0.58
10:XJ:49:VAL:HG23	14:XN:41:ARG:HB2	1.84	0.58
26:Y1:73:LEU:HD21	26:Y1:98:LEU:HD23	1.83	0.58
35:YA:495:G:N3	52:YW:61:ASN:ND2	2.51	0.58
51:YV:69:LYS:HE2	51:YV:86:GLY:HA3	1.85	0.58
1:XA:1191:A:OP1	3:XC:4:LYS:NZ	2.37	0.58
1:XA:1540:U:O2'	18:XR:55:ARG:NH2	2.36	0.58
27:Y2:65:ASN:ND2	35:YA:72:U:O4	2.36	0.58
35:YA:1689:A:H62	35:YA:1698:A:H2	1.52	0.58
35:YA:2134:A:N7	35:YA:2157:G:O2'	2.37	0.58
2:QB:185:ILE:HG22	2:QB:199:TYR:HB2	1.86	0.58
35:RA:2032:G:H22	35:RA:2572:A:H5'	1.68	0.58
4:XD:23:GLY:N	4:XD:26:CYS:SG	2.76	0.58
1:XA:1178:G:OP2	9:XI:93:ARG:NH2	2.36	0.58
35:YA:1824:G:N3	37:YD:254:THR:OG1	2.36	0.58
40:YG:118:ARG:HG3	40:YG:181:ARG:HD3	1.84	0.58
1:QA:1191:A:H5''	3:QC:4:LYS:HE3	1.84	0.58
1:QA:1318:A:H4'	19:QS:11:VAL:HG11	1.85	0.58
25:R0:48:GLY:O	25:R0:80:HIS:ND1	2.37	0.58
43:RN:54:VAL:HB	43:RN:122:VAL:HG12	1.85	0.58
45:RP:19:VAL:HG23	45:RP:27:HIS:HB3	1.86	0.58
35:RA:1812:A:H4'	37:RD:46:GLN:HE22	1.67	0.58
37:RD:43:ARG:HB2	37:RD:54:ARG:HB2	1.85	0.58
25:R0:23:VAL:HG21	35:RA:857:C:H4'	1.85	0.58
2:XB:118:LEU:HB3	2:XB:142:LEU:HD13	1.86	0.58
17:XQ:88:TYR:OH	17:XQ:92:ARG:NH1	2.36	0.58
35:YA:1667:G:O2'	35:YA:1669:A:N6	2.36	0.58
55:YZ:109:ALA:HB3	55:YZ:145:GLU:HG2	1.86	0.58
24:XY:4:ILE:HB	24:XY:76:LEU:HA	1.85	0.58
39:YF:143:ALA:HB1	39:YF:148:LEU:HB2	1.86	0.58
1:QA:958:A:OP1	24:QZ:36:ARG:NH1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:R4:16:CYS:SG	29:R4:36:CYS:HB2	2.44	0.57
6:QF:9:VAL:HB	6:QF:87:ARG:HB2	1.84	0.57
31:R6:6:ARG:NH2	35:RA:2285:C:OP2	2.37	0.57
35:RA:586:A:H5'	39:RF:89:VAL:HG11	1.86	0.57
36:YB:30:C:H1'	36:YB:57:A:H61	1.69	0.57
1:QA:316:G:OP2	1:QA:351:G:O2'	2.22	0.57
17:QQ:88:TYR:OH	17:QQ:92:ARG:NH2	2.37	0.57
35:YA:583:G:OP2	50:YU:10:ARG:NH1	2.37	0.57
53:YX:53:LYS:NZ	53:YX:55:ASN:OD1	2.36	0.57
11:QK:58:PRO:HB2	11:QK:93:GLN:HG3	1.86	0.57
29:R4:23:GLU:OE2	40:RG:6:ALA:N	2.32	0.57
49:YT:51:ARG:HG2	49:YT:98:LYS:HD2	1.86	0.57
25:R0:36:ILE:HA	25:R0:60:PHE:HA	1.87	0.57
38:RE:34:VAL:HG12	38:RE:72:VAL:HG21	1.86	0.57
1:XA:4:U:O2	8:XH:105:ARG:NH1	2.37	0.57
36:YB:50:G:OP2	48:YS:62:LYS:NZ	2.37	0.57
42:YI:80:PRO:HB2	42:YI:146:ALA:HB2	1.87	0.57
34:R9:6:SER:HB3	35:RA:2466:C:H5''	1.86	0.57
1:XA:811:C:O2'	1:XA:901:A:N1	2.38	0.57
1:XA:951:G:OP2	13:XM:102:ARG:NH1	2.37	0.57
1:QA:1030:C:N4	35:YA:2167:U:O2'	2.38	0.57
35:YA:269:U:H3	35:YA:370:G:H1	1.52	0.57
1:QA:878:G:H5'	8:QH:89:PRO:HG2	1.87	0.57
31:R6:8:LYS:HG3	31:R6:54:ILE:HD13	1.87	0.57
22:QV:19:G:O6	40:RG:83:ARG:NH2	2.37	0.57
47:RR:75:LEU:HA	47:RR:78:LYS:HB3	1.86	0.57
1:XA:972:C:H1'	10:XJ:55:LYS:HE2	1.87	0.57
13:XM:3:ARG:NH1	13:XM:8:GLU:OE2	2.37	0.57
38:YE:67:PHE:HZ	38:YE:78:LEU:HD11	1.70	0.57
46:YQ:13:GLN:O	46:YQ:72:LYS:NZ	2.37	0.57
1:QA:974:A:OP2	14:QN:41:ARG:NH1	2.38	0.57
35:RA:727:A:OP1	35:RA:1431:U:O2'	2.21	0.57
35:RA:1992:G:N2	35:RA:1996:C:O2'	2.37	0.57
51:RV:52:VAL:HG21	51:RV:55:ALA:HB3	1.86	0.57
35:YA:987:G:O2'	35:YA:1000:A:N3	2.34	0.57
27:R2:22:GLU:OE2	27:R2:68:ARG:NH2	2.37	0.57
44:RO:2:ILE:HB	44:RO:33:ALA:HB3	1.85	0.57
4:XD:57:ARG:NH2	4:XD:205:GLU:OE2	2.38	0.57
1:QA:1304:G:OP1	21:QU:2:GLY:N	2.38	0.57
34:R9:1:MET:HG2	35:RA:2477:C:H2'	1.86	0.57
35:RA:2848:G:O2'	35:RA:2867:G:N2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:RG:82:LEU:HD12	40:RG:88:ILE:HG21	1.86	0.57
35:RA:995:C:H5'	50:RU:54:LYS:HG2	1.85	0.57
36:RB:104:A:OP1	55:RZ:72:ARG:NH2	2.38	0.57
1:QA:672:U:H2'	1:QA:673:G:H8	1.69	0.56
4:QD:60:GLU:HG3	4:QD:202:LEU:HD12	1.87	0.56
45:YP:38:GLN:HB3	45:YP:45:LEU:HB3	1.86	0.56
1:QA:774:G:OP1	37:RD:202:LYS:NZ	2.38	0.56
30:Y5:49:CYS:SG	30:Y5:50:GLY:N	2.78	0.56
8:XH:51:VAL:HG11	8:XH:60:ARG:HG3	1.87	0.56
38:YE:8:LYS:NZ	38:YE:192:ASN:OD1	2.38	0.56
36:YB:37:C:O2	48:YS:95:HIS:NE2	2.38	0.56
35:RA:1102:C:H2'	35:RA:1103:A:H8	1.70	0.56
35:RA:1138:G:O2'	43:RN:102:ALA:O	2.23	0.56
1:XA:664:G:H22	1:XA:741:G:H1	1.51	0.56
35:YA:674:G:H1'	39:YF:74:ARG:HD3	1.88	0.56
49:YT:106:SER:HA	49:YT:110:ILE:HD11	1.87	0.56
55:YZ:126:VAL:HG12	55:YZ:163:LEU:HA	1.86	0.56
47:RR:86:ARG:NH2	47:RR:118:GLU:OXT	2.39	0.56
52:RW:18:ARG:HD2	52:RW:76:VAL:HB	1.87	0.56
4:XD:10:ARG:HG3	4:XD:40:PRO:HG3	1.86	0.56
5:XE:102:ALA:HB1	5:XE:106:PRO:HG2	1.88	0.56
9:XI:10:ARG:NH1	9:XI:75:ASP:OD2	2.38	0.56
35:YA:15:G:H1	35:YA:525:U:H3	1.53	0.56
35:YA:807:U:O2'	35:YA:2060:A:N1	2.38	0.56
50:YU:90:VAL:HG22	51:YV:38:LEU:HB3	1.85	0.56
13:QM:23:TYR:HD2	13:QM:67:GLU:HA	1.71	0.56
35:RA:2148:G:H2'	35:RA:2149:G:H8	1.69	0.56
35:RA:818:G:HO2'	35:RA:838:C:HO2'	1.53	0.56
1:XA:544:G:OP1	4:XD:59:ARG:NH2	2.38	0.56
26:Y1:91:LYS:O	26:Y1:95:LEU:HG	2.05	0.56
35:YA:1388:G:HO2'	35:YA:1525:G:HO2'	1.54	0.56
35:YA:996:A:OP2	50:YU:92:ARG:NH2	2.39	0.56
51:YV:85:LYS:CG	51:YV:85:LYS:CA	2.79	0.56
55:YZ:102:LEU:HD21	55:YZ:155:LEU:HD11	1.87	0.56
8:QH:34:GLU:OE1	8:QH:37:ARG:NH2	2.39	0.56
25:R0:19:LYS:NZ	35:RA:2261:C:OP1	2.35	0.56
36:RB:9:G:H1	36:RB:111:U:H3	1.52	0.56
38:RE:119:ARG:NH1	38:RE:159:HIS:O	2.39	0.56
39:YF:116:ASP:OD1	39:YF:119:ARG:NH2	2.38	0.56
52:YW:24:ILE:HD13	52:YW:36:LEU:HD11	1.88	0.56
1:QA:686:U:H1'	11:QK:42:TRP:HE1	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:1247:U:H3	1:XA:1290:G:H1	1.53	0.56
10:XJ:45:ARG:HB3	10:XJ:65:LEU:HB3	1.87	0.56
35:YA:141:A:HO2'	35:YA:1407:C:HO2'	1.52	0.56
48:YS:27:SER:HA	48:YS:88:ASP:HB3	1.87	0.56
49:YT:128:GLU:HG3	49:YT:129:ARG:HG3	1.88	0.56
1:QA:1236:A:H4'	1:QA:1304:G:H4'	1.86	0.56
1:QA:1320:C:O2	19:QS:36:ARG:NH2	2.39	0.56
35:RA:1388:G:HO2'	35:RA:1525:G:HO2'	1.54	0.56
35:RA:2445:G:OP1	39:RF:74:ARG:NH1	2.39	0.56
1:XA:405:U:O4	4:XD:2:GLY:N	2.39	0.56
7:XG:78:ARG:NH1	7:XG:154:TYR:O	2.38	0.56
41:YH:9:ILE:HD11	41:YH:69:ARG:HG2	1.88	0.56
24:QZ:57:SER:HB2	24:QZ:67:VAL:HG12	1.88	0.56
35:RA:1782:C:H1'	35:RA:2609:U:H5''	1.87	0.56
35:RA:1817:G:OP1	37:RD:88:ARG:NH2	2.39	0.56
35:RA:629:G:N3	35:RA:639:U:O2'	2.39	0.56
35:RA:958:U:OP2	46:RQ:14:ARG:NH1	2.39	0.56
9:XI:26:VAL:HG12	9:XI:61:ALA:HB3	1.87	0.56
35:YA:768:G:O2'	35:YA:1379:A:N6	2.39	0.56
1:QA:811:C:O2'	1:QA:901:A:N1	2.38	0.55
13:QM:58:GLU:O	13:QM:62:ASN:HB2	2.06	0.55
52:RW:86:LEU:HD22	52:RW:96:ILE:HD11	1.87	0.55
9:QI:25:LYS:NZ	9:QI:60:ASP:OD2	2.39	0.55
33:R8:52:LYS:H	33:R8:52:LYS:HD3	1.70	0.55
35:RA:2751:G:N2	35:RA:2751:G:OP1	2.37	0.55
26:Y1:92:LYS:NZ	26:Y1:96:LYS:NZ	2.55	0.55
32:Y7:35:ARG:HG3	32:Y7:42:LEU:HD21	1.88	0.55
1:QA:403:C:OP2	4:QD:74:GLN:NE2	2.40	0.55
1:QA:957:U:OP1	19:QS:81:ARG:NH2	2.39	0.55
44:RO:80:ASP:OD2	49:RT:64:ARG:NH2	2.40	0.55
55:YZ:108:PRO:HB3	55:YZ:144:LEU:HB2	1.87	0.55
29:R4:16:CYS:SG	29:R4:17:GLY:N	2.80	0.55
35:RA:987:G:O2'	35:RA:1000:A:N3	2.37	0.55
35:RA:1858:G:O2'	35:RA:1884:A:N6	2.39	0.55
35:RA:2472:G:H5'	35:RA:2473:U:H5''	1.89	0.55
35:YA:1139:G:O2'	35:YA:1143:A:N6	2.40	0.55
35:YA:2495:G:H5''	46:YQ:82:ARG:HG2	1.88	0.55
52:YW:22:ASP:OD1	52:YW:25:ARG:NH1	2.39	0.55
2:QB:109:SER:O	2:QB:113:HIS:ND1	2.39	0.55
42:RI:4:ILE:HG12	42:RI:18:VAL:HG12	1.88	0.55
1:QA:186(B):C:H2'	1:QA:186(C):G:H8	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:1250:G:OP2	45:RP:18:ARG:NH2	2.40	0.55
35:RA:521:G:H2'	35:RA:522:G:H8	1.72	0.55
48:RS:18:ILE:HG13	48:RS:88:ASP:HA	1.88	0.55
26:Y1:93:GLU:O	26:Y1:97:LEU:HD13	2.06	0.55
35:YA:270(E):G:H1	35:YA:270(U):C:H42	1.54	0.55
35:RA:1565:C:OP1	37:RD:4:LYS:NZ	2.37	0.55
35:YA:2749:A:H5''	41:YH:3:ARG:HE	1.72	0.55
53:YX:55:ASN:HB2	53:YX:80:ILE:HG23	1.87	0.55
1:QA:112:G:OP2	16:QP:27:LYS:NZ	2.39	0.55
35:RA:1339:G:H5''	53:RX:16:LYS:HD3	1.88	0.55
35:RA:665:C:H2'	35:RA:666:G:H8	1.71	0.55
2:XB:88:ALA:HB2	2:XB:219:VAL:HG13	1.89	0.55
24:XY:73:ASP:OD1	24:XY:73:ASP:N	2.40	0.55
35:YA:2130:U:H3	35:YA:2158:A:H1'	1.71	0.55
1:QA:1119:C:H2'	1:QA:1120:G:H8	1.71	0.55
1:QA:547:A:OP1	4:QD:73:ARG:NH2	2.40	0.55
35:RA:39:C:O2	39:RF:46:ARG:NH2	2.40	0.55
35:YA:1102:C:H2'	35:YA:1103:A:H8	1.72	0.55
35:YA:2245:U:H5''	35:YA:2246:G:H5'	1.89	0.55
48:YS:56:LEU:HD12	48:YS:69:VAL:HG23	1.88	0.55
35:RA:2291:U:O2'	35:RA:2374:C:O2	2.25	0.55
35:RA:2816:C:O2	35:RA:2883:A:O2'	2.25	0.55
41:RH:56:SER:OG	41:RH:57:ASP:N	2.39	0.55
20:XT:85:MET:HA	20:XT:88:VAL:HG22	1.89	0.55
25:Y0:51:VAL:HG21	25:Y0:79:VAL:HG23	1.89	0.55
1:QA:405:U:O4	4:QD:2:GLY:N	2.40	0.54
20:QT:89:ARG:HD2	20:QT:104:LEU:HD11	1.89	0.54
19:XS:11:VAL:HG12	19:XS:13:ASP:H	1.72	0.54
35:YA:859:G:N2	35:YA:917:A:OP2	2.40	0.54
1:QA:544:G:OP1	4:QD:59:ARG:NH2	2.38	0.54
44:RO:25:LEU:HB2	44:RO:38:VAL:HG13	1.88	0.54
25:Y0:77:ARG:NH2	35:YA:857:C:OP2	2.40	0.54
29:Y4:48:ARG:NH2	29:Y4:51:ASP:OD2	2.37	0.54
47:YR:28:LEU:HD23	47:YR:48:VAL:HG21	1.88	0.54
30:R5:16:ARG:NH2	35:RA:517:C:OP1	2.40	0.54
35:RA:392:C:H5''	35:RA:409:C:H5''	1.89	0.54
46:RQ:27:VAL:N	46:RQ:138:ASP:OD2	2.40	0.54
1:XA:1357:A:N6	1:XA:1365:G:H1	2.04	0.54
10:XJ:61:GLU:HB2	14:XN:58:LYS:HE2	1.88	0.54
38:YE:101:ARG:HH21	38:YE:171:GLU:HB2	1.72	0.54
1:QA:552:U:H2'	1:QA:553:A:H8	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:QB:16:HIS:CE1	2:QB:209:ARG:HG2	2.42	0.54
6:QF:3:ARG:NH1	6:QF:66:GLU:OE1	2.39	0.54
1:QA:963:G:H21	10:QJ:55:LYS:HG2	1.72	0.54
13:QM:88:ARG:HG2	13:QM:98:VAL:HB	1.89	0.54
26:R1:18:ILE:HG12	26:R1:37:ILE:HG12	1.89	0.54
1:XA:1304:G:OP1	21:XU:2:GLY:N	2.40	0.54
3:XC:20:SER:HB2	3:XC:40:ARG:HH22	1.72	0.54
8:XH:34:GLU:OE1	8:XH:37:ARG:NH2	2.41	0.54
35:YA:2303:G:N3	40:YG:132:ASN:ND2	2.55	0.54
1:QA:1119:C:OP1	9:QI:83:ARG:NH2	2.40	0.54
1:QA:452:A:H62	1:QA:480:U:H3	1.55	0.54
29:R4:56:VAL:O	29:R4:60:GLN:NE2	2.40	0.54
37:RD:18:VAL:HA	37:RD:211:ARG:HH22	1.73	0.54
10:XJ:51:ARG:HB2	10:XJ:60:ARG:HA	1.89	0.54
26:Y1:76:ARG:HH22	26:Y1:97:LEU:HB3	1.72	0.54
45:YP:95:VAL:HB	45:YP:125:VAL:HG12	1.89	0.54
35:YA:997:G:H5'	50:YU:93:LYS:HD2	1.89	0.54
1:QA:218:C:H5'	1:QA:466:C:H42	1.73	0.54
1:QA:262:A:H5''	20:QT:76:ALA:HB2	1.88	0.54
8:QH:106:GLY:O	8:QH:122:ARG:NH2	2.40	0.54
34:R9:25:VAL:HB	34:R9:34:GLN:HB2	1.89	0.54
1:XA:1251:A:N3	1:XA:1369:C:O2'	2.37	0.54
35:YA:219:G:N3	35:YA:234:C:O2'	2.40	0.54
1:QA:1240:U:OP1	7:QG:119:ARG:NH2	2.41	0.54
1:QA:701:C:O2'	1:QA:703:G:N3	2.41	0.54
35:RA:2547:U:O2	44:RO:23:ARG:NH2	2.41	0.54
1:XA:1502:A:H2	1:XA:1505:G:H1	1.54	0.54
2:XB:70:PHE:HD1	2:XB:163:PHE:HB3	1.73	0.54
35:YA:1980:G:O2'	35:YA:1982:C:OP2	2.22	0.54
39:YF:135:LYS:HB2	39:YF:138:GLU:HG3	1.90	0.54
41:YH:5:GLY:HA2	41:YH:69:ARG:HG3	1.88	0.54
47:YR:24:GLN:HG3	47:YR:44:LEU:HD13	1.89	0.54
1:QA:380:G:N2	1:QA:383:A:OP2	2.34	0.54
35:YA:2680:C:OP2	38:YE:111:ARG:NH2	2.41	0.54
46:YQ:116:GLU:OE2	46:YQ:119:ARG:NH1	2.41	0.54
24:QZ:59:ARG:NH2	24:QZ:62:GLU:OE1	2.41	0.54
30:R5:36:CYS:HB3	30:R5:49:CYS:HB3	1.90	0.54
36:RB:8:U:O2'	48:RS:25:ARG:NH2	2.41	0.54
1:XA:1219:U:OP1	14:XN:19:ARG:NH2	2.41	0.54
1:XA:1297:C:O2'	7:XG:114:ARG:NH1	2.41	0.54
37:YD:69:ARG:NH2	37:YD:128:GLY:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:YS:28:VAL:HG11	48:YS:98:VAL:HG12	1.89	0.54
1:QA:437:U:O2'	4:QD:123:HIS:ND1	2.39	0.54
5:QE:102:ALA:HB1	5:QE:106:PRO:HG2	1.90	0.54
10:QJ:34:VAL:HG22	10:QJ:74:ILE:HG23	1.90	0.54
40:RG:68:PRO:HB3	40:RG:92:VAL:HB	1.90	0.54
45:RP:101:VAL:HB	45:RP:106:LEU:HB3	1.90	0.54
1:QA:992:U:H3	1:QA:1044:A:H62	1.55	0.53
1:QA:401:C:O2'	1:QA:621:A:N3	2.39	0.53
1:QA:953:G:N7	13:QM:104:ARG:NH2	2.56	0.53
35:RA:974:G:O2'	35:RA:975:G:N7	2.34	0.53
53:RX:72:LYS:NZ	53:RX:75:ASP:OD1	2.38	0.53
2:XB:118:LEU:HD11	2:XB:138:LEU:HD12	1.88	0.53
39:YF:167:ALA:HB1	39:YF:173:VAL:HG11	1.89	0.53
46:YQ:137:TYR:HB3	55:YZ:76:LEU:HD21	1.90	0.53
20:QT:41:ILE:HD13	20:QT:87:LYS:HD3	1.90	0.53
35:RA:2701:C:H3'	35:RA:2702:U:H5''	1.91	0.53
35:RA:372:G:N2	35:RA:401:A:OP2	2.37	0.53
46:RQ:58:PHE:HD2	46:RQ:61:GLY:HA3	1.72	0.53
49:RT:50:ILE:HD11	49:RT:100:TYR:HA	1.89	0.53
35:YA:700:G:O2'	35:YA:1632:A:N3	2.37	0.53
35:YA:1859:A:N6	35:YA:1883:G:O2'	2.41	0.53
1:QA:1032:A:N6	35:YA:2167:U:O3'	2.42	0.53
15:QO:29:VAL:HG23	15:QO:63:ARG:HG3	1.89	0.53
35:RA:1300:U:H4'	35:RA:1301:A:H5'	1.90	0.53
1:XA:958:A:N3	1:XA:985:C:O2'	2.37	0.53
15:XO:70:LEU:HD11	15:XO:77:ARG:HE	1.73	0.53
35:YA:259:G:H21	35:YA:621:A:H8	1.57	0.53
38:YE:101:ARG:NH1	38:YE:169:ASN:O	2.42	0.53
38:YE:77:ILE:HD13	38:YE:195:LEU:HD13	1.89	0.53
32:R7:37:LYS:NZ	35:RA:468:G:OP2	2.40	0.53
55:RZ:7:ALA:HB3	55:RZ:61:LEU:HB3	1.89	0.53
1:XA:1288:A:O3'	21:XU:10:ARG:NH1	2.39	0.53
35:YA:2748:A:H8	41:YH:63:SER:HB2	1.73	0.53
44:YO:23:ARG:NH2	44:YO:28:SER:O	2.41	0.53
9:QI:42:ARG:NH1	9:QI:71:SER:OG	2.41	0.53
46:RQ:138:ASP:OD1	55:RZ:81:ARG:NH2	2.41	0.53
35:YA:2547:U:O2	44:YO:23:ARG:NH2	2.41	0.53
36:YB:47:C:OP1	48:YS:10:ARG:NH2	2.41	0.53
1:QA:973:G:O6	1:QA:974:A:N6	2.42	0.53
35:YA:1433:U:H3	35:YA:1560:G:H1	1.55	0.53
25:Y0:2:ALA:N	35:YA:2494:G:OP1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:2451:A:C2	56:ZB:3:PPU:HD2	2.43	0.53
2:QB:7:VAL:HG12	2:QB:12:GLU:OE1	2.09	0.53
9:QI:128:ARG:NH2	22:QV:33:U:OP2	2.38	0.53
33:R8:29:LYS:O	33:R8:31:HIS:N	2.32	0.53
35:RA:631:A:OP1	45:RP:64:LYS:NZ	2.41	0.53
35:RA:996:A:OP2	50:RU:92:ARG:NH2	2.42	0.53
38:RE:24:THR:HG21	38:RE:188:VAL:HG12	1.90	0.53
1:XA:1210:C:O2'	1:XA:1213:A:O2'	2.26	0.53
1:XA:1522:U:H2'	1:XA:1523:G:H8	1.74	0.53
1:XA:191:G:O2'	20:XT:101:GLY:O	2.26	0.53
35:YA:2646:C:OP2	35:YA:2732:G:O2'	2.26	0.53
38:YE:128:SER:OG	38:YE:129:HIS:N	2.40	0.53
43:YN:21:LYS:HB3	43:YN:26:LEU:HB2	1.90	0.53
5:QE:153:LYS:HE2	5:QE:155:GLU:HB3	1.89	0.53
35:RA:1490:A:O2'	37:RD:99:ASP:OD1	2.24	0.53
53:RX:57:LEU:HG	53:RX:78:LYS:HB2	1.89	0.53
1:XA:673:G:H2'	1:XA:674:G:C8	2.44	0.53
35:YA:114:U:O2'	53:YX:33:LYS:NZ	2.41	0.53
35:YA:116:C:O2'	35:YA:126:A:N3	2.36	0.53
35:YA:2287:A:H62	35:YA:2344:U:H3	1.56	0.53
35:YA:392:C:H5''	35:YA:409:C:H5''	1.91	0.53
35:YA:181:A:H1'	35:YA:435:C:H5'	1.90	0.53
44:YO:47:ILE:O	44:YO:53:LYS:NZ	2.42	0.53
42:RI:140:LEU:HD12	42:RI:142:VAL:HG12	1.90	0.53
42:RI:40:THR:HG23	42:RI:43:ASN:H	1.73	0.53
35:YA:833:U:O2	45:YP:55:ARG:NH2	2.41	0.53
44:YO:43:VAL:HG23	44:YO:54:GLU:HA	1.89	0.53
1:QA:1286:A:H4'	21:QU:26:LYS:HD2	1.91	0.53
40:RG:37:VAL:HB	40:RG:94:LEU:HB2	1.90	0.53
43:RN:15:LEU:HD22	43:RN:134:ARG:HD3	1.90	0.53
48:RS:27:SER:HA	48:RS:88:ASP:HB3	1.90	0.53
49:RT:66:VAL:HA	49:RT:71:GLY:HA2	1.91	0.53
1:XA:1492:A:H2'	35:YA:1913:A:H61	1.73	0.53
38:YE:94:GLU:O	38:YE:97:LYS:NZ	2.42	0.53
4:QD:57:ARG:NH2	4:QD:205:GLU:OE2	2.35	0.52
35:YA:1196:C:HO2'	35:YA:1228:G:HO2'	1.57	0.52
1:QA:1073:U:O2	2:QB:104:ASN:ND2	2.43	0.52
5:QE:48:ALA:HB2	5:QE:57:LYS:HE3	1.90	0.52
35:RA:998:C:OP2	50:RU:58:ARG:NH1	2.42	0.52
48:RS:26:LEU:HB3	48:RS:87:PHE:HA	1.90	0.52
52:RW:22:ASP:OD1	52:RW:25:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:XD:15:GLU:OE2	4:XD:59:ARG:NH1	2.41	0.52
35:YA:1543:A:H2'	35:YA:1544:C:H3'	1.92	0.52
35:YA:1728:G:N7	35:YA:1731:G:N2	2.50	0.52
35:YA:2251:G:OP2	46:YQ:82:ARG:NH2	2.41	0.52
1:QA:1251:A:N3	1:QA:1369:C:O2'	2.39	0.52
1:QA:450:G:OP1	16:QP:43:LYS:NZ	2.35	0.52
2:QB:87:ARG:NH1	2:QB:220:ASP:OD1	2.26	0.52
35:RA:270(J):G:N2	35:RA:270(Q):C:O2	2.42	0.52
1:XA:261:U:OP2	20:XT:79:ARG:NH2	2.42	0.52
35:YA:1889:A:N3	35:YA:2086:U:O2'	2.43	0.52
55:YZ:54:HIS:HB3	55:YZ:101:PRO:HD3	1.90	0.52
2:QB:67:THR:HG21	2:QB:155:LEU:HG	1.91	0.52
1:QA:1296:C:O3'	13:QM:13:LYS:NZ	2.42	0.52
35:RA:299:A:N1	35:RA:322:A:O2'	2.37	0.52
38:RE:36:ARG:NH2	38:RE:88:GLY:O	2.42	0.52
1:XA:514:C:H2'	1:XA:515:G:H8	1.74	0.52
2:XB:174:VAL:O	2:XB:178:ARG:HB3	2.09	0.52
5:XE:80:ILE:HG22	5:XE:91:LEU:HB2	1.90	0.52
35:YA:1654:A:O2'	38:YE:113:PHE:O	2.24	0.52
13:QM:49:THR:HG22	13:QM:51:ALA:H	1.75	0.52
29:R4:14:ILE:HG13	29:R4:31:ILE:HG13	1.92	0.52
35:RA:26:G:H1'	35:RA:515:A:H61	1.73	0.52
39:RF:116:ASP:OD2	45:RP:1:MET:N	2.36	0.52
6:XF:95:GLU:O	18:XR:32:ARG:NH1	2.42	0.52
35:YA:1827:C:OP2	37:YD:222:ARG:NH1	2.43	0.52
39:YF:160:ASN:HB3	39:YF:163:VAL:HG12	1.91	0.52
40:YG:161:THR:HG22	40:YG:163:ALA:H	1.73	0.52
1:QA:501:C:H1'	1:QA:549:C:H1'	1.91	0.52
35:RA:1864:U:H3	35:RA:1878:G:H1	1.56	0.52
35:RA:1980:G:O2'	35:RA:1982:C:OP2	2.24	0.52
25:R0:24:LYS:NZ	35:RA:2355:C:O2'	2.42	0.52
35:RA:2725:A:O2'	35:RA:2726:U:O2	2.27	0.52
35:RA:442:G:H1'	39:RF:48:THR:HG21	1.90	0.52
35:RA:581:C:H2'	35:RA:582:G:H8	1.74	0.52
51:RV:59:ALA:HB1	51:RV:94:LEU:HB3	1.91	0.52
10:XJ:13:HIS:HA	10:XJ:16:LEU:HB2	1.90	0.52
24:XY:67:VAL:HG23	24:XY:78:ALA:HB3	1.92	0.52
39:YF:185:ASP:OD1	39:YF:188:ARG:NH1	2.38	0.52
51:YV:59:ALA:HB2	51:YV:96:ILE:HD13	1.91	0.52
56:ZB:3:PPU:C9	56:ZB:3:PPU:N7	2.73	0.52
1:QA:1128:C:O2	1:QA:1146:A:N6	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:QC:139:GLN:O	3:QC:143:GLU:HB2	2.10	0.52
1:QA:1279:A:OP2	10:QJ:9:ARG:NH1	2.42	0.52
35:RA:1952:A:N3	35:RA:2560:C:O2'	2.39	0.52
44:RO:87:ILE:HD12	44:RO:91:LEU:HD13	1.92	0.52
35:YA:2849:U:OP1	49:YT:95:ARG:NH1	2.42	0.52
1:QA:1145:C:H4'	1:QA:1146:A:H8	1.75	0.52
1:QA:1241:G:H1	1:QA:1296:C:H42	1.57	0.52
4:QD:32:ALA:HA	4:QD:35:ARG:HB2	1.92	0.52
35:RA:833:U:O2	45:RP:55:ARG:NH1	2.40	0.52
9:XI:93:ARG:HH21	9:XI:97:LYS:HD2	1.75	0.52
35:YA:1798:U:OP2	37:YD:274:ARG:NH2	2.43	0.52
35:YA:994:C:OP1	50:YU:53:ARG:NH2	2.43	0.52
41:YH:54:ARG:HH22	41:YH:62:LYS:HE2	1.74	0.52
1:QA:979:C:OP1	1:QA:1223:C:N4	2.43	0.52
1:QA:1522:U:H2'	1:QA:1523:G:H8	1.74	0.52
35:RA:1689:A:H62	35:RA:1698:A:H2	1.58	0.52
1:XA:406:G:N3	4:XD:119:GLN:NE2	2.54	0.52
33:Y8:29:LYS:O	33:Y8:31:HIS:N	2.32	0.52
35:YA:1011:G:OP2	50:YU:66:ASN:ND2	2.42	0.52
35:YA:1047:G:O2'	35:YA:1110:G:N2	2.43	0.52
38:YE:36:ARG:HG2	38:YE:47:VAL:HG12	1.90	0.52
1:QA:861:G:HO2'	1:QA:874:G:HO2'	1.58	0.52
44:RO:120:GLU:OE1	49:RT:67:SER:OG	2.26	0.52
48:RS:31:SER:OG	48:RS:32:LEU:N	2.42	0.52
49:RT:64:ARG:NH1	49:RT:106:SER:OG	2.41	0.52
1:XA:1350:A:O2'	7:XG:33:ASP:OD1	2.28	0.52
35:YA:1131:G:C2	43:YN:75:TYR:HB2	2.45	0.52
35:YA:13:A:O2'	35:YA:15:G:N7	2.41	0.52
1:QA:855:G:OP2	1:QA:871:U:N3	2.43	0.51
1:QA:427:U:OP1	4:QD:13:ARG:NH2	2.42	0.51
4:QD:23:GLY:N	4:QD:26:CYS:SG	2.83	0.51
36:RB:48:A:OP2	48:RS:30:ARG:NH2	2.43	0.51
37:RD:148:GLU:HB2	37:RD:151:LYS:HD2	1.91	0.51
35:RA:2638:G:OP1	38:RE:82:ARG:NH2	2.43	0.51
45:RP:39:LYS:HE2	45:RP:45:LEU:HD11	1.91	0.51
49:RT:29:ARG:NH1	49:RT:46:GLU:OE1	2.44	0.51
1:XA:1356:G:H2'	1:XA:1357:A:H8	1.73	0.51
1:XA:714:G:H2'	1:XA:715:A:C8	2.45	0.51
35:YA:2148:G:H2'	35:YA:2149:G:H8	1.75	0.51
35:YA:2795:G:H21	35:YA:2801:A:H62	1.58	0.51
35:YA:442:G:H1'	39:YF:48:THR:HG21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:YO:3:GLN:HG2	44:YO:4:PRO:HD2	1.92	0.51
1:QA:80:G:N2	1:QA:89:U:O2	2.40	0.51
1:QA:925:G:H1	1:QA:1391:U:H3	1.56	0.51
25:R0:74:ARG:NH1	36:RB:12:C:O2	2.42	0.51
1:XA:1417:G:O2'	1:XA:1483:A:N6	2.42	0.51
1:XA:673:G:O3'	6:XF:87:ARG:NH2	2.43	0.51
35:YA:2115:G:N2	35:YA:2170:A:N7	2.58	0.51
35:YA:309:G:N3	35:YA:329:G:O2'	2.42	0.51
43:YN:133:GLN:HG2	43:YN:135:PRO:HD3	1.92	0.51
46:YQ:34:LEU:HB2	46:YQ:118:LEU:HD22	1.92	0.51
55:YZ:28:MET:HG3	55:YZ:37:VAL:HG21	1.92	0.51
1:QA:501:C:H2'	1:QA:502:G:H8	1.75	0.51
1:QA:581:G:O3'	15:QO:64:ARG:NH2	2.43	0.51
35:RA:1165:U:H3	35:RA:1184:G:H1	1.58	0.51
35:RA:1550:C:H5'	35:RA:1733:G:H22	1.76	0.51
35:RA:1889:A:N3	35:RA:2086:U:O2'	2.43	0.51
48:RS:10:ARG:NH1	48:RS:91:PRO:O	2.44	0.51
2:XB:127:ILE:O	2:XB:135:GLN:NE2	2.43	0.51
35:YA:1791:A:N6	35:YA:1828:G:O2'	2.40	0.51
35:YA:289:A:H3'	35:YA:290:G:H8	1.76	0.51
32:Y7:37:LYS:NZ	35:YA:468:G:OP2	2.38	0.51
33:R8:52:LYS:N	33:R8:52:LYS:HD3	2.25	0.51
35:RA:1385:G:O2'	35:RA:1396:U:O2	2.27	0.51
35:RA:1142(A):A:O2'	43:RN:25:ARG:NH2	2.43	0.51
1:XA:501:C:H1'	1:XA:549:C:H1'	1.93	0.51
33:Y8:29:LYS:HG3	33:Y8:30:ARG:H	1.75	0.51
46:YQ:104:PHE:HE2	46:YQ:125:LEU:HD11	1.76	0.51
51:YV:14:VAL:HG11	51:YV:57:VAL:HG11	1.93	0.51
36:YB:104:A:OP1	55:YZ:72:ARG:NH1	2.43	0.51
16:QP:5:ARG:NH2	16:QP:27:LYS:O	2.43	0.51
31:R6:6:ARG:HH12	35:RA:2285:C:H5	1.58	0.51
35:RA:1791:A:N6	35:RA:1828:G:O2'	2.43	0.51
40:RG:83:ARG:HH11	40:RG:83:ARG:HG3	1.75	0.51
2:XB:178:ARG:NH2	2:XB:198:ASP:OD1	2.44	0.51
2:XB:185:ILE:HG22	2:XB:199:TYR:HB2	1.92	0.51
24:XZ:67:VAL:HG13	24:XZ:78:ALA:HB3	1.93	0.51
35:YA:2584:U:H5'	56:ZB:3:PPU:H103	1.91	0.51
50:YU:92:ARG:CZ	51:YV:11:GLN:H	2.24	0.51
1:QA:1129:C:N4	1:QA:1142:G:O6	2.44	0.51
1:QA:537:G:H5''	12:QL:113:ARG:HH12	1.76	0.51
27:R2:18:PRO:HA	27:R2:21:LEU:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:RD:146:GLU:HB2	37:RD:189:CYS:HB3	1.92	0.51
1:XA:1125:U:O4	10:XJ:5:ARG:NH1	2.43	0.51
1:XA:1147:C:O2	9:XI:16:ARG:NH1	2.43	0.51
1:XA:501:C:H2'	1:XA:502:G:H8	1.76	0.51
13:XM:45:VAL:HA	13:XM:48:LEU:HD22	1.92	0.51
35:YA:1681:G:O2'	35:YA:1762:A:O2'	2.28	0.51
35:YA:993:G:OP1	50:YU:50:ARG:NH2	2.44	0.51
36:YB:24:G:H1'	36:YB:27:C:H41	1.74	0.51
1:QA:34:C:H2'	1:QA:35:G:H8	1.76	0.51
44:RO:76:ALA:HB3	49:RT:75:ILE:HD12	1.93	0.51
1:XA:1139:G:N2	1:XA:1143:G:O6	2.44	0.51
1:XA:1356:G:H2'	1:XA:1357:A:C8	2.45	0.51
1:XA:448:A:OP2	1:XA:485:G:N2	2.42	0.51
1:XA:618:C:H5'	1:XA:619:U:H5''	1.92	0.51
35:RA:862:G:OP1	46:RQ:18:LYS:NZ	2.38	0.51
41:RH:127:GLU:HG2	41:RH:130:ARG:HE	1.75	0.51
43:RN:14:VAL:HB	43:RN:52:VAL:HG13	1.93	0.51
1:XA:501:C:OP1	12:XL:117:ARG:NH2	2.44	0.51
35:YA:532:A:N1	35:YA:2035:G:N2	2.58	0.51
35:YA:2566:A:N1	44:YO:28:SER:OG	2.43	0.51
19:QS:10:PHE:CE1	19:QS:38:SER:HB2	2.46	0.51
42:RI:81:VAL:HG21	42:RI:88:ILE:HD13	1.91	0.51
47:RR:56:LYS:NZ	47:RR:90:ARG:O	2.44	0.51
50:RU:74:LEU:HD11	50:RU:114:LYS:HE3	1.93	0.51
11:XK:45:GLY:HA2	11:XK:48:ILE:HD12	1.93	0.51
24:QZ:12:ASP:OD1	24:QZ:81:ARG:NH1	2.44	0.51
35:RA:2468:G:OP1	46:RQ:119:ARG:NH2	2.38	0.51
35:RA:307:G:H21	35:RA:330:A:H62	1.58	0.51
1:XA:954:G:H21	1:XA:1227:A:H62	1.58	0.51
9:XI:9:ARG:HB3	9:XI:104:ARG:HE	1.74	0.51
35:YA:1799:G:OP2	37:YD:273:ARG:NH2	2.44	0.51
33:Y8:63:PRO:HB2	35:YA:593:G:H4'	1.92	0.51
35:YA:642:G:H21	35:YA:646:A:H2	1.59	0.51
1:QA:1356:G:H2'	1:QA:1357:A:C8	2.46	0.50
1:QA:782:A:H62	1:QA:800:G:N2	2.09	0.50
13:QM:15:VAL:HG23	13:QM:34:LEU:HD21	1.92	0.50
35:RA:116:C:O2'	35:RA:126:A:N3	2.40	0.50
42:RI:133:HIS:HB3	42:RI:134:PRO:HD3	1.93	0.50
4:XD:4:TYR:OH	4:XD:10:ARG:NH2	2.43	0.50
17:XQ:66:SER:O	17:XQ:70:ARG:NH1	2.44	0.50
35:YA:2099:U:O2	35:YA:2190:G:O6	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:QJ:6:ILE:HG22	10:QJ:98:ILE:HG22	1.92	0.50
10:QJ:78:ASN:HB2	10:QJ:81:THR:HG23	1.91	0.50
35:RA:1818:U:H2'	37:RD:157:ARG:HG2	1.93	0.50
44:RO:43:VAL:HG13	44:RO:54:GLU:HA	1.92	0.50
1:XA:1141:C:H2'	1:XA:1142:G:H8	1.76	0.50
1:XA:1375:A:H4'	7:XG:29:LYS:HD3	1.92	0.50
1:XA:578:C:O2'	1:XA:728:A:N3	2.40	0.50
1:XA:891:U:H2'	1:XA:892:A:H8	1.75	0.50
35:YA:1434:A:H61	35:YA:1558:A:H62	1.59	0.50
35:YA:2515:C:H2'	35:YA:2516:G:H8	1.75	0.50
42:YI:30:LEU:HB3	42:YI:36:ALA:HB3	1.93	0.50
45:YP:97:PRO:HD3	45:YP:126:VAL:HG23	1.93	0.50
1:QA:945:G:N2	1:QA:1334:G:O2'	2.44	0.50
2:QB:6:THR:O	2:QB:217:ARG:NH1	2.44	0.50
7:QG:75:VAL:HA	7:QG:88:PRO:HA	1.94	0.50
35:RA:1681:G:O2'	35:RA:1762:A:O2'	2.29	0.50
37:RD:8:PRO:HB3	37:RD:14:ARG:HB3	1.93	0.50
1:XA:924:C:O2'	1:XA:1502:A:N6	2.41	0.50
26:Y1:92:LYS:NZ	26:Y1:96:LYS:HZ2	2.09	0.50
35:YA:571:A:H5'	35:YA:2030:A:H62	1.76	0.50
35:YA:2291:U:O2'	35:YA:2374:C:O2	2.28	0.50
35:YA:302:C:OP2	54:YY:73:ARG:NH1	2.43	0.50
35:YA:2618:G:H21	38:YE:150:VAL:HG21	1.76	0.50
38:YE:36:ARG:NH1	38:YE:85:ASN:OD1	2.45	0.50
43:YN:34:LEU:HD11	43:YN:120:LEU:HB2	1.93	0.50
35:YA:1188:U:H4'	51:YV:79:VAL:HG22	1.92	0.50
54:RY:99:CYS:SG	54:RY:100:ALA:N	2.84	0.50
1:XA:1454:G:OP1	20:XT:39:LYS:NZ	2.34	0.50
5:XE:11:ILE:HD12	5:XE:105:VAL:HG13	1.94	0.50
5:XE:81:GLU:HG2	5:XE:90:VAL:HG12	1.92	0.50
35:YA:1462:C:H4'	35:YA:2703:C:H5'	1.93	0.50
35:YA:2808:U:O4	35:YA:2892:A:N7	2.45	0.50
35:YA:668:G:H2'	35:YA:670:A:H62	1.76	0.50
1:QA:978:A:OP2	1:QA:1362(A):C:N4	2.45	0.50
22:QV:8:U:H3	22:QV:14:A:H62	1.59	0.50
35:YA:2298:A:H62	35:YA:2318:G:H8	1.59	0.50
1:QA:1202:G:O4'	14:QN:29:ARG:NH1	2.44	0.50
1:QA:995:C:H2'	1:QA:996:A:H8	1.77	0.50
2:QB:163:PHE:HD1	2:QB:185:ILE:HG13	1.77	0.50
4:QD:98:GLU:HA	4:QD:103:ASN:HD22	1.76	0.50
33:R8:6:THR:HG22	33:R8:63:PRO:HD2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:1657:C:H4'	38:RE:133:LYS:HB3	1.93	0.50
35:RA:2646:C:OP2	35:RA:2732:G:O2'	2.23	0.50
35:RA:373:U:H2'	35:RA:374:A:H8	1.77	0.50
35:RA:459:U:H2'	35:RA:460:A:H8	1.77	0.50
49:RT:62:THR:HG22	49:RT:75:ILE:HG12	1.94	0.50
35:YA:372:G:N2	35:YA:401:A:OP2	2.41	0.50
1:QA:924:C:O2'	1:QA:1502:A:N6	2.44	0.50
35:RA:783:A:H4'	35:RA:2588:G:H4'	1.94	0.50
2:XB:19:HIS:ND1	2:XB:20:GLU:OE2	2.45	0.50
18:XR:38:GLU:OE1	18:XR:41:LYS:NZ	2.44	0.50
20:XT:30:LYS:HG3	20:XT:34:LYS:HE2	1.93	0.50
45:YP:52:GLU:OE1	45:YP:55:ARG:NH1	2.45	0.50
35:RA:1863:G:HO2'	35:RA:2411:A:HO2'	1.55	0.50
35:RA:2328:A:H2'	35:RA:2329:G:C8	2.47	0.50
36:RB:44:G:H1'	36:RB:47:C:H42	1.77	0.50
49:RT:26:ASP:OD1	49:RT:120:ARG:NH2	2.40	0.50
50:YU:105:VAL:HG11	51:YV:39:LEU:HD21	1.94	0.50
2:QB:113:HIS:HB3	2:QB:114:ARG:HH21	1.76	0.50
12:QL:71:PRO:O	12:QL:102:ARG:NH1	2.38	0.50
35:RA:1857:G:N2	35:RA:1885:A:H62	2.07	0.50
34:R9:30:PRO:HB2	35:RA:2527:C:H4'	1.94	0.50
37:RD:21:PHE:HB3	37:RD:24:ILE:HG12	1.93	0.50
13:XM:91:ARG:HB2	13:XM:98:VAL:HG12	1.93	0.50
1:XA:835:U:OP1	18:XR:64:ARG:NH2	2.41	0.50
35:YA:581:C:H2'	35:YA:582:G:H8	1.76	0.50
35:YA:764:A:H5'	37:YD:210:GLY:HA2	1.94	0.50
55:YZ:115:GLY:HA2	55:YZ:177:PRO:HD3	1.94	0.50
1:QA:1510:U:H2'	1:QA:1511:G:C8	2.47	0.49
35:RA:1340:U:OP2	53:RX:78:LYS:NZ	2.44	0.49
35:RA:1678:G:N2	35:RA:1989:G:H22	2.10	0.49
55:RZ:23:LYS:HD2	55:RZ:38:TYR:HE2	1.76	0.49
1:XA:643:C:H2'	1:XA:644:G:H8	1.76	0.49
1:XA:1073:U:O2	2:XB:104:ASN:ND2	2.45	0.49
5:XE:154:GLY:HA2	8:XH:64:LYS:HD3	1.93	0.49
35:YA:1598:C:O3'	53:YX:35:THR:OG1	2.29	0.49
35:YA:1607:C:N4	35:YA:1622:G:OP2	2.34	0.49
46:YQ:37:LEU:HD11	46:YQ:130:LYS:HB2	1.93	0.49
9:QI:121:ARG:NH1	9:QI:122:ALA:O	2.45	0.49
11:QK:34:ASP:OD1	11:QK:38:ASN:N	2.45	0.49
35:RA:2343:C:O2'	35:RA:2373:G:O2'	2.27	0.49
54:RY:14:LEU:HB2	54:RY:75:ILE:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:34:C:H2'	1:XA:35:G:H8	1.77	0.49
1:XA:715:A:H2'	1:XA:716:A:C8	2.47	0.49
11:XK:18:ARG:HB3	11:XK:33:THR:HG23	1.94	0.49
22:XV:9:G:O2'	22:XV:10:G:N7	2.41	0.49
26:Y1:56:GLN:HG3	26:Y1:87:PRO:HD3	1.95	0.49
35:YA:1022:G:N7	43:YN:66:LYS:NZ	2.60	0.49
31:Y6:23:THR:HG21	35:YA:2286:A:H61	1.76	0.49
1:QA:516:U:O2'	1:QA:519:C:N3	2.41	0.49
2:QB:223:ILE:HD12	2:QB:226:ARG:HG2	1.94	0.49
2:QB:8:LYS:O	2:QB:11:LEU:N	2.34	0.49
1:QA:191:G:O2'	20:QT:101:GLY:O	2.26	0.49
35:RA:527:C:N4	35:RA:2779:U:OP2	2.46	0.49
39:RF:185:ASP:OD1	39:RF:188:ARG:NH2	2.45	0.49
1:XA:412:A:OP2	4:XD:35:ARG:NH2	2.44	0.49
1:XA:530:G:N7	24:XY:59:ARG:NH1	2.59	0.49
1:XA:1249:C:O2'	9:XI:73:GLN:OE1	2.30	0.49
35:YA:1254:A:H5''	35:YA:1255:U:H5'	1.94	0.49
36:YB:13:A:N1	36:YB:69:G:O2'	2.41	0.49
38:YE:11:MET:HG2	38:YE:24:THR:HG22	1.95	0.49
1:QA:677:U:O2	1:QA:777:A:O2'	2.27	0.49
21:QU:14:TRP:HZ3	21:QU:15:ARG:HH21	1.61	0.49
35:RA:814:C:O2'	35:RA:1225:C:N3	2.44	0.49
35:RA:2749:A:H5''	41:RH:4:ILE:HD12	1.95	0.49
35:RA:679:C:H2'	35:RA:680:G:H8	1.76	0.49
15:QO:53:HIS:NE2	35:RA:715:G:O6	2.42	0.49
3:XC:141:VAL:HG11	3:XC:202:ILE:HG12	1.95	0.49
3:XC:14:ILE:HG13	3:XC:15:THR:HG23	1.94	0.49
1:XA:1119:C:OP2	9:XI:9:ARG:NH2	2.45	0.49
16:XP:33:ILE:HG22	16:XP:34:GLU:HG3	1.94	0.49
34:Y9:9:ARG:HH21	34:Y9:12:ASP:HA	1.78	0.49
35:YA:2731:G:OP1	38:YE:169:ASN:ND2	2.44	0.49
40:YG:82:LEU:HD11	40:YG:88:ILE:HD13	1.94	0.49
36:YB:90:C:OP2	46:YQ:16:ARG:NH1	2.45	0.49
35:YA:1228:G:OP2	50:YU:16:LYS:NZ	2.46	0.49
55:YZ:149:SER:OG	55:YZ:172:ALA:O	2.26	0.49
1:QA:1141:C:H2'	1:QA:1142:G:H8	1.77	0.49
1:QA:1541:U:OP2	18:QR:55:ARG:NH1	2.44	0.49
3:QC:19:GLU:HG2	3:QC:54:ARG:HE	1.77	0.49
11:QK:22:HIS:HB3	11:QK:29:ILE:HG23	1.94	0.49
17:QQ:83:ASP:OD1	17:QQ:83:ASP:N	2.45	0.49
25:R0:7:LEU:HD13	46:RQ:85:LYS:HZ1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:RQ:37:LEU:HD11	46:RQ:130:LYS:HB2	1.95	0.49
35:RA:994:C:OP1	50:RU:53:ARG:NH2	2.46	0.49
54:RY:56:PRO:HG2	54:RY:57:GLN:HE22	1.78	0.49
1:XA:824:C:H2'	1:XA:825:G:H8	1.78	0.49
35:YA:1257:C:OP1	39:YF:72:ARG:NH2	2.44	0.49
35:YA:629:G:N3	35:YA:639:U:O2'	2.43	0.49
35:YA:659:C:H2'	35:YA:660:G:H8	1.77	0.49
2:QB:74:LYS:NZ	2:QB:206:ASP:OD1	2.40	0.49
12:QL:117:ARG:HB2	12:QL:122:THR:HB	1.95	0.49
1:QA:1312:G:OP2	29:R4:62:ARG:NH2	2.45	0.49
35:RA:1454:U:O2'	35:RA:1455:G:N7	2.43	0.49
35:RA:1678:G:H21	35:RA:1989:G:H22	1.59	0.49
35:RA:2844:G:H3'	35:RA:2845:G:H8	1.77	0.49
10:XJ:25:GLU:O	10:XJ:29:ARG:HB3	2.13	0.49
35:YA:1165:U:H3	35:YA:1184:G:H1	1.61	0.49
49:YT:24:PRO:HG3	49:YT:52:ILE:HG22	1.95	0.49
52:YW:58:ALA:HB1	52:YW:64:MET:HB2	1.95	0.49
1:QA:677:U:H3	1:QA:713:G:H22	1.60	0.49
9:QL:118:LYS:H	9:QL:121:ARG:HB3	1.77	0.49
35:RA:1230:C:H2'	35:RA:1231:G:H8	1.76	0.49
35:RA:2720:U:H3	35:RA:2873:A:H2	1.58	0.49
1:XA:1353:G:OP1	21:XU:10:ARG:NH2	2.43	0.49
2:XB:219:VAL:HA	2:XB:222:ILE:HD12	1.95	0.49
35:YA:2472:G:H5'	35:YA:2473:U:H5''	1.93	0.49
44:YO:25:LEU:HB2	44:YO:38:VAL:HG13	1.94	0.49
45:YP:95:VAL:HA	45:YP:99:LEU:HD23	1.95	0.49
46:YQ:68:ILE:HG22	46:YQ:101:ARG:HE	1.77	0.49
46:YQ:141:GLN:NE2	55:YZ:74:VAL:O	2.45	0.49
51:YV:21:ARG:HA	51:YV:93:GLU:HA	1.95	0.49
1:QA:673:G:H1'	18:QR:75:ILE:HD12	1.95	0.49
35:RA:379:G:H1	35:RA:395:U:H3	1.60	0.49
42:RI:88:ILE:HB	42:RI:121:LYS:HG2	1.93	0.49
46:RQ:115:MET:HG2	46:RQ:131:ILE:HG21	1.95	0.49
46:RQ:134:ARG:HH22	55:RZ:122:ARG:HG3	1.78	0.49
35:YA:2443:C:H2'	35:YA:2444:G:H8	1.77	0.49
41:YH:7:LEU:HD12	41:YH:8:PRO:HD2	1.95	0.49
29:R4:36:CYS:SG	29:R4:37:SER:N	2.84	0.49
32:R7:13:ALA:HB2	32:R7:46:VAL:HG11	1.94	0.49
35:RA:270(N):G:H5''	42:RI:57:ARG:HH12	1.77	0.49
36:RB:39:A:O2'	36:RB:46:A:N1	2.43	0.49
1:XA:583:A:N6	1:XA:758:G:O2'	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:XL:71:PRO:HG3	12:XL:99:HIS:HD2	1.78	0.49
6:XF:100:ASN:ND2	18:XR:23:LYS:O	2.45	0.49
39:YF:117:ARG:HH21	39:YF:187:VAL:HA	1.77	0.49
1:QA:593:G:H1	1:QA:646:U:H3	1.61	0.49
1:QA:663:A:N6	1:QA:742:G:H1	2.07	0.49
6:QF:61:LEU:HD23	6:QF:63:TYR:HE2	1.77	0.49
8:QH:34:GLU:HB3	8:QH:118:VAL:HG11	1.94	0.49
30:R5:25:LEU:HD11	52:RW:41:LYS:HE2	1.94	0.49
35:RA:698:C:O2'	35:RA:734:A:N6	2.45	0.49
1:XA:1321:C:H5'	1:XA:1322:C:H2'	1.94	0.49
3:XC:139:GLN:OE1	3:XC:170:GLN:NE2	2.45	0.49
1:XA:1151:A:H5'	10:XJ:42:THR:HG23	1.95	0.49
1:QA:429:U:O2'	4:QD:22:LYS:NZ	2.45	0.48
35:RA:2747:G:N2	35:RA:2748:A:N1	2.61	0.48
53:RX:55:ASN:HB2	53:RX:80:ILE:HB	1.94	0.48
1:XA:666:G:H5'	1:XA:726:C:H1'	1.95	0.48
35:YA:321:G:O2'	35:YA:340:A:N3	2.44	0.48
35:YA:380:U:H2'	35:YA:381:G:H8	1.78	0.48
1:QA:971:G:N2	1:QA:1363:A:OP2	2.43	0.48
1:QA:673:G:H2'	1:QA:674:G:C8	2.48	0.48
2:QB:223:ILE:HG12	2:QB:230:VAL:HG22	1.95	0.48
25:R0:7:LEU:HB3	46:RQ:85:LYS:NZ	2.28	0.48
29:R4:39:CYS:O	29:R4:41:PRO:CG	2.60	0.48
1:XA:191(F):U:H2'	1:XA:191:G:H8	1.78	0.48
4:XD:23:GLY:HA3	4:XD:112:VAL:HG22	1.96	0.48
27:Y2:18:PRO:HA	27:Y2:21:LEU:HB2	1.95	0.48
35:YA:117:G:OP2	35:YA:119:A:O2'	2.30	0.48
36:YB:15:A:OP2	36:YB:107:U:O2'	2.31	0.48
50:YU:50:ARG:O	50:YU:54:LYS:NZ	2.46	0.48
1:QA:713:G:H2'	1:QA:714:G:C8	2.48	0.48
34:R9:16:VAL:HG22	34:R9:25:VAL:HG22	1.95	0.48
40:RG:18:GLU:OE2	40:RG:21:ARG:NH2	2.38	0.48
43:RN:128:HIS:CE1	43:RN:134:ARG:HG3	2.48	0.48
50:RU:34:LYS:NZ	50:RU:37:GLU:OE1	2.39	0.48
53:RX:34:ALA:O	53:RX:77:LYS:NZ	2.43	0.48
3:XC:131:ARG:NH1	3:XC:167:TRP:O	2.46	0.48
4:XD:57:ARG:HB3	4:XD:206:PHE:HB2	1.95	0.48
12:XL:47:LYS:O	24:XY:44:LYS:NZ	2.37	0.48
35:YA:184:C:O2'	35:YA:217:G:N3	2.38	0.48
35:YA:581:C:H2'	35:YA:582:G:C8	2.48	0.48
45:YP:116:GLY:O	45:YP:137:LYS:NZ	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:QD:64:LEU:HB2	4:QD:198:VAL:HG11	1.96	0.48
35:RA:2470:G:OP1	46:RQ:59:ARG:NH2	2.45	0.48
38:RE:7:VAL:HG13	38:RE:51:PHE:HE2	1.78	0.48
44:RO:8:LEU:HB2	44:RO:19:ILE:HG13	1.95	0.48
5:XE:105:VAL:HG21	5:XE:128:PRO:HB3	1.94	0.48
12:XL:75:HIS:HA	12:XL:102:ARG:HH22	1.78	0.48
25:Y0:41:ARG:HA	25:Y0:41:ARG:HE	1.77	0.48
35:YA:270(H):C:H42	35:YA:270(R):G:H1	1.60	0.48
35:YA:2816:C:O2	35:YA:2883:A:O2'	2.26	0.48
37:YD:206:LEU:HA	37:YD:211:ARG:HD2	1.94	0.48
51:YV:61:VAL:HA	51:YV:94:LEU:HD23	1.95	0.48
1:QA:501:C:H2'	1:QA:502:G:C8	2.48	0.48
8:QH:119:LEU:HD22	8:QH:123:GLU:HB3	1.96	0.48
27:R2:66:GLU:OE1	27:R2:69:ARG:NH2	2.47	0.48
35:RA:1824:G:N3	37:RD:254:THR:OG1	2.46	0.48
35:RA:2081:C:H2'	35:RA:2082:A:H8	1.79	0.48
35:RA:654(G):C:N3	35:RA:654(N):G:N1	2.61	0.48
38:RE:1:MET:N	38:RE:1:MET:SD	2.70	0.48
38:RE:35:GLN:HB2	38:RE:66:HIS:HE1	1.78	0.48
1:XA:127:G:O2'	17:XQ:2:PRO:O	2.30	0.48
35:YA:307:G:H21	35:YA:330:A:H62	1.60	0.48
35:YA:851:U:H2'	35:YA:852:G:H8	1.79	0.48
35:RA:2441:C:OP2	35:RA:2586:C:O2'	2.30	0.48
30:R5:3:LYS:HG2	35:RA:2611:U:C4	2.49	0.48
35:RA:270(G):C:H42	35:RA:270(S):G:H1	1.62	0.48
35:RA:296:C:O3'	54:RY:95:LYS:NZ	2.46	0.48
35:RA:521:G:H2'	35:RA:522:G:C8	2.49	0.48
41:RH:88:LEU:HA	41:RH:130:ARG:HA	1.96	0.48
35:RA:24:G:O2'	52:RW:78:GLU:O	2.27	0.48
13:XM:58:GLU:O	13:XM:62:ASN:HB2	2.14	0.48
45:YP:87:ASP:O	45:YP:90:ARG:NH1	2.47	0.48
1:QA:1414:U:H2'	1:QA:1415:G:H8	1.78	0.48
4:QD:18:LYS:HB3	4:QD:18:LYS:HE3	1.66	0.48
35:RA:1067:A:N6	35:RA:1068:G:O6	2.47	0.48
35:RA:1598:C:O3'	53:RX:35:THR:OG1	2.29	0.48
40:RG:113:ARG:HB2	40:RG:140:ILE:HB	1.96	0.48
1:XA:1308:U:H2'	1:XA:1309:G:H8	1.79	0.48
1:XA:501:C:H2'	1:XA:502:G:C8	2.48	0.48
25:Y0:47:PRO:HB2	48:YS:20:ARG:HH12	1.79	0.48
35:YA:1385:G:O2'	35:YA:1396:U:O2	2.29	0.48
35:YA:28:A:N6	35:YA:512:G:O2'	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:R3:44:ARG:HA	28:R3:47:VAL:HG12	1.96	0.48
38:RE:77:ILE:HG21	38:RE:195:LEU:HD22	1.95	0.48
46:RQ:135:ASP:OD2	55:RZ:81:ARG:NH1	2.43	0.48
2:XB:101:MET:HA	2:XB:108:ILE:HG13	1.95	0.48
35:YA:2685:G:H1'	35:YA:2726:U:H5	1.79	0.48
44:YO:112:MET:HA	44:YO:115:VAL:HG22	1.95	0.48
47:YR:3:HIS:O	47:YR:5:LYS:N	2.46	0.48
1:QA:738:C:H5''	6:QF:69:GLU:HB2	1.96	0.48
35:RA:1652:A:OP1	47:RR:8:ARG:NH1	2.41	0.48
36:RB:44:G:O2'	36:RB:47:C:N4	2.47	0.48
1:XA:1060:C:H2'	1:XA:1061:G:H8	1.79	0.48
12:XL:56:ALA:HB2	12:XL:70:ILE:HD11	1.95	0.48
26:Y1:71:TYR:HA	26:Y1:74:VAL:HG12	1.95	0.48
35:YA:918:A:N3	36:YB:80:U:O2'	2.41	0.48
31:R6:6:ARG:HD2	31:R6:24:GLU:HB2	1.96	0.48
35:RA:577:G:O2'	35:RA:1254:A:OP1	2.32	0.48
35:RA:1842:G:O2'	37:RD:253:GLN:NE2	2.45	0.48
35:RA:2405:G:O2'	35:RA:2412:A:N6	2.47	0.48
37:RD:182:LEU:H	37:RD:272:ALA:HB3	1.79	0.48
49:RT:106:SER:HA	49:RT:110:ILE:HD11	1.96	0.48
46:RQ:63:LYS:HD2	55:RZ:175:VAL:HG21	1.96	0.48
1:XA:1175:G:H2'	1:XA:1176:A:C8	2.49	0.48
1:XA:769:G:H4'	1:XA:1513:A:H4'	1.96	0.48
10:XJ:44:VAL:HG22	10:XJ:66:ARG:HG2	1.96	0.48
13:XM:105:THR:HG22	13:XM:106:ASN:H	1.78	0.48
1:QA:269:C:H2'	1:QA:270:A:C8	2.48	0.47
1:QA:28:G:O2'	1:QA:296:U:OP1	2.27	0.47
1:QA:745:C:OP1	1:QA:851:G:O2'	2.31	0.47
2:QB:88:ALA:HB2	2:QB:219:VAL:HG13	1.96	0.47
3:QC:20:SER:OG	3:QC:22:TRP:NE1	2.45	0.47
5:QE:50:GLU:HB3	5:QE:53:LEU:HD13	1.94	0.47
10:QJ:34:VAL:HG13	10:QJ:74:ILE:HG12	1.96	0.47
19:QS:27:GLU:HB3	19:QS:29:ARG:HH21	1.79	0.47
35:RA:27:G:N2	35:RA:513:A:OP2	2.45	0.47
35:RA:581:C:H2'	35:RA:582:G:C8	2.49	0.47
35:RA:851:U:H2'	35:RA:852:G:H8	1.78	0.47
1:XA:1413:A:H2	1:XA:1487:G:H22	1.60	0.47
1:XA:21:G:H2'	1:XA:22:G:C8	2.49	0.47
12:XL:70:ILE:HG12	12:XL:77:LEU:HD12	1.96	0.47
12:XL:32:PHE:HE1	12:XL:86:ARG:HG3	1.79	0.47
1:XA:1047:G:H5''	14:YN:4:LYS:HD2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:577:G:O2'	35:YA:1254:A:OP1	2.32	0.47
35:YA:2747:G:N2	35:YA:2748:A:N1	2.62	0.47
41:YH:89:ILE:O	41:YH:129:THR:OG1	2.33	0.47
1:QA:1009:G:O6	1:QA:1020:U:O2	2.31	0.47
1:QA:21:G:H2'	1:QA:22:G:C8	2.49	0.47
1:QA:624:C:H2'	1:QA:625:G:H8	1.79	0.47
4:QD:57:ARG:HB3	4:QD:206:PHE:HB2	1.95	0.47
8:QH:91:ARG:NH1	17:QQ:32:TYR:O	2.46	0.47
19:QS:3:ARG:HH12	19:QS:11:VAL:HG12	1.78	0.47
35:RA:1139:G:H21	35:RA:1143:A:H8	1.60	0.47
35:RA:297:C:OP1	54:RY:87:LYS:NZ	2.43	0.47
35:RA:655:A:H4'	35:RA:656:G:H5'	1.96	0.47
41:RH:52:VAL:O	41:RH:65:HIS:NE2	2.42	0.47
55:RZ:54:HIS:HB3	55:RZ:101:PRO:HD3	1.96	0.47
1:XA:1355:G:H2'	1:XA:1356:G:H8	1.79	0.47
37:YD:142:VAL:HG23	37:YD:193:VAL:HA	1.96	0.47
40:YG:67:LYS:HD2	40:YG:68:PRO:HD2	1.96	0.47
25:Y0:51:VAL:O	48:YS:20:ARG:NH2	2.48	0.47
50:YU:102:GLU:HG3	51:YV:2:PHE:HE1	1.78	0.47
56:ZB:3:PPU:CD1	56:ZB:3:PPU:N	2.73	0.47
1:QA:545:C:OP1	4:QD:61:LYS:NZ	2.48	0.47
37:RD:153:ALA:O	37:RD:157:ARG:NH1	2.47	0.47
43:RN:103:VAL:HG21	43:RN:120:LEU:HD13	1.96	0.47
35:YA:839:U:H1'	35:YA:1191:G:H1'	1.96	0.47
38:YE:170:LEU:HD23	38:YE:186:GLY:HA3	1.96	0.47
35:YA:2304:G:N2	40:YG:156:ASP:OD2	2.46	0.47
49:YT:26:ASP:HB3	49:YT:92:GLY:H	1.79	0.47
10:QJ:21:GLN:HA	10:QJ:24:VAL:HG22	1.96	0.47
18:XR:51:LEU:HD22	18:XR:55:ARG:HD2	1.95	0.47
41:YH:3:ARG:HH21	41:YH:54:ARG:HH12	1.63	0.47
50:YU:102:GLU:HG3	51:YV:2:PHE:CE1	2.49	0.47
1:QA:1210:C:O2'	1:QA:1213:A:O2'	2.30	0.47
1:QA:1323:G:H2'	1:QA:1324:A:C8	2.49	0.47
3:QC:131:ARG:NH1	3:QC:167:TRP:O	2.43	0.47
3:QC:19:GLU:O	3:QC:40:ARG:NH2	2.47	0.47
35:RA:1212:G:O2'	35:RA:1237:A:N6	2.48	0.47
35:RA:1388:G:O2'	35:RA:1525:G:O2'	2.30	0.47
35:RA:2306:C:H5'	35:RA:2307:G:H5''	1.96	0.47
35:RA:2853:C:H2'	35:RA:2854:G:H8	1.79	0.47
47:RR:104:ARG:HG3	47:RR:107:ASP:HB3	1.96	0.47
1:XA:1026:G:H22	1:XA:1035:A:H2	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:XC:164:ARG:NH1	3:XC:166:GLU:OE2	2.47	0.47
20:XT:48:LYS:HD3	20:XT:48:LYS:HA	1.56	0.47
35:YA:39:C:O2	39:YF:46:ARG:NH2	2.44	0.47
29:Y4:31:ILE:HG21	40:YG:142:PRO:HB2	1.97	0.47
1:QA:1071:C:H2'	1:QA:1072:G:H8	1.79	0.47
1:QA:961:U:OP2	1:QA:1222:G:O2'	2.33	0.47
1:QA:187:C:H2'	1:QA:188:U:H4'	1.96	0.47
1:QA:56:U:H2'	1:QA:57:G:H8	1.79	0.47
1:QA:578:C:O2'	1:QA:728:A:N3	2.39	0.47
1:QA:958:A:C5	19:QS:55:LYS:HG3	2.49	0.47
33:R8:9:GLY:O	33:R8:13:ARG:NE	2.41	0.47
30:R5:9:LYS:NZ	35:RA:2019:A:N7	2.55	0.47
39:RF:143:ALA:HB1	39:RF:148:LEU:HB2	1.95	0.47
3:XC:88:ARG:NH2	3:XC:101:LEU:O	2.48	0.47
10:XJ:6:ILE:HD12	10:XJ:98:ILE:HG22	1.97	0.47
35:YA:2144:U:H1'	35:YA:2147:G:H22	1.79	0.47
36:YB:5:C:O2'	36:YB:27:C:O2	2.30	0.47
38:YE:47:VAL:HG11	38:YE:86:PRO:HD2	1.96	0.47
40:YG:119:GLY:HA3	40:YG:181:ARG:HG3	1.97	0.47
55:YZ:4:ARG:HG2	55:YZ:58:VAL:HB	1.97	0.47
1:QA:714:G:H2'	1:QA:715:A:C8	2.50	0.47
24:QY:1:MET:HB2	24:QY:35:ARG:HG3	1.97	0.47
46:RQ:136:ALA:HB1	55:RZ:52:SER:HB2	1.96	0.47
1:XA:1236:A:H4'	1:XA:1304:G:H4'	1.95	0.47
35:YA:1394:U:O2	53:YX:16:LYS:NZ	2.42	0.47
35:YA:956:G:OP2	46:YQ:14:ARG:NH2	2.48	0.47
1:QA:1286:A:N1	21:QU:18:TYR:OH	2.37	0.47
1:QA:1417:G:O2'	1:QA:1483:A:N6	2.46	0.47
1:QA:157:G:H1	1:QA:164:U:H3	1.62	0.47
7:QG:15:ASP:HB3	7:QG:19:GLY:H	1.79	0.47
1:QA:826:C:O2	8:QH:15:ASN:ND2	2.48	0.47
35:RA:837:C:N3	35:RA:941:A:N6	2.62	0.47
35:RA:2822:G:OP1	38:RE:159:HIS:NE2	2.48	0.47
1:XA:909:A:N3	1:XA:1413:A:O2'	2.44	0.47
12:XL:113:ARG:NH2	12:XL:116:SER:OG	2.43	0.47
21:XU:6:ARG:HH21	21:XU:15:ARG:HH21	1.61	0.47
28:Y3:39:ASP:OD1	28:Y3:44:ARG:NH2	2.47	0.47
35:YA:2012:G:OP1	52:YW:11:ARG:NH2	2.47	0.47
37:YD:70:TRP:NE1	37:YD:146:GLU:OE2	2.39	0.47
41:YH:149:ARG:NH2	41:YH:167:GLU:OE2	2.47	0.47
1:QA:131:C:OP1	1:QA:190:G:N2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:QC:29:TYR:OH	14:QN:54:PRO:O	2.32	0.47
29:R4:40:HIS:N	29:R4:41:PRO:HD3	2.24	0.47
35:RA:839:U:H1'	35:RA:1191:G:H1'	1.97	0.47
35:RA:919:G:N2	35:RA:2269:A:OP2	2.44	0.47
37:RD:142:VAL:HG23	37:RD:193:VAL:HA	1.97	0.47
1:XA:45:U:H2'	1:XA:46:G:C8	2.50	0.47
3:XC:19:GLU:HG2	3:XC:54:ARG:HE	1.80	0.47
30:Y5:16:ARG:NH1	30:Y5:17:ASP:OD1	2.47	0.47
35:YA:2844:G:H3'	35:YA:2845:G:H8	1.80	0.47
1:QA:592:G:H2'	1:QA:593:G:H8	1.80	0.47
1:QA:618:C:H5'	1:QA:619:U:H5''	1.96	0.47
2:QB:171:ALA:HA	2:QB:174:VAL:HG22	1.97	0.47
12:QL:83:VAL:HG12	12:QL:107:ALA:HB2	1.95	0.47
36:RB:118:G:C2'	36:RB:119:A:O4'	2.63	0.47
40:RG:139:LEU:HD21	40:RG:149:VAL:HG21	1.96	0.47
46:RQ:39:PRO:HB3	46:RQ:99:PRO:HD3	1.97	0.47
55:RZ:181:GLU:HB2	55:RZ:183:LEU:HG	1.97	0.47
1:XA:1071:C:H2'	1:XA:1072:G:H8	1.79	0.47
1:XA:624:C:H2'	1:XA:625:G:H8	1.79	0.47
4:XD:25:ARG:NE	4:XD:30:LYS:O	2.42	0.47
35:YA:140:A:H8	35:YA:1408:C:HO2'	1.63	0.47
35:YA:1791:A:H3'	35:YA:1792:G:H8	1.80	0.47
35:YA:2692:C:H2'	35:YA:2693:A:H8	1.80	0.47
38:YE:77:ILE:HD11	38:YE:79:ARG:HH21	1.79	0.47
55:YZ:11:GLU:HA	55:YZ:36:LYS:HE2	1.97	0.47
1:QA:674:G:H2'	1:QA:675:A:C8	2.49	0.47
13:QM:19:LEU:HD11	13:QM:56:LEU:HD21	1.97	0.47
35:RA:2845:G:H2'	35:RA:2846:G:H8	1.80	0.47
37:RD:36:PRO:HG3	37:RD:63:ARG:HG3	1.98	0.47
1:XA:429:U:O2'	4:XD:22:LYS:NZ	2.48	0.47
9:XI:125:TYR:HE1	9:XI:127:LYS:HE3	1.80	0.47
13:XM:47:ASP:N	13:XM:47:ASP:OD1	2.48	0.47
26:Y1:92:LYS:HZ1	26:Y1:96:LYS:NZ	2.13	0.47
35:YA:1139:G:HO2'	35:YA:1143:A:H62	1.63	0.47
35:YA:699:A:N3	35:YA:1633:G:O2'	2.40	0.47
37:YD:69:ARG:HH11	37:YD:105:ILE:HG21	1.79	0.47
56:ZB:3:PPU:CD1	56:ZB:3:PPU:HN2	2.26	0.47
1:QA:1342:C:H2'	1:QA:1343:G:C8	2.50	0.46
1:QA:150:C:H2'	1:QA:151:A:H8	1.80	0.46
1:QA:186(B):C:H2'	1:QA:186(C):G:C8	2.49	0.46
2:QB:27:LYS:HD2	2:QB:193:ASP:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:390:C:O3'	16:QP:28:ARG:NH2	2.49	0.46
18:QR:32:ARG:HE	18:QR:65:ILE:HD11	1.79	0.46
35:RA:1230:C:H2'	35:RA:1231:G:C8	2.50	0.46
35:RA:1049:C:N4	35:RA:2751:G:O6	2.48	0.46
37:RD:9:TYR:HD1	37:RD:10:THR:HG23	1.80	0.46
38:RE:57:LYS:HA	38:RE:57:LYS:HD3	1.37	0.46
13:QM:11:ARG:NH2	40:RG:146:TYR:OH	2.41	0.46
45:RP:115:LEU:HA	45:RP:134:ALA:HB2	1.97	0.46
55:RZ:110:GLY:O	55:RZ:115:GLY:N	2.48	0.46
1:XA:1512:U:H2'	1:XA:1513:A:C8	2.50	0.46
1:XA:576:G:N2	1:XA:760:G:OP2	2.48	0.46
35:YA:2030:A:H4'	35:YA:2031:A:H8	1.79	0.46
1:QA:923:A:O2'	1:QA:1399:C:OP2	2.27	0.46
2:QB:47:THR:HA	2:QB:202:PRO:HG2	1.97	0.46
1:QA:779:C:H5''	11:QK:122:LYS:HG2	1.97	0.46
27:R2:36:ARG:NH2	53:RX:8:ILE:O	2.48	0.46
35:RA:1057:A:N6	35:RA:1088:A:OP2	2.49	0.46
35:RA:1530:G:H1	35:RA:1541:U:H3	1.62	0.46
35:RA:1667:G:O2'	35:RA:1991:U:O4	2.32	0.46
35:RA:1830:C:H2'	35:RA:1831:G:H8	1.80	0.46
35:RA:225:A:N6	35:RA:419:C:O2'	2.47	0.46
35:RA:578:A:OP1	35:RA:1255:U:O2'	2.27	0.46
37:RD:147:LEU:HD21	37:RD:183:ARG:HH22	1.80	0.46
39:RF:115:ALA:O	39:RF:119:ARG:HB2	2.15	0.46
48:RS:66:ALA:HA	48:RS:69:VAL:HG12	1.98	0.46
49:RT:96:ARG:HD2	49:RT:101:PHE:HE2	1.79	0.46
1:XA:376:G:H1	1:XA:387:U:H3	1.64	0.46
17:XQ:45:HIS:CD2	17:XQ:47:PRO:HG3	2.51	0.46
31:Y6:11:LEU:HG	31:Y6:49:HIS:HB3	1.96	0.46
35:YA:1243:G:O2'	45:YP:7:ARG:NH2	2.49	0.46
52:YW:33:ARG:NE	52:YW:52:GLU:OE2	2.46	0.46
1:QA:1435:G:H2'	1:QA:1436:U:C6	2.50	0.46
24:QY:12:ASP:O	24:QY:15:TYR:N	2.48	0.46
25:R0:50:ASN:HA	25:R0:62:LEU:HD12	1.97	0.46
35:RA:1434:A:H61	35:RA:1558:A:N6	2.14	0.46
30:R5:4:HIS:O	35:RA:2056:G:N2	2.48	0.46
45:RP:148:LEU:HA	45:RP:148:LEU:HD23	1.74	0.46
7:XG:20:ASP:HB3	7:XG:23:VAL:HG23	1.97	0.46
35:YA:30:G:O2'	35:YA:1214:A:N3	2.42	0.46
28:Y3:17:LYS:NZ	35:YA:968:G:OP1	2.47	0.46
37:YD:145:VAL:HB	37:YD:155:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:907:U:OP1	46:YQ:24:GLY:N	2.48	0.46
46:YQ:75:THR:HG21	46:YQ:87:LYS:HG2	1.96	0.46
10:QJ:43:ARG:HH11	10:QJ:43:ARG:HD2	1.47	0.46
35:RA:2849:U:H3	35:RA:2867:G:H1'	1.80	0.46
37:RD:245:PRO:HA	37:RD:246:PRO:HD3	1.85	0.46
41:RH:24:VAL:HB	41:RH:35:VAL:HG13	1.98	0.46
44:RO:98:VAL:HG11	44:RO:114:ILE:HG23	1.98	0.46
36:RB:47:C:H5'	48:RS:10:ARG:HH12	1.79	0.46
1:XA:1119:C:H2'	1:XA:1120:G:H8	1.79	0.46
1:XA:1126:U:N3	1:XA:1281:U:O4'	2.45	0.46
7:XG:15:ASP:HB3	7:XG:19:GLY:H	1.80	0.46
35:YA:247:G:OP2	35:YA:249:C:N4	2.49	0.46
39:YF:60:SER:OG	39:YF:61:GLY:N	2.48	0.46
35:YA:24:G:O2'	52:YW:78:GLU:O	2.32	0.46
4:QD:177:ASP:HB3	4:QD:182:LYS:HG2	1.98	0.46
16:QP:49:LEU:HD11	16:QP:73:LEU:HG	1.98	0.46
1:XA:579:G:H5'	1:XA:728:A:H1'	1.98	0.46
1:XA:972:C:OP2	10:XJ:57:LYS:NZ	2.46	0.46
11:XK:106:LYS:O	18:XR:87:ARG:NH1	2.48	0.46
1:QA:824:C:H2'	1:QA:825:G:H8	1.81	0.46
4:QD:133:VAL:HG12	4:QD:135:LEU:H	1.80	0.46
8:QH:104:ARG:HG3	8:QH:107:LEU:HB2	1.98	0.46
13:QM:24:GLY:O	13:QM:29:ARG:NH1	2.49	0.46
30:R5:16:ARG:NH1	30:R5:17:ASP:OD1	2.48	0.46
35:RA:2037:G:H2'	35:RA:2038:G:C8	2.51	0.46
35:RA:197:A:H62	35:RA:2430:A:H2'	1.79	0.46
35:RA:668:G:H2'	35:RA:670:A:H62	1.81	0.46
37:RD:79:VAL:O	37:RD:114:GLY:N	2.46	0.46
1:XA:376:G:O3'	16:XP:5:ARG:NH1	2.42	0.46
26:Y1:18:ILE:HG12	26:Y1:37:ILE:HG12	1.98	0.46
35:YA:2148:G:H2'	35:YA:2149:G:C8	2.51	0.46
35:YA:2693:A:H2'	35:YA:2694:G:H8	1.80	0.46
30:R5:41:PRO:O	30:R5:44:THR:OG1	2.28	0.46
4:XD:85:LYS:HD2	4:XD:92:VAL:HG11	1.98	0.46
47:YR:33:ARG:HE	47:YR:113:LEU:HD11	1.80	0.46
1:QA:662:G:H2'	1:QA:663:A:C8	2.51	0.46
35:RA:1607:C:N4	35:RA:1622:G:OP2	2.37	0.46
35:RA:2089:U:H3	35:RA:2230:G:H1	1.63	0.46
35:RA:2298:A:H62	35:RA:2318:G:H8	1.64	0.46
35:RA:300:A:OP1	54:RY:86:ARG:NH2	2.48	0.46
1:XA:1130:A:H62	1:XA:1144:G:H21	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:XY:3:LEU:HB2	24:XY:35:ARG:HH21	1.81	0.46
35:YA:1056:G:H4'	35:YA:1086:A:H1'	1.98	0.46
35:YA:2029:G:N1	35:YA:2033:A:OP1	2.32	0.46
55:YZ:146:ILE:HA	55:YZ:174:VAL:HG23	1.97	0.46
1:QA:1249:C:O2'	9:QI:73:GLN:NE2	2.48	0.46
16:QP:18:ARG:HA	16:QP:38:TYR:HA	1.98	0.46
18:QR:32:ARG:HA	18:QR:69:THR:HG21	1.98	0.46
19:QS:28:LYS:NZ	19:QS:46:GLY:O	2.31	0.46
26:R1:67:ILE:O	26:R1:70:VAL:HG12	2.15	0.46
35:RA:2124:G:H22	35:RA:2174:C:H42	1.64	0.46
35:RA:589:C:H2'	35:RA:590:A:C8	2.51	0.46
40:RG:124:SER:O	40:RG:124:SER:OG	2.34	0.46
40:RG:166:ASP:N	40:RG:166:ASP:OD1	2.49	0.46
35:RA:661:C:HO2'	45:RP:14:LYS:H	1.63	0.46
35:YA:1830:C:H2'	35:YA:1831:G:H8	1.79	0.46
35:YA:831:G:N2	45:YP:53:GLY:O	2.47	0.46
1:QA:1346:A:OP1	9:QI:120:ARG:NH1	2.48	0.46
1:QA:948:C:H2'	1:QA:949:A:H8	1.80	0.46
2:QB:53:ARG:HG2	2:QB:56:ARG:HH21	1.80	0.46
4:QD:4:TYR:OH	4:QD:10:ARG:NH2	2.49	0.46
9:QI:10:ARG:NH1	9:QI:75:ASP:OD2	2.49	0.46
35:RA:1598:C:H5'	53:RX:37:THR:HG23	1.98	0.46
35:RA:2130:U:O2	35:RA:2133:G:O2'	2.29	0.46
35:RA:29:U:H5''	50:RU:7:GLY:HA2	1.98	0.46
41:RH:130:ARG:HH11	41:RH:132:ARG:HB2	1.81	0.46
48:RS:28:VAL:HG11	48:RS:98:VAL:HG12	1.98	0.46
35:RA:138:G:N1	53:RX:44:GLU:OE1	2.38	0.46
1:XA:1510:U:H2'	1:XA:1511:G:C8	2.51	0.46
1:XA:552:U:H2'	1:XA:553:A:H8	1.81	0.46
1:XA:592:G:H2'	1:XA:593:G:H8	1.81	0.46
1:XA:806:C:H2'	1:XA:807:A:H8	1.80	0.46
1:XA:885:G:H2'	1:XA:886:G:H8	1.81	0.46
1:XA:948:C:H2'	1:XA:949:A:H8	1.81	0.46
4:XD:100:ARG:NH2	4:XD:136:PRO:O	2.49	0.46
7:XG:16:LEU:HD13	9:XI:42:ARG:HA	1.98	0.46
1:XA:128:G:O2'	17:XQ:3:LYS:NZ	2.49	0.46
25:Y0:27:GLU:HG3	25:Y0:68:GLU:HA	1.98	0.46
35:YA:1779:U:OP2	35:YA:1784:A:N6	2.40	0.46
35:YA:600:G:N2	35:YA:605:C:O3'	2.49	0.46
44:YO:19:ILE:HG22	44:YO:43:VAL:HG12	1.96	0.46
1:QA:1354:C:H2'	1:QA:1355:G:H8	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:671:G:O2'	6:QF:80:ARG:NH2	2.44	0.45
24:QY:16:TRP:NE1	24:QY:80:CYS:O	2.48	0.45
35:RA:1249:U:H2'	45:RP:18:ARG:HH22	1.81	0.45
35:RA:443:A:OP2	35:RA:615:G:N2	2.35	0.45
43:RN:35:ARG:HH11	43:RN:108:PRO:HG3	1.81	0.45
43:RN:61:ARG:HG2	43:RN:61:ARG:O	2.14	0.45
45:RP:95:VAL:HB	45:RP:125:VAL:HA	1.97	0.45
1:XA:599:C:O2'	8:XH:129:VAL:O	2.25	0.45
14:XN:26:ARG:HD3	14:XN:43:CYS:HB3	1.98	0.45
1:XA:1312:G:H5'	19:XS:5:LEU:HD11	1.98	0.45
35:YA:1262:A:OP1	52:YW:99:ARG:NH1	2.49	0.45
10:QJ:43:ARG:HH12	10:QJ:45:ARG:HB2	1.82	0.45
19:QS:6:LYS:HE3	19:QS:6:LYS:HB2	1.74	0.45
28:R3:40:THR:HG22	28:R3:42:ALA:H	1.81	0.45
35:RA:1262:A:OP2	52:RW:97:LYS:NZ	2.48	0.45
35:RA:2186:G:H2'	35:RA:2187:G:H8	1.81	0.45
35:RA:2566:A:N1	44:RO:28:SER:OG	2.42	0.45
35:RA:918:A:N3	36:RB:80:U:O2'	2.47	0.45
38:RE:10:GLY:HA3	49:RT:7:ILE:HD11	1.98	0.45
43:RN:23:LEU:HB2	43:RN:62:VAL:HG12	1.98	0.45
1:XA:684:A:O2'	11:XK:39:PRO:O	2.34	0.45
9:XI:5:TYR:HE1	9:XI:16:ARG:HB2	1.81	0.45
32:Y7:28:ARG:NH2	35:YA:1368:G:OP1	2.46	0.45
35:YA:2135:A:N6	35:YA:2156:G:H21	2.14	0.45
35:YA:2784:C:H1'	38:YE:37:ARG:HH12	1.81	0.45
4:QD:109:GLY:HA3	4:QD:165:MET:HG3	1.98	0.45
1:QA:553:A:H5''	12:QL:24:VAL:HG21	1.98	0.45
24:QZ:58:ARG:HG3	24:QZ:68:TYR:HE1	1.81	0.45
29:R4:17:GLY:N	29:R4:33:VAL:O	2.49	0.45
35:RA:1827:C:OP2	37:RD:222:ARG:NH1	2.45	0.45
35:RA:2773:C:OP1	38:RE:166:THR:OG1	2.33	0.45
35:RA:704:G:O2'	35:RA:726:G:N2	2.49	0.45
40:RG:37:VAL:HG22	40:RG:159:VAL:HG12	1.97	0.45
47:RR:2:ARG:HD2	47:RR:2:ARG:HA	1.71	0.45
1:XA:713:G:H2'	1:XA:714:G:C8	2.52	0.45
8:XH:25:ASP:HB3	8:XH:58:TYR:HD2	1.82	0.45
9:XI:21:PRO:HA	9:XI:59:PHE:HA	1.98	0.45
35:YA:2392:A:H2	35:YA:2424:C:H42	1.64	0.45
35:YA:2540:C:O2'	35:YA:2740:A:N3	2.41	0.45
36:YB:48:A:OP2	48:YS:30:ARG:NH2	2.49	0.45
1:QA:1177:G:H2'	1:QA:1178:G:C4	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:1341:U:OP2	35:RA:1394:U:O2'	2.28	0.45
35:RA:1636:C:H2'	35:RA:1637:A:C8	2.52	0.45
35:RA:1779:U:OP2	35:RA:1784:A:N6	2.38	0.45
35:RA:2591:C:H2'	35:RA:2592:G:C8	2.51	0.45
35:RA:740:U:H2'	35:RA:741:G:C8	2.51	0.45
35:YA:1028:A:N3	35:YA:2486:G:O2'	2.44	0.45
35:YA:814:C:O2'	35:YA:1225:C:N3	2.48	0.45
42:YI:76:THR:OG1	42:YI:139:GLN:NE2	2.49	0.45
54:YY:11:ASP:N	54:YY:11:ASP:OD1	2.49	0.45
1:QA:1432:G:O2'	1:QA:1468:A:N6	2.49	0.45
1:QA:985:C:H2'	1:QA:986:A:H8	1.81	0.45
20:QT:51:GLU:HA	20:QT:54:LYS:HG2	1.99	0.45
35:RA:1423:G:H2'	35:RA:1424:G:H8	1.81	0.45
35:RA:2801:A:OP1	35:RA:2895:U:O2'	2.35	0.45
40:RG:109:VAL:HG11	40:RG:142:PRO:HB3	1.98	0.45
50:RU:34:LYS:HA	50:RU:34:LYS:HD2	1.71	0.45
1:XA:17:U:H2'	1:XA:18:C:C6	2.52	0.45
1:XA:452:A:O2'	1:XA:453:A:O4'	2.33	0.45
1:XA:890:G:O2'	1:XA:906:G:O6	2.29	0.45
4:XD:81:GLU:OE1	4:XD:139:ARG:NH2	2.49	0.45
35:YA:2701:C:H3'	35:YA:2702:U:H5''	1.97	0.45
35:YA:277:C:H3'	35:YA:278:A:H8	1.81	0.45
43:YN:22:THR:OG1	43:YN:23:LEU:N	2.46	0.45
50:YU:88:ILE:HG23	50:YU:90:VAL:HG23	1.98	0.45
1:QA:377:G:H2'	1:QA:378:G:H8	1.82	0.45
37:RD:79:VAL:HG21	37:RD:111:LEU:HD11	1.98	0.45
38:RE:147:PRO:HB2	38:RE:149:ARG:HG2	1.99	0.45
42:RI:109:ILE:HD11	42:RI:130:TYR:CZ	2.52	0.45
51:RV:3:ALA:HB2	51:RV:40:LEU:HD23	1.99	0.45
5:XE:107:ARG:O	5:XE:111:GLU:HB2	2.17	0.45
1:XA:254:G:O2'	17:XQ:16:GLN:O	2.34	0.45
21:XU:26:LYS:HA	21:XU:26:LYS:HD2	1.78	0.45
35:YA:2246:G:H2'	35:YA:2247:A:H8	1.81	0.45
1:QA:309:G:O2'	1:QA:607:A:N1	2.50	0.45
29:R4:2:LYS:HA	29:R4:2:LYS:HD3	1.60	0.45
32:R7:7:PRO:HB2	35:RA:1309:G:H4'	1.98	0.45
36:RB:60:C:H2'	36:RB:61:G:H8	1.82	0.45
41:RH:121:ILE:HD11	41:RH:133:VAL:HG22	1.99	0.45
49:RT:77:PRO:HB2	49:RT:80:SER:HB2	1.99	0.45
6:XF:10:LEU:HD13	6:XF:61:LEU:HD13	1.97	0.45
35:YA:1782:C:H1'	35:YA:2609:U:H5''	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:2246:G:H2'	35:YA:2247:A:C8	2.51	0.45
35:YA:1500:G:O2'	37:YD:100:GLY:O	2.29	0.45
42:YI:78:THR:HG22	42:YI:141:LYS:HB2	1.98	0.45
43:YN:1:MET:HG2	51:YV:12:TYR:HD1	1.81	0.45
1:QA:359:U:H2'	1:QA:360:A:H8	1.82	0.45
1:QA:1327:C:H5''	21:QU:20:LYS:HE2	1.99	0.45
31:R6:34:LEU:HG	31:R6:36:LEU:HD13	1.97	0.45
35:RA:230:U:H2'	35:RA:231:C:H6	1.82	0.45
51:RV:68:LYS:H	51:RV:68:LYS:HD2	1.82	0.45
54:RY:9:LYS:NZ	54:RY:28:LYS:O	2.34	0.45
1:XA:1469:G:H2'	1:XA:1470:G:H8	1.81	0.45
35:YA:1636:C:H2'	35:YA:1637:A:C8	2.52	0.45
35:YA:582:G:H2'	35:YA:583:G:H8	1.82	0.45
52:YW:71:VAL:HA	52:YW:107:LEU:HD23	1.99	0.45
1:QA:666:G:H5'	1:QA:726:C:H1'	1.99	0.45
2:QB:201:ILE:HG21	2:QB:214:ILE:HG21	1.99	0.45
5:QE:154:GLY:HA2	8:QH:64:LYS:HE3	1.99	0.45
8:QH:104:ARG:HB3	8:QH:108:GLY:H	1.82	0.45
24:QZ:24:VAL:HA	24:QZ:27:ILE:HD12	1.99	0.45
34:R9:33:LYS:NZ	35:RA:2743:C:OP1	2.38	0.45
35:RA:1600:C:OP1	53:RX:58:HIS:NE2	2.45	0.45
1:XA:411:A:H62	1:XA:413:G:H21	1.65	0.45
16:XP:18:ARG:HH11	16:XP:35:LYS:HD2	1.82	0.45
34:Y9:27:CYS:SG	34:Y9:28:GLU:N	2.89	0.45
26:Y1:40:ARG:NH2	35:YA:2232:U:OP2	2.50	0.45
44:YO:120:GLU:OE2	49:YT:65:LYS:NZ	2.49	0.45
50:YU:91:ASP:HA	50:YU:95:LEU:HB2	1.97	0.45
1:QA:1512:U:H2'	1:QA:1513:A:C8	2.52	0.45
1:QA:922:G:H4'	5:QE:20:GLN:HA	1.99	0.45
24:QZ:4:ILE:HB	24:QZ:76:LEU:HA	1.99	0.45
35:RA:2867:G:O2'	35:RA:2868:A:O4'	2.35	0.45
45:RP:121:LYS:HB3	45:RP:123:LEU:HD22	1.98	0.45
45:RP:134:ALA:O	45:RP:138:LEU:HB2	2.17	0.45
51:RV:21:ARG:HH11	51:RV:21:ARG:HG3	1.82	0.45
55:RZ:48:PHE:HE1	55:RZ:71:VAL:HG21	1.82	0.45
2:XB:67:THR:HG21	2:XB:155:LEU:HD11	1.98	0.45
35:YA:521:G:H2'	35:YA:522:G:H8	1.82	0.45
35:YA:78:A:H2'	35:YA:79:G:H8	1.81	0.45
35:YA:848:G:H2'	35:YA:849:A:C8	2.52	0.45
35:YA:919:G:N2	35:YA:2269:A:OP2	2.51	0.45
35:YA:971:C:O2'	35:YA:983:A:N3	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:YF:113:ALA:HB2	39:YF:183:VAL:HG23	1.99	0.45
1:QA:112:G:O2'	1:QA:354:G:O2'	2.33	0.44
24:QY:42:LYS:O	24:QY:58:ARG:NH1	2.48	0.44
30:R5:12:SER:OG	35:RA:2021:C:OP1	2.34	0.44
35:RA:2680:C:H5'	38:RE:189:PRO:HA	1.97	0.44
1:XA:407:G:H2'	1:XA:408:A:H8	1.82	0.44
1:XA:401:C:O2'	1:XA:621:A:N3	2.47	0.44
26:Y1:76:ARG:NH2	26:Y1:97:LEU:HB3	2.32	0.44
35:YA:2720:U:H3	35:YA:2873:A:H2	1.65	0.44
35:YA:539:G:H2'	35:YA:540:G:H8	1.82	0.44
35:YA:589:C:H2'	35:YA:590:A:H8	1.82	0.44
7:QG:20:ASP:HB3	7:QG:23:VAL:HG12	2.00	0.44
35:RA:1399:C:H2'	35:RA:1400:G:H8	1.81	0.44
1:XA:1128:C:H1'	1:XA:1146:A:H61	1.83	0.44
1:XA:950:U:H3	1:XA:1231:G:H1	1.66	0.44
25:Y0:56:ASP:HA	35:YA:2386:C:H4'	1.98	0.44
38:YE:5:LEU:HD11	38:YE:79:ARG:HB2	1.98	0.44
1:QA:769:G:H4'	1:QA:1513:A:H4'	1.99	0.44
1:QA:17:U:H2'	1:QA:18:C:C6	2.52	0.44
6:QF:6:VAL:HB	6:QF:63:TYR:HB2	1.99	0.44
13:QM:98:VAL:HG23	13:QM:99:ARG:HG3	1.99	0.44
31:R6:9:LEU:HA	31:R6:54:ILE:HB	1.99	0.44
35:RA:1188:U:H4'	51:RV:79:VAL:HG22	1.98	0.44
35:RA:1651:G:H4'	47:RR:39:PRO:HG2	2.00	0.44
3:XC:150:LYS:HE3	3:XC:167:TRP:HE1	1.82	0.44
7:XG:26:PHE:HD1	7:XG:101:LEU:HG	1.82	0.44
9:XI:9:ARG:H	9:XI:79:LEU:HD23	1.82	0.44
35:YA:121:G:H4'	35:YA:149:A:H5'	1.99	0.44
34:Y9:6:SER:HB3	35:YA:2466:C:H5''	2.00	0.44
33:Y8:12:LYS:NZ	35:YA:249:C:O2	2.40	0.44
43:YN:54:VAL:HB	43:YN:122:VAL:HG12	2.00	0.44
25:Y0:48:GLY:O	48:YS:20:ARG:NH1	2.50	0.44
53:YX:29:TRP:HZ3	53:YX:59:VAL:HG11	1.82	0.44
1:QA:1172:C:H2'	1:QA:1173:G:H8	1.83	0.44
1:QA:1404:C:H2'	1:QA:1405:G:C8	2.53	0.44
1:QA:993:G:O2'	1:QA:994:A:N7	2.50	0.44
35:RA:1568:G:OP1	37:RD:63:ARG:NH1	2.41	0.44
35:RA:1936:A:N6	35:RA:1963:U:O2	2.49	0.44
35:RA:2246:G:H2'	35:RA:2247:A:C8	2.53	0.44
35:RA:321:G:O2'	35:RA:340:A:N3	2.47	0.44
35:RA:627:A:H4'	35:RA:628:G:H5'	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:995:C:H5'	50:RU:53:ARG:HG2	1.99	0.44
47:RR:14:SER:OG	47:RR:15:SER:N	2.50	0.44
55:RZ:70:LEU:HG	55:RZ:91:LEU:HD11	1.98	0.44
4:XD:57:ARG:HE	4:XD:205:GLU:HG3	1.82	0.44
11:XK:87:THR:HA	11:XK:91:ARG:HD2	1.97	0.44
35:YA:2451:A:C4	56:ZB:3:PPU:HD2	2.51	0.44
35:YA:2692:C:H2'	35:YA:2693:A:C8	2.52	0.44
41:YH:86:GLU:OE2	41:YH:132:ARG:NH2	2.50	0.44
48:YS:25:ARG:HG2	48:YS:88:ASP:HB2	1.99	0.44
1:QA:1179:A:H4'	9:QI:103:THR:HA	1.99	0.44
1:QA:6:G:H4'	1:QA:298:A:H4'	1.99	0.44
8:QH:86:ILE:HG22	8:QH:93:VAL:HG11	1.98	0.44
13:QM:13:LYS:HD2	13:QM:13:LYS:HA	1.72	0.44
24:QY:5:TRP:CD1	24:QZ:5:TRP:HD1	2.36	0.44
26:R1:10:LYS:NZ	26:R1:65:SER:OG	2.50	0.44
35:RA:700:G:O2'	35:RA:1632:A:N3	2.49	0.44
35:RA:2859:G:H2'	35:RA:2860:A:C8	2.52	0.44
37:RD:145:VAL:O	37:RD:155:LEU:N	2.49	0.44
38:RE:58:ARG:HD2	38:RE:58:ARG:HA	1.50	0.44
40:RG:31:VAL:O	40:RG:33:ARG:NH1	2.48	0.44
45:RP:29:LYS:HB3	45:RP:29:LYS:HE3	1.80	0.44
5:XE:51:VAL:HG23	5:XE:52:PRO:HD3	1.99	0.44
34:Y9:1:MET:HB2	35:YA:2526:G:H1'	1.98	0.44
35:YA:247:G:H4'	35:YA:386:G:C5	2.52	0.44
55:YZ:69:THR:HG22	55:YZ:90:VAL:HG12	1.98	0.44
15:QO:87:ILE:HA	15:QO:87:ILE:HD12	1.92	0.44
27:R2:4:SER:OG	27:R2:5:GLU:N	2.47	0.44
35:RA:1571:A:H2'	35:RA:1572:A:C8	2.53	0.44
35:RA:539:G:H2'	35:RA:540:G:H8	1.83	0.44
37:RD:147:LEU:HD11	37:RD:183:ARG:HH12	1.83	0.44
35:RA:675:A:H4'	39:RF:67:GLN:HE22	1.83	0.44
1:XA:450:G:H4'	16:XP:41:PRO:HB2	1.99	0.44
1:XA:745:C:OP1	1:XA:851:G:O2'	2.35	0.44
8:XH:116:LYS:HG2	8:XH:129:VAL:HG11	1.99	0.44
27:Y2:8:LYS:HA	27:Y2:11:GLU:HG2	1.98	0.44
35:YA:2329:G:H2'	35:YA:2330:G:C8	2.53	0.44
35:YA:630:G:N2	35:YA:633:A:OP2	2.38	0.44
35:YA:2208:U:O2'	37:YD:150:LYS:O	2.35	0.44
55:YZ:76:LEU:HA	55:YZ:83:PRO:HA	2.00	0.44
2:QB:80:ILE:HD13	2:QB:211:ILE:HG22	1.98	0.44
35:RA:2788:C:O2'	35:RA:2809:A:N3	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:RI:26:ALA:HA	42:RI:30:LEU:HB2	1.98	0.44
50:RU:88:ILE:HG23	50:RU:90:VAL:HG23	2.00	0.44
51:RV:85:LYS:HE2	51:RV:85:LYS:HB2	1.66	0.44
1:XA:1355:G:H2'	1:XA:1356:G:C8	2.52	0.44
1:XA:1483:A:H1'	35:YA:1948:G:H1'	1.99	0.44
2:XB:19:HIS:ND1	2:XB:205:ASP:OD1	2.50	0.44
8:XH:91:ARG:NE	17:XQ:32:TYR:O	2.51	0.44
32:Y7:7:PRO:HB2	35:YA:1309:G:H4'	1.99	0.44
35:YA:2328:A:H2'	35:YA:2329:G:C8	2.52	0.44
35:YA:2469:A:H2	35:YA:2481:G:H21	1.64	0.44
35:YA:959:A:N3	35:YA:2457:U:O2'	2.46	0.44
1:QA:1386:G:H2'	1:QA:1387:G:H8	1.82	0.44
1:QA:836:G:H1	1:QA:850:U:H3	1.65	0.44
1:QA:736:C:O2'	6:QF:90:VAL:O	2.31	0.44
1:QA:1348:U:H4'	9:QI:120:ARG:HD2	1.99	0.44
13:QM:91:ARG:HB2	13:QM:98:VAL:HG12	1.97	0.44
35:RA:1204:A:H1'	35:RA:1206:G:C5	2.52	0.44
35:RA:144:C:H2'	35:RA:145:G:H8	1.82	0.44
35:RA:2074:U:H2'	35:RA:2075:U:C6	2.53	0.44
35:RA:2183:C:H2'	35:RA:2184:G:H8	1.82	0.44
25:R0:35:ASN:ND2	35:RA:2353:G:O2'	2.51	0.44
35:RA:247:G:H4'	35:RA:386:G:C5	2.53	0.44
38:RE:154:LYS:HA	38:RE:154:LYS:HD2	1.82	0.44
42:RI:128:LEU:O	42:RI:138:ILE:N	2.51	0.44
44:RO:11:ALA:O	44:RO:99:PHE:N	2.40	0.44
33:R8:57:ARG:NH1	45:RP:52:GLU:OE2	2.48	0.44
54:RY:13:VAL:HG12	54:RY:74:PRO:HA	2.00	0.44
1:XA:1300:G:O2'	1:XA:1303:C:N4	2.51	0.44
1:XA:691:G:O6	11:XK:55:LYS:NZ	2.47	0.44
12:XL:70:ILE:HG13	12:XL:100:ILE:HD12	1.98	0.44
24:XZ:37:THR:O	24:XZ:37:THR:OG1	2.35	0.44
28:Y3:49:LYS:HE2	35:YA:851:U:H5'	1.98	0.44
35:YA:819:A:OP2	35:YA:1187:G:N2	2.40	0.44
39:YF:110:LEU:HD11	39:YF:181:LEU:HG	1.99	0.44
48:YS:36:TYR:CD1	48:YS:52:SER:HB2	2.53	0.44
1:QA:1001:G:H2'	1:QA:1002:G:C8	2.53	0.44
1:QA:1300:G:O2'	1:QA:1303:C:N4	2.44	0.44
1:QA:552:U:H2'	1:QA:553:A:C8	2.52	0.44
1:QA:877:C:H2'	1:QA:878:G:H8	1.83	0.44
2:QB:59:GLU:HG3	2:QB:221:LEU:HD21	1.99	0.44
16:QP:19:ILE:N	16:QP:37:GLY:O	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:R6:12:GLU:HB3	31:R6:19:ARG:HG3	2.00	0.44
35:RA:1181:C:H2'	35:RA:1182:A:C8	2.53	0.44
35:RA:1518:C:H2'	35:RA:1519:G:H8	1.83	0.44
35:RA:654(D):G:H1	35:RA:654(Q):C:H42	1.65	0.44
1:XA:946:A:H2'	1:XA:947:G:C8	2.52	0.44
1:XA:985:C:H2'	1:XA:986:A:C8	2.53	0.44
35:YA:2135:A:H62	35:YA:2156:G:N2	2.16	0.44
30:Y5:25:LEU:HD12	52:YW:19:LEU:HB3	1.98	0.44
1:QA:692:U:OP1	11:QK:124:LYS:NZ	2.39	0.43
4:QD:103:ASN:O	4:QD:107:ARG:HB2	2.18	0.43
4:QD:127:THR:HA	4:QD:132:ARG:HA	2.00	0.43
1:QA:717:C:O2'	11:QK:116:HIS:O	2.32	0.43
19:QS:50:ALA:HB1	19:QS:57:HIS:HB3	1.99	0.43
35:RA:1542:G:O6	35:RA:1543:A:N6	2.51	0.43
35:RA:2572:A:OP1	35:RA:2574:G:O2'	2.28	0.43
25:R0:77:ARG:NH2	35:RA:857:C:OP2	2.49	0.43
1:XA:476:G:H2'	1:XA:477:G:C8	2.53	0.43
29:Y4:51:ASP:OD1	29:Y4:51:ASP:N	2.50	0.43
29:Y4:2:LYS:HB3	29:Y4:5:ILE:HG12	2.00	0.43
33:Y8:28:GLY:HA3	33:Y8:44:LYS:HD3	2.00	0.43
35:YA:142:G:H2'	35:YA:143:C:C6	2.53	0.43
35:YA:2443:C:H2'	35:YA:2444:G:C8	2.53	0.43
35:YA:589:C:H2'	35:YA:590:A:C8	2.53	0.43
53:YX:12:VAL:HB	53:YX:27:THR:HG23	1.99	0.43
1:QA:1172:C:H2'	1:QA:1173:G:C8	2.53	0.43
1:QA:603:U:H2'	1:QA:604:G:H8	1.83	0.43
1:QA:736:C:H2'	1:QA:737:A:H8	1.83	0.43
5:QE:33:VAL:HG13	5:QE:112:LEU:HD12	1.99	0.43
35:RA:1403:C:H5''	35:RA:1471:A:H1'	2.00	0.43
35:RA:2446:G:N2	35:RA:2449:U:O2	2.51	0.43
35:RA:2696:U:H2'	35:RA:2697:G:C8	2.53	0.43
35:RA:774:A:O2'	35:RA:777:A:N3	2.51	0.43
1:XA:991:U:O4	1:XA:1213:A:N7	2.51	0.43
1:XA:403:C:OP2	4:XD:74:GLN:NE2	2.47	0.43
19:XS:11:VAL:HG11	19:XS:16:LEU:HB2	2.00	0.43
35:YA:1259:G:H2'	35:YA:1260:G:C8	2.52	0.43
46:YQ:77:LYS:NZ	46:YQ:86:GLY:O	2.49	0.43
46:YQ:60:ARG:HA	55:YZ:179:ASP:HA	2.00	0.43
1:QA:1502:A:H2	1:QA:1505:G:H1	1.65	0.43
1:QA:985:C:H2'	1:QA:986:A:C8	2.52	0.43
24:QY:5:TRP:CD1	24:QZ:5:TRP:CD1	3.05	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:1995:U:O2	44:RO:3:GLN:NE2	2.51	0.43
35:RA:244:A:H4'	45:RP:74:GLU:HB2	2.00	0.43
35:RA:2723:C:OP2	38:RE:109:LYS:NZ	2.46	0.43
35:RA:2853:C:H2'	35:RA:2854:G:C8	2.53	0.43
35:RA:859:G:O2'	35:RA:916:G:O6	2.35	0.43
38:RE:25:VAL:HG21	49:RT:7:ILE:HG12	2.00	0.43
50:RU:75:ASN:HB2	50:RU:78:THR:HG23	2.01	0.43
55:RZ:10:ARG:NH1	55:RZ:26:GLY:O	2.51	0.43
1:XA:1323:G:H2'	1:XA:1324:A:C8	2.53	0.43
1:XA:1422:G:H5''	44:YO:48:PRO:HB3	1.98	0.43
1:XA:878:G:H5'	8:XH:89:PRO:HG2	2.00	0.43
33:Y8:5:LYS:HG2	35:YA:242:G:C8	2.52	0.43
35:YA:1571:A:H2'	35:YA:1572:A:C8	2.53	0.43
35:YA:570:G:H2'	35:YA:2030:A:C5	2.53	0.43
30:Y5:16:ARG:NH2	35:YA:517:C:OP1	2.41	0.43
35:YA:861:A:N3	36:YB:79:C:O2'	2.49	0.43
36:YB:24:G:O6	36:YB:56:G:O2'	2.37	0.43
39:YF:143:ALA:O	39:YF:148:LEU:N	2.51	0.43
39:YF:113:ALA:HB1	39:YF:186:ILE:HG21	1.99	0.43
42:YI:5:LEU:HD21	42:YI:12:LEU:HB3	2.01	0.43
1:QA:514:C:H2'	1:QA:515:G:H8	1.84	0.43
1:QA:689:C:H3'	1:QA:690:G:H21	1.84	0.43
4:QD:60:GLU:OE2	4:QD:63:LYS:NZ	2.36	0.43
13:QM:12:ASN:HB3	13:QM:46:LYS:HB3	2.00	0.43
35:RA:1073:A:H2'	35:RA:1074:G:H8	1.82	0.43
35:RA:2119:A:N6	35:RA:2170:A:N7	2.66	0.43
35:RA:2438:U:O3'	35:RA:2439:A:H3'	2.18	0.43
35:RA:2873:A:H8	47:RR:6:SER:H	1.64	0.43
37:RD:147:LEU:HD12	37:RD:155:LEU:HD11	1.99	0.43
42:RI:88:ILE:HG13	42:RI:121:LYS:HA	2.00	0.43
1:XA:262:A:H5''	20:XT:76:ALA:HB2	2.00	0.43
42:YI:14:ASP:H	42:YI:17:GLN:HB3	1.84	0.43
44:YO:63:VAL:HB	44:YO:102:VAL:HG12	2.00	0.43
1:QA:1086:U:H2'	1:QA:1087:G:H8	1.84	0.43
1:QA:452:A:O2'	16:QP:72:ARG:NH1	2.51	0.43
2:QB:102:LEU:HD23	2:QB:182:ILE:HD12	2.01	0.43
2:QB:119:GLU:OE2	2:QB:153:ARG:NH2	2.51	0.43
1:QA:1309:G:OP1	13:QM:88:ARG:NH2	2.51	0.43
1:QA:390:C:H4'	16:QP:28:ARG:HH21	1.83	0.43
35:RA:2291:U:H2'	35:RA:2292:C:C6	2.54	0.43
38:RE:52:LEU:HB3	38:RE:54:GLN:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:RO:7:TYR:HE1	44:RO:44:LYS:HG3	1.83	0.43
54:RY:39:VAL:HG13	54:RY:42:VAL:HB	2.00	0.43
1:XA:1127:G:H2'	1:XA:1128:C:C6	2.53	0.43
2:XB:168:THR:HB	2:XB:192:SER:HB2	2.00	0.43
2:XB:15:VAL:HG11	2:XB:209:ARG:HB2	2.01	0.43
2:XB:55:PHE:HA	2:XB:58:ILE:HB	2.00	0.43
35:YA:2291:U:OP1	35:YA:2380:C:O2'	2.36	0.43
35:YA:303:U:H2'	35:YA:304:G:H8	1.83	0.43
35:YA:414:C:H2'	35:YA:415:A:C8	2.54	0.43
43:YN:116:LEU:HD23	43:YN:116:LEU:HA	1.89	0.43
47:YR:86:ARG:NH2	47:YR:118:GLU:OXT	2.44	0.43
55:YZ:128:VAL:HG22	55:YZ:161:VAL:HA	2.01	0.43
1:QA:324:G:OP1	20:QT:70:SER:OG	2.34	0.43
1:QA:736:C:H2'	1:QA:737:A:C8	2.53	0.43
2:QB:48:MET:HA	2:QB:51:LEU:HD12	2.00	0.43
24:QZ:19:THR:OG1	24:QZ:20:ASP:N	2.51	0.43
35:RA:1070:A:H5'	35:RA:1071:G:H5''	2.00	0.43
35:RA:1332:G:H8	35:RA:1332:G:H2'	1.74	0.43
35:RA:2845:G:H2'	35:RA:2846:G:C8	2.53	0.43
35:RA:380:U:H2'	35:RA:381:G:H8	1.83	0.43
35:RA:755:C:H2'	35:RA:756:C:C6	2.53	0.43
1:XA:1404:C:H2'	1:XA:1405:G:C8	2.54	0.43
4:XD:122:ARG:HA	4:XD:122:ARG:HD2	1.80	0.43
24:XY:5:TRP:HB2	24:XZ:3:LEU:HB2	2.01	0.43
35:YA:2657:A:O3'	41:YH:160:LYS:NZ	2.49	0.43
35:YA:221:A:H61	35:YA:265:A:H8	1.65	0.43
35:YA:2871:C:OP1	47:YR:50:HIS:NE2	2.50	0.43
35:YA:874:G:H2'	35:YA:875:G:H8	1.84	0.43
42:YI:10:GLU:O	42:YI:11:ASN:ND2	2.51	0.43
1:QA:1355:G:H2'	1:QA:1356:G:H8	1.84	0.43
1:QA:216:G:H2'	1:QA:217:C:C6	2.54	0.43
1:QA:946:A:H2'	1:QA:947:G:C8	2.53	0.43
8:QH:23:SER:OG	8:QH:24:THR:N	2.52	0.43
20:QT:71:THR:HG22	20:QT:72:LEU:HG	2.00	0.43
43:RN:15:LEU:HD23	43:RN:136:GLU:HG2	1.99	0.43
45:RP:64:LYS:O	45:RP:66:GLY:N	2.52	0.43
28:Y3:8:LEU:HG	28:Y3:28:LEU:HD13	2.01	0.43
35:YA:2591:C:H2'	35:YA:2592:G:C8	2.54	0.43
35:YA:221:A:N1	35:YA:265:A:O2'	2.52	0.43
35:YA:1614:A:C6	52:YW:91:GLY:HA2	2.54	0.43
1:QA:413:G:O2'	1:QA:428:G:N2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:QD:108:LEU:HD12	4:QD:174:LEU:HD13	2.00	0.43
1:QA:8:A:N6	4:QD:205:GLU:O	2.51	0.43
11:QK:62:GLN:HG3	11:QK:97:ALA:HB2	2.01	0.43
35:RA:1203:G:O6	35:RA:1204:A:N6	2.52	0.43
35:RA:1380:G:O2'	35:RA:1569:A:N6	2.52	0.43
35:RA:1800:C:H42	35:RA:1817:G:N2	2.17	0.43
35:RA:589:C:H2'	35:RA:590:A:H8	1.84	0.43
35:RA:630:G:N2	35:RA:633:A:OP2	2.47	0.43
36:RB:24:G:H1'	36:RB:27:C:H41	1.83	0.43
35:RA:1792:G:H5'	37:RD:205:VAL:HG13	2.00	0.43
43:RN:23:LEU:HD13	43:RN:60:ILE:HD12	2.01	0.43
51:RV:14:VAL:HB	51:RV:96:ILE:HG12	2.00	0.43
1:XA:56:U:H2'	1:XA:57:G:H8	1.82	0.43
1:XA:677:U:O2	1:XA:777:A:O2'	2.34	0.43
8:XH:26:VAL:O	8:XH:59:LEU:N	2.46	0.43
25:Y0:68:GLU:HG3	25:Y0:80:HIS:HB2	2.01	0.43
29:Y4:14:ILE:HB	29:Y4:22:ILE:HB	1.99	0.43
35:YA:1073:A:H2'	35:YA:1074:G:C8	2.54	0.43
35:YA:1434:A:H61	35:YA:1558:A:N6	2.16	0.43
35:YA:373:U:H2'	35:YA:374:A:H8	1.84	0.43
41:YH:3:ARG:HA	41:YH:3:ARG:HD3	1.46	0.43
50:YU:43:GLY:HA3	51:YV:73:SER:OG	2.18	0.43
1:QA:1065:U:O5'	1:QA:1190:G:N2	2.51	0.43
9:QL:5:TYR:HE1	9:QL:16:ARG:HB2	1.84	0.43
12:QL:59:ARG:HA	12:QL:65:GLU:HA	2.01	0.43
1:QA:376:G:H5''	16:QP:5:ARG:HB2	2.01	0.43
35:RA:1568:G:H5''	37:RD:61:LEU:HD23	2.01	0.43
35:RA:2784:C:O2	38:RE:37:ARG:NH2	2.52	0.43
36:RB:90:C:OP2	46:RQ:16:ARG:NH2	2.34	0.43
41:RH:59:ARG:HA	41:RH:62:LYS:HD2	1.99	0.43
46:RQ:109:VAL:HB	46:RQ:114:ALA:HB2	2.01	0.43
1:XA:1218:C:H2'	1:XA:1219:U:C6	2.54	0.43
1:XA:279:A:OP2	17:XQ:95:TYR:OH	2.28	0.43
1:XA:368:U:C1'	1:XA:368:U:C2	3.02	0.43
6:XF:37:VAL:HA	6:XF:65:VAL:HG12	2.00	0.43
1:XA:1202:G:O4'	14:XN:29:ARG:NH1	2.52	0.43
26:Y1:8:SER:HB3	26:Y1:66:HIS:CD2	2.53	0.43
35:YA:1899:G:H21	35:YA:1902:C:N4	2.16	0.43
15:XO:88:ARG:NH2	35:YA:714:U:OP2	2.49	0.43
35:YA:822:U:H2'	35:YA:823:G:H8	1.83	0.43
40:YG:41:GLN:HG2	40:YG:43:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:244:A:H4'	45:YP:74:GLU:HB2	2.01	0.43
8:QH:109:ILE:HG22	8:QH:137:VAL:HB	2.01	0.43
12:QL:32:PHE:HE1	12:QL:86:ARG:HG3	1.84	0.43
30:R5:7:PRO:O	35:RA:2016:U:O2'	2.32	0.43
33:R8:29:LYS:HG3	33:R8:30:ARG:H	1.83	0.43
35:RA:2543:G:H2'	35:RA:2544:G:C8	2.54	0.43
35:RA:443:A:C8	39:RF:45:ARG:HG3	2.54	0.43
45:RP:97:PRO:O	45:RP:98:GLU:HG3	2.18	0.43
36:RB:113:C:H4'	48:RS:46:VAL:HG22	2.01	0.43
50:RU:92:ARG:NH1	51:RV:11:GLN:O	2.52	0.43
1:XA:1308:U:H2'	1:XA:1309:G:C8	2.54	0.43
1:XA:974:A:OP2	14:XN:41:ARG:NH1	2.45	0.43
5:XE:5:ASP:OD1	5:XE:5:ASP:N	2.52	0.43
35:YA:1278:A:H2'	35:YA:1279:G:C8	2.53	0.43
35:YA:230:U:H2'	35:YA:231:C:H6	1.84	0.43
35:YA:642:G:N2	35:YA:645:C:OP2	2.51	0.43
36:YB:14:U:O2'	36:YB:107:U:O2'	2.35	0.43
1:QA:45:U:H2'	1:QA:46:G:C8	2.54	0.42
7:QG:62:PHE:HD1	7:QG:124:LEU:HD21	1.84	0.42
1:QA:636:U:H5'	17:QQ:2:PRO:HG3	2.00	0.42
19:QS:19:VAL:HA	19:QS:22:LEU:HB2	2.00	0.42
35:RA:1316:U:H2'	35:RA:1317:A:C8	2.54	0.42
37:RD:60:ARG:NH1	37:RD:86:PRO:O	2.52	0.42
38:RE:111:ARG:HA	47:RR:2:ARG:HH12	1.83	0.42
1:XA:1326:C:OP2	21:XU:6:ARG:NH1	2.51	0.42
10:XJ:24:VAL:HG13	10:XJ:34:VAL:HG21	2.01	0.42
35:YA:1113:U:H2'	35:YA:1114:G:C8	2.54	0.42
35:YA:1316:U:H2'	35:YA:1317:A:H8	1.82	0.42
35:YA:223:A:O2'	35:YA:420:C:O2	2.32	0.42
36:YB:80:U:H2'	36:YB:81:G:H21	1.82	0.42
1:QA:1412:C:H2'	1:QA:1413:A:C8	2.54	0.42
1:QA:448:A:OP2	1:QA:485:G:N2	2.39	0.42
6:QF:79:LEU:HB3	6:QF:88:VAL:HG21	2.00	0.42
35:RA:2314:C:H2'	35:RA:2315:G:H8	1.84	0.42
35:RA:2779:U:H2'	35:RA:2779:U:H6	1.73	0.42
36:RB:49:C:OP2	48:RS:30:ARG:NH1	2.52	0.42
37:RD:264:LYS:HD3	37:RD:266:SER:HB3	2.00	0.42
35:RA:873:G:O3'	46:RQ:63:LYS:NZ	2.50	0.42
1:XA:1030:C:H42	1:XA:1032:A:H62	1.67	0.42
1:XA:1244:C:H2'	1:XA:1245:A:H8	1.84	0.42
1:XA:1392:G:N2	1:XA:1502:A:H8	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:516:U:O2'	1:XA:519:C:N3	2.43	0.42
9:XI:95:LYS:HE2	9:XI:95:LYS:HB2	1.88	0.42
13:XM:25:ILE:HD11	13:XM:64:TRP:HE1	1.84	0.42
24:XZ:33:ASP:OD1	24:XZ:37:THR:OG1	2.28	0.42
25:Y0:36:ILE:HD13	25:Y0:60:PHE:HB3	2.02	0.42
35:YA:1278:A:H2'	35:YA:1279:G:H8	1.84	0.42
35:YA:1342:A:H2	35:YA:1602:U:H3	1.66	0.42
35:YA:2074:U:H2'	35:YA:2075:U:C6	2.54	0.42
35:YA:964:C:O2'	35:YA:2273:A:N3	2.38	0.42
35:YA:859:G:O2'	35:YA:916:G:O6	2.34	0.42
40:YG:32:PRO:HB2	40:YG:172:LEU:HD22	2.01	0.42
1:QA:1342:C:H2'	1:QA:1343:G:H8	1.85	0.42
3:QC:180:ALA:HB1	3:QC:182:ILE:HG23	2.01	0.42
8:QH:21:LYS:O	8:QH:65:TYR:OH	2.30	0.42
12:QL:60:LEU:HD22	12:QL:85:ILE:HG21	2.01	0.42
13:QM:49:THR:HB	13:QM:52:GLU:HG3	2.02	0.42
24:QY:44:LYS:CE	24:QY:59:ARG:HE	2.32	0.42
37:RD:108:PRO:HB3	37:RD:143:HIS:CE1	2.53	0.42
37:RD:108:PRO:HD2	37:RD:111:LEU:HD22	2.02	0.42
1:XA:407:G:H2'	1:XA:408:A:C8	2.54	0.42
1:XA:922:G:OP1	5:XE:20:GLN:NE2	2.48	0.42
12:XL:104:VAL:HG12	12:XL:105:TYR:H	1.84	0.42
17:XQ:44:ALA:HB1	17:XQ:73:VAL:HG22	2.01	0.42
24:XY:34:THR:OG1	24:XY:58:ARG:NH1	2.51	0.42
24:XZ:19:THR:OG1	24:XZ:20:ASP:N	2.52	0.42
28:Y3:15:TYR:HA	28:Y3:16:PRO:HD3	1.92	0.42
35:YA:1020:A:N1	35:YA:1141:U:H2'	2.34	0.42
35:YA:1353:A:H2'	35:YA:1354:A:C8	2.53	0.42
35:YA:1568:G:H4'	37:YD:59:LYS:HB3	2.01	0.42
35:YA:2438:U:O3'	35:YA:2439:A:H3'	2.19	0.42
35:YA:2693:A:H2'	35:YA:2694:G:C8	2.54	0.42
35:YA:2853:C:H2'	35:YA:2854:G:H8	1.85	0.42
1:QA:1218:C:H2'	1:QA:1219:U:C6	2.54	0.42
1:QA:508:C:O2	1:QA:510:A:N6	2.52	0.42
1:QA:938:A:N3	1:QA:1376:U:O2'	2.44	0.42
6:QF:76:ALA:O	6:QF:80:ARG:NE	2.50	0.42
35:RA:1353:A:H2'	35:RA:1354:A:C8	2.55	0.42
1:XA:1129:C:H4'	1:XA:1130:A:H5'	2.01	0.42
1:XA:1539:C:H42	23:XX:7:G:H1	1.65	0.42
1:XA:41:G:H2'	1:XA:42:G:H8	1.84	0.42
2:XB:70:PHE:CD1	2:XB:163:PHE:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y0:48:GLY:HA3	25:Y0:80:HIS:CE1	2.54	0.42
26:Y1:21:ARG:HD3	26:Y1:35:THR:HG21	2.01	0.42
35:YA:439:G:H2'	35:YA:440:G:C8	2.55	0.42
43:YN:40:PRO:HB3	50:YU:68:ALA:HB2	2.00	0.42
3:QC:65:ALA:HA	3:QC:100:ALA:HB3	2.01	0.42
18:QR:44:LEU:HD21	18:QR:74:ARG:HH21	1.85	0.42
27:R2:41:ILE:HG21	27:R2:44:LEU:HD22	2.02	0.42
35:RA:23:G:OP1	35:RA:504:U:N3	2.43	0.42
35:RA:2416:C:H5''	45:RP:64:LYS:HE2	2.00	0.42
35:RA:2258:C:O2'	35:RA:2427:C:OP2	2.34	0.42
42:RI:114:LEU:HD12	42:RI:130:TYR:HB2	2.01	0.42
43:RN:85:ILE:HD11	43:RN:89:LYS:HG2	2.01	0.42
2:XB:208:ILE:HA	2:XB:211:ILE:HD12	2.00	0.42
6:XF:22:GLU:OE2	6:XF:82:ARG:NH2	2.45	0.42
11:XK:38:ASN:HA	11:XK:39:PRO:HD3	1.88	0.42
14:XN:12:ARG:HH21	14:XN:14:PRO:HD3	1.85	0.42
26:Y1:73:LEU:HD12	26:Y1:97:LEU:HB2	2.01	0.42
35:YA:2469:A:N6	35:YA:2481:G:O2'	2.53	0.42
35:YA:2683:C:O2	44:YO:70:LYS:NZ	2.43	0.42
35:YA:2791:C:O2	35:YA:2805:G:N2	2.51	0.42
44:YO:68:GLU:HG3	44:YO:78:ARG:HD3	2.01	0.42
48:YS:66:ALA:HA	48:YS:69:VAL:HG12	2.01	0.42
1:XA:1432:G:OP1	49:YT:108:ARG:N	2.53	0.42
1:QA:522:C:H41	12:QL:53:ARG:NH2	2.18	0.42
8:QH:36:LEU:HD12	8:QH:59:LEU:HD23	2.01	0.42
16:QP:8:ARG:HB3	16:QP:28:ARG:NH1	2.35	0.42
18:QR:60:ALA:O	18:QR:64:ARG:NH1	2.53	0.42
35:RA:1882:C:H3'	35:RA:1883:G:H8	1.84	0.42
35:RA:1858:G:H2'	35:RA:1883:G:H22	1.84	0.42
35:RA:2328:A:H2'	35:RA:2329:G:H8	1.85	0.42
35:RA:2515:C:H2'	35:RA:2516:G:H8	1.84	0.42
35:RA:2692:C:H2'	35:RA:2693:A:H8	1.84	0.42
35:RA:679:C:H2'	35:RA:680:G:C8	2.54	0.42
35:RA:948:G:N2	35:RA:985:C:OP2	2.51	0.42
43:RN:137:LYS:HD3	43:RN:137:LYS:HA	1.77	0.42
35:RA:807:U:OP2	45:RP:41:ARG:NH1	2.53	0.42
52:RW:13:SER:HA	52:RW:14:PRO:HD3	1.92	0.42
3:XC:11:ARG:NH2	3:XC:177:THR:O	2.47	0.42
35:YA:1400:G:H2'	35:YA:1401:G:C8	2.55	0.42
35:YA:1568:G:H5''	37:YD:61:LEU:HG	2.01	0.42
35:YA:2745:C:O2	41:YH:139:GLN:NE2	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:YB:66:A:H61	36:YB:107:U:H2'	1.85	0.42
44:YO:78:ARG:HH12	49:YT:75:ILE:HD11	1.84	0.42
47:YR:58:GLY:HA2	47:YR:80:PHE:HE2	1.84	0.42
1:QA:123:C:H2'	1:QA:124:G:H8	1.84	0.42
1:QA:406:G:H2'	1:QA:407:G:H8	1.85	0.42
1:QA:522:C:H41	12:QL:53:ARG:HH22	1.68	0.42
13:QM:7:VAL:HB	13:QM:9:ILE:HG12	2.01	0.42
35:RA:1205:U:C4	39:RF:171:PRO:HA	2.55	0.42
35:RA:2392:A:H2	35:RA:2424:C:H42	1.67	0.42
35:RA:2052:G:O2'	38:RE:143:ASN:O	2.30	0.42
1:XA:1058:G:H1	1:XA:1199:U:H3	1.67	0.42
1:XA:1172:C:H2'	1:XA:1173:G:H8	1.84	0.42
1:XA:985:C:H2'	1:XA:986:A:H8	1.83	0.42
16:XP:26:ARG:HD3	16:XP:26:ARG:HA	1.91	0.42
24:XZ:49:LYS:HA	24:XZ:49:LYS:HD3	1.81	0.42
35:YA:2162:G:O2'	35:YA:2173:A:OP2	2.27	0.42
35:YA:380:U:H2'	35:YA:381:G:C8	2.54	0.42
35:YA:38:A:H2'	35:YA:39:C:C6	2.55	0.42
35:YA:597:U:H3	35:YA:660:G:H1	1.67	0.42
54:YY:83:THR:OG1	54:YY:84:ARG:N	2.52	0.42
1:QA:1010:G:H2'	1:QA:1011:G:H8	1.84	0.42
1:QA:1298:C:H4'	1:QA:1299:A:C4	2.54	0.42
1:QA:1512:U:H2'	1:QA:1513:A:H8	1.84	0.42
1:QA:700:G:H4'	1:QA:704:A:H1'	2.00	0.42
2:QB:74:LYS:NZ	2:QB:205:ASP:O	2.44	0.42
13:QM:13:LYS:HA	13:QM:44:ARG:HH11	1.84	0.42
35:RA:1259:G:H2'	35:RA:1260:G:C8	2.55	0.42
35:RA:576:U:H2'	35:RA:577:G:C8	2.55	0.42
35:RA:822:U:H2'	35:RA:823:G:H8	1.84	0.42
35:RA:890:A:H2'	35:RA:892:G:C8	2.55	0.42
38:RE:41:LYS:HB3	38:RE:41:LYS:HE2	1.87	0.42
40:RG:109:VAL:O	40:RG:113:ARG:HG2	2.19	0.42
1:XA:1378:C:O2	7:XG:76:ARG:NH2	2.49	0.42
11:XK:80:VAL:HG13	11:XK:103:LEU:HD12	2.01	0.42
13:XM:51:ALA:HA	13:XM:54:VAL:HG12	2.02	0.42
33:Y8:37:SER:HB3	33:Y8:40:GLU:HG3	2.01	0.42
35:YA:1021:A:OP2	43:YN:65:LYS:NZ	2.42	0.42
35:YA:1225:C:H2'	35:YA:1226:G:C8	2.54	0.42
35:YA:1568:G:OP2	37:YD:63:ARG:NH2	2.41	0.42
35:YA:1363:C:O2'	35:YA:1809:A:N3	2.44	0.42
37:YD:133:LEU:HD23	37:YD:136:ILE:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:958:U:OP2	46:YQ:14:ARG:NH1	2.52	0.42
52:YW:110:LYS:HD3	52:YW:110:LYS:HA	1.90	0.42
55:YZ:51:ALA:HB1	55:YZ:55:HIS:HB2	2.02	0.42
55:YZ:6:LYS:HD2	55:YZ:6:LYS:HA	1.83	0.42
1:QA:1356:G:H2'	1:QA:1357:A:H8	1.85	0.42
1:QA:413:G:N2	1:QA:429:U:OP2	2.44	0.42
4:QD:119:GLN:O	4:QD:123:HIS:N	2.49	0.42
35:RA:137(A):G:O2'	35:RA:138:G:N2	2.53	0.42
35:RA:863:A:H2'	35:RA:864:G:C8	2.55	0.42
40:RG:36:LYS:HE2	40:RG:95:ARG:HH12	1.85	0.42
1:XA:1151:A:H5'	10:XJ:41:PRO:HA	2.01	0.42
2:XB:69:LEU:HB3	2:XB:162:ILE:HG22	2.00	0.42
2:XB:208:ILE:HG13	2:XB:208:ILE:H	1.65	0.42
5:XE:53:LEU:HA	5:XE:56:GLN:HG2	2.02	0.42
9:XI:42:ARG:NH1	9:XI:71:SER:OG	2.53	0.42
35:YA:1212:G:O2'	35:YA:1237:A:N6	2.52	0.42
35:YA:1482:U:O4	35:YA:1512:G:O6	2.37	0.42
39:YF:63:LYS:HE2	39:YF:67:GLN:HB2	2.02	0.42
39:YF:64:ILE:HG13	39:YF:64:ILE:H	1.71	0.42
54:YY:14:LEU:HD22	54:YY:82:PRO:HG3	2.00	0.42
1:QA:1060:C:H2'	1:QA:1061:G:H8	1.84	0.42
8:QH:19:VAL:HG13	8:QH:21:LYS:HG3	2.02	0.42
13:QM:47:ASP:OD1	13:QM:47:ASP:N	2.52	0.42
1:QA:1226:C:OP1	13:QM:91:ARG:NH1	2.53	0.42
40:RG:82:LEU:HD11	40:RG:88:ILE:HD13	2.01	0.42
45:RP:91:PHE:HE2	45:RP:95:VAL:HG22	1.85	0.42
1:XA:41:G:H2'	1:XA:42:G:C8	2.55	0.42
10:XJ:42:THR:HG22	10:XJ:68:HIS:HA	2.01	0.42
20:XT:89:ARG:HG3	20:XT:104:LEU:HD21	2.01	0.42
35:YA:151:C:H2'	35:YA:152:G:H8	1.83	0.42
25:Y0:39:ARG:HH21	35:YA:2355:C:H1'	1.84	0.42
35:YA:2688:U:OP1	35:YA:2713:A:N6	2.52	0.42
35:YA:530:G:N2	35:YA:2022:U:OP1	2.53	0.42
35:YA:78:A:H2'	35:YA:79:G:C8	2.55	0.42
13:XM:94:ARG:NH2	35:YA:887:A:OP1	2.46	0.42
41:YH:94:TYR:OH	41:YH:152:ARG:NH1	2.53	0.42
52:YW:13:SER:HA	52:YW:14:PRO:HD3	1.94	0.42
1:QA:404:U:H2'	1:QA:405:U:H6	1.84	0.41
6:QF:15:ASP:OD2	6:QF:17:SER:OG	2.38	0.41
6:QF:46:ARG:HD2	6:QF:46:ARG:HA	1.88	0.41
11:QK:38:ASN:HA	11:QK:39:PRO:HD3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:R2:28:LYS:HA	27:R2:28:LYS:HD3	1.90	0.41
35:RA:1569:A:H5'	37:RD:61:LEU:HD21	2.02	0.41
35:RA:1754:C:N3	35:RA:2716:U:O2'	2.48	0.41
35:RA:532:A:H4'	35:RA:533:G:C8	2.55	0.41
35:RA:1567:A:H3'	37:RD:86:PRO:HG3	2.02	0.41
1:XA:891:U:H2'	1:XA:892:A:C8	2.54	0.41
1:XA:980:C:H1'	14:YN:19:ARG:HA	2.02	0.41
7:XG:29:LYS:HD2	7:XG:29:LYS:HA	1.90	0.41
11:XK:108:ILE:O	18:XR:87:ARG:N	2.51	0.41
19:XS:2:PRO:HB2	19:XS:3:ARG:H	1.61	0.41
35:YA:2329:G:H2'	35:YA:2330:G:H8	1.84	0.41
35:YA:299:A:N1	35:YA:322:A:O2'	2.42	0.41
35:YA:414:C:H2'	35:YA:415:A:H8	1.84	0.41
35:YA:820:A:H4'	35:YA:836:G:N2	2.35	0.41
40:YG:166:ASP:OD1	40:YG:166:ASP:N	2.53	0.41
49:YT:19:LEU:HA	49:YT:20:PRO:HD3	1.90	0.41
55:YZ:124:ILE:HG22	55:YZ:126:VAL:HG13	2.01	0.41
1:QA:619:U:N3	4:QD:134:ASP:OD1	2.53	0.41
5:QE:105:VAL:HG11	5:QE:128:PRO:HB3	2.01	0.41
5:QE:152:ARG:NH2	8:QH:107:LEU:O	2.53	0.41
35:RA:2591:C:H2'	35:RA:2592:G:H8	1.84	0.41
35:RA:2681:C:OP2	38:RE:109:LYS:NZ	2.42	0.41
41:RH:89:ILE:HG23	41:RH:162:ILE:HG22	2.01	0.41
1:XA:1240:U:OP1	7:XG:119:ARG:NH2	2.53	0.41
1:XA:1412:C:H2'	1:XA:1413:A:C8	2.55	0.41
1:XA:56:U:H2'	1:XA:57:G:C8	2.55	0.41
1:XA:977:A:O2'	1:XA:981:U:O4	2.38	0.41
1:XA:194:C:H5''	20:XT:65:LYS:HG3	2.02	0.41
1:XA:1493:A:O2'	23:XX:20:A3P:H8	2.20	0.41
35:YA:30:G:H2'	35:YA:31:C:C6	2.55	0.41
39:YF:46:ARG:HD2	39:YF:46:ARG:HA	1.86	0.41
40:YG:72:ARG:HG2	40:YG:72:ARG:HH11	1.85	0.41
25:Y0:5:LYS:HD3	46:YQ:80:GLU:HG3	2.02	0.41
55:YZ:179:ASP:OD1	55:YZ:180:VAL:N	2.53	0.41
1:QA:1182:G:H5''	1:QA:1183:A:H5'	2.02	0.41
35:RA:2033:A:O2'	35:RA:2035:G:OP2	2.34	0.41
35:RA:219:G:N3	35:RA:234:C:O2'	2.48	0.41
35:RA:2836:U:H2'	35:RA:2837:G:C8	2.55	0.41
35:RA:329:G:O6	54:RY:19:LYS:N	2.54	0.41
35:RA:223:A:O2'	35:RA:420:C:O2	2.36	0.41
51:RV:34:GLU:OE2	51:RV:100:ARG:NH2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:269:C:H2'	1:XA:270:A:C8	2.55	0.41
18:XR:26:LEU:HD11	18:XR:39:VAL:HG13	2.03	0.41
19:XS:27:GLU:HG2	19:XS:29:ARG:NH1	2.35	0.41
24:XZ:81:ARG:HG2	24:XZ:82:TYR:H	1.85	0.41
32:Y7:10:ARG:HD2	35:YA:125:G:C6	2.55	0.41
36:YB:114:G:H2'	36:YB:115:G:H8	1.85	0.41
47:YR:66:VAL:HG21	47:YR:80:PHE:HE1	1.85	0.41
55:YZ:119:GLU:HB2	55:YZ:122:ARG:HH11	1.85	0.41
1:QA:359:U:H2'	1:QA:360:A:C8	2.56	0.41
3:QC:16:ARG:HD2	3:QC:16:ARG:HA	1.68	0.41
1:QA:933:G:O6	7:QG:3:ARG:NH2	2.53	0.41
8:QH:69:ARG:NH2	8:QH:75:ARG:O	2.53	0.41
10:QJ:4:ILE:HG23	10:QJ:74:ILE:HB	2.01	0.41
31:R6:25:LYS:HE2	31:R6:25:LYS:HB2	1.67	0.41
35:RA:1687:G:O2'	35:RA:1701:A:N6	2.47	0.41
35:RA:2314:C:H5'	40:RG:38:VAL:HG11	2.02	0.41
45:RP:46:LYS:HD2	45:RP:46:LYS:HA	1.96	0.41
35:RA:196:A:O5'	45:RP:46:LYS:NZ	2.53	0.41
47:RR:13:HIS:CE1	47:RR:16:HIS:HB2	2.55	0.41
50:RU:90:VAL:C	50:RU:92:ARG:H	2.23	0.41
1:XA:1096:C:H2'	1:XA:1097:C:H6	1.86	0.41
5:XE:106:PRO:HB3	5:XE:135:THR:HG21	2.01	0.41
7:XG:13:GLN:HA	7:XG:14:PRO:HD3	1.91	0.41
18:XR:31:LEU:HD12	18:XR:66:LEU:HB2	2.03	0.41
20:XT:29:LYS:O	20:XT:33:ILE:HG12	2.21	0.41
33:Y8:10:ALA:HB3	33:Y8:62:LEU:HD21	2.02	0.41
35:YA:1769:G:O2'	35:YA:1958:C:OP1	2.32	0.41
35:YA:2471:C:H3'	35:YA:2472:G:H8	1.84	0.41
48:YS:34:HIS:CD2	48:YS:54:LEU:HD12	2.56	0.41
17:QQ:45:HIS:CD2	17:QQ:47:PRO:HG3	2.55	0.41
18:QR:53:ARG:HH21	18:QR:59:SER:HA	1.86	0.41
35:RA:177:G:H3'	35:RA:178:G:H8	1.84	0.41
35:RA:2788:C:H5'	38:RE:61:ARG:HH12	1.86	0.41
40:RG:40:ASN:HB3	40:RG:156:ASP:HB2	2.02	0.41
49:RT:5:ALA:HA	49:RT:8:LYS:HB3	2.03	0.41
1:XA:390:C:H2'	1:XA:391:G:C8	2.55	0.41
3:XC:40:ARG:HG2	3:XC:55:VAL:HG21	2.01	0.41
8:XH:29:SER:HB3	8:XH:32:LYS:HG3	2.03	0.41
17:XQ:53:LEU:HD23	17:XQ:85:VAL:HG11	2.02	0.41
35:YA:1403:C:H5''	35:YA:1471:A:H1'	2.02	0.41
35:YA:2850:A:N7	35:YA:2868:A:O2'	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:806:C:O2	35:YA:2444:G:O2'	2.36	0.41
35:YA:970:C:H2'	35:YA:971:C:C6	2.56	0.41
41:YH:54:ARG:NH2	41:YH:57:ASP:OD1	2.54	0.41
49:YT:62:THR:HG22	49:YT:75:ILE:HG12	2.02	0.41
50:YU:92:ARG:NH2	51:YV:11:GLN:H	2.18	0.41
35:YA:1187:G:H5''	51:YV:81:TYR:CE1	2.55	0.41
1:QA:1354:C:H2'	1:QA:1355:G:C8	2.56	0.41
1:QA:454:C:H41	1:QA:478:A:H61	1.68	0.41
1:QA:524:G:H2'	1:QA:525:C:C6	2.56	0.41
27:R2:14:ARG:HG2	27:R2:63:VAL:HG21	2.03	0.41
28:R3:8:LEU:HG	28:R3:28:LEU:HD12	2.01	0.41
30:R5:30:LEU:HD12	30:R5:39:MET:HB3	2.02	0.41
33:R8:58:ILE:HA	33:R8:61:LEU:HD12	2.03	0.41
35:RA:1771:C:H2'	35:RA:1772:G:C8	2.56	0.41
35:RA:414:C:H2'	35:RA:415:A:C8	2.55	0.41
47:RR:24:GLN:HG3	47:RR:44:LEU:HD13	2.02	0.41
1:XA:1251:A:H2'	1:XA:1252:A:C8	2.56	0.41
1:XA:1436:U:OP1	20:XT:23:ARG:NH2	2.53	0.41
1:XA:359:U:H2'	1:XA:360:A:C8	2.56	0.41
1:XA:45:U:H2'	1:XA:46:G:H8	1.85	0.41
1:XA:524:G:H2'	1:XA:525:C:C6	2.55	0.41
1:XA:736:C:H2'	1:XA:737:A:C8	2.55	0.41
9:XI:49:PRO:HA	9:XI:52:ALA:HB3	2.03	0.41
14:YN:37:PHE:HB3	14:YN:39:LEU:HD13	2.03	0.41
17:XQ:18:THR:OG1	17:XQ:69:LYS:NZ	2.39	0.41
26:Y1:60:PHE:HE1	26:Y1:91:LYS:HG3	1.86	0.41
35:YA:2291:U:H2'	35:YA:2292:C:C6	2.55	0.41
1:QA:919:A:O2'	1:QA:1080:A:N1	2.43	0.41
8:QH:41:ARG:NH2	8:QH:123:GLU:OE1	2.53	0.41
10:QJ:8:LEU:HB3	10:QJ:70:ARG:HB2	2.02	0.41
35:RA:1231:G:H2'	35:RA:1232:G:H8	1.85	0.41
35:RA:121:G:H4'	35:RA:149:A:H5'	2.02	0.41
35:RA:570:G:H2'	35:RA:2030:A:C5	2.55	0.41
38:RE:64:LYS:HA	38:RE:64:LYS:HD3	1.73	0.41
49:RT:85:LYS:NZ	49:RT:87:ASP:OD2	2.46	0.41
1:XA:1127:G:H21	1:XA:1147:C:H42	1.67	0.41
1:XA:1182:G:H4'	1:XA:1183:A:H5'	2.03	0.41
3:XC:91:LEU:HB3	3:XC:99:VAL:HG11	2.03	0.41
20:XT:26:ASN:HB2	20:XT:71:THR:HG23	2.03	0.41
30:Y5:3:LYS:H	35:YA:2577:A:H4'	1.85	0.41
35:YA:1423:G:H2'	35:YA:1424:G:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:33:U:O4	35:YA:446:G:O2'	2.33	0.41
35:YA:679:C:H2'	35:YA:680:G:H8	1.86	0.41
39:YF:155:LEU:HD11	39:YF:176:LEU:HB2	2.03	0.41
1:QA:116:A:H61	1:QA:313:A:H1'	1.85	0.41
1:QA:362:G:N2	1:QA:365:U:OP2	2.52	0.41
1:QA:377:G:H2'	1:QA:378:G:C8	2.56	0.41
1:QA:652:U:O3'	8:QH:56:LYS:NZ	2.54	0.41
1:QA:652:U:O4	1:QA:752:G:O2'	2.32	0.41
13:QM:23:TYR:CE2	13:QM:71:ARG:HG3	2.55	0.41
29:R4:2:LYS:O	29:R4:4:GLY:N	2.53	0.41
44:RO:22:ILE:HD11	44:RO:42:SER:HB2	2.02	0.41
46:RQ:116:GLU:O	46:RQ:120:ILE:HG12	2.20	0.41
1:XA:1127:G:N2	1:XA:1147:C:H42	2.19	0.41
1:XA:142:G:H2'	1:XA:143:A:C8	2.56	0.41
1:XA:898:G:N2	1:XA:901:A:OP2	2.48	0.41
10:XJ:66:ARG:HD2	14:XN:57:ARG:HH22	1.85	0.41
1:XA:195:A:H4'	20:XT:68:LYS:HE3	2.03	0.41
23:XX:14:A:H2'	23:XX:15:A:H8	1.86	0.41
35:YA:2001:A:H2'	35:YA:2002:G:C8	2.56	0.41
35:YA:2103:C:N4	35:YA:2187:G:O6	2.54	0.41
35:YA:2749:A:O2'	41:YH:59:ARG:NE	2.48	0.41
35:YA:764:A:H2	37:YD:219:PRO:HG3	1.85	0.41
1:QA:1228:C:H4'	13:QM:116:THR:HA	2.02	0.41
1:QA:1427:U:H2'	1:QA:1428:A:C8	2.56	0.41
1:QA:189:U:O4	17:QQ:63:ARG:N	2.53	0.41
9:QI:102:LEU:HA	9:QI:102:LEU:HD23	1.81	0.41
13:QM:121:LYS:HD2	13:QM:121:LYS:HA	1.81	0.41
22:QV:9:G:O2'	22:QV:10:G:N7	2.46	0.41
28:R3:29:ARG:N	28:R3:33:GLN:OE1	2.50	0.41
29:R4:13:ARG:HD3	29:R4:13:ARG:HA	1.94	0.41
35:RA:1336:A:H2'	35:RA:1337:G:C8	2.56	0.41
35:RA:2186:G:H2'	35:RA:2187:G:C8	2.56	0.41
35:RA:922:U:H2'	35:RA:923:C:C6	2.56	0.41
37:RD:77:ALA:HA	37:RD:97:TYR:HA	2.02	0.41
35:RA:2723:C:P	38:RE:109:LYS:HZ3	2.44	0.41
38:RE:25:VAL:HG11	49:RT:10:VAL:HG11	2.03	0.41
1:XA:708:C:H2'	1:XA:709:G:H8	1.86	0.41
1:XA:790:A:OP1	22:XV:38:A:O2'	2.34	0.41
1:XA:806:C:H2'	1:XA:807:A:C8	2.56	0.41
1:XA:892:A:H2'	1:XA:893:C:C6	2.56	0.41
3:XC:152:ILE:HG12	3:XC:167:TRP:HD1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:1657:C:H2'	35:YA:1658:C:C6	2.55	0.41
35:YA:2853:C:H2'	35:YA:2854:G:C8	2.56	0.41
38:YE:7:VAL:HG13	38:YE:51:PHE:HE2	1.86	0.41
39:YF:24:LEU:HA	39:YF:25:PRO:HD3	1.94	0.41
40:YG:64:THR:HG23	40:YG:66:GLN:H	1.86	0.41
42:YI:14:ASP:H	42:YI:17:GLN:CB	2.34	0.41
35:YA:195:A:H5''	45:YP:46:LYS:NZ	2.36	0.41
1:QA:80:G:H1	1:QA:89:U:H3	1.68	0.41
7:QG:88:PRO:HG2	7:QG:152:ALA:HB2	2.03	0.41
8:QH:86:ILE:HD12	8:QH:133:LEU:HD22	2.03	0.41
8:QH:36:LEU:HA	8:QH:36:LEU:HD23	1.92	0.41
13:QM:3:ARG:HA	13:QM:8:GLU:HA	2.03	0.41
35:RA:1278:A:H2'	35:RA:1279:G:C8	2.56	0.41
35:RA:824:A:H1'	35:RA:2358:G:N7	2.36	0.41
35:RA:2597:G:H2'	35:RA:2598:A:C8	2.55	0.41
42:RI:72:LEU:HG	42:RI:138:ILE:HG13	2.01	0.41
2:XB:15:VAL:HG11	2:XB:210:SER:N	2.35	0.41
6:XF:45:LEU:HD12	6:XF:59:TYR:HD1	1.86	0.41
10:XJ:78:ASN:OD1	10:XJ:78:ASN:N	2.50	0.41
35:YA:453:C:O2	35:YA:457:A:O2'	2.35	0.41
1:QA:1119:C:H2'	1:QA:1120:G:C8	2.55	0.41
1:QA:1199:U:O2'	1:QA:1202:G:OP1	2.35	0.41
1:QA:41:G:H2'	1:QA:42:G:H8	1.85	0.41
13:QM:84:ILE:HD13	19:QS:65:ASN:HD21	1.86	0.41
25:R0:39:ARG:HD3	25:R0:39:ARG:HA	1.88	0.41
19:QS:42:PRO:HD3	29:R4:63:TYR:OH	2.20	0.41
35:RA:1400:G:H2'	35:RA:1401:G:C8	2.55	0.41
35:RA:635:C:O2'	35:RA:639:U:OP1	2.37	0.41
35:RA:861:A:N3	36:RB:79:C:O2'	2.53	0.41
36:RB:60:C:H2'	36:RB:61:G:C8	2.56	0.41
38:RE:34:VAL:HG12	38:RE:72:VAL:HG11	2.02	0.41
46:RQ:31:ASP:OD1	55:RZ:122:ARG:NH2	2.47	0.41
50:RU:32:PHE:CZ	50:RU:36:ARG:HD2	2.56	0.41
1:XA:1435:G:H2'	1:XA:1436:U:C6	2.56	0.41
1:XA:1513:A:H2'	1:XA:1514:C:C6	2.55	0.41
35:YA:2698:U:H2'	35:YA:2699:C:C6	2.56	0.41
35:YA:680:G:H2'	35:YA:681:G:C8	2.55	0.41
35:YA:992:C:H2'	35:YA:993:G:H8	1.85	0.41
52:YW:68:ARG:NE	52:YW:110:LYS:O	2.48	0.41
35:YA:1262:A:OP2	52:YW:97:LYS:NZ	2.54	0.41
1:QA:1037:C:H2'	1:QA:1038:C:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:125:U:H2'	1:QA:126:G:C8	2.55	0.40
4:QD:122:ARG:HA	4:QD:122:ARG:HD2	1.94	0.40
16:QP:18:ARG:HH11	16:QP:35:LYS:HD2	1.86	0.40
18:QR:40:LEU:HB3	18:QR:79:LEU:HD21	2.02	0.40
35:RA:1316:U:H2'	35:RA:1317:A:H8	1.86	0.40
26:R1:11:ARG:NH2	35:RA:1365:A:O2'	2.52	0.40
35:RA:1399:C:H2'	35:RA:1400:G:C8	2.56	0.40
35:RA:1409:C:H2'	35:RA:1410:G:H8	1.86	0.40
35:RA:1449:A:C4	35:RA:1529:A:H2	2.39	0.40
35:RA:1889:A:H2'	35:RA:1890:A:C8	2.56	0.40
35:RA:463:G:N2	35:RA:466:A:OP2	2.42	0.40
35:RA:764:A:H5'	37:RD:210:GLY:HA2	2.02	0.40
48:RS:39:ILE:HD12	48:RS:85:VAL:HG11	2.02	0.40
1:XA:1311:G:OP1	29:Y4:58:ARG:NH2	2.54	0.40
1:XA:1441:G:O2'	1:XA:1446:A:N6	2.49	0.40
1:XA:269:C:H2'	1:XA:270:A:H8	1.86	0.40
7:XG:94:ARG:NH1	7:XG:98:SER:OG	2.54	0.40
9:XI:42:ARG:NH2	9:XI:75:ASP:OD1	2.52	0.40
35:YA:141:A:C8	35:YA:1408:C:H1'	2.56	0.40
35:YA:2037:G:H2'	35:YA:2038:G:C8	2.56	0.40
39:YF:48:THR:O	39:YF:48:THR:OG1	2.39	0.40
40:YG:29:TRP:O	40:YG:33:ARG:NH1	2.54	0.40
46:YQ:116:GLU:HA	46:YQ:119:ARG:HG2	2.03	0.40
49:YT:80:SER:HA	49:YT:81:PRO:HD3	1.92	0.40
50:YU:90:VAL:HG11	51:YV:39:LEU:HB2	2.04	0.40
54:YY:81:LYS:HD2	54:YY:82:PRO:HD2	2.03	0.40
1:QA:401:C:H2'	1:QA:402:G:H8	1.86	0.40
1:QA:1101:A:N6	2:QB:176:GLU:OE2	2.54	0.40
3:QC:164:ARG:NH1	3:QC:166:GLU:OE2	2.37	0.40
6:QF:3:ARG:HB3	6:QF:93:SER:HB2	2.03	0.40
19:QS:10:PHE:HE1	19:QS:38:SER:HB2	1.85	0.40
25:R0:49:LYS:HB3	25:R0:80:HIS:HD1	1.85	0.40
35:RA:582:G:H2'	35:RA:583:G:C8	2.56	0.40
27:R2:65:ASN:ND2	35:RA:72:U:O4	2.54	0.40
38:RE:114:ALA:HB1	38:RE:118:LYS:HD2	2.02	0.40
1:XA:1159:U:O2'	1:XA:1160:G:N7	2.53	0.40
1:XA:881:G:OP2	12:XL:12:ARG:NH2	2.54	0.40
1:XA:927:G:H1	1:XA:1390:U:H3	1.68	0.40
1:XA:993:G:O2'	1:XA:994:A:N7	2.54	0.40
2:XB:16:HIS:ND1	2:XB:17:PHE:O	2.54	0.40
4:XD:102:ASP:N	4:XD:102:ASP:OD1	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:XG:15:ASP:OD1	7:XG:44:TYR:OH	2.38	0.40
2:XB:178:ARG:NH1	8:XH:74:PRO:HB3	2.36	0.40
20:XT:27:LYS:HD3	20:XT:27:LYS:HA	1.92	0.40
20:XT:50:GLU:HB3	20:XT:99:LEU:HD21	2.04	0.40
35:YA:1652:A:OP1	47:YR:8:ARG:NH1	2.44	0.40
35:YA:2327:A:H2'	35:YA:2328:A:C8	2.56	0.40
35:YA:698:C:O2'	35:YA:734:A:N6	2.55	0.40
35:YA:969:U:H2'	35:YA:970:C:C6	2.56	0.40
39:YF:155:LEU:HD23	39:YF:186:ILE:HD13	2.02	0.40
42:YI:79:ILE:HG22	42:YI:81:VAL:HG13	2.03	0.40
47:YR:58:GLY:HA2	47:YR:80:PHE:CE2	2.56	0.40
53:YX:31:HIS:HB3	53:YX:34:ALA:HB2	2.03	0.40
55:YZ:48:PHE:HE1	55:YZ:71:VAL:HG21	1.86	0.40
1:QA:1488:G:H2'	1:QA:1489:G:C8	2.56	0.40
1:QA:954:G:H21	1:QA:1227:A:N6	2.19	0.40
2:QB:133:LYS:HD2	2:QB:133:LYS:HA	1.91	0.40
11:QK:70:LYS:HA	11:QK:70:LYS:HD3	1.87	0.40
23:QX:6:G:H2'	23:QX:7:G:C8	2.57	0.40
33:R8:46:ARG:HA	33:R8:46:ARG:HD2	1.83	0.40
35:RA:1529:A:H62	35:RA:1542:G:N2	2.19	0.40
35:RA:270(I):G:H2'	35:RA:270(J):G:C8	2.57	0.40
35:RA:2728:U:H2'	35:RA:2729:G:C8	2.56	0.40
35:RA:663:G:H5''	45:RP:17:LYS:HD3	2.04	0.40
35:RA:807:U:H2'	35:RA:808:G:H8	1.85	0.40
36:RB:9:G:H5'	48:RS:25:ARG:HH22	1.86	0.40
38:RE:67:PHE:HD1	38:RE:67:PHE:HA	1.75	0.40
43:RN:16:ILE:HB	43:RN:54:VAL:HG22	2.03	0.40
1:XA:1354:C:H2'	1:XA:1355:G:H8	1.86	0.40
1:XA:7:G:O2'	5:XE:120:THR:O	2.40	0.40
7:XG:78:ARG:HE	7:XG:80:VAL:HG23	1.87	0.40
1:XA:1314:C:N4	19:XS:2:PRO:O	2.55	0.40
26:Y1:73:LEU:HD13	26:Y1:73:LEU:HA	1.82	0.40
13:XM:3:ARG:NH1	29:Y4:34:GLU:OE2	2.54	0.40
35:YA:1411:C:H2'	35:YA:1412:A:H8	1.86	0.40
31:Y6:6:ARG:NH1	35:YA:2285:C:OP2	2.53	0.40
35:YA:576:U:H2'	35:YA:577:G:C8	2.56	0.40
35:YA:787:U:H5''	35:YA:788:A:H5'	2.04	0.40
43:YN:96:GLU:HG3	43:YN:122:VAL:HG23	2.04	0.40
1:QA:1128:C:H1'	1:QA:1146:A:H61	1.86	0.40
1:QA:603:U:H2'	1:QA:604:G:C8	2.57	0.40
4:QD:88:VAL:HG13	4:QD:91:SER:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:R3:18:ASP:N	28:R3:18:ASP:OD1	2.54	0.40
34:R9:6:SER:OG	34:R9:6:SER:O	2.40	0.40
35:RA:1935:G:H1'	35:RA:1964:G:N2	2.37	0.40
35:RA:37:C:H2'	35:RA:38:A:C8	2.57	0.40
35:RA:616:A:C4	39:RF:180:GLY:HA3	2.56	0.40
35:RA:78:A:H2'	35:RA:79:G:H8	1.85	0.40
36:RB:105:G:H2'	36:RB:106:G:H8	1.85	0.40
35:RA:323:G:H2'	39:RF:169:ASN:ND2	2.37	0.40
40:RG:124:SER:OG	40:RG:132:ASN:O	2.38	0.40
42:RI:65:ALA:HB1	42:RI:134:PRO:HD2	2.03	0.40
50:RU:61:TRP:HB3	50:RU:93:LYS:O	2.22	0.40
1:XA:1064:G:H1'	1:XA:1066:C:C6	2.56	0.40
1:XA:1064:G:O6	1:XA:1193:G:N1	2.54	0.40
1:XA:1287:A:H2	1:XA:1353:G:H1'	1.86	0.40
1:XA:719:C:N3	18:XR:74:ARG:NH1	2.49	0.40
19:XS:40:ILE:HG12	19:XS:71:LEU:HG	2.03	0.40
26:Y1:92:LYS:HZ3	26:Y1:96:LYS:NZ	2.19	0.40
29:Y4:37:SER:HB3	40:YG:108:ASN:HA	2.04	0.40
31:Y6:17:LYS:HD3	31:Y6:17:LYS:HA	1.85	0.40
35:YA:1060:U:H5'	35:YA:1061:U:H5	1.86	0.40
35:YA:588:U:H1'	39:YF:90:PHE:HB3	2.04	0.40
40:YG:59:GLU:OE1	40:YG:153:ARG:NH2	2.55	0.40
51:YV:12:TYR:CD1	51:YV:20:LEU:HD11	2.56	0.40
55:YZ:72:ARG:NH2	55:YZ:97:GLU:O	2.54	0.40
1:QA:1070:U:OP1	5:QE:18:ARG:NH2	2.45	0.40
1:QA:272:C:H2'	1:QA:273:A:H8	1.87	0.40
1:QA:411:A:H62	1:QA:413:G:H21	1.70	0.40
14:QN:27:CYS:SG	14:QN:28:GLY:N	2.94	0.40
19:QS:10:PHE:HB2	19:QS:39:THR:HB	2.02	0.40
34:R9:2:LYS:HE2	34:R9:33:LYS:HG2	2.04	0.40
35:RA:448:U:C4	35:RA:583:G:H1'	2.57	0.40
35:RA:848:G:H2'	35:RA:849:A:C8	2.57	0.40
1:XA:674:G:H2'	1:XA:675:A:C8	2.51	0.40
1:XA:737:A:H2'	1:XA:738:C:C6	2.56	0.40
6:XF:30:LEU:HD23	6:XF:75:LEU:HD11	2.03	0.40
13:XM:15:VAL:HA	13:XM:18:ALA:HB3	2.02	0.40
35:YA:1901:A:OP2	37:YD:255:LYS:NZ	2.37	0.40
35:YA:2025:C:H2'	35:YA:2026:C:C6	2.56	0.40
30:Y5:29:THR:HG21	35:YA:2815:C:H5'	2.03	0.40
35:YA:2006:C:O2'	35:YA:2823:A:N3	2.51	0.40
35:YA:639:U:H2'	35:YA:640:C:C6	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:YF:6:VAL:HB	39:YF:24:LEU:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	233/256 (91%)	202 (87%)	27 (12%)	4 (2%)	9	42
2	XB	234/256 (91%)	211 (90%)	21 (9%)	2 (1%)	17	56
3	QC	203/239 (85%)	186 (92%)	17 (8%)	0	100	100
3	XC	203/239 (85%)	188 (93%)	14 (7%)	1 (0%)	29	68
4	QD	206/209 (99%)	193 (94%)	11 (5%)	2 (1%)	15	54
4	XD	206/209 (99%)	187 (91%)	17 (8%)	2 (1%)	15	54
5	QE	149/162 (92%)	140 (94%)	9 (6%)	0	100	100
5	XE	149/162 (92%)	142 (95%)	7 (5%)	0	100	100
6	QF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
6	XF	99/101 (98%)	99 (100%)	0	0	100	100
7	QG	153/156 (98%)	144 (94%)	8 (5%)	1 (1%)	22	61
7	XG	153/156 (98%)	147 (96%)	6 (4%)	0	100	100
8	QH	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
8	XH	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
9	QI	125/128 (98%)	112 (90%)	13 (10%)	0	100	100
9	XI	124/128 (97%)	113 (91%)	11 (9%)	0	100	100
10	QJ	97/105 (92%)	85 (88%)	12 (12%)	0	100	100
10	XJ	94/105 (90%)	80 (85%)	13 (14%)	1 (1%)	14	52
11	QK	117/129 (91%)	107 (92%)	10 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	XK	114/129 (88%)	105 (92%)	9 (8%)	0	100	100
12	QL	123/132 (93%)	110 (89%)	11 (9%)	2 (2%)	9	43
12	XL	120/132 (91%)	103 (86%)	16 (13%)	1 (1%)	19	58
13	QM	118/126 (94%)	102 (86%)	13 (11%)	3 (2%)	5	34
13	XM	117/126 (93%)	96 (82%)	21 (18%)	0	100	100
14	QN	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	9	42
14	XN	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	9	42
15	QO	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
15	XO	85/89 (96%)	84 (99%)	1 (1%)	0	100	100
16	QP	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
16	XP	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
17	QQ	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
17	XQ	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
18	QR	68/88 (77%)	64 (94%)	4 (6%)	0	100	100
18	XR	68/88 (77%)	64 (94%)	4 (6%)	0	100	100
19	QS	81/93 (87%)	69 (85%)	11 (14%)	1 (1%)	13	50
19	XS	81/93 (87%)	75 (93%)	6 (7%)	0	100	100
20	QT	97/106 (92%)	90 (93%)	7 (7%)	0	100	100
20	XT	97/106 (92%)	88 (91%)	6 (6%)	3 (3%)	4	30
21	QU	23/27 (85%)	20 (87%)	2 (9%)	1 (4%)	2	22
21	XU	23/27 (85%)	22 (96%)	0	1 (4%)	2	22
24	QY	82/84 (98%)	70 (85%)	10 (12%)	2 (2%)	6	35
24	QZ	82/84 (98%)	72 (88%)	10 (12%)	0	100	100
24	XY	82/84 (98%)	71 (87%)	8 (10%)	3 (4%)	3	26
24	XZ	82/84 (98%)	70 (85%)	11 (13%)	1 (1%)	13	50
25	R0	79/85 (93%)	72 (91%)	6 (8%)	1 (1%)	12	48
25	Y0	80/85 (94%)	72 (90%)	8 (10%)	0	100	100
26	R1	92/98 (94%)	82 (89%)	10 (11%)	0	100	100
26	Y1	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	14	52
27	R2	67/72 (93%)	61 (91%)	5 (8%)	1 (2%)	10	45
27	Y2	67/72 (93%)	63 (94%)	2 (3%)	2 (3%)	4	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	R3	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
28	Y3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
29	R4	67/71 (94%)	46 (69%)	17 (25%)	4 (6%)	1	15
29	Y4	67/71 (94%)	54 (81%)	12 (18%)	1 (2%)	10	45
30	R5	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
30	Y5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
31	R6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
31	Y6	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
32	R7	45/49 (92%)	45 (100%)	0	0	100	100
32	Y7	46/49 (94%)	46 (100%)	0	0	100	100
33	R8	62/65 (95%)	54 (87%)	6 (10%)	2 (3%)	4	29
33	Y8	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	4	29
34	R9	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
34	Y9	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
37	RD	270/276 (98%)	244 (90%)	22 (8%)	4 (2%)	10	45
37	YD	272/276 (99%)	263 (97%)	9 (3%)	0	100	100
38	RE	203/206 (98%)	179 (88%)	20 (10%)	4 (2%)	7	39
38	YE	202/206 (98%)	191 (95%)	9 (4%)	2 (1%)	15	54
39	RF	200/210 (95%)	195 (98%)	5 (2%)	0	100	100
39	YF	200/210 (95%)	184 (92%)	14 (7%)	2 (1%)	15	54
40	RG	179/182 (98%)	152 (85%)	24 (13%)	3 (2%)	9	42
40	YG	179/182 (98%)	151 (84%)	26 (14%)	2 (1%)	14	52
41	RH	172/180 (96%)	137 (80%)	29 (17%)	6 (4%)	3	27
41	YH	172/180 (96%)	164 (95%)	8 (5%)	0	100	100
42	RI	143/148 (97%)	117 (82%)	20 (14%)	6 (4%)	3	23
42	YI	144/148 (97%)	123 (85%)	19 (13%)	2 (1%)	11	46
43	RN	136/140 (97%)	117 (86%)	17 (12%)	2 (2%)	10	45
43	YN	136/140 (97%)	118 (87%)	16 (12%)	2 (2%)	10	45
44	RO	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
44	YO	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	19	58
45	RP	148/150 (99%)	125 (84%)	19 (13%)	4 (3%)	5	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	YP	147/150 (98%)	138 (94%)	7 (5%)	2 (1%)	11	46
46	RQ	139/141 (99%)	121 (87%)	13 (9%)	5 (4%)	3	26
46	YQ	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
47	RR	115/118 (98%)	108 (94%)	6 (5%)	1 (1%)	17	56
47	YR	115/118 (98%)	103 (90%)	11 (10%)	1 (1%)	17	56
48	RS	109/112 (97%)	93 (85%)	15 (14%)	1 (1%)	17	56
48	YS	109/112 (97%)	93 (85%)	16 (15%)	0	100	100
49	RT	135/146 (92%)	119 (88%)	15 (11%)	1 (1%)	22	61
49	YT	135/146 (92%)	119 (88%)	16 (12%)	0	100	100
50	RU	115/118 (98%)	106 (92%)	8 (7%)	1 (1%)	17	56
50	YU	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	17	56
51	RV	99/101 (98%)	90 (91%)	9 (9%)	0	100	100
51	YV	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	15	54
52	RW	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
52	YW	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
53	RX	90/96 (94%)	86 (96%)	4 (4%)	0	100	100
53	YX	90/96 (94%)	86 (96%)	3 (3%)	1 (1%)	14	52
54	RY	105/110 (96%)	94 (90%)	11 (10%)	0	100	100
54	YY	105/110 (96%)	101 (96%)	3 (3%)	1 (1%)	15	54
55	RZ	181/206 (88%)	166 (92%)	13 (7%)	2 (1%)	14	52
55	YZ	181/206 (88%)	168 (93%)	13 (7%)	0	100	100
All	All	11789/12464 (95%)	10734 (91%)	950 (8%)	105 (1%)	17	56

All (105) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	208	ILE
14	QN	17	LYS
21	QU	3	LYS
24	QY	82	TYR
27	R2	47	ASN
29	R4	40	HIS
33	R8	29	LYS
33	R8	30	ARG
41	RH	152	ARG

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Mol	Chain	Res	Type
42	RI	132	PRO
42	RI	143	SER
42	RI	144	VAL
43	RN	22	THR
45	RP	27	HIS
45	RP	57	THR
45	RP	108	LYS
46	RQ	85	LYS
55	RZ	53	ILE
2	XB	236	TYR
12	XL	105	TYR
14	XN	17	LYS
20	XT	73	HIS
21	XU	3	LYS
24	XY	82	TYR
33	Y8	30	ARG
42	YI	145	VAL
43	YN	22	THR
47	YR	4	LEU
51	YV	49	THR
4	QD	155	LEU
12	QL	105	TYR
12	QL	128	ALA
29	R4	3	GLU
29	R4	11	PRO
29	R4	41	PRO
37	RD	238	GLY
37	RD	243	GLY
38	RE	145	LYS
41	RH	10	PRO
41	RH	86	GLU
50	RU	92	ARG
4	XD	155	LEU
24	XZ	50	HIS
26	Y1	83	GLU
27	Y2	71	ASN
33	Y8	29	LYS
39	YF	129	PHE
40	YG	137	GLU
42	YI	15	VAL
45	YP	36	LYS
50	YU	92	ARG

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Mol	Chain	Res	Type
2	QB	9	GLU
4	QD	156	GLU
13	QM	12	ASN
19	QS	28	LYS
24	QY	50	HIS
37	RD	36	PRO
38	RE	55	ASN
38	RE	74	PRO
40	RG	117	PHE
46	RQ	25	ASP
47	RR	4	LEU
55	RZ	52	SER
10	XJ	56	HIS
29	Y4	47	GLN
53	YX	68	ARG
25	R0	47	PRO
38	RE	83	ASP
40	RG	81	LYS
40	RG	116	ASP
41	RH	15	VAL
41	RH	87	LEU
42	RI	134	PRO
4	XD	156	GLU
24	XY	50	HIS
24	XY	83	HIS
39	YF	67	GLN
40	YG	81	LYS
7	QG	8	GLU
13	QM	67	GLU
42	RI	10	GLU
42	RI	133	HIS
43	RN	36	GLY
45	RP	36	LYS
46	RQ	105	GLU
27	Y2	70	GLN
38	YE	30	PRO
43	YN	23	LEU
45	YP	29	LYS
2	QB	231	GLU
2	QB	233	SER
13	QM	9	ILE
41	RH	154	PRO

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Mol	Chain	Res	Type
46	RQ	67	ARG
48	RS	57	LYS
49	RT	109	GLU
2	XB	233	SER
3	XC	4	LYS
38	YE	145	LYS
44	YO	97	ARG
46	RQ	66	ILE
54	YY	10	GLY
20	XT	98	PRO
37	RD	123	ALA
20	XT	96	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	203/220 (92%)	196 (97%)	7 (3%)	37	68
2	XB	204/220 (93%)	201 (98%)	3 (2%)	65	84
3	QC	159/188 (85%)	154 (97%)	5 (3%)	40	70
3	XC	159/188 (85%)	155 (98%)	4 (2%)	47	75
4	QD	180/181 (99%)	175 (97%)	5 (3%)	43	72
4	XD	180/181 (99%)	178 (99%)	2 (1%)	73	88
5	QE	116/123 (94%)	115 (99%)	1 (1%)	78	90
5	XE	116/123 (94%)	112 (97%)	4 (3%)	37	68
6	QF	90/90 (100%)	89 (99%)	1 (1%)	73	88
6	XF	90/90 (100%)	90 (100%)	0	100	100
7	QG	126/127 (99%)	121 (96%)	5 (4%)	31	64
7	XG	126/127 (99%)	121 (96%)	5 (4%)	31	64
8	QH	118/119 (99%)	115 (98%)	3 (2%)	47	75
8	XH	118/119 (99%)	117 (99%)	1 (1%)	81	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	QI	98/99 (99%)	92 (94%)	6 (6%)	18	51
9	XI	97/99 (98%)	96 (99%)	1 (1%)	76	88
10	QJ	89/92 (97%)	84 (94%)	5 (6%)	21	54
10	XJ	86/92 (94%)	85 (99%)	1 (1%)	71	87
11	QK	90/99 (91%)	88 (98%)	2 (2%)	52	78
11	XK	88/99 (89%)	87 (99%)	1 (1%)	73	88
12	QL	104/109 (95%)	102 (98%)	2 (2%)	57	80
12	XL	103/109 (94%)	101 (98%)	2 (2%)	57	80
13	QM	96/101 (95%)	95 (99%)	1 (1%)	76	88
13	XM	95/101 (94%)	91 (96%)	4 (4%)	30	63
14	QN	49/50 (98%)	47 (96%)	2 (4%)	30	63
14	XN	49/50 (98%)	49 (100%)	0	100	100
15	QO	79/80 (99%)	79 (100%)	0	100	100
15	XO	79/80 (99%)	78 (99%)	1 (1%)	69	86
16	QP	72/74 (97%)	72 (100%)	0	100	100
16	XP	72/74 (97%)	70 (97%)	2 (3%)	43	72
17	QQ	95/97 (98%)	94 (99%)	1 (1%)	73	88
17	XQ	95/97 (98%)	93 (98%)	2 (2%)	53	79
18	QR	61/77 (79%)	58 (95%)	3 (5%)	25	59
18	XR	61/77 (79%)	60 (98%)	1 (2%)	62	83
19	QS	72/80 (90%)	69 (96%)	3 (4%)	30	63
19	XS	69/80 (86%)	69 (100%)	0	100	100
20	QT	76/82 (93%)	76 (100%)	0	100	100
20	XT	76/82 (93%)	76 (100%)	0	100	100
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	20 (100%)	0	100	100
24	QY	78/78 (100%)	74 (95%)	4 (5%)	24	57
24	QZ	78/78 (100%)	73 (94%)	5 (6%)	17	50
24	XY	78/78 (100%)	78 (100%)	0	100	100
24	XZ	78/78 (100%)	74 (95%)	4 (5%)	24	57
25	R0	65/67 (97%)	64 (98%)	1 (2%)	65	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	Y0	65/67 (97%)	62 (95%)	3 (5%)	27	61
26	R1	79/83 (95%)	78 (99%)	1 (1%)	69	86
26	Y1	82/83 (99%)	82 (100%)	0	100	100
27	R2	64/67 (96%)	63 (98%)	1 (2%)	62	83
27	Y2	64/67 (96%)	63 (98%)	1 (2%)	62	83
28	R3	51/52 (98%)	50 (98%)	1 (2%)	55	79
28	Y3	51/52 (98%)	50 (98%)	1 (2%)	55	79
29	R4	62/63 (98%)	54 (87%)	8 (13%)	4	22
29	Y4	62/63 (98%)	60 (97%)	2 (3%)	39	69
30	R5	51/52 (98%)	51 (100%)	0	100	100
30	Y5	51/52 (98%)	50 (98%)	1 (2%)	55	79
31	R6	51/52 (98%)	49 (96%)	2 (4%)	32	64
31	Y6	51/52 (98%)	49 (96%)	2 (4%)	32	64
32	R7	40/42 (95%)	40 (100%)	0	100	100
32	Y7	41/42 (98%)	41 (100%)	0	100	100
33	R8	54/55 (98%)	50 (93%)	4 (7%)	13	44
33	Y8	54/55 (98%)	52 (96%)	2 (4%)	34	65
34	R9	34/34 (100%)	33 (97%)	1 (3%)	42	71
34	Y9	34/34 (100%)	34 (100%)	0	100	100
37	RD	214/218 (98%)	209 (98%)	5 (2%)	50	77
37	YD	216/218 (99%)	214 (99%)	2 (1%)	78	90
38	RE	165/166 (99%)	160 (97%)	5 (3%)	41	71
38	YE	164/166 (99%)	163 (99%)	1 (1%)	86	94
39	RF	161/166 (97%)	160 (99%)	1 (1%)	86	94
39	YF	161/166 (97%)	160 (99%)	1 (1%)	86	94
40	RG	155/156 (99%)	149 (96%)	6 (4%)	32	64
40	YG	155/156 (99%)	150 (97%)	5 (3%)	39	69
41	RH	145/148 (98%)	140 (97%)	5 (3%)	37	68
41	YH	144/148 (97%)	142 (99%)	2 (1%)	67	85
42	RI	122/124 (98%)	117 (96%)	5 (4%)	30	63
42	YI	122/124 (98%)	119 (98%)	3 (2%)	47	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	RN	117/119 (98%)	114 (97%)	3 (3%)	46	74
43	YN	117/119 (98%)	117 (100%)	0	100	100
44	RO	100/100 (100%)	99 (99%)	1 (1%)	76	88
44	YO	100/100 (100%)	98 (98%)	2 (2%)	55	79
45	RP	116/116 (100%)	114 (98%)	2 (2%)	60	82
45	YP	115/116 (99%)	114 (99%)	1 (1%)	78	90
46	RQ	111/111 (100%)	107 (96%)	4 (4%)	35	66
46	YQ	111/111 (100%)	111 (100%)	0	100	100
47	RR	100/101 (99%)	100 (100%)	0	100	100
47	YR	100/101 (99%)	98 (98%)	2 (2%)	55	79
48	RS	87/88 (99%)	83 (95%)	4 (5%)	27	61
48	YS	87/88 (99%)	84 (97%)	3 (3%)	37	68
49	RT	120/127 (94%)	114 (95%)	6 (5%)	24	58
49	YT	120/127 (94%)	117 (98%)	3 (2%)	47	75
50	RU	93/94 (99%)	92 (99%)	1 (1%)	73	88
50	YU	93/94 (99%)	92 (99%)	1 (1%)	73	88
51	RV	82/82 (100%)	76 (93%)	6 (7%)	14	45
51	YV	82/82 (100%)	80 (98%)	2 (2%)	49	76
52	RW	92/92 (100%)	90 (98%)	2 (2%)	52	78
52	YW	92/92 (100%)	90 (98%)	2 (2%)	52	78
53	RX	74/78 (95%)	74 (100%)	0	100	100
53	YX	74/78 (95%)	72 (97%)	2 (3%)	44	73
54	RY	88/91 (97%)	88 (100%)	0	100	100
54	YY	88/91 (97%)	87 (99%)	1 (1%)	73	88
55	RZ	162/179 (90%)	160 (99%)	2 (1%)	71	87
55	YZ	162/179 (90%)	159 (98%)	3 (2%)	57	80
All	All	10001/10378 (96%)	9777 (98%)	224 (2%)	52	78

All (224) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	QB	11	LEU
2	QB	17	PHE

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Mol	Chain	Res	Type
2	QB	21	ARG
2	QB	114	ARG
2	QB	132	LYS
2	QB	209	ARG
2	QB	226	ARG
3	QC	11	ARG
3	QC	16	ARG
3	QC	105	GLU
3	QC	132	ARG
3	QC	193	TYR
4	QD	17	VAL
4	QD	21	LEU
4	QD	31	CYS
4	QD	33	MET
4	QD	107	ARG
5	QE	47	LYS
6	QF	80	ARG
7	QG	10	ARG
7	QG	53	LYS
7	QG	79	ARG
7	QG	114	ARG
7	QG	155	ARG
8	QH	29	SER
8	QH	50	ARG
8	QH	104	ARG
9	QI	4	TYR
9	QI	16	ARG
9	QI	18	PHE
9	QI	20	ARG
9	QI	26	VAL
9	QI	70	LYS
10	QJ	25	GLU
10	QJ	43	ARG
10	QJ	55	LYS
10	QJ	60	ARG
10	QJ	79	ARG
11	QK	12	ARG
11	QK	92	GLU
12	QL	59	ARG
12	QL	117	ARG
13	QM	11	ARG
14	QN	12	ARG

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Mol	Chain	Res	Type
14	QN	50	LYS
17	QQ	101	ARG
18	QR	34	TYR
18	QR	54	ARG
18	QR	83	GLU
19	QS	3	ARG
19	QS	12	ASP
19	QS	28	LYS
24	QY	6	SER
24	QY	11	ASP
24	QY	18	GLU
24	QY	25	LYS
24	QZ	7	GLU
24	QZ	21	LYS
24	QZ	22	ARG
24	QZ	36	ARG
24	QZ	63	GLU
25	R0	14	ARG
26	R1	57	GLU
27	R2	23	LYS
28	R3	30	ARG
29	R4	1	MET
29	R4	11	PRO
29	R4	13	ARG
29	R4	39	CYS
29	R4	42	PHE
29	R4	46	GLN
29	R4	48	ARG
29	R4	63	TYR
31	R6	10	LEU
31	R6	25	LYS
33	R8	35	GLN
33	R8	46	ARG
33	R8	52	LYS
33	R8	65	GLU
34	R9	9	ARG
37	RD	7	LYS
37	RD	24	ILE
37	RD	25	THR
37	RD	43	ARG
37	RD	273	ARG
38	RE	1	MET

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Mol	Chain	Res	Type
38	RE	59	VAL
38	RE	64	LYS
38	RE	79	ARG
38	RE	152	LYS
39	RF	99	TYR
40	RG	33	ARG
40	RG	55	LYS
40	RG	83	ARG
40	RG	115	ARG
40	RG	118	ARG
40	RG	146	TYR
41	RH	51	ARG
41	RH	69	ARG
41	RH	97	ARG
41	RH	152	ARG
41	RH	154	PRO
42	RI	85	GLU
42	RI	86	THR
42	RI	130	TYR
42	RI	136	VAL
42	RI	138	ILE
43	RN	12	ARG
43	RN	61	ARG
43	RN	115	ARG
44	RO	31	LYS
45	RP	29	LYS
45	RP	76	LYS
46	RQ	5	ARG
46	RQ	87	LYS
46	RQ	91	GLU
46	RQ	93	TYR
48	RS	20	ARG
48	RS	23	ARG
48	RS	76	LYS
48	RS	112	PHE
49	RT	95	ARG
49	RT	96	ARG
49	RT	101	PHE
49	RT	108	ARG
49	RT	109	GLU
49	RT	128	GLU
50	RU	90	VAL

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Mol	Chain	Res	Type
51	RV	19	LYS
51	RV	21	ARG
51	RV	39	LEU
51	RV	72	VAL
51	RV	79	VAL
51	RV	95	LEU
52	RW	18	ARG
52	RW	113	LYS
55	RZ	80	ARG
55	RZ	135	GLU
2	XB	17	PHE
2	XB	122	PHE
2	XB	236	TYR
3	XC	72	LYS
3	XC	85	ARG
3	XC	111	LEU
3	XC	132	ARG
4	XD	76	ARG
4	XD	118	ARG
5	XE	24	ARG
5	XE	43	LEU
5	XE	63	ARG
5	XE	155	GLU
7	XG	48	LYS
7	XG	57	GLU
7	XG	78	ARG
7	XG	94	ARG
7	XG	111	ARG
8	XH	60	ARG
9	XI	114	TYR
10	XJ	29	ARG
11	XK	96	ARG
12	XL	17	LYS
12	XL	98	TYR
13	XM	13	LYS
13	XM	36	LYS
13	XM	58	GLU
13	XM	102	ARG
15	XO	79	ARG
16	XP	26	ARG
16	XP	32	TYR
17	XQ	52	LYS

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Mol	Chain	Res	Type
17	XQ	92	ARG
18	XR	42	ARG
24	XZ	8	GLU
24	XZ	22	ARG
24	XZ	40	GLU
24	XZ	82	TYR
25	Y0	14	ARG
25	Y0	41	ARG
25	Y0	82	ARG
27	Y2	7	ARG
28	Y3	30	ARG
29	Y4	48	ARG
29	Y4	67	TYR
30	Y5	37	LYS
31	Y6	4	GLU
31	Y6	12	GLU
33	Y8	48	PHE
33	Y8	50	LEU
37	YD	63	ARG
37	YD	88	ARG
38	YE	73	GLU
39	YF	127	GLU
40	YG	18	GLU
40	YG	33	ARG
40	YG	51	ARG
40	YG	55	LYS
40	YG	72	ARG
41	YH	3	ARG
41	YH	13	LYS
42	YI	10	GLU
42	YI	11	ASN
42	YI	12	LEU
44	YO	64	ARG
44	YO	108	GLU
45	YP	108	LYS
47	YR	57	ARG
47	YR	88	ARG
48	YS	23	ARG
48	YS	106	ARG
48	YS	111	GLU
49	YT	96	ARG
49	YT	111	ARG

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Mol	Chain	Res	Type
49	YT	133	GLU
50	YU	44	ASN
51	YV	5	VAL
51	YV	18	LEU
52	YW	41	LYS
52	YW	60	ASN
53	YX	57	LEU
53	YX	68	ARG
54	YY	87	LYS
55	YZ	29	TYR
55	YZ	156	LYS
55	YZ	168	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	QB	16	HIS
9	QI	3	GLN
37	RD	46	GLN
55	RZ	151	HIS
13	XM	101	GLN
40	YG	132	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1508/1521 (99%)	293 (19%)	33 (2%)
1	XA	1505/1521 (98%)	301 (20%)	40 (2%)
22	QV	77/77 (100%)	8 (10%)	1 (1%)
22	XV	77/77 (100%)	9 (11%)	1 (1%)
23	QX	16/20 (80%)	7 (43%)	2 (12%)
23	XX	16/20 (80%)	8 (50%)	0
35	RA	2888/2915 (99%)	623 (21%)	37 (1%)
35	YA	2875/2915 (98%)	578 (20%)	28 (0%)
36	RB	119/124 (95%)	24 (20%)	1 (0%)
36	YB	119/124 (95%)	17 (14%)	1 (0%)
56	ZA	1/3 (33%)	0	0
56	ZB	1/3 (33%)	0	0
All	All	9202/9320 (98%)	1868 (20%)	144 (1%)

All (1868) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	4	U
1	QA	5	U
1	QA	6	G
1	QA	22	G
1	QA	32	A
1	QA	39	G
1	QA	47	C
1	QA	48	C
1	QA	50	A
1	QA	51	A
1	QA	61	G
1	QA	66	G
1	QA	79	G
1	QA	80	G
1	QA	89	U
1	QA	90	C
1	QA	92	G
1	QA	93	U
1	QA	101	A
1	QA	116	A
1	QA	120	A
1	QA	121	C
1	QA	131	C
1	QA	182	U
1	QA	185	A
1	QA	188	U
1	QA	189	U
1	QA	190	G
1	QA	191(A)	G
1	QA	191(D)	U
1	QA	191(E)	G
1	QA	195	A
1	QA	197	A
1	QA	198	G
1	QA	208	U
1	QA	209	U
1	QA	210	U
1	QA	220	G
1	QA	247	G
1	QA	251	G
1	QA	266	G
1	QA	267	C

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Mol	Chain	Res	Type
1	QA	270	A
1	QA	275	G
1	QA	281	G
1	QA	289	G
1	QA	321	A
1	QA	328	C
1	QA	332	G
1	QA	345	C
1	QA	346	G
1	QA	347	G
1	QA	350	G
1	QA	351	G
1	QA	352	C
1	QA	353	A
1	QA	354	G
1	QA	356	A
1	QA	367	U
1	QA	372	C
1	QA	373	A
1	QA	384	G
1	QA	397	A
1	QA	398	C
1	QA	406	G
1	QA	412	A
1	QA	414	A
1	QA	422	C
1	QA	423	G
1	QA	424	G
1	QA	429	U
1	QA	439	A
1	QA	452	A
1	QA	465	A
1	QA	466	C
1	QA	467	G
1	QA	478	A
1	QA	482	A
1	QA	484	G
1	QA	485	G
1	QA	494	U
1	QA	497	U
1	QA	505	G
1	QA	511	C

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Mol	Chain	Res	Type
1	QA	518	C
1	QA	519	C
1	QA	521	G
1	QA	527	G
1	QA	530	G
1	QA	531	U
1	QA	532	A
1	QA	533	A
1	QA	545	C
1	QA	547	A
1	QA	548	G
1	QA	559	A
1	QA	564	C
1	QA	572	A
1	QA	573	A
1	QA	576	G
1	QA	577	G
1	QA	579	G
1	QA	596	C
1	QA	607	A
1	QA	618	C
1	QA	630	G
1	QA	642	A
1	QA	652	U
1	QA	653	A
1	QA	665	A
1	QA	686	U
1	QA	688	G
1	QA	702	A
1	QA	703	G
1	QA	704	A
1	QA	721	G
1	QA	722	A
1	QA	723	U
1	QA	724	G
1	QA	731	G
1	QA	749	C
1	QA	755	G
1	QA	760	G
1	QA	774	G
1	QA	777	A
1	QA	786	G

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Mol	Chain	Res	Type
1	QA	793	U
1	QA	794	A
1	QA	813	U
1	QA	816	A
1	QA	817	C
1	QA	818	G
1	QA	819	A
1	QA	821	G
1	QA	828	A
1	QA	841	U
1	QA	842	C
1	QA	843	U
1	QA	848	C
1	QA	859	A
1	QA	872	A
1	QA	884	U
1	QA	914	A
1	QA	916	G
1	QA	926	G
1	QA	927	G
1	QA	934	C
1	QA	935	A
1	QA	942	G
1	QA	960	U
1	QA	961	U
1	QA	966	G
1	QA	968	A
1	QA	969	A
1	QA	972	C
1	QA	974	A
1	QA	975	A
1	QA	976	G
1	QA	977	A
1	QA	980	C
1	QA	982	U
1	QA	991	U
1	QA	992	U
1	QA	993	G
1	QA	994	A
1	QA	999	U
1	QA	1000	A
1	QA	1001	G

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Mol	Chain	Res	Type
1	QA	1003	G
1	QA	1004	A
1	QA	1005	A
1	QA	1006	C
1	QA	1007	C
1	QA	1008	C
1	QA	1009	G
1	QA	1024	G
1	QA	1025	U
1	QA	1026	G
1	QA	1029	G
1	QA	1030	C
1	QA	1031	G
1	QA	1032	A
1	QA	1032(A)	G
1	QA	1033	G
1	QA	1034	G
1	QA	1036	G
1	QA	1039	C
1	QA	1046	A
1	QA	1053	G
1	QA	1054	C
1	QA	1055	A
1	QA	1064	G
1	QA	1065	U
1	QA	1066	C
1	QA	1068	G
1	QA	1070	U
1	QA	1081	G
1	QA	1086	U
1	QA	1094	G
1	QA	1095	U
1	QA	1101	A
1	QA	1108	G
1	QA	1117	G
1	QA	1118	C
1	QA	1124	G
1	QA	1125	U
1	QA	1127	G
1	QA	1129	C
1	QA	1130	A
1	QA	1131	G

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Mol	Chain	Res	Type
1	QA	1136	U
1	QA	1137	C
1	QA	1138	G
1	QA	1139	G
1	QA	1140	C
1	QA	1146	A
1	QA	1157	A
1	QA	1158	C
1	QA	1159	U
1	QA	1160	G
1	QA	1171	G
1	QA	1177	G
1	QA	1178	G
1	QA	1181	G
1	QA	1182	G
1	QA	1183	A
1	QA	1187	G
1	QA	1196	U
1	QA	1212	U
1	QA	1213	A
1	QA	1227	A
1	QA	1233	G
1	QA	1238	A
1	QA	1240	U
1	QA	1241	G
1	QA	1257	U
1	QA	1258	G
1	QA	1260	C
1	QA	1268	A
1	QA	1270	C
1	QA	1273	G
1	QA	1278	U
1	QA	1280	A
1	QA	1281	U
1	QA	1285	A
1	QA	1286	A
1	QA	1287	A
1	QA	1288	A
1	QA	1300	G
1	QA	1303	C
1	QA	1305	G
1	QA	1318	A

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Mol	Chain	Res	Type
1	QA	1319	A
1	QA	1320	C
1	QA	1323	G
1	QA	1331	G
1	QA	1335	C
1	QA	1346	A
1	QA	1347	G
1	QA	1348	U
1	QA	1353	G
1	QA	1368	G
1	QA	1370	G
1	QA	1398	A
1	QA	1406	U
1	QA	1419	G
1	QA	1442	G
1	QA	1446	A
1	QA	1450	U
1	QA	1451	A
1	QA	1452	C
1	QA	1453	G
1	QA	1454	G
1	QA	1492	A
1	QA	1493	A
1	QA	1497	G
1	QA	1499	A
1	QA	1504	G
1	QA	1506	U
1	QA	1517	G
1	QA	1519	A
1	QA	1520	G
1	QA	1529	G
1	QA	1530	G
1	QA	1532	U
1	QA	1533	C
1	QA	1534	A
1	QA	1536	C
1	QA	1537	U
1	QA	1538	C
1	QA	1539	C
1	QA	1540	U
1	QA	1541	U
22	QV	2	G

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Mol	Chain	Res	Type
22	QV	20	U
22	QV	21	A
22	QV	22	G
22	QV	46	G
22	QV	47	U
22	QV	49	G
22	QV	76	A
23	QX	8	A
23	QX	10	G
23	QX	11	U
23	QX	12	A
23	QX	13	A
23	QX	14	A
23	QX	19	U
35	RA	9	U
35	RA	15	G
35	RA	27	G
35	RA	34	C
35	RA	35	G
35	RA	46	C
35	RA	60	G
35	RA	61	G
35	RA	64	A
35	RA	71	A
35	RA	74	A
35	RA	75	G
35	RA	83	G
35	RA	91	A
35	RA	95	G
35	RA	99	U
35	RA	101	G
35	RA	102	G
35	RA	118	A
35	RA	119	A
35	RA	120	U
35	RA	125	G
35	RA	129	C
35	RA	139	G
35	RA	140	A
35	RA	144	C
35	RA	155	C
35	RA	172	C

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Mol	Chain	Res	Type
35	RA	173	G
35	RA	174	C
35	RA	175	G
35	RA	181	A
35	RA	182	A
35	RA	196	A
35	RA	199	A
35	RA	204	A
35	RA	205	G
35	RA	215	G
35	RA	216	A
35	RA	221	A
35	RA	222	A
35	RA	228	A
35	RA	229	A
35	RA	233	A
35	RA	245	G
35	RA	248	G
35	RA	252	G
35	RA	265	A
35	RA	266	G
35	RA	270(B)	A
35	RA	270(J)	G
35	RA	270(K)	C
35	RA	270(L)	U
35	RA	270(M)	U
35	RA	270(N)	G
35	RA	270(O)	U
35	RA	270(P)	C
35	RA	270(Q)	C
35	RA	270(Z)	U
35	RA	271(C)	U
35	RA	271	G
35	RA	273(D)	C
35	RA	274	G
35	RA	275	G
35	RA	278	A
35	RA	283	A
35	RA	289	A
35	RA	311	A
35	RA	316	C
35	RA	324	A

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Mol	Chain	Res	Type
35	RA	329	G
35	RA	330	A
35	RA	332	A
35	RA	345	A
35	RA	353	G
35	RA	355	G
35	RA	358	U
35	RA	362	U
35	RA	363	G
35	RA	363(D)	G
35	RA	371	A
35	RA	372	G
35	RA	373	U
35	RA	386	G
35	RA	388	G
35	RA	396	G
35	RA	405	U
35	RA	406	G
35	RA	411	G
35	RA	412	A
35	RA	428	A
35	RA	443	A
35	RA	444	C
35	RA	448	U
35	RA	451	C
35	RA	456	C
35	RA	457	A
35	RA	467	G
35	RA	470	A
35	RA	481	G
35	RA	494	G
35	RA	505	A
35	RA	508	G
35	RA	509	C
35	RA	512	G
35	RA	513	A
35	RA	529	A
35	RA	531	C
35	RA	532	A
35	RA	533	G
35	RA	537	C
35	RA	549	G

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Mol	Chain	Res	Type
35	RA	563	G
35	RA	573	G
35	RA	575	A
35	RA	587	C
35	RA	588	U
35	RA	603	A
35	RA	607	U
35	RA	613	U
35	RA	614	U
35	RA	615	G
35	RA	617	G
35	RA	622	G
35	RA	627	A
35	RA	634	C
35	RA	637	A
35	RA	645	C
35	RA	646	A
35	RA	651	G
35	RA	654	A
35	RA	654(A)	G
35	RA	654(B)	C
35	RA	654(G)	C
35	RA	654(Q)	C
35	RA	654(R)	C
35	RA	654(S)	G
35	RA	654(T)	C
35	RA	686	G
35	RA	708	C
35	RA	717	G
35	RA	722	A
35	RA	730	C
35	RA	753	C
35	RA	765	G
35	RA	775	G
35	RA	776	G
35	RA	782	A
35	RA	784	A
35	RA	785	G
35	RA	788	A
35	RA	789	A
35	RA	792	G
35	RA	793	A

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Mol	Chain	Res	Type
35	RA	805	G
35	RA	812	C
35	RA	819	A
35	RA	827	U
35	RA	828	U
35	RA	830	G
35	RA	831	G
35	RA	845	G
35	RA	846	C
35	RA	854	G
35	RA	856	C
35	RA	857	C
35	RA	859	G
35	RA	866	A
35	RA	872	A
35	RA	878	A
35	RA	882	G
35	RA	883	G
35	RA	884	C
35	RA	886	C
35	RA	888	C
35	RA	889	C
35	RA	890	A
35	RA	894	C
35	RA	895	U
35	RA	896	A
35	RA	897	C
35	RA	899	A
35	RA	900	A
35	RA	910	A
35	RA	915	C
35	RA	917	A
35	RA	919	G
35	RA	928	G
35	RA	932	G
35	RA	938	G
35	RA	941	A
35	RA	945	A
35	RA	946	G
35	RA	953	A
35	RA	957	A
35	RA	959	A

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Mol	Chain	Res	Type
35	RA	961	C
35	RA	968	G
35	RA	973	A
35	RA	974	G
35	RA	983	A
35	RA	990	A
35	RA	991	C
35	RA	996	A
35	RA	1012	U
35	RA	1013	C
35	RA	1015	G
35	RA	1017	G
35	RA	1022	G
35	RA	1023	U
35	RA	1025	G
35	RA	1026	U
35	RA	1027	A
35	RA	1033	U
35	RA	1034	G
35	RA	1044	G
35	RA	1046	A
35	RA	1047	G
35	RA	1049	C
35	RA	1053	C
35	RA	1061	U
35	RA	1065	U
35	RA	1067	A
35	RA	1070	A
35	RA	1071	G
35	RA	1073	A
35	RA	1075	C
35	RA	1083	U
35	RA	1086	A
35	RA	1087	G
35	RA	1088	A
35	RA	1089	G
35	RA	1095	A
35	RA	1096	A
35	RA	1111	A
35	RA	1130	U
35	RA	1131	G
35	RA	1135	C

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Mol	Chain	Res	Type
35	RA	1136	G
35	RA	1139	G
35	RA	1141	U
35	RA	1142(A)	A
35	RA	1143	A
35	RA	1148	A
35	RA	1155	A
35	RA	1156	A
35	RA	1173	G
35	RA	1174	A
35	RA	1175	U
35	RA	1176	G
35	RA	1177	A
35	RA	1178	C
35	RA	1180	C
35	RA	1195	G
35	RA	1203	G
35	RA	1204	A
35	RA	1205	U
35	RA	1210	A
35	RA	1212	G
35	RA	1220	A
35	RA	1221	C
35	RA	1224	G
35	RA	1236	G
35	RA	1247	A
35	RA	1250	G
35	RA	1252	G
35	RA	1253	A
35	RA	1255	U
35	RA	1256	G
35	RA	1265	A
35	RA	1272	A
35	RA	1275	A
35	RA	1281	G
35	RA	1286	A
35	RA	1300	U
35	RA	1301	A
35	RA	1308	A
35	RA	1311	G
35	RA	1314	C
35	RA	1319	G

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Mol	Chain	Res	Type
35	RA	1329	U
35	RA	1341	U
35	RA	1352	U
35	RA	1359	A
35	RA	1365	A
35	RA	1368	G
35	RA	1378	A
35	RA	1379	A
35	RA	1380	G
35	RA	1384	A
35	RA	1385	G
35	RA	1391	U
35	RA	1395	A
35	RA	1407	C
35	RA	1408	C
35	RA	1416	G
35	RA	1417	C
35	RA	1419	A
35	RA	1420	U
35	RA	1421	G
35	RA	1428	C
35	RA	1437	C
35	RA	1444(A)	A
35	RA	1449	A
35	RA	1449(A)	G
35	RA	1453	A
35	RA	1455	G
35	RA	1458	C
35	RA	1461	G
35	RA	1466	G
35	RA	1467	C
35	RA	1471	A
35	RA	1475	G
35	RA	1476	C
35	RA	1478	G
35	RA	1482	U
35	RA	1483	G
35	RA	1487	G
35	RA	1488	G
35	RA	1490	A
35	RA	1493	C
35	RA	1497	U

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Mol	Chain	Res	Type
35	RA	1505	C
35	RA	1509	C
35	RA	1510	A
35	RA	1521	G
35	RA	1523	U
35	RA	1526	G
35	RA	1535	U
35	RA	1536	A
35	RA	1537	C
35	RA	1538	G
35	RA	1540	G
35	RA	1543	A
35	RA	1544	C
35	RA	1545	A
35	RA	1547	C
35	RA	1554	A
35	RA	1558	A
35	RA	1559	G
35	RA	1560	G
35	RA	1566	A
35	RA	1569	A
35	RA	1578	U
35	RA	1580	A
35	RA	1585	C
35	RA	1586	A
35	RA	1587	A
35	RA	1592	C
35	RA	1598	C
35	RA	1603	A
35	RA	1608	A
35	RA	1640	C
35	RA	1648	C
35	RA	1651	G
35	RA	1654	A
35	RA	1674	G
35	RA	1688	U
35	RA	1695	G
35	RA	1696	G
35	RA	1698	A
35	RA	1699	G
35	RA	1700	A
35	RA	1725	G

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Mol	Chain	Res	Type
35	RA	1728	G
35	RA	1729	A
35	RA	1730	U
35	RA	1731	G
35	RA	1743	G
35	RA	1756	G
35	RA	1762	A
35	RA	1763	G
35	RA	1764	G
35	RA	1769	G
35	RA	1773	A
35	RA	1776	G
35	RA	1780	A
35	RA	1782	C
35	RA	1791	A
35	RA	1800	C
35	RA	1801	G
35	RA	1802	A
35	RA	1811	G
35	RA	1816	G
35	RA	1820	U
35	RA	1828	G
35	RA	1829	A
35	RA	1847	A
35	RA	1853	A
35	RA	1858	G
35	RA	1864	U
35	RA	1869	G
35	RA	1872	A
35	RA	1878	G
35	RA	1881	C
35	RA	1882	C
35	RA	1888	G
35	RA	1889	A
35	RA	1903	G
35	RA	1906	G
35	RA	1913	A
35	RA	1927	A
35	RA	1929	G
35	RA	1930	G
35	RA	1931	U
35	RA	1936	A

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Mol	Chain	Res	Type
35	RA	1938	A
35	RA	1941	C
35	RA	1948	G
35	RA	1955	U
35	RA	1963	U
35	RA	1965	C
35	RA	1966	A
35	RA	1967	C
35	RA	1970	A
35	RA	1971	A
35	RA	1972	A
35	RA	1980	G
35	RA	1982	C
35	RA	1992	G
35	RA	1993	U
35	RA	1996	C
35	RA	2004	G
35	RA	2020	A
35	RA	2021	C
35	RA	2022	U
35	RA	2023	G
35	RA	2026	C
35	RA	2031	A
35	RA	2032	G
35	RA	2033	A
35	RA	2034	U
35	RA	2043	C
35	RA	2052	G
35	RA	2055	C
35	RA	2056	G
35	RA	2059	A
35	RA	2060	A
35	RA	2061	G
35	RA	2062	A
35	RA	2063	C
35	RA	2069	G
35	RA	2092	U
35	RA	2093	G
35	RA	2111	C
35	RA	2112	G
35	RA	2113	U
35	RA	2116	G

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Mol	Chain	Res	Type
35	RA	2117	A
35	RA	2119	A
35	RA	2127	G
35	RA	2128	C
35	RA	2130	U
35	RA	2131	G
35	RA	2132	U
35	RA	2134	A
35	RA	2136	C
35	RA	2139	C
35	RA	2145	C
35	RA	2147	G
35	RA	2148	G
35	RA	2153	G
35	RA	2161	C
35	RA	2165	G
35	RA	2167	U
35	RA	2168	G
35	RA	2169	A
35	RA	2170	A
35	RA	2171	A
35	RA	2173	A
35	RA	2178	C
35	RA	2189	U
35	RA	2190	G
35	RA	2192	G
35	RA	2198	A
35	RA	2210	G
35	RA	2212	A
35	RA	2213	U
35	RA	2215	G
35	RA	2225	A
35	RA	2226	C
35	RA	2238	G
35	RA	2239	G
35	RA	2243	U
35	RA	2246	G
35	RA	2275	C
35	RA	2278	A
35	RA	2279	G
35	RA	2280	G
35	RA	2282	G

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Mol	Chain	Res	Type
35	RA	2283	C
35	RA	2302	G
35	RA	2305	A
35	RA	2306	C
35	RA	2307	G
35	RA	2308	G
35	RA	2309	A
35	RA	2311	A
35	RA	2312	U
35	RA	2319	G
35	RA	2320	A
35	RA	2321	G
35	RA	2325	G
35	RA	2334	G
35	RA	2343	C
35	RA	2347	C
35	RA	2350	C
35	RA	2354	G
35	RA	2358	G
35	RA	2372	G
35	RA	2382	G
35	RA	2383	G
35	RA	2385	C
35	RA	2392	A
35	RA	2394	C
35	RA	2402	C
35	RA	2403	C
35	RA	2406	U
35	RA	2410	G
35	RA	2411	A
35	RA	2422	A
35	RA	2423	U
35	RA	2425	A
35	RA	2428	G
35	RA	2429	G
35	RA	2430	A
35	RA	2435	A
35	RA	2439	A
35	RA	2440	C
35	RA	2441	C
35	RA	2445	G
35	RA	2448	A

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Mol	Chain	Res	Type
35	RA	2450	A
35	RA	2469	A
35	RA	2471	C
35	RA	2472	G
35	RA	2475	C
35	RA	2476	A
35	RA	2482	G
35	RA	2491	U
35	RA	2502	G
35	RA	2505	G
35	RA	2518	A
35	RA	2519	U
35	RA	2524	G
35	RA	2527	C
35	RA	2529	G
35	RA	2535	G
35	RA	2540	C
35	RA	2542	A
35	RA	2543	G
35	RA	2554	U
35	RA	2566	A
35	RA	2567	G
35	RA	2569	G
35	RA	2572	A
35	RA	2573	C
35	RA	2578	G
35	RA	2585	U
35	RA	2602	A
35	RA	2609	U
35	RA	2610	C
35	RA	2612	C
35	RA	2615	U
35	RA	2629	A
35	RA	2630	G
35	RA	2646	C
35	RA	2654	A
35	RA	2655	G
35	RA	2665	A
35	RA	2673	G
35	RA	2682	U
35	RA	2689	U
35	RA	2690	C

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Mol	Chain	Res	Type
35	RA	2702	U
35	RA	2703	C
35	RA	2712	U
35	RA	2712(A)	A
35	RA	2713	A
35	RA	2714	G
35	RA	2726	U
35	RA	2733	A
35	RA	2744	G
35	RA	2748	A
35	RA	2752	C
35	RA	2757	A
35	RA	2758	A
35	RA	2761	G
35	RA	2762	G
35	RA	2765	A
35	RA	2766	G
35	RA	2777	G
35	RA	2778	A
35	RA	2779	U
35	RA	2780	G
35	RA	2787	C
35	RA	2790	A
35	RA	2797	U
35	RA	2799	A
35	RA	2807	G
35	RA	2808	U
35	RA	2818	G
35	RA	2820	A
35	RA	2821	A
35	RA	2823	A
35	RA	2827	C
35	RA	2830	G
35	RA	2833	G
35	RA	2834	G
35	RA	2835	A
35	RA	2846	G
35	RA	2850	A
35	RA	2860	A
35	RA	2867	G
35	RA	2868	A
35	RA	2872	G

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Mol	Chain	Res	Type
35	RA	2873	A
35	RA	2876	G
35	RA	2877	G
35	RA	2879	C
35	RA	2880	C
35	RA	2892	A
35	RA	2893	G
36	RB	2	C
36	RB	8	U
36	RB	13	A
36	RB	15	A
36	RB	19	G
36	RB	25	A
36	RB	27	C
36	RB	40	U
36	RB	41	U
36	RB	42	C
36	RB	45	A
36	RB	47	C
36	RB	53	A
36	RB	67	G
36	RB	73	A
36	RB	81	G
36	RB	88	C
36	RB	89	G
36	RB	92	G
36	RB	105	G
36	RB	108	C
36	RB	109	G
36	RB	117	G
36	RB	119	A
1	XA	5	U
1	XA	6	G
1	XA	9	G
1	XA	32	A
1	XA	39	G
1	XA	47	C
1	XA	48	C
1	XA	51	A
1	XA	61	G
1	XA	64	G
1	XA	65	U

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Mol	Chain	Res	Type
1	XA	66	G
1	XA	75	C
1	XA	76	G
1	XA	79	G
1	XA	91	C
1	XA	93	U
1	XA	101	A
1	XA	108	G
1	XA	116	A
1	XA	120	A
1	XA	121	C
1	XA	129(A)	G
1	XA	144	G
1	XA	146	G
1	XA	163	C
1	XA	169	C
1	XA	182	U
1	XA	184	G
1	XA	185	A
1	XA	186(F)	C
1	XA	188	U
1	XA	189	U
1	XA	191(A)	G
1	XA	191(D)	U
1	XA	195	A
1	XA	197	A
1	XA	198	G
1	XA	208	U
1	XA	209	U
1	XA	210	U
1	XA	216	G
1	XA	244	U
1	XA	247	G
1	XA	251	G
1	XA	266	G
1	XA	267	C
1	XA	270	A
1	XA	275	G
1	XA	279	A
1	XA	280	C
1	XA	281	G
1	XA	289	G

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Mol	Chain	Res	Type
1	XA	298	A
1	XA	316	G
1	XA	321	A
1	XA	328	C
1	XA	329	A
1	XA	332	G
1	XA	345	C
1	XA	346	G
1	XA	347	G
1	XA	351	G
1	XA	352	C
1	XA	353	A
1	XA	354	G
1	XA	367	U
1	XA	368	U
1	XA	372	C
1	XA	373	A
1	XA	384	G
1	XA	388	G
1	XA	390	C
1	XA	397	A
1	XA	398	C
1	XA	406	G
1	XA	411	A
1	XA	412	A
1	XA	422	C
1	XA	423	G
1	XA	424	G
1	XA	429	U
1	XA	442	C
1	XA	467	G
1	XA	477	G
1	XA	482	A
1	XA	484	G
1	XA	485	G
1	XA	492	G
1	XA	496	A
1	XA	497	U
1	XA	505	G
1	XA	511	C
1	XA	518	C
1	XA	521	G

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Mol	Chain	Res	Type
1	XA	527	G
1	XA	530	G
1	XA	531	U
1	XA	532	A
1	XA	533	A
1	XA	547	A
1	XA	548	G
1	XA	559	A
1	XA	564	C
1	XA	572	A
1	XA	573	A
1	XA	576	G
1	XA	577	G
1	XA	579	G
1	XA	595	G
1	XA	596	C
1	XA	630	G
1	XA	653	A
1	XA	665	A
1	XA	666	G
1	XA	688	G
1	XA	701	C
1	XA	702	A
1	XA	703	G
1	XA	704	A
1	XA	721	G
1	XA	724	G
1	XA	731	G
1	XA	749	C
1	XA	755	G
1	XA	760	G
1	XA	792	A
1	XA	793	U
1	XA	794	A
1	XA	812	C
1	XA	813	U
1	XA	816	A
1	XA	817	C
1	XA	819	A
1	XA	821	G
1	XA	828	A
1	XA	836	G

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Mol	Chain	Res	Type
1	XA	841	U
1	XA	842	C
1	XA	843	U
1	XA	848	C
1	XA	859	A
1	XA	870	U
1	XA	914	A
1	XA	922	G
1	XA	926	G
1	XA	927	G
1	XA	934	C
1	XA	935	A
1	XA	960	U
1	XA	961	U
1	XA	968	A
1	XA	969	A
1	XA	972	C
1	XA	974	A
1	XA	976	G
1	XA	977	A
1	XA	980	C
1	XA	989	C
1	XA	991	U
1	XA	992	U
1	XA	993	G
1	XA	994	A
1	XA	999	U
1	XA	1000	A
1	XA	1001	G
1	XA	1002	G
1	XA	1004	A
1	XA	1005	A
1	XA	1006	C
1	XA	1007	C
1	XA	1008	C
1	XA	1009	G
1	XA	1010	G
1	XA	1020	U
1	XA	1024	G
1	XA	1028(A)	C
1	XA	1029	G
1	XA	1031	G

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Mol	Chain	Res	Type
1	XA	1032(A)	G
1	XA	1033	G
1	XA	1034	G
1	XA	1036	G
1	XA	1038	C
1	XA	1039	C
1	XA	1042	G
1	XA	1046	A
1	XA	1053	G
1	XA	1054	C
1	XA	1055	A
1	XA	1064	G
1	XA	1065	U
1	XA	1066	C
1	XA	1068	G
1	XA	1070	U
1	XA	1081	G
1	XA	1094	G
1	XA	1101	A
1	XA	1108	G
1	XA	1117	G
1	XA	1118	C
1	XA	1124	G
1	XA	1125	U
1	XA	1127	G
1	XA	1130	A
1	XA	1131	G
1	XA	1136	U
1	XA	1137	C
1	XA	1138	G
1	XA	1139	G
1	XA	1140	C
1	XA	1146	A
1	XA	1147	C
1	XA	1157	A
1	XA	1158	C
1	XA	1159	U
1	XA	1160	G
1	XA	1171	G
1	XA	1176	A
1	XA	1177	G
1	XA	1178	G

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Mol	Chain	Res	Type
1	XA	1181	G
1	XA	1183	A
1	XA	1184	G
1	XA	1191	A
1	XA	1196	U
1	XA	1212	U
1	XA	1213	A
1	XA	1214	C
1	XA	1225	A
1	XA	1226	C
1	XA	1227	A
1	XA	1238	A
1	XA	1240	U
1	XA	1241	G
1	XA	1255	G
1	XA	1257	U
1	XA	1258	G
1	XA	1260	C
1	XA	1270	C
1	XA	1273	G
1	XA	1278	U
1	XA	1280	A
1	XA	1281	U
1	XA	1285	A
1	XA	1286	A
1	XA	1287	A
1	XA	1288	A
1	XA	1300	G
1	XA	1301	U
1	XA	1303	C
1	XA	1305	G
1	XA	1306	A
1	XA	1319	A
1	XA	1320	C
1	XA	1323	G
1	XA	1331	G
1	XA	1345	U
1	XA	1346	A
1	XA	1347	G
1	XA	1353	G
1	XA	1362(A)	C
1	XA	1363	A

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Mol	Chain	Res	Type
1	XA	1370	G
1	XA	1381	U
1	XA	1394	A
1	XA	1397	C
1	XA	1398	A
1	XA	1400	C
1	XA	1419	G
1	XA	1442	G
1	XA	1446	A
1	XA	1450	U
1	XA	1451	A
1	XA	1452	C
1	XA	1453	G
1	XA	1454	G
1	XA	1487	G
1	XA	1492	A
1	XA	1493	A
1	XA	1497	G
1	XA	1499	A
1	XA	1504	G
1	XA	1505	G
1	XA	1506	U
1	XA	1507	A
1	XA	1517	G
1	XA	1519	A
1	XA	1520	G
1	XA	1529	G
1	XA	1530	G
1	XA	1531	A
1	XA	1532	U
1	XA	1533	C
1	XA	1534	A
1	XA	1535	C
1	XA	1536	C
1	XA	1537	U
1	XA	1538	C
1	XA	1540	U
1	XA	1541	U
22	XV	2	G
22	XV	18	G
22	XV	20	U
22	XV	21	A

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Mol	Chain	Res	Type
22	XV	22	G
22	XV	42	G
22	XV	47	U
22	XV	49	G
22	XV	76	A
23	XX	5	A
23	XX	8	A
23	XX	10	G
23	XX	11	U
23	XX	12	A
23	XX	13	A
23	XX	14	A
23	XX	19	U
35	YA	9	U
35	YA	27	G
35	YA	34	C
35	YA	46	C
35	YA	55	G
35	YA	64	A
35	YA	69	C
35	YA	71	A
35	YA	74	A
35	YA	75	G
35	YA	83	G
35	YA	85	G
35	YA	102	G
35	YA	118	A
35	YA	119	A
35	YA	120	U
35	YA	123	G
35	YA	125	G
35	YA	138	G
35	YA	140	A
35	YA	149	A
35	YA	154	G
35	YA	155	C
35	YA	156	U
35	YA	157	U
35	YA	175	G
35	YA	196	A
35	YA	199	A
35	YA	204	A

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Mol	Chain	Res	Type
35	YA	215	G
35	YA	216	A
35	YA	221	A
35	YA	222	A
35	YA	229	A
35	YA	233	A
35	YA	241	A
35	YA	248	G
35	YA	249	C
35	YA	252	G
35	YA	261	G
35	YA	265	A
35	YA	266	G
35	YA	267	C
35	YA	270(B)	A
35	YA	270(C)	C
35	YA	270(J)	G
35	YA	270(K)	C
35	YA	270(N)	G
35	YA	270(O)	U
35	YA	270(Z)	U
35	YA	271(C)	U
35	YA	271	G
35	YA	274	G
35	YA	275	G
35	YA	278	A
35	YA	279	C
35	YA	283	A
35	YA	287	C
35	YA	289	A
35	YA	290	G
35	YA	311	A
35	YA	317	G
35	YA	324	A
35	YA	329	G
35	YA	330	A
35	YA	332	A
35	YA	352	G
35	YA	356	G
35	YA	363	G
35	YA	363(A)	A
35	YA	363(E)	U

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Mol	Chain	Res	Type
35	YA	363(F)	A
35	YA	372	G
35	YA	373	U
35	YA	380	U
35	YA	386	G
35	YA	395	U
35	YA	405	U
35	YA	406	G
35	YA	411	G
35	YA	412	A
35	YA	428	A
35	YA	444	C
35	YA	448	U
35	YA	454	A
35	YA	456	C
35	YA	457	A
35	YA	470	A
35	YA	481	G
35	YA	494	G
35	YA	501	A
35	YA	504	U
35	YA	505	A
35	YA	508	G
35	YA	509	C
35	YA	512	G
35	YA	525	U
35	YA	526	A
35	YA	529	A
35	YA	531	C
35	YA	532	A
35	YA	533	G
35	YA	562	U
35	YA	563	G
35	YA	571	A
35	YA	573	G
35	YA	575	A
35	YA	588	U
35	YA	603	A
35	YA	604	G
35	YA	607	U
35	YA	613	U
35	YA	614	U

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Mol	Chain	Res	Type
35	YA	615	G
35	YA	617	G
35	YA	622	G
35	YA	624	C
35	YA	627	A
35	YA	637	A
35	YA	645	C
35	YA	646	A
35	YA	666	G
35	YA	668	G
35	YA	669	G
35	YA	670	A
35	YA	686	G
35	YA	717	G
35	YA	722	A
35	YA	730	C
35	YA	753	C
35	YA	776	G
35	YA	782	A
35	YA	784	A
35	YA	785	G
35	YA	788	A
35	YA	789	A
35	YA	792	G
35	YA	793	A
35	YA	805	G
35	YA	812	C
35	YA	819	A
35	YA	827	U
35	YA	832	G
35	YA	856	C
35	YA	857	C
35	YA	859	G
35	YA	869	G
35	YA	882	G
35	YA	883	G
35	YA	884	C
35	YA	885	C
35	YA	886	C
35	YA	888	C
35	YA	889	C
35	YA	890	A

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Mol	Chain	Res	Type
35	YA	894	C
35	YA	896	A
35	YA	897	C
35	YA	906	G
35	YA	910	A
35	YA	915	C
35	YA	917	A
35	YA	919	G
35	YA	928	G
35	YA	932	G
35	YA	938	G
35	YA	941	A
35	YA	945	A
35	YA	946	G
35	YA	953	A
35	YA	961	C
35	YA	973	A
35	YA	974	G
35	YA	975	G
35	YA	980	A
35	YA	983	A
35	YA	990	A
35	YA	991	C
35	YA	996	A
35	YA	999	U
35	YA	1000	A
35	YA	1005	C
35	YA	1012	U
35	YA	1013	C
35	YA	1017	G
35	YA	1020	A
35	YA	1022	G
35	YA	1023	U
35	YA	1024	G
35	YA	1025	G
35	YA	1026	U
35	YA	1027	A
35	YA	1033	U
35	YA	1044	G
35	YA	1046	A
35	YA	1047	G
35	YA	1048	A

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Mol	Chain	Res	Type
35	YA	1060	U
35	YA	1061	U
35	YA	1064	C
35	YA	1066	U
35	YA	1070	A
35	YA	1073	A
35	YA	1083	U
35	YA	1085	A
35	YA	1086	A
35	YA	1087	G
35	YA	1088	A
35	YA	1089	G
35	YA	1093	G
35	YA	1094	U
35	YA	1095	A
35	YA	1096	A
35	YA	1099	G
35	YA	1122	G
35	YA	1126	A
35	YA	1128	A
35	YA	1130	U
35	YA	1135	C
35	YA	1136	G
35	YA	1139	G
35	YA	1141	U
35	YA	1142(A)	A
35	YA	1148	A
35	YA	1156	A
35	YA	1170	G
35	YA	1173	G
35	YA	1174	A
35	YA	1175	U
35	YA	1177	A
35	YA	1178	C
35	YA	1179	C
35	YA	1180	C
35	YA	1195	G
35	YA	1204	A
35	YA	1205	U
35	YA	1210	A
35	YA	1212	G
35	YA	1220	A

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Mol	Chain	Res	Type
35	YA	1236	G
35	YA	1247	A
35	YA	1248	G
35	YA	1252	G
35	YA	1253	A
35	YA	1255	U
35	YA	1256	G
35	YA	1265	A
35	YA	1272	A
35	YA	1281	G
35	YA	1294	U
35	YA	1300	U
35	YA	1301	A
35	YA	1308	A
35	YA	1311	G
35	YA	1314	C
35	YA	1329	U
35	YA	1330	C
35	YA	1352	U
35	YA	1359	A
35	YA	1360	A
35	YA	1368	G
35	YA	1370	C
35	YA	1378	A
35	YA	1379	A
35	YA	1380	G
35	YA	1384	A
35	YA	1385	G
35	YA	1391	U
35	YA	1395	A
35	YA	1406	U
35	YA	1416	G
35	YA	1419	A
35	YA	1420	U
35	YA	1421	G
35	YA	1428	C
35	YA	1437	C
35	YA	1444(A)	A
35	YA	1445	C
35	YA	1449	A
35	YA	1449(A)	G
35	YA	1455	G

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Mol	Chain	Res	Type
35	YA	1459	G
35	YA	1460	A
35	YA	1461	G
35	YA	1467	C
35	YA	1471	A
35	YA	1475	G
35	YA	1480	G
35	YA	1482	U
35	YA	1483	G
35	YA	1488	G
35	YA	1490	A
35	YA	1493	C
35	YA	1509	C
35	YA	1510	A
35	YA	1516	U
35	YA	1522	G
35	YA	1523	U
35	YA	1535	U
35	YA	1536	A
35	YA	1537	C
35	YA	1538	G
35	YA	1540	G
35	YA	1543	A
35	YA	1544	C
35	YA	1545	A
35	YA	1547	C
35	YA	1554	A
35	YA	1558	A
35	YA	1559	G
35	YA	1560	G
35	YA	1566	A
35	YA	1569	A
35	YA	1578	U
35	YA	1580	A
35	YA	1585	C
35	YA	1586	A
35	YA	1598	C
35	YA	1608	A
35	YA	1613	G
35	YA	1618	A
35	YA	1634	A
35	YA	1640	C

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Mol	Chain	Res	Type
35	YA	1648	C
35	YA	1654	A
35	YA	1667	G
35	YA	1674	G
35	YA	1696	G
35	YA	1700	A
35	YA	1703	G
35	YA	1725	G
35	YA	1728	G
35	YA	1729	A
35	YA	1743	G
35	YA	1753	G
35	YA	1754	C
35	YA	1756	G
35	YA	1762	A
35	YA	1763	G
35	YA	1764	G
35	YA	1773	A
35	YA	1774	C
35	YA	1780	A
35	YA	1782	C
35	YA	1791	A
35	YA	1800	C
35	YA	1801	G
35	YA	1802	A
35	YA	1816	G
35	YA	1820	U
35	YA	1828	G
35	YA	1829	A
35	YA	1835	G
35	YA	1847	A
35	YA	1858	G
35	YA	1872	A
35	YA	1878	G
35	YA	1881	C
35	YA	1882	C
35	YA	1888	G
35	YA	1889	A
35	YA	1903	G
35	YA	1906	G
35	YA	1910	G
35	YA	1913	A

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Mol	Chain	Res	Type
35	YA	1929	G
35	YA	1930	G
35	YA	1936	A
35	YA	1938	A
35	YA	1955	U
35	YA	1963	U
35	YA	1964	G
35	YA	1966	A
35	YA	1967	C
35	YA	1970	A
35	YA	1971	A
35	YA	1972	A
35	YA	1980	G
35	YA	1982	C
35	YA	1992	G
35	YA	1993	U
35	YA	2020	A
35	YA	2021	C
35	YA	2023	G
35	YA	2027	G
35	YA	2031	A
35	YA	2032	G
35	YA	2033	A
35	YA	2043	C
35	YA	2052	G
35	YA	2055	C
35	YA	2056	G
35	YA	2059	A
35	YA	2060	A
35	YA	2061	G
35	YA	2062	A
35	YA	2069	G
35	YA	2093	G
35	YA	2099	U
35	YA	2111	C
35	YA	2112	G
35	YA	2113	U
35	YA	2114	A
35	YA	2116	G
35	YA	2117	A
35	YA	2119	A
35	YA	2120	G

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Mol	Chain	Res	Type
35	YA	2123	G
35	YA	2126	A
35	YA	2128	C
35	YA	2130	U
35	YA	2131	G
35	YA	2132	U
35	YA	2134	A
35	YA	2140	C
35	YA	2145	C
35	YA	2147	G
35	YA	2148	G
35	YA	2157	G
35	YA	2161	C
35	YA	2167	U
35	YA	2168	G
35	YA	2169	A
35	YA	2170	A
35	YA	2171	A
35	YA	2173	A
35	YA	2174	C
35	YA	2177	C
35	YA	2189	U
35	YA	2190	G
35	YA	2191	G
35	YA	2192	G
35	YA	2198	A
35	YA	2210	G
35	YA	2211	G
35	YA	2212	A
35	YA	2215	G
35	YA	2225	A
35	YA	2226	C
35	YA	2238	G
35	YA	2239	G
35	YA	2266	A
35	YA	2275	C
35	YA	2278	A
35	YA	2283	C
35	YA	2287	A
35	YA	2288	A
35	YA	2305	A
35	YA	2306	C

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Mol	Chain	Res	Type
35	YA	2307	G
35	YA	2308	G
35	YA	2309	A
35	YA	2312	U
35	YA	2316	C
35	YA	2318	G
35	YA	2320	A
35	YA	2325	G
35	YA	2334	G
35	YA	2335	A
35	YA	2336	A
35	YA	2343	C
35	YA	2346	A
35	YA	2347	C
35	YA	2350	C
35	YA	2354	G
35	YA	2358	G
35	YA	2383	G
35	YA	2385	C
35	YA	2392	A
35	YA	2402	C
35	YA	2403	C
35	YA	2406	U
35	YA	2410	G
35	YA	2422	A
35	YA	2423	U
35	YA	2424	C
35	YA	2425	A
35	YA	2429	G
35	YA	2430	A
35	YA	2435	A
35	YA	2439	A
35	YA	2440	C
35	YA	2441	C
35	YA	2448	A
35	YA	2450	A
35	YA	2469	A
35	YA	2472	G
35	YA	2474	C
35	YA	2475	C
35	YA	2476	A
35	YA	2478	A

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Mol	Chain	Res	Type
35	YA	2484	G
35	YA	2491	U
35	YA	2494	G
35	YA	2498	C
35	YA	2502	G
35	YA	2505	G
35	YA	2518	A
35	YA	2529	G
35	YA	2535	G
35	YA	2542	A
35	YA	2543	G
35	YA	2554	U
35	YA	2566	A
35	YA	2567	G
35	YA	2572	A
35	YA	2573	C
35	YA	2578	G
35	YA	2602	A
35	YA	2609	U
35	YA	2611	U
35	YA	2612	C
35	YA	2629	A
35	YA	2630	G
35	YA	2645	G
35	YA	2646	C
35	YA	2655	G
35	YA	2665	A
35	YA	2673	G
35	YA	2682	U
35	YA	2686	G
35	YA	2689	U
35	YA	2690	C
35	YA	2691	C
35	YA	2702	U
35	YA	2703	C
35	YA	2712	U
35	YA	2713	A
35	YA	2714	G
35	YA	2724	C
35	YA	2725	A
35	YA	2726	U
35	YA	2732	G

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Mol	Chain	Res	Type
35	YA	2733	A
35	YA	2734	A
35	YA	2739	U
35	YA	2744	G
35	YA	2748	A
35	YA	2751	G
35	YA	2752	C
35	YA	2754	U
35	YA	2757	A
35	YA	2762	G
35	YA	2764	A
35	YA	2766	G
35	YA	2777	G
35	YA	2778	A
35	YA	2779	U
35	YA	2780	G
35	YA	2790	A
35	YA	2791	C
35	YA	2792	G
35	YA	2807	G
35	YA	2808	U
35	YA	2811	G
35	YA	2818	G
35	YA	2820	A
35	YA	2821	A
35	YA	2823	A
35	YA	2830	G
35	YA	2832	U
35	YA	2833	G
35	YA	2834	G
35	YA	2835	A
35	YA	2846	G
35	YA	2848	G
35	YA	2849	U
35	YA	2850	A
35	YA	2860	A
35	YA	2872	G
35	YA	2873	A
35	YA	2879	C
35	YA	2880	C
35	YA	2892	A
35	YA	2893	G

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Mol	Chain	Res	Type
35	YA	2894	G
35	YA	2896	C
35	YA	2897	U
36	YB	8	U
36	YB	13	A
36	YB	14	U
36	YB	15	A
36	YB	16	G
36	YB	25	A
36	YB	42	C
36	YB	44	G
36	YB	45	A
36	YB	57	A
36	YB	67	G
36	YB	73	A
36	YB	81	G
36	YB	88	C
36	YB	109	G
36	YB	112	G
36	YB	119	A

All (144) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	QA	5	U
1	QA	31	G
1	QA	60	A
1	QA	115	G
1	QA	181	G
1	QA	190	G
1	QA	197	A
1	QA	201	C
1	QA	208	U
1	QA	250	A
1	QA	428	G
1	QA	484	G
1	QA	496	A
1	QA	518	C
1	QA	547	A
1	QA	687	A
1	QA	748	C
1	QA	792	A

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Mol	Chain	Res	Type
1	QA	812	C
1	QA	841	U
1	QA	913	A
1	QA	960	U
1	QA	992	U
1	QA	1038	C
1	QA	1065	U
1	QA	1067	A
1	QA	1137	C
1	QA	1182	G
1	QA	1346	A
1	QA	1347	G
1	QA	1498	U
1	QA	1528	U
1	QA	1532	U
22	QV	1	C
23	QX	9	G
23	QX	11	U
35	RA	90	U
35	RA	119	A
35	RA	128	C
35	RA	227	A
35	RA	372	G
35	RA	387	U
35	RA	404	C
35	RA	587	C
35	RA	752	A
35	RA	845	G
35	RA	856	C
35	RA	877	U
35	RA	1022	G
35	RA	1085	A
35	RA	1171	G
35	RA	1204	A
35	RA	1300	U
35	RA	1427	A
35	RA	1558	A
35	RA	1559	G
35	RA	1653	G
35	RA	1694	C
35	RA	1699	G
35	RA	1819	A

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Mol	Chain	Res	Type
35	RA	1930	G
35	RA	1992	G
35	RA	2092	U
35	RA	2144	U
35	RA	2191	G
35	RA	2211	G
35	RA	2439	A
35	RA	2447	G
35	RA	2481	G
35	RA	2689	U
35	RA	2776	A
35	RA	2849	U
35	RA	2859	G
36	RB	66	A
1	XA	5	U
1	XA	60	A
1	XA	92	G
1	XA	115	G
1	XA	181	G
1	XA	197	A
1	XA	201	C
1	XA	243	A
1	XA	250	A
1	XA	279	A
1	XA	315	A
1	XA	328	C
1	XA	428	G
1	XA	547	A
1	XA	595	G
1	XA	687	A
1	XA	703	G
1	XA	748	C
1	XA	792	A
1	XA	812	C
1	XA	913	A
1	XA	960	U
1	XA	992	U
1	XA	1000	A
1	XA	1004	A
1	XA	1033	G
1	XA	1038	C
1	XA	1054	C

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Mol	Chain	Res	Type
1	XA	1065	U
1	XA	1067	A
1	XA	1124	G
1	XA	1137	C
1	XA	1139	G
1	XA	1157	A
1	XA	1182	G
1	XA	1190	G
1	XA	1300	G
1	XA	1305	G
1	XA	1498	U
1	XA	1532	U
22	XV	1	C
35	YA	119	A
35	YA	372	G
35	YA	587	C
35	YA	603	A
35	YA	752	A
35	YA	827	U
35	YA	856	C
35	YA	1022	G
35	YA	1171	G
35	YA	1379	A
35	YA	1427	A
35	YA	1558	A
35	YA	1559	G
35	YA	1653	G
35	YA	1819	A
35	YA	2144	U
35	YA	2166	G
35	YA	2191	G
35	YA	2211	G
35	YA	2225	A
35	YA	2439	A
35	YA	2447	G
35	YA	2610	C
35	YA	2689	U
35	YA	2776	A
35	YA	2848	G
35	YA	2849	U
35	YA	2859	G
36	YB	66	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	A3P	XX	20	23	23,28,29	5.22	7 (30%)	23,42,45	1.53	3 (13%)
23	A3P	QX	20	23	23,28,29	5.26	7 (30%)	23,42,45	1.49	4 (17%)
56	PPU	ZB	3	56,35	32,40,41	0.85	2 (6%)	33,57,60	1.87	10 (30%)
56	PPU	ZA	3	56,35	32,40,41	0.90	0	33,57,60	1.80	7 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	A3P	XX	20	23	-	1/8/30/31	0/3/3/3
23	A3P	QX	20	23	-	2/8/30/31	0/3/3/3
56	PPU	ZB	3	56,35	-	14/21/43/44	0/4/4/4
56	PPU	ZA	3	56,35	-	6/21/43/44	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	QX	20	A3P	O4'-C1'	18.93	1.67	1.41
23	XX	20	A3P	O4'-C1'	18.45	1.66	1.41
23	XX	20	A3P	C2'-C1'	-13.73	1.32	1.53
23	QX	20	A3P	C2'-C1'	-13.44	1.33	1.53
23	XX	20	A3P	O4'-C4'	-5.92	1.31	1.45
23	QX	20	A3P	O4'-C4'	-5.91	1.31	1.45
23	QX	20	A3P	P1-O3'	4.79	1.68	1.59
23	XX	20	A3P	P1-O3'	4.10	1.67	1.59
23	XX	20	A3P	O3'-C3'	-3.45	1.31	1.44
23	QX	20	A3P	O3'-C3'	-3.23	1.32	1.44
23	XX	20	A3P	C6-N6	3.22	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	QX	20	A3P	C6-N6	2.85	1.44	1.34
23	XX	20	A3P	C3'-C4'	2.15	1.58	1.52
56	ZB	3	PPU	C2'-C1'	-2.05	1.50	1.53
23	QX	20	A3P	C2'-C3'	2.03	1.57	1.52
56	ZB	3	PPU	C5-C4	2.03	1.46	1.40

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	XX	20	A3P	N3-C2-N1	-4.92	120.98	128.68
56	ZA	3	PPU	N1-C6-N6	4.77	122.08	117.06
56	ZB	3	PPU	CG-CB-CA	-4.38	105.02	114.13
23	QX	20	A3P	N3-C2-N1	-4.07	122.32	128.68
56	ZB	3	PPU	N1-C6-N6	3.96	121.22	117.06
56	ZA	3	PPU	C3'-N3'-C	-3.92	117.30	123.21
56	ZA	3	PPU	C9-N6-C6	-3.78	108.08	119.51
56	ZA	3	PPU	CA-C-N3'	3.69	121.27	116.15
56	ZB	3	PPU	C10-N6-C6	-3.49	108.95	119.51
56	ZB	3	PPU	C9-N6-C6	-3.46	109.03	119.51
23	XX	20	A3P	C3'-C2'-C1'	3.24	107.07	99.89
56	ZA	3	PPU	C10-N6-C6	-3.06	110.24	119.51
56	ZA	3	PPU	N3-C2-N1	-3.04	123.92	128.68
23	XX	20	A3P	C4-C5-N7	-2.99	106.28	109.40
56	ZB	3	PPU	N3-C2-N1	-2.96	124.05	128.68
56	ZB	3	PPU	C4-C5-N7	-2.82	106.46	109.40
23	QX	20	A3P	C4-C5-N7	-2.79	106.49	109.40
23	QX	20	A3P	C3'-C2'-C1'	2.67	105.80	99.89
56	ZB	3	PPU	CB-CA-C	2.61	115.07	108.97
56	ZB	3	PPU	CA-C-N3'	-2.58	112.57	116.15
23	QX	20	A3P	C2'-C3'-C4'	2.43	107.53	103.22
56	ZB	3	PPU	C3'-N3'-C	2.39	126.82	123.21
56	ZB	3	PPU	C10-N6-C9	-2.36	108.53	116.12
56	ZA	3	PPU	C4-C5-N7	-2.26	107.04	109.40

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	XX	20	A3P	C3'-O3'-P1-O1P
56	ZB	3	PPU	N3'-C-CA-N
56	ZB	3	PPU	O-C-CA-CB
56	ZB	3	PPU	N3'-C-CA-CB

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Mol	Chain	Res	Type	Atoms
56	ZB	3	PPU	CA-C-N3'-C3'
56	ZB	3	PPU	C5-C6-N6-C10
56	ZA	3	PPU	N-CA-CB-CG
56	ZA	3	PPU	C-CA-CB-CG
56	ZA	3	PPU	C5-C6-N6-C9
56	ZB	3	PPU	O-C-N3'-C3'
56	ZB	3	PPU	CE1-CZ-OC-CM
56	ZA	3	PPU	CE1-CZ-OC-CM
56	ZB	3	PPU	CE2-CZ-OC-CM
56	ZA	3	PPU	CE2-CZ-OC-CM
56	ZB	3	PPU	N1-C6-N6-C10
23	QX	20	A3P	C3'-C4'-C5'-O5'
56	ZB	3	PPU	C5-C6-N6-C9
56	ZA	3	PPU	C5-C6-N6-C10
56	ZB	3	PPU	CA-CB-CG-CD1
56	ZB	3	PPU	CA-CB-CG-CD2
56	ZB	3	PPU	O-C-CA-N
23	QX	20	A3P	O4'-C4'-C5'-O5'
56	ZB	3	PPU	C2'-C3'-N3'-C

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	XX	20	A3P	2	0
23	QX	20	A3P	1	0
56	ZB	3	PPU	7	0
56	ZA	3	PPU	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 900 ligands modelled in this entry, 898 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	SF4	XD	301	4	0,12,12	0.00	-	-		
58	SF4	QD	302	4	0,12,12	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SF4	XD	301	4	-	-	0/6/5/5
58	SF4	QD	302	4	-	-	0/6/5/5

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.