Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2023 – 10:46 AM EDT

PDB ID	:	8FON
Title	:	Crystal structure of tRNA^Lys(SUU) bound to AUA codon in the ribosomal P site
Authors	:	Nguyen, H.A.; Hoffer, E.D.; Maehigashi, T.; Fagan, C.E.; Dunham, C.M.
Deposited on	:	2023-01-02
Resolution	:	3.64 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

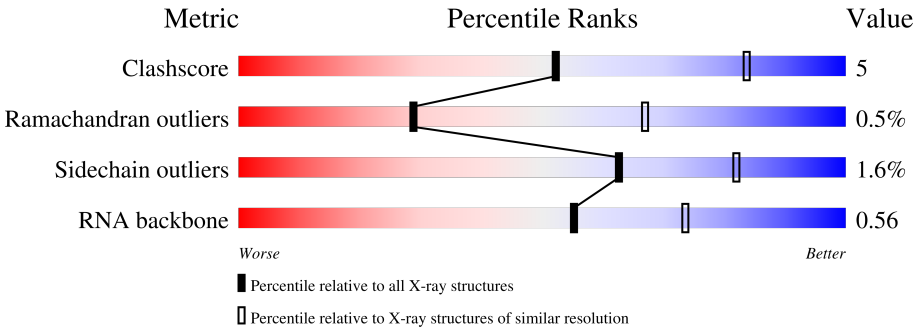
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.64 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	1439 (3.78-3.50)
Ramachandran outliers	138981	1391 (3.78-3.50)
Sidechain outliers	138945	1391 (3.78-3.50)
RNA backbone	3102	1019 (4.26-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	QA	1522	61% 31% 6% ••
1	XA	1522	59% 34% 6% ••
2	QB	256	77% 14% 8%
2	XB	256	82% 10% 8%
3	QC	239	69% 16% 14%
3	XC	239	72% 13% • 14%

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Mol	Chain	Length	Quality of chain
4	QD	209	82% 18%
4	XD	209	77% 22%
5	QE	162	83% 10% 7%
5	XE	162	81% 12% 7%
6	QF	101	91% 9%
6	XF	101	86% 14%
7	QG	156	91% 7%
7	XG	156	85% 15%
8	QH	138	88% 11%
8	XH	138	87% 12%
9	QI	128	62% 35%
9	XI	128	79% 20%
10	QJ	105	73% 21% 6%
10	XJ	105	72% 19% 9%
11	QK	129	77% 16% 8%
11	XK	129	71% 19% 10%
12	QL	131	79% 16% 5%
12	XL	131	78% 15% 7%
13	QM	126	69% 25% 5%
13	XM	126	81% 13% 6%
14	QN	61	79% 18%
14	XN	61	80% 16%
15	QO	89	90% 9%
15	XO	89	90% 8%
16	QP	88	83% 13% 5%

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Mol	Chain	Length	Quality of chain
16	XP	88	84% 10% 5%
17	QQ	105	85% 10% 5%
17	XQ	105	86% 10% 5%
18	QR	88	68% 11% 20%
18	XR	88	66% 14% 20%
19	QS	93	73% 16% 11%
19	XS	93	70% 19% 10%
20	QT	106	79% 14% 7%
20	XT	106	81% 12% 7%
21	QU	27	89% 7%
21	XU	27	74% 19% 7%
22	QV	76	58% 29% 8%
22	XV	76	61% 26% 7%
23	QX	23	9% 87%
23	XX	23	61% 26% 13%
24	R0	85	71% 19% 11%
24	Y0	85	71% 18% 12%
25	R1	98	80% 19%
25	Y1	98	74% 20% 5%
26	R2	72	75% 21%
26	Y2	72	83% 10% 6%
27	R3	60	85% 13%
27	Y3	60	67% 22% 10%
28	R4	71	82% 15%
28	Y4	71	82% 13%

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Mol	Chain	Length	Quality of chain
29	R5	60	92% 7%
29	Y5	60	90% 8%
30	R6	54	81% 17%
30	Y6	54	81% 17%
31	R7	49	84% 12%
31	Y7	49	90% 8%
32	R8	65	57% 29% 12%
32	Y8	65	78% 20%
33	R9	37	81% 19%
33	Y9	37	73% 27%
34	RA	2915	63% 29% 6%
34	YA	2915	63% 29% 6%
35	RB	122	70% 23% 5%
35	YB	122	70% 23% 5%
36	RD	276	80% 19%
36	YD	276	83% 15%
37	RE	206	79% 19%
37	YE	206	88% 10%
38	RF	210	79% 17%
38	YF	210	86% 10%
39	RG	182	70% 26%
39	YG	182	70% 26%
40	RH	180	66% 28%
40	YH	180	81% 14%
41	RI	148	70% 24% 5%

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Mol	Chain	Length	Quality of chain
41	YI	148	77% 16% 5%
42	RN	140	82% 14%
42	YN	140	84% 15%
43	RO	122	80% 20%
43	YO	122	80% 20%
44	RP	150	83% 15%
44	YP	150	83% 13%
45	RQ	141	77% 23%
45	YQ	141	76% 23%
46	RR	118	86% 14%
46	YR	118	82% 17%
47	RS	112	75% 23%
47	YS	112	79% 20%
48	RT	146	76% 16% 6%
48	YT	146	69% 24% 6%
49	RU	118	85% 13%
49	YU	118	77% 19%
50	RV	101	72% 25%
50	YV	101	87% 11%
51	RW	113	88% 12%
51	YW	113	84% 15%
52	RX	96	85% 10%
52	YX	96	82% 14%
53	RY	110	86% 11%
53	YY	110	83% 15%

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Mol	Chain	Length	Quality of chain
54	RZ	206	
54	YZ	206	
55	XY	17	
56	Z6	3	
56	Z8	3	

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 292577 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	1500	Total	C	N	O	P	0	0	0
			32247	14353	5981	10414	1499			
1	XA	1511	Total	C	N	O	P	0	0	0
			32471	14454	6014	10493	1510			

- 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	84	Total	C	N	O	S	0	0	0
			674	430	126	116	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 217	C 134	N 52	O 31	0	0	0
21	XU	25	Total 217	C 134	N 52	O 31	0	0	0

- Molecule 22 is a RNA chain called P-site tRNA^Lys(SUU).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	74	Total 1584	C 710	N 278	O 523	P 73	0	0	0
22	XV	74	Total 1584	C 710	N 278	O 523	P 73	0	0	0

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	3	Total 65	C 29	N 12	O 21	P 3	0	0	0
23	XX	23	Total 499	C 223	N 96	O 157	P 23	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	R0	76	Total 603	C 372	N 128	O 102	S 1	0	0	0
24	Y0	75	Total 599	C 370	N 127	O 101	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	R1	97	Total 763	C 481	N 150	O 131	S 1	0	0	0
25	Y1	93	Total 729	C 457	N 145	O 126	S 1	0	0	0

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Y2	68	Total	C	N	O	S	0	0	0
			575	355	117	102	1			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	R6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
30	Y6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			

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

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

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

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

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

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

- Molecule 34 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	RA	2881	Total	C	N	O	P	0	0	0
			62051	27618	11609	19944	2880			
34	YA	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			

- Molecule 35 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	RB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			
35	YB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 36 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	RD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
36	YD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

- Molecule 37 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	RE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
37	YE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 38 is a protein called 50S ribosomal protein L4.

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

- Molecule 39 is a protein called 50S ribosomal protein L5.

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

- Molecule 40 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	RH	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
40	YH	173	Total	C	N	O	S	0	0	0
			1330	845	250	234	1			

- Molecule 41 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	RI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
41	YI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 42 is a protein called 50S ribosomal protein L13.

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

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

- Molecule 43 is a protein called 50S ribosomal protein L14.

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

- Molecule 44 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	RP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
44	YP	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			

- Molecule 45 is a protein called 50S ribosomal protein L16.

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

- Molecule 46 is a protein called 50S ribosomal protein L17.

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

- Molecule 47 is a protein called 50S ribosomal protein L18.

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

- Molecule 48 is a protein called 50S ribosomal protein L19.

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

- Molecule 49 is a protein called 50S ribosomal protein L20.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L22.

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

- Molecule 52 is a protein called 50S ribosomal protein L23.

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

- Molecule 53 is a protein called 50S ribosomal protein L24.

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

- Molecule 54 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	RZ	203	Total	C	N	O	S	0	0	0
			1601	1020	283	295	3			
54	YZ	203	Total	C	N	O	S	0	0	0
			1601	1020	283	295	3			

- Molecule 55 is a RNA chain called A-site ASL^Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	XY	17	Total	C	N	O	P	0	0	0
			362	163	68	115	16			

- Molecule 56 is a RNA chain called CC-puro.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	Z6	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			
56	Z8	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	73	Total	Mg	0	0
			73	73		
57	QF	1	Total	Mg	0	0
			1	1		
57	QH	1	Total	Mg	0	0
			1	1		
57	QJ	1	Total	Mg	0	0
			1	1		
57	QM	1	Total	Mg	0	0
			1	1		
57	QV	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	R0	1	Total Mg 1 1	0	0
57	R1	1	Total Mg 1 1	0	0
57	R3	1	Total Mg 1 1	0	0
57	RA	483	Total Mg 483 483	0	0
57	RB	7	Total Mg 7 7	0	0
57	RE	4	Total Mg 4 4	0	0
57	RN	1	Total Mg 1 1	0	0
57	RO	1	Total Mg 1 1	0	0
57	RP	3	Total Mg 3 3	0	0
57	RQ	3	Total Mg 3 3	0	0
57	RR	1	Total Mg 1 1	0	0
57	RT	1	Total Mg 1 1	0	0
57	RY	1	Total Mg 1 1	0	0
57	XA	73	Total Mg 73 73	0	0
57	XE	1	Total Mg 1 1	0	0
57	XK	1	Total Mg 1 1	0	0
57	XL	1	Total Mg 1 1	0	0
57	XM	1	Total Mg 1 1	0	0
57	XQ	1	Total Mg 1 1	0	0
57	XS	1	Total Mg 1 1	0	0
57	Y0	2	Total Mg 2 2	0	0

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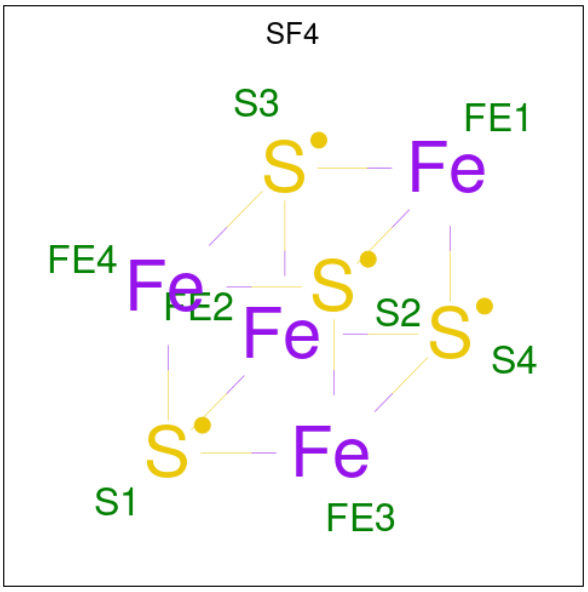
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	Y1	1	Total Mg 1 1	0	0
57	Y7	1	Total Mg 1 1	0	0
57	Y8	1	Total Mg 1 1	0	0
57	YA	538	Total Mg 538 538	0	0
57	YB	13	Total Mg 13 13	0	0
57	YD	3	Total Mg 3 3	0	0
57	YE	4	Total Mg 4 4	0	0
57	YN	1	Total Mg 1 1	0	0
57	YO	1	Total Mg 1 1	0	0
57	YP	1	Total Mg 1 1	0	0
57	YQ	3	Total Mg 3 3	0	0
57	YR	2	Total Mg 2 2	0	0
57	YX	2	Total Mg 2 2	0	0
57	YY	1	Total Mg 1 1	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	QN	1	Total Zn 1 1	0	0
59	R4	1	Total Zn 1 1	0	0
59	R5	1	Total Zn 1 1	0	0
59	R6	1	Total Zn 1 1	0	0
59	R9	1	Total Zn 1 1	0	0
59	RY	1	Total Zn 1 1	0	0
59	XN	1	Total Zn 1 1	0	0
59	Y4	1	Total Zn 1 1	0	0
59	Y5	1	Total Zn 1 1	0	0
59	Y6	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	Y9	1	Total Zn 1 1	0	0
59	YY	1	Total Zn 1 1	0	0

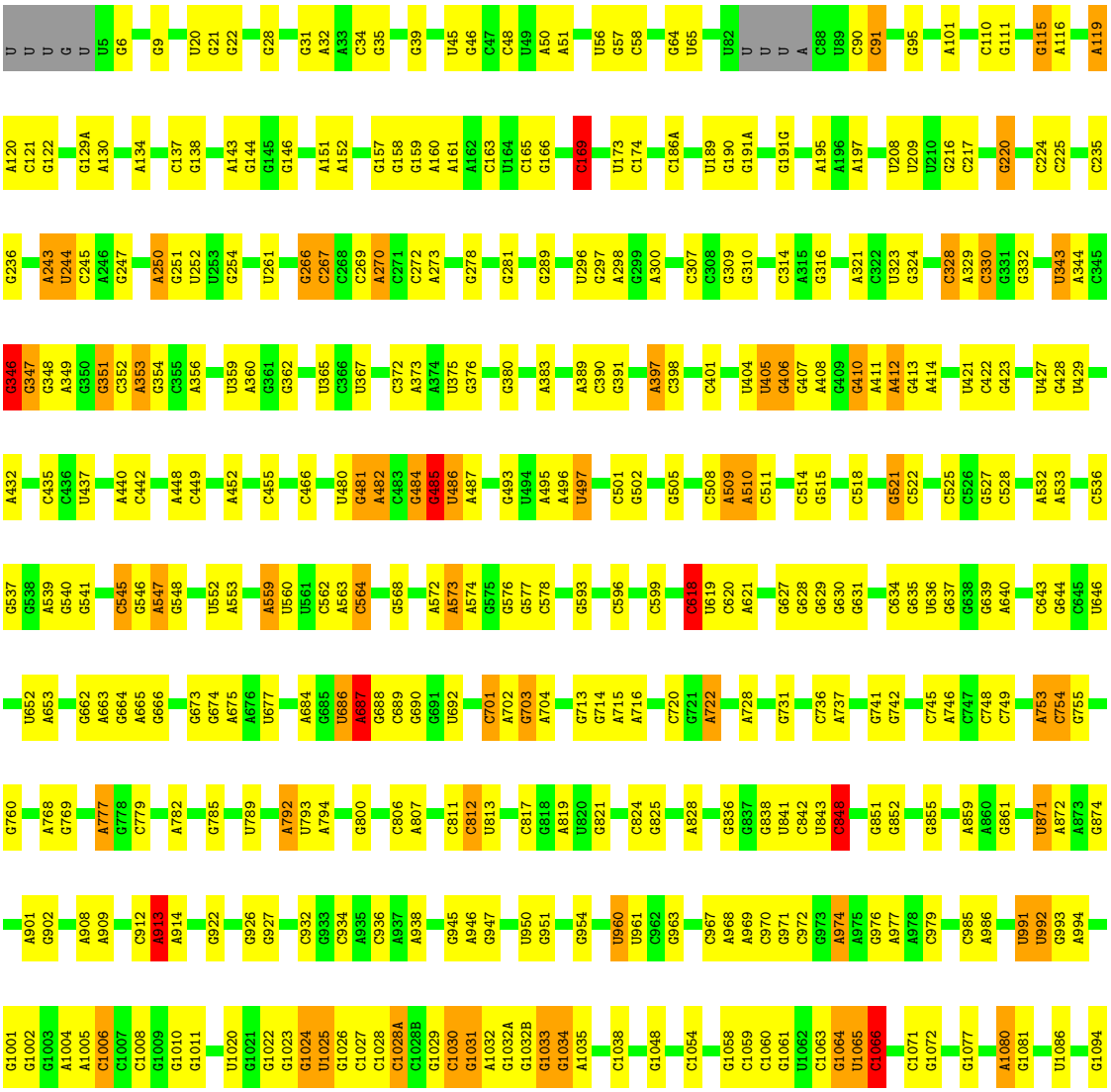
3 Residue-property plots (i)

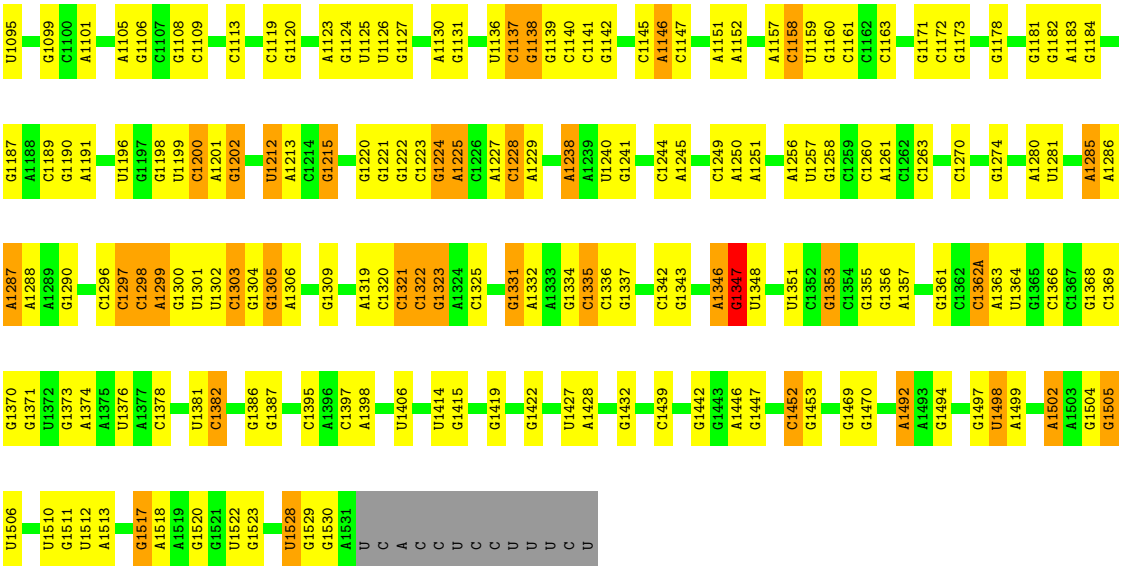
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

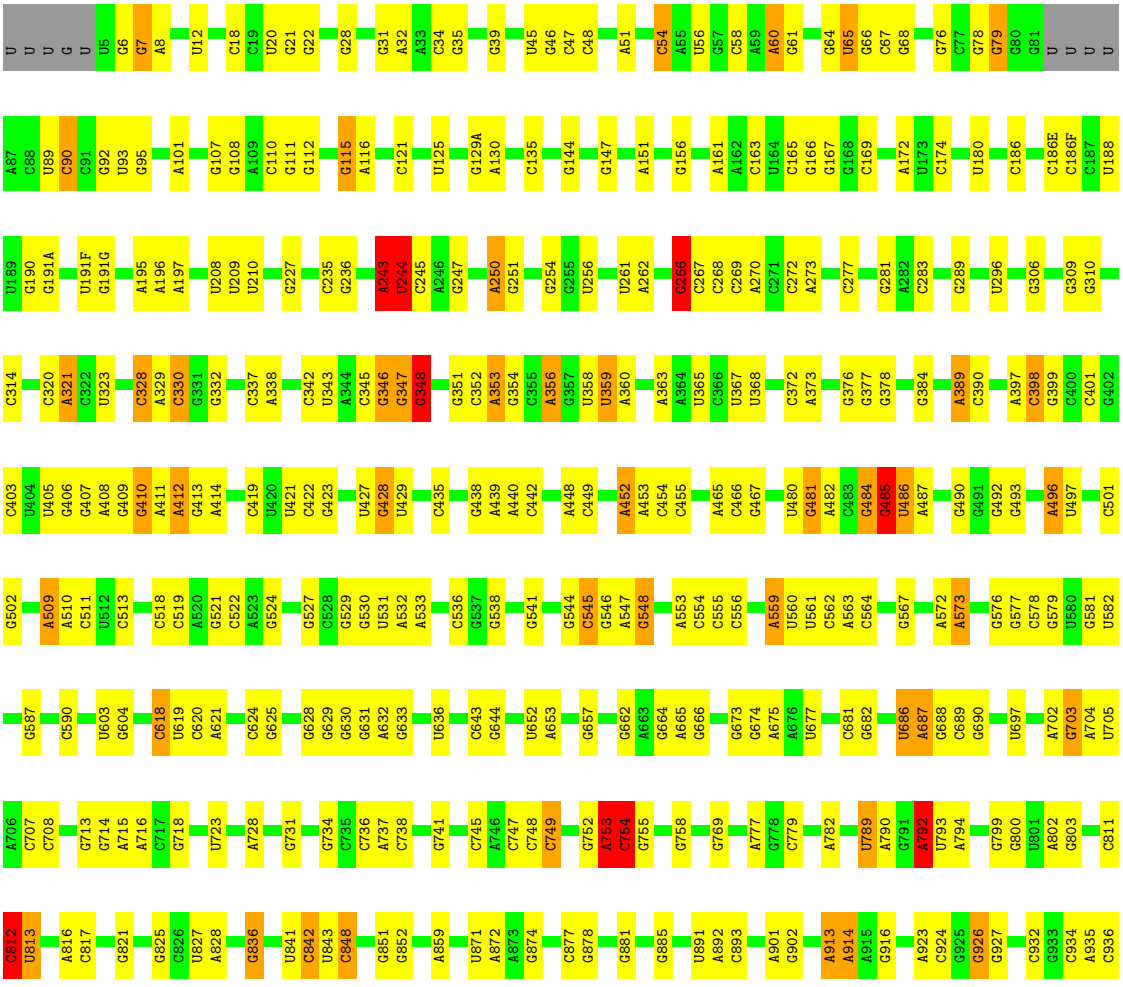
Chain QA:

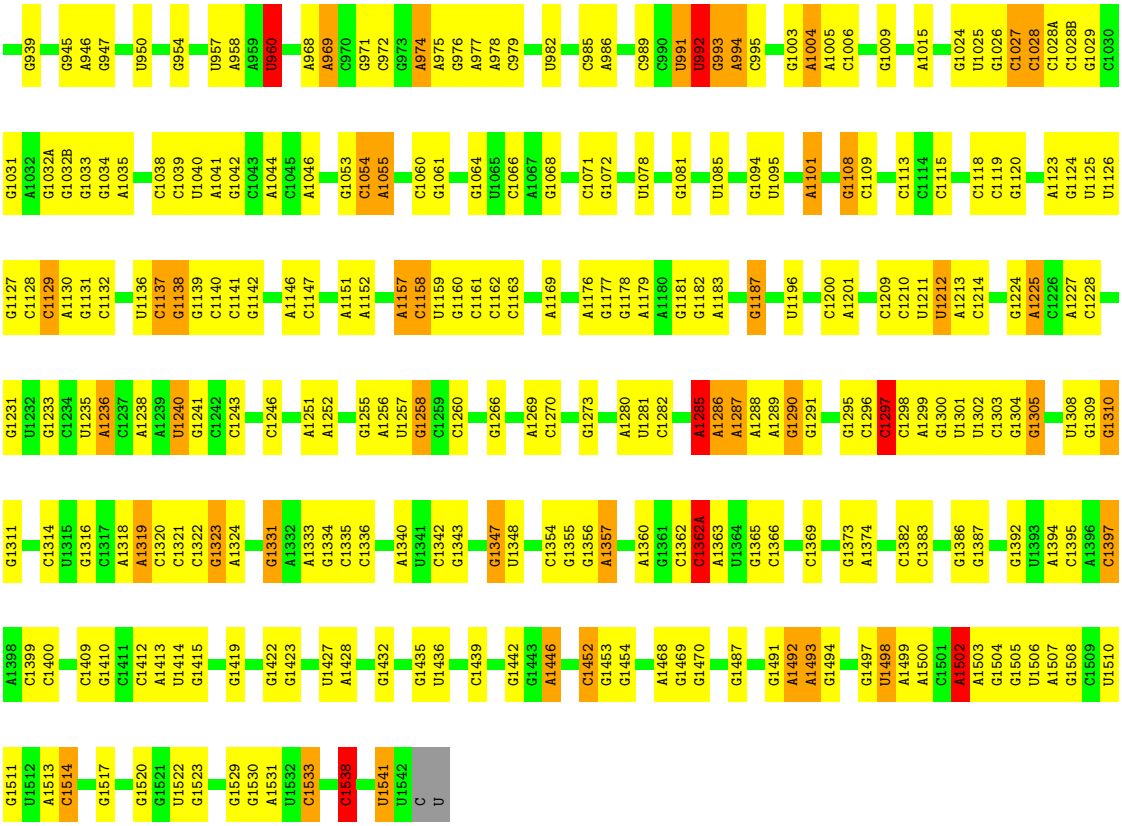




• Molecule 1: 16S rRNA

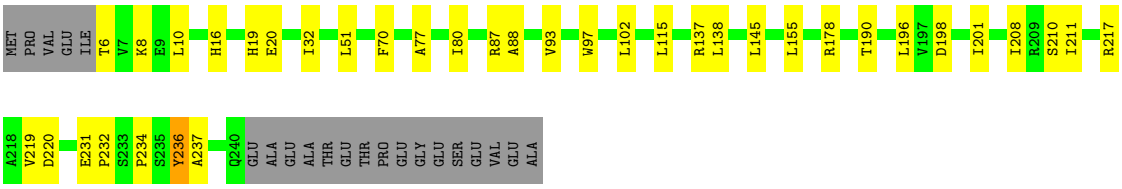
Chain XA:





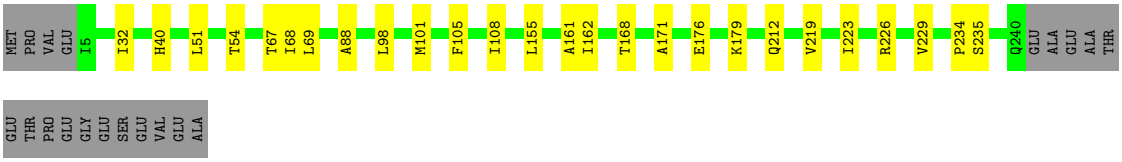
• Molecule 2: 30S ribosomal protein S2

Chain QB:



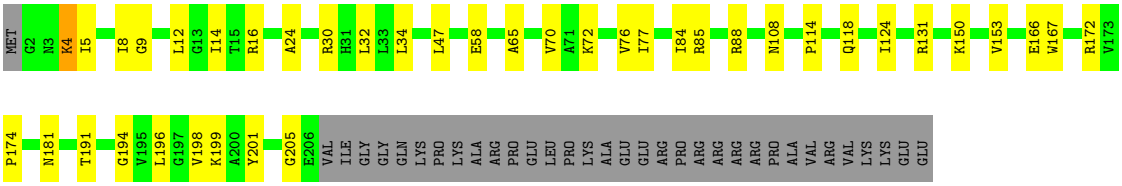
• Molecule 2: 30S ribosomal protein S2

Chain XB:



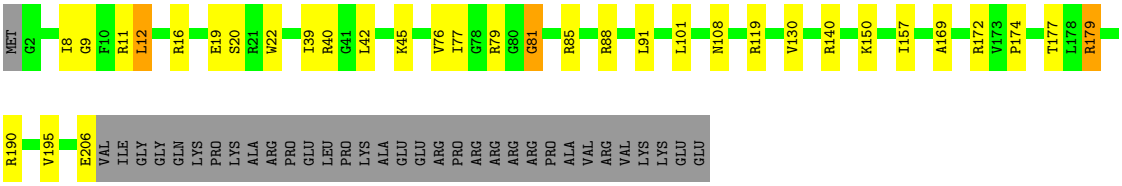
• Molecule 3: 30S ribosomal protein S3

Chain QC:



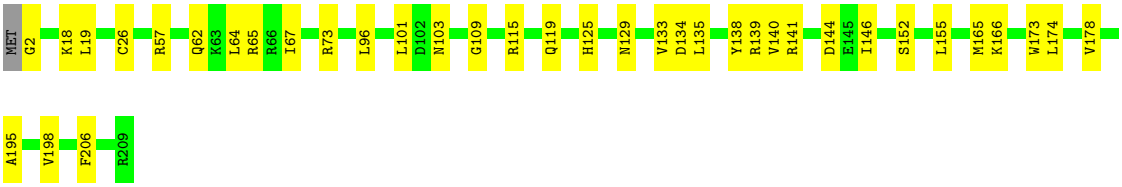
• Molecule 3: 30S ribosomal protein S3

Chain XC:



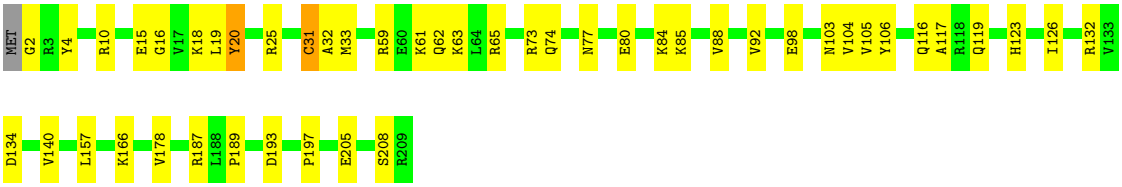
• Molecule 4: 30S ribosomal protein S4

Chain QD:



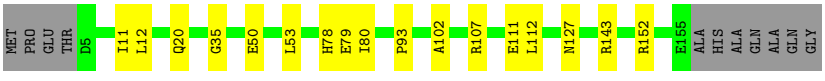
• Molecule 4: 30S ribosomal protein S4

Chain XD:



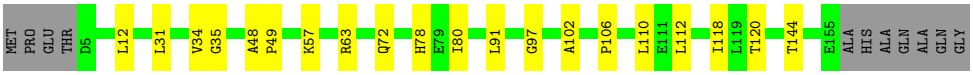
• Molecule 5: 30S ribosomal protein S5

Chain QE:



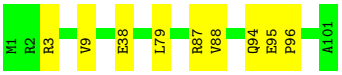
• Molecule 5: 30S ribosomal protein S5

Chain XE:



• Molecule 6: 30S ribosomal protein S6

Chain QF:

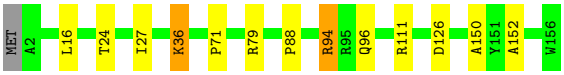


• Molecule 6: 30S ribosomal protein S6

Chain XF:

• Molecule 7: 30S ribosomal protein S7

Chain QG:



• Molecule 7: 30S ribosomal protein S7

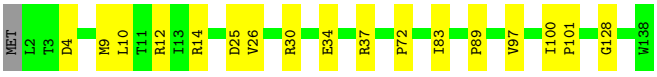
Chain XG:

• Molecule 8: 30S ribosomal protein S8

Chain QH:

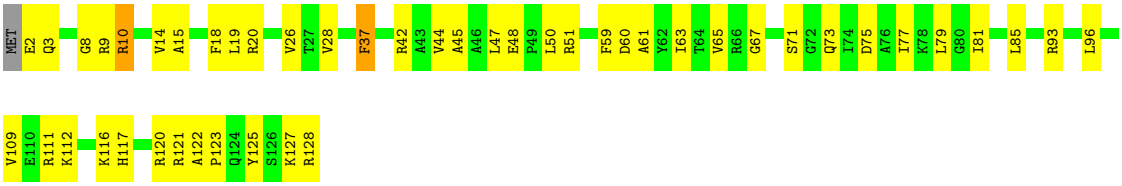
• Molecule 8: 30S ribosomal protein S8

Chain XH:



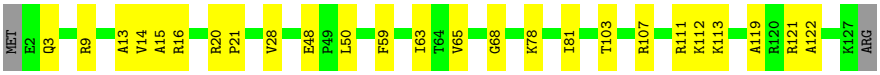
• Molecule 9: 30S ribosomal protein S9

Chain QI:



• Molecule 9: 30S ribosomal protein S9

Chain XI:



• Molecule 10: 30S ribosomal protein S10

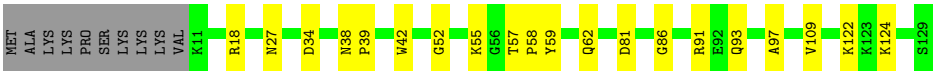
Chain QJ:

• Molecule 10: 30S ribosomal protein S10

Chain XJ:

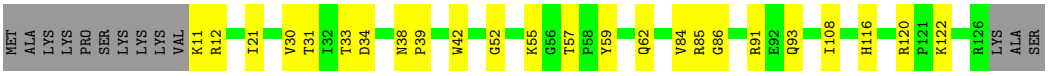
• Molecule 11: 30S ribosomal protein S11

Chain QK:



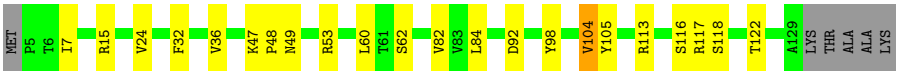
• Molecule 11: 30S ribosomal protein S11

Chain XK:



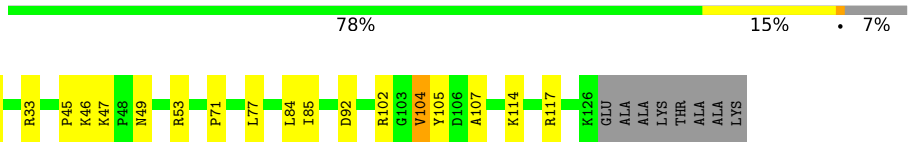
• Molecule 12: 30S ribosomal protein S12

Chain QL:



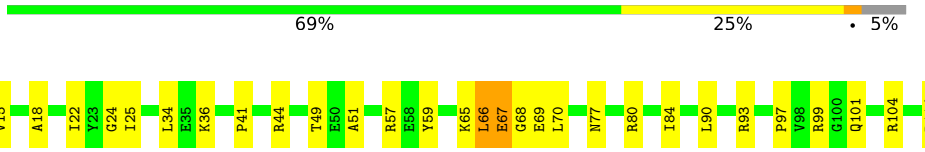
• Molecule 12: 30S ribosomal protein S12

Chain XL:



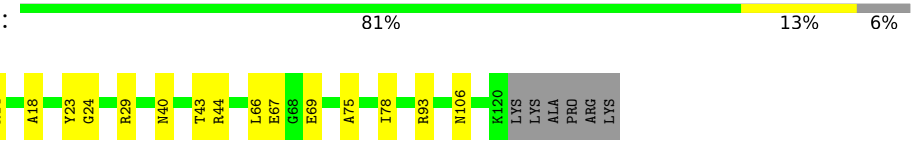
• Molecule 13: 30S ribosomal protein S13

Chain QM:



• Molecule 13: 30S ribosomal protein S13

Chain XM:

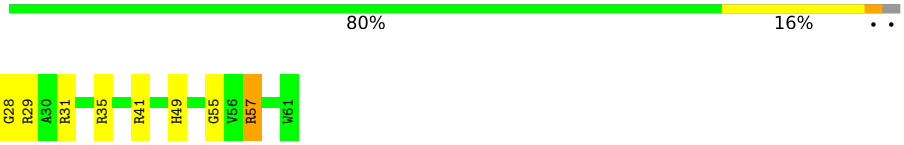


• Molecule 14: 30S ribosomal protein S14 type Z

Chain QN:

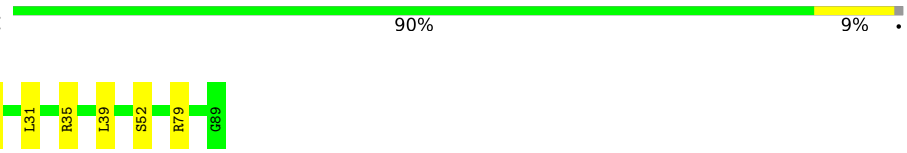
• Molecule 14: 30S ribosomal protein S14 type Z

Chain XN:



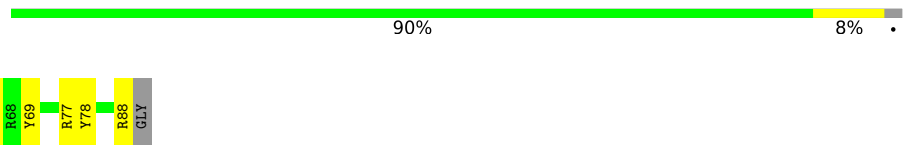
• Molecule 15: 30S ribosomal protein S15

Chain QO:



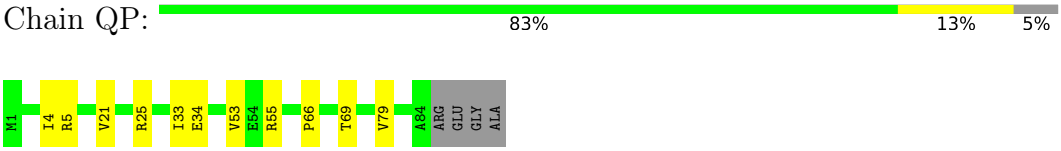
• Molecule 15: 30S ribosomal protein S15

Chain XO:



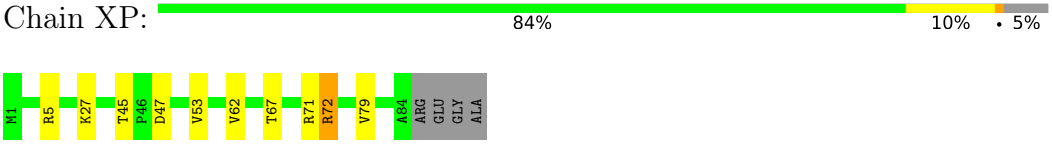
• Molecule 16: 30S ribosomal protein S16

Chain QP:



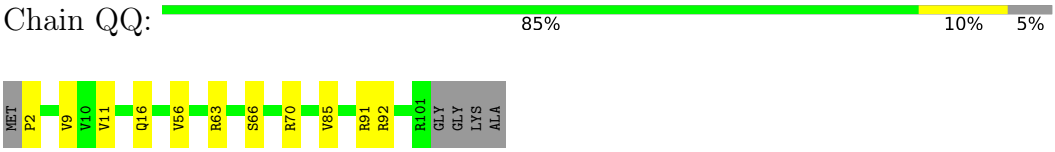
• Molecule 16: 30S ribosomal protein S16

Chain XP:



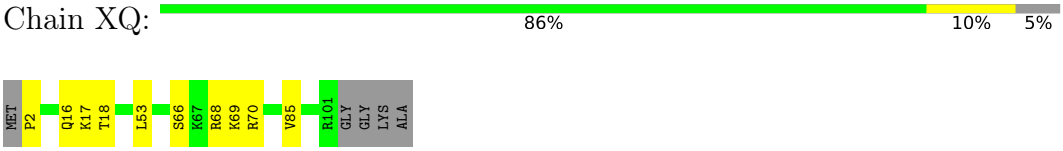
• Molecule 17: 30S ribosomal protein S17

Chain QQ:



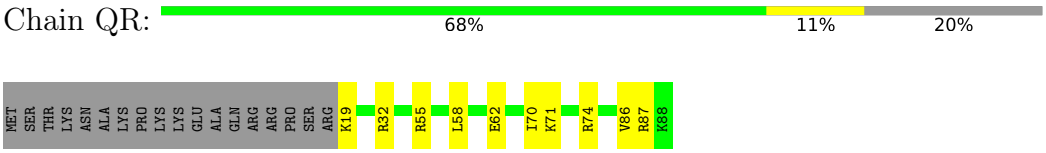
• Molecule 17: 30S ribosomal protein S17

Chain XQ:



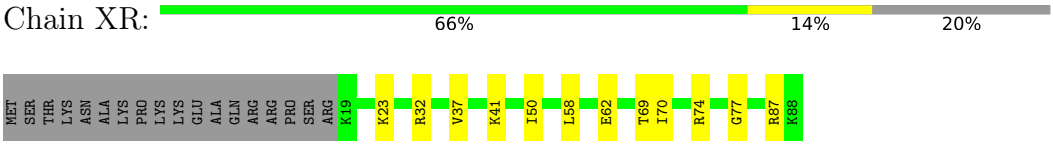
• Molecule 18: 30S ribosomal protein S18

Chain QR:



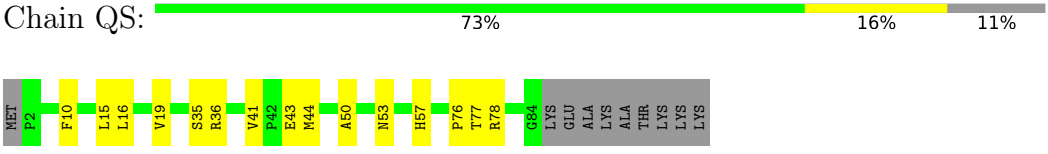
• Molecule 18: 30S ribosomal protein S18

Chain XR:



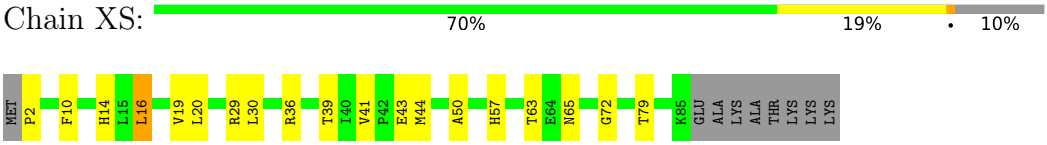
• Molecule 19: 30S ribosomal protein S19

Chain QS:



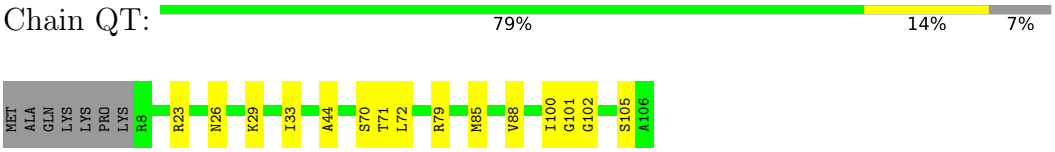
• Molecule 19: 30S ribosomal protein S19

Chain XS:



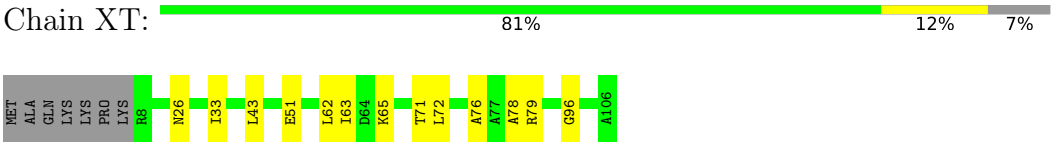
• Molecule 20: 30S ribosomal protein S20

Chain QT:



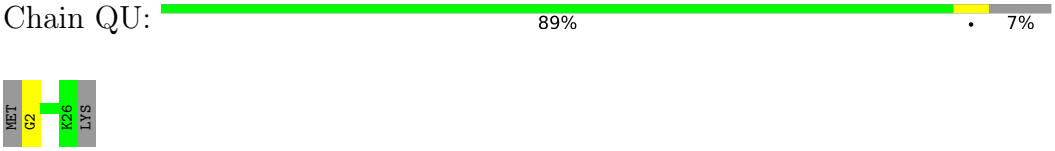
• Molecule 20: 30S ribosomal protein S20

Chain XT:



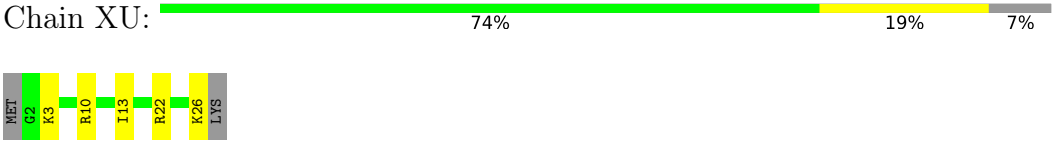
• Molecule 21: 30S ribosomal protein Thx

Chain QU:



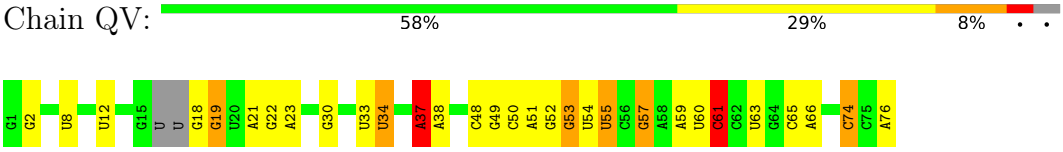
• Molecule 21: 30S ribosomal protein Thx

Chain XU:



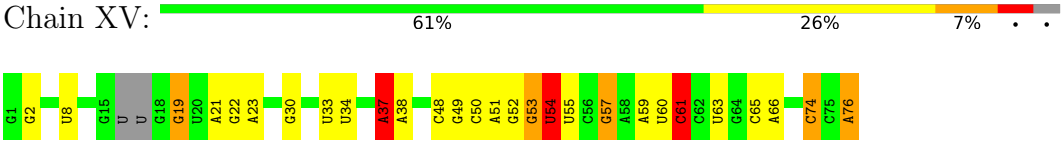
• Molecule 22: P-site tRNA^Lys(SUU)

Chain QV:



• Molecule 22: P-site tRNA^Lys(SUU)

Chain XV:



• Molecule 23: mRNA

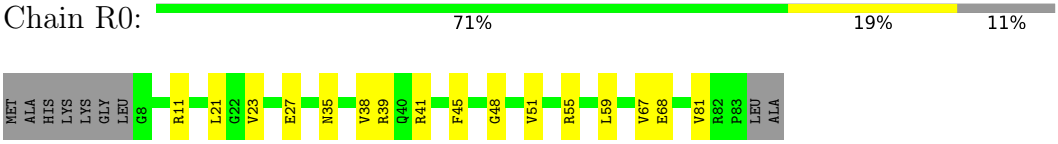
Chain QX:

• Molecule 23: mRNA

Chain XX:

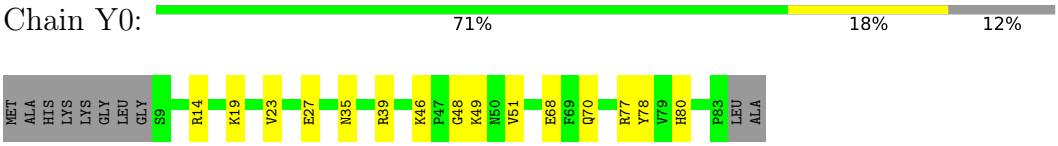
• Molecule 24: 50S ribosomal protein L27

Chain R0:



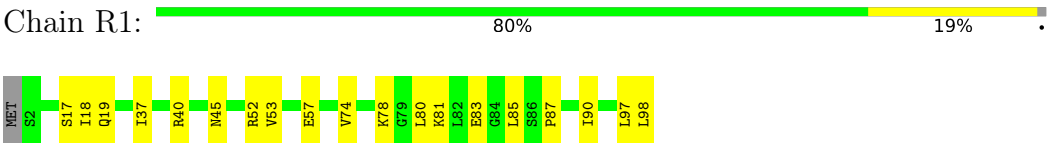
• Molecule 24: 50S ribosomal protein L27

Chain Y0:



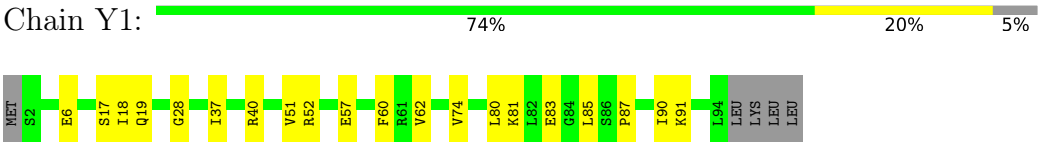
• Molecule 25: 50S ribosomal protein L28

Chain R1:



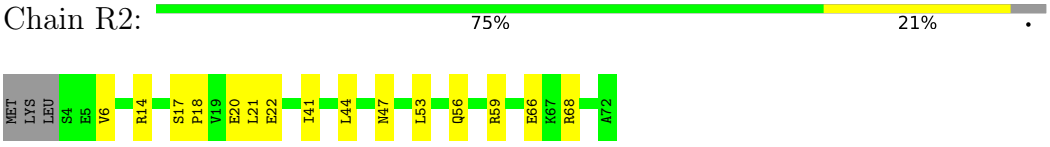
• Molecule 25: 50S ribosomal protein L28

Chain Y1:



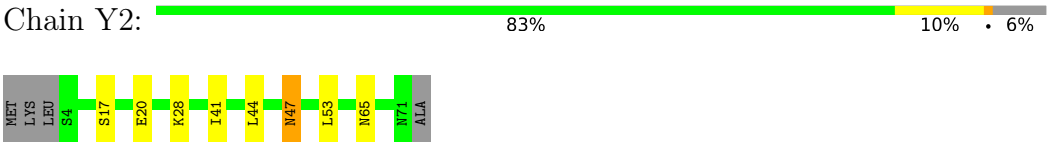
• Molecule 26: 50S ribosomal protein L29

Chain R2:



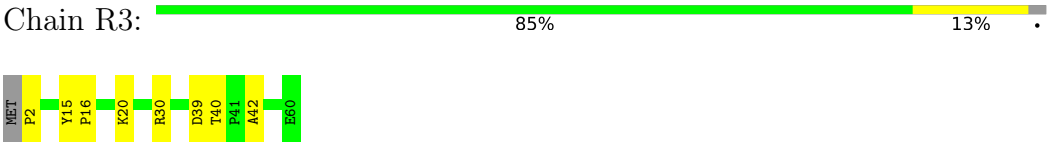
• Molecule 26: 50S ribosomal protein L29

Chain Y2:



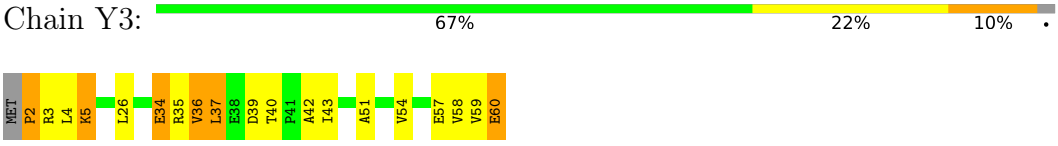
• Molecule 27: 50S ribosomal protein L30

Chain R3:



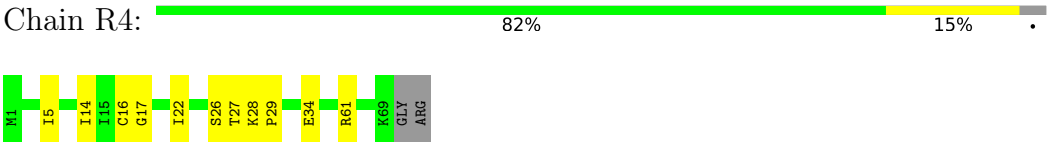
• Molecule 27: 50S ribosomal protein L30

Chain Y3:



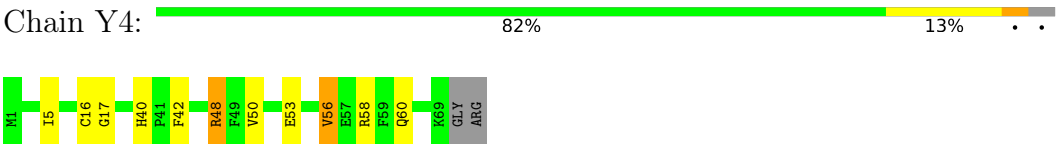
• Molecule 28: 50S ribosomal protein L31

Chain R4:



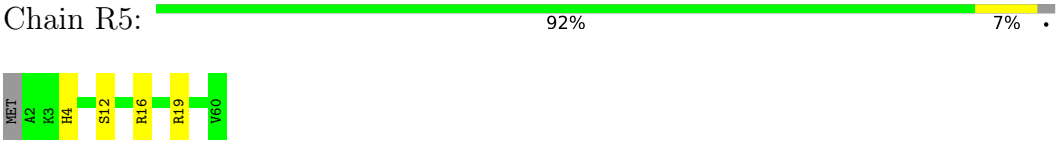
• Molecule 28: 50S ribosomal protein L31

Chain Y4:



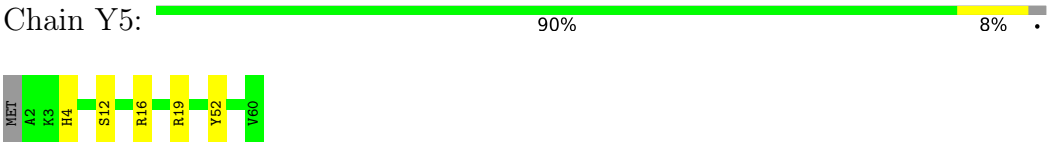
• Molecule 29: 50S ribosomal protein L32

Chain R5:



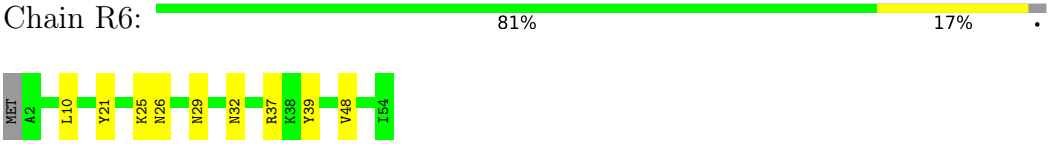
• Molecule 29: 50S ribosomal protein L32

Chain Y5:



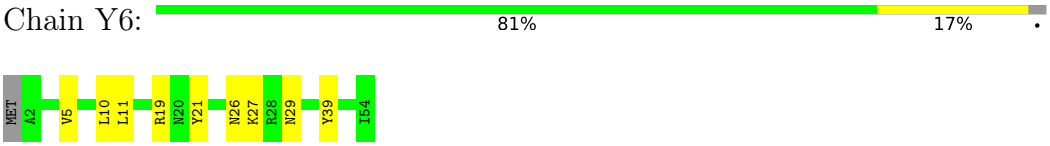
• Molecule 30: 50S ribosomal protein L33

Chain R6:



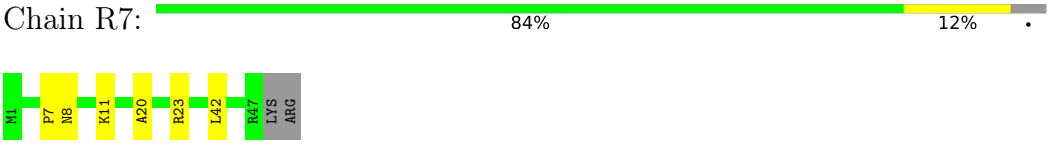
• Molecule 30: 50S ribosomal protein L33

Chain Y6:



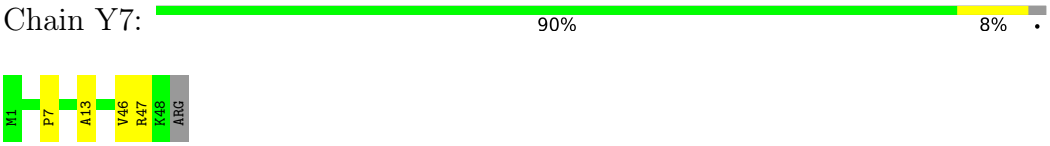
• Molecule 31: 50S ribosomal protein L34

Chain R7:



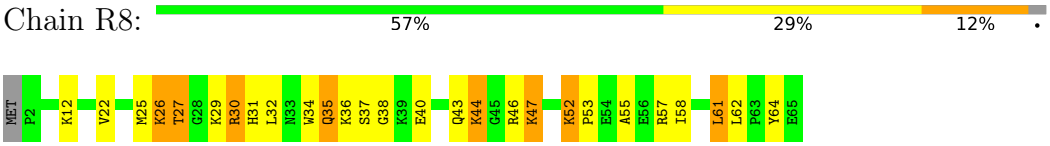
• Molecule 31: 50S ribosomal protein L34

Chain Y7:



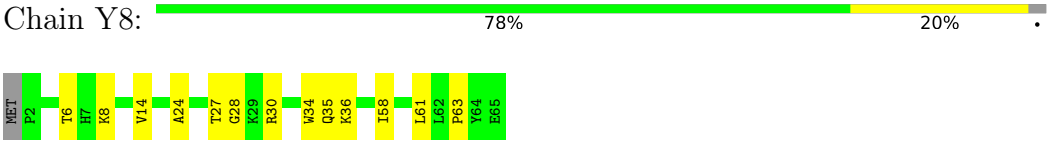
• Molecule 32: 50S ribosomal protein L35

Chain R8:



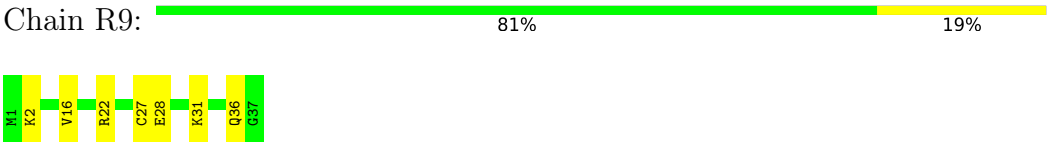
• Molecule 32: 50S ribosomal protein L35

Chain Y8:



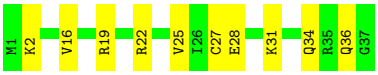
• Molecule 33: 50S ribosomal protein L36

Chain R9:



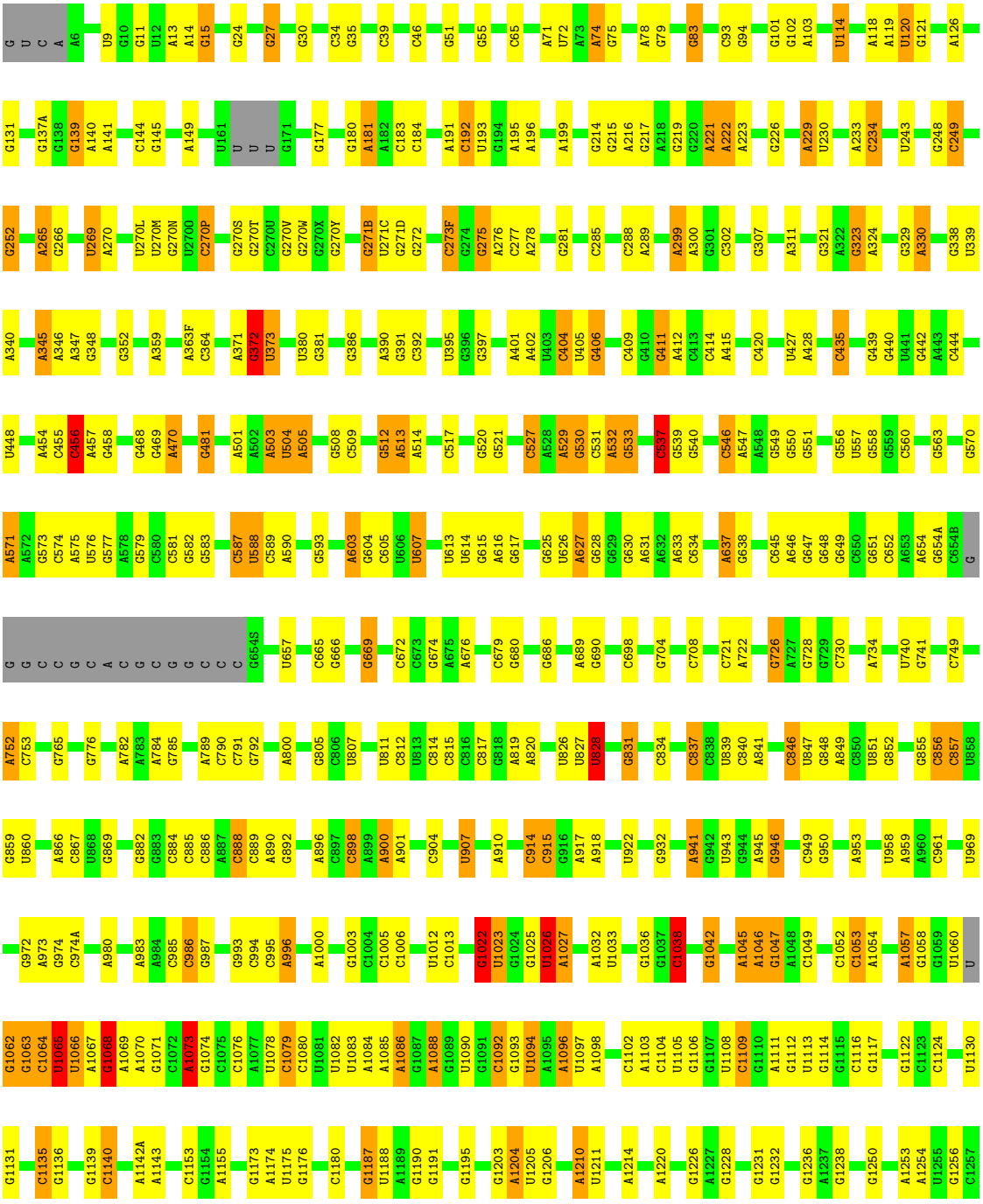
• Molecule 33: 50S ribosomal protein L36

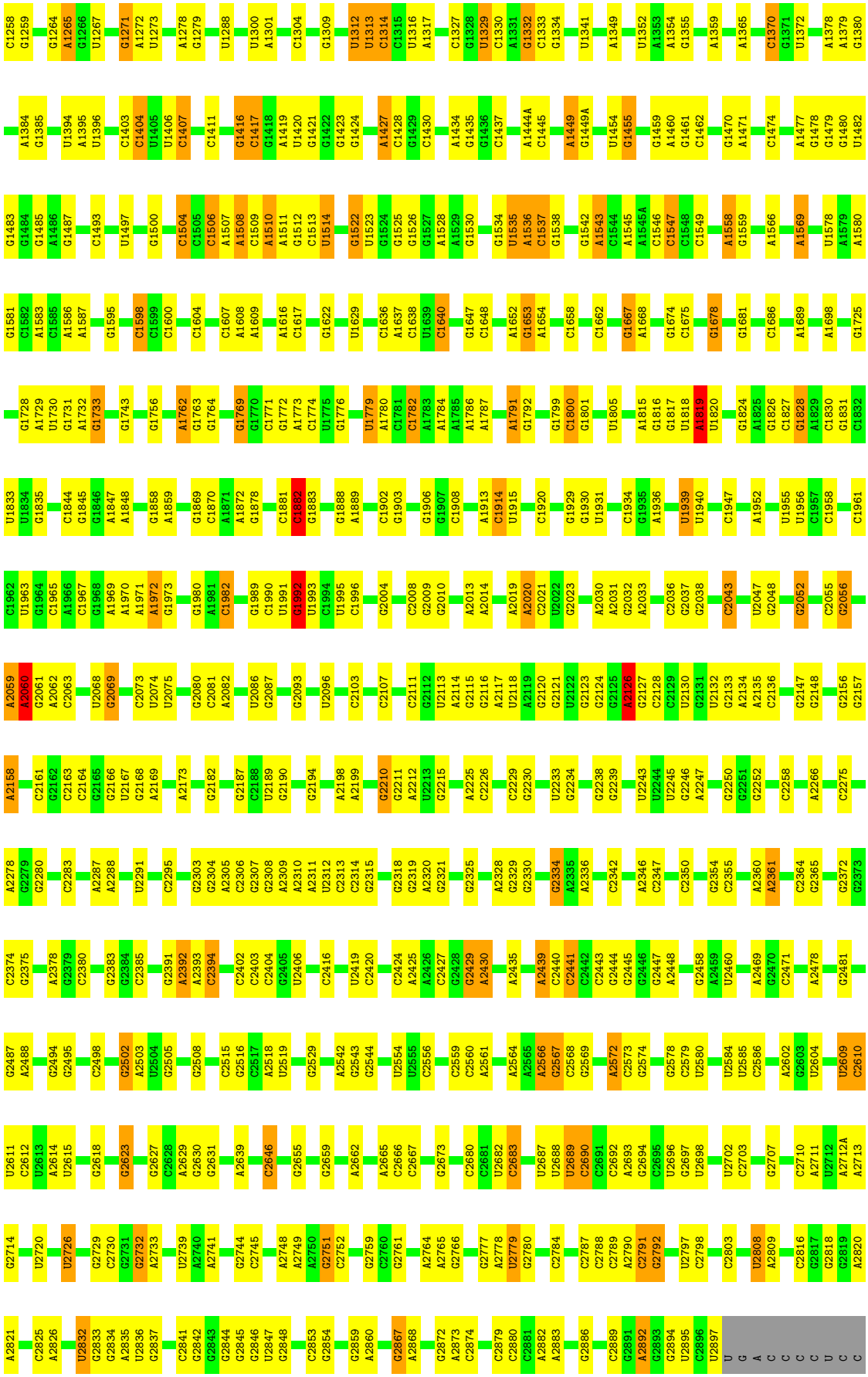
Chain Y9:



• Molecule 34: 23S rRNA

Chain RA:

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A1384 G1385 U1394 A1395 U1396 C1403 C1404 U1405 U1406 C1407 C1411 G1416 C1417 G1418 A1419 U1420 G1421 G1422 G1423 G1424 A1427 C1428 G1429 C1430 A1434 G1435 G1436 C1437 A1444A C1445 A1449 G1449A U1454 G1455 G1459 A1460 G1461 C1462 G1470 A1471 C1474 A1477 G1478 G1479 G1480 U1482
G1483 G1484 G1485 A1486 G1487 C1493 U1497 G1500 C1504 C1505 C1506 A1507 A1508 C1509 A1510 A1511 G1512 C1513 U1514 G1522 U1523 G1524 G1525 G1526 G1527 A1528 A1529 G1530 G1534 U1535 A1536 C1537 G1538 G1542 A1543 C1544 A1545 A1545A C1546 C1547 C1548 C1549 A1558 G1559 A1566 A1569 U1578 A1579 A1580
G1581 C1582 A1583 C1585 A1586 A1587 G1595 C1598 C1599 C1600 C1604 C1607 A1608 A1609 A1616 C1617 G1622 U1629 C1636 A1637 C1638 U1639 C1640 C1647 C1648 A1652 G1653 A1654 C1658 C1662 G1667 A1668 G1674 C1675 G1678 G1681 C1686 A1689 A1698 G1725
G1728 A1729 U1730 G1731 A1732 G1733 G1743 G1756 A1762 G1763 G1764 G1769 G1770 C1771 G1772 A1773 C1774 U1775 G1776 U1779 A1780 C1781 C1782 A1783 A1784 A1785 A1786 A1787 A1791 G1792 G1799 C1800 G1801 U1805 A1815 G1816 G1817 U1818 A1819 U1820 G1824 A1825 G1826 C1827 G1828 A1829 C1830 G1831 C1832
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C1962 U1963 G1964 C1965 A1966 C1967 G1968 A1969 A1970 A1971 A1972 G1973 G1980 A1981 C1982 G1989 C1990 U1991 G1992 U1993 C1994 U1995 C1996 G2004 C2008 G2009 G2010 A2013 A2014 A2019 A2020 C2021 U2022 G2023 A2030 A2031 G2032 A2033 C2036 G2037 G2038 C2043 U2047 G2048 G2052 C2055 G2056
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A2158 C2161 G2162 C2163 C2164 G2165 G2166 U2167 G2168 A2169 A2173 G2182 G2187 C2188 U2189 G2190 G2194 A2198 A2199 G2210 G2211 A2212 U2213 G2215 A2225 C2226 C2229 G2230 U2233 G2234 G2238 G2239 U2243 U2244 U2245 G2246 A2247 G2250 G2251 G2252 C2258 A2266 C2275
A2278 G2279 G2280 C2283 A2287 A2288 U2291 C2295 G2303 G2304 A2305 C2306 G2307 G2308 A2309 A2310 A2311 U2312 C2313 C2314 G2315 G2318 G2319 A2320 G2321 G2325 A2328 G2329 G2330 G2334 A2335 A2336 C2342 A2346 C2347 C2350 G2354 C2355 A2360 A2361 C2364 G2365 G2372 G2373
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U2611 C2612 U2613 A2614 U2615 G2618 G2623 G2627 C2628 A2629 G2630 G2631 A2639 C2646 G2655 G2659 A2662 A2665 C2666 C2667 G2673 C2680 C2681 U2682 C2683 U2687 U2688 U2689 C2690 C2691 C2692 A2693 G2694 C2695 U2696 G2697 U2698 U2702 C2703 G2707 C2710 A2711 U2712 A2712A A2713
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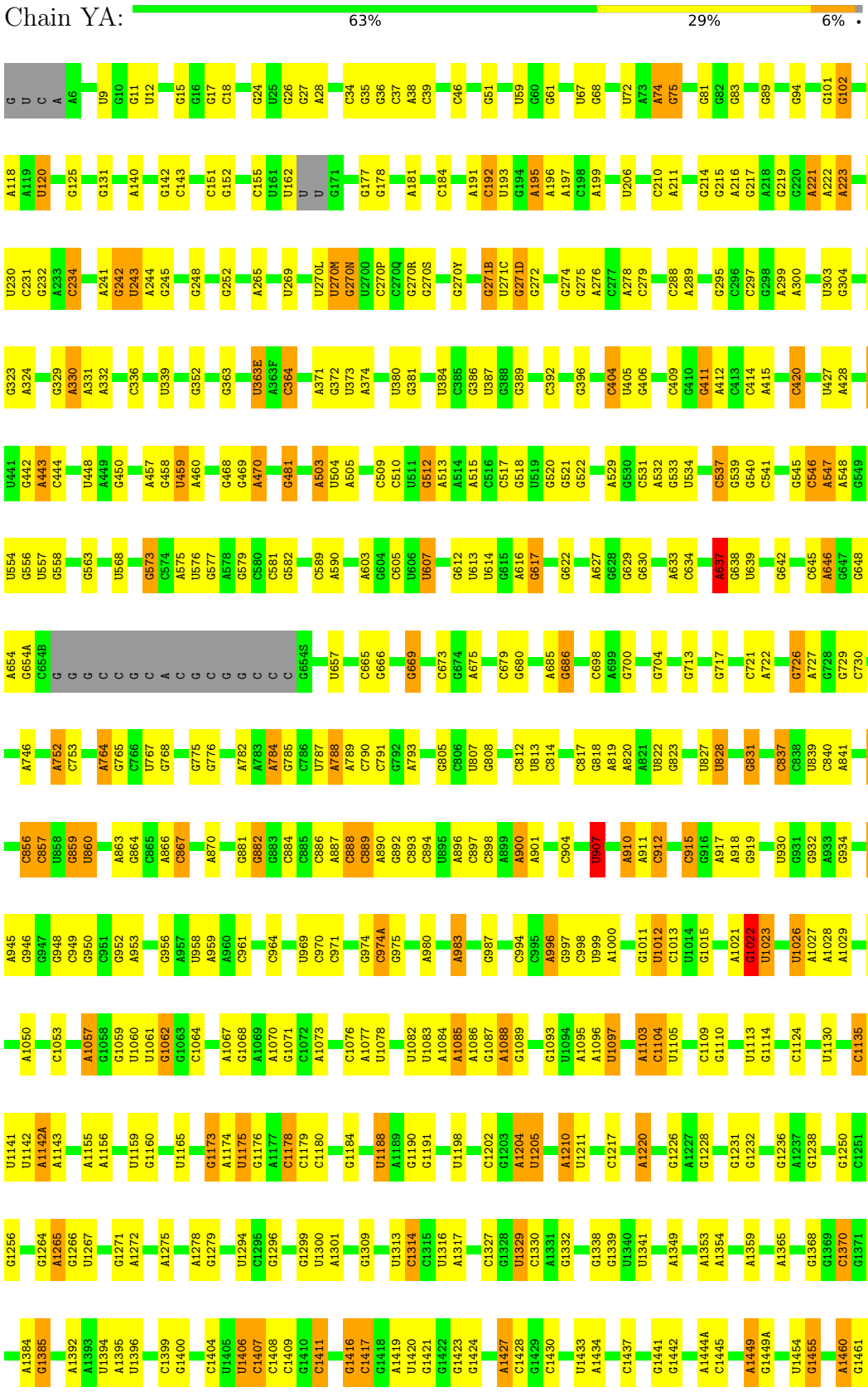
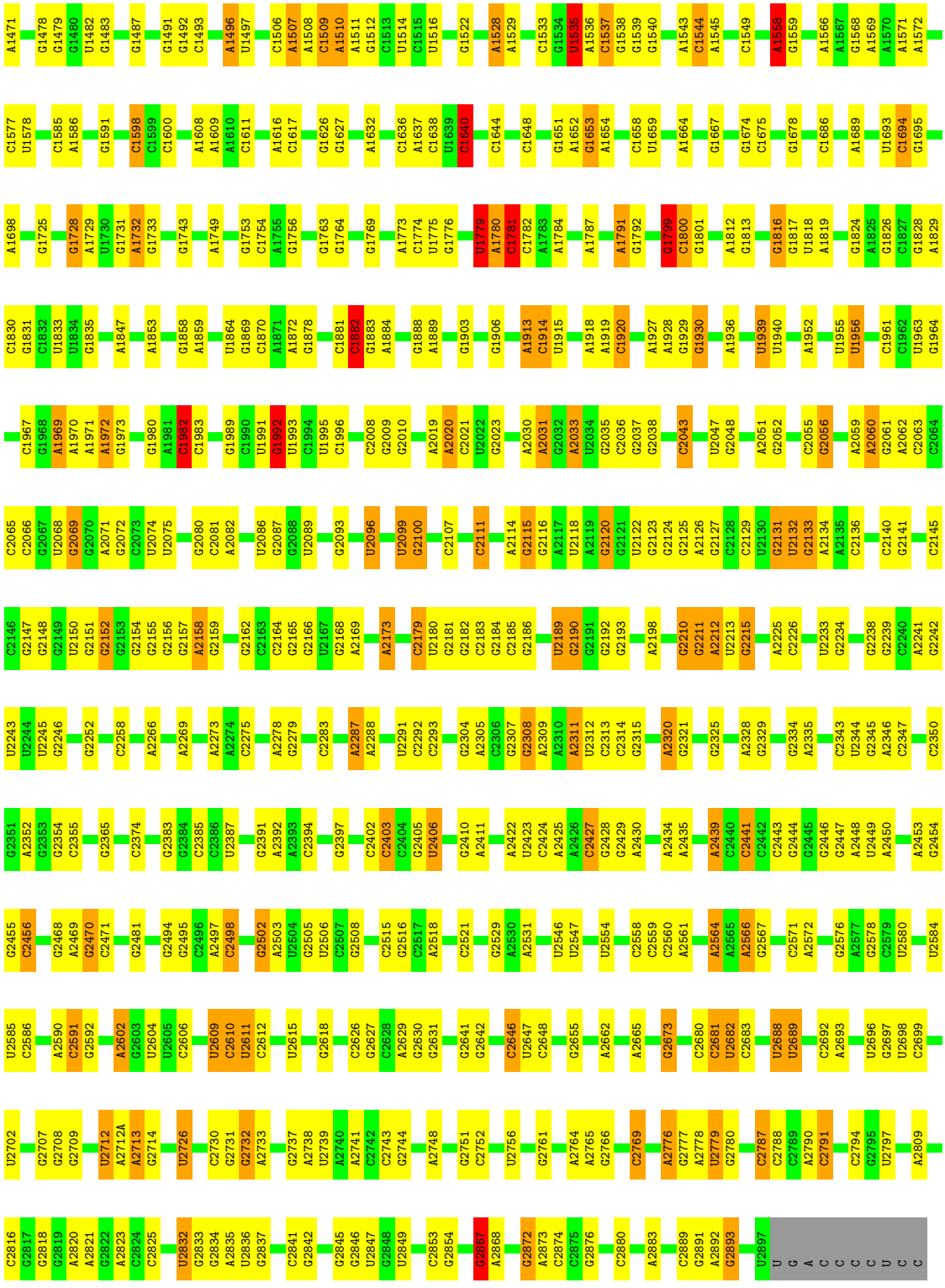
A2821 C2825 A2826 U2832 G2833 G2834 A2835 U2836 G2837 C2841 G2842 G2843 G2844 G2845 G2846 U2847 G2848 C2853 G2854 G2859 A2860 G2867 A2868 G2872 A2873 C2874 C2879 C2880 C2881 A2882 A2883 G2886 C2889 G2891 A2892 G2893 G2894 U2895 C2896 U2897 U G A C C C C U C C

• Molecule 34: 23S rRNA

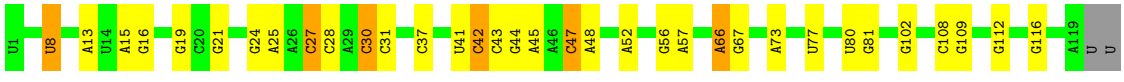
Chain YA:





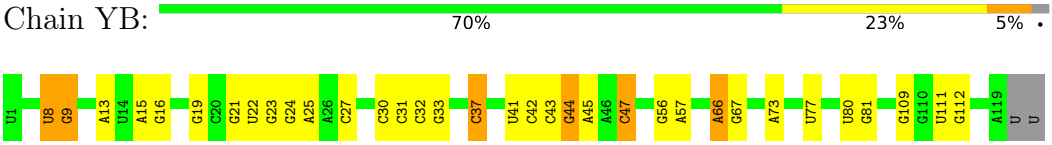
• Molecule 35: 5S rRNA

Chain RB:



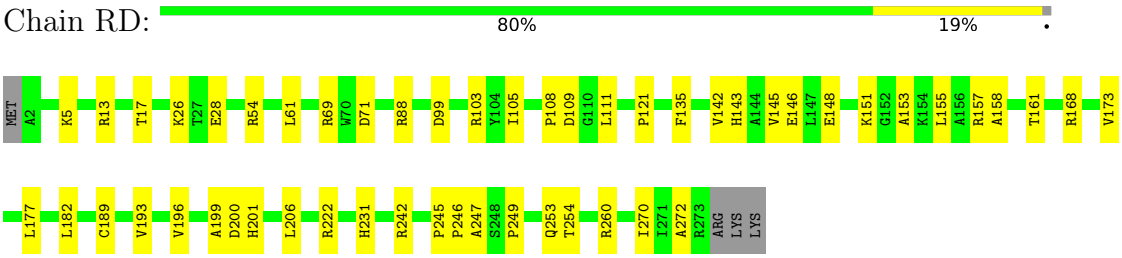
• Molecule 35: 5S rRNA

Chain YB:



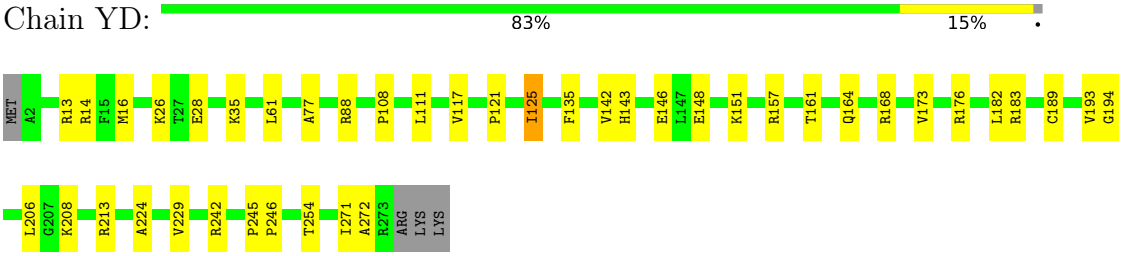
• Molecule 36: 50S ribosomal protein L2

Chain RD:



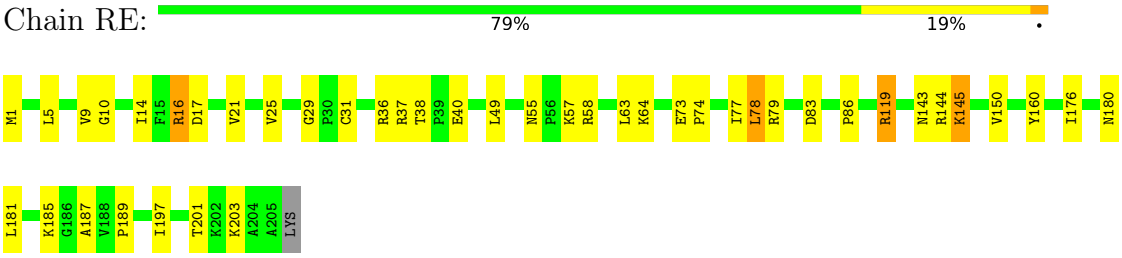
• Molecule 36: 50S ribosomal protein L2

Chain YD:



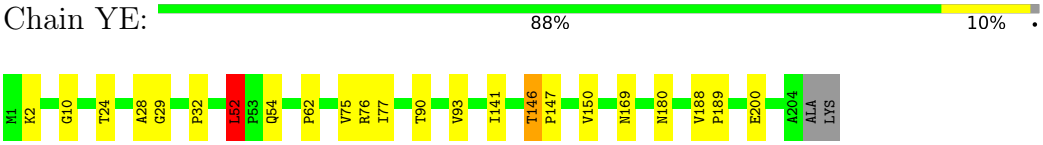
• Molecule 37: 50S ribosomal protein L3

Chain RE:



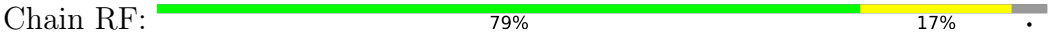
• Molecule 37: 50S ribosomal protein L3

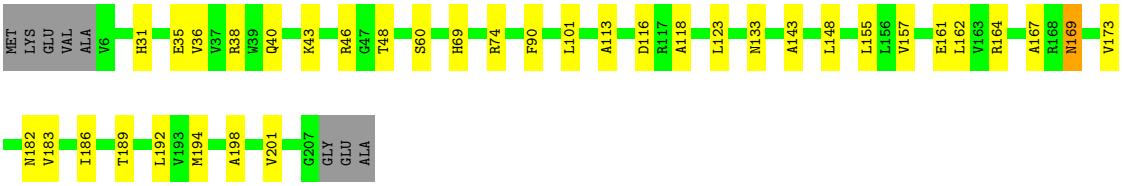
Chain YE:



• Molecule 38: 50S ribosomal protein L4

Chain RF:



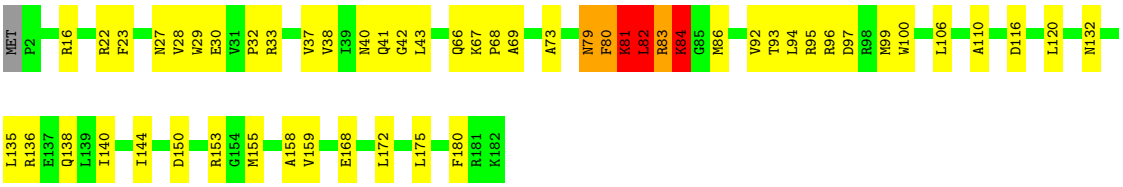


• Molecule 38: 50S ribosomal protein L4

Chain YF:

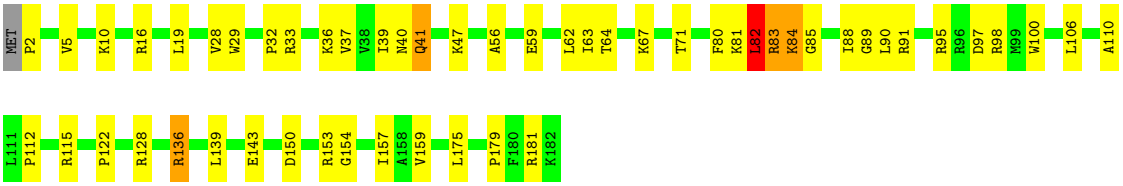
• Molecule 39: 50S ribosomal protein L5

Chain RG:



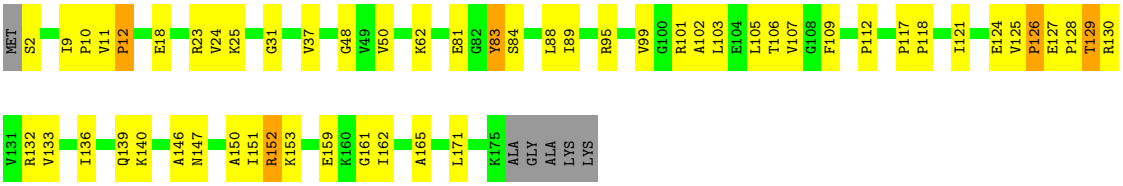
• Molecule 39: 50S ribosomal protein L5

Chain YG:



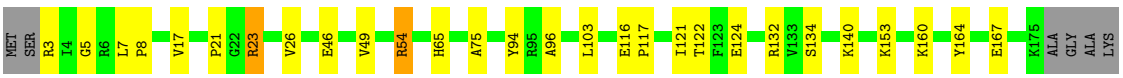
• Molecule 40: 50S ribosomal protein L6

Chain RH:



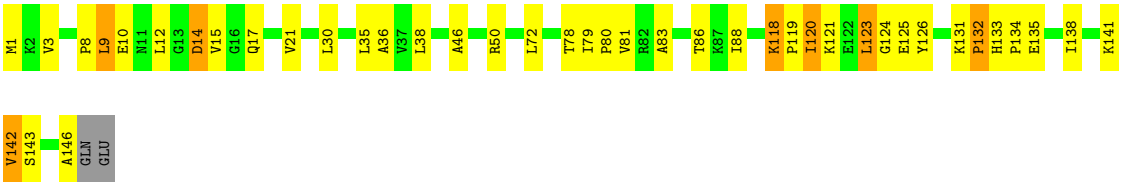
• Molecule 40: 50S ribosomal protein L6

Chain YH:



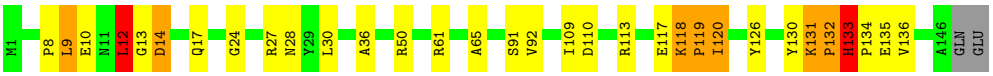
• Molecule 41: 50S ribosomal protein L9

Chain RI:



• Molecule 41: 50S ribosomal protein L9

Chain YI:



• Molecule 42: 50S ribosomal protein L13

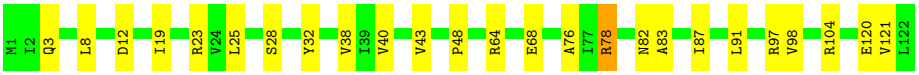
Chain RN:

• Molecule 42: 50S ribosomal protein L13

Chain YN:

• Molecule 43: 50S ribosomal protein L14

Chain RO:

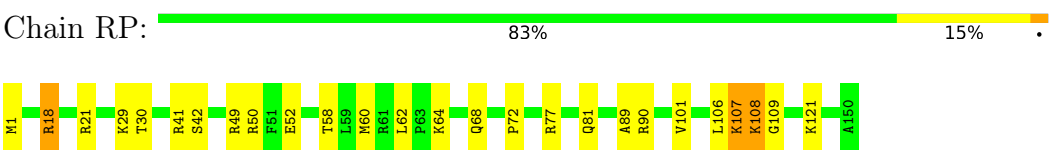


• Molecule 43: 50S ribosomal protein L14

Chain YO:

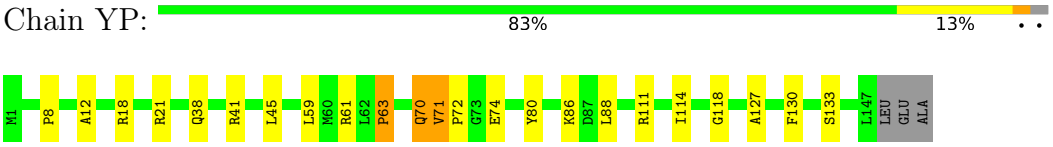
• Molecule 44: 50S ribosomal protein L15

Chain RP:



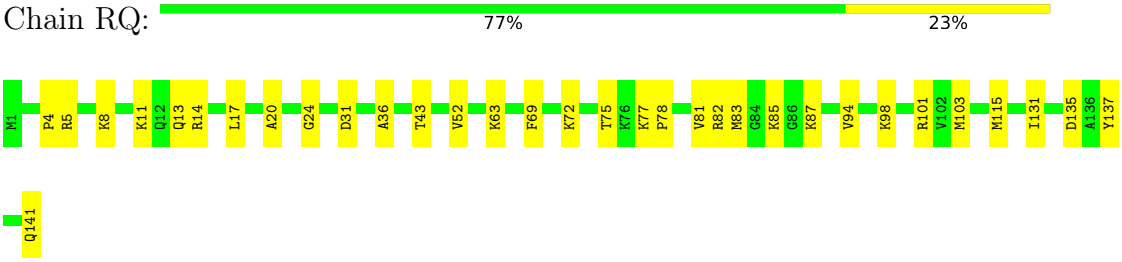
• Molecule 44: 50S ribosomal protein L15

Chain YP:



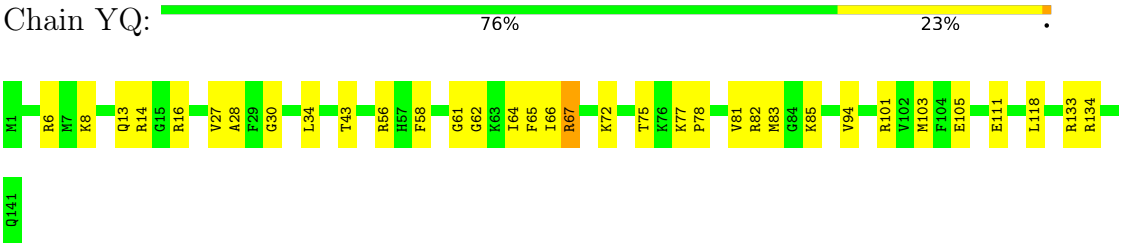
• Molecule 45: 50S ribosomal protein L16

Chain RQ:



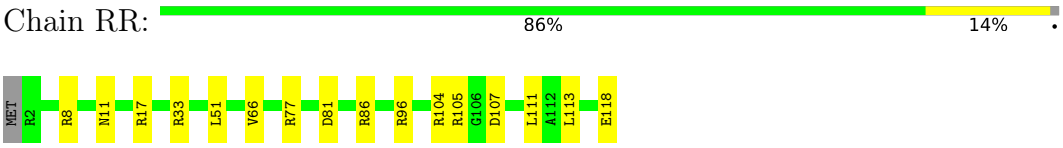
• Molecule 45: 50S ribosomal protein L16

Chain YQ:



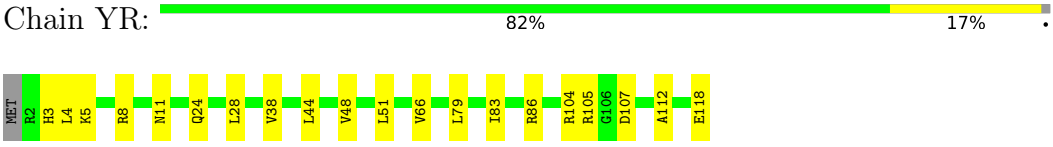
• Molecule 46: 50S ribosomal protein L17

Chain RR:



• Molecule 46: 50S ribosomal protein L17

Chain YR:



• Molecule 47: 50S ribosomal protein L18

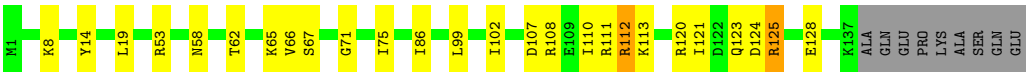
Chain RS:

• Molecule 47: 50S ribosomal protein L18

Chain YS:

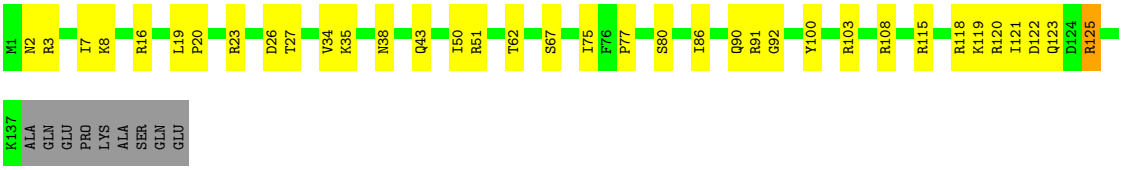
• Molecule 48: 50S ribosomal protein L19

Chain RT:



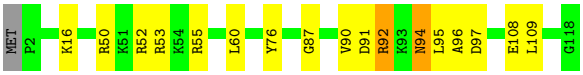
• Molecule 48: 50S ribosomal protein L19

Chain YT:



• Molecule 49: 50S ribosomal protein L20

Chain RU:

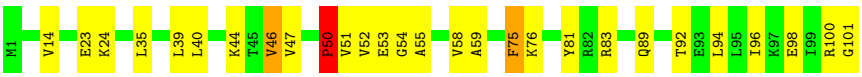


• Molecule 49: 50S ribosomal protein L20

Chain YU:

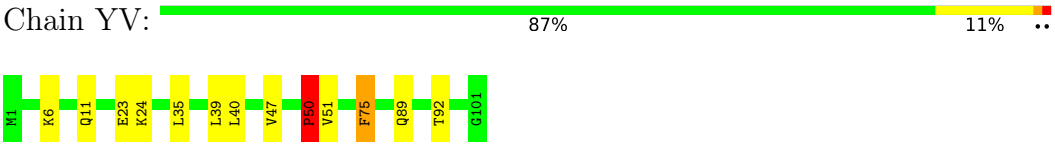
• Molecule 50: 50S ribosomal protein L21

Chain RV:



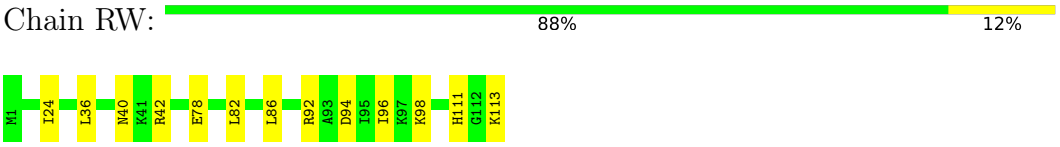
• Molecule 50: 50S ribosomal protein L21

Chain YV:



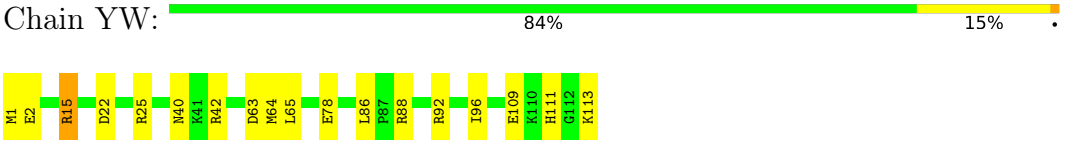
• Molecule 51: 50S ribosomal protein L22

Chain RW:



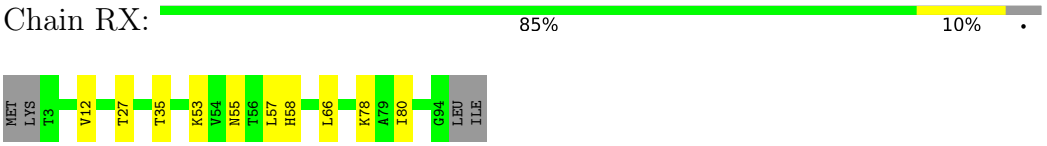
• Molecule 51: 50S ribosomal protein L22

Chain YW:



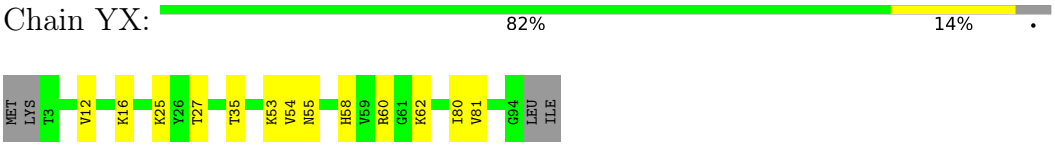
• Molecule 52: 50S ribosomal protein L23

Chain RX:



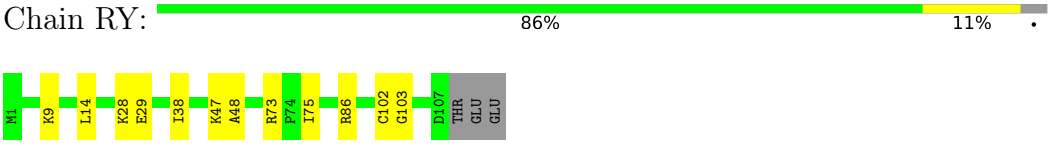
• Molecule 52: 50S ribosomal protein L23

Chain YX:



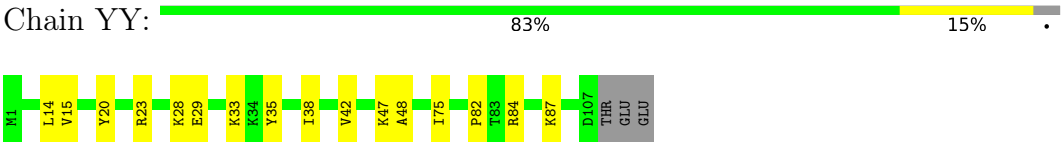
• Molecule 53: 50S ribosomal protein L24

Chain RY:



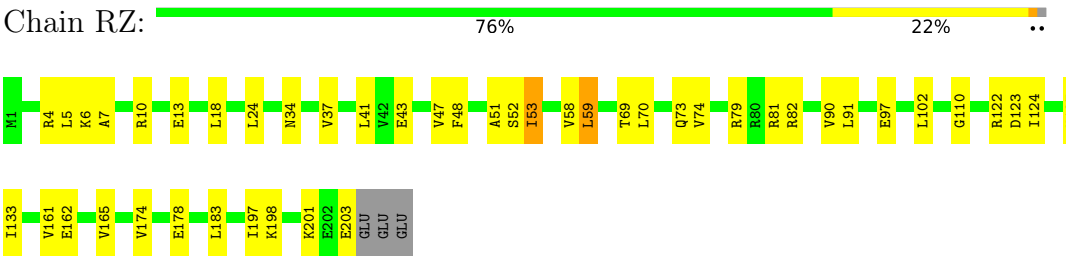
• Molecule 53: 50S ribosomal protein L24

Chain YY:



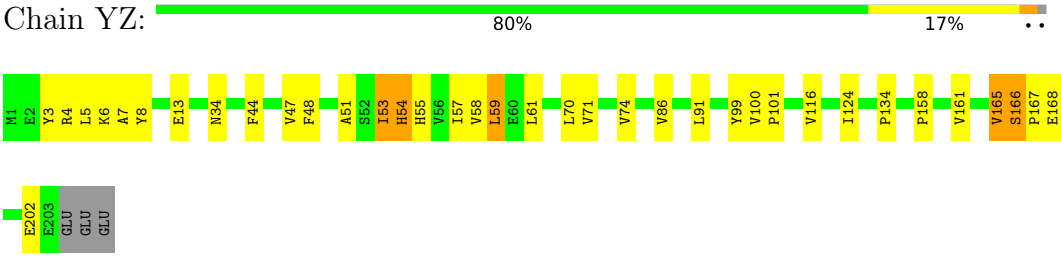
• Molecule 54: 50S ribosomal protein L25

Chain RZ:



• Molecule 54: 50S ribosomal protein L25

Chain YZ:

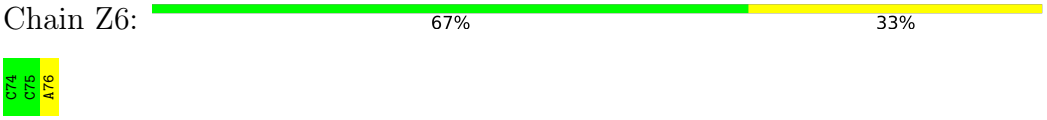


• Molecule 55: A-site ASL^Phe

Chain XY:

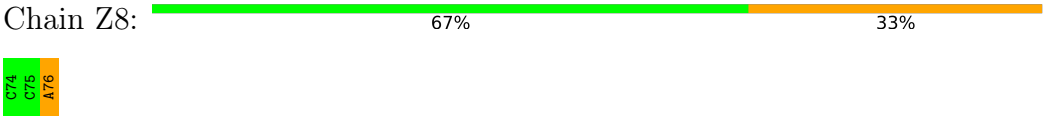
• Molecule 56: CC-puro

Chain Z6:



• Molecule 56: CC-puro

Chain Z8:



4 Data and refinement statistics (i)

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	210.56Å 447.23Å 618.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	174.01 – 3.64	Depositor
% Data completeness (in resolution range)	95.7 (174.01-3.64)	Depositor
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.232 , 0.278	Depositor
Wilson B-factor (Å^2)	105.8	Xtriage
Anisotropy	0.167	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	292577	wwPDB-VP
Average B, all atoms (Å^2)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PPU, MG, MNU, T6A, SF4, ZN

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	0.33	0/36098	1.06	143/56341 (0.3%)
1	XA	0.33	0/36346	1.06	155/56725 (0.3%)
2	QB	0.29	0/1942	0.54	0/2619
2	XB	0.28	0/1950	0.55	0/2630
3	QC	0.28	0/1629	0.54	0/2195
3	XC	0.28	0/1629	0.57	0/2195
4	QD	0.28	0/1733	0.50	0/2318
4	XD	0.30	0/1733	0.52	0/2318
5	QE	0.27	0/1171	0.53	0/1576
5	XE	0.27	0/1171	0.55	0/1576
6	QF	0.25	0/856	0.51	0/1154
6	XF	0.25	0/856	0.50	0/1154
7	QG	0.26	0/1276	0.49	0/1709
7	XG	0.27	0/1276	0.54	0/1709
8	QH	0.25	0/1128	0.49	0/1517
8	XH	0.25	0/1128	0.51	0/1517
9	QI	0.53	3/1029 (0.3%)	0.73	2/1379 (0.1%)
9	XI	0.32	0/1017	0.61	0/1365
10	QJ	0.28	0/814	0.56	1/1095 (0.1%)
10	XJ	0.27	0/790	0.59	0/1063
11	QK	0.26	0/900	0.50	0/1213
11	XK	0.27	0/879	0.49	0/1187
12	QL	0.30	0/991	0.57	0/1327
12	XL	0.30	0/972	0.56	0/1301
13	QM	0.30	0/965	0.58	0/1292
13	XM	0.28	0/956	0.62	0/1281
14	QN	0.35	0/501	0.58	0/664
14	XN	0.31	0/501	0.62	0/664
15	QO	0.25	0/745	0.49	0/992
15	XO	0.25	0/740	0.45	0/987
16	QP	0.26	0/721	0.51	0/970
16	XP	0.26	0/721	0.49	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
17	QQ	0.25	0/847	0.49	0/1131
17	XQ	0.26	0/847	0.50	0/1131
18	QR	0.28	0/579	0.61	0/768
18	XR	0.27	0/579	0.56	0/768
19	QS	0.28	0/680	0.59	0/915
19	XS	0.27	0/689	0.62	1/926 (0.1%)
20	QT	0.29	0/765	0.56	0/1007
20	XT	0.29	0/765	0.55	0/1007
21	QU	0.25	0/221	0.44	0/288
21	XU	0.23	0/221	0.48	0/288
22	QV	0.43	1/1706 (0.1%)	1.22	13/2652 (0.5%)
22	XV	0.39	0/1706	1.20	13/2652 (0.5%)
23	QX	0.35	0/72	1.01	0/110
23	XX	0.32	0/560	1.09	2/872 (0.2%)
24	R0	0.25	0/611	0.49	0/814
24	Y0	0.26	0/607	0.47	0/809
25	R1	0.28	0/770	0.56	0/1022
25	Y1	0.28	0/736	0.55	0/978
26	R2	0.26	0/583	0.54	0/771
26	Y2	0.27	0/577	0.51	0/764
27	R3	0.26	0/474	0.52	0/635
27	Y3	0.35	0/474	0.61	0/635
28	R4	0.29	0/578	0.60	0/776
28	Y4	0.29	0/578	0.57	0/776
29	R5	0.26	0/473	0.50	0/639
29	Y5	0.25	0/473	0.49	0/639
30	R6	0.24	0/460	0.50	0/613
30	Y6	0.25	0/460	0.47	0/613
31	R7	0.25	0/417	0.44	0/550
31	Y7	0.24	0/426	0.44	0/561
32	R8	0.40	0/525	0.72	0/691
32	Y8	0.27	0/525	0.51	0/691
33	R9	0.23	0/310	0.48	0/407
33	Y9	0.23	0/310	0.46	0/407
34	RA	0.35	0/69498	1.08	333/108491 (0.3%)
34	YA	0.34	0/69543	1.07	307/108563 (0.3%)
35	RB	0.35	0/2878	1.13	18/4490 (0.4%)
35	YB	0.36	0/2878	1.13	17/4490 (0.4%)
36	RD	0.29	0/2165	0.54	0/2919
36	YD	0.30	0/2165	0.53	0/2919
37	RE	0.35	0/1601	0.64	1/2160 (0.0%)
37	YE	0.30	0/1596	0.55	0/2153
38	RF	0.30	0/1620	0.61	0/2194

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	YF	0.29	0/1620	0.60	0/2194
39	RG	0.31	0/1499	0.61	0/2016
39	YG	0.33	0/1499	0.61	0/2016
40	RH	0.36	0/1362	0.71	1/1841 (0.1%)
40	YH	0.28	0/1356	0.52	0/1833
41	RI	0.36	0/1151	0.66	0/1558
41	YI	0.41	1/1151 (0.1%)	0.65	0/1558
42	RN	0.29	0/1131	0.53	0/1525
42	YN	0.27	0/1131	0.53	0/1525
43	RO	0.28	0/943	0.52	0/1269
43	YO	0.27	0/943	0.52	0/1269
44	RP	0.31	0/1162	0.66	0/1544
44	YP	0.30	0/1139	0.59	0/1514
45	RQ	0.30	0/1143	0.60	0/1527
45	YQ	0.31	0/1143	0.60	0/1527
46	RR	0.26	0/974	0.57	0/1302
46	YR	0.27	0/974	0.57	0/1302
47	RS	0.31	0/892	0.68	1/1187 (0.1%)
47	YS	0.30	0/892	0.64	1/1187 (0.1%)
48	RT	0.30	0/1155	0.59	0/1542
48	YT	0.29	0/1155	0.58	0/1542
49	RU	0.30	0/982	0.59	1/1306 (0.1%)
49	YU	0.33	0/982	0.64	1/1306 (0.1%)
50	RV	0.34	0/790	0.70	2/1057 (0.2%)
50	YV	0.34	0/790	0.73	3/1057 (0.3%)
51	RW	0.26	0/911	0.51	0/1220
51	YW	0.29	0/911	0.54	0/1220
52	RX	0.27	0/739	0.53	1/993 (0.1%)
52	YX	0.27	0/739	0.52	0/993
53	RY	0.26	0/831	0.51	0/1108
53	YY	0.27	0/831	0.51	0/1108
54	RZ	0.32	0/1634	0.64	2/2216 (0.1%)
54	YZ	0.31	0/1634	0.56	0/2216
55	XY	0.34	0/405	1.11	0/630
56	Z6	0.44	0/40	1.44	0/60
56	Z8	0.40	0/40	1.28	0/60
All	All	0.33	5/316386 (0.0%)	0.96	1019/473016 (0.2%)

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
27	Y3	0	1
37	YE	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	YI	133	HIS	C-N	8.27	1.50	1.34
9	QI	10	ARG	CZ-NH1	6.74	1.41	1.33
9	QI	37	PHE	CA-CB	6.25	1.67	1.53
9	QI	10	ARG	CA-CB	5.60	1.66	1.53
22	QV	53	G	C2-N3	-5.05	1.28	1.32

All (1019) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	XV	53	G	OP1-P-O3'	-14.20	73.97	105.20
1	QA	1158	C	N1-C2-O2	12.73	126.54	118.90
1	QA	1158	C	C2-N1-C1'	12.38	132.42	118.80
22	QV	53	G	C2-N3-C4	12.10	117.95	111.90
35	RB	31	C	C2-N1-C1'	10.59	130.45	118.80
1	QA	1301	U	N1-C2-O2	10.51	130.16	122.80
34	RA	828	U	C2-N1-C1'	10.51	130.31	117.70
1	QA	1301	U	C2-N1-C1'	10.39	130.17	117.70
34	RA	546	C	N1-C2-O2	10.38	125.13	118.90
34	YA	1313	U	N1-C2-O2	10.01	129.81	122.80
35	YB	31	C	C2-N1-C1'	9.98	129.78	118.80
34	YA	1313	U	C2-N1-C1'	9.93	129.61	117.70
1	QA	1158	C	N3-C2-O2	-9.88	114.99	121.90
34	RA	828	U	N1-C2-O2	9.85	129.69	122.80
22	QV	53	G	N3-C4-C5	-9.54	123.83	128.60
34	RA	546	C	C2-N1-C1'	9.47	129.22	118.80
35	RB	31	C	N1-C2-O2	9.46	124.57	118.90
34	YA	1313	U	N3-C2-O2	-9.38	115.63	122.20
35	YB	31	C	N1-C2-O2	9.38	124.53	118.90
1	QA	1301	U	N3-C2-O2	-9.36	115.65	122.20
34	RA	1396	U	N3-C2-O2	-9.32	115.68	122.20
1	QA	307	C	N1-C2-O2	9.25	124.45	118.90
34	YA	828	U	C2-N1-C1'	9.19	128.72	117.70
22	XV	53	G	C2-N3-C4	9.12	116.46	111.90
34	RA	1313	U	N3-C2-O2	-9.05	115.86	122.20
34	RA	1313	U	C2-N1-C1'	9.00	128.50	117.70
34	RA	1313	U	N1-C2-O2	8.98	129.09	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	QA	328	C	N1-C2-O2	8.97	124.28	118.90
1	XA	358	U	N3-C2-O2	-8.95	115.94	122.20
34	RA	828	U	N3-C2-O2	-8.91	115.97	122.20
34	YA	860	U	N3-C2-O2	-8.78	116.05	122.20
34	YA	1914	C	C2-N1-C1'	8.72	128.39	118.80
34	RA	1914	C	N1-C2-O2	8.66	124.10	118.90
34	RA	1407	C	C2-N1-C1'	8.65	128.31	118.80
34	YA	1407	C	C2-N1-C1'	8.64	128.31	118.80
34	RA	1396	U	N1-C2-O2	8.57	128.80	122.80
1	XA	330	C	N1-C2-O2	8.57	124.04	118.90
1	QA	328	C	C2-N1-C1'	8.55	128.21	118.80
1	QA	1158	C	C6-N1-C1'	-8.55	110.54	120.80
34	RA	1774	C	C6-N1-C2	-8.47	116.91	120.30
34	RA	1882	C	C2-N1-C1'	8.44	128.09	118.80
34	YA	1535	U	C2-N1-C1'	8.43	127.82	117.70
22	QV	53	G	N1-C6-O6	-8.38	114.87	119.90
34	YA	120	U	N1-C2-O2	8.37	128.66	122.80
34	RA	856	C	C6-N1-C2	-8.36	116.96	120.30
34	RA	1108	U	N1-C2-O2	8.35	128.65	122.80
1	XA	135	C	C6-N1-C2	-8.32	116.97	120.30
34	YA	1535	U	N1-C2-O2	8.30	128.61	122.80
34	RA	546	C	N3-C2-O2	-8.30	116.09	121.90
34	YA	120	U	N3-C2-O2	-8.28	116.40	122.20
34	RA	1108	U	C2-N1-C1'	8.27	127.62	117.70
34	RA	546	C	C6-N1-C2	-8.24	117.01	120.30
22	XV	54	U	OP1-P-OP2	8.23	131.95	119.60
1	QA	1158	C	C6-N1-C2	-8.21	117.02	120.30
1	XA	358	U	N1-C2-O2	8.15	128.50	122.80
1	XA	979	C	C6-N1-C2	-8.12	117.05	120.30
34	RA	1774	C	N1-C2-O2	7.98	123.69	118.90
1	QA	1066	C	N1-C2-O2	7.95	123.67	118.90
1	QA	1381	U	N1-C2-O2	7.94	128.36	122.80
34	YA	120	U	C2-N1-C1'	7.90	127.18	117.70
1	XA	812	C	P-O3'-C3'	7.89	129.17	119.70
34	YA	856	C	C6-N1-C2	-7.88	117.15	120.30
1	QA	307	C	N3-C2-O2	-7.85	116.41	121.90
34	YA	828	U	N1-C2-O2	7.84	128.29	122.80
34	YA	1640	C	N1-C2-O2	7.84	123.60	118.90
34	RA	1914	C	C2-N1-C1'	7.83	127.42	118.80
34	RA	1109	C	N1-C2-O2	7.82	123.59	118.90
34	RA	2666	C	N1-C2-O2	7.81	123.59	118.90
34	RA	1108	U	N3-C2-O2	-7.81	116.73	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	QV	53	G	C8-N9-C4	-7.80	103.28	106.40
34	YA	1774	C	N3-C2-O2	-7.77	116.46	121.90
34	YA	1535	U	N3-C2-O2	-7.76	116.77	122.20
1	XA	449	C	C2-N1-C1'	7.73	127.30	118.80
1	QA	1066	C	C2-N1-C1'	7.72	127.30	118.80
34	RA	1956	U	N3-C2-O2	-7.72	116.80	122.20
34	RA	1314	C	C2-N1-C1'	7.72	127.29	118.80
34	YA	1882	C	C2-N1-C1'	7.72	127.29	118.80
34	YA	2456	C	C5-C6-N1	7.69	124.84	121.00
35	RB	31	C	C6-N1-C2	-7.62	117.25	120.30
1	QA	1381	U	N3-C2-O2	-7.62	116.86	122.20
34	RA	435	C	N1-C2-O2	7.62	123.47	118.90
34	RA	1065	U	N3-C2-O2	-7.59	116.89	122.20
34	RA	1774	C	N3-C2-O2	-7.59	116.59	121.90
35	RB	27	C	N1-C2-O2	7.59	123.45	118.90
34	YA	1774	C	N1-C2-O2	7.58	123.45	118.90
35	YB	31	C	C6-N1-C2	-7.57	117.27	120.30
34	YA	867	C	N1-C2-O2	7.57	123.44	118.90
34	YA	1914	C	N1-C2-O2	7.55	123.43	118.90
1	QA	1028(A)	C	N1-C2-O2	7.53	123.42	118.90
34	YA	1407	C	C6-N1-C2	-7.51	117.29	120.30
34	RA	373	U	N1-C2-O2	7.50	128.05	122.80
34	YA	2210	G	C4-N9-C1'	7.49	136.24	126.50
34	RA	120	U	N1-C2-O2	7.47	128.03	122.80
34	YA	1956	U	N3-C2-O2	-7.45	116.98	122.20
47	YS	110	LEU	CA-CB-CG	7.44	132.40	115.30
34	RA	373	U	C2-N1-C1'	7.42	126.60	117.70
34	YA	1920	C	C5-C6-N1	7.42	124.71	121.00
34	RA	2832	U	P-O3'-C3'	7.42	128.60	119.70
34	RA	1640	C	N1-C2-O2	7.40	123.34	118.90
1	XA	449	C	N1-C2-O2	7.40	123.34	118.90
34	YA	1406	U	C2-N1-C1'	7.38	126.56	117.70
34	RA	2210	G	C4-N9-C1'	7.37	136.08	126.50
34	RA	120	U	N3-C2-O2	-7.35	117.05	122.20
1	XA	747	C	N1-C2-O2	7.35	123.31	118.90
34	RA	120	U	C2-N1-C1'	7.34	126.51	117.70
34	RA	1038	C	N1-C2-O2	7.34	123.30	118.90
34	RA	1065	U	P-O3'-C3'	7.31	128.48	119.70
1	QA	110	C	N1-C2-O2	7.30	123.28	118.90
34	YA	435	C	N1-C2-O2	7.30	123.28	118.90
35	RB	31	C	C6-N1-C1'	-7.29	112.06	120.80
34	RA	1065	U	C6-N1-C2	-7.28	116.63	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	XA	1113	C	C6-N1-C2	-7.28	117.39	120.30
34	RA	456	C	N1-C2-O2	7.28	123.27	118.90
1	XA	747	C	N3-C2-O2	-7.27	116.81	121.90
1	XA	110	C	N1-C2-O2	7.26	123.26	118.90
22	XV	53	G	N3-C4-C5	-7.23	124.98	128.60
34	RA	2874	C	C2-N1-C1'	7.23	126.76	118.80
34	YA	1204	A	O4'-C1'-N9	7.20	113.96	108.20
1	QA	330	C	N1-C2-O2	7.19	123.21	118.90
34	RA	2321	G	N3-C4-C5	-7.19	125.01	128.60
34	YA	2063	C	N1-C2-O2	7.18	123.21	118.90
34	RA	2868	A	C8-N9-C4	-7.18	102.93	105.80
34	YA	1411	C	C2-N1-C1'	7.17	126.68	118.80
1	QA	1297	C	P-O3'-C3'	7.16	128.29	119.70
1	XA	1158	C	C2-N1-C1'	7.16	126.67	118.80
1	QA	1065	U	P-O3'-C3'	7.14	128.27	119.70
34	RA	373	U	N3-C2-O2	-7.14	117.20	122.20
35	YB	31	C	N3-C2-O2	-7.14	116.90	121.90
1	QA	328	C	P-O3'-C3'	7.13	128.26	119.70
22	QV	61	C	N3-C4-C5	-7.13	119.05	121.90
34	RA	856	C	C5-C6-N1	7.13	124.56	121.00
1	QA	90	C	C2-N1-C1'	7.11	126.62	118.80
34	YA	2874	C	C2-N1-C1'	7.10	126.61	118.80
34	YA	837	C	N1-C2-O2	7.09	123.16	118.90
34	YA	828	U	N3-C2-O2	-7.08	117.24	122.20
1	XA	1028(A)	C	C6-N1-C2	-7.04	117.48	120.30
34	YA	2321	G	N3-C4-C5	-7.04	125.08	128.60
1	QA	1158	C	C5-C6-N1	7.04	124.52	121.00
34	YA	607	U	N1-C2-O2	7.03	127.72	122.80
1	XA	979	C	N3-C2-O2	-7.03	116.98	121.90
34	RA	1065	U	C5-C6-N1	7.00	126.20	122.70
34	YA	860	U	C2-N1-C1'	6.99	126.09	117.70
34	RA	1956	U	N1-C2-O2	6.99	127.69	122.80
34	RA	828	U	C6-N1-C1'	-6.97	111.44	121.20
1	XA	410	G	OP1-P-O3'	6.96	120.51	105.20
1	QA	1528	U	P-O3'-C3'	6.95	128.03	119.70
34	RA	837	C	C6-N1-C2	-6.95	117.52	120.30
34	RA	1022	G	P-O3'-C3'	6.93	128.02	119.70
34	YA	234	C	N1-C2-O2	6.93	123.06	118.90
1	QA	250	A	P-O3'-C3'	6.92	128.00	119.70
35	RB	31	C	N3-C2-O2	-6.92	117.06	121.90
34	RA	1314	C	C5-C6-N1	6.92	124.46	121.00
34	YA	1406	U	N1-C2-O2	6.92	127.64	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	YA	1558	A	P-O3'-C3'	6.91	127.99	119.70
34	YA	2210	G	N3-C4-C5	-6.91	125.15	128.60
34	RA	1396	U	C2-N1-C1'	6.89	125.97	117.70
1	QA	169	C	N1-C2-O2	6.89	123.03	118.90
1	QA	1163	C	C2-N1-C1'	6.89	126.38	118.80
1	XA	992	U	P-O3'-C3'	6.89	127.97	119.70
34	YA	2063	C	N3-C2-O2	-6.89	117.08	121.90
34	YA	2832	U	P-O3'-C3'	6.88	127.96	119.70
34	YA	1202	C	N1-C2-O2	6.88	123.03	118.90
34	YA	846	C	P-O3'-C3'	6.88	127.95	119.70
1	QA	792	A	P-O3'-C3'	6.87	127.95	119.70
1	QA	992	U	P-O3'-C3'	6.87	127.94	119.70
34	RA	1064	C	C6-N1-C2	-6.87	117.55	120.30
34	RA	1396	U	C6-N1-C2	-6.87	116.88	121.00
34	YA	2394	C	N1-C2-O2	6.87	123.02	118.90
1	QA	913	A	P-O3'-C3'	6.87	127.94	119.70
1	QA	1498	U	P-O3'-C3'	6.87	127.94	119.70
1	XA	1533	C	C2-N1-C1'	6.86	126.35	118.80
34	RA	2126	A	P-O3'-C3'	6.86	127.93	119.70
34	RA	1404	C	C2-N1-C1'	6.86	126.34	118.80
34	RA	1514	U	N1-C2-O2	6.86	127.60	122.80
1	QA	1066	C	C5-C6-N1	6.85	124.43	121.00
34	YA	1022	G	P-O3'-C3'	6.85	127.92	119.70
34	RA	1109	C	C2-N1-C1'	6.85	126.33	118.80
35	YB	27	C	N1-C2-O2	6.85	123.01	118.90
34	RA	546	C	C5-C6-N1	6.84	124.42	121.00
34	RA	1314	C	C6-N1-C2	-6.84	117.56	120.30
34	RA	2394	C	N1-C2-O2	6.83	123.00	118.90
1	XA	454	C	N1-C2-O2	6.83	123.00	118.90
1	XA	979	C	N1-C2-O2	6.83	123.00	118.90
34	YA	1956	U	N1-C2-O2	6.82	127.57	122.80
34	YA	1026	U	P-O3'-C3'	6.82	127.88	119.70
1	XA	1027	C	P-O3'-C3'	6.81	127.87	119.70
34	RA	1407	C	C6-N1-C2	-6.80	117.58	120.30
1	XA	135	C	N1-C2-O2	6.79	122.98	118.90
1	XA	687	A	P-O3'-C3'	6.79	127.85	119.70
34	RA	1064	C	C5-C6-N1	6.79	124.40	121.00
1	QA	1301	U	C6-N1-C1'	-6.79	111.70	121.20
34	YA	1462	C	N1-C2-O2	6.79	122.97	118.90
1	XA	812	C	OP2-P-O3'	6.79	120.13	105.20
34	RA	1558	A	P-O3'-C3'	6.78	127.84	119.70
34	YA	2584	U	C2-N1-C1'	6.78	125.84	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	YA	2456	C	C6-N1-C2	-6.77	117.59	120.30
1	QA	328	C	N3-C2-O2	-6.77	117.16	121.90
1	XA	328	C	P-O3'-C3'	6.77	127.82	119.70
34	YA	2403	C	C5-C6-N1	6.77	124.38	121.00
34	RA	1914	C	N3-C2-O2	-6.76	117.17	121.90
34	RA	904	C	C2-N1-C1'	6.76	126.24	118.80
1	XA	1224	G	N3-C4-N9	-6.75	121.95	126.00
1	XA	1297	C	P-O3'-C3'	6.75	127.80	119.70
1	QA	1285	A	P-O3'-C3'	6.75	127.79	119.70
34	YA	607	U	N3-C2-O2	-6.74	117.48	122.20
22	XV	53	G	C8-N9-C4	-6.74	103.70	106.40
34	YA	2210	G	N3-C4-N9	6.74	130.04	126.00
1	QA	252	U	C2-N1-C1'	6.73	125.78	117.70
1	QA	812	C	P-O3'-C3'	6.73	127.78	119.70
34	RA	2745	C	C6-N1-C2	-6.73	117.61	120.30
34	RA	637	A	P-O3'-C3'	6.73	127.78	119.70
34	RA	607	U	N1-C2-O2	6.73	127.51	122.80
34	YA	2321	G	C4-N9-C1'	6.72	135.24	126.50
34	YA	2681	C	P-O3'-C3'	6.72	127.77	119.70
34	RA	867	C	N1-C2-O2	6.71	122.93	118.90
1	XA	328	C	N1-C2-O2	6.71	122.93	118.90
1	XA	358	U	C2-N1-C1'	6.71	125.75	117.70
1	XA	1362(A)	C	N3-C2-O2	-6.71	117.20	121.90
34	YA	856	C	C2-N1-C1'	6.71	126.18	118.80
1	XA	283	C	N1-C2-O2	6.70	122.92	118.90
35	YB	31	C	C6-N1-C1'	-6.70	112.76	120.80
1	QA	1066	C	C6-N1-C2	-6.70	117.62	120.30
34	RA	613	U	N1-C2-O2	6.70	127.49	122.80
34	YA	12	U	N3-C2-O2	-6.69	117.52	122.20
34	YA	837	C	C6-N1-C2	-6.69	117.62	120.30
34	YA	404	C	P-O3'-C3'	6.68	127.72	119.70
34	YA	2179	C	N1-C2-O2	6.67	122.90	118.90
34	YA	856	C	C5-C6-N1	6.67	124.34	121.00
34	YA	637	A	P-O3'-C3'	6.67	127.71	119.70
1	QA	58	C	C6-N1-C2	-6.67	117.63	120.30
1	XA	1498	U	P-O3'-C3'	6.65	127.68	119.70
34	RA	2321	G	C4-N9-C1'	6.65	135.15	126.50
22	XV	61	C	N3-C4-C5	-6.65	119.24	121.90
22	QV	61	C	C6-N1-C2	-6.64	117.64	120.30
1	XA	1285	A	P-O3'-C3'	6.64	127.67	119.70
34	RA	234	C	N1-C2-O2	6.63	122.88	118.90
34	RA	2688	U	N3-C2-O2	-6.63	117.56	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	XA	1533	C	C6-N1-C2	-6.63	117.65	120.30
34	YA	837	C	N3-C2-O2	-6.63	117.26	121.90
34	RA	192	C	N1-C2-O2	6.62	122.87	118.90
34	RA	613	U	C2-N1-C1'	6.62	125.64	117.70
34	RA	1092	C	C6-N1-C2	-6.62	117.65	120.30
1	XA	135	C	N3-C2-O2	-6.61	117.27	121.90
1	QA	687	A	P-O3'-C3'	6.61	127.63	119.70
1	QA	1346	A	P-O3'-C3'	6.59	127.61	119.70
34	RA	846	C	P-O3'-C3'	6.58	127.60	119.70
34	YA	1407	C	C5-C6-N1	6.58	124.29	121.00
1	XA	58	C	C6-N1-C2	-6.56	117.67	120.30
22	XV	61	C	C6-N1-C2	-6.56	117.68	120.30
1	QA	252	U	N1-C2-O2	6.56	127.39	122.80
1	QA	484	G	P-O3'-C3'	6.56	127.57	119.70
34	RA	1931	U	N1-C2-O2	6.55	127.38	122.80
34	RA	1686	C	C2-N1-C1'	6.54	125.99	118.80
34	YA	271(B)	G	P-O3'-C3'	6.54	127.55	119.70
34	RA	404	C	P-O3'-C3'	6.54	127.54	119.70
34	YA	1640	C	C2-N1-C1'	6.53	125.99	118.80
34	RA	2210	G	N3-C4-N9	6.53	129.92	126.00
34	RA	1931	U	N3-C2-O2	-6.53	117.63	122.20
34	YA	1313	U	C6-N1-C1'	-6.52	112.07	121.20
1	XA	932	C	C2-N1-C1'	6.51	125.96	118.80
34	YA	2043	C	C2-N1-C1'	6.50	125.95	118.80
1	XA	60	A	P-O3'-C3'	6.50	127.50	119.70
1	QA	252	U	N3-C2-O2	-6.50	117.65	122.20
19	XS	16	LEU	CA-CB-CG	6.49	130.24	115.30
34	RA	1640	C	C6-N1-C2	-6.49	117.70	120.30
34	RA	1312	U	P-O3'-C3'	6.48	127.47	119.70
34	YA	2063	C	C6-N1-C2	-6.48	117.71	120.30
22	QV	53	G	N3-C2-N2	-6.47	115.37	119.90
1	XA	484	G	P-O3'-C3'	6.47	127.46	119.70
34	RA	2666	C	N3-C2-O2	-6.47	117.37	121.90
34	YA	860	U	N1-C2-O2	6.46	127.32	122.80
35	YB	37	C	N1-C2-O2	6.46	122.77	118.90
34	YA	192	C	N1-C2-O2	6.45	122.77	118.90
1	QA	509	A	OP1-P-O3'	6.45	119.39	105.20
34	RA	2210	G	N3-C4-C5	-6.45	125.38	128.60
34	RA	435	C	N3-C2-O2	-6.43	117.40	121.90
34	YA	1180	C	C2-N1-C1'	6.43	125.87	118.80
34	RA	1934	C	C2-N1-C1'	6.42	125.87	118.80
22	XV	53	G	N3-C2-N2	-6.42	115.40	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	YA	242	G	P-O3'-C3'	6.42	127.41	119.70
34	YA	1417	C	C5-C6-N1	6.42	124.21	121.00
34	YA	904	C	C2-N1-C1'	6.42	125.86	118.80
34	RA	2808	U	N1-C2-O2	6.41	127.28	122.80
1	QA	346	G	N3-C4-C5	-6.41	125.40	128.60
1	QA	1301	U	C5-C6-N1	6.41	125.90	122.70
49	YU	40	PHE	N-CA-CB	6.40	122.11	110.60
34	RA	1049	C	N1-C2-O2	6.39	122.74	118.90
34	RA	1774	C	C2-N1-C1'	6.39	125.83	118.80
34	RA	752	A	P-O3'-C3'	6.39	127.37	119.70
1	XA	330	C	N3-C2-O2	-6.39	117.43	121.90
34	RA	1881	C	C2-N1-C1'	6.38	125.82	118.80
34	YA	1915	U	N1-C2-O2	6.38	127.27	122.80
34	RA	1506	C	N3-C2-O2	-6.38	117.44	121.90
34	RA	708	C	C2-N1-C1'	6.36	125.80	118.80
34	RA	1065	U	N1-C2-O2	6.36	127.25	122.80
34	RA	2295	C	O5'-P-OP2	-6.36	99.98	105.70
1	QA	753	A	P-O3'-C3'	6.36	127.33	119.70
1	XA	449	C	N3-C2-O2	-6.36	117.45	121.90
34	YA	1774	C	C6-N1-C2	-6.36	117.76	120.30
34	RA	837	C	N3-C2-O2	-6.35	117.45	121.90
34	YA	1686	C	C2-N1-C1'	6.35	125.78	118.80
34	RA	1406	U	C2-N1-C1'	6.34	125.31	117.70
34	YA	974(A)	C	N1-C2-O2	6.33	122.70	118.90
34	RA	192	C	N3-C2-O2	-6.33	117.47	121.90
34	YA	1653	G	P-O3'-C3'	6.33	127.30	119.70
34	RA	2868	A	N7-C8-N9	6.33	116.96	113.80
34	YA	228	A	C2-N3-C4	6.33	113.77	110.60
34	YA	231	C	C2-N1-C1'	6.33	125.76	118.80
1	QA	307	C	C2-N1-C1'	6.33	125.76	118.80
34	RA	1109	C	N3-C2-O2	-6.33	117.47	121.90
34	RA	420	C	C2-N1-C1'	6.32	125.75	118.80
1	QA	346	G	C2-N3-C4	6.32	115.06	111.90
34	RA	837	C	N1-C2-O2	6.32	122.69	118.90
1	XA	481	G	P-O3'-C3'	6.32	127.28	119.70
1	XA	1113	C	C5-C6-N1	6.31	124.16	121.00
1	QA	1147	C	N1-C2-O2	6.30	122.68	118.90
1	XA	913	A	P-O3'-C3'	6.30	127.26	119.70
34	RA	530	G	O4'-C1'-N9	6.30	113.24	108.20
34	YA	856	C	N1-C2-O2	6.30	122.68	118.90
1	XA	620	C	N1-C2-O2	6.28	122.67	118.90
34	RA	1116	C	C2-N1-C1'	6.28	125.70	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	XV	53	G	OP2-P-O3'	-6.28	91.39	105.20
34	YA	867	C	N3-C2-O2	-6.27	117.51	121.90
34	RA	2688	U	C2-N1-C1'	6.27	125.22	117.70
34	YA	510	C	N1-C2-O2	6.27	122.66	118.90
1	QA	1381	U	C2-N1-C1'	6.27	125.22	117.70
35	RB	31	C	C5-C6-N1	6.26	124.13	121.00
34	RA	1961	C	N3-C2-O2	-6.26	117.52	121.90
1	QA	620	C	N1-C2-O2	6.26	122.66	118.90
34	YA	2129	C	N1-C2-O2	6.25	122.65	118.90
9	QI	10	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	QA	328	C	C6-N1-C2	-6.25	117.80	120.30
34	RA	1038	C	C6-N1-C2	-6.25	117.80	120.30
1	XA	1383	C	N1-C2-O2	6.25	122.65	118.90
34	YA	2210	G	C8-N9-C1'	-6.25	118.88	127.00
1	QA	1505	G	N3-C4-N9	-6.24	122.25	126.00
1	XA	1290	G	N3-C4-N9	6.23	129.74	126.00
34	YA	1882	C	C6-N1-C2	-6.23	117.81	120.30
34	YA	2065	C	C6-N1-C2	-6.23	117.81	120.30
34	RA	915	C	C2-N1-C1'	6.23	125.65	118.80
34	YA	669	G	C4-N9-C1'	6.23	134.60	126.50
1	XA	1158	C	N1-C2-O2	6.23	122.64	118.90
1	QA	1059	C	C6-N1-C2	-6.22	117.81	120.30
34	RA	1064	C	N1-C2-O2	6.22	122.63	118.90
1	XA	455	C	N1-C2-O2	6.22	122.63	118.90
1	QA	1263	C	C2-N1-C1'	6.22	125.64	118.80
34	YA	1644	C	N3-C2-O2	-6.22	117.55	121.90
34	YA	1406	U	C5-C6-N1	6.21	125.81	122.70
34	RA	512	G	P-O3'-C3'	6.21	127.15	119.70
34	YA	1528	A	N7-C8-N9	6.21	116.90	113.80
1	XA	115	G	P-O3'-C3'	6.20	127.14	119.70
34	YA	893	C	N1-C2-O2	6.20	122.62	118.90
34	YA	2739	U	N1-C2-O2	6.20	127.14	122.80
34	RA	1406	U	N1-C2-O2	6.20	127.14	122.80
34	RA	1920	C	C5-C6-N1	6.20	124.10	121.00
50	RV	35	LEU	CA-CB-CG	6.20	129.56	115.30
1	XA	485	G	P-O3'-C3'	6.20	127.14	119.70
1	XA	522	C	N1-C2-O2	6.20	122.62	118.90
34	RA	243	U	N1-C2-O2	6.19	127.13	122.80
34	RA	1915	U	N1-C2-O2	6.19	127.13	122.80
1	XA	753	A	P-O3'-C3'	6.18	127.12	119.70
34	RA	537	C	C6-N1-C2	-6.18	117.83	120.30
34	RA	2043	C	C2-N1-C1'	6.18	125.60	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	RA	2210	G	C8-N9-C1'	-6.18	118.97	127.00
34	RA	1407	C	C5-C6-N1	6.18	124.09	121.00
34	RA	2808	U	N3-C2-O2	-6.17	117.88	122.20
1	QA	449	C	C2-N1-C1'	6.17	125.59	118.80
34	YA	752	A	P-O3'-C3'	6.17	127.10	119.70
34	RA	456	C	C2-N1-C1'	6.16	125.58	118.80
35	RB	77	U	N1-C2-O2	6.16	127.11	122.80
34	RA	1653	G	P-O3'-C3'	6.15	127.08	119.70
34	YA	859	G	P-O3'-C3'	6.15	127.08	119.70
34	RA	537	C	C2-N1-C1'	6.15	125.56	118.80
34	RA	1267	U	C2-N1-C1'	6.14	125.07	117.70
34	YA	1914	C	N3-C2-O2	-6.14	117.60	121.90
1	QA	115	G	P-O3'-C3'	6.14	127.07	119.70
1	XA	110	C	N3-C2-O2	-6.14	117.61	121.90
34	YA	2867	G	P-O3'-C3'	6.14	127.06	119.70
34	RA	222	A	P-O3'-C3'	6.13	127.06	119.70
34	RA	2043	C	C6-N1-C2	-6.13	117.85	120.30
1	XA	90	C	N1-C2-O2	6.13	122.58	118.90
34	YA	2776	A	P-O3'-C3'	6.13	127.05	119.70
50	YV	35	LEU	CA-CB-CG	6.13	129.39	115.30
1	XA	346	G	C4-N9-C1'	6.13	134.46	126.50
1	QA	58	C	C5-C6-N1	6.12	124.06	121.00
34	RA	1774	C	C5-C6-N1	6.12	124.06	121.00
34	RA	420	C	C6-N1-C2	-6.11	117.86	120.30
1	QA	91	C	C2-N1-C1'	6.11	125.52	118.80
1	XA	509	A	OP1-P-O3'	6.11	118.64	105.20
34	RA	907	U	N3-C2-O2	-6.10	117.93	122.20
22	QV	55	U	C5-C6-N1	6.10	125.75	122.70
1	XA	346	G	N3-C4-C5	-6.09	125.55	128.60
1	XA	454	C	N3-C2-O2	-6.09	117.63	121.90
34	RA	2107	C	C2-N1-C1'	6.09	125.50	118.80
34	RA	1396	U	C5-C6-N1	6.09	125.74	122.70
34	YA	1549	C	C2-N1-C1'	6.09	125.50	118.80
34	YA	1516	U	C2-N1-C1'	6.09	125.01	117.70
34	RA	2161	C	C2-N1-C1'	6.09	125.50	118.80
34	RA	229	A	P-O3'-C3'	6.08	127.00	119.70
34	YA	229	A	P-O3'-C3'	6.08	127.00	119.70
34	RA	1961	C	N1-C2-O2	6.08	122.55	118.90
34	YA	2712	U	P-O3'-C3'	6.08	126.99	119.70
1	XA	1161	C	N1-C2-O2	6.07	122.54	118.90
1	XA	1140	C	C2-N1-C1'	6.06	125.47	118.80
1	XA	1224	G	C4-N9-C1'	-6.06	118.62	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	QA	485	G	P-O3'-C3'	6.06	126.97	119.70
34	YA	1085	A	P-O3'-C3'	6.06	126.97	119.70
34	YA	828	U	C6-N1-C1'	-6.06	112.72	121.20
34	YA	1658	C	C5-C6-N1	6.06	124.03	121.00
34	YA	1914	C	C6-N1-C1'	-6.06	113.53	120.80
34	YA	2889	C	C2-N1-C1'	6.05	125.46	118.80
34	RA	1882	C	N1-C2-O2	6.05	122.53	118.90
34	RA	503	A	P-O3'-C3'	6.05	126.96	119.70
1	XA	979	C	C2-N1-C1'	6.05	125.45	118.80
34	YA	1640	C	C6-N1-C2	-6.04	117.88	120.30
34	RA	1882	C	C6-N1-C2	-6.04	117.88	120.30
34	YA	192	C	N3-C2-O2	-6.04	117.67	121.90
34	YA	1694	C	P-O3'-C3'	6.04	126.94	119.70
34	RA	193	U	N1-C2-O2	6.04	127.03	122.80
34	RA	221	A	P-O3'-C3'	6.04	126.94	119.70
34	YA	537	C	C5-C6-N1	6.03	124.01	121.00
1	QA	482	A	C8-N9-C4	-6.03	103.39	105.80
34	RA	613	U	N3-C2-O2	-6.03	117.98	122.20
1	QA	1347	G	P-O3'-C3'	6.02	126.93	119.70
1	XA	412	A	P-O3'-C3'	6.02	126.93	119.70
1	QA	412	A	P-O3'-C3'	6.02	126.92	119.70
34	RA	1404	C	C6-N1-C2	-6.02	117.89	120.30
34	YA	537	C	C2-N1-C1'	6.02	125.42	118.80
34	YA	2559	C	C6-N1-C2	-6.02	117.89	120.30
35	YB	27	C	C2-N1-C1'	6.02	125.42	118.80
1	QA	442	C	C2-N1-C1'	6.01	125.42	118.80
34	RA	114	U	C2-N1-C1'	6.01	124.92	117.70
34	YA	915	C	C2-N1-C1'	6.01	125.41	118.80
34	YA	1544	C	N1-C2-O2	6.01	122.50	118.90
35	YB	31	C	C5-C6-N1	6.01	124.00	121.00
34	RA	1038	C	C2-N1-C1'	6.00	125.39	118.80
34	RA	2584	U	C2-N1-C1'	6.00	124.89	117.70
34	RA	2689	U	P-O3'-C3'	5.99	126.89	119.70
1	XA	266	G	P-O3'-C3'	5.99	126.89	119.70
1	QA	960	U	N1-C2-O2	5.99	126.99	122.80
34	YA	2874	C	C6-N1-C2	-5.99	117.90	120.30
34	RA	1658	C	C5-C6-N1	5.99	124.00	121.00
34	YA	2648	C	C5-C6-N1	5.99	124.00	121.00
34	YA	420	C	C2-N1-C1'	5.99	125.39	118.80
34	YA	907	U	N3-C2-O2	-5.99	118.01	122.20
35	YB	66	A	P-O3'-C3'	5.98	126.88	119.70
35	RB	66	A	P-O3'-C3'	5.98	126.88	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	XV	53	G	N1-C6-O6	-5.98	116.31	119.90
34	YA	1915	U	N3-C2-O2	-5.98	118.01	122.20
34	YA	1404	C	C2-N1-C1'	5.98	125.38	118.80
34	RA	339	U	N3-C2-O2	-5.97	118.02	122.20
34	YA	752	A	OP2-P-O3'	5.97	118.35	105.20
34	RA	537	C	C5-C6-N1	5.97	123.99	121.00
1	XA	1028	C	N1-C2-O2	5.97	122.48	118.90
34	YA	1314	C	C2-N1-C1'	5.97	125.37	118.80
34	RA	898	C	N1-C2-O2	5.97	122.48	118.90
34	RA	1915	U	N3-C2-O2	-5.97	118.02	122.20
35	RB	30	C	C6-N1-C2	-5.97	117.91	120.30
34	RA	860	U	C2-N1-C1'	5.96	124.86	117.70
34	YA	1370	C	C2-N1-C1'	5.96	125.36	118.80
34	YA	1881	C	C2-N1-C1'	5.96	125.36	118.80
34	RA	1640	C	N3-C2-O2	-5.96	117.73	121.90
34	RA	1267	U	N1-C2-O2	5.96	126.97	122.80
34	RA	2559	C	C2-N1-C1'	5.96	125.35	118.80
35	RB	77	U	N3-C2-O2	-5.95	118.03	122.20
1	QA	1066	C	N3-C2-O2	-5.95	117.74	121.90
1	XA	1452	C	N1-C2-O2	5.95	122.47	118.90
34	YA	243	U	N3-C2-O2	-5.94	118.04	122.20
1	QA	119	A	P-O3'-C3'	5.94	126.83	119.70
1	QA	404	U	N3-C2-O2	-5.94	118.04	122.20
34	RA	1534	G	N3-C4-C5	-5.94	125.63	128.60
34	YA	2403	C	C2-N1-C1'	5.93	125.32	118.80
34	RA	2610	C	P-O3'-C3'	5.93	126.81	119.70
1	XA	1290	G	C4-N9-C1'	5.92	134.20	126.50
1	QA	110	C	N3-C2-O2	-5.92	117.75	121.90
34	RA	1052	C	C6-N1-C2	-5.92	117.93	120.30
34	YA	2403	C	C6-N1-C2	-5.92	117.93	120.30
34	RA	372	G	P-O3'-C3'	5.92	126.80	119.70
34	RA	192	C	C6-N1-C2	-5.92	117.93	120.30
34	RA	546	C	C6-N1-C1'	-5.91	113.71	120.80
34	YA	2096	U	N1-C2-O2	5.91	126.94	122.80
34	YA	2559	C	C2-N1-C1'	5.90	125.30	118.80
34	YA	1920	C	C6-N1-C2	-5.90	117.94	120.30
34	RA	2683	C	N1-C2-O2	5.90	122.44	118.90
34	YA	1528	A	C8-N9-C4	-5.90	103.44	105.80
34	RA	1417	C	C5-C6-N1	5.90	123.95	121.00
34	RA	2726	U	C2-N1-C1'	5.90	124.78	117.70
34	YA	12	U	C2-N1-C1'	5.90	124.78	117.70
35	RB	27	C	N3-C2-O2	-5.89	117.78	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	RA	2060	A	P-O3'-C3'	5.88	126.76	119.70
34	YA	435	C	N3-C2-O2	-5.88	117.78	121.90
34	RA	1882	C	C5-C6-N1	5.88	123.94	121.00
1	QA	1163	C	C6-N1-C2	-5.87	117.95	120.30
34	RA	2688	U	N1-C2-O2	5.87	126.91	122.80
34	RA	2825	C	N1-C2-O2	5.87	122.42	118.90
34	YA	1514	U	N1-C2-O2	5.87	126.91	122.80
34	YA	243	U	N1-C2-O2	5.87	126.91	122.80
34	YA	510	C	C2-N1-C1'	5.87	125.25	118.80
34	YA	721	C	C2-N1-C1'	5.86	125.25	118.80
34	YA	2825	C	N1-C2-O2	5.86	122.42	118.90
34	RA	1188	U	N1-C2-O2	5.86	126.90	122.80
34	RA	1462	C	N1-C2-O2	5.86	122.41	118.90
34	YA	1799	G	P-O3'-C3'	5.85	126.72	119.70
1	XA	244	U	P-O3'-C3'	5.85	126.72	119.70
34	YA	221	A	P-O3'-C3'	5.85	126.72	119.70
34	YA	503	A	P-O3'-C3'	5.85	126.72	119.70
35	YB	77	U	N1-C2-O2	5.85	126.89	122.80
34	YA	1406	U	N3-C2-O2	-5.84	118.11	122.20
34	RA	1267	U	N3-C2-O2	-5.84	118.11	122.20
34	RA	1427	A	P-O3'-C3'	5.84	126.71	119.70
34	YA	1427	A	P-O3'-C3'	5.84	126.70	119.70
34	YA	1640	C	N3-C2-O2	-5.83	117.82	121.90
22	QV	18	G	N3-C4-N9	-5.83	122.50	126.00
1	XA	1028	C	N3-C2-O2	-5.83	117.82	121.90
34	YA	1516	U	N3-C2-O2	-5.83	118.12	122.20
1	QA	1038	C	C2-N1-C1'	5.83	125.21	118.80
34	RA	1474	C	C2-N1-C1'	5.83	125.21	118.80
34	YA	2787	C	C2-N1-C1'	5.83	125.21	118.80
34	RA	669	G	C4-N9-C1'	5.82	134.07	126.50
34	RA	1640	C	C2-N1-C1'	5.81	125.19	118.80
34	YA	2566	A	P-O3'-C3'	5.81	126.68	119.70
34	RA	193	U	N3-C2-O2	-5.81	118.13	122.20
34	RA	1534	G	N3-C4-N9	5.81	129.49	126.00
1	XA	960	U	C2-N1-C1'	5.81	124.67	117.70
34	RA	1675	C	N1-C2-O2	5.81	122.39	118.90
1	XA	346	G	N3-C4-N9	5.81	129.48	126.00
1	XA	754	C	C2-N1-C1'	5.81	125.19	118.80
34	YA	2063	C	C2-N1-C1'	5.80	125.18	118.80
1	QA	307	C	C6-N1-C2	-5.80	117.98	120.30
34	YA	907	U	N1-C2-O2	5.80	126.86	122.80
34	YA	2688	U	N3-C2-O2	-5.80	118.14	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	RA	1833	U	N3-C2-O2	-5.79	118.14	122.20
34	RA	2874	C	C6-N1-C2	-5.79	117.98	120.30
34	YA	195	A	P-O3'-C3'	5.79	126.65	119.70
1	QA	1200	C	P-O3'-C3'	5.79	126.65	119.70
34	RA	721	C	C2-N1-C1'	5.79	125.17	118.80
1	QA	244	U	P-O3'-C3'	5.79	126.65	119.70
1	QA	789	U	C2-N1-C1'	5.79	124.64	117.70
1	XA	348	G	N1-C6-O6	-5.79	116.43	119.90
34	YA	1411	C	C6-N1-C2	-5.79	117.98	120.30
34	YA	1462	C	N3-C2-O2	-5.79	117.85	121.90
34	RA	1920	C	C6-N1-C2	-5.78	117.99	120.30
1	XA	180	U	N3-C2-O2	-5.78	118.15	122.20
34	YA	2739	U	N3-C2-O2	-5.78	118.15	122.20
1	XA	522	C	C2-N1-C1'	5.78	125.15	118.80
34	YA	12	U	N1-C2-O2	5.78	126.84	122.80
22	QV	61	C	C2-N3-C4	5.77	122.79	119.90
34	RA	2394	C	N3-C2-O2	-5.77	117.86	121.90
35	YB	37	C	N3-C2-O2	-5.77	117.86	121.90
1	QA	328	C	C5-C6-N1	5.77	123.89	121.00
34	RA	1406	U	N3-C2-O2	-5.77	118.16	122.20
34	RA	607	U	N3-C2-O2	-5.76	118.17	122.20
34	RA	2439	A	P-O3'-C3'	5.76	126.62	119.70
1	XA	410	G	P-O3'-C3'	5.76	126.62	119.70
1	QA	328	C	C6-N1-C1'	-5.76	113.89	120.80
34	RA	2566	A	P-O3'-C3'	5.76	126.61	119.70
34	YA	1644	C	N1-C2-O2	5.76	122.36	118.90
1	XA	703	G	P-O3'-C3'	5.75	126.61	119.70
1	XA	1224	G	C8-N9-C1'	5.75	134.48	127.00
34	RA	856	C	N1-C2-O2	5.75	122.35	118.90
34	RA	1407	C	N1-C2-O2	5.75	122.35	118.90
34	RA	2808	U	C2-N1-C1'	5.75	124.60	117.70
34	RA	1065	U	C2-N1-C1'	5.74	124.59	117.70
34	RA	1514	U	N3-C2-O2	-5.74	118.18	122.20
34	YA	1506	C	N1-C2-O2	5.74	122.34	118.90
1	QA	749	C	N1-C2-O2	5.74	122.34	118.90
34	YA	1992	G	P-O3'-C3'	5.74	126.58	119.70
1	QA	1228	C	C2-N1-C1'	5.73	125.11	118.80
34	RA	1882	C	C6-N1-C1'	-5.72	113.93	120.80
1	XA	1290	G	N3-C4-C5	-5.72	125.74	128.60
34	YA	2726	U	C2-N1-C1'	5.72	124.57	117.70
34	RA	587	C	P-O3'-C3'	5.72	126.56	119.70
34	YA	193	U	N1-C2-O2	5.72	126.80	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	RA	1038	C	N3-C2-O2	-5.72	117.90	121.90
1	QA	266	G	P-O3'-C3'	5.71	126.56	119.70
34	RA	271(B)	G	P-O3'-C3'	5.71	126.56	119.70
34	YA	2343	C	N1-C2-O2	5.71	122.33	118.90
34	RA	752	A	OP2-P-O3'	5.71	117.77	105.20
34	YA	1267	U	N3-C2-O2	-5.71	118.20	122.20
34	RA	1604	C	C6-N1-C2	-5.71	118.02	120.30
1	XA	1028(B)	C	C6-N1-C2	-5.71	118.02	120.30
1	QA	1225	A	C4-N9-C1'	5.70	136.56	126.30
1	XA	186(E)	C	C6-N1-C2	-5.70	118.02	120.30
34	YA	2065	C	C5-C6-N1	5.70	123.85	121.00
34	RA	373	U	C5-C6-N1	5.69	125.55	122.70
23	XX	-12	C	C6-N1-C2	-5.69	118.02	120.30
34	YA	1097	U	N1-C2-O2	5.69	126.78	122.80
9	QI	37	PHE	CB-CG-CD1	5.69	124.78	120.80
34	YA	2584	U	N3-C2-O2	-5.69	118.22	122.20
34	RA	1819	A	P-O3'-C3'	5.68	126.52	119.70
1	QA	1028(A)	C	N3-C2-O2	-5.68	117.92	121.90
34	RA	1313	U	C6-N1-C1'	-5.68	113.25	121.20
34	RA	1437	C	C2-N1-C1'	5.68	125.05	118.80
34	YA	1267	U	C2-N1-C1'	5.68	124.51	117.70
1	XA	789	U	C2-N1-C1'	5.68	124.51	117.70
1	XA	1395	C	C2-N1-C1'	5.68	125.04	118.80
34	YA	1776	G	C4-N9-C1'	5.68	133.88	126.50
1	QA	1325	C	C6-N1-C2	-5.67	118.03	120.30
34	RA	1462	C	N3-C2-O2	-5.67	117.93	121.90
34	RA	1514	U	C2-N1-C1'	5.67	124.51	117.70
1	QA	528	C	N1-C2-O2	5.67	122.30	118.90
34	RA	2556	C	N1-C2-O2	5.67	122.30	118.90
1	QA	932	C	C2-N1-C1'	5.67	125.03	118.80
1	QA	1382	C	N1-C2-O2	5.67	122.30	118.90
34	RA	1038	C	C5-C6-N1	5.67	123.83	121.00
1	XA	54	C	C6-N1-C2	-5.67	118.03	120.30
1	XA	135	C	C2-N1-C1'	5.67	125.03	118.80
1	XA	1502	A	N7-C8-N9	5.67	116.63	113.80
1	QA	243	A	P-O3'-C3'	5.66	126.50	119.70
34	RA	1506	C	N1-C2-O2	5.66	122.30	118.90
37	RE	78	LEU	CA-CB-CG	5.66	128.33	115.30
1	XA	1397	C	N1-C2-O2	5.66	122.30	118.90
34	RA	2226	C	N1-C2-O2	5.65	122.29	118.90
34	RA	1314	C	N1-C2-O2	5.65	122.29	118.90
34	RA	1407	C	C6-N1-C1'	-5.65	114.02	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	QV	53	G	N1-C2-N2	5.65	121.28	116.20
34	YA	363(E)	U	N3-C2-O2	-5.63	118.26	122.20
50	YV	75	PHE	CB-CG-CD1	5.63	124.74	120.80
1	QA	1362(A)	C	N3-C2-O2	-5.63	117.96	121.90
34	RA	1992	G	P-O3'-C3'	5.63	126.45	119.70
34	YA	2779	U	N1-C2-O2	5.62	126.74	122.80
34	RA	1506	C	C6-N1-C2	-5.62	118.05	120.30
1	QA	1452	C	N1-C2-O2	5.62	122.27	118.90
34	YA	860	U	C6-N1-C2	-5.62	117.63	121.00
1	XA	1310	G	P-O3'-C3'	5.62	126.44	119.70
34	RA	273(F)	C	C2-N1-C1'	5.62	124.98	118.80
22	XV	54	U	O5'-P-OP1	5.61	117.44	110.70
34	RA	2667	C	N1-C2-O2	5.61	122.27	118.90
1	QA	703	G	P-O3'-C3'	5.61	126.43	119.70
35	YB	77	U	N3-C2-O2	-5.61	118.27	122.20
23	XX	-5	G	P-O3'-C3'	5.61	126.43	119.70
34	YA	537	C	C6-N1-C2	-5.61	118.06	120.30
34	RA	2096	U	N1-C2-O2	5.61	126.73	122.80
35	RB	37	C	N1-C2-O2	5.61	122.27	118.90
1	QA	1263	C	N1-C2-O2	5.61	122.26	118.90
34	RA	907	U	N1-C2-O2	5.60	126.72	122.80
34	YA	2584	U	N1-C2-O2	5.60	126.72	122.80
22	QV	53	G	N9-C4-C5	5.60	107.64	105.40
1	XA	454	C	C6-N1-C2	-5.60	118.06	120.30
34	YA	363(E)	U	N1-C2-O2	5.60	126.72	122.80
34	YA	1516	U	N1-C2-O2	5.59	126.72	122.80
1	XA	243	A	P-O3'-C3'	5.59	126.41	119.70
34	YA	234	C	N3-C2-O2	-5.59	117.98	121.90
34	YA	1914	C	O4'-C1'-N1	5.59	112.67	108.20
34	RA	2720	U	N3-C2-O2	-5.58	118.29	122.20
34	YA	2688	U	C2-N1-C1'	5.58	124.40	117.70
1	XA	250	A	P-O3'-C3'	5.58	126.39	119.70
1	QA	330	C	N3-C2-O2	-5.58	118.00	121.90
34	RA	1549	C	C2-N1-C1'	5.58	124.93	118.80
1	QA	1198	G	N1-C6-O6	-5.57	116.56	119.90
34	YA	1914	C	C6-N1-C2	-5.57	118.07	120.30
34	RA	1934	C	C6-N1-C2	-5.57	118.07	120.30
1	QA	749	C	N3-C2-O2	-5.56	118.01	121.90
34	YA	817	C	C6-N1-C2	-5.56	118.08	120.30
34	RA	1404	C	C5-C6-N1	5.56	123.78	121.00
1	QA	1439	C	C2-N1-C1'	5.55	124.91	118.80
34	YA	1407	C	N1-C2-O2	5.55	122.23	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	XA	135	C	C5-C6-N1	5.55	123.78	121.00
34	RA	273(F)	C	C6-N1-C2	-5.55	118.08	120.30
1	XA	545	C	C6-N1-C2	-5.55	118.08	120.30
1	XA	1439	C	C2-N1-C1'	5.55	124.90	118.80
34	YA	1294	U	N3-C2-O2	-5.55	118.32	122.20
1	QA	482	A	N7-C8-N9	5.54	116.57	113.80
34	RA	2803	C	N1-C2-O2	5.54	122.22	118.90
34	YA	2825	C	C6-N1-C2	-5.54	118.08	120.30
34	RA	275	G	OP1-P-O3'	5.54	117.38	105.20
34	YA	1644	C	C6-N1-C2	-5.53	118.09	120.30
34	YA	1097	U	N3-C2-O2	-5.53	118.33	122.20
34	YA	2712	U	N3-C2-O2	-5.53	118.33	122.20
34	RA	1073	A	P-O3'-C3'	5.53	126.34	119.70
34	RA	2321	G	C2-N3-C4	5.53	114.67	111.90
1	XA	1028	C	C6-N1-C2	-5.53	118.09	120.30
1	XA	789	U	N3-C2-O2	-5.53	118.33	122.20
34	RA	1805	U	N3-C2-O2	-5.52	118.33	122.20
1	QA	525	C	C5-C6-N1	5.52	123.76	121.00
34	RA	817	C	C6-N1-C2	-5.52	118.09	120.30
34	RA	2043	C	C5-C6-N1	5.52	123.76	121.00
34	RA	1210	A	P-O3'-C3'	5.52	126.32	119.70
1	QA	405	U	N1-C2-O2	5.52	126.66	122.80
1	QA	754	C	C2-N1-C1'	5.52	124.87	118.80
1	QA	528	C	C2-N1-C1'	5.51	124.86	118.80
34	RA	828	U	C5-C6-N1	5.51	125.45	122.70
34	RA	867	C	N3-C2-O2	-5.51	118.04	121.90
34	RA	93	C	C6-N1-C2	-5.51	118.10	120.30
34	YA	2726	U	N3-C2-O2	-5.51	118.35	122.20
34	YA	2066	C	N1-C2-O2	5.50	122.20	118.90
1	QA	404	U	N1-C2-O2	5.50	126.65	122.80
1	XA	365	U	C2-N1-C1'	5.50	124.30	117.70
34	YA	2179	C	N3-C2-O2	-5.50	118.05	121.90
50	YV	75	PHE	CB-CG-CD2	-5.50	116.95	120.80
34	YA	1640	C	C5-C6-N1	5.49	123.75	121.00
34	YA	1549	C	C6-N1-C2	-5.49	118.10	120.30
34	RA	2321	G	N3-C4-N9	5.49	129.29	126.00
34	RA	1513	C	C2-N1-C1'	5.49	124.83	118.80
1	QA	1161	C	N1-C2-O2	5.48	122.19	118.90
34	YA	2591	C	C5-C6-N1	5.48	123.74	121.00
34	YA	1407	C	C6-N1-C1'	-5.47	114.23	120.80
1	QA	90	C	C6-N1-C2	-5.47	118.11	120.30
1	XA	1028(A)	C	N3-C2-O2	-5.47	118.07	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	RA	1931	U	C2-N1-C1'	5.47	124.26	117.70
34	RA	2739	U	N1-C2-O2	5.47	126.63	122.80
34	RA	1026	U	OP1-P-O3'	5.46	117.22	105.20
47	RS	56	LEU	CA-CB-CG	5.46	127.87	115.30
1	XA	960	U	N1-C2-O2	5.46	126.63	122.80
1	XA	1228	C	C2-N1-C1'	5.46	124.81	118.80
34	YA	114	U	C2-N1-C1'	5.46	124.26	117.70
34	YA	2226	C	N1-C2-O2	5.46	122.18	118.90
1	QA	497	U	N1-C2-O2	5.46	126.62	122.80
34	RA	2787	C	N1-C2-O2	5.46	122.17	118.90
34	YA	1430	C	C5-C6-N1	5.46	123.73	121.00
1	XA	991	U	N1-C2-O2	5.46	126.62	122.80
34	YA	529	A	N7-C8-N9	5.45	116.53	113.80
34	YA	1437	C	C2-N1-C1'	5.45	124.80	118.80
1	QA	1303	C	N1-C2-O2	5.45	122.17	118.90
34	YA	1437	C	C6-N1-C2	-5.45	118.12	120.30
34	YA	2591	C	C6-N1-C2	-5.45	118.12	120.30
34	YA	1509	C	OP1-P-O3'	5.45	117.18	105.20
22	XV	53	G	N1-C2-N2	5.44	121.10	116.20
1	XA	435	C	C2-N1-C1'	5.44	124.79	118.80
34	RA	2073	C	C6-N1-C2	-5.44	118.12	120.30
34	YA	1833	U	N3-C2-O2	-5.43	118.40	122.20
1	QA	1395	C	N1-C2-O2	5.43	122.16	118.90
34	YA	1178	C	P-O3'-C3'	5.43	126.22	119.70
34	YA	243	U	C2-N1-C1'	5.43	124.21	117.70
1	XA	330	C	C6-N1-C2	-5.42	118.13	120.30
34	YA	1882	C	N1-C2-O2	5.42	122.15	118.90
34	RA	1062	G	N3-C4-N9	5.42	129.25	126.00
1	XA	449	C	C6-N1-C2	-5.42	118.13	120.30
49	RU	60	LEU	CA-CB-CG	5.41	127.75	115.30
34	YA	1178	C	C6-N1-C2	-5.41	118.14	120.30
34	RA	270(P)	C	N1-C2-O2	5.41	122.15	118.90
34	RA	234	C	N3-C2-O2	-5.41	118.11	121.90
34	YA	1012	U	OP2-P-O3'	5.41	117.10	105.20
34	RA	856	C	C2-N1-C1'	5.41	124.75	118.80
34	YA	1411	C	N1-C2-O2	5.41	122.14	118.90
34	YA	1882	C	C5-C6-N1	5.40	123.70	121.00
1	QA	1505	G	C8-N9-C1'	5.40	134.02	127.00
1	XA	1161	C	C2-N1-C1'	5.39	124.73	118.80
1	QA	1109	C	N1-C2-O2	5.39	122.13	118.90
34	RA	1062	G	N3-C4-C5	-5.39	125.91	128.60
34	YA	2321	G	C8-N9-C4	-5.38	104.25	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	RA	1135	C	N1-C2-O2	5.38	122.13	118.90
34	RA	1474	C	C6-N1-C2	-5.38	118.15	120.30
34	YA	193	U	N3-C2-O2	-5.38	118.43	122.20
1	QA	754	C	N1-C2-O2	5.38	122.13	118.90
1	XA	180	U	N1-C2-O2	5.38	126.56	122.80
34	YA	1267	U	N1-C2-O2	5.38	126.56	122.80
1	QA	353	A	OP2-P-O3'	5.37	117.02	105.20
34	YA	1506	C	C2-N1-C1'	5.37	124.71	118.80
1	XA	186(F)	C	N3-C2-O2	-5.37	118.14	121.90
34	RA	1065	U	O4'-C1'-N1	5.37	112.49	108.20
34	RA	1914	C	C6-N1-C1'	-5.37	114.36	120.80
35	RB	27	C	C2-N1-C1'	5.37	124.70	118.80
34	YA	1332	G	C4-N9-C1'	5.37	133.48	126.50
1	QA	1505	G	C4-N9-C1'	-5.37	119.53	126.50
34	YA	2179	C	C2-N1-C1'	5.36	124.70	118.80
34	RA	1052	C	C2-N1-C1'	5.36	124.70	118.80
34	YA	1202	C	N3-C2-O2	-5.36	118.15	121.90
1	XA	991	U	N3-C2-O2	-5.36	118.45	122.20
34	YA	1535	U	C6-N1-C1'	-5.36	113.70	121.20
34	YA	1992	G	OP2-P-O3'	5.36	116.98	105.20
1	XA	1026	G	N3-C4-N9	5.35	129.21	126.00
34	RA	435	C	C6-N1-C2	-5.35	118.16	120.30
34	RA	1629	U	N3-C2-O2	-5.35	118.46	122.20
1	XA	545	C	C5-C6-N1	5.35	123.67	121.00
34	YA	1982	C	C2-N1-C1'	5.34	124.68	118.80
34	RA	1640	C	C5-C6-N1	5.34	123.67	121.00
34	RA	1881	C	C6-N1-C2	-5.34	118.16	120.30
1	XA	1538	C	N1-C2-O2	5.34	122.10	118.90
34	YA	1433	U	N1-C2-O2	5.34	126.54	122.80
34	RA	1332	G	C4-N9-C1'	5.34	133.44	126.50
34	RA	708	C	C6-N1-C2	-5.33	118.17	120.30
34	RA	915	C	C6-N1-C2	-5.33	118.17	120.30
1	XA	1026	G	N3-C4-C5	-5.33	125.94	128.60
34	RA	2321	G	C8-N9-C4	-5.33	104.27	106.40
34	YA	1549	C	C5-C6-N1	5.33	123.66	121.00
1	XA	1533	C	C5-C6-N1	5.33	123.66	121.00
1	QA	563	A	C4-N9-C1'	5.32	135.88	126.30
34	YA	2089	U	N1-C2-O2	5.32	126.53	122.80
1	XA	342	C	C6-N1-C2	-5.32	118.17	120.30
34	YA	1332	G	N7-C8-N9	5.32	115.76	113.10
34	YA	2712	U	N1-C2-O2	5.31	126.52	122.80
34	YA	2779	U	C2-N1-C1'	5.31	124.07	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	YA	206	U	N1-C2-O2	5.31	126.52	122.80
34	YA	1514	U	C2-N1-C1'	5.31	124.07	117.70
34	YA	2471	C	C2-N1-C1'	5.31	124.64	118.80
34	YA	613	U	C2-N1-C1'	5.30	124.07	117.70
1	XA	697	U	N3-C2-O2	-5.30	118.49	122.20
34	RA	1109	C	C6-N1-C2	-5.30	118.18	120.30
34	YA	459	U	N1-C2-O2	5.30	126.51	122.80
1	QA	346	G	N3-C4-N9	5.29	129.18	126.00
34	RA	2063	C	C6-N1-C2	-5.29	118.18	120.30
34	RA	1057	A	P-O3'-C3'	5.29	126.05	119.70
34	YA	1779	U	C2-N1-C1'	5.29	124.05	117.70
1	QA	596	C	C6-N1-C2	-5.29	118.19	120.30
1	XA	1357	A	N7-C8-N9	5.29	116.44	113.80
34	YA	2089	U	N3-C2-O2	-5.29	118.50	122.20
1	QA	449	C	N1-C2-O2	5.28	122.07	118.90
1	QA	618	C	N1-C2-O2	5.28	122.07	118.90
1	XA	390	C	C2-N1-C1'	5.28	124.61	118.80
34	RA	243	U	N3-C2-O2	-5.28	118.50	122.20
1	QA	1303	C	N3-C2-O2	-5.28	118.20	121.90
1	XA	1225	A	C4-N9-C1'	5.28	135.80	126.30
34	RA	1049	C	N3-C2-O2	-5.28	118.21	121.90
1	XA	991	U	C2-N1-C1'	5.28	124.03	117.70
1	QA	1260	C	N3-C2-O2	-5.27	118.21	121.90
54	RZ	59	LEU	CA-CB-CG	5.27	127.42	115.30
1	XA	1452	C	C2-N1-C1'	5.27	124.60	118.80
34	RA	1370	C	C2-N1-C1'	5.27	124.60	118.80
1	QA	545	C	C6-N1-C2	-5.27	118.19	120.30
1	XA	390	C	C6-N1-C2	-5.27	118.19	120.30
34	YA	1961	C	N1-C2-O2	5.27	122.06	118.90
34	YA	2889	C	C6-N1-C2	-5.27	118.19	120.30
34	RA	285	C	C2-N1-C1'	5.27	124.59	118.80
34	RA	456	C	N3-C2-O2	-5.27	118.21	121.90
1	XA	186(E)	C	N3-C2-O2	-5.26	118.22	121.90
1	XA	328	C	N3-C2-O2	-5.26	118.22	121.90
34	RA	1686	C	C6-N1-C2	-5.26	118.19	120.30
34	RA	1116	C	N1-C2-O2	5.26	122.06	118.90
34	YA	2683	C	N1-C2-O2	5.26	122.06	118.90
34	RA	2584	U	N3-C2-O2	-5.26	118.52	122.20
1	XA	1163	C	C2-N1-C1'	5.25	124.58	118.80
34	YA	1076	C	N1-C2-O2	5.25	122.05	118.90
34	YA	1313	U	C5-C6-N1	5.25	125.33	122.70
34	YA	1404	C	C6-N1-C2	-5.25	118.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	RA	2889	C	C2-N1-C1'	5.25	124.57	118.80
34	RA	74	A	P-O3'-C3'	5.24	125.99	119.70
34	RA	1947	C	C2-N1-C1'	5.24	124.57	118.80
34	RA	2666	C	C6-N1-C2	-5.24	118.20	120.30
34	YA	363(E)	U	C2-N1-C1'	5.24	123.99	117.70
34	RA	1026	U	P-O3'-C3'	5.24	125.99	119.70
34	RA	2703	C	C2-N1-C1'	5.24	124.56	118.80
34	RA	2825	C	C6-N1-C2	-5.24	118.20	120.30
1	XA	893	C	C5-C6-N1	5.24	123.62	121.00
1	XA	58	C	C5-C6-N1	5.24	123.62	121.00
1	QA	217	C	C2-N1-C1'	5.24	124.56	118.80
1	QA	267	C	O5'-P-OP1	-5.24	100.99	105.70
34	RA	1062	G	C4-N9-C1'	5.24	133.31	126.50
34	YA	893	C	C2-N1-C1'	5.23	124.56	118.80
34	YA	2794	C	C6-N1-C2	-5.23	118.21	120.30
34	RA	1304	C	C2-N1-C1'	5.23	124.56	118.80
34	YA	2162	G	N3-C4-C5	-5.23	125.98	128.60
34	RA	1068	G	O5'-P-OP2	-5.23	101.00	105.70
34	YA	1198	U	N3-C2-O2	-5.23	118.54	122.20
34	RA	1180	C	C2-N1-C1'	5.23	124.55	118.80
1	QA	1163	C	N1-C2-O2	5.22	122.03	118.90
34	YA	1411	C	C5-C6-N1	5.22	123.61	121.00
34	RA	1116	C	C6-N1-C2	-5.22	118.21	120.30
34	YA	669	G	C8-N9-C1'	-5.22	120.21	127.00
34	YA	2394	C	N3-C2-O2	-5.22	118.25	121.90
34	RA	1934	C	C5-C6-N1	5.22	123.61	121.00
34	RA	2666	C	C2-N1-C1'	5.22	124.54	118.80
22	QV	55	U	C6-N1-C2	-5.21	117.87	121.00
34	RA	1915	U	C2-N1-C1'	5.21	123.95	117.70
34	YA	339	U	N3-C2-O2	-5.21	118.55	122.20
34	YA	2794	C	C2-N1-C1'	5.21	124.53	118.80
34	RA	846	C	N1-C2-O2	5.21	122.03	118.90
34	RA	1513	C	N1-C2-O2	5.21	122.03	118.90
34	RA	2703	C	N1-C2-O2	5.21	122.03	118.90
34	YA	1180	C	N1-C2-O2	5.21	122.03	118.90
1	XA	449	C	C6-N1-C1'	-5.21	114.55	120.80
52	RX	66	LEU	CA-CB-CG	5.20	127.27	115.30
1	XA	697	U	N1-C2-O2	5.20	126.44	122.80
34	YA	1064	C	C6-N1-C2	-5.20	118.22	120.30
34	RA	456	C	C6-N1-C2	-5.20	118.22	120.30
34	RA	898	C	N3-C2-O2	-5.20	118.26	121.90
34	YA	721	C	C6-N1-C2	-5.20	118.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	QJ	85	LEU	CA-CB-CG	5.20	127.26	115.30
34	YA	1781	C	N1-C2-O2	5.20	122.02	118.90
34	RA	856	C	P-O3'-C3'	5.20	125.94	119.70
1	XA	1158	C	N3-C2-O2	-5.20	118.26	121.90
34	YA	904	C	C6-N1-C2	-5.19	118.22	120.30
34	RA	1914	C	C6-N1-C2	-5.19	118.22	120.30
1	XA	792	A	O4'-C1'-N9	5.19	112.35	108.20
34	YA	2320	A	C2-N3-C4	5.19	113.19	110.60
1	XA	1033	G	N3-C2-N2	5.19	123.53	119.90
35	YB	27	C	N3-C2-O2	-5.19	118.27	121.90
1	QA	1147	C	N3-C2-O2	-5.19	118.27	121.90
34	RA	1092	C	C5-C6-N1	5.18	123.59	121.00
35	RB	47	C	N1-C2-O2	5.18	122.01	118.90
1	XA	1224	G	N3-C4-C5	5.18	131.19	128.60
1	QA	1038	C	C6-N1-C2	-5.18	118.23	120.30
34	YA	2096	U	N3-C2-O2	-5.18	118.58	122.20
1	QA	1063	C	C6-N1-C2	-5.17	118.23	120.30
34	RA	2720	U	N1-C2-O2	5.17	126.42	122.80
34	YA	481	G	O4'-C1'-N9	5.17	112.34	108.20
34	RA	2730	C	C2-N1-C1'	5.17	124.48	118.80
34	YA	1105	U	N3-C2-O2	-5.17	118.58	122.20
1	XA	1140	C	C6-N1-C2	-5.16	118.23	120.30
34	YA	2068	U	C5-C6-N1	5.16	125.28	122.70
34	YA	930	U	N1-C2-O2	5.16	126.41	122.80
34	RA	2610	C	OP2-P-O3'	5.16	116.55	105.20
34	YA	2321	G	N3-C4-N9	5.16	129.10	126.00
1	QA	960	U	C2-N1-C1'	5.16	123.89	117.70
34	RA	481	G	O4'-C1'-N9	5.15	112.32	108.20
34	RA	1108	U	C6-N1-C1'	-5.15	113.99	121.20
1	XA	1246	C	C6-N1-C2	-5.15	118.24	120.30
34	RA	275	G	P-O3'-C3'	5.15	125.88	119.70
1	XA	509	A	P-O3'-C3'	5.15	125.88	119.70
1	XA	1109	C	N1-C2-O2	5.15	121.99	118.90
34	YA	271(B)	G	OP2-P-O3'	5.15	116.53	105.20
34	YA	2610	C	P-O3'-C3'	5.15	125.88	119.70
34	YA	2779	U	N3-C2-O2	-5.15	118.59	122.20
34	RA	1947	C	C6-N1-C2	-5.15	118.24	120.30
1	XA	1362	C	C6-N1-C2	-5.15	118.24	120.30
34	YA	2129	C	N3-C2-O2	-5.15	118.30	121.90
34	YA	2832	U	OP2-P-O3'	5.15	116.52	105.20
1	QA	960	U	N3-C2-O2	-5.14	118.60	122.20
34	YA	2402	C	P-O3'-C3'	5.14	125.87	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	QA	1198	G	N9-C4-C5	5.14	107.46	105.40
1	XA	989	C	C6-N1-C2	-5.14	118.24	120.30
34	YA	867	C	C2-N1-C1'	5.14	124.45	118.80
1	QA	936	C	N1-C2-O2	5.13	121.98	118.90
1	XA	705	U	N3-C2-O2	-5.13	118.61	122.20
1	XA	1147	C	N1-C2-O2	5.13	121.98	118.90
35	YB	27	C	C6-N1-C2	-5.13	118.25	120.30
34	RA	508	G	N3-C4-C5	-5.13	126.04	128.60
34	RA	1304	C	C6-N1-C2	-5.13	118.25	120.30
34	RA	456	C	C5-C6-N1	5.13	123.56	121.00
34	YA	828	U	C5-C6-N1	5.13	125.26	122.70
1	QA	1301	U	C6-N1-C2	-5.12	117.93	121.00
1	XA	1290	G	C8-N9-C1'	-5.12	120.34	127.00
34	YA	1920	C	C2-N1-C1'	5.12	124.43	118.80
1	XA	1004	A	C2-N3-C4	5.12	113.16	110.60
34	YA	529	A	C4-N9-C1'	5.12	135.51	126.30
34	YA	912	C	C2-N1-C1'	5.12	124.43	118.80
34	RA	2096	U	N3-C2-O2	-5.12	118.62	122.20
34	YA	2099	U	N1-C2-O2	5.12	126.38	122.80
1	QA	1290	G	N3-C4-C5	-5.11	126.04	128.60
34	RA	914	C	C6-N1-C2	-5.11	118.25	120.30
34	YA	269	U	N3-C2-O2	-5.11	118.62	122.20
34	YA	2043	C	C5-C6-N1	5.11	123.56	121.00
34	YA	384	U	N1-C2-O2	5.11	126.38	122.80
34	YA	2343	C	N3-C2-O2	-5.11	118.33	121.90
34	YA	1314	C	C6-N1-C2	-5.10	118.26	120.30
1	QA	405	U	N3-C2-O2	-5.10	118.63	122.20
1	QA	497	U	N3-C2-O2	-5.10	118.63	122.20
34	YA	2683	C	C6-N1-C2	-5.10	118.26	120.30
34	YA	2752	C	C6-N1-C2	-5.10	118.26	120.30
34	RA	183	C	N1-C2-O2	5.10	121.96	118.90
34	YA	2769	C	C2-N1-C1'	5.09	124.40	118.80
50	RV	50	PRO	N-CA-CB	-5.09	97.00	102.60
1	QA	481	G	P-O3'-C3'	5.09	125.80	119.70
35	YB	47	C	N1-C2-O2	5.08	121.95	118.90
34	RA	1675	C	N3-C2-O2	-5.08	118.34	121.90
34	RA	986	C	C6-N1-C2	-5.08	118.27	120.30
34	RA	846	C	N3-C2-O2	-5.08	118.34	121.90
1	XA	989	C	C2-N1-C1'	5.08	124.39	118.80
22	XV	61	C	C2-N3-C4	5.08	122.44	119.90
34	YA	1776	G	N3-C4-N9	5.08	129.05	126.00
34	YA	2726	U	N1-C2-O2	5.08	126.35	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	RB	77	U	C2-N1-C1'	5.08	123.79	117.70
34	YA	2471	C	N1-C2-O2	5.08	121.95	118.90
34	YA	364	C	C6-N1-C2	-5.07	118.27	120.30
54	RZ	201	LYS	CA-CB-CG	5.07	124.56	113.40
34	YA	2043	C	C6-N1-C2	-5.07	118.27	120.30
34	YA	1188	U	N1-C2-O2	5.07	126.35	122.80
34	YA	1675	C	N1-C2-O2	5.07	121.94	118.90
1	XA	1514	C	C5-C6-N1	5.06	123.53	121.00
34	RA	898	C	C6-N1-C2	-5.06	118.28	120.30
35	RB	30	C	C2-N1-C1'	5.06	124.36	118.80
34	YA	2179	C	C6-N1-C2	-5.06	118.28	120.30
34	RA	1535	U	C2-N1-C1'	5.05	123.76	117.70
1	XA	283	C	N3-C2-O2	-5.05	118.36	121.90
35	YB	37	C	C6-N1-C2	-5.05	118.28	120.30
34	YA	856	C	P-O3'-C3'	5.05	125.76	119.70
1	QA	1158	C	C2-N3-C4	5.05	122.42	119.90
34	RA	269	U	N3-C2-O2	-5.05	118.67	122.20
1	XA	620	C	N3-C2-O2	-5.05	118.37	121.90
34	RA	243	U	C5-C6-N1	5.04	125.22	122.70
1	XA	455	C	N3-C2-O2	-5.04	118.37	121.90
34	RA	1430	C	C5-C6-N1	5.04	123.52	121.00
34	RA	2825	C	N3-C2-O2	-5.04	118.37	121.90
1	XA	1383	C	N3-C2-O2	-5.04	118.37	121.90
34	YA	1314	C	C5-C6-N1	5.04	123.52	121.00
1	QA	510	A	O5'-P-OP1	-5.04	101.16	105.70
1	XA	1140	C	N1-C2-O2	5.04	121.92	118.90
34	YA	898	C	C2-N1-C1'	5.04	124.34	118.80
34	RA	860	U	N3-C2-O2	-5.04	118.67	122.20
35	RB	37	C	N3-C2-O2	-5.04	118.38	121.90
34	RA	904	C	C6-N1-C2	-5.03	118.29	120.30
34	YA	2068	U	N1-C2-O2	5.03	126.32	122.80
34	YA	974(A)	C	N3-C2-O2	-5.03	118.38	121.90
34	RA	345	A	P-O3'-C3'	5.03	125.74	119.70
40	RH	128	PRO	C-N-CA	5.03	134.27	121.70
34	YA	1460	A	P-O3'-C3'	5.03	125.74	119.70
34	RA	339	U	N1-C2-O2	5.03	126.32	122.80
34	RA	1678	G	N3-C2-N2	-5.03	116.38	119.90
34	RA	2752	C	N1-C2-O2	5.03	121.92	118.90
34	YA	2682	U	N1-C2-O2	5.03	126.32	122.80
1	XA	346	G	C8-N9-C1'	-5.03	120.47	127.00
34	RA	1053	C	P-O3'-C3'	5.02	125.73	119.70
34	YA	1105	U	C2-N1-C1'	5.02	123.73	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	QA	722	A	C2-N3-C4	5.02	113.11	110.60
34	RA	2471	C	C2-N1-C1'	5.02	124.33	118.80
34	RA	2556	C	N3-C2-O2	-5.02	118.39	121.90
1	XA	328	C	C2-N1-C1'	5.02	124.32	118.80
34	YA	999	U	N3-C2-O2	-5.02	118.69	122.20
34	YA	1135	C	N1-C2-O2	5.02	121.91	118.90
1	XA	330	C	C2-N1-C1'	5.02	124.32	118.80
34	YA	930	U	C2-N1-C1'	5.02	123.72	117.70
34	RA	1332	G	N7-C8-N9	5.02	115.61	113.10
1	XA	689	C	C2-N1-C1'	5.01	124.32	118.80
34	RA	1992	G	OP2-P-O3'	5.01	116.23	105.20
34	YA	1509	C	P-O3'-C3'	5.01	125.72	119.70
34	RA	195	A	P-O3'-C3'	5.01	125.71	119.70
34	RA	1052	C	N1-C2-O2	5.01	121.91	118.90
34	RA	1786	A	C4-N9-C1'	5.01	135.32	126.30
1	XA	536	C	C6-N1-C2	-5.01	118.30	120.30
34	YA	1433	U	N3-C2-O2	-5.01	118.69	122.20
34	RA	1417	C	C2-N1-C1'	5.01	124.31	118.80
34	RA	2739	U	N3-C2-O2	-5.01	118.69	122.20
34	YA	970	C	C5-C6-N1	5.01	123.50	121.00
1	QA	652	U	N3-C2-O2	-5.01	118.69	122.20
34	RA	114	U	N1-C2-O2	5.01	126.30	122.80
1	QA	848	C	N1-C2-O2	5.00	121.90	118.90
1	QA	1224	G	N3-C4-N9	-5.00	123.00	126.00
34	RA	1079	C	C6-N1-C2	-5.00	118.30	120.30
34	YA	893	C	N3-C2-O2	-5.00	118.40	121.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	Y3	34	GLU	Mainchain
37	YE	146	THR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16278	248	0
1	XA	32471	0	16395	253	0
2	QB	1907	0	1958	20	0
2	XB	1915	0	1969	19	0
3	QC	1605	0	1668	30	0
3	XC	1605	0	1668	20	0
4	QD	1703	0	1767	21	0
4	XD	1703	0	1767	46	0
5	QE	1155	0	1213	12	0
5	XE	1155	0	1213	12	0
6	QF	843	0	857	5	0
6	XF	843	0	857	10	0
7	QG	1257	0	1296	11	0
7	XG	1257	0	1296	13	0
8	QH	1108	0	1165	14	0
8	XH	1108	0	1165	11	0
9	QI	1010	0	1037	31	0
9	XI	998	0	1024	16	0
10	QJ	801	0	849	15	0
10	XJ	777	0	816	14	0
11	QK	885	0	904	16	0
11	XK	864	0	881	16	0
12	QL	975	0	1062	20	0
12	XL	956	0	1046	24	0
13	QM	955	0	1021	29	0
13	XM	946	0	1008	13	0
14	QN	492	0	531	8	0
14	XN	492	0	529	8	0
15	QO	734	0	771	4	0
15	XO	729	0	768	5	0
16	QP	705	0	725	8	0
16	XP	705	0	725	8	0
17	QQ	834	0	904	7	0
17	XQ	834	0	904	7	0
18	QR	574	0	644	6	0
18	XR	574	0	644	11	0
19	QS	665	0	686	13	0
19	XS	674	0	699	11	0
20	QT	763	0	861	11	0
20	XT	763	0	861	8	0
21	QU	217	0	234	1	0
21	XU	217	0	234	5	0
22	QV	1584	0	808	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	XV	1584	0	808	14	0
23	QX	65	0	33	1	0
23	XX	499	0	249	6	0
24	R0	603	0	620	12	0
24	Y0	599	0	617	11	0
25	R1	763	0	848	12	0
25	Y1	729	0	802	11	0
26	R2	581	0	629	8	0
26	Y2	575	0	624	7	0
27	R3	469	0	518	4	0
27	Y3	469	0	518	22	0
28	R4	565	0	557	6	0
28	Y4	565	0	559	7	0
29	R5	459	0	478	4	0
29	Y5	459	0	477	6	0
30	R6	453	0	477	5	0
30	Y6	453	0	476	5	0
31	R7	409	0	454	4	0
31	Y7	418	0	467	3	0
32	R8	517	0	582	45	0
32	Y8	517	0	582	9	0
33	R9	307	0	337	5	0
33	Y9	307	0	336	8	0
34	RA	62051	0	31279	371	0
34	YA	62091	0	31298	424	0
35	RB	2573	0	1306	16	0
35	YB	2573	0	1306	11	0
36	RD	2115	0	2195	43	0
36	YD	2115	0	2195	37	0
37	RE	1568	0	1634	29	0
37	YE	1563	0	1629	19	0
38	RF	1585	0	1632	23	0
38	YF	1585	0	1632	16	0
39	RG	1474	0	1535	51	0
39	YG	1474	0	1535	45	0
40	RH	1336	0	1418	47	0
40	YH	1330	0	1413	15	0
41	RI	1136	0	1223	32	0
41	YI	1136	0	1223	55	0
42	RN	1104	0	1180	29	0
42	YN	1104	0	1180	11	0
43	RO	933	0	996	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	YO	933	0	996	19	0
44	RP	1145	0	1228	35	0
44	YP	1122	0	1204	22	0
45	RQ	1122	0	1179	24	0
45	YQ	1122	0	1179	28	0
46	RR	960	0	1021	11	0
46	YR	960	0	1021	11	0
47	RS	882	0	943	19	0
47	YS	882	0	943	17	0
48	RT	1141	0	1202	29	0
48	YT	1141	0	1202	32	0
49	RU	964	0	1022	26	0
49	YU	964	0	1022	50	0
50	RV	779	0	852	31	0
50	YV	779	0	852	16	0
51	RW	900	0	964	9	0
51	YW	900	0	964	29	0
52	RX	725	0	778	6	0
52	YX	725	0	778	10	0
53	RY	818	0	910	8	0
53	YY	818	0	911	11	0
54	RZ	1601	0	1630	32	0
54	YZ	1601	0	1630	30	0
55	XY	362	0	186	4	0
56	Z6	74	0	51	0	0
56	Z8	74	0	51	2	0
57	QA	73	0	0	0	0
57	QF	1	0	0	0	0
57	QH	1	0	0	0	0
57	QJ	1	0	0	0	0
57	QM	1	0	0	0	0
57	QV	1	0	0	0	0
57	R0	1	0	0	0	0
57	R1	1	0	0	0	0
57	R3	1	0	0	0	0
57	RA	483	0	0	0	0
57	RB	7	0	0	0	0
57	RE	4	0	0	0	0
57	RN	1	0	0	0	0
57	RO	1	0	0	0	0
57	RP	3	0	0	0	0
57	RQ	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	RR	1	0	0	0	0
57	RT	1	0	0	0	0
57	RY	1	0	0	0	0
57	XA	73	0	0	0	0
57	XE	1	0	0	0	0
57	XK	1	0	0	0	0
57	XL	1	0	0	0	0
57	XM	1	0	0	0	0
57	XQ	1	0	0	0	0
57	XS	1	0	0	0	0
57	Y0	2	0	0	0	0
57	Y1	1	0	0	0	0
57	Y7	1	0	0	0	0
57	Y8	1	0	0	0	0
57	YA	538	0	0	0	0
57	YB	13	0	0	0	0
57	YD	3	0	0	0	0
57	YE	4	0	0	0	0
57	YN	1	0	0	0	0
57	YO	1	0	0	0	0
57	YP	1	0	0	0	0
57	YQ	3	0	0	0	0
57	YR	2	0	0	0	0
57	YX	2	0	0	0	0
57	YY	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	RY	1	0	0	0	0
59	XN	1	0	0	0	0
59	Y4	1	0	0	0	0
59	Y5	1	0	0	0	0
59	Y6	1	0	0	0	0
59	Y9	1	0	0	0	0
59	YY	1	0	0	0	0
All	All	292577	0	198284	2581	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 (2581) 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:YW:1:MET:HG3	51:YW:64:MET:CE	1.51	1.41
50:YV:40:LEU:CD2	50:YV:47:VAL:HG12	1.52	1.40
4:XD:19:LEU:CD2	4:XD:197:PRO:HG3	1.59	1.33
1:QA:1189:C:H5"	3:QC:5:ILE:CD1	1.56	1.33
41:YI:61:ARG:HB2	41:YI:133:HIS:CE1	1.73	1.23
51:YW:1:MET:CG	51:YW:64:MET:HE2	1.70	1.19
13:QM:24:GLY:HA3	13:QM:66:LEU:CD2	1.71	1.18
42:RN:112:LEU:O	42:RN:116:LEU:HD12	1.41	1.17
41:YI:14:ASP:OD1	41:YI:17:GLN:HG2	1.45	1.16
51:YW:1:MET:C	51:YW:64:MET:HE1	1.67	1.15
32:R8:25:MET:HE1	44:RP:64:LYS:HD2	1.16	1.15
49:RU:92:ARG:HG2	49:RU:95:LEU:CD2	1.77	1.14
41:YI:61:ARG:CB	41:YI:133:HIS:CE1	2.29	1.14
36:RD:121:PRO:HB3	36:RD:135:PHE:CE2	1.82	1.13
41:YI:92:VAL:O	41:YI:120:ILE:HG22	1.46	1.13
2:XB:212:GLN:NE2	2:XB:235:SER:HB3	1.65	1.11
36:RD:121:PRO:HB3	36:RD:135:PHE:HE2	1.14	1.11
42:RN:23:LEU:HD12	42:RN:60:ILE:CD1	1.81	1.10
12:XL:46:LYS:HG2	12:XL:47:LYS:H	1.05	1.09
48:YT:120:ARG:HA	48:YT:123:GLN:HG3	1.30	1.09
51:YW:1:MET:CG	51:YW:64:MET:CE	2.28	1.09
2:XB:212:GLN:CD	2:XB:235:SER:HB3	1.71	1.09
4:XD:19:LEU:HD21	4:XD:197:PRO:HG3	1.34	1.08
34:YA:997:G:OP1	49:YU:93:LYS:HB2	1.50	1.08
41:YI:61:ARG:HB2	41:YI:133:HIS:HE1	1.06	1.08
41:RI:123:LEU:HD12	41:RI:123:LEU:H	1.16	1.08
51:YW:1:MET:HG3	51:YW:64:MET:HE2	1.15	1.06
41:YI:118:LYS:HB3	41:YI:119:PRO:HD3	1.36	1.05
50:RV:52:VAL:HG21	50:RV:55:ALA:HB3	1.36	1.05
41:YI:92:VAL:HB	41:YI:120:ILE:CG2	1.86	1.04
13:QM:24:GLY:HA3	13:QM:66:LEU:HD22	1.04	1.04
44:RP:101:VAL:HB	44:RP:106:LEU:HB3	1.40	1.04
50:YV:40:LEU:HD22	50:YV:47:VAL:HG12	1.39	1.04
48:RT:107:ASP:O	48:RT:110:ILE:HG22	1.58	1.03
1:QA:1189:C:H5"	3:QC:5:ILE:HD12	1.37	1.03
34:RA:2361:A:H5"	34:RA:2361:A:H8	1.24	1.02
41:YI:92:VAL:HB	41:YI:120:ILE:HG23	1.40	1.02
34:YA:996:A:O2'	49:YU:92:ARG:HD2	1.60	1.01
49:RU:91:ASP:HA	49:RU:95:LEU:HB2	1.43	1.01
41:YI:118:LYS:HB3	41:YI:119:PRO:CD	1.90	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:RN:23:LEU:CD1	42:RN:60:ILE:HD12	1.92	1.00
42:RN:23:LEU:HD12	42:RN:60:ILE:HD12	1.00	1.00
41:YI:120:ILE:HD11	41:YI:126:TYR:CE2	1.96	1.00
51:YW:1:MET:HG3	51:YW:64:MET:HE3	1.39	0.99
32:R8:61:LEU:HD12	34:RA:593:G:H4'	1.45	0.99
34:RA:2135:A:H62	34:RA:2156:G:N2	1.61	0.99
34:YA:997:G:H5'	49:YU:92:ARG:HB2	1.45	0.98
35:RB:8:U:H3	35:RB:112:G:H1	1.03	0.98
32:R8:61:LEU:CD1	34:RA:593:G:H4'	1.94	0.98
49:YU:92:ARG:NH1	49:YU:95:LEU:CD1	2.26	0.97
39:RG:83:ARG:HB3	39:RG:83:ARG:HH11	1.24	0.97
4:XD:19:LEU:HD22	4:XD:197:PRO:HG3	1.44	0.97
41:YI:120:ILE:HD11	41:YI:126:TYR:CD2	2.00	0.97
51:YW:1:MET:C	51:YW:64:MET:CE	2.33	0.97
4:XD:19:LEU:HD21	4:XD:197:PRO:CG	1.95	0.96
32:R8:25:MET:CE	44:RP:64:LYS:HD2	1.95	0.96
32:R8:27:THR:HG23	34:RA:2392:A:O2'	1.64	0.96
2:XB:212:GLN:CD	2:XB:235:SER:CB	2.34	0.95
4:XD:19:LEU:CD2	4:XD:197:PRO:CG	2.43	0.95
41:RI:132:PRO:HD2	41:RI:134:PRO:O	1.63	0.95
13:QM:24:GLY:CA	13:QM:66:LEU:HD22	1.96	0.95
50:YV:40:LEU:HD23	50:YV:47:VAL:HG12	1.49	0.95
34:RA:2135:A:N6	34:RA:2156:G:H21	1.63	0.94
34:YA:1359:A:H62	34:YA:1372:U:H3	0.99	0.94
41:YI:133:HIS:HB3	41:YI:134:PRO:HD3	1.48	0.94
50:YV:40:LEU:CD2	50:YV:47:VAL:CG1	2.46	0.93
34:YA:2096:U:H3	34:YA:2193:G:H1	1.15	0.93
12:XL:84:LEU:CB	12:XL:104:VAL:HG11	1.98	0.93
12:XL:46:LYS:HG2	12:XL:47:LYS:N	1.84	0.93
34:YA:997:G:OP1	49:YU:93:LYS:HE2	1.68	0.93
51:YW:1:MET:O	51:YW:64:MET:HE1	1.67	0.92
39:YG:84:LYS:HA	39:YG:84:LYS:NZ	1.85	0.92
41:RI:120:ILE:HD11	41:RI:126:TYR:CE2	2.05	0.91
40:RH:9:ILE:CG2	40:RH:10:PRO:CD	2.48	0.91
45:YQ:27:VAL:HA	45:YQ:105:GLU:OE2	1.69	0.91
4:XD:31:CYS:O	4:XD:31:CYS:SG	2.29	0.91
41:YI:61:ARG:HB3	41:YI:133:HIS:CE1	2.06	0.90
40:RH:9:ILE:CG2	40:RH:10:PRO:HD2	2.02	0.90
27:Y3:5:LYS:HA	27:Y3:36:VAL:HG12	1.49	0.90
32:R8:61:LEU:HD11	34:RA:593:G:O2'	1.72	0.90
27:Y3:5:LYS:HB2	27:Y3:36:VAL:CG1	2.01	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:YI:133:HIS:CB	41:YI:134:PRO:CD	2.50	0.90
50:RV:52:VAL:HG23	50:RV:55:ALA:H	1.36	0.89
41:YI:9:LEU:H	41:YI:9:LEU:HD12	1.37	0.89
34:YA:1359:A:N6	34:YA:1372:U:H3	1.70	0.89
32:R8:57:ARG:O	32:R8:61:LEU:CD2	2.21	0.89
34:RA:2808:U:C2	34:RA:2892:A:N6	2.41	0.89
1:XA:1357:A:H61	1:XA:1365:G:H1	1.20	0.89
34:YA:2099:U:H3	34:YA:2190:G:H1	1.16	0.89
37:YE:28:ALA:O	37:YE:93:VAL:CG1	2.20	0.89
37:YE:28:ALA:O	37:YE:93:VAL:HG13	1.74	0.88
32:R8:52:LYS:H	32:R8:53:PRO:CD	1.85	0.88
48:YT:119:LYS:O	48:YT:123:GLN:HG3	1.74	0.88
40:RH:12:PRO:HG3	40:RH:48:GLY:HA2	1.54	0.87
41:YI:133:HIS:CB	41:YI:134:PRO:HD3	2.03	0.87
48:YT:120:ARG:HA	48:YT:123:GLN:CG	2.04	0.87
40:RH:9:ILE:HG22	40:RH:10:PRO:HD2	1.57	0.87
44:RP:107:LYS:HB3	44:RP:107:LYS:HZ3	1.39	0.87
1:QA:1189:C:C5'	3:QC:5:ILE:CD1	2.49	0.87
1:QA:1189:C:H5"	3:QC:5:ILE:HD13	1.53	0.86
27:Y3:5:LYS:HB2	27:Y3:36:VAL:HG12	1.57	0.86
39:RG:84:LYS:HA	39:RG:84:LYS:CE	2.03	0.86
45:YQ:27:VAL:HG13	45:YQ:105:GLU:OE2	1.76	0.85
34:RA:2135:A:H62	34:RA:2156:G:H21	0.88	0.85
54:YZ:7:ALA:HB2	54:YZ:59:LEU:HD12	1.57	0.85
49:RU:92:ARG:HG2	49:RU:95:LEU:HD21	1.59	0.84
44:RP:101:VAL:CB	44:RP:106:LEU:HB3	2.05	0.84
13:QM:66:LEU:HD23	13:QM:70:LEU:HD22	1.59	0.84
27:Y3:5:LYS:CA	27:Y3:36:VAL:HG12	2.08	0.83
12:XL:84:LEU:HB3	12:XL:104:VAL:HG11	1.60	0.83
39:RG:83:ARG:HH11	39:RG:83:ARG:CB	1.92	0.83
35:YB:8:U:H3	35:YB:112:G:H1	1.23	0.83
49:YU:92:ARG:HH12	49:YU:95:LEU:HG	1.41	0.83
32:R8:57:ARG:O	32:R8:61:LEU:HD23	1.78	0.83
32:R8:52:LYS:N	32:R8:53:PRO:CD	2.42	0.83
39:RG:84:LYS:HA	39:RG:84:LYS:HE3	1.59	0.83
4:XD:19:LEU:HD11	4:XD:63:LYS:HG3	1.61	0.83
41:YI:8:PRO:HG3	41:YI:14:ASP:HA	1.61	0.82
49:YU:87:GLY:O	50:YV:50:PRO:HD3	1.79	0.82
41:RI:86:THR:HA	41:RI:123:LEU:HD13	1.62	0.82
48:YT:120:ARG:CA	48:YT:123:GLN:HG3	2.10	0.82
13:QM:24:GLY:CA	13:QM:66:LEU:CD2	2.57	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:YW:1:MET:CB	51:YW:64:MET:CE	2.58	0.81
49:YU:92:ARG:HH12	49:YU:95:LEU:CD1	1.94	0.81
44:RP:101:VAL:HB	44:RP:106:LEU:CB	2.11	0.81
12:XL:84:LEU:HB2	12:XL:104:VAL:HG11	1.61	0.80
34:YA:2069:G:N2	34:YA:2443:C:C2	2.49	0.80
45:YQ:27:VAL:CA	45:YQ:105:GLU:OE2	2.28	0.80
32:R8:52:LYS:N	32:R8:53:PRO:HD2	1.97	0.80
40:RH:9:ILE:HG22	40:RH:10:PRO:CD	2.10	0.80
27:Y3:5:LYS:CB	27:Y3:36:VAL:HG12	2.12	0.80
49:YU:92:ARG:HH11	49:YU:95:LEU:HD12	1.46	0.80
40:RH:9:ILE:HG23	40:RH:10:PRO:CD	2.11	0.80
34:YA:2308:G:N1	39:YG:80:PHE:HZ	1.78	0.80
54:RZ:48:PHE:HA	54:RZ:51:ALA:HB3	1.62	0.80
49:YU:92:ARG:HH12	49:YU:95:LEU:CG	1.95	0.79
34:RA:2361:A:H5"	34:RA:2361:A:C8	2.15	0.79
49:YU:92:ARG:NH1	49:YU:95:LEU:HD12	1.97	0.79
22:XV:54:U:H5"	54:YZ:202:GLU:HA	1.65	0.79
48:YT:119:LYS:O	48:YT:123:GLN:CG	2.31	0.79
50:RV:44:LYS:O	50:RV:46:VAL:HG12	1.82	0.79
41:YI:61:ARG:CB	41:YI:133:HIS:HE1	1.79	0.78
41:YI:118:LYS:CB	41:YI:119:PRO:CD	2.60	0.78
40:RH:12:PRO:HG3	40:RH:48:GLY:CA	2.14	0.77
36:YD:121:PRO:HB3	36:YD:135:PHE:CD2	2.19	0.77
37:RE:55:ASN:OD1	37:RE:58:ARG:HD2	1.84	0.77
41:RI:123:LEU:H	41:RI:123:LEU:CD1	1.93	0.77
36:YD:121:PRO:HB3	36:YD:135:PHE:CE2	2.18	0.77
34:YA:2304:G:H22	34:YA:2312:U:H3	1.33	0.77
42:RN:115:ARG:HG2	42:RN:115:ARG:HH11	1.50	0.77
50:YV:40:LEU:HD21	50:YV:47:VAL:HG12	1.65	0.77
48:RT:121:ILE:O	48:RT:125:ARG:HG2	1.84	0.76
41:YI:131:LYS:HB3	41:YI:135:GLU:HA	1.66	0.76
54:YZ:53:ILE:HG22	54:YZ:71:VAL:HG13	1.66	0.76
1:XA:452:A:H62	1:XA:480:U:H3	1.33	0.76
39:RG:81:LYS:HE3	39:RG:83:ARG:HD2	1.68	0.76
37:RE:16:ARG:HG3	37:RE:16:ARG:O	1.86	0.76
48:RT:120:ARG:HG2	48:RT:123:GLN:OE1	1.84	0.76
54:YZ:124:ILE:HD11	54:YZ:165:VAL:HG11	1.66	0.76
41:RI:83:ALA:HB1	41:RI:123:LEU:HD21	1.68	0.76
27:Y3:37:LEU:HD12	27:Y3:37:LEU:N	2.01	0.76
39:YG:84:LYS:HA	39:YG:84:LYS:HZ3	1.51	0.76
41:YI:65:ALA:CB	41:YI:132:PRO:HG2	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:2245:U:H5'	34:RA:2246:G:H5'	1.68	0.75
34:YA:411:G:N2	44:YP:71:VAL:HG11	2.01	0.75
49:YU:87:GLY:O	50:YV:50:PRO:CD	2.34	0.75
49:RU:92:ARG:HG2	49:RU:95:LEU:HD23	1.67	0.75
42:RN:23:LEU:HD11	42:RN:98:VAL:HG22	1.69	0.75
13:QM:66:LEU:CD2	13:QM:70:LEU:HD22	2.17	0.74
48:RT:112:ARG:HH11	48:RT:112:ARG:HG3	1.51	0.74
39:YG:82:LEU:HD11	39:YG:88:ILE:HD13	1.67	0.74
41:YI:14:ASP:OD1	41:YI:17:GLN:CG	2.32	0.74
1:QA:440:A:H62	1:QA:493:G:H21	1.36	0.74
34:YA:2406:U:C4	44:YP:72:PRO:HD2	2.22	0.74
49:RU:87:GLY:O	50:RV:50:PRO:HD2	1.88	0.74
45:YQ:27:VAL:CG1	45:YQ:105:GLU:OE2	2.36	0.74
40:RH:147:ASN:O	40:RH:151:ILE:HG13	1.87	0.74
50:YV:40:LEU:HD22	50:YV:47:VAL:CG1	2.16	0.74
44:RP:101:VAL:HB	44:RP:106:LEU:HD23	1.70	0.73
40:RH:9:ILE:HG21	40:RH:50:VAL:H	1.54	0.73
41:RI:132:PRO:CD	41:RI:134:PRO:O	2.35	0.73
49:RU:92:ARG:CG	49:RU:95:LEU:CD2	2.63	0.73
26:Y2:47:ASN:HD22	34:YA:94:G:H21	1.37	0.72
34:YA:2245:U:H5'	34:YA:2246:G:H5'	1.70	0.72
41:YI:132:PRO:HD2	41:YI:134:PRO:O	1.89	0.72
34:RA:2508:G:H1	34:RA:2580:U:H3	1.37	0.72
50:RV:52:VAL:HG21	50:RV:55:ALA:CB	2.15	0.72
34:YA:2069:G:C2	34:YA:2443:C:C2	2.78	0.72
48:YT:120:ARG:HG2	48:YT:123:GLN:OE1	1.89	0.72
22:QV:52:G:H21	54:RZ:198:LYS:HE3	1.54	0.72
34:YA:2406:U:H2'	34:YA:2406:U:OP2	1.90	0.71
34:YA:2308:G:N1	39:YG:80:PHE:CZ	2.59	0.71
39:YG:47:LYS:HD2	39:YG:81:LYS:HB2	1.73	0.71
1:XA:1357:A:N6	1:XA:1365:G:H1	1.88	0.71
12:XL:46:LYS:CG	12:XL:47:LYS:H	1.93	0.71
50:RV:51:VAL:HG12	50:RV:53:GLU:H	1.56	0.71
34:RA:2808:U:N3	34:RA:2892:A:N6	2.39	0.71
41:YI:9:LEU:HD12	41:YI:9:LEU:N	2.06	0.71
42:RN:112:LEU:O	42:RN:116:LEU:CD1	2.31	0.71
47:YS:74:ALA:HB1	47:YS:107:GLU:HB3	1.73	0.71
32:R8:37:SER:O	32:R8:40:GLU:N	2.21	0.70
51:YW:2:GLU:N	51:YW:64:MET:HE3	2.07	0.70
48:RT:102:ILE:HB	48:RT:110:ILE:HD13	1.74	0.70
4:XD:19:LEU:HD22	4:XD:197:PRO:CG	2.18	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:YZ:48:PHE:HA	54:YZ:51:ALA:HB3	1.73	0.70
35:RB:80:U:H2'	35:RB:81:G:H21	1.55	0.70
22:QV:34:MNU:HN3	23:QX:3:G:H1	1.37	0.70
50:RV:52:VAL:CG2	50:RV:55:ALA:HB3	2.18	0.70
19:XS:19:VAL:HG11	19:XS:44:MET:HG2	1.73	0.70
35:YB:80:U:H2'	35:YB:81:G:H21	1.57	0.70
34:YA:996:A:O2'	49:YU:92:ARG:CD	2.37	0.70
49:YU:91:ASP:O	49:YU:95:LEU:HB2	1.92	0.70
32:R8:35:GLN:OE1	32:R8:35:GLN:HA	1.91	0.69
27:Y3:2:PRO:HA	27:Y3:39:ASP:HB3	1.73	0.69
12:QL:117:ARG:HB2	12:QL:122:THR:HB	1.75	0.69
1:XA:664:G:H22	1:XA:741:G:H1	1.41	0.69
39:YG:84:LYS:HA	39:YG:84:LYS:HZ2	1.55	0.69
41:RI:8:PRO:HD3	41:RI:15:VAL:HG22	1.73	0.69
41:YI:65:ALA:HB1	41:YI:132:PRO:HG2	1.73	0.69
1:XA:438:G:H21	1:XA:496:A:H62	1.40	0.69
47:YS:74:ALA:CB	47:YS:107:GLU:HB3	2.23	0.69
49:YU:95:LEU:HD11	50:YV:11:GLN:HB2	1.73	0.69
51:YW:1:MET:CB	51:YW:64:MET:HE1	2.22	0.69
34:RA:1038:C:H42	34:RA:1117:G:H1	1.41	0.69
2:QB:231:GLU:HG3	2:QB:232:PRO:HD2	1.75	0.68
27:Y3:3:ARG:CB	27:Y3:60:GLU:OXT	2.41	0.68
41:YI:92:VAL:O	41:YI:120:ILE:CG2	2.36	0.68
22:XV:74:C:H42	34:YA:2252:G:H1	1.40	0.68
36:RD:109:ASP:N	36:RD:196:VAL:O	2.27	0.68
41:RI:120:ILE:CD1	41:RI:126:TYR:CE2	2.76	0.68
49:YU:92:ARG:NH1	49:YU:95:LEU:HG	2.07	0.68
32:R8:30:ARG:NH2	44:RP:62:LEU:HD12	2.08	0.68
42:RN:114:ARG:HB3	42:RN:114:ARG:HH11	1.57	0.68
1:QA:1492:A:OP2	12:QL:47:LYS:HE2	1.93	0.68
44:RP:107:LYS:HB3	44:RP:107:LYS:NZ	2.08	0.68
34:YA:997:G:OP1	49:YU:93:LYS:CE	2.42	0.68
25:Y1:83:GLU:HG2	25:Y1:85:LEU:H	1.58	0.67
34:RA:1062:G:H22	34:RA:1088:A:H62	1.42	0.67
41:YI:14:ASP:OD1	41:YI:14:ASP:N	2.24	0.67
41:YI:133:HIS:HB2	41:YI:134:PRO:CD	2.25	0.67
1:XA:827:U:O2	1:XA:874:G:N2	2.27	0.67
35:YB:30:C:H1'	35:YB:57:A:H61	1.60	0.67
42:RN:112:LEU:C	42:RN:116:LEU:HD12	2.13	0.67
44:RP:101:VAL:HB	44:RP:106:LEU:CD2	2.25	0.67
50:RV:52:VAL:CG2	50:RV:55:ALA:H	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:2361:A:H8	34:RA:2361:A:C5'	2.04	0.67
39:RG:83:ARG:HB3	39:RG:83:ARG:NH1	2.06	0.67
3:XC:81:GLY:O	3:XC:85:ARG:HG2	1.95	0.66
29:R5:19:ARG:NH2	34:RA:1264:G:OP1	2.29	0.66
54:RZ:4:ARG:HG2	54:RZ:58:VAL:HB	1.78	0.66
34:YA:67:U:H3	34:YA:74:A:H2	1.41	0.66
32:R8:27:THR:CG2	34:RA:2392:A:O2'	2.41	0.66
41:RI:83:ALA:CB	41:RI:123:LEU:HD21	2.26	0.66
1:XA:111:G:H1	1:XA:330:C:H41	1.44	0.66
1:XA:954:G:H21	1:XA:1227:A:H62	1.44	0.66
4:XD:19:LEU:CD1	4:XD:63:LYS:HG3	2.25	0.66
40:RH:12:PRO:CG	40:RH:48:GLY:HA2	2.26	0.66
4:XD:18:LYS:HB3	4:XD:33:MET:SD	2.36	0.66
32:Y8:14:VAL:HG23	32:Y8:24:ALA:HB2	1.77	0.66
24:R0:27:GLU:HG3	24:R0:68:GLU:HA	1.77	0.66
36:RD:121:PRO:CB	36:RD:135:PHE:HE2	2.01	0.66
1:QA:689:C:H3'	1:QA:690:G:H21	1.60	0.65
1:QA:1322:C:OP2	19:QS:78:ARG:NH1	2.29	0.65
24:Y0:27:GLU:HG3	24:Y0:68:GLU:HA	1.77	0.65
34:YA:1995:U:O2	43:YO:3:GLN:NE2	2.29	0.65
1:QA:1322:C:OP2	19:QS:78:ARG:NH2	2.29	0.65
42:RN:110:GLY:O	42:RN:114:ARG:NH1	2.29	0.65
47:RS:10:ARG:NH1	47:RS:91:PRO:O	2.29	0.65
32:R8:30:ARG:HH21	44:RP:62:LEU:HD12	1.62	0.65
40:RH:9:ILE:HD12	40:RH:50:VAL:O	1.96	0.65
2:XB:212:GLN:CD	2:XB:235:SER:HB2	2.15	0.65
34:YA:1568:G:H5"	36:YD:61:LEU:HD23	1.78	0.65
40:RH:9:ILE:HG23	40:RH:10:PRO:HD3	1.77	0.65
11:QK:18:ARG:HG2	11:QK:81:ASP:HB2	1.77	0.65
13:QM:80:ARG:HH12	13:QM:84:ILE:HD13	1.61	0.65
54:YZ:54:HIS:ND1	54:YZ:101:PRO:HG3	2.11	0.65
34:RA:855:G:H1	34:RA:922:U:H3	1.45	0.65
25:Y1:18:ILE:HG12	25:Y1:37:ILE:HG12	1.79	0.65
49:YU:92:ARG:NH1	49:YU:95:LEU:HD11	2.10	0.65
1:QA:664:G:H22	1:QA:741:G:H1	1.43	0.65
9:XI:3:GLN:HG2	9:XI:20:ARG:HB2	1.79	0.64
54:YZ:54:HIS:HB3	54:YZ:101:PRO:HD3	1.80	0.64
34:RA:2751:G:N7	40:RH:2:SER:N	2.45	0.64
1:XA:686:U:H1'	11:XK:42:TRP:HE1	1.62	0.64
1:QA:1066:C:N4	1:QA:1191:A:N6	2.46	0.64
13:XM:14:ARG:H	13:XM:44:ARG:HG3	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:RG:84:LYS:HE3	39:RG:84:LYS:CA	2.28	0.64
1:QA:686:U:H1'	11:QK:42:TRP:HE1	1.62	0.64
17:QQ:66:SER:O	17:QQ:70:ARG:NH1	2.31	0.64
32:R8:61:LEU:HD13	34:RA:593:G:H4'	1.79	0.64
1:XA:950:U:H3	1:XA:1231:G:H1	1.46	0.64
32:R8:30:ARG:HG3	32:R8:30:ARG:O	1.97	0.64
1:XA:1502:A:H2	1:XA:1505:G:H1	1.46	0.64
1:QA:1492:A:OP2	12:QL:47:LYS:CE	2.46	0.64
19:QS:19:VAL:HG21	19:QS:44:MET:HG2	1.80	0.64
2:XB:212:GLN:OE1	2:XB:235:SER:CB	2.46	0.64
4:XD:20:TYR:CE1	4:XD:106:TYR:OH	2.51	0.64
41:YI:61:ARG:CB	41:YI:133:HIS:ND1	2.61	0.64
1:QA:152:A:H62	1:QA:169:C:H42	1.44	0.64
4:XD:16:GLY:C	4:XD:33:MET:HE1	2.18	0.64
4:XD:19:LEU:HD11	4:XD:63:LYS:CG	2.28	0.64
1:QA:1086:U:H3	1:QA:1099:G:H22	1.46	0.63
34:RA:1678:G:N2	34:RA:1990:C:O2	2.31	0.63
1:QA:1322:C:H6	1:QA:1322:C:OP1	1.80	0.63
3:XC:20:SER:HB2	3:XC:40:ARG:HH22	1.62	0.63
36:YD:182:LEU:H	36:YD:272:ALA:HB3	1.63	0.63
49:YU:92:ARG:NH1	49:YU:95:LEU:CG	2.59	0.63
19:XS:41:VAL:HG12	19:XS:43:GLU:H	1.63	0.63
32:R8:12:LYS:HG2	44:RP:68:GLN:HG2	1.79	0.63
4:QD:62:GLN:HE22	4:QD:65:ARG:HH21	1.47	0.63
41:YI:91:SER:HB2	41:YI:119:PRO:HB2	1.79	0.63
32:R8:40:GLU:O	32:R8:44:LYS:HD3	1.99	0.63
1:XA:545:C:OP1	4:XD:61:LYS:NZ	2.32	0.63
49:YU:92:ARG:HG3	49:YU:92:ARG:O	1.98	0.63
25:R1:83:GLU:HG2	25:R1:85:LEU:H	1.62	0.63
1:XA:1422:G:H5"	43:YO:48:PRO:HB3	1.80	0.63
42:YN:133:GLN:HG2	42:YN:135:PRO:HD3	1.80	0.63
1:QA:674:G:H2'	1:QA:675:A:H8	1.64	0.63
34:RA:2393:A:C8	34:RA:2393:A:H5"	2.34	0.63
17:XQ:66:SER:O	17:XQ:70:ARG:NH1	2.32	0.63
41:YI:133:HIS:HB2	41:YI:134:PRO:HD2	1.80	0.63
48:YT:51:ARG:HH21	48:YT:62:THR:HG21	1.63	0.63
3:QC:114:PRO:O	3:QC:118:GLN:HB2	1.99	0.62
51:YW:1:MET:CB	51:YW:64:MET:HE2	2.26	0.62
1:QA:1189:C:H5"	3:QC:5:ILE:HD11	1.73	0.62
34:RA:2360:A:H8	34:RA:2360:A:O5'	1.81	0.62
1:XA:439:A:OP2	1:XA:493:G:N1	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:YI:117:GLU:OE1	41:YI:117:GLU:N	2.19	0.62
22:QV:74:C:H42	34:RA:2252:G:H1	1.47	0.62
29:R5:16:ARG:NH2	34:RA:517:C:OP1	2.33	0.62
9:XI:121:ARG:NH1	9:XI:122:ALA:O	2.33	0.62
34:RA:2068:U:H3	34:RA:2430:A:H2	1.47	0.62
34:YA:996:A:H4'	49:YU:92:ARG:NE	2.14	0.62
41:RI:79:ILE:HG22	41:RI:79:ILE:O	2.00	0.62
34:YA:1250:G:OP2	44:YP:18:ARG:NH2	2.32	0.62
34:YA:2443:C:H2'	34:YA:2444:G:H8	1.65	0.62
34:YA:2392:A:H1'	44:YP:61:ARG:HE	1.64	0.62
54:YZ:124:ILE:CD1	54:YZ:165:VAL:HG11	2.29	0.62
10:XJ:6:ILE:HD11	10:XJ:96:ILE:HB	1.81	0.62
54:YZ:166:SER:HB3	54:YZ:168:GLU:H	1.65	0.62
1:QA:1422:G:H5"	43:RO:48:PRO:HB3	1.81	0.62
36:YD:125:ILE:HD13	36:YD:125:ILE:N	2.16	0.61
1:QA:1222:G:H5"	19:QS:78:ARG:HE	1.64	0.61
9:QI:8:GLY:HA2	9:QI:79:LEU:HD23	1.83	0.61
36:RD:161:THR:O	36:RD:196:VAL:HG23	2.00	0.61
1:XA:562:C:H1'	12:XL:15:ARG:HD2	1.82	0.61
34:YA:300:A:OP2	53:YY:84:ARG:NH2	2.34	0.61
14:QN:24:CYS:HB3	14:QN:28:GLY:H	1.65	0.61
34:RA:676:A:H8	34:RA:2069:G:H21	1.47	0.61
34:YA:83:G:H1	34:YA:102:G:HO2'	1.48	0.61
34:YA:2406:U:O4	44:YP:70:GLN:NE2	2.34	0.61
32:R8:52:LYS:H	32:R8:53:PRO:HD3	1.61	0.61
34:RA:27:G:N2	34:RA:513:A:OP2	2.32	0.61
16:XP:53:VAL:HG13	16:XP:79:VAL:HG12	1.82	0.61
10:QJ:24:VAL:HG21	10:QJ:36:GLY:HA2	1.81	0.61
42:YN:15:LEU:HD22	42:YN:134:ARG:HD2	1.83	0.61
42:RN:114:ARG:HH11	42:RN:114:ARG:CG	2.13	0.61
45:RQ:36:ALA:HB2	45:RQ:103:MET:CE	2.31	0.61
34:YA:997:G:OP1	49:YU:93:LYS:CB	2.39	0.61
1:QA:410:G:H21	1:QA:432:A:H62	1.49	0.61
34:RA:1652:A:OP1	46:RR:8:ARG:NH1	2.34	0.61
42:RN:23:LEU:CD1	42:RN:60:ILE:CD1	2.66	0.60
34:YA:2731:G:OP1	37:YE:169:ASN:ND2	2.34	0.60
41:YI:120:ILE:HG23	41:YI:120:ILE:O	2.00	0.60
12:QL:36:VAL:HG22	12:QL:82:VAL:HG22	1.83	0.60
34:RA:2618:G:H21	37:RE:150:VAL:HG21	1.66	0.60
6:QF:3:ARG:NH1	6:QF:38:GLU:OE2	2.34	0.60
34:RA:1187:G:H5'	50:RV:81:TYR:HE1	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:674:G:H2'	1:XA:675:A:H8	1.67	0.60
36:YD:125:ILE:O	36:YD:125:ILE:HG22	2.00	0.60
28:R4:16:CYS:SG	28:R4:17:GLY:N	2.74	0.60
32:R8:52:LYS:HZ2	34:RA:834:C:H4'	1.67	0.60
34:RA:1069:A:H2'	34:RA:1073:A:H62	1.67	0.60
26:Y2:47:ASN:ND2	34:YA:94:G:N3	2.50	0.60
1:QA:1522:U:H2'	1:QA:1523:G:H8	1.66	0.60
41:RI:131:LYS:HG3	41:RI:135:GLU:OE1	2.02	0.60
4:QD:57:ARG:HB3	4:QD:206:PHE:HB2	1.83	0.60
34:RA:1902:C:OP1	36:RD:242:ARG:NH1	2.34	0.60
37:YE:28:ALA:O	37:YE:93:VAL:HG12	1.99	0.60
34:RA:321:G:O2'	34:RA:340:A:N3	2.34	0.60
53:RY:9:LYS:NZ	53:RY:28:LYS:O	2.35	0.60
5:XE:102:ALA:HB1	5:XE:106:PRO:HG2	1.83	0.60
34:YA:2069:G:N2	34:YA:2443:C:O2	2.34	0.60
34:RA:2759:G:H21	40:RH:139:GLN:HE21	1.49	0.60
37:YE:29:GLY:CA	37:YE:180:ASN:HB3	2.31	0.59
1:QA:1066:C:H42	1:QA:1191:A:N6	2.00	0.59
40:RH:118:PRO:HG2	40:RH:121:ILE:HD13	1.83	0.59
46:RR:86:ARG:NH2	46:RR:118:GLU:OXT	2.35	0.59
34:YA:994:C:OP1	49:YU:53:ARG:NH2	2.35	0.59
43:YO:104:ARG:HH21	48:YT:34:VAL:HG11	1.68	0.59
34:RA:1779:U:OP2	34:RA:1784:A:N6	2.32	0.59
34:RA:2303:G:N3	39:RG:132:ASN:ND2	2.50	0.59
24:Y0:39:ARG:HH21	34:YA:2355:C:H1'	1.65	0.59
34:YA:1728:G:H8	34:YA:1732:A:H62	1.48	0.59
34:YA:2287:A:H62	34:YA:2344:U:H3	1.50	0.59
34:RA:2759:G:H21	40:RH:139:GLN:NE2	2.00	0.59
36:RD:108:PRO:HA	36:RD:196:VAL:O	2.03	0.59
39:RG:150:ASP:HB3	39:RG:153:ARG:HH22	1.67	0.59
1:XA:8:A:N6	4:XD:205:GLU:O	2.35	0.59
34:RA:1047:G:H21	34:RA:1111:A:H62	1.50	0.59
28:Y4:53:GLU:OE2	28:Y4:60:GLN:NE2	2.35	0.59
35:YB:111:U:H2'	35:YB:112:G:H8	1.68	0.59
14:QN:24:CYS:SG	14:QN:25:VAL:N	2.76	0.59
34:RA:571:A:H5'	34:RA:2030:A:H62	1.67	0.59
37:RE:5:LEU:HG	37:RE:49:LEU:HD23	1.82	0.59
54:RZ:47:VAL:O	54:RZ:51:ALA:N	2.33	0.59
1:QA:111:G:H1	1:QA:330:C:H41	1.50	0.59
34:RA:2130:U:O2	34:RA:2158:A:N6	2.35	0.59
48:RT:112:ARG:HH11	48:RT:112:ARG:CG	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:1165:U:H3	34:YA:1184:G:H1	1.50	0.59
39:YG:82:LEU:CD1	39:YG:88:ILE:HD13	2.33	0.59
1:QA:1190:G:OP2	3:QC:5:ILE:HD12	2.02	0.59
1:QA:1077:G:N2	1:QA:1080:A:OP2	2.36	0.59
37:RE:78:LEU:HG	37:RE:79:ARG:HG2	1.84	0.59
43:RO:68:GLU:OE2	43:RO:78:ARG:NH1	2.36	0.59
48:RT:125:ARG:O	48:RT:128:GLU:N	2.36	0.59
50:RV:46:VAL:O	50:RV:46:VAL:HG22	2.01	0.59
8:XH:12:ARG:NH1	8:XH:25:ASP:O	2.34	0.59
18:XR:32:ARG:HA	18:XR:69:THR:HG21	1.85	0.59
41:YI:61:ARG:HB3	41:YI:133:HIS:ND1	2.18	0.59
32:R8:25:MET:HE2	44:RP:64:LYS:HB2	1.84	0.59
54:RZ:5:LEU:H	54:RZ:59:LEU:HA	1.67	0.59
54:RZ:127:LYS:HB3	54:RZ:162:GLU:HB2	1.84	0.59
3:XC:88:ARG:HG2	3:XC:101:LEU:HD13	1.85	0.59
1:QA:278:G:OP2	17:QQ:92:ARG:NH2	2.37	0.58
1:QA:521:G:HO2'	1:QA:536:C:HO2'	1.50	0.58
1:QA:1199:U:O2'	1:QA:1202:G:OP1	2.21	0.58
4:QD:18:LYS:NZ	4:QD:26:CYS:SG	2.76	0.58
32:R8:43:GLN:NE2	34:RA:2365:G:O6	2.35	0.58
35:RB:48:A:OP2	47:RS:30:ARG:NH2	2.36	0.58
12:XL:33:ARG:H	12:XL:85:ILE:HG22	1.67	0.58
34:RA:1859:A:N6	34:RA:1883:G:O2'	2.37	0.58
1:XA:403:C:OP2	4:XD:74:GLN:NE2	2.33	0.58
1:XA:544:G:OP1	4:XD:59:ARG:NH2	2.36	0.58
1:XA:825:G:O2'	8:XH:12:ARG:NH2	2.34	0.58
28:Y4:56:VAL:HG11	28:Y4:58:ARG:HE	1.68	0.58
39:YG:63:ILE:HG13	39:YG:64:THR:HG23	1.85	0.58
34:RA:11:G:H22	34:RA:2627:G:H5"	1.68	0.58
38:RF:157:VAL:HB	38:RF:194:MET:HG2	1.84	0.58
1:XA:261:U:OP2	20:XT:79:ARG:NH2	2.36	0.58
8:XH:10:LEU:HD22	8:XH:83:ILE:HD11	1.85	0.58
32:Y8:30:ARG:HH21	44:YP:63:PRO:HB2	1.68	0.58
34:YA:997:G:C5'	49:YU:92:ARG:HB2	2.27	0.58
43:YO:104:ARG:NH2	48:YT:43:GLN:OE1	2.37	0.58
34:RA:1817:G:OP1	36:RD:88:ARG:NH2	2.35	0.58
34:RA:2788:C:O2'	34:RA:2809:A:N3	2.35	0.58
40:RH:83:TYR:HD2	40:RH:83:TYR:O	1.86	0.58
54:RZ:7:ALA:HB2	54:RZ:59:LEU:HB3	1.84	0.58
1:XA:1119:C:H2'	1:XA:1120:G:H8	1.69	0.58
11:XK:62:GLN:HB3	11:XK:93:GLN:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:1359:A:N7	34:YA:1372:U:O4	2.36	0.58
35:YB:9:G:OP1	47:YS:15:ARG:NH1	2.37	0.58
1:QA:316:G:OP2	1:QA:351:G:O2'	2.22	0.58
9:QI:47:LEU:HD22	9:QI:50:LEU:HD22	1.84	0.58
34:RA:307:G:H21	34:RA:330:A:H62	1.50	0.58
34:RA:2848:G:O2'	34:RA:2867:G:N2	2.36	0.58
25:Y1:87:PRO:HA	25:Y1:90:ILE:HG22	1.85	0.58
34:YA:1830:C:H2'	34:YA:1831:G:H8	1.69	0.58
34:YA:2069:G:C2	34:YA:2443:C:O2	2.56	0.58
45:YQ:28:ALA:N	45:YQ:105:GLU:OE2	2.37	0.58
1:QA:437:U:H3	1:QA:495:A:H62	1.51	0.58
34:RA:2784:C:O2'	37:RE:37:ARG:NH1	2.36	0.58
43:YO:3:GLN:HE21	43:YO:32:TYR:HE1	1.51	0.58
1:QA:945:G:N2	1:QA:1334:G:O2'	2.36	0.58
19:QS:53:ASN:HB2	19:QS:77:THR:HG22	1.85	0.58
49:RU:95:LEU:HD22	49:RU:95:LEU:N	2.18	0.58
53:RY:47:LYS:NZ	53:RY:48:ALA:O	2.36	0.58
34:YA:698:C:O2'	34:YA:734:A:N6	2.36	0.58
34:RA:2729:G:H1'	37:RE:187:ALA:HB2	1.86	0.58
35:RB:43:C:O2	39:RG:95:ARG:NH1	2.36	0.58
45:YQ:67:ARG:HD2	45:YQ:105:GLU:OE1	2.03	0.58
1:QA:1366:C:O2'	10:QJ:60:ARG:NH2	2.36	0.58
32:R8:52:LYS:H	32:R8:53:PRO:HD2	1.58	0.58
32:R8:61:LEU:CD1	34:RA:593:G:C4'	2.78	0.58
34:RA:184:C:O2'	34:RA:217:G:N3	2.36	0.58
39:RG:73:ALA:HB2	39:RG:82:LEU:HD21	1.85	0.58
1:XA:452:A:O2'	16:XP:72:ARG:NH1	2.37	0.58
9:QI:3:GLN:NE2	9:QI:18:PHE:CG	2.72	0.58
36:RD:168:ARG:HG2	36:RD:173:VAL:HG12	1.85	0.58
1:XA:12:U:H3	1:XA:22:G:H1	1.52	0.58
34:YA:1327:C:O2'	46:YR:105:ARG:NH1	2.37	0.58
34:RA:527:C:N4	34:RA:2779:U:OP2	2.37	0.57
1:XA:926:G:O2'	23:XX:-3:A:N1	2.37	0.57
1:XA:1266:G:N2	1:XA:1269:A:OP2	2.35	0.57
14:XN:55:GLY:O	14:XN:57:ARG:NH1	2.36	0.57
1:QA:1502:A:H2	1:QA:1505:G:H22	1.52	0.57
42:RN:18:ALA:HA	42:RN:21:LYS:HE3	1.86	0.57
27:Y3:3:ARG:HB3	27:Y3:60:GLU:OXT	2.03	0.57
33:Y9:36:GLN:NE2	34:YA:1124:C:O2	2.38	0.57
34:YA:1454:U:O2'	34:YA:1455:G:N7	2.33	0.57
41:YI:65:ALA:HB2	41:YI:132:PRO:HG2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:XI:48:GLU:HB2	9:XI:78:LYS:HE3	1.87	0.57
41:YI:133:HIS:CB	41:YI:134:PRO:HD2	2.34	0.57
34:RA:2572:A:H5"	34:RA:2574:G:H4'	1.87	0.57
38:RF:133:ASN:H	38:RF:162:LEU:HD13	1.69	0.57
1:QA:559:A:H4'	1:QA:560:U:H3'	1.86	0.57
39:RG:66:GLN:NE2	39:RG:93:THR:O	2.38	0.57
40:RH:9:ILE:HG23	40:RH:50:VAL:O	2.05	0.57
54:RZ:110:GLY:HA3	54:RZ:174:VAL:HG11	1.85	0.57
51:YW:1:MET:CA	51:YW:64:MET:HE1	2.33	0.57
34:RA:300:A:OP1	53:RY:86:ARG:NH2	2.38	0.57
34:YA:1859:A:N6	34:YA:1883:G:O2'	2.38	0.57
49:YU:92:ARG:HH11	49:YU:92:ARG:HG2	1.70	0.57
2:QB:178:ARG:NH2	2:QB:196:LEU:O	2.38	0.57
34:RA:141:A:H8	34:RA:1595:G:H21	1.51	0.57
34:RA:2816:C:O2	34:RA:2883:A:O2'	2.23	0.57
43:RO:68:GLU:HG3	43:RO:78:ARG:HD2	1.87	0.57
1:XA:553:A:H5"	12:XL:24:VAL:HG21	1.86	0.57
2:XB:223:ILE:HG13	2:XB:229:VAL:HG22	1.86	0.57
19:XS:50:ALA:HB1	19:XS:57:HIS:HB3	1.86	0.57
34:YA:589:C:H2'	34:YA:590:A:H8	1.69	0.57
34:YA:1510:A:O2'	34:YA:1512:G:N7	2.37	0.57
34:YA:1817:G:OP1	36:YD:88:ARG:NH2	2.37	0.57
39:YG:36:LYS:HE2	39:YG:95:ARG:HH22	1.70	0.57
39:YG:41:GLN:HE21	39:YG:90:LEU:HD12	1.69	0.57
42:RN:115:ARG:HG2	42:RN:115:ARG:NH1	2.16	0.57
1:XA:1295:G:O2'	13:XM:14:ARG:NH1	2.38	0.57
34:YA:2406:U:N3	44:YP:72:PRO:HD2	2.19	0.57
44:YP:18:ARG:HH21	44:YP:21:ARG:HE	1.53	0.57
1:QA:1306:A:N6	1:QA:1331:G:O2'	2.37	0.57
34:RA:458:G:N2	34:RA:470:A:OP2	2.37	0.57
34:RA:2882:A:OP1	46:RR:96:ARG:NH1	2.36	0.57
1:XA:1286:A:H5"	21:XU:26:LYS:HD2	1.87	0.57
7:XG:30:ILE:HD12	7:XG:32:ARG:HH12	1.70	0.57
34:YA:2107:C:O2	34:YA:2182:G:N2	2.38	0.57
1:QA:811:C:O2'	1:QA:901:A:N1	2.38	0.57
13:QM:49:THR:HG22	13:QM:51:ALA:H	1.70	0.57
13:QM:97:PRO:HB2	13:QM:101:GLN:HG3	1.85	0.57
34:RA:674:G:H1'	38:RF:74:ARG:HD3	1.86	0.57
34:RA:1327:C:O2'	46:RR:105:ARG:NH1	2.37	0.57
42:RN:114:ARG:HH11	42:RN:114:ARG:CB	2.17	0.57
34:YA:2470:G:H5'	45:YQ:56:ARG:HH21	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:YY:47:LYS:NZ	53:YY:48:ALA:O	2.38	0.57
1:QA:254:G:O2'	17:QQ:16:GLN:O	2.23	0.56
20:QT:44:ALA:HB2	20:QT:88:VAL:HG23	1.86	0.56
22:QV:63:U:OP1	24:R0:11:ARG:NH1	2.37	0.56
34:RA:665:C:H2'	34:RA:666:G:H8	1.70	0.56
1:XA:227:G:N2	16:XP:62:VAL:O	2.37	0.56
4:XD:4:TYR:OH	4:XD:10:ARG:NH2	2.38	0.56
34:YA:998:C:OP2	49:YU:58:ARG:NH1	2.38	0.56
34:YA:2030:A:H4'	34:YA:2031:A:H8	1.70	0.56
1:QA:406:G:H21	4:QD:119:GLN:HE22	1.51	0.56
34:RA:2361:A:C8	34:RA:2361:A:C5'	2.85	0.56
36:RD:71:ASP:HB2	36:RD:103:ARG:HH12	1.69	0.56
39:RG:116:ASP:OD1	39:RG:116:ASP:O	2.22	0.56
2:XB:68:ILE:HG12	2:XB:161:ALA:HB3	1.87	0.56
25:Y1:80:LEU:HD12	25:Y1:81:LYS:HG2	1.87	0.56
47:YS:78:LEU:HD21	47:YS:108:GLY:HA3	1.87	0.56
1:QA:440:A:H62	1:QA:493:G:N2	2.01	0.56
1:QA:1321:C:H5"	1:QA:1322:C:H5"	1.87	0.56
32:R8:58:ILE:HG22	44:RP:49:ARG:HH11	1.71	0.56
34:RA:807:U:O2'	34:RA:2060:A:N1	2.37	0.56
34:RA:2334:G:H5'	47:RS:9:ARG:HG2	1.86	0.56
50:RV:76:LYS:H	50:RV:81:TYR:HB3	1.71	0.56
54:RZ:10:ARG:NH2	54:RZ:37:VAL:O	2.39	0.56
1:XA:64:G:H5"	1:XA:65:U:H5'	1.88	0.56
1:XA:538:G:H5"	12:XL:114:LYS:HB2	1.87	0.56
12:XL:71:PRO:O	12:XL:102:ARG:NH1	2.38	0.56
34:YA:392:C:H5"	34:YA:409:C:H5"	1.87	0.56
34:YA:2876:G:H5'	48:YT:2:ASN:HB3	1.88	0.56
44:YP:127:ALA:HB3	44:YP:130:PHE:HE1	1.69	0.56
45:YQ:43:THR:HG22	45:YQ:94:VAL:HG12	1.86	0.56
37:YE:29:GLY:HA2	37:YE:180:ASN:HB3	1.87	0.56
39:YG:136:ARG:HA	39:YG:154:GLY:HA3	1.88	0.56
33:R9:36:GLN:NE2	34:RA:1124:C:O2	2.39	0.56
11:XK:57:THR:HG22	11:XK:59:TYR:H	1.69	0.56
39:YG:10:LYS:NZ	39:YG:175:LEU:O	2.38	0.56
1:QA:35:G:N3	12:QL:118:SER:OG	2.39	0.56
50:RV:23:GLU:OE2	50:RV:89:GLN:NE2	2.39	0.56
34:YA:888:C:H3'	34:YA:889:C:H4'	1.87	0.56
39:YG:29:TRP:O	39:YG:33:ARG:NH1	2.38	0.56
1:QA:1137:C:O2	1:QA:1138:G:N2	2.39	0.56
39:RG:80:PHE:CD1	39:RG:80:PHE:N	2.73	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:RW:82:LEU:HB2	51:RW:98:LYS:HB2	1.88	0.56
1:XA:79:G:H1	1:XA:90:C:H42	1.53	0.56
1:XA:971:G:N2	1:XA:1363:A:OP2	2.38	0.56
41:YI:133:HIS:HB3	41:YI:134:PRO:CD	2.21	0.56
1:QA:1031:G:H2'	1:QA:1032:A:H8	1.70	0.56
1:QA:1119:C:OP2	9:QI:9:ARG:NH2	2.39	0.56
13:QM:24:GLY:HA3	13:QM:66:LEU:HD21	1.80	0.56
38:RF:161:GLU:OE1	38:RF:164:ARG:NH2	2.39	0.56
1:XA:1321:C:H5"	1:XA:1322:C:H2'	1.88	0.56
1:XA:1347:G:N2	1:XA:1374:A:OP2	2.39	0.56
22:XV:63:U:O2	54:YZ:198:LYS:NZ	2.38	0.56
34:YA:336:C:O2'	53:YY:35:TYR:OH	2.24	0.56
1:QA:1414:U:H2'	1:QA:1415:G:H8	1.69	0.56
9:QI:121:ARG:NH1	9:QI:122:ALA:O	2.39	0.56
31:R7:7:PRO:HB2	34:RA:1309:G:H4'	1.88	0.56
34:RA:814:C:H1'	34:RA:1226:G:H21	1.71	0.56
34:RA:1359:A:H62	34:RA:1372:U:H3	1.53	0.56
54:RZ:5:LEU:HD12	54:RZ:43:GLU:HB3	1.87	0.56
1:XA:1179:A:H4'	9:XI:103:THR:HA	1.87	0.56
1:XA:1356:G:H2'	1:XA:1357:A:H8	1.71	0.56
16:XP:45:THR:HG22	16:XP:47:ASP:H	1.71	0.56
45:YQ:8:LYS:HA	54:YZ:197:ILE:HB	1.88	0.56
25:R1:18:ILE:HG12	25:R1:37:ILE:HG12	1.88	0.56
32:Y8:8:LYS:NZ	34:YA:245:G:O6	2.39	0.56
34:YA:2602:A:N6	56:Z8:76:PPU:OP2	2.39	0.56
50:YV:47:VAL:HG23	50:YV:47:VAL:O	2.04	0.56
50:RV:47:VAL:O	50:RV:47:VAL:HG22	2.05	0.55
4:XD:20:TYR:O	4:XD:20:TYR:CD1	2.59	0.55
43:YO:76:ALA:HB3	48:YT:75:ILE:HD12	1.87	0.55
17:QQ:9:VAL:HG22	17:QQ:56:VAL:HG22	1.87	0.55
34:YA:729:G:C6	34:YA:1775:U:C4	2.93	0.55
35:YB:43:C:H4'	39:YG:98:ARG:HH12	1.69	0.55
36:YD:168:ARG:HG2	36:YD:173:VAL:HG12	1.88	0.55
2:QB:231:GLU:HG3	2:QB:232:PRO:CD	2.36	0.55
34:RA:1800:C:H42	34:RA:1817:G:N2	2.05	0.55
34:RA:1992:G:N2	34:RA:1996:C:O2'	2.40	0.55
40:RH:83:TYR:N	40:RH:83:TYR:CD2	2.72	0.55
49:RU:90:VAL:HG22	50:RV:39:LEU:HD12	1.89	0.55
34:YA:26:G:H1'	34:YA:515:A:H61	1.70	0.55
34:YA:807:U:O2'	34:YA:2060:A:N1	2.39	0.55
49:YU:90:VAL:HG22	50:YV:39:LEU:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1261:A:H62	1:QA:1274:G:H21	1.53	0.55
1:XA:1055:A:H8	1:XA:1055:A:O5'	1.89	0.55
4:XD:73:ARG:O	4:XD:77:ASN:ND2	2.39	0.55
24:Y0:51:VAL:O	47:YS:20:ARG:NH2	2.38	0.55
39:YG:97:ASP:H	39:YG:100:TRP:HD1	1.54	0.55
1:QA:261:U:OP2	20:QT:79:ARG:NH2	2.39	0.55
34:RA:2126:A:N6	34:RA:2163:C:O2'	2.39	0.55
39:RG:83:ARG:HH11	39:RG:83:ARG:CG	2.20	0.55
49:RU:87:GLY:O	50:RV:50:PRO:CD	2.53	0.55
1:XA:34:C:H2'	1:XA:35:G:H8	1.72	0.55
1:XA:1119:C:OP2	9:XI:9:ARG:NH2	2.39	0.55
41:YI:130:TYR:O	41:YI:136:VAL:HG13	2.06	0.55
51:YW:2:GLU:N	51:YW:64:MET:CE	2.68	0.55
53:YY:15:VAL:HG21	53:YY:42:VAL:HG11	1.87	0.55
34:RA:1546:C:H5'	34:RA:1547:C:H5'	1.88	0.55
34:RA:2502:G:H5"	34:RA:2503:A:H5"	1.88	0.55
39:RG:95:ARG:HB3	39:RG:96:ARG:HG2	1.87	0.55
40:RH:107:VAL:O	40:RH:152:ARG:NH1	2.39	0.55
34:YA:2183:C:H2'	34:YA:2184:G:H8	1.71	0.55
40:YH:96:ALA:HB1	40:YH:103:LEU:HD11	1.88	0.55
9:QI:9:ARG:HG2	9:QI:14:VAL:HG12	1.88	0.55
34:RA:1329:U:H5"	34:RA:1330:C:H5	1.72	0.55
34:RA:1818:U:H2'	36:RD:157:ARG:HG2	1.89	0.55
1:XA:643:C:H2'	1:XA:644:G:H8	1.71	0.55
1:XA:1503:A:C4	1:XA:1531:A:C2	2.95	0.55
9:XI:13:ALA:HB2	9:XI:68:GLY:HA3	1.88	0.55
10:XJ:44:VAL:HG22	10:XJ:66:ARG:HG2	1.88	0.55
34:YA:2680:C:H5'	37:YE:189:PRO:HA	1.88	0.55
1:QA:954:G:H21	1:QA:1227:A:H62	1.55	0.55
34:RA:900:A:H3'	34:RA:901:A:H8	1.72	0.55
35:RB:44:G:H1'	35:RB:47:C:H42	1.71	0.55
24:Y0:77:ARG:NH2	34:YA:857:C:OP2	2.39	0.55
45:YQ:30:GLY:O	45:YQ:134:ARG:NH2	2.38	0.55
1:QA:677:U:H3	1:QA:713:G:H22	1.55	0.55
1:QA:974:A:N3	14:QN:31:ARG:NH1	2.55	0.55
34:RA:1800:C:H42	34:RA:1817:G:H22	1.54	0.55
40:RH:121:ILE:HD11	40:RH:140:LYS:HB3	1.88	0.55
43:RO:23:ARG:NH2	43:RO:28:SER:O	2.40	0.55
47:RS:23:ARG:NH1	47:RS:85:VAL:O	2.40	0.55
54:RZ:52:SER:O	54:RZ:52:SER:OG	2.17	0.55
1:XA:20:U:O2'	1:XA:573:A:N6	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:XV:19:G:N3	22:XV:57:G:N2	2.54	0.55
34:YA:581:C:H2'	34:YA:582:G:H8	1.72	0.55
34:YA:958:U:OP2	45:YQ:14:ARG:NH1	2.39	0.55
34:YA:1939:U:OP1	34:YA:2604:U:O2'	2.24	0.55
34:YA:2446:G:N2	34:YA:2449:U:O2	2.40	0.55
42:YN:16:ILE:HG21	42:YN:26:LEU:HD11	1.89	0.55
1:QA:152:A:H62	1:QA:169:C:N4	2.04	0.55
10:QJ:51:ARG:O	14:QN:45:ARG:NH1	2.39	0.55
34:RA:65:C:H1'	34:RA:456:C:H42	1.71	0.55
47:RS:71:ARG:NH1	47:RS:75:GLU:OE2	2.40	0.55
34:YA:793:A:OP2	34:YA:2071:A:O2'	2.25	0.55
35:YB:33:G:H5'	39:YG:2:PRO:HG3	1.89	0.55
1:QA:720:C:O2	18:QR:71:LYS:NZ	2.34	0.54
1:QA:1028(A):C:H42	1:QA:1032(B):G:H1	1.55	0.54
13:QM:68:GLY:O	39:RG:116:ASP:HB2	2.06	0.54
34:RA:1607:C:N4	34:RA:1622:G:OP2	2.36	0.54
34:RA:2306:C:N4	39:RG:42:GLY:O	2.40	0.54
1:XA:254:G:O2'	17:XQ:16:GLN:O	2.24	0.54
1:XA:587:G:N2	1:XA:754:C:OP2	2.38	0.54
1:XA:618:C:H5'	1:XA:619:U:H5"	1.88	0.54
33:Y9:2:LYS:NZ	33:Y9:31:LYS:O	2.38	0.54
34:YA:2111:C:H5	34:YA:2145:C:H42	1.55	0.54
34:YA:2115:G:N2	34:YA:2165:G:N7	2.56	0.54
54:YZ:7:ALA:HB2	54:YZ:59:LEU:CD1	2.34	0.54
22:QV:19:G:N3	22:QV:57:G:N2	2.55	0.54
34:RA:137(A):G:O6	34:RA:139:G:O2'	2.21	0.54
50:RV:58:VAL:HB	50:RV:98:GLU:HB2	1.88	0.54
28:Y4:42:PHE:HE2	39:YG:179:PRO:HB2	1.73	0.54
34:YA:2150:U:H2'	34:YA:2151:G:H8	1.73	0.54
1:QA:825:G:O2'	8:QH:12:ARG:NH2	2.37	0.54
10:QJ:54:PHE:HB2	10:QJ:55:LYS:HD3	1.87	0.54
32:R8:34:TRP:HB3	34:RA:2420:C:OP1	2.06	0.54
34:RA:392:C:H5"	34:RA:409:C:H5"	1.88	0.54
22:QV:65:C:H2'	22:QV:66:A:H8	1.73	0.54
32:R8:57:ARG:O	32:R8:61:LEU:HD21	2.07	0.54
34:YA:288:C:H2'	34:YA:289:A:H8	1.72	0.54
34:YA:1600:C:OP1	52:YX:58:HIS:NE2	2.38	0.54
39:YG:84:LYS:HG3	39:YG:84:LYS:O	2.08	0.54
54:YZ:3:TYR:HB2	54:YZ:57:ILE:HG13	1.89	0.54
13:QM:80:ARG:NH1	13:QM:80:ARG:O	2.39	0.54
18:QR:70:ILE:O	18:QR:74:ARG:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:XG:15:ASP:HB3	7:XG:19:GLY:H	1.73	0.54
9:XI:112:LYS:HA	9:XI:119:ALA:HB2	1.88	0.54
34:RA:2318:G:N2	34:RA:2318:G:OP2	2.41	0.54
38:RF:116:ASP:OD2	44:RP:1:MET:N	2.40	0.54
40:RH:109:PHE:CE1	40:RH:152:ARG:HD2	2.42	0.54
20:XT:71:THR:OG1	20:XT:72:LEU:N	2.39	0.54
25:Y1:52:ARG:HH11	25:Y1:57:GLU:HB2	1.73	0.54
27:Y3:3:ARG:HG2	27:Y3:60:GLU:OXT	2.08	0.54
28:Y4:16:CYS:SG	28:Y4:17:GLY:N	2.81	0.54
34:YA:2688:U:OP1	34:YA:2713:A:N6	2.40	0.54
1:QA:1190:G:OP1	3:QC:5:ILE:HB	2.07	0.54
8:QH:4:ASP:HB2	8:QH:89:PRO:HG3	1.90	0.54
9:QI:44:VAL:O	9:QI:51:ARG:NH2	2.41	0.54
30:R6:26:ASN:ND2	30:R6:29:ASN:OD1	2.40	0.54
39:RG:32:PRO:HB2	39:RG:172:LEU:HD13	1.89	0.54
24:Y0:48:GLY:O	47:YS:20:ARG:NH1	2.40	0.54
51:YW:1:MET:HB3	51:YW:64:MET:CE	2.36	0.54
54:YZ:158:PRO:HG2	54:YZ:161:VAL:HG21	1.89	0.54
1:QA:1296:C:OP1	13:QM:44:ARG:NH2	2.41	0.54
4:QD:166:LYS:HA	4:QD:178:VAL:HG21	1.90	0.54
10:QJ:49:VAL:HG23	14:QN:41:ARG:HB2	1.90	0.54
11:QK:52:GLY:H	11:QK:55:LYS:HE2	1.73	0.54
34:YA:882:G:H22	34:YA:894:C:H42	1.55	0.54
1:QA:405:U:O4	4:QD:2:GLY:N	2.41	0.54
34:RA:987:G:O2'	34:RA:1000:A:N3	2.39	0.54
34:RA:996:A:H4'	49:RU:92:ARG:HE	1.72	0.54
34:RA:1102:C:H2'	34:RA:1103:A:H8	1.72	0.54
34:RA:2328:A:H2'	34:RA:2329:G:C8	2.43	0.54
41:RI:86:THR:HA	41:RI:123:LEU:CD1	2.37	0.54
1:XA:992:U:H3	1:XA:1044:A:H62	1.54	0.54
32:Y8:27:THR:HG22	44:YP:63:PRO:HD3	1.90	0.54
33:Y9:27:CYS:SG	33:Y9:28:GLU:N	2.81	0.54
34:RA:603:A:N1	34:RA:625:G:O2'	2.39	0.54
34:RA:994:C:OP1	49:RU:53:ARG:NH2	2.41	0.54
34:RA:2120:G:N2	34:RA:2121:G:O6	2.41	0.54
34:RA:2134:A:N7	34:RA:2157:G:O2'	2.41	0.54
35:RB:30:C:H1'	35:RB:57:A:H61	1.73	0.54
36:RD:158:ALA:O	36:RD:196:VAL:HG21	2.08	0.54
34:YA:1359:A:N6	34:YA:1372:U:N3	2.40	0.54
34:YA:1816:G:O6	36:YD:35:LYS:NZ	2.40	0.54
37:YE:52:LEU:HD13	37:YE:52:LEU:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:643:C:H2'	1:QA:644:G:H8	1.73	0.53
19:QS:50:ALA:HB1	19:QS:57:HIS:HB3	1.90	0.53
32:R8:61:LEU:HD12	34:RA:593:G:C4'	2.29	0.53
10:XJ:49:VAL:HG23	14:XN:41:ARG:HB2	1.90	0.53
24:Y0:70:GLN:OE1	24:Y0:80:HIS:NE2	2.40	0.53
34:YA:1479:G:N7	34:YA:1510:A:N6	2.56	0.53
34:YA:2122:U:H2'	34:YA:2123:G:H8	1.72	0.53
24:R0:48:GLY:O	47:RS:20:ARG:NH1	2.40	0.53
45:RQ:77:LYS:NZ	45:RQ:83:MET:O	2.38	0.53
1:XA:1538:C:H42	23:XX:-11:A:H61	1.55	0.53
34:YA:1385:G:O2'	34:YA:1396:U:O2	2.26	0.53
40:YH:94:TYR:OH	40:YH:160:LYS:NZ	2.42	0.53
49:YU:87:GLY:O	50:YV:50:PRO:HD2	2.09	0.53
49:YU:108:GLU:OE2	49:YU:112:ARG:NH1	2.41	0.53
1:XA:1034:G:H2'	1:XA:1035:A:H8	1.72	0.53
1:XA:1432:G:O2'	1:XA:1468:A:N6	2.41	0.53
11:XK:34:ASP:OD1	11:XK:38:ASN:N	2.39	0.53
34:YA:2120:G:H21	34:YA:2179:C:H41	1.55	0.53
2:QB:88:ALA:HB2	2:QB:219:VAL:HG13	1.91	0.53
27:R3:15:TYR:O	27:R3:20:LYS:NZ	2.41	0.53
40:RH:125:VAL:O	40:RH:125:VAL:HG12	2.07	0.53
6:XF:94:GLN:OE1	18:XR:32:ARG:NH1	2.40	0.53
34:YA:2071:A:H2'	34:YA:2072:G:H8	1.73	0.53
40:YH:124:GLU:HB2	40:YH:132:ARG:HB3	1.90	0.53
1:QA:768:A:N3	1:QA:1512:U:O2'	2.42	0.53
26:R2:47:ASN:ND2	34:RA:94:G:N3	2.56	0.53
32:R8:58:ILE:HA	32:R8:61:LEU:HD21	1.91	0.53
34:RA:577:G:O2'	34:RA:1254:A:OP1	2.26	0.53
48:RT:124:ASP:OD1	48:RT:124:ASP:N	2.42	0.53
1:XA:974:A:OP2	14:XN:41:ARG:NH1	2.41	0.53
1:XA:1015:A:OP1	19:XS:14:HIS:NE2	2.42	0.53
34:YA:987:G:O2'	34:YA:1000:A:N3	2.37	0.53
38:YF:101:LEU:O	38:YF:106:ARG:NH1	2.41	0.53
50:YV:23:GLU:OE2	50:YV:89:GLN:NE2	2.41	0.53
1:QA:1373:G:H5'	7:QG:36:LYS:HG2	1.91	0.53
15:QO:39:LEU:HD11	15:QO:52:SER:HB3	1.91	0.53
38:RF:143:ALA:HB1	38:RF:148:LEU:HB2	1.90	0.53
44:RP:101:VAL:CB	44:RP:106:LEU:HD23	2.38	0.53
48:RT:19:LEU:HD22	48:RT:86:ILE:HG22	1.90	0.53
53:RY:29:GLU:HB3	53:RY:38:ILE:HD12	1.90	0.53
13:XM:24:GLY:O	13:XM:29:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Y5:12:SER:HB3	34:YA:2020:A:H5'	1.90	0.53
30:Y6:26:ASN:ND2	30:Y6:29:ASN:OD1	2.40	0.53
33:Y9:2:LYS:HB2	33:Y9:34:GLN:HG2	1.91	0.53
34:YA:629:G:N3	34:YA:639:U:O2'	2.41	0.53
34:YA:2743:C:O2'	40:YH:153:LYS:NZ	2.41	0.53
1:QA:1251:A:N3	1:QA:1369:C:O2'	2.35	0.53
9:QI:65:VAL:HG21	9:QI:73:GLN:HG3	1.91	0.53
34:RA:372:G:N2	34:RA:401:A:OP2	2.39	0.53
34:RA:1140:C:OP2	42:RN:66:LYS:NZ	2.39	0.53
34:RA:1228:G:OP2	49:RU:16:LYS:NZ	2.40	0.53
37:RE:64:LYS:O	37:RE:73:GLU:OE2	2.27	0.53
42:YN:86:PRO:HD2	42:YN:89:LYS:HE2	1.91	0.53
1:QA:1032(B):G:O6	1:QA:1034:G:N2	2.41	0.53
1:QA:1305:G:N2	1:QA:1332:A:OP2	2.41	0.53
4:QD:140:VAL:HG11	4:QD:146:ILE:HD11	1.90	0.53
16:QP:4:ILE:HG12	16:QP:21:VAL:HG12	1.89	0.53
1:XA:993:G:O2'	1:XA:994:A:N7	2.38	0.53
4:XD:20:TYR:HE1	4:XD:106:TYR:OH	1.89	0.53
25:Y1:19:GLN:HG3	34:YA:2080:G:H5'	1.90	0.53
34:RA:625:G:O6	44:RP:107:LYS:HD3	2.09	0.53
34:RA:1939:U:OP1	34:RA:2604:U:O2'	2.26	0.53
37:RE:1:MET:N	37:RE:83:ASP:O	2.42	0.53
1:XA:842:C:O2'	1:XA:848:C:N4	2.42	0.53
13:XM:10:PRO:HB2	13:XM:18:ALA:HB1	1.90	0.53
54:YZ:53:ILE:HD11	54:YZ:99:TYR:HB2	1.91	0.53
10:QJ:9:ARG:HB2	10:QJ:95:GLU:HB2	1.91	0.53
13:QM:65:LYS:O	13:QM:66:LEU:HG	2.09	0.53
32:R8:61:LEU:CD1	34:RA:593:G:O2'	2.51	0.53
34:RA:1094:U:OP1	34:RA:1096:A:N6	2.42	0.53
34:RA:2392:A:H1'	44:RP:60:MET:HG2	1.90	0.53
37:RE:9:VAL:HB	37:RE:25:VAL:HG23	1.91	0.53
39:RG:95:ARG:HA	39:RG:99:MET:HE3	1.91	0.53
52:RX:53:LYS:NZ	52:RX:55:ASN:OD1	2.42	0.53
4:XD:105:VAL:HG23	4:XD:117:ALA:HB1	1.91	0.53
7:XG:88:PRO:HG2	7:XG:152:ALA:HB2	1.91	0.53
38:YF:165:ARG:HG2	38:YF:168:ARG:HH12	1.74	0.53
41:YI:118:LYS:HB3	41:YI:119:PRO:HD2	1.87	0.53
49:YU:92:ARG:HH11	49:YU:92:ARG:CG	2.22	0.53
51:YW:1:MET:HB3	51:YW:64:MET:HE1	1.91	0.53
51:YW:64:MET:HA	51:YW:109:GLU:OE2	2.09	0.53
1:QA:20:U:O2'	1:QA:573:A:N6	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:QM:15:VAL:HA	13:QM:18:ALA:HB3	1.91	0.52
26:R2:22:GLU:OE2	26:R2:68:ARG:NH2	2.42	0.52
34:RA:820:A:N3	34:RA:943:U:O2'	2.40	0.52
54:RZ:6:LYS:HD2	54:RZ:43:GLU:HG3	1.90	0.52
27:Y3:5:LYS:HA	27:Y3:36:VAL:CG1	2.30	0.52
48:YT:16:ARG:HH21	48:YT:19:LEU:HD21	1.73	0.52
48:YT:118:ARG:HA	48:YT:121:ILE:HB	1.91	0.52
49:YU:49:HIS:HA	49:YU:52:ARG:HB3	1.91	0.52
1:QA:1321:C:O2	19:QS:36:ARG:NH2	2.42	0.52
45:RQ:81:VAL:O	45:RQ:82:ARG:NE	2.39	0.52
48:RT:62:THR:HG22	48:RT:75:ILE:HG12	1.91	0.52
50:RV:24:LYS:HA	50:RV:92:THR:HG23	1.92	0.52
1:XA:1255:G:O2'	1:XA:1258:G:N3	2.39	0.52
32:Y8:58:ILE:HG12	44:YP:59:LEU:HD12	1.91	0.52
1:QA:1119:C:H2'	1:QA:1120:G:H8	1.74	0.52
1:QA:1141:C:H2'	1:QA:1142:G:H8	1.73	0.52
24:R0:38:VAL:HG21	24:R0:45:PHE:HD2	1.74	0.52
43:RO:19:ILE:HG22	43:RO:43:VAL:HA	1.92	0.52
1:XA:21:G:H21	1:XA:914:A:H62	1.56	0.52
34:YA:458:G:N2	34:YA:470:A:OP2	2.42	0.52
34:YA:2392:A:H2	34:YA:2424:C:H42	1.57	0.52
39:YG:39:ILE:HG12	39:YG:157:ILE:HG12	1.90	0.52
43:YO:64:ARG:HB2	43:YO:83:ALA:HB3	1.91	0.52
7:QG:16:LEU:HD11	9:QI:45:ALA:HB2	1.91	0.52
34:RA:1250:G:OP2	44:RP:18:ARG:NH2	2.42	0.52
34:RA:2258:C:O2'	34:RA:2427:C:OP2	2.25	0.52
47:RS:26:LEU:HB2	47:RS:87:PHE:HA	1.90	0.52
1:XA:1095:U:OP1	1:XA:1108:G:N2	2.37	0.52
1:XA:1240:U:H3	7:XG:32:ARG:HD2	1.74	0.52
1:XA:1360:A:OP2	14:XN:35:ARG:NH2	2.42	0.52
34:YA:89:G:OP1	53:YY:33:LYS:NZ	2.41	0.52
34:YA:820:A:N3	34:YA:943:U:O2'	2.38	0.52
34:YA:2010:G:H5"	51:YW:42:ARG:HB2	1.92	0.52
1:QA:297:G:N2	1:QA:300:A:OP2	2.42	0.52
36:RD:108:PRO:C	36:RD:196:VAL:O	2.47	0.52
1:XA:619:U:N3	4:XD:134:ASP:OD1	2.38	0.52
1:XA:957:U:H4'	19:XS:79:THR:HG23	1.90	0.52
3:XC:172:ARG:HG2	3:XC:174:PRO:HD3	1.90	0.52
8:XH:4:ASP:HB2	8:XH:89:PRO:HG3	1.91	0.52
16:QP:4:ILE:HB	16:QP:66:PRO:HB3	1.91	0.52
34:RA:2683:C:OP1	48:RT:53:ARG:NH2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:RT:121:ILE:O	48:RT:125:ARG:CG	2.55	0.52
1:XA:129(A):G:N2	1:XA:188:U:O2'	2.43	0.52
1:XA:414:A:OP2	1:XA:428:G:N2	2.43	0.52
34:YA:1664:A:H61	34:YA:1996:C:N4	2.08	0.52
1:QA:501:C:H2'	1:QA:502:G:H8	1.75	0.52
9:QI:10:ARG:HH12	9:QI:79:LEU:HD22	1.73	0.52
9:QI:109:VAL:O	9:QI:111:ARG:NH2	2.42	0.52
28:R4:14:ILE:HB	28:R4:22:ILE:HB	1.90	0.52
34:RA:530:G:O2'	34:RA:532:A:N7	2.43	0.52
34:RA:1791:A:H4'	36:RD:206:LEU:HB2	1.91	0.52
22:XV:52:G:H21	54:YZ:198:LYS:HE3	1.75	0.52
27:Y3:3:ARG:HG3	27:Y3:59:VAL:HB	1.90	0.52
34:YA:1496:A:H8	34:YA:1577:C:HO2'	1.58	0.52
37:YE:10:GLY:HA3	48:YT:8:LYS:HD3	1.90	0.52
9:QI:19:LEU:HD11	9:QI:81:ILE:HD13	1.92	0.52
13:QM:93:ARG:NH1	34:RA:888:C:OP2	2.43	0.52
42:RN:133:GLN:HG2	42:RN:135:PRO:HD3	1.92	0.52
48:RT:111:ARG:C	48:RT:113:LYS:H	2.14	0.52
1:XA:713:G:H2'	1:XA:714:G:C8	2.45	0.52
1:XA:945:G:N2	1:XA:1334:G:O2'	2.43	0.52
1:XA:1522:U:H2'	1:XA:1523:G:H8	1.74	0.52
2:XB:67:THR:HG21	2:XB:155:LEU:HG	1.92	0.52
22:XV:65:C:H2'	22:XV:66:A:H8	1.75	0.52
32:Y8:6:THR:HG22	32:Y8:63:PRO:HD2	1.90	0.52
36:YD:146:GLU:HB2	36:YD:189:CYS:HB3	1.91	0.52
41:YI:13:GLY:HA3	41:YI:17:GLN:HB2	1.92	0.52
5:QE:152:ARG:NH1	8:QH:42:GLU:O	2.43	0.52
37:RE:5:LEU:HD23	37:RE:197:ILE:HG22	1.92	0.52
40:RH:9:ILE:HG23	40:RH:10:PRO:HD2	1.75	0.52
40:RH:153:LYS:HG2	40:RH:161:GLY:HA2	1.92	0.52
43:RO:8:LEU:HD13	43:RO:82:ASN:HB3	1.91	0.52
47:RS:95:HIS:HA	47:RS:99:LYS:HE3	1.92	0.52
48:RT:65:LYS:HE3	48:RT:67:SER:HB2	1.92	0.52
49:RU:92:ARG:NH2	49:RU:94:ASN:OD1	2.43	0.52
1:XA:1235:U:H5"	21:XU:3:LYS:HD2	1.90	0.52
22:XV:76:A:OP1	34:YA:2439:A:N6	2.42	0.52
35:YB:44:G:H1'	35:YB:47:C:H42	1.74	0.52
1:QA:401:C:O2'	1:QA:621:A:N3	2.37	0.52
6:QF:79:LEU:HB3	6:QF:88:VAL:HG21	1.92	0.52
25:R1:52:ARG:HH11	25:R1:57:GLU:HB2	1.75	0.52
34:RA:996:A:OP2	49:RU:92:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:673:G:H2'	1:XA:674:G:C8	2.44	0.52
1:XA:1071:C:H2'	1:XA:1072:G:H8	1.74	0.52
1:XA:1236:A:H4'	1:XA:1304:G:H4'	1.92	0.52
34:YA:746:A:HO2'	34:YA:2611:U:HO2'	1.56	0.52
51:YW:88:ARG:HB2	51:YW:92:ARG:HB3	1.91	0.52
1:QA:684:A:O2'	11:QK:39:PRO:O	2.27	0.51
9:QI:48:GLU:OE2	9:QI:51:ARG:NH2	2.42	0.51
16:QP:53:VAL:HG13	16:QP:79:VAL:HG22	1.91	0.51
42:RN:47:ALA:O	42:RN:119:ARG:NH1	2.40	0.51
43:RO:3:GLN:HE21	43:RO:32:TYR:HE1	1.59	0.51
1:XA:745:C:OP1	1:XA:851:G:O2'	2.28	0.51
27:Y3:51:ALA:HA	27:Y3:54:VAL:HG12	1.92	0.51
34:YA:996:A:HO2'	49:YU:92:ARG:HD2	1.70	0.51
34:YA:1689:A:H62	34:YA:1698:A:H2	1.57	0.51
34:YA:2008:C:H2'	34:YA:2009:G:H8	1.76	0.51
7:QG:150:ALA:HB1	11:QK:57:THR:HG21	1.92	0.51
16:QP:21:VAL:HG23	16:QP:33:ILE:HB	1.92	0.51
34:RA:890:A:H2'	34:RA:892:G:H8	1.75	0.51
9:XI:21:PRO:HA	9:XI:59:PHE:HA	1.91	0.51
14:XN:29:ARG:HG2	14:XN:31:ARG:H	1.74	0.51
34:YA:442:G:H1'	38:YF:48:THR:HG21	1.91	0.51
34:YA:1022:G:N2	34:YA:1023:U:O4	2.43	0.51
43:YO:19:ILE:HG22	43:YO:43:VAL:HA	1.93	0.51
1:QA:1382:C:O2'	7:QG:79:ARG:NH1	2.43	0.51
27:R3:2:PRO:HD2	27:R3:39:ASP:HB3	1.92	0.51
30:R6:25:LYS:NZ	30:R6:32:ASN:O	2.35	0.51
34:RA:537:C:OP1	34:RA:995:C:N4	2.36	0.51
34:RA:589:C:H2'	34:RA:590:A:H8	1.74	0.51
36:RD:69:ARG:HD3	36:RD:105:ILE:HD13	1.91	0.51
1:XA:1314:C:N4	19:XS:2:PRO:O	2.44	0.51
2:XB:69:LEU:HB3	2:XB:162:ILE:HG22	1.92	0.51
19:XS:29:ARG:HH21	19:XS:30:LEU:HD23	1.75	0.51
34:YA:581:C:H2'	34:YA:582:G:C8	2.46	0.51
34:YA:2069:G:C2	34:YA:2443:C:N3	2.78	0.51
1:QA:343:U:O2	1:QA:346:G:N2	2.31	0.51
1:QA:1304:G:OP1	21:QU:2:GLY:N	2.43	0.51
34:RA:144:C:H2'	34:RA:145:G:H8	1.76	0.51
37:RE:63:LEU:O	37:RE:73:GLU:OE2	2.27	0.51
43:RO:64:ARG:HB2	43:RO:83:ALA:HB3	1.92	0.51
8:XH:9:MET:HG3	8:XH:26:VAL:HG11	1.92	0.51
9:XI:15:ALA:HA	9:XI:65:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Y5:16:ARG:NH2	34:YA:517:C:OP1	2.42	0.51
32:Y8:28:GLY:O	32:Y8:36:LYS:NZ	2.41	0.51
34:YA:612:G:N2	34:YA:616:A:O2'	2.43	0.51
34:YA:637:A:OP1	44:YP:133:SER:OG	2.27	0.51
34:YA:964:C:O2'	34:YA:2273:A:N3	2.40	0.51
34:YA:2328:A:H2'	34:YA:2329:G:C8	2.46	0.51
34:YA:2788:C:O2'	34:YA:2809:A:N3	2.39	0.51
45:RQ:141:GLN:NE2	54:RZ:123:ASP:OD1	2.43	0.51
1:XA:1414:U:H2'	1:XA:1415:G:H8	1.74	0.51
11:XK:62:GLN:OE1	11:XK:93:GLN:NE2	2.40	0.51
23:XX:-12:C:H2'	23:XX:-11:A:H8	1.75	0.51
34:YA:2033:A:O2'	34:YA:2035:G:OP2	2.24	0.51
34:YA:2816:C:O2	34:YA:2883:A:O2'	2.26	0.51
34:RA:1047:G:H21	34:RA:1111:A:N6	2.08	0.51
34:RA:1333:C:H2'	34:RA:1334:G:H8	1.76	0.51
34:RA:1454:U:O2'	34:RA:1455:G:N7	2.40	0.51
40:RH:124:GLU:HB3	40:RH:132:ARG:HB2	1.91	0.51
26:Y2:47:ASN:HD22	34:YA:94:G:N2	2.06	0.51
42:YN:96:GLU:HB2	42:YN:122:VAL:HG12	1.93	0.51
49:YU:96:ALA:O	49:YU:99:ALA:HB3	2.11	0.51
1:QA:514:C:H2'	1:QA:515:G:H8	1.76	0.51
3:QC:153:VAL:HG22	3:QC:198:VAL:HG22	1.92	0.51
8:QH:10:LEU:HD22	8:QH:83:ILE:HD11	1.93	0.51
10:QJ:43:ARG:HB2	10:QJ:67:THR:HB	1.92	0.51
34:RA:252:G:OP2	44:RP:50:ARG:NH1	2.43	0.51
34:RA:1536:A:OP2	34:RA:1537:C:N4	2.43	0.51
34:RA:2515:C:H2'	34:RA:2516:G:H8	1.75	0.51
34:RA:2682:U:O3'	48:RT:58:ASN:ND2	2.44	0.51
34:RA:2845:G:H2'	34:RA:2846:G:H8	1.76	0.51
39:RG:27:ASN:HB3	39:RG:30:GLU:HG3	1.93	0.51
34:YA:1930:G:N2	34:YA:1969:A:OP2	2.35	0.51
45:YQ:81:VAL:O	45:YQ:82:ARG:NE	2.40	0.51
1:QA:235:C:H2'	1:QA:236:G:H8	1.76	0.51
33:R9:27:CYS:SG	33:R9:28:GLU:N	2.83	0.51
34:RA:1689:A:H62	34:RA:1698:A:H2	1.58	0.51
34:RA:2393:A:H5"	34:RA:2393:A:H8	1.74	0.51
1:XA:978:A:OP2	1:XA:1362(A):C:N4	2.36	0.51
34:YA:1652:A:OP1	46:YR:8:ARG:NH1	2.43	0.51
34:YA:2258:C:O2'	34:YA:2427:C:OP2	2.27	0.51
49:YU:94:ASN:C	49:YU:96:ALA:H	2.13	0.51
32:R8:12:LYS:NZ	34:RA:249:C:O2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:1305:G:H22	1:XA:1331:G:H2'	1.74	0.51
1:QA:689:C:OP1	11:QK:27:ASN:ND2	2.40	0.51
34:RA:1047:G:N2	34:RA:1111:A:H62	2.08	0.51
34:RA:1500:G:N2	36:RD:99:ASP:O	2.43	0.51
46:RR:51:LEU:HD22	46:RR:66:VAL:HG13	1.92	0.51
1:XA:407:G:H2'	1:XA:408:A:H8	1.74	0.51
4:XD:80:GLU:OE1	4:XD:84:LYS:NZ	2.43	0.51
19:XS:36:ARG:NH2	19:XS:72:GLY:O	2.44	0.51
34:YA:1693:U:O2	36:YD:14:ARG:NH1	2.44	0.51
1:QA:165:C:H2'	1:QA:166:G:H8	1.76	0.50
1:QA:191(G):G:O2'	20:QT:101:GLY:O	2.29	0.50
1:QA:1010:G:H2'	1:QA:1011:G:H8	1.75	0.50
34:RA:557:U:H2'	34:RA:558:G:H8	1.76	0.50
34:RA:1542:G:O6	34:RA:1543:A:N6	2.43	0.50
34:RA:2059:A:HO2'	38:RF:69:HIS:HD1	1.58	0.50
51:RW:86:LEU:HD22	51:RW:96:ILE:HD11	1.93	0.50
34:YA:223:A:O2'	34:YA:420:C:O2	2.28	0.50
34:YA:1667:G:O2'	34:YA:1991:U:O4	2.29	0.50
34:YA:1799:G:O2'	36:YD:183:ARG:NH1	2.44	0.50
46:YR:86:ARG:NH2	46:YR:118:GLU:OXT	2.38	0.50
1:QA:1347:G:N2	1:QA:1374:A:OP2	2.39	0.50
3:QC:34:LEU:HD13	14:QN:25:VAL:HG11	1.94	0.50
26:R2:41:ILE:HD11	26:R2:44:LEU:HD12	1.92	0.50
37:RE:14:ILE:HG23	48:RT:14:TYR:HE2	1.76	0.50
40:RH:88:LEU:HA	40:RH:130:ARG:HA	1.92	0.50
1:QA:56:U:H2'	1:QA:57:G:H8	1.76	0.50
4:QD:129:ASN:HD21	4:QD:144:ASP:HA	1.76	0.50
10:QJ:6:ILE:HG23	10:QJ:72:VAL:HB	1.93	0.50
11:QK:57:THR:HG22	11:QK:59:TYR:H	1.77	0.50
11:QK:109:VAL:HG12	18:QR:86:VAL:HA	1.94	0.50
34:RA:65:C:O2'	34:RA:456:C:N3	2.39	0.50
34:RA:1022:G:N2	34:RA:1023:U:O4	2.41	0.50
34:RA:2680:C:H5'	37:RE:189:PRO:HA	1.93	0.50
45:RQ:36:ALA:HB2	45:RQ:103:MET:HE1	1.93	0.50
45:RQ:36:ALA:HB2	45:RQ:103:MET:HE2	1.92	0.50
13:XM:69:GLU:HG2	28:Y4:50:VAL:HG21	1.93	0.50
34:YA:244:A:H4'	44:YP:74:GLU:HB2	1.92	0.50
34:YA:1316:U:H2'	34:YA:1317:A:H8	1.76	0.50
41:YI:24:GLY:O	41:YI:28:ASN:HB2	2.11	0.50
1:QA:954:G:O6	13:QM:104:ARG:NH1	2.44	0.50
1:QA:1229:A:OP1	13:QM:114:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:QH:12:ARG:NH1	8:QH:25:ASP:O	2.39	0.50
25:R1:98:LEU:O	34:RA:269:U:O2'	2.30	0.50
32:R8:46:ARG:NH2	34:RA:631:A:OP1	2.45	0.50
34:RA:826:U:OP1	34:RA:2429:G:OP1	2.30	0.50
1:XA:7:G:O2'	5:XE:120:THR:O	2.30	0.50
1:XA:191(F):U:H2'	1:XA:191(G):G:H8	1.77	0.50
1:XA:993:G:H2'	1:XA:995:C:H41	1.76	0.50
2:XB:32:ILE:HD11	2:XB:40:HIS:HB3	1.92	0.50
4:XD:98:GLU:HA	4:XD:103:ASN:HD22	1.75	0.50
34:YA:2515:C:H2'	34:YA:2516:G:H8	1.76	0.50
39:YG:122:PRO:HD3	39:YG:181:ARG:HB2	1.94	0.50
41:YI:130:TYR:O	41:YI:136:VAL:CG1	2.59	0.50
44:YP:38:GLN:HG3	44:YP:45:LEU:HD23	1.94	0.50
51:YW:2:GLU:CA	51:YW:64:MET:HE3	2.42	0.50
37:RE:31:CYS:HB3	37:RE:49:LEU:HG	1.93	0.50
39:RG:37:VAL:HG22	39:RG:159:VAL:HG23	1.93	0.50
41:RI:3:VAL:HG12	41:RI:38:LEU:HA	1.94	0.50
1:XA:1356:G:H2'	1:XA:1357:A:C8	2.46	0.50
9:XI:9:ARG:HG2	9:XI:14:VAL:HG12	1.94	0.50
27:Y3:5:LYS:HE3	27:Y3:34:GLU:OE2	2.10	0.50
35:YB:37:C:O2	47:YS:95:HIS:NE2	2.42	0.50
38:YF:164:ARG:O	38:YF:168:ARG:HB2	2.11	0.50
38:RF:36:VAL:HG22	38:RF:101:LEU:HD21	1.94	0.50
45:RQ:63:LYS:HA	54:RZ:178:GLU:HG2	1.92	0.50
1:XA:924:C:O2'	1:XA:1502:A:N6	2.43	0.50
1:QA:1497:G:H1'	1:QA:1518:A:H2	1.76	0.50
15:QO:16:ALA:HB1	15:QO:21:ASP:HB3	1.93	0.50
20:QT:85:MET:HA	20:QT:88:VAL:HG12	1.94	0.50
34:RA:581:C:H2'	34:RA:582:G:H8	1.77	0.50
38:RF:155:LEU:HB2	38:RF:189:THR:HG21	1.94	0.50
42:RN:114:ARG:NH1	42:RN:114:ARG:CG	2.73	0.50
1:XA:1251:A:N3	1:XA:1369:C:O2'	2.36	0.50
1:XA:1347:G:H5"	9:XI:107:ARG:HB2	1.94	0.50
1:XA:1432:G:OP1	48:YT:108:ARG:N	2.44	0.50
25:Y1:51:VAL:HG11	25:Y1:74:VAL:HG21	1.94	0.50
34:YA:630:G:N2	34:YA:633:A:OP2	2.36	0.50
34:YA:1329:U:H5"	34:YA:1330:C:H5	1.76	0.50
34:YA:1341:U:OP2	34:YA:1394:U:O2'	2.26	0.50
34:YA:1598:C:O3'	52:YX:35:THR:OG1	2.28	0.50
34:YA:1791:A:H3'	34:YA:1792:G:H8	1.76	0.50
1:QA:1058:G:OP1	3:QC:199:LYS:NZ	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1071:C:H2'	1:QA:1072:G:H8	1.77	0.50
5:QE:35:GLY:HA3	5:QE:112:LEU:HB3	1.92	0.50
34:RA:181:A:H1'	34:RA:435:C:H5'	1.93	0.50
34:RA:560:C:H4'	49:RU:52:ARG:HH12	1.76	0.50
34:RA:1652:A:N6	46:RR:11:ASN:OD1	2.42	0.50
45:RQ:135:ASP:OD2	54:RZ:81:ARG:NH2	2.45	0.50
1:XA:578:C:O2'	1:XA:728:A:N3	2.38	0.50
1:XA:1469:G:H2'	1:XA:1470:G:H8	1.76	0.50
1:XA:1503:A:C5	1:XA:1531:A:C2	3.00	0.50
34:YA:605:C:O2	34:YA:657:U:O2'	2.29	0.50
47:YS:39:ILE:HD12	47:YS:85:VAL:HG11	1.94	0.50
3:QC:9:GLY:HA2	3:QC:12:LEU:HG	1.94	0.50
13:QM:24:GLY:CA	13:QM:66:LEU:HD21	2.39	0.50
13:QM:36:LYS:HD2	13:QM:59:TYR:HE1	1.77	0.50
14:QN:37:PHE:HD2	14:QN:44:LEU:HD22	1.77	0.50
34:RA:302:C:OP2	53:RY:73:ARG:NH1	2.39	0.50
34:RA:1341:U:OP2	34:RA:1394:U:O2'	2.28	0.50
1:XA:376:G:H5"	16:XP:5:ARG:HB2	1.94	0.50
2:XB:212:GLN:OE1	2:XB:235:SER:HB2	2.09	0.50
24:Y0:23:VAL:HG21	34:YA:857:C:H4'	1.94	0.50
34:YA:577:G:O2'	34:YA:1254:A:OP1	2.29	0.50
34:YA:665:C:H2'	34:YA:666:G:H8	1.77	0.50
38:YF:110:LEU:HD11	38:YF:181:LEU:HD13	1.94	0.50
41:YI:120:ILE:C	41:YI:120:ILE:HD12	2.32	0.50
48:YT:119:LYS:O	48:YT:123:GLN:HG2	2.10	0.50
1:QA:1066:C:N4	1:QA:1191:A:H62	2.10	0.49
1:QA:1250:A:OP1	9:QI:67:GLY:N	2.41	0.49
9:QI:26:VAL:HG22	9:QI:61:ALA:HB3	1.94	0.49
9:QI:63:ILE:HG21	9:QI:77:ILE:HG12	1.93	0.49
34:RA:581:C:H2'	34:RA:582:G:C8	2.47	0.49
34:RA:1882:C:H3'	34:RA:1883:G:H8	1.77	0.49
34:RA:2841:C:H2'	34:RA:2842:G:H8	1.77	0.49
1:XA:1101:A:N6	2:XB:176:GLU:OE2	2.45	0.49
29:Y5:19:ARG:NH2	34:YA:1264:G:OP1	2.34	0.49
45:YQ:77:LYS:NZ	45:YQ:83:MET:O	2.44	0.49
1:QA:713:G:H2'	1:QA:714:G:C8	2.47	0.49
41:RI:88:ILE:HD12	41:RI:121:LYS:HA	1.94	0.49
1:XA:107:G:H3'	1:XA:108:G:H21	1.77	0.49
1:XA:581:G:OP1	15:XO:65:ARG:NH1	2.44	0.49
27:Y3:37:LEU:HB2	27:Y3:43:ILE:HG21	1.94	0.49
34:YA:2508:G:H1	34:YA:2580:U:H3	1.58	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:2571:C:O2'	37:YE:146:THR:O	2.30	0.49
46:YR:28:LEU:HD23	46:YR:48:VAL:HG11	1.93	0.49
1:QA:938:A:N3	1:QA:1376:U:O2'	2.39	0.49
34:RA:30:G:O2'	34:RA:1214:A:N3	2.39	0.49
4:XD:105:VAL:HG11	4:XD:126:ILE:HD13	1.94	0.49
4:XD:187:ARG:NH1	4:XD:193:ASP:OD2	2.45	0.49
30:Y6:5:VAL:HA	30:Y6:27:LYS:HE2	1.94	0.49
34:YA:270(R):G:H2'	34:YA:270(S):G:H8	1.77	0.49
34:YA:1538:G:H2'	34:YA:1539:G:H8	1.77	0.49
38:YF:157:VAL:HG21	38:YF:181:LEU:HD23	1.93	0.49
1:QA:440:A:N6	1:QA:493:G:H21	2.06	0.49
1:QA:742:G:OP2	15:QO:35:ARG:NH2	2.44	0.49
3:QC:85:ARG:HG3	3:QC:88:ARG:HH21	1.78	0.49
13:QM:34:LEU:HD13	13:QM:41:PRO:HG3	1.93	0.49
39:RG:16:ARG:HH21	39:RG:28:VAL:HG22	1.78	0.49
42:RN:112:LEU:HG	42:RN:116:LEU:HD11	1.93	0.49
34:YA:546:C:OP1	34:YA:547:A:N6	2.45	0.49
34:YA:1983:C:H4'	34:YA:2606:C:H4'	1.93	0.49
40:YH:7:LEU:HD12	40:YH:8:PRO:HD2	1.93	0.49
44:YP:86:LYS:HB3	44:YP:118:GLY:HA3	1.93	0.49
1:QA:1406:U:O2	1:QA:1517:G:N2	2.41	0.49
5:QE:50:GLU:HB2	5:QE:53:LEU:HD13	1.94	0.49
8:QH:91:ARG:HB2	12:QL:7:ILE:HG13	1.94	0.49
33:R9:2:LYS:NZ	33:R9:31:LYS:O	2.41	0.49
34:RA:299:A:H5'	53:RY:86:ARG:HH21	1.78	0.49
34:RA:1045:A:H5"	34:RA:1046:A:H5'	1.95	0.49
34:RA:1510:A:O2'	34:RA:1512:G:N7	2.44	0.49
34:RA:2047:U:H2'	34:RA:2048:G:H8	1.77	0.49
41:RI:124:GLY:H	41:RI:142:VAL:HG13	1.78	0.49
45:RQ:52:VAL:HG13	54:RZ:183:LEU:HD13	1.95	0.49
1:XA:256:U:OP1	17:XQ:17:LYS:NZ	2.43	0.49
1:XA:266:G:H5'	1:XA:268:C:H41	1.77	0.49
10:XJ:9:ARG:HB2	10:XJ:95:GLU:HB3	1.93	0.49
34:YA:28:A:N6	34:YA:512:G:O2'	2.45	0.49
34:YA:2211:G:H21	34:YA:2212:A:H2	1.59	0.49
53:YY:29:GLU:HB3	53:YY:38:ILE:HD12	1.94	0.49
1:QA:1322:C:O2	1:QA:1322:C:H2'	2.11	0.49
1:QA:1355:G:H2'	1:QA:1356:G:H8	1.77	0.49
34:RA:1678:G:H22	34:RA:1989:G:N2	2.10	0.49
42:RN:114:ARG:NH1	42:RN:114:ARG:HG2	2.27	0.49
43:RO:104:ARG:NH1	43:RO:121:VAL:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:1296:C:OP1	13:XM:44:ARG:NH2	2.42	0.49
3:XC:11:ARG:NH2	3:XC:177:THR:O	2.34	0.49
10:XJ:44:VAL:HG11	10:XJ:46:ARG:HH21	1.77	0.49
34:YA:270(M):U:OP2	41:YI:50:ARG:NH1	2.46	0.49
34:YA:1491:G:H2'	34:YA:1492:G:H8	1.77	0.49
34:YA:2081:C:H2'	34:YA:2082:A:H8	1.76	0.49
34:YA:2468:G:O2'	34:YA:2481:G:N2	2.46	0.49
1:QA:522:C:H41	12:QL:53:ARG:HH22	1.60	0.49
13:QM:22:ILE:HB	13:QM:25:ILE:HB	1.95	0.49
49:RU:109:LEU:HD23	50:RV:47:VAL:HG21	1.93	0.49
1:XA:28:G:O2'	1:XA:296:U:OP1	2.29	0.49
25:Y1:6:GLU:HB3	25:Y1:91:LYS:HD2	1.94	0.49
27:Y3:3:ARG:CG	27:Y3:59:VAL:HB	2.43	0.49
34:YA:2311:A:H1'	39:YG:82:LEU:HD11	1.94	0.49
1:QA:745:C:OP1	1:QA:851:G:O2'	2.30	0.49
30:R6:37:ARG:HA	30:R6:48:VAL:HA	1.93	0.49
51:RW:92:ARG:NH1	51:RW:94:ASP:OD1	2.46	0.49
1:XA:347:G:H1'	1:XA:348:G:H5'	1.94	0.49
1:XA:1068:G:OP1	1:XA:1387:G:O2'	2.31	0.49
13:XM:7:VAL:HG23	39:YG:115:ARG:HH22	1.77	0.49
31:Y7:7:PRO:HB2	34:YA:1309:G:H4'	1.94	0.49
34:YA:2125:G:O2'	34:YA:2173:A:N6	2.46	0.49
34:YA:2154:G:H2'	34:YA:2155:G:H8	1.78	0.49
34:YA:2185:C:H2'	34:YA:2186:G:H8	1.77	0.49
44:YP:80:TYR:HE1	44:YP:111:ARG:HD2	1.78	0.49
1:QA:562:C:H1'	12:QL:15:ARG:HD2	1.94	0.49
2:QB:137:ARG:HG3	2:QB:138:LEU:HD12	1.95	0.49
12:QL:49:ASN:ND2	12:QL:92:ASP:OD2	2.43	0.49
34:RA:589:C:H2'	34:RA:590:A:C8	2.48	0.49
36:RD:5:LYS:HG2	36:RD:17:THR:HG22	1.95	0.49
37:RE:57:LYS:HA	37:RE:57:LYS:HE3	1.95	0.49
39:RG:23:PHE:HE2	39:RG:168:GLU:HA	1.78	0.49
41:RI:1:MET:N	41:RI:21:VAL:O	2.38	0.49
1:XA:8:A:N6	4:XD:208:SER:O	2.45	0.49
34:YA:1826:G:O2'	36:YD:242:ARG:NH2	2.44	0.49
34:YA:1952:A:N3	34:YA:2560:C:O2'	2.41	0.49
34:YA:2495:G:H5"	45:YQ:81:VAL:HG12	1.95	0.49
34:YA:2707:G:H2'	34:YA:2708:G:H8	1.78	0.49
1:QA:1322:C:OP2	19:QS:78:ARG:CZ	2.61	0.49
1:QA:1386:G:H2'	1:QA:1387:G:H8	1.78	0.49
34:RA:1066:U:O2'	34:RA:1068:G:OP2	2.23	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:RE:10:GLY:HA3	48:RT:8:LYS:HD3	1.95	0.49
40:RH:103:LEU:HD22	40:RH:105:LEU:HD23	1.95	0.49
11:XK:86:GLY:O	11:XK:91:ARG:NH1	2.43	0.49
33:Y9:22:ARG:HH12	34:YA:2741:A:H5"	1.78	0.49
34:YA:181:A:H1'	34:YA:435:C:H5'	1.95	0.49
34:YA:839:U:H1'	34:YA:1191:G:H1'	1.93	0.49
39:YG:83:ARG:C	39:YG:85:GLY:H	2.17	0.49
1:QA:1005:A:OP2	1:QA:1006:C:N4	2.46	0.48
1:QA:1342:C:H2'	1:QA:1343:G:C8	2.47	0.48
4:QD:64:LEU:HB2	4:QD:198:VAL:HG11	1.95	0.48
9:QI:28:VAL:HG22	9:QI:63:ILE:HB	1.94	0.48
9:QI:117:HIS:HE1	9:QI:123:PRO:HB3	1.77	0.48
34:RA:2646:C:OP2	34:RA:2732:G:O2'	2.27	0.48
36:RD:142:VAL:HG23	36:RD:193:VAL:HA	1.94	0.48
37:RE:38:THR:OG1	37:RE:40:GLU:OE1	2.30	0.48
39:RG:120:LEU:HB2	39:RG:180:PHE:HA	1.95	0.48
1:XA:923:A:O2'	1:XA:1399:C:OP2	2.27	0.48
9:XI:111:ARG:O	9:XI:113:LYS:NZ	2.38	0.48
12:XL:84:LEU:HD22	12:XL:104:VAL:HG21	1.95	0.48
34:YA:27:G:N2	34:YA:513:A:OP2	2.46	0.48
34:YA:265:A:N1	34:YA:427:U:O2'	2.40	0.48
34:YA:1882:C:H3'	34:YA:1883:G:H8	1.78	0.48
48:YT:77:PRO:HB2	48:YT:80:SER:HB2	1.95	0.48
34:RA:1288:U:O3'	34:RA:1647:G:N2	2.46	0.48
34:RA:2844:G:H3'	34:RA:2845:G:H8	1.78	0.48
36:RD:108:PRO:HD2	36:RD:111:LEU:HD22	1.94	0.48
1:XA:1123:A:H4'	10:XJ:36:GLY:HA3	1.95	0.48
1:XA:1500:A:H5"	1:XA:1508:G:H5"	1.95	0.48
3:XC:81:GLY:O	3:XC:85:ARG:CG	2.61	0.48
13:XM:93:ARG:HH21	34:YA:887:A:H5'	1.78	0.48
34:YA:918:A:N3	35:YB:80:U:O2'	2.44	0.48
1:QA:662:G:O2'	1:QA:836:G:OP1	2.28	0.48
15:QO:8:LYS:HG3	15:QO:31:LEU:HD11	1.95	0.48
48:RT:112:ARG:CG	48:RT:112:ARG:NH1	2.73	0.48
34:YA:837:C:N3	34:YA:941:A:N6	2.61	0.48
36:YD:125:ILE:N	36:YD:125:ILE:CD1	2.76	0.48
38:YF:101:LEU:HD23	38:YF:106:ARG:HG2	1.94	0.48
45:YQ:28:ALA:HB3	45:YQ:67:ARG:HH12	1.78	0.48
3:QC:58:GLU:HB3	3:QC:65:ALA:HB3	1.95	0.48
4:QD:133:VAL:HG12	4:QD:135:LEU:H	1.77	0.48
34:RA:24:G:O2'	51:RW:78:GLU:O	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:265:A:N6	34:RA:427:U:O2'	2.47	0.48
34:RA:630:G:N2	34:RA:633:A:OP2	2.39	0.48
34:RA:1800:C:N4	34:RA:1817:G:H22	2.11	0.48
36:RD:182:LEU:H	36:RD:272:ALA:HB3	1.78	0.48
40:RH:109:PHE:CZ	40:RH:152:ARG:HD2	2.49	0.48
1:XA:277:C:H5"	17:XQ:68:ARG:HH21	1.78	0.48
1:XA:452:A:N6	1:XA:480:U:H3	2.06	0.48
3:XC:130:VAL:HG21	3:XC:157:ILE:HG23	1.96	0.48
36:YD:77:ALA:HB3	36:YD:117:VAL:HG13	1.95	0.48
1:QA:1127:G:N2	1:QA:1145:C:O2	2.40	0.48
9:QI:8:GLY:O	9:QI:15:ALA:N	2.45	0.48
10:QJ:8:LEU:HB3	10:QJ:16:LEU:HD11	1.96	0.48
34:RA:71:A:H62	34:RA:114:U:H1'	1.79	0.48
34:RA:918:A:N3	35:RB:80:U:O2'	2.42	0.48
39:RG:29:TRP:O	39:RG:33:ARG:NH1	2.45	0.48
39:RG:83:ARG:NH1	39:RG:83:ARG:CG	2.77	0.48
43:RO:12:ASP:HB3	43:RO:98:VAL:HG12	1.96	0.48
49:RU:92:ARG:CG	49:RU:95:LEU:HD23	2.37	0.48
34:YA:1113:U:H2'	34:YA:1114:G:C8	2.49	0.48
34:YA:2047:U:H2'	34:YA:2048:G:H8	1.77	0.48
34:YA:2315:G:OP1	39:YG:36:LYS:NZ	2.39	0.48
34:YA:2647:U:O2	34:YA:2673:G:O6	2.32	0.48
41:YI:30:LEU:HB3	41:YI:36:ALA:HB3	1.96	0.48
20:QT:100:ILE:HG13	20:QT:102:GLY:H	1.78	0.48
34:RA:9:U:OP1	42:RN:115:ARG:NH2	2.46	0.48
34:RA:2495:G:H5"	45:RQ:81:VAL:HG12	1.95	0.48
40:RH:9:ILE:HG22	40:RH:10:PRO:N	2.29	0.48
54:RZ:69:THR:HG22	54:RZ:90:VAL:HG22	1.95	0.48
1:XA:1243:C:OP2	21:XU:10:ARG:NH2	2.47	0.48
4:XD:88:VAL:HG12	5:XE:97:GLY:HA3	1.94	0.48
36:YD:26:LYS:NZ	36:YD:28:GLU:O	2.42	0.48
3:QC:150:LYS:HB3	3:QC:201:TYR:HB2	1.95	0.48
34:RA:1485:G:H1	34:RA:1504:C:H42	1.60	0.48
35:RB:102:G:N3	54:RZ:73:GLN:NE2	2.54	0.48
37:RE:21:VAL:HG23	37:RE:185:LYS:HE3	1.94	0.48
1:XA:559:A:H4'	1:XA:560:U:H3'	1.95	0.48
1:XA:811:C:O2'	1:XA:901:A:N1	2.42	0.48
1:XA:1187:G:H4'	9:XI:111:ARG:HH21	1.79	0.48
12:XL:114:LYS:O	12:XL:117:ARG:NH1	2.46	0.48
22:XV:37:T6A:HN1	22:XV:38:A:H1'	1.79	0.48
39:YG:5:VAL:HG11	39:YG:100:TRP:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:YT:50:ILE:HD11	48:YT:100:TYR:HA	1.95	0.48
1:QA:619:U:N3	4:QD:134:ASP:OD1	2.39	0.48
1:QA:963:G:H21	10:QJ:55:LYS:HE3	1.78	0.48
1:QA:1323:G:N2	1:QA:1361:G:O2'	2.47	0.48
1:QA:1492:A:OP1	12:QL:47:LYS:HG3	2.13	0.48
11:QK:34:ASP:OD1	11:QK:38:ASN:N	2.47	0.48
34:RA:514:A:N3	34:RA:581:C:O2'	2.41	0.48
45:RQ:24:GLY:H	45:RQ:101:ARG:HD2	1.79	0.48
1:XA:165:C:H2'	1:XA:166:G:H8	1.79	0.48
1:XA:1141:C:H2'	1:XA:1142:G:H8	1.78	0.48
4:XD:16:GLY:O	4:XD:33:MET:HE1	2.14	0.48
45:YQ:75:THR:HG21	45:YQ:85:LYS:HE3	1.96	0.48
1:QA:1250:A:H2	1:QA:1370:G:H1'	1.79	0.48
2:QB:8:LYS:HG3	2:QB:10:LEU:H	1.79	0.48
12:QL:113:ARG:HH21	12:QL:116:SER:HB2	1.78	0.48
32:R8:27:THR:HB	34:RA:2361:A:P	2.54	0.48
34:RA:679:C:H2'	34:RA:680:G:C8	2.49	0.48
34:RA:1316:U:H2'	34:RA:1317:A:H8	1.79	0.48
39:RG:106:LEU:HA	39:RG:110:ALA:HB3	1.95	0.48
44:RP:18:ARG:HE	44:RP:21:ARG:HG3	1.78	0.48
45:RQ:8:LYS:HA	54:RZ:197:ILE:HB	1.96	0.48
30:Y6:21:TYR:OH	30:Y6:39:TYR:O	2.32	0.48
34:YA:589:C:H2'	34:YA:590:A:C8	2.48	0.48
34:YA:617:G:OP1	38:YF:40:GLN:NE2	2.47	0.48
36:YD:148:GLU:OE1	36:YD:151:LYS:NZ	2.38	0.48
2:QB:6:THR:O	2:QB:217:ARG:NH1	2.47	0.48
34:RA:83:G:O2'	34:RA:102:G:N2	2.46	0.48
36:RD:247:ALA:HA	36:RD:253:GLN:HA	1.96	0.48
48:RT:102:ILE:HB	48:RT:110:ILE:CD1	2.42	0.48
34:YA:679:C:H2'	34:YA:680:G:H8	1.78	0.48
36:YD:108:PRO:HD2	36:YD:111:LEU:HD22	1.95	0.48
38:YF:198:ALA:HA	38:YF:201:VAL:HG12	1.95	0.48
40:YH:3:ARG:HH21	40:YH:5:GLY:H	1.59	0.48
1:QA:618:C:H5'	1:QA:619:U:H5"	1.96	0.47
3:QC:84:ILE:HG23	3:QC:85:ARG:HD2	1.95	0.47
6:QF:9:VAL:HB	6:QF:87:ARG:HB2	1.95	0.47
11:QK:62:GLN:HG3	11:QK:97:ALA:HB2	1.96	0.47
28:R4:26:SER:OG	28:R4:27:THR:N	2.47	0.47
34:RA:550:G:H2'	34:RA:551:G:H8	1.80	0.47
34:RA:1449:A:O2'	34:RA:1530:G:N2	2.45	0.47
34:RA:1972:A:H2'	34:RA:1973:G:H8	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:2791:C:H4'	34:RA:2792:G:H5'	1.96	0.47
41:RI:125:GLU:OE1	41:RI:141:LYS:HG2	2.14	0.47
50:RV:47:VAL:O	50:RV:47:VAL:HG13	2.13	0.47
3:XC:190:ARG:HA	3:XC:195:VAL:HG22	1.95	0.47
42:YN:14:VAL:HG21	42:YN:33:LEU:HD23	1.96	0.47
49:YU:91:ASP:OD1	49:YU:96:ALA:HA	2.13	0.47
1:QA:28:G:O2'	1:QA:296:U:OP1	2.32	0.47
1:QA:1343:G:H4'	9:QI:122:ALA:HB3	1.95	0.47
9:QI:85:LEU:HD11	9:QI:96:LEU:HD11	1.95	0.47
34:RA:672:C:OP2	44:RP:42:SER:OG	2.31	0.47
34:RA:1278:A:H2'	34:RA:1279:G:C8	2.49	0.47
40:RH:12:PRO:HG3	40:RH:48:GLY:O	2.13	0.47
40:RH:24:VAL:HG13	40:RH:37:VAL:HG21	1.96	0.47
41:RI:9:LEU:HD13	41:RI:9:LEU:HA	1.70	0.47
55:XY:28:G:H2'	55:XY:29:G:H8	1.79	0.47
34:YA:59:U:H3	34:YA:68:G:H1	1.63	0.47
34:YA:151:C:H2'	34:YA:152:G:H8	1.79	0.47
34:YA:764:A:N3	36:YD:213:ARG:NH1	2.61	0.47
43:YO:87:ILE:HD12	43:YO:91:LEU:HA	1.96	0.47
1:QA:1189:C:C5'	3:QC:5:ILE:HD13	2.33	0.47
1:QA:1368:G:O2'	10:QJ:46:ARG:NH2	2.47	0.47
2:QB:87:ARG:NH1	2:QB:220:ASP:OD1	2.47	0.47
3:QC:172:ARG:HG2	3:QC:174:PRO:HD3	1.96	0.47
5:QE:79:GLU:HG2	8:QH:104:ARG:HH11	1.78	0.47
5:QE:107:ARG:O	5:QE:111:GLU:HB2	2.13	0.47
34:RA:219:G:N3	34:RA:234:C:O2'	2.47	0.47
34:RA:837:C:N3	34:RA:941:A:N6	2.61	0.47
36:RD:146:GLU:HB2	36:RD:189:CYS:HB3	1.97	0.47
38:RF:113:ALA:HB2	38:RF:183:VAL:HG23	1.96	0.47
1:XA:1510:U:H2'	1:XA:1511:G:C8	2.48	0.47
34:YA:303:U:H2'	34:YA:304:G:H8	1.78	0.47
34:YA:443:A:H2'	38:YF:45:ARG:HH12	1.79	0.47
34:YA:704:G:O2'	34:YA:726:G:N2	2.47	0.47
34:YA:1791:A:N6	34:YA:1828:G:O2'	2.39	0.47
34:YA:2521:C:O2'	34:YA:2564:A:N3	2.44	0.47
1:QA:34:C:H2'	1:QA:35:G:H8	1.78	0.47
1:QA:346:G:H1'	1:QA:347:G:H5'	1.96	0.47
1:QA:501:C:H2'	1:QA:502:G:C8	2.49	0.47
1:QA:1510:U:H2'	1:QA:1511:G:H8	1.79	0.47
2:QB:77:ALA:HB2	2:QB:211:ILE:HD13	1.96	0.47
34:RA:807:U:OP2	44:RP:41:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:2627:G:N2	34:RA:2777:G:OP2	2.44	0.47
37:RE:201:THR:HG22	37:RE:203:LYS:H	1.78	0.47
45:RQ:31:ASP:OD1	54:RZ:122:ARG:NH2	2.46	0.47
1:XA:946:A:O2'	1:XA:1333:A:N3	2.43	0.47
1:XA:1210:C:HO2'	1:XA:1213:A:HO2'	1.61	0.47
5:XE:12:LEU:HB3	5:XE:31:LEU:HB3	1.96	0.47
34:YA:1678:G:N2	34:YA:1989:G:H22	2.13	0.47
54:YZ:47:VAL:O	54:YZ:51:ALA:N	2.47	0.47
25:R1:78:LYS:HD3	34:RA:270(S):G:H1'	1.97	0.47
29:R5:4:HIS:O	34:RA:2056:G:N2	2.47	0.47
34:RA:1478:G:H2'	34:RA:1479:G:H8	1.80	0.47
39:RG:38:VAL:HB	39:RG:158:ALA:HB3	1.97	0.47
43:RO:25:LEU:HB2	43:RO:38:VAL:HG13	1.95	0.47
43:RO:87:ILE:HD12	43:RO:91:LEU:HA	1.96	0.47
1:XA:419:C:OP1	1:XA:513:C:O2'	2.32	0.47
34:YA:956:G:OP2	45:YQ:14:ARG:NH2	2.48	0.47
34:YA:2140:C:H2'	34:YA:2141:G:H8	1.79	0.47
34:YA:2308:G:C2	39:YG:80:PHE:HZ	2.32	0.47
39:YG:82:LEU:HD23	39:YG:82:LEU:N	2.28	0.47
9:QI:116:LYS:HE3	9:QI:120:ARG:HA	1.95	0.47
44:RP:107:LYS:NZ	44:RP:107:LYS:CB	2.73	0.47
4:XD:98:GLU:HG2	4:XD:189:PRO:HG3	1.95	0.47
34:YA:822:U:H2'	34:YA:823:G:H8	1.80	0.47
34:YA:2692:C:H2'	34:YA:2693:A:H8	1.79	0.47
36:YD:121:PRO:HB3	36:YD:135:PHE:HE2	1.76	0.47
39:YG:71:THR:N	39:YG:89:GLY:O	2.46	0.47
43:YO:25:LEU:HB2	43:YO:38:VAL:HG13	1.96	0.47
51:YW:1:MET:O	51:YW:64:MET:CE	2.49	0.47
1:QA:401:C:OP2	4:QD:73:ARG:NH1	2.48	0.47
1:QA:714:G:H2'	1:QA:715:A:C8	2.49	0.47
1:QA:979:C:OP1	1:QA:1223:C:N4	2.48	0.47
1:QA:1356:G:H2'	1:QA:1357:A:C8	2.49	0.47
19:QS:53:ASN:ND2	19:QS:76:PRO:O	2.45	0.47
34:RA:180:G:N1	34:RA:214:G:N7	2.54	0.47
34:RA:728:G:H5"	36:RD:13:ARG:HH21	1.79	0.47
36:RD:26:LYS:NZ	36:RD:28:GLU:O	2.41	0.47
48:RT:120:ARG:HA	48:RT:123:GLN:HB2	1.95	0.47
51:RW:111:HIS:CD2	51:RW:113:LYS:H	2.32	0.47
53:RY:14:LEU:HB2	53:RY:75:ILE:HD11	1.97	0.47
1:XA:21:G:H2'	1:XA:22:G:C8	2.50	0.47
1:XA:359:U:H2'	1:XA:360:A:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:715:A:H2'	1:XA:716:A:C8	2.49	0.47
3:XC:150:LYS:HG3	3:XC:169:ALA:HB2	1.97	0.47
11:XK:21:ILE:HB	11:XK:84:VAL:HG12	1.96	0.47
27:Y3:5:LYS:HG2	27:Y3:57:GLU:HB3	1.97	0.47
34:YA:83:G:O2'	34:YA:102:G:N2	2.47	0.47
34:YA:1571:A:H2'	34:YA:1572:A:H8	1.80	0.47
34:YA:2293:C:O2'	47:YS:93:LYS:NZ	2.42	0.47
36:YD:143:HIS:ND1	36:YD:194:GLY:O	2.43	0.47
39:YG:19:LEU:HD13	39:YG:32:PRO:HD2	1.96	0.47
48:YT:26:ASP:HB2	48:YT:91:ARG:HA	1.96	0.47
49:YU:90:VAL:HG11	50:YV:40:LEU:HG	1.97	0.47
52:YX:54:VAL:HG22	52:YX:81:VAL:HG23	1.95	0.47
1:QA:323:U:OP1	20:QT:26:ASN:ND2	2.45	0.47
3:QC:47:LEU:HD22	3:QC:76:VAL:HG22	1.96	0.47
25:R1:97:LEU:HD22	34:RA:270(T):G:H5"	1.96	0.47
27:R3:40:THR:HG22	27:R3:42:ALA:H	1.80	0.47
34:RA:679:C:H2'	34:RA:680:G:H8	1.79	0.47
34:RA:1638:C:O2	34:RA:2698:U:O2'	2.33	0.47
36:RD:121:PRO:CB	36:RD:135:PHE:CE2	2.75	0.47
10:XJ:57:LYS:HE2	10:XJ:60:ARG:HH22	1.80	0.47
34:YA:1972:A:H2'	34:YA:1973:G:H8	1.80	0.47
34:YA:2069:G:N1	34:YA:2443:C:N3	2.63	0.47
32:R8:27:THR:HG23	34:RA:2392:A:HO2'	1.75	0.47
34:RA:579:G:O2'	34:RA:2019:A:OP1	2.32	0.47
34:RA:1278:A:H2'	34:RA:1279:G:H8	1.79	0.47
34:RA:1830:C:H2'	34:RA:1831:G:H8	1.80	0.47
38:RF:40:GLN:HE22	38:RF:182:ASN:HB2	1.79	0.47
1:XA:401:C:O2'	1:XA:621:A:N3	2.41	0.47
1:XA:939:G:H21	1:XA:1374:A:H61	1.62	0.47
1:XA:1209:C:O2'	1:XA:1214:C:N4	2.44	0.47
13:XM:75:ALA:HA	13:XM:78:ILE:HG12	1.96	0.47
16:XP:5:ARG:NH2	16:XP:27:LYS:O	2.48	0.47
34:YA:1278:A:H2'	34:YA:1279:G:H8	1.80	0.47
34:YA:2646:C:OP2	34:YA:2732:G:O2'	2.27	0.47
39:YG:37:VAL:HG22	39:YG:159:VAL:HG12	1.96	0.47
48:YT:19:LEU:HD22	48:YT:86:ILE:HG22	1.96	0.47
1:QA:269:C:H2'	1:QA:270:A:H8	1.80	0.47
1:QA:362:G:N2	1:QA:365:U:OP2	2.46	0.47
7:QG:88:PRO:HG2	7:QG:152:ALA:HB2	1.97	0.47
34:RA:2052:G:H4'	37:RE:143:ASN:H	1.78	0.47
41:RI:80:PRO:HB2	41:RI:146:ALA:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:RI:120:ILE:CD1	41:RI:126:TYR:CD2	2.98	0.47
41:RI:123:LEU:HD12	41:RI:123:LEU:N	2.02	0.47
1:XA:636:U:H5'	17:XQ:2:PRO:HG3	1.96	0.47
1:XA:1366:C:O2'	10:XJ:60:ARG:NH1	2.48	0.47
12:XL:77:LEU:HD21	12:XL:107:ALA:HB2	1.97	0.47
34:YA:270(N):G:O4'	41:YI:50:ARG:NH2	2.48	0.47
34:YA:743:G:O2'	34:YA:1659:U:OP1	2.29	0.47
34:YA:900:A:H3'	34:YA:901:A:H8	1.80	0.47
34:YA:1231:G:H2'	34:YA:1232:G:H8	1.79	0.47
34:YA:1441:G:H2'	34:YA:1442:G:H8	1.79	0.47
34:YA:1664:A:H61	34:YA:1996:C:H42	1.63	0.47
44:YP:71:VAL:HG13	44:YP:72:PRO:HA	1.97	0.47
48:YT:35:LYS:HE3	48:YT:38:ASN:HA	1.97	0.47
54:YZ:5:LEU:HD11	54:YZ:44:PHE:HA	1.97	0.47
1:QA:578:C:O2'	1:QA:728:A:N3	2.42	0.46
2:QB:198:ASP:OD1	8:QH:68:ARG:NH1	2.43	0.46
31:R7:8:ASN:HB3	31:R7:11:LYS:HB3	1.97	0.46
34:RA:839:U:H1'	34:RA:1191:G:H1'	1.97	0.46
34:RA:1508:A:O2'	34:RA:1509:C:O4'	2.33	0.46
34:RA:2696:U:H2'	34:RA:2697:G:C8	2.50	0.46
39:RG:135:LEU:HD13	39:RG:140:ILE:HD11	1.95	0.46
14:XN:27:CYS:SG	14:XN:28:GLY:N	2.88	0.46
34:YA:554:U:H2'	34:YA:556:G:C8	2.50	0.46
34:YA:952:G:OP1	45:YQ:16:ARG:NH1	2.48	0.46
34:YA:1228:G:OP2	49:YU:16:LYS:NZ	2.39	0.46
42:YN:6:PRO:HG3	42:YN:41:ASP:HB2	1.96	0.46
45:YQ:111:GLU:OE1	45:YQ:133:ARG:NH2	2.48	0.46
34:RA:2375:G:N2	34:RA:2378:A:OP2	2.41	0.46
40:RH:146:ALA:O	40:RH:150:ALA:HB3	2.15	0.46
41:RI:30:LEU:HB3	41:RI:36:ALA:HB3	1.97	0.46
4:XD:166:LYS:HB2	4:XD:178:VAL:HG11	1.98	0.46
8:XH:34:GLU:OE1	8:XH:37:ARG:NH2	2.48	0.46
31:Y7:13:ALA:HB2	31:Y7:46:VAL:HG11	1.97	0.46
33:Y9:16:VAL:HG22	33:Y9:25:VAL:HG22	1.97	0.46
34:YA:1103:A:H5'	34:YA:1104:C:H5	1.79	0.46
1:QA:56:U:H2'	1:QA:57:G:C8	2.51	0.46
34:RA:347:A:H2'	34:RA:348:G:H8	1.80	0.46
34:RA:402:A:N3	34:RA:406:G:O2'	2.46	0.46
34:RA:1636:C:H2'	34:RA:1637:A:C8	2.51	0.46
35:RB:28:C:H5"	47:RS:29:PHE:HE2	1.78	0.46
36:RD:148:GLU:HB2	36:RD:151:LYS:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:RE:74:PRO:HG2	37:RE:77:ILE:HG22	1.96	0.46
50:RV:51:VAL:C	50:RV:53:GLU:H	2.18	0.46
1:XA:125:U:O3'	1:XA:633:G:N2	2.49	0.46
1:XA:452:A:H2'	1:XA:453:A:H8	1.81	0.46
10:XJ:23:ILE:HD12	10:XJ:85:LEU:HD11	1.96	0.46
34:YA:1818:U:H2'	36:YD:157:ARG:HG2	1.96	0.46
51:YW:111:HIS:HD2	51:YW:113:LYS:H	1.63	0.46
54:YZ:53:ILE:C	54:YZ:55:HIS:H	2.19	0.46
1:QA:1510:U:H2'	1:QA:1511:G:C8	2.50	0.46
4:QD:19:LEU:HD22	4:QD:67:ILE:HD11	1.98	0.46
34:RA:2416:C:O3'	44:RP:64:LYS:NZ	2.48	0.46
34:RA:2561:A:H4'	43:RO:40:VAL:HG11	1.98	0.46
34:YA:1266:G:O5'	51:YW:15:ARG:NH2	2.48	0.46
34:YA:2630:G:H2'	34:YA:2631:G:H8	1.79	0.46
1:QA:673:G:H2'	1:QA:674:G:C8	2.50	0.46
1:QA:967:C:O2'	9:QI:125:TYR:OH	2.30	0.46
1:QA:985:C:H2'	1:QA:986:A:H8	1.79	0.46
1:QA:1309:G:N7	13:QM:99:ARG:NH2	2.63	0.46
13:QM:13:LYS:HD3	13:QM:44:ARG:HD3	1.98	0.46
33:R9:22:ARG:HH12	34:RA:2741:A:H5"	1.80	0.46
1:XA:675:A:H1'	11:XK:116:HIS:CD2	2.51	0.46
7:XG:35:LYS:HD3	7:XG:38:LEU:HD12	1.97	0.46
34:YA:270(R):G:H2'	34:YA:270(S):G:C8	2.50	0.46
34:YA:867:C:N3	34:YA:912:C:O2'	2.43	0.46
34:YA:1819:A:H5"	36:YD:161:THR:HG21	1.98	0.46
41:YI:12:LEU:HD23	41:YI:12:LEU:HA	1.75	0.46
1:QA:824:C:H2'	1:QA:825:G:H8	1.80	0.46
34:RA:458:G:O2'	34:RA:469:G:O6	2.32	0.46
43:RO:120:GLU:OE1	48:RT:67:SER:OG	2.34	0.46
1:XA:405:U:O4	4:XD:2:GLY:N	2.49	0.46
13:XM:7:VAL:HG11	39:YG:139:LEU:HD13	1.98	0.46
34:YA:534:U:H5'	49:YU:42:ALA:HB1	1.98	0.46
34:YA:648:G:H2'	34:YA:649:G:H8	1.81	0.46
34:YA:2849:U:O4	48:YT:23:ARG:NH1	2.42	0.46
41:YI:92:VAL:CB	41:YI:120:ILE:CG2	2.77	0.46
41:YI:109:ILE:HB	41:YI:130:TYR:CZ	2.51	0.46
1:QA:159:G:O2'	1:QA:161:A:N7	2.45	0.46
1:QA:376:G:H5"	16:QP:5:ARG:HB2	1.97	0.46
1:QA:407:G:H2'	1:QA:408:A:C8	2.51	0.46
1:QA:946:A:H2'	1:QA:947:G:C8	2.51	0.46
1:QA:1033:G:H2'	1:QA:1034:G:H4'	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1105:A:H2'	1:QA:1106:G:H8	1.81	0.46
11:QK:58:PRO:HB2	11:QK:93:GLN:HG3	1.96	0.46
13:QM:3:ARG:HE	13:QM:9:ILE:HG21	1.80	0.46
32:R8:52:LYS:NZ	34:RA:834:C:H4'	2.31	0.46
34:RA:941:A:N3	34:RA:1190:G:O2'	2.48	0.46
38:RF:31:HIS:NE2	38:RF:35:GLU:OE2	2.48	0.46
40:RH:84:SER:HB2	40:RH:133:VAL:O	2.16	0.46
40:RH:159:GLU:HG3	40:RH:171:LEU:HD11	1.97	0.46
1:XA:243:A:H4'	1:XA:244:U:H3'	1.97	0.46
1:XA:448:A:OP2	1:XA:485:G:N2	2.43	0.46
1:XA:1342:C:H2'	1:XA:1343:G:H8	1.79	0.46
1:XA:1491:G:H5'	12:XL:47:LYS:HE3	1.98	0.46
2:XB:105:PHE:HA	2:XB:108:ILE:HG22	1.98	0.46
34:YA:414:C:H2'	34:YA:415:A:C8	2.51	0.46
34:YA:2133:G:O2'	34:YA:2158:A:N1	2.48	0.46
34:YA:2405:G:O2'	34:YA:2411:A:N6	2.48	0.46
38:YF:167:ALA:HB1	38:YF:173:VAL:HG11	1.98	0.46
46:YR:24:GLN:HG3	46:YR:44:LEU:HD13	1.97	0.46
49:YU:62:ILE:HD11	49:YU:93:LYS:HD2	1.97	0.46
54:YZ:100:VAL:HG21	54:YZ:134:PRO:HG2	1.96	0.46
24:R0:35:ASN:HD22	34:RA:2354:G:H4'	1.81	0.46
40:RH:89:ILE:O	40:RH:129:THR:OG1	2.34	0.46
40:RH:101:ARG:HE	40:RH:117:PRO:HG2	1.81	0.46
1:XA:54:C:N4	1:XA:353:A:OP2	2.43	0.46
3:XC:9:GLY:HA2	3:XC:12:LEU:HG	1.97	0.46
5:XE:34:VAL:HG11	5:XE:63:ARG:HE	1.81	0.46
19:XS:63:THR:OG1	19:XS:65:ASN:OD1	2.34	0.46
34:YA:1338:G:N7	52:YX:62:LYS:NZ	2.53	0.46
34:YA:1824:G:N3	36:YD:254:THR:OG1	2.48	0.46
1:QA:21:G:H2'	1:QA:22:G:C8	2.50	0.46
1:QA:922:G:H4'	5:QE:20:GLN:HA	1.98	0.46
34:RA:13:A:O2'	34:RA:15:G:N7	2.46	0.46
35:RB:8:U:O2	35:RB:112:G:N2	2.38	0.46
53:RY:102:CYS:SG	53:RY:103:GLY:N	2.89	0.46
1:XA:714:G:H2'	1:XA:715:A:C8	2.50	0.46
4:XD:62:GLN:HE22	4:XD:65:ARG:HH21	1.63	0.46
5:XE:91:LEU:HD13	5:XE:120:THR:HG22	1.98	0.46
34:YA:1800:C:H42	34:YA:1817:G:N2	2.14	0.46
34:YA:2115:G:N2	34:YA:2164:C:OP2	2.48	0.46
52:YX:12:VAL:HB	52:YX:27:THR:HG23	1.98	0.46
54:YZ:70:LEU:HG	54:YZ:91:LEU:HD21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1034:G:H2'	1:QA:1035:A:C8	2.51	0.46
18:QR:58:LEU:HD23	18:QR:62:GLU:HB3	1.98	0.46
19:QS:41:VAL:HG12	19:QS:43:GLU:H	1.81	0.46
39:RG:82:LEU:HD23	39:RG:82:LEU:HA	1.81	0.46
3:XC:20:SER:OG	3:XC:22:TRP:NE1	2.49	0.46
34:YA:75:G:H22	34:YA:111:A:H2	1.64	0.46
52:YX:55:ASN:HB2	52:YX:80:ILE:HG23	1.98	0.46
54:YZ:74:VAL:HG23	54:YZ:86:VAL:HG22	1.97	0.46
3:QC:131:ARG:NH2	3:QC:166:GLU:OE2	2.49	0.45
24:R0:21:LEU:HD21	24:R0:41:ARG:HH11	1.80	0.45
30:R6:21:TYR:OH	30:R6:39:TYR:O	2.34	0.45
32:R8:30:ARG:CZ	44:RP:62:LEU:HD12	2.45	0.45
34:RA:414:C:H2'	34:RA:415:A:H8	1.82	0.45
34:RA:1086:A:OP1	34:RA:1104:C:O2'	2.27	0.45
34:RA:1791:A:H3'	34:RA:1792:G:H8	1.80	0.45
1:XA:186:C:H5'	20:XT:78:ALA:HB1	1.97	0.45
1:XA:377:G:H2'	1:XA:378:G:H8	1.80	0.45
1:XA:452:A:H4'	16:XP:72:ARG:HH12	1.81	0.45
1:XA:957:U:H3	1:XA:960:U:H5"	1.81	0.45
1:XA:1342:C:H2'	1:XA:1343:G:C8	2.51	0.45
8:XH:97:VAL:HG21	8:XH:128:GLY:HA2	1.98	0.45
13:XM:40:ASN:HB2	13:XM:43:THR:HG23	1.97	0.45
19:XS:16:LEU:O	19:XS:20:LEU:HB2	2.16	0.45
27:Y3:2:PRO:HA	27:Y3:39:ASP:CB	2.45	0.45
34:YA:767:U:H2'	34:YA:768:G:H8	1.82	0.45
34:YA:1278:A:H2'	34:YA:1279:G:C8	2.52	0.45
34:YA:1571:A:H2'	34:YA:1572:A:C8	2.51	0.45
34:YA:2100:G:O6	34:YA:2189:U:O2	2.34	0.45
54:YZ:53:ILE:C	54:YZ:53:ILE:HD12	2.36	0.45
1:QA:677:U:O2	1:QA:777:A:O2'	2.33	0.45
7:QG:16:LEU:HD12	9:QI:44:VAL:HG23	1.98	0.45
34:RA:2010:G:H5"	51:RW:42:ARG:HB2	1.98	0.45
41:RI:9:LEU:CD2	41:RI:35:LEU:HD13	2.46	0.45
41:RI:80:PRO:HA	41:RI:143:SER:HB2	1.98	0.45
1:XA:398:C:H2'	1:XA:399:G:H8	1.81	0.45
1:XA:1129:C:O2	1:XA:1132:C:N4	2.50	0.45
1:XA:1137:C:O2'	1:XA:1138:G:N2	2.49	0.45
1:XA:1323:G:H2'	1:XA:1324:A:C8	2.51	0.45
1:XA:1423:G:H5'	43:YO:49:ARG:HH12	1.79	0.45
3:XC:39:ILE:HD12	3:XC:91:LEU:HD22	1.97	0.45
12:XL:49:ASN:ND2	12:XL:92:ASP:OD2	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:XX:-14:G:H2'	23:XX:-13:G:C8	2.52	0.45
1:QA:390:C:H2'	1:QA:391:G:C8	2.51	0.45
34:RA:390:A:H4'	34:RA:391:G:H5'	1.98	0.45
34:RA:1105:U:H2'	34:RA:1106:G:H8	1.81	0.45
34:RA:1815:A:OP2	36:RD:54:ARG:NH2	2.49	0.45
39:RG:73:ALA:HB1	39:RG:82:LEU:HD13	1.99	0.45
40:RH:9:ILE:CG2	40:RH:50:VAL:O	2.64	0.45
45:RQ:75:THR:HG21	45:RQ:85:LYS:HE3	1.97	0.45
47:RS:66:ALA:HA	47:RS:69:VAL:HG12	1.98	0.45
1:XA:309:G:H2'	1:XA:310:G:H8	1.81	0.45
5:XE:35:GLY:HA3	5:XE:112:LEU:HB3	1.97	0.45
9:XI:28:VAL:HA	9:XI:63:ILE:HB	1.97	0.45
16:XP:67:THR:O	16:XP:71:ARG:N	2.44	0.45
26:Y2:65:ASN:ND2	34:YA:72:U:O4	2.48	0.45
34:YA:704:G:H1'	34:YA:727:A:H61	1.80	0.45
34:YA:776:G:N7	34:YA:793:A:O2'	2.49	0.45
34:RA:985:C:H2'	34:RA:986:C:H6	1.80	0.45
34:RA:1824:G:N3	36:RD:254:THR:OG1	2.49	0.45
1:XA:45:U:H2'	1:XA:46:G:H8	1.80	0.45
20:XT:62:LEU:HA	20:XT:65:LYS:HB2	1.98	0.45
40:YH:21:PRO:O	40:YH:23:ARG:NH1	2.49	0.45
43:YO:97:ARG:H	43:YO:117:LEU:HD13	1.81	0.45
45:YQ:27:VAL:C	45:YQ:105:GLU:OE2	2.55	0.45
51:YW:86:LEU:HD22	51:YW:96:ILE:HD11	1.97	0.45
1:QA:272:C:H2'	1:QA:273:A:H8	1.82	0.45
1:QA:546:G:H4'	1:QA:548:G:H4'	1.99	0.45
1:QA:715:A:H2'	1:QA:716:A:C8	2.51	0.45
1:QA:1376:U:OP1	7:QG:94:ARG:NH1	2.48	0.45
34:RA:605:C:O2	34:RA:657:U:O2'	2.34	0.45
34:RA:2229:C:H2'	34:RA:2230:G:H8	1.81	0.45
34:RA:2328:A:H2'	34:RA:2329:G:H8	1.79	0.45
43:RO:104:ARG:HH11	43:RO:121:VAL:HG12	1.81	0.45
49:RU:108:GLU:OE1	50:RV:47:VAL:HG11	2.17	0.45
1:XA:748:C:H1'	1:XA:749:C:H5	1.80	0.45
1:XA:1060:C:H2'	1:XA:1061:G:H8	1.82	0.45
9:XI:50:LEU:HD22	9:XI:81:ILE:HG21	1.98	0.45
18:XR:70:ILE:O	18:XR:74:ARG:HB2	2.16	0.45
34:YA:971:C:O2'	34:YA:983:A:N3	2.39	0.45
35:YB:23:G:H2'	35:YB:24:G:C5	2.51	0.45
1:QA:972:C:OP2	10:QJ:57:LYS:NZ	2.38	0.45
22:QV:22:G:H2'	22:QV:23:A:H8	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:R0:39:ARG:HH21	34:RA:2355:C:H1'	1.82	0.45
34:RA:576:U:H2'	34:RA:577:G:C8	2.51	0.45
35:RB:24:G:H1'	35:RB:27:C:H41	1.82	0.45
36:RD:145:VAL:HB	36:RD:155:LEU:HB2	1.98	0.45
41:RI:9:LEU:HD21	41:RI:35:LEU:HD13	1.98	0.45
44:RP:52:GLU:OE2	44:RP:58:THR:OG1	2.33	0.45
1:XA:34:C:H2'	1:XA:35:G:C8	2.51	0.45
1:XA:707:C:OP1	11:XK:85:ARG:NH1	2.48	0.45
1:XA:718:G:O6	18:XR:74:ARG:NH1	2.50	0.45
1:XA:1240:U:OP1	7:XG:119:ARG:NH2	2.49	0.45
31:Y7:47:ARG:HH12	52:YX:60:ARG:HH22	1.62	0.45
34:YA:458:G:O2'	34:YA:469:G:O6	2.30	0.45
34:YA:576:U:H2'	34:YA:577:G:C8	2.52	0.45
34:YA:2074:U:H2'	34:YA:2075:U:C6	2.51	0.45
50:YV:24:LYS:HA	50:YV:92:THR:HG23	1.98	0.45
1:QA:1113:C:H4'	3:QC:14:ILE:HG13	1.99	0.45
2:QB:93:VAL:HG11	2:QB:97:TRP:HD1	1.81	0.45
3:QC:77:ILE:HD12	3:QC:84:ILE:HG21	1.98	0.45
34:RA:1153:C:H5'	49:RU:76:TYR:HE2	1.81	0.45
34:RA:1952:A:N3	34:RA:2560:C:O2'	2.40	0.45
34:RA:2008:C:H2'	34:RA:2009:G:H8	1.82	0.45
34:RA:2659:G:N2	34:RA:2662:A:OP2	2.50	0.45
45:RQ:137:TYR:HD1	54:RZ:74:VAL:HG11	1.81	0.45
46:RR:33:ARG:HD3	46:RR:113:LEU:HD11	1.99	0.45
50:RV:51:VAL:C	50:RV:53:GLU:N	2.70	0.45
1:XA:662:G:O2'	1:XA:836:G:OP1	2.35	0.45
1:XA:769:G:H4'	1:XA:1513:A:H4'	1.99	0.45
34:YA:1826:G:OP1	36:YD:224:ALA:N	2.50	0.45
49:YU:74:LEU:HD21	49:YU:110:VAL:HG13	1.98	0.45
1:QA:143:A:H2	1:QA:220:G:H1	1.64	0.45
1:QA:1030:C:O2'	1:QA:1031:G:O4'	2.34	0.45
2:QB:51:LEU:HD23	2:QB:201:ILE:HD12	1.98	0.45
4:QD:125:HIS:HD1	4:QD:152:SER:HB3	1.81	0.45
16:QP:34:GLU:OE2	16:QP:55:ARG:NH2	2.47	0.45
24:R0:67:VAL:HG22	24:R0:81:VAL:HG22	1.97	0.45
34:RA:1732:A:H3'	34:RA:1733:G:H8	1.81	0.45
34:RA:2123:G:H2'	34:RA:2124:G:H8	1.81	0.45
34:RA:2579:C:H2'	34:RA:2580:U:H6	1.82	0.45
48:RT:111:ARG:C	48:RT:113:LYS:N	2.70	0.45
49:RU:92:ARG:HG2	49:RU:95:LEU:HD22	1.88	0.45
1:XA:269:C:H2'	1:XA:270:A:H8	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Y6:11:LEU:HB2	30:Y6:21:TYR:HB2	1.97	0.45
34:YA:1491:G:H2'	34:YA:1492:G:C8	2.52	0.45
34:YA:1782:C:H1'	34:YA:2609:U:H5"	1.98	0.45
42:YN:23:LEU:HB2	42:YN:62:VAL:HG12	1.99	0.45
47:YS:71:ARG:O	47:YS:107:GLU:OE1	2.34	0.45
1:QA:593:G:H1	1:QA:646:U:H3	1.65	0.45
1:QA:736:C:H2'	1:QA:737:A:C8	2.52	0.45
1:QA:1023:G:H3'	1:QA:1024:G:H5"	1.98	0.45
1:QA:1060:C:H2'	1:QA:1061:G:H8	1.81	0.45
1:QA:1151:A:H2'	1:QA:1152:A:C8	2.51	0.45
5:QE:102:ALA:O	5:QE:107:ARG:NH2	2.50	0.45
22:QV:37:T6A:HN1	22:QV:38:A:H1'	1.82	0.45
34:RA:958:U:OP2	45:RQ:14:ARG:NH1	2.49	0.45
36:RD:108:PRO:CA	36:RD:196:VAL:O	2.65	0.45
1:XA:272:C:H2'	1:XA:273:A:H8	1.82	0.45
1:XA:546:G:H4'	1:XA:548:G:H4'	1.98	0.45
28:Y4:40:HIS:CD2	39:YG:112:PRO:HB3	2.52	0.45
34:YA:414:C:O2	34:YA:1864:U:O2'	2.33	0.45
34:YA:890:A:H2'	34:YA:892:G:H8	1.82	0.45
34:YA:919:G:N2	34:YA:2269:A:OP2	2.50	0.45
34:YA:1449:A:C4	34:YA:1529:A:H2	2.35	0.45
51:YW:111:HIS:CD2	51:YW:113:LYS:H	2.34	0.45
1:QA:861:G:O2'	1:QA:874:G:O2'	2.35	0.45
1:QA:970:C:N4	9:QI:128:ARG:O	2.42	0.45
1:QA:985:C:H2'	1:QA:986:A:C8	2.52	0.45
34:RA:414:C:H2'	34:RA:415:A:C8	2.52	0.45
34:RA:740:U:H2'	34:RA:741:G:C8	2.51	0.45
34:RA:1316:U:H2'	34:RA:1317:A:C8	2.52	0.45
34:RA:1667:G:O2'	34:RA:1991:U:O4	2.31	0.45
34:RA:1819:A:H5"	36:RD:161:THR:HG21	1.99	0.45
34:RA:2404:C:O3'	44:RP:77:ARG:NH2	2.50	0.45
34:RA:2544:G:H1'	34:RA:2646:C:H4'	1.99	0.45
34:RA:2623:G:OP1	34:RA:2826:A:O2'	2.27	0.45
39:RG:73:ALA:HB1	39:RG:82:LEU:CD1	2.47	0.45
1:XA:356:A:N3	1:XA:368:U:O2'	2.40	0.45
1:XA:407:G:H2'	1:XA:408:A:C8	2.51	0.45
55:XY:37:A:O2'	34:YA:1913:A:N1	2.42	0.45
27:Y3:3:ARG:CG	27:Y3:60:GLU:OXT	2.64	0.45
34:YA:297:C:OP1	53:YY:87:LYS:NZ	2.42	0.45
34:YA:679:C:H2'	34:YA:680:G:C8	2.51	0.45
34:YA:784:A:N6	34:YA:2072:G:O2'	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:2071:A:H2'	34:YA:2072:G:C8	2.52	0.45
34:YA:2291:U:O2'	34:YA:2374:C:O2	2.35	0.45
34:YA:2590:A:H2'	34:YA:2591:C:H6	1.82	0.45
37:YE:2:LYS:HG2	37:YE:200:GLU:HB2	1.99	0.45
39:YG:106:LEU:HA	39:YG:110:ALA:HB3	1.98	0.45
47:YS:26:LEU:HB3	47:YS:87:PHE:HA	1.99	0.45
22:QV:65:C:H2'	22:QV:66:A:C8	2.52	0.44
34:RA:281:G:H21	34:RA:359:A:H62	1.65	0.44
34:RA:2318:G:H1	47:RS:2:ALA:HA	1.82	0.44
35:RB:8:U:O4	35:RB:112:G:O6	2.35	0.44
38:RF:40:GLN:HA	38:RF:43:LYS:HG2	1.99	0.44
11:XK:52:GLY:H	11:XK:55:LYS:HE2	1.82	0.44
34:YA:17:G:H4'	49:YU:25:TRP:HE1	1.82	0.44
34:YA:818:G:N1	34:YA:1188:U:OP2	2.35	0.44
34:YA:975:G:N2	34:YA:1156:A:O2'	2.50	0.44
34:YA:2737:G:H2'	34:YA:2738:A:C8	2.52	0.44
53:YY:20:TYR:HB3	53:YY:23:ARG:HG3	1.99	0.44
1:QA:407:G:H2'	1:QA:408:A:H8	1.81	0.44
1:QA:806:C:H2'	1:QA:807:A:H8	1.82	0.44
2:QB:70:PHE:O	2:QB:93:VAL:N	2.46	0.44
24:R0:55:ARG:NH1	34:RA:2364:C:OP1	2.48	0.44
29:R5:12:SER:HB3	34:RA:2020:A:H5'	1.99	0.44
34:RA:604:G:OP1	44:RP:90:ARG:NH1	2.50	0.44
34:RA:2123:G:H2'	34:RA:2124:G:C8	2.52	0.44
39:RG:68:PRO:HB3	39:RG:92:VAL:HB	1.98	0.44
39:RG:81:LYS:HA	39:RG:81:LYS:HD2	1.57	0.44
50:RV:55:ALA:HA	50:RV:101:GLY:HA2	2.00	0.44
52:RX:12:VAL:HB	52:RX:27:THR:HG23	1.99	0.44
1:XA:707:C:H2'	1:XA:708:C:H6	1.82	0.44
1:XA:1541:U:H3	23:XX:-14:G:H1	1.66	0.44
3:XC:19:GLU:O	3:XC:40:ARG:NH2	2.50	0.44
10:XJ:23:ILE:HG23	10:XJ:85:LEU:HD11	1.99	0.44
29:Y5:4:HIS:O	34:YA:2056:G:N2	2.50	0.44
34:YA:81:G:HO2'	34:YA:295:G:HO2'	1.61	0.44
36:YD:108:PRO:HB3	36:YD:143:HIS:CE1	2.52	0.44
51:YW:1:MET:HG2	51:YW:64:MET:HE2	1.84	0.44
54:YZ:6:LYS:HD3	54:YZ:8:TYR:CZ	2.52	0.44
1:QA:407:G:OP1	4:QD:115:ARG:NH1	2.50	0.44
1:QA:687:A:N6	1:QA:701:C:O4'	2.51	0.44
25:R1:19:GLN:HG3	34:RA:2080:G:H5'	1.98	0.44
34:RA:851:U:H2'	34:RA:852:G:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:RE:144:ARG:HB3	37:RE:145:LYS:H	1.70	0.44
49:RU:109:LEU:CD2	50:RV:47:VAL:HG21	2.47	0.44
1:XA:22:G:H4'	1:XA:885:G:C8	2.52	0.44
1:XA:67:C:H2'	1:XA:68:G:C8	2.52	0.44
1:XA:438:G:N2	1:XA:496:A:H62	2.13	0.44
1:XA:501:C:H2'	1:XA:502:G:H8	1.82	0.44
1:XA:579:G:H5'	1:XA:728:A:H1'	1.99	0.44
17:XQ:53:LEU:HD23	17:XQ:85:VAL:HG11	1.99	0.44
22:XV:22:G:H2'	22:XV:23:A:H8	1.82	0.44
25:Y1:17:SER:HB2	25:Y1:40:ARG:HD2	2.00	0.44
27:Y3:37:LEU:N	27:Y3:37:LEU:CD1	2.73	0.44
34:YA:729:G:C6	34:YA:1775:U:N3	2.85	0.44
34:YA:1399:C:H2'	34:YA:1400:G:H8	1.81	0.44
34:YA:2151:G:H2'	34:YA:2152:G:H8	1.81	0.44
45:YQ:65:PHE:HD2	45:YQ:105:GLU:O	2.00	0.44
1:QA:448:A:OP2	1:QA:485:G:N2	2.39	0.44
1:QA:782:A:H62	1:QA:800:G:H21	1.66	0.44
3:QC:124:ILE:HG21	3:QC:196:LEU:HG	1.99	0.44
19:QS:15:LEU:HD11	19:QS:35:SER:HB3	1.98	0.44
34:RA:1470:G:O2'	34:RA:1522:G:O6	2.33	0.44
34:RA:1598:C:O3'	52:RX:35:THR:OG1	2.36	0.44
34:RA:1995:U:O2	43:RO:3:GLN:NE2	2.36	0.44
34:RA:2037:G:H2'	34:RA:2038:G:C8	2.53	0.44
34:RA:2378:A:H4'	47:RS:23:ARG:NH1	2.33	0.44
49:RU:94:ASN:C	49:RU:96:ALA:H	2.21	0.44
54:RZ:48:PHE:HE1	54:RZ:53:ILE:HG22	1.82	0.44
1:XA:1386:G:H2'	1:XA:1387:G:H8	1.81	0.44
6:XF:48:LEU:HD22	18:XR:77:GLY:HA3	1.98	0.44
22:XV:50:C:H2'	22:XV:51:A:C8	2.53	0.44
26:Y2:17:SER:HB3	26:Y2:20:GLU:HG2	1.99	0.44
34:YA:373:U:H2'	34:YA:374:A:H8	1.81	0.44
34:YA:807:U:H2'	34:YA:808:G:H8	1.82	0.44
41:YI:118:LYS:CB	41:YI:119:PRO:HD2	2.42	0.44
4:QD:195:ALA:HB1	6:XF:16:GLN:HG3	1.98	0.44
34:RA:1380:G:O2'	34:RA:1569:A:N6	2.50	0.44
34:RA:2250:G:C4	45:RQ:82:ARG:HG3	2.53	0.44
36:RD:245:PRO:HA	36:RD:246:PRO:HD3	1.83	0.44
41:RI:118:LYS:HB3	41:RI:118:LYS:HE3	1.50	0.44
42:RN:47:ALA:HB2	42:RN:112:LEU:HD11	1.98	0.44
1:XA:166:G:H2'	1:XA:167:G:H8	1.83	0.44
1:XA:486:U:H2'	1:XA:487:A:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:674:G:H2'	1:XA:675:A:C8	2.49	0.44
1:XA:738:C:H5"	6:XF:69:GLU:HB2	2.00	0.44
1:XA:1492:A:OP2	12:XL:47:LYS:HG2	2.17	0.44
7:XG:111:ARG:NH2	7:XG:126:ASP:OD2	2.41	0.44
11:XK:108:ILE:O	18:XR:87:ARG:N	2.45	0.44
33:Y9:19:ARG:NE	34:YA:2756:U:OP2	2.39	0.44
34:YA:219:G:N3	34:YA:234:C:O2'	2.49	0.44
34:YA:1651:G:N7	46:YR:11:ASN:ND2	2.65	0.44
39:YG:59:GLU:OE1	39:YG:153:ARG:NH2	2.39	0.44
1:QA:537:G:H5"	12:QL:113:ARG:HH12	1.83	0.44
10:QJ:34:VAL:HG23	10:QJ:74:ILE:HA	2.00	0.44
25:R1:45:ASN:HB2	34:RA:397:G:H5"	1.99	0.44
26:R2:6:VAL:HG13	26:R2:59:ARG:HE	1.82	0.44
28:R4:5:ILE:O	39:RG:67:LYS:NZ	2.51	0.44
34:RA:39:C:O2	38:RF:46:ARG:NH2	2.50	0.44
34:RA:288:C:H2'	34:RA:289:A:H8	1.83	0.44
34:RA:468:G:H5"	38:RF:60:SER:HB2	2.00	0.44
34:RA:1026:U:H1'	34:RA:1027:A:H5"	1.99	0.44
34:RA:1600:C:OP1	52:RX:58:HIS:NE2	2.32	0.44
34:RA:2291:U:O2'	34:RA:2374:C:O2	2.34	0.44
34:RA:2304:G:H22	34:RA:2312:U:H3	1.65	0.44
38:RF:167:ALA:HB1	38:RF:173:VAL:HG11	1.98	0.44
1:XA:235:C:H2'	1:XA:236:G:H8	1.81	0.44
1:XA:1354:C:H2'	1:XA:1355:G:H8	1.83	0.44
14:XN:23:ARG:NH1	14:XN:28:GLY:O	2.51	0.44
34:YA:1416:G:H2'	34:YA:1417:C:C6	2.53	0.44
34:YA:2867:G:OP2	48:YT:119:LYS:NZ	2.38	0.44
36:YD:121:PRO:HB3	36:YD:135:PHE:HD2	1.77	0.44
1:QA:1249:C:N4	1:QA:1288:A:OP2	2.51	0.44
12:QL:47:LYS:N	12:QL:48:PRO:HD2	2.33	0.44
33:R9:16:VAL:HG11	34:RA:1032:A:H4'	2.00	0.44
34:RA:323:G:H2'	38:RF:169:ASN:ND2	2.33	0.44
34:RA:2246:G:H2'	34:RA:2247:A:C8	2.53	0.44
36:RD:155:LEU:HD23	36:RD:177:LEU:HD11	1.99	0.44
41:RI:14:ASP:OD1	41:RI:17:GLN:OE1	2.35	0.44
2:XB:179:LYS:HA	8:XH:72:PRO:HD3	1.99	0.44
5:XE:110:LEU:HD13	5:XE:118:ILE:HD13	1.98	0.44
34:YA:814:C:H1'	34:YA:1226:G:H21	1.82	0.44
34:YA:1638:C:O2	34:YA:2698:U:O2'	2.35	0.44
34:YA:2352:A:N6	34:YA:2365:G:O2'	2.51	0.44
40:YH:121:ILE:HD11	40:YH:140:LYS:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:YN:128:HIS:NE2	42:YN:134:ARG:HD3	2.32	0.44
2:QB:80:ILE:HD11	2:QB:208:ILE:HG23	1.99	0.44
32:R8:55:ALA:HB1	44:RP:49:ARG:O	2.17	0.44
34:RA:1042:G:O6	34:RA:1113:U:O2	2.36	0.44
34:RA:1231:G:H2'	34:RA:1232:G:H8	1.83	0.44
34:RA:1569:A:H4'	36:RD:61:LEU:HD11	1.99	0.44
48:RT:125:ARG:O	48:RT:128:GLU:HB3	2.18	0.44
1:XA:18:C:H4'	1:XA:1078:U:H3	1.81	0.44
1:XA:877:C:H2'	1:XA:878:G:H8	1.83	0.44
3:XC:76:VAL:HG23	3:XC:77:ILE:HG13	2.00	0.44
15:XO:67:LEU:HB3	15:XO:78:TYR:HE1	1.82	0.44
34:YA:389:G:N1	44:YP:71:VAL:O	2.43	0.44
34:YA:1316:U:H2'	34:YA:1317:A:C8	2.52	0.44
34:YA:2099:U:O4	34:YA:2190:G:O6	2.36	0.44
34:YA:2453:A:H2'	34:YA:2454:G:H8	1.83	0.44
37:YE:52:LEU:CD2	37:YE:77:ILE:HD12	2.48	0.44
39:YG:16:ARG:HH21	39:YG:28:VAL:HG22	1.81	0.44
39:YG:41:GLN:NE2	39:YG:56:ALA:HB1	2.33	0.44
53:YY:28:LYS:N	53:YY:38:ILE:O	2.44	0.44
1:QA:634:C:H2'	1:QA:635:G:H8	1.83	0.44
1:QA:838:G:H1	1:QA:848:C:H42	1.66	0.44
7:QG:111:ARG:NH2	7:QG:126:ASP:OD2	2.44	0.44
25:R1:53:VAL:HG13	25:R1:74:VAL:HG13	2.00	0.44
34:RA:1139:G:O2'	34:RA:1143:A:N1	2.41	0.44
37:RE:36:ARG:HH12	37:RE:86:PRO:HD2	1.83	0.44
1:XA:320:C:H2'	1:XA:321:A:C8	2.53	0.44
1:XA:1491:G:C5'	12:XL:47:LYS:HE3	2.48	0.44
3:XC:42:LEU:HA	3:XC:45:LYS:HG2	2.00	0.44
34:YA:307:G:H21	34:YA:330:A:H62	1.66	0.44
34:YA:1353:A:H2'	34:YA:1354:A:C8	2.53	0.44
34:YA:2561:A:H4'	43:YO:40:VAL:HG11	2.00	0.44
41:YI:130:TYR:O	41:YI:136:VAL:O	2.36	0.44
52:YX:25:LYS:HB3	52:YX:80:ILE:HD11	2.00	0.44
54:YZ:4:ARG:HG2	54:YZ:58:VAL:HB	2.00	0.44
1:QA:452:A:H62	1:QA:480:U:H3	1.64	0.43
1:QA:946:A:H2'	1:QA:947:G:H8	1.82	0.43
26:R2:18:PRO:HA	26:R2:21:LEU:HD12	2.00	0.43
32:R8:36:LYS:HB3	32:R8:40:GLU:HG2	1.99	0.43
34:RA:1354:A:H3'	34:RA:1355:G:H8	1.83	0.43
34:RA:2329:G:H2'	34:RA:2330:G:C8	2.53	0.43
34:RA:2859:G:H2'	34:RA:2860:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:RR:104:ARG:HG3	46:RR:107:ASP:HB3	2.00	0.43
2:XB:98:LEU:HB2	2:XB:101:MET:HE2	2.00	0.43
24:Y0:46:LYS:HD2	24:Y0:78:TYR:HE1	1.82	0.43
34:YA:177:G:H3'	34:YA:178:G:H8	1.83	0.43
34:YA:787:U:H5"	34:YA:788:A:H5'	2.00	0.43
34:YA:847:U:H3	34:YA:934:G:N2	2.16	0.43
34:YA:949:C:H2'	34:YA:950:G:H8	1.83	0.43
34:YA:2391:G:O2'	34:YA:2422:A:N7	2.51	0.43
34:YA:2845:G:H2'	34:YA:2846:G:C8	2.53	0.43
43:YO:120:GLU:OE1	48:YT:67:SER:OG	2.32	0.43
47:YS:18:ILE:HG13	47:YS:88:ASP:HA	1.99	0.43
48:YT:20:PRO:HD2	48:YT:86:ILE:HG23	2.00	0.43
1:QA:1022:G:H2'	1:QA:1023:G:H8	1.84	0.43
4:QD:109:GLY:HA3	4:QD:165:MET:HG2	1.99	0.43
22:QV:50:C:H2'	22:QV:51:A:C8	2.52	0.43
30:R6:10:LEU:HD21	34:RA:2419:U:H4'	2.00	0.43
34:RA:520:G:H2'	34:RA:521:G:H8	1.83	0.43
34:RA:704:G:O2'	34:RA:726:G:N2	2.48	0.43
34:RA:2578:G:OP1	34:RA:2614:A:N6	2.51	0.43
35:RB:116:G:H4'	47:RS:54:LEU:HD22	2.00	0.43
1:XA:262:A:H5"	20:XT:76:ALA:HB2	2.01	0.43
1:XA:802:A:H3'	1:XA:803:G:H8	1.81	0.43
6:XF:97:PHE:HB2	18:XR:32:ARG:HE	1.84	0.43
24:Y0:49:LYS:HE2	47:YS:43:GLU:HG3	2.00	0.43
34:YA:37:C:H2'	34:YA:38:A:H8	1.83	0.43
34:YA:414:C:H2'	34:YA:415:A:H8	1.83	0.43
34:YA:996:A:H4'	49:YU:92:ARG:HE	1.79	0.43
34:YA:2791:C:H5	34:YA:2893:G:H3'	1.83	0.43
34:YA:2841:C:H2'	34:YA:2842:G:H8	1.81	0.43
40:YH:17:VAL:HG22	40:YH:26:VAL:HG12	2.01	0.43
40:YH:122:THR:HB	40:YH:134:SER:HB2	1.99	0.43
49:YU:83:LEU:HD12	49:YU:113:ALA:HB2	2.00	0.43
51:YW:1:MET:C	51:YW:64:MET:HE3	2.22	0.43
1:QA:45:U:H2'	1:QA:46:G:C8	2.53	0.43
1:QA:692:U:OP1	11:QK:124:LYS:NZ	2.42	0.43
1:QA:1298:C:H4'	1:QA:1299:A:C8	2.53	0.43
8:QH:9:MET:HG3	8:QH:26:VAL:HG11	1.99	0.43
34:RA:1203:G:O6	34:RA:1204:A:N6	2.52	0.43
34:RA:1435:G:N2	34:RA:1477:A:O2'	2.50	0.43
1:XA:946:A:H2'	1:XA:947:G:C8	2.53	0.43
13:XM:23:TYR:HD2	13:XM:67:GLU:HA	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:520:G:H2'	34:YA:521:G:H8	1.83	0.43
34:YA:907:U:O2'	45:YQ:101:ARG:NH2	2.48	0.43
34:YA:1173:G:N2	34:YA:1175:U:O4	2.44	0.43
34:YA:2630:G:H2'	34:YA:2631:G:C8	2.53	0.43
34:YA:2853:C:H2'	34:YA:2854:G:H8	1.83	0.43
41:YI:131:LYS:CB	41:YI:135:GLU:HA	2.43	0.43
45:YQ:34:LEU:HB2	45:YQ:118:LEU:HD22	2.00	0.43
1:QA:1172:C:H2'	1:QA:1173:G:H8	1.83	0.43
1:QA:1221:G:OP1	1:QA:1321:C:N4	2.51	0.43
34:RA:2749:A:H4'	40:RH:62:LYS:HB3	1.99	0.43
37:RE:176:ILE:HB	37:RE:181:LEU:HB2	1.99	0.43
3:XC:88:ARG:HE	3:XC:101:LEU:HB2	1.84	0.43
12:XL:104:VAL:HG13	12:XL:105:TYR:CD2	2.52	0.43
29:Y5:52:TYR:OH	34:YA:2883:A:OP1	2.34	0.43
34:YA:1139:G:O2'	34:YA:1143:A:N1	2.38	0.43
34:YA:1339:G:H5"	52:YX:16:LYS:HD3	2.00	0.43
34:YA:1853:A:N3	34:YA:2233:U:O2'	2.41	0.43
36:YD:108:PRO:HG2	36:YD:111:LEU:HB2	2.01	0.43
45:YQ:58:PHE:HD2	45:YQ:61:GLY:HA3	1.82	0.43
52:YX:53:LYS:NZ	52:YX:55:ASN:OD1	2.51	0.43
1:QA:636:U:H2'	1:QA:637:G:H8	1.82	0.43
1:QA:1492:A:OP2	12:QL:47:LYS:HE3	2.16	0.43
2:QB:19:HIS:ND1	2:QB:20:GLU:OE2	2.51	0.43
3:QC:8:ILE:HG23	3:QC:16:ARG:HG2	1.98	0.43
25:R1:80:LEU:HD12	25:R1:81:LYS:HG3	2.01	0.43
31:R7:20:ALA:HA	31:R7:23:ARG:HD3	2.01	0.43
34:RA:2845:G:H2'	34:RA:2846:G:C8	2.54	0.43
48:RT:107:ASP:O	48:RT:110:ILE:CG2	2.47	0.43
52:RX:55:ASN:HB2	52:RX:80:ILE:HG23	2.01	0.43
1:XA:296:U:O2'	1:XA:556:C:O2	2.34	0.43
11:XK:33:THR:HA	11:XK:39:PRO:HA	2.00	0.43
18:XR:50:ILE:HG13	18:XR:74:ARG:HH22	1.83	0.43
27:Y3:40:THR:HG22	27:Y3:42:ALA:H	1.84	0.43
39:YG:83:ARG:C	39:YG:85:GLY:N	2.70	0.43
44:YP:88:LEU:HD11	44:YP:114:ILE:HD12	2.00	0.43
48:YT:3:ARG:HG3	48:YT:7:ILE:HG12	2.00	0.43
1:QA:397:A:N7	1:QA:547:A:O2'	2.46	0.43
1:QA:1432:G:OP1	48:RT:108:ARG:N	2.48	0.43
13:QM:90:LEU:HD23	13:QM:93:ARG:HE	1.84	0.43
34:RA:749:C:H5'	34:RA:1271:G:H1'	2.00	0.43
34:RA:1155:A:H5"	49:RU:55:ARG:CZ	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:1769:G:O2'	34:RA:1958:C:OP1	2.30	0.43
40:RH:9:ILE:CG2	40:RH:50:VAL:H	2.26	0.43
50:RV:52:VAL:C	50:RV:54:GLY:H	2.22	0.43
52:RX:57:LEU:HG	52:RX:78:LYS:HB2	2.00	0.43
19:XS:10:PHE:HB2	19:XS:39:THR:HG22	2.01	0.43
34:YA:807:U:OP2	44:YP:41:ARG:NH2	2.51	0.43
34:YA:1779:U:OP2	34:YA:1784:A:N6	2.39	0.43
36:YD:142:VAL:HG23	36:YD:193:VAL:HA	2.01	0.43
1:QA:375:U:OP1	16:QP:69:THR:OG1	2.28	0.43
1:QA:1048:G:H1'	1:QA:1215:G:H5"	2.01	0.43
1:QA:1355:G:H2'	1:QA:1356:G:C8	2.54	0.43
1:QA:1414:U:H2'	1:QA:1415:G:C8	2.53	0.43
19:QS:10:PHE:HE2	19:QS:16:LEU:HB2	1.84	0.43
34:RA:78:A:H2'	34:RA:79:G:H8	1.83	0.43
34:RA:848:G:H2'	34:RA:849:A:C8	2.53	0.43
34:RA:1844:C:H2'	34:RA:1845:G:H8	1.84	0.43
34:RA:2103:C:N4	34:RA:2187:G:O6	2.52	0.43
54:RZ:97:GLU:HA	54:RZ:127:LYS:HA	2.00	0.43
54:RZ:102:LEU:HD11	54:RZ:124:ILE:HB	1.99	0.43
1:XA:563:A:H2'	1:XA:567:G:C8	2.53	0.43
1:XA:652:U:O4	1:XA:752:G:O2'	2.25	0.43
1:XA:1151:A:O2'	10:XJ:70:ARG:NH2	2.52	0.43
55:XY:34:G:H2'	55:XY:35:A:C8	2.54	0.43
34:YA:784:A:C5	36:YD:229:VAL:HG21	2.54	0.43
34:YA:1021:A:H61	34:YA:1142(A):A:H61	1.66	0.43
34:YA:1800:C:H42	34:YA:1817:G:H22	1.65	0.43
1:QA:427:U:O2'	1:QA:541:G:OP1	2.28	0.43
1:QA:1010:G:H2'	1:QA:1011:G:C8	2.53	0.43
1:QA:1469:G:H2'	1:QA:1470:G:H8	1.84	0.43
5:QE:78:HIS:HB3	8:QH:107:LEU:HD12	2.01	0.43
9:QI:20:ARG:O	9:QI:60:ASP:N	2.52	0.43
34:RA:2458:G:O2'	34:RA:2460:U:O4	2.33	0.43
1:XA:359:U:H2'	1:XA:360:A:H8	1.84	0.43
1:XA:1492:A:P	12:XL:47:LYS:HG2	2.58	0.43
2:XB:223:ILE:HA	2:XB:226:ARG:HB3	2.00	0.43
4:XD:20:TYR:CD1	4:XD:106:TYR:OH	2.70	0.43
34:YA:2241:A:H2'	34:YA:2242:G:C8	2.54	0.43
34:YA:2626:C:H2'	34:YA:2627:G:C8	2.54	0.43
34:YA:2689:U:OP2	34:YA:2872:G:N2	2.50	0.43
42:YN:47:ALA:HB2	42:YN:112:LEU:HD11	2.00	0.43
46:YR:51:LEU:HD22	46:YR:66:VAL:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:YZ:59:LEU:HA	54:YZ:59:LEU:HD13	1.72	0.43
1:QA:309:G:H2'	1:QA:310:G:H8	1.83	0.43
2:QB:115:LEU:HD13	2:QB:145:LEU:HB3	2.01	0.43
3:QC:4:LYS:HA	3:QC:4:LYS:HD3	1.65	0.43
7:QG:24:THR:HA	7:QG:27:ILE:HG22	2.00	0.43
9:QI:19:LEU:HD23	9:QI:59:PHE:HD2	1.84	0.43
9:QI:125:TYR:HE2	9:QI:127:LYS:HD3	1.83	0.43
25:R1:17:SER:HB2	25:R1:40:ARG:HD2	2.01	0.43
34:RA:442:G:H1'	38:RF:48:THR:HG21	2.01	0.43
34:RA:1771:C:H2'	34:RA:1772:G:C8	2.54	0.43
34:RA:1827:C:OP2	36:RD:222:ARG:NH1	2.51	0.43
34:RA:2487:G:H2'	34:RA:2488:A:H8	1.83	0.43
40:RH:99:VAL:HG23	40:RH:102:ALA:HB3	2.00	0.43
41:RI:131:LYS:CG	41:RI:135:GLU:OE1	2.66	0.43
46:RR:77:ARG:O	46:RR:81:ASP:HB2	2.19	0.43
48:RT:120:ARG:HA	48:RT:123:GLN:OE1	2.18	0.43
6:XF:10:LEU:HD13	6:XF:61:LEU:HD13	2.00	0.43
7:XG:136:LYS:HA	7:XG:139:GLU:HG2	2.01	0.43
34:YA:557:U:H2'	34:YA:558:G:H8	1.83	0.43
34:YA:870:A:OP1	45:YQ:6:ARG:NH2	2.50	0.43
34:YA:1057:A:N6	34:YA:1087:G:OP2	2.52	0.43
49:YU:93:LYS:HB2	49:YU:93:LYS:HE2	1.36	0.43
3:QC:191:THR:OG1	3:QC:194:GLY:O	2.35	0.43
5:QE:143:ARG:NE	8:QH:77:GLU:OE2	2.51	0.43
7:QG:71:PRO:O	7:QG:96:GLN:NE2	2.52	0.43
9:QI:42:ARG:NH2	9:QI:71:SER:O	2.52	0.43
31:R7:42:LEU:HD12	34:RA:126:A:H61	1.83	0.43
34:RA:993:G:OP1	49:RU:50:ARG:NH2	2.46	0.43
34:RA:1416:G:H2'	34:RA:1417:C:C6	2.54	0.43
39:RG:82:LEU:HD23	39:RG:86:MET:HB3	2.00	0.43
45:RQ:43:THR:HG22	45:RQ:94:VAL:HG12	2.01	0.43
1:XA:269:C:H2'	1:XA:270:A:C8	2.53	0.43
1:XA:452:A:N7	1:XA:480:U:O4	2.52	0.43
1:XA:790:A:OP1	22:XV:38:A:O2'	2.28	0.43
1:XA:946:A:H2'	1:XA:947:G:H8	1.83	0.43
1:XA:1469:G:H2'	1:XA:1470:G:C8	2.54	0.43
5:XE:78:HIS:HE1	5:XE:80:ILE:HD13	1.84	0.43
26:Y2:28:LYS:HD2	26:Y2:53:LEU:HD11	2.00	0.43
34:YA:775:G:H4'	34:YA:776:G:H5'	1.99	0.43
34:YA:1028:A:H2'	34:YA:1029:A:C8	2.54	0.43
34:YA:2531:A:H61	34:YA:2662:A:H61	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:2692:C:H2'	34:YA:2693:A:C8	2.54	0.43
45:YQ:27:VAL:HG13	45:YQ:105:GLU:CG	2.49	0.43
26:R2:17:SER:HB3	26:R2:20:GLU:HG2	2.00	0.42
34:RA:2304:G:N2	34:RA:2312:U:H3	2.17	0.42
50:RV:75:PHE:HA	50:RV:81:TYR:HD2	1.83	0.42
1:XA:427:U:O2'	1:XA:541:G:OP1	2.28	0.42
1:XA:1316:G:N2	1:XA:1319:A:OP2	2.43	0.42
23:XX:-12:C:H2'	23:XX:-11:A:C8	2.52	0.42
34:YA:468:G:H5"	38:YF:60:SER:HB2	2.00	0.42
34:YA:521:G:H2'	34:YA:522:G:H8	1.84	0.42
34:YA:1434:A:H61	34:YA:1558:A:N6	2.17	0.42
34:YA:1507:A:O2'	34:YA:1509:C:O2	2.34	0.42
34:YA:2315:G:H21	39:YG:128:ARG:HH22	1.67	0.42
40:YH:46:GLU:HB2	40:YH:49:VAL:HB	2.01	0.42
49:YU:96:ALA:O	49:YU:99:ALA:CB	2.66	0.42
1:QA:912:C:H2'	1:QA:913:A:C8	2.53	0.42
1:QA:1064:G:H1'	1:QA:1066:C:C6	2.54	0.42
1:QA:1238:A:OP1	1:QA:1335:C:O2'	2.27	0.42
10:QJ:30:SER:O	10:QJ:78:ASN:ND2	2.51	0.42
34:RA:121:G:H4'	34:RA:149:A:H5'	2.01	0.42
34:RA:191:A:H2'	34:RA:192:C:H6	1.84	0.42
39:RG:73:ALA:HB2	39:RG:82:LEU:CD2	2.49	0.42
47:RS:85:VAL:HG23	47:RS:112:PHE:HE1	1.84	0.42
1:XA:736:C:H2'	1:XA:737:A:H8	1.84	0.42
1:XA:891:U:H2'	1:XA:892:A:H8	1.85	0.42
1:XA:1233:G:O2'	1:XA:1365:G:OP1	2.30	0.42
22:XV:50:C:H2'	22:XV:51:A:H8	1.85	0.42
34:YA:39:C:O2	38:YF:46:ARG:NH2	2.48	0.42
34:YA:2233:U:H2'	34:YA:2234:G:C8	2.54	0.42
34:YA:2591:C:H2'	34:YA:2592:G:C8	2.54	0.42
36:YD:164:GLN:OE1	36:YD:176:ARG:NH2	2.47	0.42
47:YS:66:ALA:HA	47:YS:69:VAL:HG12	2.00	0.42
54:YZ:53:ILE:C	54:YZ:55:HIS:N	2.72	0.42
1:QA:269:C:H2'	1:QA:270:A:C8	2.54	0.42
1:QA:908:A:H2'	1:QA:909:A:H8	1.83	0.42
1:QA:1221:G:H4'	19:QS:77:THR:HG21	2.01	0.42
4:QD:96:LEU:HD22	4:QD:139:ARG:HE	1.84	0.42
5:QE:11:ILE:HG23	5:QE:12:LEU:HD23	2.00	0.42
24:R0:51:VAL:O	47:RS:20:ARG:NH2	2.49	0.42
43:RO:76:ALA:HB3	48:RT:75:ILE:HD12	2.01	0.42
48:RT:66:VAL:HA	48:RT:71:GLY:HA2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:RZ:70:LEU:HB2	54:RZ:91:LEU:HD21	2.01	0.42
1:XA:936:C:O2	1:XA:1382:C:N4	2.49	0.42
1:XA:1503:A:C6	1:XA:1531:A:H2	2.37	0.42
7:XG:30:ILE:HG23	7:XG:39:ALA:HB1	2.02	0.42
7:XG:140:ASP:O	7:XG:143:ARG:HG2	2.19	0.42
34:YA:142:G:H2'	34:YA:143:C:H6	1.85	0.42
34:YA:197:A:H2	34:YA:2434:A:H62	1.68	0.42
34:YA:210:C:H2'	34:YA:211:A:C8	2.54	0.42
34:YA:579:G:O2'	34:YA:2019:A:OP1	2.34	0.42
34:YA:675:A:N3	34:YA:2443:C:O2'	2.47	0.42
34:YA:863:A:H2'	34:YA:864:G:C8	2.54	0.42
34:YA:2030:A:H4'	34:YA:2031:A:C8	2.53	0.42
34:YA:2618:G:H21	37:YE:150:VAL:HG21	1.84	0.42
48:YT:92:GLY:O	48:YT:120:ARG:NH2	2.52	0.42
1:QA:300:A:O2'	1:QA:564:C:N3	2.41	0.42
34:RA:529:A:H8	34:RA:530:G:C6	2.38	0.42
34:RA:1005:C:H2'	34:RA:1006:C:C6	2.55	0.42
34:RA:2693:A:H2'	34:RA:2694:G:H8	1.84	0.42
36:RD:199:ALA:C	36:RD:201:HIS:N	2.73	0.42
38:RF:118:ALA:HB2	38:RF:123:LEU:HD23	2.01	0.42
51:RW:111:HIS:HD2	51:RW:113:LYS:H	1.67	0.42
54:RZ:13:GLU:HB3	54:RZ:18:LEU:HD11	2.01	0.42
1:XA:1211:U:H5'	1:XA:1212:U:H5'	2.01	0.42
1:XA:1492:A:OP1	12:XL:47:LYS:HG3	2.19	0.42
2:XB:88:ALA:HB2	2:XB:219:VAL:HG13	2.00	0.42
3:XC:179:ARG:HB2	3:XC:206:GLU:HG3	2.02	0.42
20:XT:43:LEU:HD23	20:XT:51:GLU:HG3	2.01	0.42
34:YA:142:G:H2'	34:YA:143:C:C6	2.55	0.42
34:YA:2181:G:H2'	34:YA:2182:G:C8	2.54	0.42
38:YF:12:LEU:HB3	38:YF:126:VAL:HA	2.02	0.42
40:YH:54:ARG:HD2	40:YH:65:HIS:CG	2.54	0.42
54:YZ:166:SER:HB3	54:YZ:168:GLU:N	2.32	0.42
1:QA:390:C:H2'	1:QA:391:G:H8	1.85	0.42
1:QA:1022:G:H2'	1:QA:1023:G:C8	2.55	0.42
1:QA:1287:A:H2	1:QA:1353:G:H1'	1.84	0.42
12:QL:84:LEU:HB2	12:QL:104:VAL:HG21	2.01	0.42
34:RA:1689:A:OP2	34:RA:1698:A:N6	2.50	0.42
34:RA:2836:U:H2'	34:RA:2837:G:C8	2.55	0.42
38:RF:198:ALA:HA	38:RF:201:VAL:HG12	2.01	0.42
1:XA:490:G:OP2	4:XD:132:ARG:NH2	2.52	0.42
1:XA:736:C:O2'	6:XF:90:VAL:O	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:812:C:H4'	1:XA:813:U:H5'	2.00	0.42
4:XD:116:GLN:HE21	4:XD:157:LEU:HD21	1.83	0.42
6:XF:35:ALA:HB1	6:XF:65:VAL:HG11	2.01	0.42
7:XG:76:ARG:O	7:XG:87:VAL:N	2.45	0.42
34:YA:729:G:C5	36:YD:208:LYS:HB2	2.54	0.42
34:YA:848:G:H2'	34:YA:849:A:C8	2.54	0.42
34:YA:948:G:H1	34:YA:969:U:H3	1.67	0.42
34:YA:2313:C:H5"	39:YG:91:ARG:HD3	2.01	0.42
6:QF:94:GLN:OE1	18:QR:32:ARG:NH1	2.50	0.42
8:QH:12:ARG:HD2	8:QH:26:VAL:HG12	2.02	0.42
13:QM:57:ARG:NH2	28:R4:34:GLU:O	2.53	0.42
18:QR:86:VAL:HG12	18:QR:87:ARG:HG2	2.01	0.42
34:RA:840:C:H2'	34:RA:841:A:H8	1.82	0.42
34:RA:2036:C:H2'	34:RA:2037:G:H8	1.84	0.42
40:RH:18:GLU:HB2	40:RH:25:LYS:HB2	2.02	0.42
46:RR:104:ARG:HE	46:RR:111:LEU:HD21	1.85	0.42
50:RV:59:ALA:HB1	50:RV:94:LEU:HB3	2.02	0.42
1:XA:681:C:H2'	1:XA:682:G:H8	1.85	0.42
1:XA:782:A:H62	1:XA:800:G:H21	1.67	0.42
1:XA:851:G:H2'	1:XA:852:G:H8	1.85	0.42
1:XA:969:A:OP1	10:XJ:55:LYS:NZ	2.51	0.42
1:XA:1054:C:OP2	1:XA:1054:C:H4'	2.20	0.42
1:XA:1054:C:C5	55:XY:34:G:H1'	2.55	0.42
1:XA:1118:C:H1'	1:XA:1179:A:C5	2.55	0.42
1:XA:1157:A:N6	1:XA:1178:G:N3	2.68	0.42
1:XA:1427:U:H2'	1:XA:1428:A:C8	2.55	0.42
4:XD:20:TYR:HE1	4:XD:106:TYR:HH	1.56	0.42
32:Y8:58:ILE:HA	32:Y8:61:LEU:HD12	2.02	0.42
34:YA:36:G:N3	34:YA:450:G:O2'	2.50	0.42
34:YA:1062:G:C8	34:YA:1088:A:H2'	2.55	0.42
34:YA:1636:C:H2'	34:YA:1637:A:C8	2.55	0.42
34:YA:2546:U:H5"	34:YA:2547:U:H5'	2.01	0.42
34:YA:2707:G:H2'	34:YA:2708:G:C8	2.55	0.42
1:QA:599:C:O2'	8:QH:129:VAL:O	2.31	0.42
28:R4:28:LYS:HA	28:R4:29:PRO:HD3	1.92	0.42
32:R8:26:LYS:HG2	32:R8:47:LYS:HD2	2.01	0.42
34:RA:946:G:O6	34:RA:972:G:N2	2.53	0.42
35:RB:8:U:P	47:RS:15:ARG:HH22	2.43	0.42
40:RH:106:THR:HG22	40:RH:112:PRO:HB3	2.01	0.42
45:RQ:20:ALA:HB3	54:RZ:79:ARG:HE	1.85	0.42
50:RV:14:VAL:HB	50:RV:96:ILE:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:RZ:48:PHE:CZ	54:RZ:53:ILE:HG23	2.55	0.42
1:XA:554:C:H2'	1:XA:555:C:H6	1.84	0.42
20:XT:33:ILE:HD12	20:XT:63:ILE:HG13	2.01	0.42
34:YA:439:G:H2'	34:YA:440:G:C8	2.55	0.42
34:YA:1309:G:O2'	34:YA:1611:C:O2'	2.32	0.42
34:YA:1626:G:H5"	34:YA:1627:G:H5'	2.02	0.42
34:YA:2311:A:H1'	39:YG:82:LEU:CD1	2.48	0.42
34:YA:2455:G:H2'	34:YA:2456:C:C6	2.54	0.42
40:YH:26:VAL:HG21	40:YH:75:ALA:HB1	2.01	0.42
48:YT:122:ASP:HA	48:YT:125:ARG:HD2	2.00	0.42
49:YU:28:ARG:NH1	49:YU:38:THR:OG1	2.47	0.42
1:QA:224:C:H2'	1:QA:225:C:H6	1.85	0.42
26:R2:53:LEU:HA	26:R2:56:GLN:HG2	2.02	0.42
34:RA:627:A:H4'	34:RA:628:G:H5'	2.02	0.42
45:RQ:11:LYS:HZ1	45:RQ:87:LYS:HD3	1.85	0.42
1:XA:45:U:H2'	1:XA:46:G:C8	2.55	0.42
1:XA:628:G:H2'	1:XA:629:G:C8	2.54	0.42
3:XC:8:ILE:HG23	3:XC:16:ARG:HE	1.85	0.42
8:XH:14:ARG:NH2	8:XH:83:ILE:O	2.43	0.42
34:YA:380:U:H2'	34:YA:381:G:H8	1.84	0.42
34:YA:573:G:N1	34:YA:2031:A:OP2	2.38	0.42
34:YA:1980:G:O2'	34:YA:1982:C:OP2	2.35	0.42
34:YA:2441:C:OP2	34:YA:2586:C:O2'	2.37	0.42
41:YI:110:ASP:N	41:YI:130:TYR:OH	2.42	0.42
1:QA:165:C:H2'	1:QA:166:G:C8	2.55	0.42
1:QA:769:G:H4'	1:QA:1513:A:H4'	2.02	0.42
1:QA:1368:G:H5"	9:QI:112:LYS:HB3	2.02	0.42
2:QB:97:TRP:HZ2	2:QB:102:LEU:HD13	1.84	0.42
3:QC:181:ASN:ND2	3:QC:205:GLY:O	2.53	0.42
12:QL:32:PHE:HB3	12:QL:84:LEU:HD11	2.02	0.42
20:QT:71:THR:HG22	20:QT:72:LEU:HD12	2.01	0.42
34:RA:698:C:O2'	34:RA:734:A:N6	2.43	0.42
34:RA:1423:G:H2'	34:RA:1424:G:H8	1.85	0.42
38:RF:186:ILE:HD12	38:RF:192:LEU:HD11	2.01	0.42
42:RN:115:ARG:O	42:RN:115:ARG:HG3	2.20	0.42
47:RS:4:LEU:N	47:RS:4:LEU:CD1	2.82	0.42
49:RU:95:LEU:HD22	49:RU:95:LEU:H	1.82	0.42
1:XA:1252:A:H61	1:XA:1285:A:H61	1.66	0.42
2:XB:168:THR:HA	2:XB:171:ALA:HB2	2.02	0.42
3:XC:119:ARG:HG2	3:XC:140:ARG:HH12	1.85	0.42
4:XD:15:GLU:OE2	4:XD:59:ARG:NH1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:210:C:H2'	34:YA:211:A:H8	1.85	0.42
34:YA:1113:U:H2'	34:YA:1114:G:H8	1.85	0.42
34:YA:2696:U:H2'	34:YA:2697:G:C8	2.55	0.42
39:YG:62:LEU:HG	39:YG:143:GLU:HB3	2.00	0.42
48:YT:120:ARG:HA	48:YT:123:GLN:CD	2.39	0.42
53:YY:14:LEU:HD22	53:YY:82:PRO:HG3	2.01	0.42
1:QA:324:G:OP1	20:QT:70:SER:OG	2.38	0.42
13:QM:67:GLU:HB3	13:QM:68:GLY:H	1.62	0.42
34:RA:2690:C:OP1	46:RR:17:ARG:NH2	2.53	0.42
36:RD:153:ALA:O	36:RD:157:ARG:NH1	2.53	0.42
39:RG:73:ALA:CB	39:RG:82:LEU:CD1	2.97	0.42
39:RG:79:ASN:HB2	39:RG:80:PHE:CD1	2.55	0.42
44:RP:89:ALA:O	44:RP:121:LYS:NZ	2.46	0.42
1:XA:603:U:H2'	1:XA:604:G:C8	2.55	0.42
34:YA:2787:C:H1'	37:YE:62:PRO:HG3	2.00	0.42
44:YP:8:PRO:HB2	44:YP:12:ALA:HB3	2.02	0.42
1:QA:137:C:H2'	1:QA:138:G:H8	1.85	0.41
1:QA:1060:C:H2'	1:QA:1061:G:C8	2.54	0.41
3:QC:70:VAL:HG12	3:QC:72:LYS:H	1.85	0.41
11:QK:86:GLY:O	11:QK:91:ARG:NH1	2.53	0.41
14:QN:48:ALA:HB2	14:QN:53:LEU:HD12	2.02	0.41
34:RA:532:A:H4'	34:RA:533:G:C8	2.55	0.41
34:RA:1105:U:H2'	34:RA:1106:G:C8	2.55	0.41
34:RA:2074:U:H2'	34:RA:2075:U:C6	2.55	0.41
35:RB:43:C:O2	39:RG:93:THR:OG1	2.34	0.41
40:RH:83:TYR:O	40:RH:83:TYR:CD2	2.70	0.41
41:RI:9:LEU:HB2	41:RI:12:LEU:HB2	2.02	0.41
42:RN:6:PRO:HG3	42:RN:41:ASP:HB2	2.01	0.41
47:RS:28:VAL:HG11	47:RS:98:VAL:HG12	2.02	0.41
54:RZ:5:LEU:HB2	54:RZ:59:LEU:HD23	2.02	0.41
1:XA:337:C:H2'	1:XA:338:A:H8	1.85	0.41
1:XA:1128:C:H5'	9:XI:16:ARG:HH22	1.85	0.41
34:YA:459:U:H2'	34:YA:460:A:H8	1.85	0.41
34:YA:550:G:H2'	34:YA:551:G:H8	1.85	0.41
34:YA:1159:U:H2'	34:YA:1160:G:H8	1.85	0.41
34:YA:1296:G:OP1	34:YA:2709:G:O2'	2.27	0.41
34:YA:2502:G:H5"	34:YA:2503:A:H5"	2.01	0.41
43:YO:68:GLU:HG3	43:YO:78:ARG:HD3	2.01	0.41
47:YS:15:ARG:NE	47:YS:88:ASP:OD1	2.53	0.41
49:YU:92:ARG:NH1	49:YU:92:ARG:CG	2.79	0.41
1:QA:45:U:H2'	1:QA:46:G:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:359:U:H2'	1:QA:360:A:H8	1.85	0.41
1:QA:1066:C:N4	1:QA:1191:A:C6	2.82	0.41
1:QA:1351:U:H3	1:QA:1371:G:H1	1.67	0.41
9:QI:10:ARG:HG3	9:QI:75:ASP:HB3	2.01	0.41
34:RA:270(V):G:H2'	34:RA:270(W):G:H8	1.86	0.41
34:RA:557:U:H2'	34:RA:558:G:C8	2.54	0.41
34:RA:582:G:H2'	34:RA:583:G:H8	1.84	0.41
34:RA:811:U:H2'	44:RP:21:ARG:HA	2.03	0.41
34:RA:2567:G:H2'	34:RA:2568:C:C6	2.55	0.41
36:RD:260:ARG:HH22	36:RD:270:ILE:HD12	1.84	0.41
40:RH:88:LEU:HD22	40:RH:165:ALA:HB2	2.02	0.41
54:RZ:203:GLU:H	54:RZ:203:GLU:HG2	1.68	0.41
17:XQ:18:THR:OG1	17:XQ:69:LYS:NZ	2.45	0.41
18:XR:58:LEU:HD23	18:XR:62:GLU:HB3	2.02	0.41
34:YA:184:C:O2'	34:YA:217:G:N3	2.43	0.41
34:YA:331:A:H62	34:YA:1210:A:H8	1.66	0.41
34:YA:685:A:OP1	34:YA:686:G:N2	2.50	0.41
34:YA:910:A:H2'	34:YA:911:A:C8	2.55	0.41
34:YA:2086:U:H2'	34:YA:2087:G:C8	2.55	0.41
41:YI:12:LEU:HB3	41:YI:13:GLY:H	1.57	0.41
46:YR:38:VAL:HG22	46:YR:112:ALA:HB2	2.01	0.41
49:YU:96:ALA:O	49:YU:99:ALA:N	2.39	0.41
53:YY:14:LEU:HB2	53:YY:75:ILE:HD11	2.02	0.41
2:QB:236:TYR:HB2	2:QB:237:ALA:H	1.57	0.41
22:QV:12:U:OP1	34:RA:1908:C:O2'	2.38	0.41
34:RA:2086:U:H2'	34:RA:2087:G:C8	2.55	0.41
34:RA:2692:C:H2'	34:RA:2693:A:H8	1.85	0.41
39:RG:37:VAL:O	39:RG:94:LEU:N	2.47	0.41
39:RG:138:GLN:HG2	39:RG:144:ILE:HG21	2.01	0.41
42:RN:16:ILE:HG21	42:RN:26:LEU:HD11	2.01	0.41
2:XB:51:LEU:HA	2:XB:54:THR:HG22	2.01	0.41
34:YA:1299:G:H22	34:YA:1640:C:H5'	1.85	0.41
34:YA:2392:A:H8	44:YP:61:ARG:HG2	1.85	0.41
34:YA:2641:G:H2'	34:YA:2642:G:H8	1.85	0.41
47:YS:34:HIS:O	47:YS:97:ARG:NH2	2.54	0.41
54:YZ:59:LEU:HB3	54:YZ:61:LEU:HD12	2.03	0.41
2:QB:16:HIS:HA	2:QB:210:SER:HB2	2.02	0.41
2:QB:32:ILE:HD11	2:QB:190:THR:HG22	2.01	0.41
11:QK:38:ASN:HA	11:QK:39:PRO:HD3	1.90	0.41
22:QV:60:U:H5"	22:QV:61:C:C5	2.56	0.41
34:RA:1826:G:H4'	36:RD:242:ARG:HH21	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:2233:U:H2'	34:RA:2234:G:C8	2.56	0.41
39:RG:73:ALA:CB	39:RG:82:LEU:HD11	2.50	0.41
40:RH:31:GLY:HA3	40:RH:136:ILE:HD13	2.02	0.41
45:RQ:4:PRO:HG3	45:RQ:69:PHE:HE2	1.86	0.41
1:XA:112:G:H4'	1:XA:389:A:H4'	2.02	0.41
4:XD:19:LEU:HD21	4:XD:197:PRO:HG2	1.93	0.41
4:XD:19:LEU:CD1	4:XD:63:LYS:CG	2.94	0.41
4:XD:119:GLN:HG2	4:XD:123:HIS:CD2	2.56	0.41
15:XO:88:ARG:NH1	34:YA:713:G:OP2	2.41	0.41
32:Y8:34:TRP:CE2	32:Y8:35:GLN:HG3	2.55	0.41
34:YA:642:G:H21	34:YA:646:A:H2	1.67	0.41
34:YA:949:C:H2'	34:YA:950:G:C8	2.55	0.41
34:YA:1408:C:H2'	34:YA:1409:C:C6	2.55	0.41
34:YA:1423:G:H2'	34:YA:1424:G:H8	1.84	0.41
36:YD:182:LEU:HB2	36:YD:271:ILE:HB	2.01	0.41
1:QA:130:A:H5'	17:QQ:63:ARG:HH11	1.85	0.41
1:QA:636:U:H5'	17:QQ:2:PRO:HG3	2.02	0.41
1:QA:991:U:O4	1:QA:1212:U:O2'	2.28	0.41
1:QA:1123:A:H4'	10:QJ:36:GLY:HA3	2.03	0.41
1:QA:1427:U:H2'	1:QA:1428:A:C8	2.56	0.41
3:QC:24:ALA:HB2	3:QC:32:LEU:HD22	2.01	0.41
34:RA:1980:G:O2'	34:RA:1982:C:OP2	2.36	0.41
41:RI:72:LEU:HG	41:RI:138:ILE:HD13	2.02	0.41
44:RP:29:LYS:HD2	44:RP:30:THR:HG23	2.01	0.41
45:RQ:13:GLN:O	45:RQ:72:LYS:NZ	2.42	0.41
1:XA:323:U:OP1	20:XT:26:ASN:ND2	2.45	0.41
1:XA:337:C:H2'	1:XA:338:A:C8	2.56	0.41
1:XA:1071:C:H5"	5:XE:49:PRO:HG2	2.02	0.41
26:Y2:41:ILE:HD11	26:Y2:44:LEU:HD12	2.01	0.41
34:YA:1800:C:O2	34:YA:1817:G:O6	2.38	0.41
34:YA:2853:C:H2'	34:YA:2854:G:C8	2.55	0.41
37:YE:52:LEU:HB3	37:YE:76:ARG:HD3	2.02	0.41
1:QA:628:G:H2'	1:QA:629:G:C8	2.55	0.41
1:QA:636:U:H2'	1:QA:637:G:C8	2.55	0.41
12:QL:24:VAL:HG13	12:QL:98:TYR:HE1	1.85	0.41
20:QT:26:ASN:HA	20:QT:29:LYS:HG2	2.01	0.41
34:RA:380:U:H2'	34:RA:381:G:H8	1.86	0.41
34:RA:828:U:H4'	34:RA:831:G:N1	2.36	0.41
34:RA:1525:G:H2'	34:RA:1526:G:C8	2.56	0.41
34:RA:2445:G:P	38:RF:74:ARG:HH22	2.43	0.41
34:RA:2639:A:O2'	42:RN:97:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:RE:63:LEU:O	37:RE:73:GLU:CD	2.59	0.41
50:RV:52:VAL:HG23	50:RV:54:GLY:H	1.84	0.41
54:RZ:128:VAL:HG11	54:RZ:133:ILE:HA	2.02	0.41
1:XA:624:C:H2'	1:XA:625:G:H8	1.85	0.41
1:XA:1297:C:H42	7:XG:115:ARG:HH21	1.68	0.41
1:XA:1347:G:H22	1:XA:1373:G:H3'	1.85	0.41
1:XA:1409:C:H2'	1:XA:1410:G:H8	1.86	0.41
1:XA:1412:C:H2'	1:XA:1413:A:C8	2.55	0.41
11:XK:31:THR:HA	11:XK:42:TRP:HA	2.01	0.41
25:Y1:60:PHE:HB3	25:Y1:62:VAL:HG13	2.02	0.41
34:YA:941:A:O2'	34:YA:1190:G:O3'	2.36	0.41
34:YA:1205:U:C4	38:YF:171:PRO:HA	2.56	0.41
34:YA:2312:U:O2	39:YG:40:ASN:ND2	2.53	0.41
34:YA:2836:U:H2'	34:YA:2837:G:C8	2.55	0.41
1:QA:522:C:H41	12:QL:53:ARG:NH2	2.18	0.41
34:RA:270:A:OP2	34:RA:270(Y):G:N1	2.53	0.41
34:RA:504:U:H5"	34:RA:505:A:H5'	2.01	0.41
36:RD:199:ALA:C	36:RD:201:HIS:H	2.24	0.41
39:RG:73:ALA:HB2	39:RG:82:LEU:HD11	2.03	0.41
40:RH:153:LYS:HD3	40:RH:162:ILE:HG13	2.02	0.41
1:XA:736:C:H2'	1:XA:737:A:C8	2.55	0.41
1:XA:985:C:H2'	1:XA:986:A:C8	2.56	0.41
1:XA:1392:G:N2	1:XA:1502:A:H8	2.19	0.41
1:XA:1513:A:H2'	1:XA:1514:C:C6	2.55	0.41
12:XL:45:PRO:HG3	12:XL:53:ARG:HD3	2.02	0.41
29:Y5:19:ARG:HH21	34:YA:1265:A:H3'	1.86	0.41
42:YN:47:ALA:O	42:YN:119:ARG:NH1	2.51	0.41
43:YO:1:MET:HB2	43:YO:32:TYR:HB3	2.01	0.41
45:YQ:62:GLY:HA2	54:YZ:116:VAL:HG21	2.02	0.41
1:QA:627:G:H2'	1:QA:628:G:H8	1.85	0.41
1:QA:950:U:H2'	1:QA:951:G:C8	2.56	0.41
34:RA:1063:G:OP1	34:RA:1065:U:O2'	2.34	0.41
34:RA:2683:C:H5'	48:RT:58:ASN:HD22	1.84	0.41
34:RA:2853:C:H2'	34:RA:2854:G:C8	2.56	0.41
36:RD:108:PRO:HB3	36:RD:143:HIS:CE1	2.56	0.41
39:RG:22:ARG:HH12	39:RG:175:LEU:HD11	1.85	0.41
39:RG:135:LEU:HB2	39:RG:155:MET:HB3	2.01	0.41
1:XA:409:G:H5"	4:XD:25:ARG:HG3	2.02	0.41
4:XD:61:LYS:HE3	4:XD:61:LYS:HB3	1.91	0.41
5:XE:72:GLN:HE22	5:XE:144:THR:HG22	1.86	0.41
13:XM:66:LEU:HB3	13:XM:67:GLU:H	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:XR:37:VAL:O	18:XR:41:LYS:N	2.53	0.41
22:XV:65:C:H2'	22:XV:66:A:C8	2.55	0.41
33:Y9:25:VAL:HB	33:Y9:34:GLN:HB2	2.02	0.41
34:YA:545:G:N2	34:YA:548:A:OP2	2.45	0.41
34:YA:1508:A:O2'	34:YA:1509:C:O4'	2.38	0.41
34:YA:1535:U:H5'	34:YA:1537:C:N3	2.36	0.41
50:YV:6:LYS:HB2	50:YV:39:LEU:HD21	2.03	0.41
1:QA:134:A:H61	16:QP:25:ARG:NH1	2.18	0.41
1:QA:348:G:H2'	1:QA:349:A:H8	1.85	0.41
1:QA:514:C:H2'	1:QA:515:G:C8	2.54	0.41
1:QA:539:A:H2'	1:QA:540:G:C8	2.56	0.41
1:QA:639:G:H2'	1:QA:640:A:H8	1.86	0.41
5:QE:78:HIS:HE1	5:QE:80:ILE:HD13	1.85	0.41
6:QF:95:GLU:HA	6:QF:96:PRO:HD3	1.95	0.41
7:QG:27:ILE:HD12	7:QG:27:ILE:HA	1.89	0.41
24:R0:38:VAL:HB	24:R0:59:LEU:HD12	2.02	0.41
32:R8:46:ARG:NH1	34:RA:630:G:OP1	2.53	0.41
34:RA:689:A:H2'	34:RA:690:G:C8	2.56	0.41
34:RA:1258:C:H2'	34:RA:1259:G:C8	2.56	0.41
34:RA:1791:A:H5'	36:RD:206:LEU:HD12	2.02	0.41
34:RA:2081:C:H2'	34:RA:2082:A:H8	1.85	0.41
34:RA:2441:C:OP2	34:RA:2586:C:O2'	2.30	0.41
34:RA:2696:U:H2'	34:RA:2697:G:H8	1.84	0.41
37:RE:29:GLY:HA2	37:RE:180:ASN:HB3	2.02	0.41
42:RN:21:LYS:HE2	42:RN:21:LYS:HB2	1.82	0.41
1:XA:590:C:OP1	8:XH:30:ARG:N	2.50	0.41
1:XA:1119:C:H2'	1:XA:1120:G:C8	2.54	0.41
1:XA:1287:A:H2'	1:XA:1288:A:C8	2.56	0.41
1:XA:1288:A:H2'	1:XA:1289:A:C8	2.56	0.41
1:XA:1308:U:H2'	1:XA:1309:G:H8	1.85	0.41
1:XA:1507:A:H2'	1:XA:1508:G:C8	2.56	0.41
3:XC:9:GLY:HA3	14:XN:49:HIS:HA	2.03	0.41
4:XD:104:VAL:HG21	4:XD:140:VAL:HG21	2.02	0.41
5:XE:48:ALA:HB2	5:XE:57:LYS:HE3	2.03	0.41
10:XJ:51:ARG:CZ	10:XJ:61:GLU:HB3	2.51	0.41
27:Y3:26:LEU:O	27:Y3:35:ARG:HG2	2.21	0.41
34:YA:271(D):G:H2'	34:YA:272:G:C8	2.56	0.41
34:YA:288:C:H2'	34:YA:289:A:C8	2.55	0.41
34:YA:813:U:H2'	34:YA:814:C:C6	2.56	0.41
34:YA:996:A:O2'	49:YU:92:ARG:NE	2.54	0.41
34:YA:1441:G:H2'	34:YA:1442:G:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:1800:C:N3	34:YA:1817:G:N1	2.68	0.41
34:YA:1812:A:H2'	34:YA:1813:G:H8	1.86	0.41
34:YA:1817:G:OP2	36:YD:157:ARG:NH2	2.54	0.41
34:YA:1918:A:O2'	34:YA:1920:C:N4	2.54	0.41
34:YA:2051:A:H4'	37:YE:141:ILE:HG12	2.03	0.41
34:YA:2096:U:O4	34:YA:2193:G:O6	2.39	0.41
34:YA:2708:G:H2'	34:YA:2709:G:H8	1.86	0.41
40:YH:164:TYR:HB2	40:YH:167:GLU:HB2	2.02	0.41
41:YI:13:GLY:HA2	41:YI:17:GLN:HG3	2.02	0.41
43:YO:8:LEU:HB2	43:YO:19:ILE:HG13	2.03	0.41
45:YQ:13:GLN:O	45:YQ:72:LYS:NZ	2.43	0.41
51:YW:22:ASP:OD1	51:YW:25:ARG:NH1	2.49	0.41
1:QA:34:C:H2'	1:QA:35:G:C8	2.55	0.41
1:QA:186(A):C:O2	20:QT:105:SER:OG	2.32	0.41
1:QA:662:G:H2'	1:QA:663:A:C8	2.55	0.41
1:QA:1228:C:H4'	13:QM:116:THR:HA	2.03	0.41
3:QC:150:LYS:HE3	3:QC:167:TRP:HE1	1.85	0.41
12:QL:60:LEU:HD12	12:QL:62:SER:H	1.86	0.41
24:R0:23:VAL:HG21	34:RA:857:C:H4'	2.03	0.41
34:RA:1662:C:O2'	34:RA:2687:U:OP1	2.37	0.41
34:RA:2314:C:H2'	34:RA:2315:G:C8	2.55	0.41
34:RA:2329:G:H2'	34:RA:2330:G:H8	1.86	0.41
34:RA:2406:U:C2	44:RP:72:PRO:HB2	2.56	0.41
34:RA:2710:C:H2'	34:RA:2711:A:C8	2.56	0.41
35:RB:42:C:H5"	39:RG:69:ALA:HB2	2.02	0.41
41:RI:46:ALA:O	41:RI:50:ARG:HG2	2.21	0.41
47:RS:10:ARG:HG2	47:RS:13:ARG:HH22	1.86	0.41
49:RU:90:VAL:HG11	50:RV:40:LEU:HG	2.02	0.41
1:XA:76:G:H1	1:XA:93:U:H3	1.68	0.41
6:XF:99:ALA:HB1	18:XR:23:LYS:HE3	2.03	0.41
7:XG:13:GLN:HA	7:XG:14:PRO:HD3	1.95	0.41
15:XO:17:ARG:HH12	15:XO:77:ARG:NH1	2.19	0.41
24:Y0:35:ASN:HD22	34:YA:2354:G:H4'	1.87	0.41
25:Y1:28:GLY:HA2	34:YA:2397:G:H5"	2.03	0.41
30:Y6:10:LEU:HD13	30:Y6:19:ARG:HD3	2.02	0.41
34:YA:24:G:O2'	51:YW:78:GLU:O	2.35	0.41
34:YA:303:U:H2'	34:YA:304:G:C8	2.56	0.41
34:YA:700:G:O2'	34:YA:1632:A:N3	2.47	0.41
34:YA:2123:G:H2'	34:YA:2124:G:H8	1.86	0.41
36:YD:13:ARG:NH1	36:YD:16:MET:SD	2.94	0.41
43:YO:78:ARG:HH21	48:YT:103:ARG:NH2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:486:U:H2'	1:QA:487:A:H8	1.86	0.40
1:QA:552:U:H2'	1:QA:553:A:H8	1.85	0.40
1:QA:851:G:H2'	1:QA:852:G:H8	1.85	0.40
1:QA:1492:A:OP1	12:QL:47:LYS:CG	2.69	0.40
4:QD:101:LEU:HB2	4:QD:138:TYR:HB3	2.03	0.40
5:QE:93:PRO:HG2	8:QH:105:ARG:HE	1.86	0.40
20:QT:29:LYS:O	20:QT:33:ILE:HG12	2.21	0.40
34:RA:626:U:O4	44:RP:81:GLN:NE2	2.52	0.40
34:RA:949:C:H2'	34:RA:950:G:C8	2.56	0.40
34:RA:1782:C:H1'	34:RA:2609:U:H5"	2.03	0.40
1:XA:881:G:P	12:XL:12:ARG:HH22	2.45	0.40
1:XA:1151:A:H2'	1:XA:1152:A:C8	2.56	0.40
1:XA:1286:A:N3	21:XU:22:ARG:NH2	2.69	0.40
1:XA:1492:A:H2'	1:XA:1493:A:C4	2.55	0.40
4:XD:85:LYS:HD2	4:XD:92:VAL:HG11	2.03	0.40
11:XK:21:ILE:HG12	11:XK:30:VAL:HG12	2.03	0.40
21:XU:10:ARG:HG2	21:XU:13:ILE:HD12	2.03	0.40
24:Y0:19:LYS:NZ	34:YA:2387:U:O2'	2.54	0.40
34:YA:513:A:O2'	34:YA:1217:C:OP1	2.34	0.40
34:YA:840:C:H2'	34:YA:841:A:H8	1.86	0.40
34:YA:2036:C:H2'	34:YA:2037:G:H8	1.85	0.40
34:YA:2698:U:H2'	34:YA:2699:C:C6	2.56	0.40
40:YH:116:GLU:HA	40:YH:117:PRO:HD3	1.95	0.40
47:YS:78:LEU:HD11	47:YS:108:GLY:O	2.21	0.40
48:YT:27:THR:HB	48:YT:90:GLN:HB3	2.03	0.40
1:QA:690:G:H22	11:QK:55:LYS:NZ	2.19	0.40
1:QA:1356:G:H2'	1:QA:1357:A:H8	1.85	0.40
25:R1:87:PRO:HA	25:R1:90:ILE:HG22	2.02	0.40
27:R3:16:PRO:HA	34:RA:969:U:H5'	2.04	0.40
34:RA:1681:G:O2'	34:RA:1762:A:O2'	2.25	0.40
34:RA:2014:A:H4'	51:RW:92:ARG:HH12	1.86	0.40
37:RE:57:LYS:HA	37:RE:57:LYS:CE	2.49	0.40
42:RN:35:ARG:HH21	42:RN:42:TRP:HZ2	1.69	0.40
45:RQ:115:MET:HG2	45:RQ:131:ILE:HG21	2.04	0.40
1:XA:165:C:H2'	1:XA:166:G:C8	2.56	0.40
1:XA:677:U:H3	1:XA:713:G:H22	1.69	0.40
1:XA:779:C:H5"	11:XK:122:LYS:HG2	2.03	0.40
1:XA:1446:A:H4'	48:YT:125:ARG:HH12	1.86	0.40
34:YA:191:A:H2'	34:YA:192:C:H6	1.87	0.40
34:YA:1780:A:O2'	34:YA:1781:C:O2	2.36	0.40
34:YA:1791:A:H4'	36:YD:206:LEU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:2590:A:H2'	34:YA:2591:C:C6	2.56	0.40
36:YD:245:PRO:HA	36:YD:246:PRO:HD3	1.79	0.40
46:YR:3:HIS:O	46:YR:5:LYS:N	2.53	0.40
1:QA:539:A:H2'	1:QA:540:G:H8	1.86	0.40
1:QA:1220:G:H2'	1:QA:1221:G:H8	1.85	0.40
32:R8:61:LEU:HD22	32:R8:61:LEU:HA	1.91	0.40
34:RA:570:G:H2'	34:RA:2030:A:C5	2.57	0.40
34:RA:588:U:H1'	38:RF:90:PHE:HB3	2.02	0.40
34:RA:648:G:H2'	34:RA:649:G:H8	1.85	0.40
34:RA:815:C:OP2	50:RV:83:ARG:NH1	2.54	0.40
34:RA:2443:C:H2'	34:RA:2444:G:C8	2.57	0.40
34:RA:2630:G:H2'	34:RA:2631:G:C8	2.55	0.40
37:RE:119:ARG:HG3	37:RE:160:TYR:HB2	2.02	0.40
39:RG:41:GLN:HE22	39:RG:43:LEU:HD21	1.87	0.40
39:RG:97:ASP:HA	39:RG:100:TRP:HD1	1.86	0.40
1:XA:1095:U:OP2	1:XA:1108:G:N1	2.49	0.40
1:XA:1435:G:H2'	1:XA:1436:U:C6	2.56	0.40
1:XA:1492:A:OP1	12:XL:47:LYS:CG	2.69	0.40
8:XH:100:ILE:HA	8:XH:101:PRO:HD3	1.93	0.40
11:XK:11:LYS:HD2	11:XK:12:ARG:HB2	2.04	0.40
22:XV:60:U:H5"	22:XV:61:C:C5	2.56	0.40
34:YA:271(D):G:H2'	34:YA:272:G:H8	1.86	0.40
34:YA:673:C:H5"	38:YF:81:PRO:HD2	2.03	0.40
34:YA:1434:A:H61	34:YA:1558:A:H62	1.69	0.40
34:YA:2020:A:H4'	49:YU:25:TRP:HZ3	1.85	0.40
34:YA:2037:G:H2'	34:YA:2038:G:C8	2.57	0.40
37:YE:24:THR:HG21	37:YE:188:VAL:HB	2.03	0.40
39:YG:150:ASP:OD1	39:YG:153:ARG:NH1	2.55	0.40
1:QA:380:G:N2	1:QA:383:A:OP2	2.40	0.40
1:QA:779:C:H5"	11:QK:122:LYS:HG2	2.04	0.40
1:QA:855:G:OP2	1:QA:871:U:N3	2.42	0.40
1:QA:1145:C:H4'	1:QA:1146:A:H8	1.86	0.40
1:QA:1244:C:H2'	1:QA:1245:A:C8	2.57	0.40
17:QQ:11:VAL:HG12	17:QQ:85:VAL:HG22	2.04	0.40
26:R2:14:ARG:NH1	26:R2:66:GLU:OE1	2.53	0.40
32:R8:31:HIS:ND1	32:R8:32:LEU:HG	2.36	0.40
34:RA:439:G:H2'	34:RA:440:G:C8	2.57	0.40
34:RA:1113:U:H2'	34:RA:1114:G:C8	2.56	0.40
34:RA:1265:A:H61	34:RA:2013:A:H5"	1.86	0.40
34:RA:2291:U:OP1	34:RA:2380:C:O2'	2.38	0.40
34:RA:2487:G:H2'	34:RA:2488:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:2841:C:H2'	34:RA:2842:G:C8	2.57	0.40
39:RG:106:LEU:HD12	39:RG:110:ALA:HB3	2.04	0.40
51:RW:24:ILE:HD13	51:RW:36:LEU:HD11	2.03	0.40
1:XA:582:U:OP2	1:XA:758:G:N1	2.42	0.40
1:XA:753:A:OP1	15:XO:69:TYR:OH	2.33	0.40
10:XJ:52:GLY:HA2	10:XJ:53:PRO:HD3	1.91	0.40
28:Y4:5:ILE:HD12	39:YG:67:LYS:HE2	2.04	0.40
34:YA:551:G:H5'	34:YA:1220:A:H1'	2.03	0.40
34:YA:828:U:H4'	34:YA:831:G:N1	2.36	0.40
34:YA:1062:G:H1'	34:YA:1088:A:C5	2.57	0.40
34:YA:1927:A:H2'	34:YA:1928:A:C8	2.56	0.40
34:YA:2212:A:H1'	34:YA:2215:G:C5	2.56	0.40
34:YA:2506:U:O2	56:Z8:76:PPU:O2'	2.38	0.40
34:YA:2730:C:H2'	34:YA:2731:G:H8	1.86	0.40
37:YE:32:PRO:HA	37:YE:90:THR:HA	2.02	0.40
46:YR:104:ARG:HG3	46:YR:107:ASP:HB3	2.04	0.40
1:QA:745:C:H2'	1:QA:746:A:C8	2.57	0.40
1:QA:1025:U:O2'	1:QA:1026:G:O4'	2.37	0.40
4:QD:152:SER:HA	4:QD:155:LEU:HD13	2.03	0.40
4:QD:173:TRP:CD1	4:QD:174:LEU:HG	2.56	0.40
32:R8:22:VAL:HB	32:R8:53:PRO:HB3	2.03	0.40
34:RA:271(D):G:H2'	34:RA:272:G:H8	1.87	0.40
34:RA:411:G:OP2	34:RA:2406:U:O2'	2.32	0.40
34:RA:1791:A:N6	34:RA:1828:G:O2'	2.50	0.40
36:RD:231:HIS:CD2	36:RD:249:PRO:HG3	2.56	0.40
45:RQ:17:LEU:HA	45:RQ:98:LYS:HE2	2.04	0.40
54:RZ:24:LEU:HD13	54:RZ:41:LEU:HD12	2.04	0.40
1:XA:789:U:H1'	1:XA:792:A:H2	1.87	0.40
6:XF:80:ARG:NE	6:XF:88:VAL:HB	2.37	0.40
34:YA:18:C:O2'	34:YA:553:U:OP1	2.40	0.40
34:YA:1888:G:OP2	34:YA:1888:G:N2	2.51	0.40
34:YA:1992:G:N2	34:YA:1996:C:O2'	2.55	0.40
34:YA:2131:G:H4'	34:YA:2132:U:H4'	2.03	0.40
34:YA:2154:G:H2'	34:YA:2155:G:C8	2.57	0.40
34:YA:2291:U:H2'	34:YA:2292:C:C6	2.56	0.40
34:YA:2314:C:H2'	34:YA:2315:G:H8	1.87	0.40
34:YA:2497:A:H1'	34:YA:2498:C:H5	1.85	0.40
37:YE:54:GLN:NE2	37:YE:76:ARG:HG2	2.37	0.40
43:YO:111:PHE:HB3	43:YO:114:ILE:HD12	2.04	0.40
46:YR:79:LEU:HD12	46:YR:83:ILE:HB	2.04	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%)	210 (90%)	22 (9%)	1 (0%)	34 70
2	XB	234/256 (91%)	211 (90%)	22 (9%)	1 (0%)	34 70
3	QC	203/239 (85%)	195 (96%)	8 (4%)	0	100 100
3	XC	203/239 (85%)	191 (94%)	10 (5%)	2 (1%)	15 54
4	QD	206/209 (99%)	202 (98%)	4 (2%)	0	100 100
4	XD	206/209 (99%)	195 (95%)	9 (4%)	2 (1%)	15 54
5	QE	149/162 (92%)	145 (97%)	4 (3%)	0	100 100
5	XE	149/162 (92%)	140 (94%)	9 (6%)	0	100 100
6	QF	99/101 (98%)	97 (98%)	2 (2%)	0	100 100
6	XF	99/101 (98%)	99 (100%)	0	0	100 100
7	QG	153/156 (98%)	149 (97%)	4 (3%)	0	100 100
7	XG	153/156 (98%)	151 (99%)	2 (1%)	0	100 100
8	QH	135/138 (98%)	132 (98%)	3 (2%)	0	100 100
8	XH	135/138 (98%)	128 (95%)	7 (5%)	0	100 100
9	QI	125/128 (98%)	116 (93%)	9 (7%)	0	100 100
9	XI	124/128 (97%)	114 (92%)	10 (8%)	0	100 100
10	QJ	97/105 (92%)	88 (91%)	9 (9%)	0	100 100
10	XJ	94/105 (90%)	85 (90%)	9 (10%)	0	100 100
11	QK	117/129 (91%)	111 (95%)	6 (5%)	0	100 100
11	XK	114/129 (88%)	106 (93%)	8 (7%)	0	100 100
12	QL	123/131 (94%)	115 (94%)	7 (6%)	1 (1%)	19 58
12	XL	120/131 (92%)	109 (91%)	11 (9%)	0	100 100
13	QM	118/126 (94%)	103 (87%)	13 (11%)	2 (2%)	9 43
13	XM	117/126 (93%)	102 (87%)	14 (12%)	1 (1%)	17 56
14	QN	58/61 (95%)	52 (90%)	5 (9%)	1 (2%)	9 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
14	XN	58/61 (95%)	52 (90%)	5 (9%)	1 (2%)	9 43
15	QO	86/89 (97%)	84 (98%)	2 (2%)	0	100 100
15	XO	85/89 (96%)	82 (96%)	3 (4%)	0	100 100
16	QP	82/88 (93%)	79 (96%)	3 (4%)	0	100 100
16	XP	82/88 (93%)	79 (96%)	3 (4%)	0	100 100
17	QQ	98/105 (93%)	96 (98%)	2 (2%)	0	100 100
17	XQ	98/105 (93%)	96 (98%)	2 (2%)	0	100 100
18	QR	68/88 (77%)	65 (96%)	3 (4%)	0	100 100
18	XR	68/88 (77%)	66 (97%)	2 (3%)	0	100 100
19	QS	81/93 (87%)	75 (93%)	6 (7%)	0	100 100
19	XS	82/93 (88%)	72 (88%)	10 (12%)	0	100 100
20	QT	97/106 (92%)	90 (93%)	7 (7%)	0	100 100
20	XT	97/106 (92%)	86 (89%)	10 (10%)	1 (1%)	15 54
21	QU	23/27 (85%)	22 (96%)	1 (4%)	0	100 100
21	XU	23/27 (85%)	22 (96%)	1 (4%)	0	100 100
24	R0	74/85 (87%)	71 (96%)	3 (4%)	0	100 100
24	Y0	73/85 (86%)	71 (97%)	2 (3%)	0	100 100
25	R1	95/98 (97%)	84 (88%)	11 (12%)	0	100 100
25	Y1	91/98 (93%)	81 (89%)	10 (11%)	0	100 100
26	R2	67/72 (93%)	63 (94%)	4 (6%)	0	100 100
26	Y2	66/72 (92%)	64 (97%)	2 (3%)	0	100 100
27	R3	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
27	Y3	57/60 (95%)	54 (95%)	3 (5%)	0	100 100
28	R4	67/71 (94%)	56 (84%)	11 (16%)	0	100 100
28	Y4	67/71 (94%)	53 (79%)	13 (19%)	1 (2%)	10 46
29	R5	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
29	Y5	57/60 (95%)	56 (98%)	1 (2%)	0	100 100
30	R6	51/54 (94%)	51 (100%)	0	0	100 100
30	Y6	51/54 (94%)	51 (100%)	0	0	100 100
31	R7	45/49 (92%)	44 (98%)	1 (2%)	0	100 100
31	Y7	46/49 (94%)	46 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
32	R8	62/65 (95%)	50 (81%)	8 (13%)	4 (6%)	1 16
32	Y8	62/65 (95%)	60 (97%)	2 (3%)	0	100 100
33	R9	35/37 (95%)	35 (100%)	0	0	100 100
33	Y9	35/37 (95%)	35 (100%)	0	0	100 100
36	RD	270/276 (98%)	254 (94%)	15 (6%)	1 (0%)	34 70
36	YD	270/276 (98%)	257 (95%)	13 (5%)	0	100 100
37	RE	203/206 (98%)	170 (84%)	33 (16%)	0	100 100
37	YE	202/206 (98%)	189 (94%)	11 (5%)	2 (1%)	15 54
38	RF	200/210 (95%)	185 (92%)	15 (8%)	0	100 100
38	YF	200/210 (95%)	183 (92%)	17 (8%)	0	100 100
39	RG	179/182 (98%)	159 (89%)	17 (10%)	3 (2%)	9 43
39	YG	179/182 (98%)	160 (89%)	18 (10%)	1 (1%)	25 63
40	RH	172/180 (96%)	152 (88%)	17 (10%)	3 (2%)	9 43
40	YH	171/180 (95%)	164 (96%)	7 (4%)	0	100 100
41	RI	144/148 (97%)	127 (88%)	14 (10%)	3 (2%)	7 39
41	YI	144/148 (97%)	127 (88%)	12 (8%)	5 (4%)	3 29
42	RN	136/140 (97%)	122 (90%)	13 (10%)	1 (1%)	22 61
42	YN	136/140 (97%)	120 (88%)	15 (11%)	1 (1%)	22 61
43	RO	120/122 (98%)	112 (93%)	8 (7%)	0	100 100
43	YO	120/122 (98%)	114 (95%)	6 (5%)	0	100 100
44	RP	148/150 (99%)	126 (85%)	20 (14%)	2 (1%)	11 47
44	YP	145/150 (97%)	137 (94%)	7 (5%)	1 (1%)	22 61
45	RQ	139/141 (99%)	122 (88%)	16 (12%)	1 (1%)	22 61
45	YQ	139/141 (99%)	122 (88%)	15 (11%)	2 (1%)	11 47
46	RR	115/118 (98%)	108 (94%)	7 (6%)	0	100 100
46	YR	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	17 56
47	RS	109/112 (97%)	90 (83%)	17 (16%)	2 (2%)	8 42
47	YS	109/112 (97%)	94 (86%)	15 (14%)	0	100 100
48	RT	135/146 (92%)	122 (90%)	13 (10%)	0	100 100
48	YT	135/146 (92%)	124 (92%)	11 (8%)	0	100 100
49	RU	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	17 56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
49	YU	115/118 (98%)	105 (91%)	8 (7%)	2 (2%)	9 43
50	RV	99/101 (98%)	86 (87%)	11 (11%)	2 (2%)	7 40
50	YV	99/101 (98%)	87 (88%)	11 (11%)	1 (1%)	15 54
51	RW	111/113 (98%)	106 (96%)	5 (4%)	0	100 100
51	YW	111/113 (98%)	105 (95%)	5 (4%)	1 (1%)	17 56
52	RX	90/96 (94%)	87 (97%)	3 (3%)	0	100 100
52	YX	90/96 (94%)	87 (97%)	3 (3%)	0	100 100
53	RY	105/110 (96%)	100 (95%)	5 (5%)	0	100 100
53	YY	105/110 (96%)	103 (98%)	2 (2%)	0	100 100
54	RZ	201/206 (98%)	186 (92%)	14 (7%)	1 (0%)	29 67
54	YZ	201/206 (98%)	186 (92%)	12 (6%)	3 (2%)	10 46
All	All	11484/12126 (95%)	10639 (93%)	787 (7%)	58 (0%)	29 67

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	R8	62	LEU
40	RH	12	PRO
41	RI	132	PRO
44	RP	108	LYS
50	RV	46	VAL
50	RV	50	PRO
41	YI	118	LYS
41	YI	132	PRO
50	YV	50	PRO
14	QN	17	LYS
32	R8	27	THR
39	RG	82	LEU
39	RG	84	LYS
41	RI	119	PRO
47	RS	4	LEU
4	XD	20	TYR
4	XD	32	ALA
37	YE	147	PRO
44	YP	63	PRO
49	YU	95	LEU
54	YZ	13	GLU
54	YZ	166	SER

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Mol	Chain	Res	Type
2	QB	234	PRO
13	QM	66	LEU
40	RH	129	THR
49	RU	97	ASP
2	XB	234	PRO
49	YU	93	LYS
12	QL	105	TYR
39	RG	81	LYS
40	RH	126	PRO
14	XN	17	LYS
41	YI	12	LEU
45	YQ	67	ARG
13	QM	69	GLU
32	R8	52	LYS
36	RD	200	ASP
42	RN	23	LEU
3	XC	12	LEU
28	Y4	48	ARG
37	YE	52	LEU
46	YR	4	LEU
51	YW	65	LEU
41	RI	133	HIS
47	RS	88	ASP
13	XM	106	ASN
39	YG	82	LEU
41	YI	10	GLU
42	YN	22	THR
32	R8	38	GLY
44	RP	109	GLY
54	RZ	53	ILE
20	XT	96	GLY
45	RQ	78	PRO
3	XC	81	GLY
41	YI	119	PRO
45	YQ	78	PRO
54	YZ	167	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	QB	203/220 (92%)	201 (99%)	2 (1%)	76 88
2	XB	204/220 (93%)	204 (100%)	0	100 100
3	QC	159/188 (85%)	156 (98%)	3 (2%)	57 79
3	XC	159/188 (85%)	156 (98%)	3 (2%)	57 79
4	QD	180/181 (99%)	178 (99%)	2 (1%)	73 87
4	XD	180/181 (99%)	179 (99%)	1 (1%)	86 94
5	QE	116/123 (94%)	115 (99%)	1 (1%)	78 89
5	XE	116/123 (94%)	116 (100%)	0	100 100
6	QF	90/90 (100%)	90 (100%)	0	100 100
6	XF	90/90 (100%)	89 (99%)	1 (1%)	73 87
7	QG	126/127 (99%)	124 (98%)	2 (2%)	62 82
7	XG	126/127 (99%)	124 (98%)	2 (2%)	62 82
8	QH	118/119 (99%)	117 (99%)	1 (1%)	81 91
8	XH	118/119 (99%)	118 (100%)	0	100 100
9	QI	98/99 (99%)	95 (97%)	3 (3%)	40 70
9	XI	97/99 (98%)	97 (100%)	0	100 100
10	QJ	89/92 (97%)	89 (100%)	0	100 100
10	XJ	86/92 (94%)	85 (99%)	1 (1%)	71 86
11	QK	90/99 (91%)	90 (100%)	0	100 100
11	XK	88/99 (89%)	87 (99%)	1 (1%)	73 87
12	QL	104/108 (96%)	103 (99%)	1 (1%)	76 88
12	XL	103/108 (95%)	102 (99%)	1 (1%)	76 88
13	QM	96/101 (95%)	94 (98%)	2 (2%)	53 77
13	XM	95/101 (94%)	95 (100%)	0	100 100
14	QN	49/50 (98%)	47 (96%)	2 (4%)	30 63
14	XN	49/50 (98%)	48 (98%)	1 (2%)	55 78
15	QO	79/80 (99%)	78 (99%)	1 (1%)	69 85
15	XO	79/80 (99%)	79 (100%)	0	100 100
16	QP	72/74 (97%)	72 (100%)	0	100 100
16	XP	72/74 (97%)	71 (99%)	1 (1%)	67 84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	QQ	95/97 (98%)	94 (99%)	1 (1%)	73 87
17	XQ	95/97 (98%)	95 (100%)	0	100 100
18	QR	61/77 (79%)	59 (97%)	2 (3%)	38 68
18	XR	61/77 (79%)	61 (100%)	0	100 100
19	QS	72/80 (90%)	72 (100%)	0	100 100
19	XS	73/80 (91%)	73 (100%)	0	100 100
20	QT	76/82 (93%)	75 (99%)	1 (1%)	69 85
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	R0	61/67 (91%)	61 (100%)	0	100 100
24	Y0	61/67 (91%)	60 (98%)	1 (2%)	62 82
25	R1	82/83 (99%)	82 (100%)	0	100 100
25	Y1	78/83 (94%)	78 (100%)	0	100 100
26	R2	64/67 (96%)	64 (100%)	0	100 100
26	Y2	64/67 (96%)	63 (98%)	1 (2%)	62 82
27	R3	51/52 (98%)	50 (98%)	1 (2%)	55 78
27	Y3	51/52 (98%)	44 (86%)	7 (14%)	3 22
28	R4	62/63 (98%)	61 (98%)	1 (2%)	62 82
28	Y4	62/63 (98%)	60 (97%)	2 (3%)	39 69
29	R5	51/52 (98%)	51 (100%)	0	100 100
29	Y5	51/52 (98%)	51 (100%)	0	100 100
30	R6	51/52 (98%)	51 (100%)	0	100 100
30	Y6	51/52 (98%)	51 (100%)	0	100 100
31	R7	40/42 (95%)	40 (100%)	0	100 100
31	Y7	41/42 (98%)	41 (100%)	0	100 100
32	R8	54/55 (98%)	46 (85%)	8 (15%)	3 19
32	Y8	54/55 (98%)	54 (100%)	0	100 100
33	R9	34/34 (100%)	34 (100%)	0	100 100
33	Y9	34/34 (100%)	34 (100%)	0	100 100
36	RD	214/218 (98%)	214 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
36	YD	214/218 (98%)	213 (100%)	1 (0%)	88 95
37	RE	165/166 (99%)	161 (98%)	4 (2%)	49 74
37	YE	165/166 (99%)	163 (99%)	2 (1%)	71 86
38	RF	161/166 (97%)	159 (99%)	2 (1%)	71 86
38	YF	161/166 (97%)	160 (99%)	1 (1%)	86 94
39	RG	155/156 (99%)	147 (95%)	8 (5%)	23 57
39	YG	155/156 (99%)	150 (97%)	5 (3%)	39 69
40	RH	145/148 (98%)	137 (94%)	8 (6%)	21 55
40	YH	144/148 (97%)	142 (99%)	2 (1%)	67 84
41	RI	122/124 (98%)	113 (93%)	9 (7%)	13 45
41	YI	122/124 (98%)	114 (93%)	8 (7%)	16 50
42	RN	117/119 (98%)	113 (97%)	4 (3%)	37 68
42	YN	117/119 (98%)	117 (100%)	0	100 100
43	RO	100/100 (100%)	98 (98%)	2 (2%)	55 78
43	YO	100/100 (100%)	100 (100%)	0	100 100
44	RP	116/116 (100%)	113 (97%)	3 (3%)	46 73
44	YP	114/116 (98%)	112 (98%)	2 (2%)	59 80
45	RQ	111/111 (100%)	110 (99%)	1 (1%)	78 89
45	YQ	111/111 (100%)	108 (97%)	3 (3%)	44 72
46	RR	100/101 (99%)	100 (100%)	0	100 100
46	YR	100/101 (99%)	100 (100%)	0	100 100
47	RS	87/88 (99%)	86 (99%)	1 (1%)	73 87
47	YS	87/88 (99%)	86 (99%)	1 (1%)	73 87
48	RT	120/127 (94%)	117 (98%)	3 (2%)	47 74
48	YT	120/127 (94%)	118 (98%)	2 (2%)	60 81
49	RU	93/94 (99%)	91 (98%)	2 (2%)	52 76
49	YU	93/94 (99%)	91 (98%)	2 (2%)	52 76
50	RV	82/82 (100%)	79 (96%)	3 (4%)	34 65
50	YV	82/82 (100%)	79 (96%)	3 (4%)	34 65
51	RW	92/92 (100%)	91 (99%)	1 (1%)	73 87
51	YW	92/92 (100%)	89 (97%)	3 (3%)	38 68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	RX	74/78 (95%)	74 (100%)	0	100	100
52	YX	74/78 (95%)	74 (100%)	0	100	100
53	RY	88/91 (97%)	88 (100%)	0	100	100
53	YY	88/91 (97%)	88 (100%)	0	100	100
54	RZ	174/179 (97%)	170 (98%)	4 (2%)	50	75
54	YZ	174/179 (97%)	169 (97%)	5 (3%)	42	71
All	All	9706/10064 (96%)	9554 (98%)	152 (2%)	62	82

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	QB	155	LEU
2	QB	236	TYR
3	QC	4	LYS
3	QC	30	ARG
3	QC	108	ASN
4	QD	103	ASN
4	QD	141	ARG
5	QE	127	ASN
7	QG	36	LYS
7	QG	94	ARG
8	QH	91	ARG
9	QI	2	GLU
9	QI	37	PHE
9	QI	93	ARG
12	QL	104	VAL
13	QM	67	GLU
13	QM	77	ASN
14	QN	27	CYS
14	QN	45	ARG
15	QO	79	ARG
17	QQ	91	ARG
18	QR	19	LYS
18	QR	55	ARG
20	QT	23	ARG
27	R3	30	ARG
28	R4	61	ARG
32	R8	26	LYS
32	R8	29	LYS
32	R8	30	ARG

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Mol	Chain	Res	Type
32	R8	35	GLN
32	R8	44	LYS
32	R8	47	LYS
32	R8	61	LEU
32	R8	64	TYR
37	RE	16	ARG
37	RE	17	ASP
37	RE	119	ARG
37	RE	145	LYS
38	RF	38	ARG
38	RF	169	ASN
39	RG	40	ASN
39	RG	79	ASN
39	RG	80	PHE
39	RG	81	LYS
39	RG	82	LEU
39	RG	83	ARG
39	RG	84	LYS
39	RG	136	ARG
40	RH	11	VAL
40	RH	23	ARG
40	RH	81	GLU
40	RH	83	TYR
40	RH	95	ARG
40	RH	126	PRO
40	RH	127	GLU
40	RH	152	ARG
41	RI	9	LEU
41	RI	10	GLU
41	RI	14	ASP
41	RI	78	THR
41	RI	81	VAL
41	RI	118	LYS
41	RI	120	ILE
41	RI	123	LEU
41	RI	142	VAL
42	RN	21	LYS
42	RN	22	THR
42	RN	114	ARG
42	RN	116	LEU
43	RO	78	ARG
43	RO	97	ARG

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Mol	Chain	Res	Type
44	RP	18	ARG
44	RP	107	LYS
44	RP	108	LYS
45	RQ	5	ARG
47	RS	57	LYS
48	RT	99	LEU
48	RT	112	ARG
48	RT	125	ARG
49	RU	92	ARG
49	RU	94	ASN
50	RV	50	PRO
50	RV	75	PHE
50	RV	100	ARG
51	RW	40	ASN
54	RZ	34	ASN
54	RZ	82	ARG
54	RZ	161	VAL
54	RZ	165	VAL
3	XC	79	ARG
3	XC	108	ASN
3	XC	179	ARG
4	XD	31	CYS
6	XF	28	ARG
7	XG	79	ARG
7	XG	94	ARG
10	XJ	47	PHE
11	XK	120	ARG
12	XL	104	VAL
14	XN	57	ARG
16	XP	72	ARG
24	Y0	14	ARG
26	Y2	47	ASN
27	Y3	2	PRO
27	Y3	4	LEU
27	Y3	5	LYS
27	Y3	36	VAL
27	Y3	37	LEU
27	Y3	58	VAL
27	Y3	60	GLU
28	Y4	48	ARG
28	Y4	56	VAL
36	YD	125	ILE

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Mol	Chain	Res	Type
37	YE	52	LEU
37	YE	75	VAL
38	YF	38	ARG
39	YG	41	GLN
39	YG	82	LEU
39	YG	83	ARG
39	YG	84	LYS
39	YG	136	ARG
40	YH	23	ARG
40	YH	54	ARG
41	YI	9	LEU
41	YI	12	LEU
41	YI	14	ASP
41	YI	27	ARG
41	YI	113	ARG
41	YI	120	ILE
41	YI	131	LYS
41	YI	133	HIS
44	YP	70	GLN
44	YP	71	VAL
45	YQ	64	ILE
45	YQ	66	ILE
45	YQ	103	MET
47	YS	106	ARG
48	YT	115	ARG
48	YT	125	ARG
49	YU	40	PHE
49	YU	93	LYS
50	YV	50	PRO
50	YV	51	VAL
50	YV	75	PHE
51	YW	15	ARG
51	YW	40	ASN
51	YW	63	ASP
54	YZ	34	ASN
54	YZ	53	ILE
54	YZ	54	HIS
54	YZ	59	LEU
54	YZ	165	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
30	R6	26	ASN
30	R6	29	ASN
39	RG	66	GLN
39	RG	79	ASN
40	RH	139	GLN
41	RI	17	GLN
48	RT	58	ASN
51	RW	111	HIS
7	XG	28	ASN
28	Y4	40	HIS
30	Y6	26	ASN
30	Y6	29	ASN
39	YG	41	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1522 (98%)	266 (17%)	30 (2%)
1	XA	1509/1522 (99%)	293 (19%)	25 (1%)
22	QV	71/76 (93%)	17 (23%)	0
22	XV	71/76 (93%)	17 (23%)	0
23	QX	2/23 (8%)	0	0
23	XX	22/23 (95%)	4 (18%)	2 (9%)
34	RA	2877/2915 (98%)	549 (19%)	37 (1%)
34	YA	2880/2915 (98%)	511 (17%)	37 (1%)
35	RB	119/122 (97%)	16 (13%)	1 (0%)
35	YB	119/122 (97%)	18 (15%)	1 (0%)
55	XY	16/17 (94%)	3 (18%)	0
56	Z6	1/3 (33%)	0	0
56	Z8	1/3 (33%)	0	0
All	All	9186/9339 (98%)	1694 (18%)	133 (1%)

All (1694) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	9	G
1	QA	31	G
1	QA	32	A
1	QA	39	G
1	QA	48	C
1	QA	50	A

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Mol	Chain	Res	Type
1	QA	51	A
1	QA	64	G
1	QA	65	U
1	QA	91	C
1	QA	95	G
1	QA	101	A
1	QA	116	A
1	QA	120	A
1	QA	121	C
1	QA	122	G
1	QA	129(A)	G
1	QA	144	G
1	QA	146	G
1	QA	151	A
1	QA	157	G
1	QA	158	G
1	QA	160	A
1	QA	163	C
1	QA	169	C
1	QA	173	U
1	QA	174	C
1	QA	189	U
1	QA	190	G
1	QA	191(A)	G
1	QA	195	A
1	QA	197	A
1	QA	208	U
1	QA	209	U
1	QA	216	G
1	QA	220	G
1	QA	244	U
1	QA	245	C
1	QA	247	G
1	QA	250	A
1	QA	251	G
1	QA	267	C
1	QA	270	A
1	QA	281	G
1	QA	289	G
1	QA	298	A
1	QA	314	C
1	QA	321	A

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Mol	Chain	Res	Type
1	QA	328	C
1	QA	329	A
1	QA	332	G
1	QA	343	U
1	QA	344	A
1	QA	346	G
1	QA	347	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	389	A
1	QA	397	A
1	QA	398	C
1	QA	406	G
1	QA	411	A
1	QA	412	A
1	QA	413	G
1	QA	414	A
1	QA	421	U
1	QA	422	C
1	QA	423	G
1	QA	428	G
1	QA	429	U
1	QA	435	C
1	QA	455	C
1	QA	466	C
1	QA	482	A
1	QA	485	G
1	QA	486	U
1	QA	496	A
1	QA	497	U
1	QA	505	G
1	QA	508	C
1	QA	509	A
1	QA	510	A
1	QA	511	C
1	QA	518	C

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Mol	Chain	Res	Type
1	QA	521	G
1	QA	527	G
1	QA	532	A
1	QA	533	A
1	QA	545	C
1	QA	547	A
1	QA	559	A
1	QA	564	C
1	QA	568	G
1	QA	572	A
1	QA	573	A
1	QA	574	A
1	QA	576	G
1	QA	577	G
1	QA	618	C
1	QA	630	G
1	QA	631	G
1	QA	653	A
1	QA	665	A
1	QA	666	G
1	QA	686	U
1	QA	688	G
1	QA	701	C
1	QA	702	A
1	QA	703	G
1	QA	704	A
1	QA	722	A
1	QA	731	G
1	QA	748	C
1	QA	754	C
1	QA	755	G
1	QA	760	G
1	QA	777	A
1	QA	785	G
1	QA	792	A
1	QA	793	U
1	QA	794	A
1	QA	813	U
1	QA	817	C
1	QA	819	A
1	QA	821	G
1	QA	828	A

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Mol	Chain	Res	Type
1	QA	841	U
1	QA	842	C
1	QA	843	U
1	QA	848	C
1	QA	859	A
1	QA	871	U
1	QA	872	A
1	QA	902	G
1	QA	914	A
1	QA	926	G
1	QA	927	G
1	QA	934	C
1	QA	960	U
1	QA	961	U
1	QA	968	A
1	QA	969	A
1	QA	971	G
1	QA	974	A
1	QA	976	G
1	QA	977	A
1	QA	991	U
1	QA	992	U
1	QA	993	G
1	QA	994	A
1	QA	1001	G
1	QA	1002	G
1	QA	1004	A
1	QA	1006	C
1	QA	1008	C
1	QA	1020	U
1	QA	1024	G
1	QA	1025	U
1	QA	1027	C
1	QA	1028	C
1	QA	1029	G
1	QA	1030	C
1	QA	1031	G
1	QA	1032(A)	G
1	QA	1033	G
1	QA	1034	G
1	QA	1054	C
1	QA	1064	G

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Mol	Chain	Res	Type
1	QA	1065	U
1	QA	1066	C
1	QA	1080	A
1	QA	1081	G
1	QA	1094	G
1	QA	1095	U
1	QA	1101	A
1	QA	1108	G
1	QA	1124	G
1	QA	1125	U
1	QA	1126	U
1	QA	1130	A
1	QA	1131	G
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	1178	G
1	QA	1181	G
1	QA	1182	G
1	QA	1183	A
1	QA	1184	G
1	QA	1187	G
1	QA	1196	U
1	QA	1201	A
1	QA	1202	G
1	QA	1212	U
1	QA	1213	A
1	QA	1215	G
1	QA	1224	G
1	QA	1225	A
1	QA	1238	A
1	QA	1240	U
1	QA	1241	G
1	QA	1256	A

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Mol	Chain	Res	Type
1	QA	1257	U
1	QA	1258	G
1	QA	1270	C
1	QA	1280	A
1	QA	1281	U
1	QA	1286	A
1	QA	1287	A
1	QA	1297	C
1	QA	1298	C
1	QA	1299	A
1	QA	1300	G
1	QA	1302	U
1	QA	1303	C
1	QA	1305	G
1	QA	1319	A
1	QA	1320	C
1	QA	1321	C
1	QA	1322	C
1	QA	1323	G
1	QA	1331	G
1	QA	1335	C
1	QA	1336	C
1	QA	1337	G
1	QA	1346	A
1	QA	1347	G
1	QA	1348	U
1	QA	1353	G
1	QA	1362(A)	C
1	QA	1363	A
1	QA	1364	U
1	QA	1378	C
1	QA	1397	C
1	QA	1398	A
1	QA	1419	G
1	QA	1442	G
1	QA	1446	A
1	QA	1447	G
1	QA	1452	C
1	QA	1453	G
1	QA	1492	A
1	QA	1494	G
1	QA	1499	A

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Mol	Chain	Res	Type
1	QA	1502	A
1	QA	1504	G
1	QA	1506	U
1	QA	1517	G
1	QA	1520	G
1	QA	1529	G
1	QA	1530	G
22	QV	2	G
22	QV	8	U
22	QV	19	G
22	QV	21	A
22	QV	30	G
22	QV	33	U
22	QV	37	T6A
22	QV	48	C
22	QV	49	G
22	QV	53	G
22	QV	54	U
22	QV	55	U
22	QV	57	G
22	QV	59	A
22	QV	61	C
22	QV	74	C
22	QV	76	A
34	RA	14	A
34	RA	15	G
34	RA	27	G
34	RA	34	C
34	RA	35	G
34	RA	46	C
34	RA	51	G
34	RA	55	G
34	RA	72	U
34	RA	74	A
34	RA	75	G
34	RA	83	G
34	RA	101	G
34	RA	103	A
34	RA	118	A
34	RA	119	A
34	RA	120	U
34	RA	131	G

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Mol	Chain	Res	Type
34	RA	139	G
34	RA	140	A
34	RA	177	G
34	RA	181	A
34	RA	196	A
34	RA	199	A
34	RA	215	G
34	RA	216	A
34	RA	221	A
34	RA	222	A
34	RA	223	A
34	RA	226	G
34	RA	229	A
34	RA	230	U
34	RA	233	A
34	RA	248	G
34	RA	249	C
34	RA	252	G
34	RA	265	A
34	RA	266	G
34	RA	270(L)	U
34	RA	270(M)	U
34	RA	270(N)	G
34	RA	270(P)	C
34	RA	271(C)	U
34	RA	273(F)	C
34	RA	275	G
34	RA	276	A
34	RA	277	C
34	RA	278	A
34	RA	299	A
34	RA	311	A
34	RA	323	G
34	RA	324	A
34	RA	329	G
34	RA	330	A
34	RA	338	G
34	RA	346	A
34	RA	352	G
34	RA	363(F)	A
34	RA	364	C
34	RA	371	A

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Mol	Chain	Res	Type
34	RA	372	G
34	RA	373	U
34	RA	386	G
34	RA	395	U
34	RA	405	U
34	RA	406	G
34	RA	411	G
34	RA	412	A
34	RA	428	A
34	RA	444	C
34	RA	448	U
34	RA	454	A
34	RA	455	C
34	RA	456	C
34	RA	457	A
34	RA	470	A
34	RA	481	G
34	RA	501	A
34	RA	504	U
34	RA	505	A
34	RA	509	C
34	RA	513	A
34	RA	527	C
34	RA	529	A
34	RA	531	C
34	RA	532	A
34	RA	533	G
34	RA	537	C
34	RA	539	G
34	RA	540	G
34	RA	546	C
34	RA	547	A
34	RA	549	G
34	RA	556	G
34	RA	563	G
34	RA	571	A
34	RA	573	G
34	RA	574	C
34	RA	575	A
34	RA	588	U
34	RA	603	A
34	RA	607	U

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Mol	Chain	Res	Type
34	RA	614	U
34	RA	615	G
34	RA	616	A
34	RA	617	G
34	RA	627	A
34	RA	634	C
34	RA	637	A
34	RA	638	G
34	RA	645	C
34	RA	646	A
34	RA	647	G
34	RA	651	G
34	RA	652	C
34	RA	654	A
34	RA	654(A)	G
34	RA	669	G
34	RA	686	G
34	RA	722	A
34	RA	726	G
34	RA	730	C
34	RA	753	C
34	RA	765	G
34	RA	776	G
34	RA	782	A
34	RA	784	A
34	RA	785	G
34	RA	789	A
34	RA	790	C
34	RA	791	C
34	RA	792	G
34	RA	800	A
34	RA	805	G
34	RA	812	C
34	RA	819	A
34	RA	827	U
34	RA	828	U
34	RA	831	G
34	RA	847	U
34	RA	856	C
34	RA	857	C
34	RA	859	G
34	RA	866	A

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Mol	Chain	Res	Type
34	RA	869	G
34	RA	882	G
34	RA	884	C
34	RA	885	C
34	RA	886	C
34	RA	888	C
34	RA	889	C
34	RA	896	A
34	RA	898	C
34	RA	900	A
34	RA	907	U
34	RA	910	A
34	RA	914	C
34	RA	915	C
34	RA	917	A
34	RA	932	G
34	RA	941	A
34	RA	945	A
34	RA	946	G
34	RA	953	A
34	RA	959	A
34	RA	961	C
34	RA	973	A
34	RA	974	G
34	RA	974(A)	C
34	RA	980	A
34	RA	983	A
34	RA	996	A
34	RA	1003	G
34	RA	1012	U
34	RA	1013	C
34	RA	1022	G
34	RA	1023	U
34	RA	1025	G
34	RA	1026	U
34	RA	1027	A
34	RA	1033	U
34	RA	1036	G
34	RA	1038	C
34	RA	1042	G
34	RA	1045	A
34	RA	1046	A

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Mol	Chain	Res	Type
34	RA	1047	G
34	RA	1054	A
34	RA	1058	G
34	RA	1060	U
34	RA	1063	G
34	RA	1064	C
34	RA	1065	U
34	RA	1066	U
34	RA	1067	A
34	RA	1068	G
34	RA	1070	A
34	RA	1071	G
34	RA	1073	A
34	RA	1074	G
34	RA	1076	C
34	RA	1078	U
34	RA	1079	C
34	RA	1080	C
34	RA	1082	U
34	RA	1083	U
34	RA	1084	A
34	RA	1085	A
34	RA	1086	A
34	RA	1088	A
34	RA	1090	U
34	RA	1092	C
34	RA	1093	G
34	RA	1094	U
34	RA	1096	A
34	RA	1097	U
34	RA	1098	A
34	RA	1109	C
34	RA	1112	G
34	RA	1122	G
34	RA	1130	U
34	RA	1131	G
34	RA	1135	C
34	RA	1136	G
34	RA	1140	C
34	RA	1142(A)	A
34	RA	1173	G
34	RA	1174	A

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Mol	Chain	Res	Type
34	RA	1175	U
34	RA	1176	G
34	RA	1187	G
34	RA	1195	G
34	RA	1204	A
34	RA	1205	U
34	RA	1206	G
34	RA	1210	A
34	RA	1211	U
34	RA	1220	A
34	RA	1236	G
34	RA	1238	G
34	RA	1253	A
34	RA	1256	G
34	RA	1265	A
34	RA	1271	G
34	RA	1272	A
34	RA	1273	U
34	RA	1300	U
34	RA	1301	A
34	RA	1312	U
34	RA	1313	U
34	RA	1314	C
34	RA	1329	U
34	RA	1332	G
34	RA	1349	A
34	RA	1352	U
34	RA	1365	A
34	RA	1370	C
34	RA	1378	A
34	RA	1379	A
34	RA	1384	A
34	RA	1385	G
34	RA	1395	A
34	RA	1403	C
34	RA	1404	C
34	RA	1407	C
34	RA	1411	C
34	RA	1416	G
34	RA	1419	A
34	RA	1420	U
34	RA	1421	G

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Mol	Chain	Res	Type
34	RA	1428	C
34	RA	1434	A
34	RA	1444(A)	A
34	RA	1445	C
34	RA	1449	A
34	RA	1449(A)	G
34	RA	1455	G
34	RA	1459	G
34	RA	1460	A
34	RA	1461	G
34	RA	1471	A
34	RA	1480	G
34	RA	1482	U
34	RA	1483	G
34	RA	1487	G
34	RA	1493	C
34	RA	1497	U
34	RA	1504	C
34	RA	1506	C
34	RA	1507	A
34	RA	1508	A
34	RA	1510	A
34	RA	1511	A
34	RA	1514	U
34	RA	1522	G
34	RA	1523	U
34	RA	1528	A
34	RA	1535	U
34	RA	1536	A
34	RA	1537	C
34	RA	1538	G
34	RA	1543	A
34	RA	1545	A
34	RA	1547	C
34	RA	1558	A
34	RA	1559	G
34	RA	1566	A
34	RA	1569	A
34	RA	1578	U
34	RA	1580	A
34	RA	1581	G
34	RA	1583	A

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Mol	Chain	Res	Type
34	RA	1586	A
34	RA	1587	A
34	RA	1598	C
34	RA	1608	A
34	RA	1609	A
34	RA	1616	A
34	RA	1617	C
34	RA	1640	C
34	RA	1648	C
34	RA	1654	A
34	RA	1667	G
34	RA	1668	A
34	RA	1674	G
34	RA	1725	G
34	RA	1728	G
34	RA	1729	A
34	RA	1730	U
34	RA	1731	G
34	RA	1733	G
34	RA	1743	G
34	RA	1756	G
34	RA	1762	A
34	RA	1763	G
34	RA	1764	G
34	RA	1769	G
34	RA	1773	A
34	RA	1776	G
34	RA	1779	U
34	RA	1780	A
34	RA	1782	C
34	RA	1787	A
34	RA	1791	A
34	RA	1799	G
34	RA	1800	C
34	RA	1801	G
34	RA	1816	G
34	RA	1820	U
34	RA	1828	G
34	RA	1835	G
34	RA	1847	A
34	RA	1848	A
34	RA	1858	G

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Mol	Chain	Res	Type
34	RA	1869	G
34	RA	1870	C
34	RA	1872	A
34	RA	1878	G
34	RA	1882	C
34	RA	1888	G
34	RA	1889	A
34	RA	1903	G
34	RA	1906	G
34	RA	1913	A
34	RA	1914	C
34	RA	1929	G
34	RA	1930	G
34	RA	1936	A
34	RA	1939	U
34	RA	1940	U
34	RA	1955	U
34	RA	1963	U
34	RA	1965	C
34	RA	1967	C
34	RA	1969	A
34	RA	1970	A
34	RA	1971	A
34	RA	1972	A
34	RA	1982	C
34	RA	1992	G
34	RA	1993	U
34	RA	2004	G
34	RA	2020	A
34	RA	2021	C
34	RA	2023	G
34	RA	2031	A
34	RA	2032	G
34	RA	2033	A
34	RA	2043	C
34	RA	2052	G
34	RA	2055	C
34	RA	2056	G
34	RA	2059	A
34	RA	2060	A
34	RA	2061	G
34	RA	2062	A

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Mol	Chain	Res	Type
34	RA	2069	G
34	RA	2093	G
34	RA	2111	C
34	RA	2113	U
34	RA	2114	A
34	RA	2115	G
34	RA	2116	G
34	RA	2117	A
34	RA	2118	U
34	RA	2126	A
34	RA	2127	G
34	RA	2128	C
34	RA	2132	U
34	RA	2133	G
34	RA	2136	C
34	RA	2147	G
34	RA	2148	G
34	RA	2158	A
34	RA	2164	C
34	RA	2166	G
34	RA	2167	U
34	RA	2168	G
34	RA	2169	A
34	RA	2173	A
34	RA	2182	G
34	RA	2189	U
34	RA	2190	G
34	RA	2194	G
34	RA	2198	A
34	RA	2199	A
34	RA	2210	G
34	RA	2211	G
34	RA	2212	A
34	RA	2215	G
34	RA	2225	A
34	RA	2238	G
34	RA	2239	G
34	RA	2243	U
34	RA	2266	A
34	RA	2275	C
34	RA	2278	A
34	RA	2280	G

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Mol	Chain	Res	Type
34	RA	2283	C
34	RA	2287	A
34	RA	2288	A
34	RA	2305	A
34	RA	2307	G
34	RA	2308	G
34	RA	2309	A
34	RA	2310	A
34	RA	2311	A
34	RA	2313	C
34	RA	2319	G
34	RA	2320	A
34	RA	2325	G
34	RA	2334	G
34	RA	2336	A
34	RA	2342	C
34	RA	2346	A
34	RA	2347	C
34	RA	2350	C
34	RA	2361	A
34	RA	2372	G
34	RA	2383	G
34	RA	2385	C
34	RA	2391	G
34	RA	2392	A
34	RA	2394	C
34	RA	2402	C
34	RA	2403	C
34	RA	2424	C
34	RA	2425	A
34	RA	2429	G
34	RA	2430	A
34	RA	2435	A
34	RA	2439	A
34	RA	2440	C
34	RA	2441	C
34	RA	2447	G
34	RA	2448	A
34	RA	2469	A
34	RA	2478	A
34	RA	2481	G
34	RA	2494	G

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Mol	Chain	Res	Type
34	RA	2498	C
34	RA	2502	G
34	RA	2505	G
34	RA	2518	A
34	RA	2519	U
34	RA	2529	G
34	RA	2542	A
34	RA	2543	G
34	RA	2554	U
34	RA	2564	A
34	RA	2567	G
34	RA	2569	G
34	RA	2572	A
34	RA	2573	C
34	RA	2585	U
34	RA	2602	A
34	RA	2609	U
34	RA	2611	U
34	RA	2612	C
34	RA	2615	U
34	RA	2623	G
34	RA	2629	A
34	RA	2646	C
34	RA	2655	G
34	RA	2665	A
34	RA	2673	G
34	RA	2689	U
34	RA	2690	C
34	RA	2702	U
34	RA	2707	G
34	RA	2712(A)	A
34	RA	2713	A
34	RA	2714	G
34	RA	2726	U
34	RA	2732	G
34	RA	2733	A
34	RA	2744	G
34	RA	2748	A
34	RA	2751	G
34	RA	2761	G
34	RA	2764	A
34	RA	2765	A

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Mol	Chain	Res	Type
34	RA	2766	G
34	RA	2778	A
34	RA	2779	U
34	RA	2780	G
34	RA	2789	C
34	RA	2790	A
34	RA	2791	C
34	RA	2792	G
34	RA	2797	U
34	RA	2798	C
34	RA	2818	G
34	RA	2820	A
34	RA	2821	A
34	RA	2833	G
34	RA	2834	G
34	RA	2835	A
34	RA	2847	U
34	RA	2867	G
34	RA	2872	G
34	RA	2873	A
34	RA	2879	C
34	RA	2880	C
34	RA	2886	G
34	RA	2892	A
34	RA	2894	G
34	RA	2895	U
34	RA	2897	U
35	RB	8	U
35	RB	13	A
35	RB	15	A
35	RB	16	G
35	RB	19	G
35	RB	21	G
35	RB	25	A
35	RB	41	U
35	RB	42	C
35	RB	45	A
35	RB	52	A
35	RB	56	G
35	RB	67	G
35	RB	73	A
35	RB	108	C

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Mol	Chain	Res	Type
35	RB	109	G
1	XA	6	G
1	XA	7	G
1	XA	31	G
1	XA	32	A
1	XA	39	G
1	XA	47	C
1	XA	48	C
1	XA	51	A
1	XA	56	U
1	XA	61	G
1	XA	65	U
1	XA	66	G
1	XA	79	G
1	XA	89	U
1	XA	92	G
1	XA	95	G
1	XA	101	A
1	XA	116	A
1	XA	121	C
1	XA	130	A
1	XA	144	G
1	XA	147	G
1	XA	151	A
1	XA	156	G
1	XA	161	A
1	XA	163	C
1	XA	169	C
1	XA	172	A
1	XA	174	C
1	XA	190	G
1	XA	191(A)	G
1	XA	195	A
1	XA	196	A
1	XA	197	A
1	XA	208	U
1	XA	209	U
1	XA	210	U
1	XA	244	U
1	XA	245	C
1	XA	247	G
1	XA	251	G

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Mol	Chain	Res	Type
1	XA	267	C
1	XA	281	G
1	XA	289	G
1	XA	306	G
1	XA	314	C
1	XA	321	A
1	XA	328	C
1	XA	329	A
1	XA	332	G
1	XA	343	U
1	XA	345	C
1	XA	346	G
1	XA	347	G
1	XA	348	G
1	XA	351	G
1	XA	352	C
1	XA	353	A
1	XA	354	G
1	XA	356	A
1	XA	359	U
1	XA	363	A
1	XA	367	U
1	XA	372	C
1	XA	373	A
1	XA	384	G
1	XA	389	A
1	XA	397	A
1	XA	398	C
1	XA	406	G
1	XA	411	A
1	XA	412	A
1	XA	413	G
1	XA	421	U
1	XA	422	C
1	XA	423	G
1	XA	428	G
1	XA	429	U
1	XA	440	A
1	XA	442	C
1	XA	452	A
1	XA	465	A
1	XA	466	C

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Mol	Chain	Res	Type
1	XA	467	G
1	XA	482	A
1	XA	484	G
1	XA	485	G
1	XA	486	U
1	XA	492	G
1	XA	496	A
1	XA	497	U
1	XA	509	A
1	XA	510	A
1	XA	511	C
1	XA	518	C
1	XA	519	C
1	XA	521	G
1	XA	524	G
1	XA	527	G
1	XA	529	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	561	U
1	XA	564	C
1	XA	572	A
1	XA	573	A
1	XA	576	G
1	XA	577	G
1	XA	618	C
1	XA	630	G
1	XA	631	G
1	XA	632	A
1	XA	653	A
1	XA	657	G
1	XA	665	A
1	XA	666	G
1	XA	686	U
1	XA	688	G
1	XA	690	G
1	XA	702	A

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Mol	Chain	Res	Type
1	XA	703	G
1	XA	704	A
1	XA	723	U
1	XA	731	G
1	XA	734	G
1	XA	749	C
1	XA	754	C
1	XA	755	G
1	XA	777	A
1	XA	792	A
1	XA	793	U
1	XA	794	A
1	XA	799	G
1	XA	813	U
1	XA	816	A
1	XA	817	C
1	XA	821	G
1	XA	828	A
1	XA	836	G
1	XA	841	U
1	XA	842	C
1	XA	843	U
1	XA	848	C
1	XA	859	A
1	XA	871	U
1	XA	872	A
1	XA	902	G
1	XA	914	A
1	XA	916	G
1	XA	926	G
1	XA	927	G
1	XA	934	C
1	XA	935	A
1	XA	958	A
1	XA	960	U
1	XA	968	A
1	XA	969	A
1	XA	972	C
1	XA	974	A
1	XA	975	A
1	XA	976	G
1	XA	977	A

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Mol	Chain	Res	Type
1	XA	982	U
1	XA	991	U
1	XA	992	U
1	XA	993	G
1	XA	994	A
1	XA	1003	G
1	XA	1004	A
1	XA	1005	A
1	XA	1006	C
1	XA	1009	G
1	XA	1024	G
1	XA	1025	U
1	XA	1028	C
1	XA	1029	G
1	XA	1031	G
1	XA	1032(A)	G
1	XA	1032(B)	G
1	XA	1038	C
1	XA	1039	C
1	XA	1040	U
1	XA	1041	A
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	1066	C
1	XA	1081	G
1	XA	1085	U
1	XA	1094	G
1	XA	1101	A
1	XA	1108	G
1	XA	1115	C
1	XA	1124	G
1	XA	1125	U
1	XA	1126	U
1	XA	1127	G
1	XA	1129	C
1	XA	1130	A
1	XA	1131	G
1	XA	1136	U

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Mol	Chain	Res	Type
1	XA	1137	C
1	XA	1138	G
1	XA	1139	G
1	XA	1146	A
1	XA	1157	A
1	XA	1158	C
1	XA	1159	U
1	XA	1160	G
1	XA	1162	C
1	XA	1169	A
1	XA	1176	A
1	XA	1177	G
1	XA	1181	G
1	XA	1182	G
1	XA	1183	A
1	XA	1187	G
1	XA	1196	U
1	XA	1200	C
1	XA	1201	A
1	XA	1212	U
1	XA	1225	A
1	XA	1236	A
1	XA	1238	A
1	XA	1240	U
1	XA	1241	G
1	XA	1256	A
1	XA	1257	U
1	XA	1258	G
1	XA	1260	C
1	XA	1270	C
1	XA	1273	G
1	XA	1280	A
1	XA	1281	U
1	XA	1282	C
1	XA	1286	A
1	XA	1287	A
1	XA	1290	G
1	XA	1291	G
1	XA	1298	C
1	XA	1299	A
1	XA	1300	G
1	XA	1301	U

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Mol	Chain	Res	Type
1	XA	1302	U
1	XA	1303	C
1	XA	1305	G
1	XA	1310	G
1	XA	1311	G
1	XA	1318	A
1	XA	1319	A
1	XA	1320	C
1	XA	1323	G
1	XA	1331	G
1	XA	1335	C
1	XA	1336	C
1	XA	1340	A
1	XA	1347	G
1	XA	1348	U
1	XA	1362(A)	C
1	XA	1394	A
1	XA	1397	C
1	XA	1400	C
1	XA	1419	G
1	XA	1442	G
1	XA	1446	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	1494	G
1	XA	1497	G
1	XA	1498	U
1	XA	1499	A
1	XA	1502	A
1	XA	1504	G
1	XA	1506	U
1	XA	1517	G
1	XA	1520	G
1	XA	1529	G
1	XA	1530	G
1	XA	1533	C
1	XA	1538	C
1	XA	1541	U

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Mol	Chain	Res	Type
22	XV	2	G
22	XV	8	U
22	XV	19	G
22	XV	21	A
22	XV	30	G
22	XV	33	U
22	XV	37	T6A
22	XV	48	C
22	XV	49	G
22	XV	53	G
22	XV	54	U
22	XV	55	U
22	XV	57	G
22	XV	59	A
22	XV	61	C
22	XV	74	C
22	XV	76	A
23	XX	-4	U
23	XX	-3	A
23	XX	-2	A
23	XX	4	U
55	XY	28	G
55	XY	30	G
55	XY	43	C
34	YA	9	U
34	YA	11	G
34	YA	15	G
34	YA	34	C
34	YA	35	G
34	YA	46	C
34	YA	51	G
34	YA	61	G
34	YA	74	A
34	YA	75	G
34	YA	101	G
34	YA	102	G
34	YA	118	A
34	YA	120	U
34	YA	125	G
34	YA	131	G
34	YA	140	A
34	YA	155	C

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Mol	Chain	Res	Type
34	YA	162	U
34	YA	196	A
34	YA	199	A
34	YA	214	G
34	YA	215	G
34	YA	216	A
34	YA	221	A
34	YA	222	A
34	YA	223	A
34	YA	226	G
34	YA	228	A
34	YA	229	A
34	YA	230	U
34	YA	232	G
34	YA	242	G
34	YA	243	U
34	YA	248	G
34	YA	252	G
34	YA	270(L)	U
34	YA	270(M)	U
34	YA	270(N)	G
34	YA	270(P)	C
34	YA	270(Y)	G
34	YA	271(B)	G
34	YA	271(C)	U
34	YA	271(D)	G
34	YA	274	G
34	YA	275	G
34	YA	276	A
34	YA	278	A
34	YA	279	C
34	YA	299	A
34	YA	311	A
34	YA	323	G
34	YA	324	A
34	YA	329	G
34	YA	330	A
34	YA	332	A
34	YA	352	G
34	YA	363	G
34	YA	363(E)	U
34	YA	364	C

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Mol	Chain	Res	Type
34	YA	371	A
34	YA	372	G
34	YA	386	G
34	YA	387	U
34	YA	396	G
34	YA	404	C
34	YA	405	U
34	YA	406	G
34	YA	411	G
34	YA	412	A
34	YA	428	A
34	YA	443	A
34	YA	444	C
34	YA	448	U
34	YA	457	A
34	YA	470	A
34	YA	481	G
34	YA	504	U
34	YA	505	A
34	YA	509	C
34	YA	512	G
34	YA	518	G
34	YA	531	C
34	YA	532	A
34	YA	533	G
34	YA	537	C
34	YA	539	G
34	YA	540	G
34	YA	541	C
34	YA	546	C
34	YA	547	A
34	YA	563	G
34	YA	568	U
34	YA	573	G
34	YA	575	A
34	YA	603	A
34	YA	607	U
34	YA	614	U
34	YA	617	G
34	YA	622	G
34	YA	627	A
34	YA	634	C

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Mol	Chain	Res	Type
34	YA	637	A
34	YA	638	G
34	YA	645	C
34	YA	646	A
34	YA	651	G
34	YA	654	A
34	YA	654(A)	G
34	YA	669	G
34	YA	686	G
34	YA	717	G
34	YA	722	A
34	YA	726	G
34	YA	730	C
34	YA	753	C
34	YA	764	A
34	YA	765	G
34	YA	782	A
34	YA	784	A
34	YA	785	G
34	YA	788	A
34	YA	789	A
34	YA	790	C
34	YA	791	C
34	YA	805	G
34	YA	812	C
34	YA	819	A
34	YA	827	U
34	YA	831	G
34	YA	847	U
34	YA	856	C
34	YA	857	C
34	YA	860	U
34	YA	866	A
34	YA	881	G
34	YA	882	G
34	YA	884	C
34	YA	886	C
34	YA	888	C
34	YA	889	C
34	YA	896	A
34	YA	897	C
34	YA	900	A

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Mol	Chain	Res	Type
34	YA	907	U
34	YA	910	A
34	YA	915	C
34	YA	917	A
34	YA	932	G
34	YA	941	A
34	YA	945	A
34	YA	946	G
34	YA	953	A
34	YA	959	A
34	YA	961	C
34	YA	974	G
34	YA	974(A)	C
34	YA	980	A
34	YA	983	A
34	YA	996	A
34	YA	1011	G
34	YA	1012	U
34	YA	1013	C
34	YA	1015	G
34	YA	1022	G
34	YA	1023	U
34	YA	1026	U
34	YA	1027	A
34	YA	1033	U
34	YA	1046	A
34	YA	1047	G
34	YA	1050	A
34	YA	1053	C
34	YA	1057	A
34	YA	1059	G
34	YA	1060	U
34	YA	1061	U
34	YA	1062	G
34	YA	1067	A
34	YA	1068	G
34	YA	1070	A
34	YA	1071	G
34	YA	1073	A
34	YA	1077	A
34	YA	1078	U
34	YA	1082	U

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Mol	Chain	Res	Type
34	YA	1083	U
34	YA	1084	A
34	YA	1085	A
34	YA	1086	A
34	YA	1088	A
34	YA	1089	G
34	YA	1093	G
34	YA	1095	A
34	YA	1096	A
34	YA	1097	U
34	YA	1103	A
34	YA	1104	C
34	YA	1110	G
34	YA	1130	U
34	YA	1135	C
34	YA	1136	G
34	YA	1139	G
34	YA	1141	U
34	YA	1142	U
34	YA	1142(A)	A
34	YA	1155	A
34	YA	1173	G
34	YA	1174	A
34	YA	1175	U
34	YA	1176	G
34	YA	1179	C
34	YA	1204	A
34	YA	1205	U
34	YA	1210	A
34	YA	1211	U
34	YA	1220	A
34	YA	1236	G
34	YA	1238	G
34	YA	1252	G
34	YA	1253	A
34	YA	1256	G
34	YA	1265	A
34	YA	1271	G
34	YA	1272	A
34	YA	1275	A
34	YA	1300	U
34	YA	1301	A

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Mol	Chain	Res	Type
34	YA	1314	C
34	YA	1329	U
34	YA	1349	A
34	YA	1365	A
34	YA	1368	G
34	YA	1370	C
34	YA	1378	A
34	YA	1379	A
34	YA	1384	A
34	YA	1385	G
34	YA	1392	A
34	YA	1395	A
34	YA	1406	U
34	YA	1407	C
34	YA	1411	C
34	YA	1416	G
34	YA	1419	A
34	YA	1420	U
34	YA	1421	G
34	YA	1428	C
34	YA	1444(A)	A
34	YA	1445	C
34	YA	1449	A
34	YA	1449(A)	G
34	YA	1455	G
34	YA	1460	A
34	YA	1461	G
34	YA	1467	C
34	YA	1471	A
34	YA	1478	G
34	YA	1482	U
34	YA	1483	G
34	YA	1487	G
34	YA	1493	C
34	YA	1496	A
34	YA	1497	U
34	YA	1507	A
34	YA	1510	A
34	YA	1511	A
34	YA	1522	G
34	YA	1528	A
34	YA	1533	C

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Mol	Chain	Res	Type
34	YA	1535	U
34	YA	1536	A
34	YA	1537	C
34	YA	1540	G
34	YA	1543	A
34	YA	1544	C
34	YA	1545	A
34	YA	1558	A
34	YA	1559	G
34	YA	1566	A
34	YA	1569	A
34	YA	1578	U
34	YA	1585	C
34	YA	1586	A
34	YA	1591	G
34	YA	1598	C
34	YA	1608	A
34	YA	1609	A
34	YA	1616	A
34	YA	1617	C
34	YA	1640	C
34	YA	1648	C
34	YA	1654	A
34	YA	1674	G
34	YA	1695	G
34	YA	1725	G
34	YA	1728	G
34	YA	1729	A
34	YA	1731	G
34	YA	1732	A
34	YA	1733	G
34	YA	1743	G
34	YA	1749	A
34	YA	1753	G
34	YA	1754	C
34	YA	1756	G
34	YA	1763	G
34	YA	1764	G
34	YA	1769	G
34	YA	1773	A
34	YA	1779	U
34	YA	1780	A

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Mol	Chain	Res	Type
34	YA	1781	C
34	YA	1787	A
34	YA	1791	A
34	YA	1799	G
34	YA	1800	C
34	YA	1801	G
34	YA	1816	G
34	YA	1829	A
34	YA	1835	G
34	YA	1847	A
34	YA	1858	G
34	YA	1869	G
34	YA	1870	C
34	YA	1872	A
34	YA	1878	G
34	YA	1882	C
34	YA	1884	A
34	YA	1889	A
34	YA	1903	G
34	YA	1906	G
34	YA	1913	A
34	YA	1914	C
34	YA	1919	A
34	YA	1929	G
34	YA	1930	G
34	YA	1936	A
34	YA	1939	U
34	YA	1940	U
34	YA	1955	U
34	YA	1956	U
34	YA	1963	U
34	YA	1964	G
34	YA	1967	C
34	YA	1969	A
34	YA	1970	A
34	YA	1971	A
34	YA	1972	A
34	YA	1982	C
34	YA	1992	G
34	YA	1993	U
34	YA	2020	A
34	YA	2021	C

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Mol	Chain	Res	Type
34	YA	2023	G
34	YA	2031	A
34	YA	2033	A
34	YA	2043	C
34	YA	2052	G
34	YA	2055	C
34	YA	2056	G
34	YA	2059	A
34	YA	2060	A
34	YA	2061	G
34	YA	2062	A
34	YA	2069	G
34	YA	2093	G
34	YA	2100	G
34	YA	2111	C
34	YA	2114	A
34	YA	2115	G
34	YA	2116	G
34	YA	2118	U
34	YA	2120	G
34	YA	2126	A
34	YA	2127	G
34	YA	2131	G
34	YA	2132	U
34	YA	2133	G
34	YA	2134	A
34	YA	2136	C
34	YA	2147	G
34	YA	2148	G
34	YA	2152	G
34	YA	2156	G
34	YA	2157	G
34	YA	2158	A
34	YA	2159	G
34	YA	2166	G
34	YA	2168	G
34	YA	2169	A
34	YA	2173	A
34	YA	2180	U
34	YA	2189	U
34	YA	2190	G
34	YA	2192	G

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Mol	Chain	Res	Type
34	YA	2198	A
34	YA	2210	G
34	YA	2211	G
34	YA	2212	A
34	YA	2213	U
34	YA	2215	G
34	YA	2225	A
34	YA	2238	G
34	YA	2239	G
34	YA	2243	U
34	YA	2266	A
34	YA	2275	C
34	YA	2278	A
34	YA	2279	G
34	YA	2283	C
34	YA	2287	A
34	YA	2288	A
34	YA	2305	A
34	YA	2307	G
34	YA	2308	G
34	YA	2309	A
34	YA	2311	A
34	YA	2320	A
34	YA	2325	G
34	YA	2334	G
34	YA	2335	A
34	YA	2345	G
34	YA	2346	A
34	YA	2347	C
34	YA	2350	C
34	YA	2383	G
34	YA	2385	C
34	YA	2403	C
34	YA	2406	U
34	YA	2410	G
34	YA	2423	U
34	YA	2425	A
34	YA	2427	C
34	YA	2428	G
34	YA	2429	G
34	YA	2430	A
34	YA	2435	A

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Mol	Chain	Res	Type
34	YA	2439	A
34	YA	2441	C
34	YA	2447	G
34	YA	2448	A
34	YA	2450	A
34	YA	2469	A
34	YA	2470	G
34	YA	2494	G
34	YA	2498	C
34	YA	2502	G
34	YA	2505	G
34	YA	2518	A
34	YA	2529	G
34	YA	2554	U
34	YA	2558	C
34	YA	2564	A
34	YA	2566	A
34	YA	2567	G
34	YA	2572	A
34	YA	2576	G
34	YA	2578	G
34	YA	2585	U
34	YA	2602	A
34	YA	2609	U
34	YA	2611	U
34	YA	2612	C
34	YA	2615	U
34	YA	2629	A
34	YA	2646	C
34	YA	2655	G
34	YA	2665	A
34	YA	2673	G
34	YA	2682	U
34	YA	2689	U
34	YA	2702	U
34	YA	2712	U
34	YA	2712(A)	A
34	YA	2713	A
34	YA	2714	G
34	YA	2726	U
34	YA	2732	G
34	YA	2733	A

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Mol	Chain	Res	Type
34	YA	2744	G
34	YA	2748	A
34	YA	2751	G
34	YA	2761	G
34	YA	2764	A
34	YA	2765	A
34	YA	2766	G
34	YA	2769	C
34	YA	2777	G
34	YA	2778	A
34	YA	2779	U
34	YA	2780	G
34	YA	2790	A
34	YA	2791	C
34	YA	2797	U
34	YA	2818	G
34	YA	2820	A
34	YA	2821	A
34	YA	2823	A
34	YA	2833	G
34	YA	2834	G
34	YA	2835	A
34	YA	2847	U
34	YA	2867	G
34	YA	2868	A
34	YA	2872	G
34	YA	2873	A
34	YA	2880	C
34	YA	2891	G
34	YA	2892	A
34	YA	2893	G
35	YB	8	U
35	YB	9	G
35	YB	13	A
35	YB	15	A
35	YB	16	G
35	YB	19	G
35	YB	21	G
35	YB	22	U
35	YB	25	A
35	YB	32	C
35	YB	41	U

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Mol	Chain	Res	Type
35	YB	42	C
35	YB	44	G
35	YB	45	A
35	YB	56	G
35	YB	67	G
35	YB	73	A
35	YB	109	G

All (133) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	QA	64	G
1	QA	115	G
1	QA	119	A
1	QA	243	A
1	QA	244	U
1	QA	250	A
1	QA	266	G
1	QA	328	C
1	QA	410	G
1	QA	412	A
1	QA	481	G
1	QA	484	G
1	QA	485	G
1	QA	509	A
1	QA	687	A
1	QA	703	G
1	QA	753	A
1	QA	792	A
1	QA	812	C
1	QA	913	A
1	QA	992	U
1	QA	1065	U
1	QA	1200	C
1	QA	1285	A
1	QA	1297	C
1	QA	1336	C
1	QA	1346	A
1	QA	1347	G
1	QA	1498	U
1	QA	1528	U
34	RA	221	A

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Mol	Chain	Res	Type
34	RA	222	A
34	RA	229	A
34	RA	271(B)	G
34	RA	345	A
34	RA	372	G
34	RA	404	C
34	RA	503	A
34	RA	512	G
34	RA	587	C
34	RA	637	A
34	RA	752	A
34	RA	846	C
34	RA	856	C
34	RA	1022	G
34	RA	1026	U
34	RA	1053	C
34	RA	1057	A
34	RA	1065	U
34	RA	1067	A
34	RA	1073	A
34	RA	1204	A
34	RA	1210	A
34	RA	1312	U
34	RA	1427	A
34	RA	1558	A
34	RA	1653	G
34	RA	1819	A
34	RA	1992	G
34	RA	2060	A
34	RA	2126	A
34	RA	2361	A
34	RA	2439	A
34	RA	2566	A
34	RA	2610	C
34	RA	2689	U
34	RA	2832	U
35	RB	66	A
1	XA	60	A
1	XA	78	G
1	XA	115	G
1	XA	243	A
1	XA	244	U

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Mol	Chain	Res	Type
1	XA	250	A
1	XA	266	G
1	XA	328	C
1	XA	410	G
1	XA	412	A
1	XA	481	G
1	XA	484	G
1	XA	485	G
1	XA	509	A
1	XA	687	A
1	XA	703	G
1	XA	753	A
1	XA	812	C
1	XA	913	A
1	XA	992	U
1	XA	1027	C
1	XA	1285	A
1	XA	1297	C
1	XA	1310	G
1	XA	1498	U
23	XX	-5	G
23	XX	-3	A
34	YA	195	A
34	YA	221	A
34	YA	229	A
34	YA	241	A
34	YA	242	G
34	YA	271(B)	G
34	YA	278	A
34	YA	404	C
34	YA	503	A
34	YA	637	A
34	YA	752	A
34	YA	846	C
34	YA	856	C
34	YA	859	G
34	YA	974	G
34	YA	1022	G
34	YA	1026	U
34	YA	1085	A
34	YA	1109	C
34	YA	1178	C

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Mol	Chain	Res	Type
34	YA	1204	A
34	YA	1210	A
34	YA	1427	A
34	YA	1460	A
34	YA	1558	A
34	YA	1653	G
34	YA	1694	C
34	YA	1799	G
34	YA	1992	G
34	YA	2406	U
34	YA	2566	A
34	YA	2610	C
34	YA	2681	C
34	YA	2712	U
34	YA	2776	A
34	YA	2832	U
34	YA	2867	G
35	YB	66	A

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

6 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	$\#\|Z\| > 2$
22	T6A	QV	37	22	27,34,35	0.97	1 (3%)	29,49,52	1.72	6 (20%)
22	T6A	XV	37	22	27,34,35	0.95	2 (7%)	29,49,52	1.61	5 (17%)
22	MNU	XV	34	22,23	20,24,25	1.32	3 (15%)	28,34,37	1.82	8 (28%)
56	PPU	Z6	76	34,56	32,40,41	0.87	1 (3%)	33,57,60	1.49	7 (21%)
22	MNU	QV	34	22,23	20,24,25	1.30	3 (15%)	28,34,37	1.63	8 (28%)
56	PPU	Z8	76	34,56	32,40,41	0.89	1 (3%)	33,57,60	1.56	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
22	T6A	QV	37	22	-	13/19/41/42	0/3/3/3
22	T6A	XV	37	22	-	14/19/41/42	0/3/3/3
22	MNU	XV	34	22,23	-	0/9/28/29	0/2/2/2
56	PPU	Z6	76	34,56	-	4/21/43/44	0/4/4/4
22	MNU	QV	34	22,23	-	0/9/28/29	0/2/2/2
56	PPU	Z8	76	34,56	-	3/21/43/44	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	XV	34	MNU	C2-N1	3.13	1.43	1.38
22	QV	34	MNU	C2-N1	2.92	1.43	1.38
22	QV	34	MNU	C4-N3	-2.85	1.33	1.38
22	XV	34	MNU	C4-N3	-2.83	1.33	1.38
56	Z8	76	PPU	C5-C4	2.68	1.48	1.40
56	Z6	76	PPU	C5-C4	2.61	1.47	1.40
22	QV	37	T6A	C5-C4	2.53	1.47	1.40
22	XV	37	T6A	C5-C4	2.43	1.47	1.40
22	QV	34	MNU	C2-N3	-2.18	1.34	1.38
22	XV	34	MNU	C2-N3	-2.05	1.34	1.38
22	XV	37	T6A	C10-N6	-2.03	1.33	1.37

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	QV	37	T6A	C2-N1-C6	5.54	121.34	116.59
22	XV	37	T6A	C2-N1-C6	5.26	121.10	116.59
22	XV	34	MNU	N3-C2-N1	4.45	120.79	114.89
56	Z6	76	PPU	N1-C6-N6	4.30	121.58	117.06
22	QV	34	MNU	N3-C2-N1	4.27	120.55	114.89
56	Z8	76	PPU	N1-C6-N6	4.20	121.48	117.06
22	XV	34	MNU	C1'-N1-C2	4.12	125.03	117.57
22	QV	37	T6A	N6-C10-N11	3.93	119.25	113.76
22	XV	34	MNU	C4-N3-C2	-3.73	122.52	127.35
22	QV	34	MNU	C4-N3-C2	-3.29	123.09	127.35
22	QV	34	MNU	C1'-N1-C2	3.23	123.42	117.57
22	QV	37	T6A	N3-C2-N1	-3.22	123.65	128.68
22	XV	37	T6A	N6-C10-N11	3.13	118.13	113.76
56	Z8	76	PPU	C4-C5-N7	-3.09	106.18	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	Z8	76	PPU	C10-N6-C9	-3.05	106.29	116.12
22	XV	34	MNU	O2-C2-N3	-3.04	115.84	121.50
56	Z6	76	PPU	C4-C5-N7	-3.04	106.23	109.40
56	Z6	76	PPU	C9-N6-C6	-3.03	110.33	119.51
56	Z8	76	PPU	N3-C2-N1	-3.03	123.94	128.68
22	XV	37	T6A	N3-C2-N1	-3.02	123.96	128.68
56	Z8	76	PPU	C10-N6-C6	-2.91	110.71	119.51
22	QV	34	MNU	O2-C2-N3	-2.89	116.11	121.50
22	XV	34	MNU	C1'-N1-C6	-2.89	116.32	121.12
56	Z6	76	PPU	C10-N6-C6	-2.88	110.80	119.51
22	XV	34	MNU	O4-C4-C5	-2.75	120.86	124.96
56	Z6	76	PPU	C10-N6-C9	-2.74	107.28	116.12
56	Z8	76	PPU	C9-N6-C6	-2.74	111.22	119.51
22	XV	34	MNU	C6-N1-C2	-2.68	118.58	121.30
56	Z8	76	PPU	C3'-N3'-C	-2.64	119.23	123.21
22	XV	37	T6A	N6-C6-N1	2.62	122.23	118.72
22	QV	34	MNU	O4-C4-C5	-2.61	121.07	124.96
56	Z6	76	PPU	N3-C2-N1	-2.52	124.73	128.68
22	XV	34	MNU	C5-C4-N3	2.49	118.47	114.97
22	QV	34	MNU	C6-N1-C2	-2.46	118.80	121.30
22	QV	37	T6A	O10-C10-N6	-2.43	119.51	123.62
22	XV	37	T6A	C4-C5-N7	-2.37	106.93	109.40
22	QV	37	T6A	C4-C5-N7	-2.33	106.97	109.40
22	QV	34	MNU	C5-C4-N3	2.29	118.18	114.97
56	Z6	76	PPU	C3'-N3'-C	-2.12	120.02	123.21
22	QV	34	MNU	C1'-N1-C6	-2.05	117.71	121.12
22	QV	37	T6A	N6-C6-N1	2.00	121.40	118.72

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	QV	37	T6A	O10-C10-N6-C6
22	QV	37	T6A	N11-C10-N6-C6
22	QV	37	T6A	N6-C10-N11-C12
22	QV	37	T6A	O10-C10-N11-C12
22	QV	37	T6A	N11-C12-C13-ODA
22	QV	37	T6A	N11-C12-C13-ODB
22	XV	37	T6A	C5-C6-N6-C10
22	XV	37	T6A	O10-C10-N6-C6
22	XV	37	T6A	N11-C10-N6-C6
22	XV	37	T6A	N6-C10-N11-C12

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Mol	Chain	Res	Type	Atoms
22	XV	37	T6A	O10-C10-N11-C12
22	XV	37	T6A	N11-C12-C13-ODA
22	XV	37	T6A	N11-C12-C13-ODB
56	Z6	76	PPU	C5-C6-N6-C9
56	Z6	76	PPU	CE1-CZ-OC-CM
56	Z8	76	PPU	CE1-CZ-OC-CM
22	QV	37	T6A	C3'-C4'-C5'-O5'
22	XV	37	T6A	C3'-C4'-C5'-O5'
56	Z6	76	PPU	CE2-CZ-OC-CM
56	Z8	76	PPU	CE2-CZ-OC-CM
22	XV	37	T6A	C4'-C5'-O5'-P
22	QV	37	T6A	O4'-C4'-C5'-O5'
22	XV	37	T6A	O4'-C4'-C5'-O5'
22	QV	37	T6A	C5-C6-N6-C10
56	Z6	76	PPU	N1-C6-N6-C9
22	QV	37	T6A	C4'-C5'-O5'-P
22	QV	37	T6A	C13-C12-N11-C10
22	XV	37	T6A	N1-C6-N6-C10
56	Z8	76	PPU	C5-C6-N6-C9
22	QV	37	T6A	C13-C12-C14-O14
22	XV	37	T6A	C13-C12-C14-O14
22	XV	37	T6A	C13-C12-C14-C15
22	XV	37	T6A	C13-C12-N11-C10
22	QV	37	T6A	N1-C6-N6-C10

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	QV	37	T6A	1	0
22	XV	37	T6A	1	0
22	QV	34	MNU	1	0
56	Z8	76	PPU	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1253 ligands modelled in this entry, 1251 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	-	0,12,12	-	-	-		
58	SF4	QD	301	4	0,12,12	-	-	-		

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

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