



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2020 – 09:03 AM BST

PDB ID : 6OJ2
Title : Crystal structure of tRNA^{Ala}(GGC) bound to the near-cognate 70S A-site
Authors : Nguyen, H.A.; Sunita, S.; Dunham, C.M.
Deposited on : 2019-04-10
Resolution : 3.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : **FAILED**
buster-report : 1.1.7 (2018)
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) : 2.13

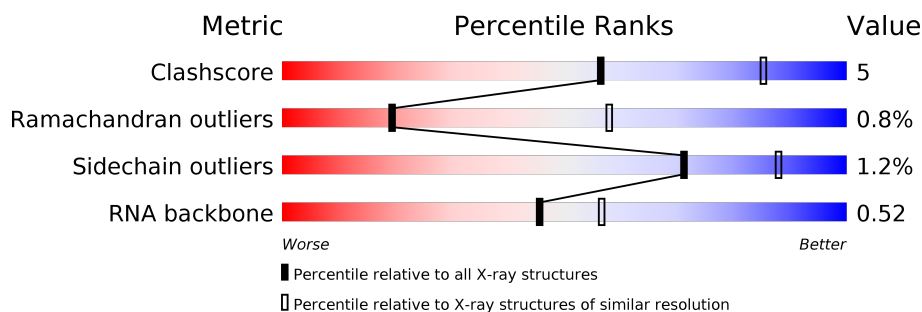
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)















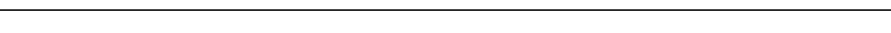




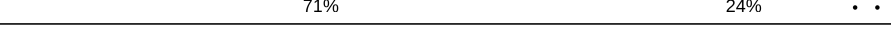



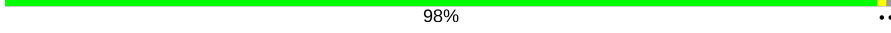

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	QA	1522	66% 27% 6% ..
1	XA	1522	64% 28% 5% ..
2	QB	256	71% 21% 7%
2	XB	256	72% 20% 7%
3	QC	239	73% 12% 14%
3	XC	239	70% 16% 14%
4	QD	209	84% 14% .

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Mol	Chain	Length	Quality of chain
4	XD	209	 79% 19% .
5	QE	162	 78% 15% 7%
5	XE	162	 73% 20% 7%
6	QF	101	 92% 7% .
6	XF	101	 86% 14%
7	QG	156	 85% 15% .
7	XG	156	 85% 14% .
8	QH	138	 78% 22%
8	XH	138	 75% 25%
9	QI	128	 75% 23% ..
9	XI	128	 77% 22% ..
10	QJ	105	 76% 18% 6%
10	XJ	105	 70% 24% 6%
11	QK	129	 80% 12% 8%
11	XK	129	 77% 16% 8%
12	QL	131	 77% 18% . 5%
12	XL	131	 76% 18% .. 5%
13	QM	126	 64% 31% . .
13	XM	126	 71% 24% . .
14	QN	61	 64% 31% . .
14	XN	61	 79% 20% .
15	QO	89	 87% 10% ..
15	XO	89	 98% ..
16	QP	88	 81% 14% . 5%
16	XP	88	 82% 13% . 5%















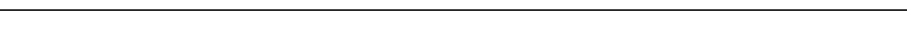




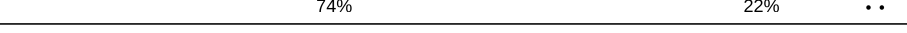





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Mol	Chain	Length	Quality of chain
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QW	76	
23	XW	76	
24	QX	19	
24	XX	19	
25	QY	76	
25	XY	76	
26	R0	85	
26	Y0	85	
27	R1	98	
27	Y1	98	
28	R2	72	
28	Y2	72	
29	R3	60	















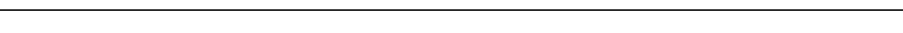




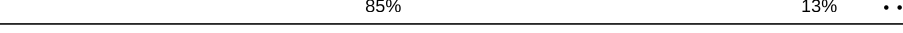





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Mol	Chain	Length	Quality of chain
29	Y3	60	
30	R4	71	
30	Y4	71	
31	R5	60	
31	Y5	60	
32	R6	54	
32	Y6	54	
33	R7	49	
33	Y7	49	
34	R8	65	
34	Y8	65	
35	R9	37	
35	Y9	37	
36	RA	2915	
36	YA	2915	
37	RB	122	
37	YB	122	
38	RD	276	
38	YD	276	
39	RE	206	
39	YE	206	
40	RF	210	
40	YF	210	
41	RG	182	
41	YG	182	






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Mol	Chain	Length	Quality of chain
42	RH	180	 77% 17% • 6%
42	YH	180	 71% 23% • 6%
43	RI	148	 86% 13% •
43	YI	148	 79% 19% ••
44	RN	140	 90% 9% •
44	YN	140	 81% 14% ••
45	RO	122	 79% 19% •
45	YO	122	 76% 23% •
46	RP	150	 79% 21% •
46	YP	150	 83% 17% •
47	RQ	141	 81% 18% ••
47	YQ	141	 72% 27% •
48	RR	118	 79% 19% •
48	YR	118	 85% 14% •
49	RS	112	 79% 18% ••
49	YS	112	 79% 20% ••
50	RT	146	 69% 24% • 6%
50	YT	146	 70% 24% 6%
51	RU	118	 85% 13% ••
51	YU	118	 75% 19% •••
52	RV	101	 84% 16%
52	YV	101	 88% 12%
53	RW	113	 86% 14%
53	YW	113	 84% 16%
54	RX	96	 82% 14% •

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Mol	Chain	Length	Quality of chain
54	YX	96	 82% 14% •
55	RY	110	 72% 17% • 7%
55	YY	110	 73% 18% • 7%
56	RZ	206	 62% 26% 11%
56	YZ	206	 68% 18% • 11%

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 298371 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	1500	Total	C	N	O	P	0	0	0
			32249	14354	5984	10412	1499			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	QB	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			
2	XB	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	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
			1674	1050	333	284	7			
4	XD	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	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	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	XH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- 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	127	Total	C	N	O		0	0	0
			1010	639	197	174				

- 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	99	Total	C	N	O	S	0	0	0
			801	504	157	139	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	119	Total	C	N	O	S	0	0	0
			885	549	168	165	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	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	QM	121	Total	C	N	O	S	0	0	0
			964	597	199	166	2			
13	XM	121	Total	C	N	O	S	0	0	0
			964	597	199	166	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	88	Total	C	N	O	S	0	0	0
			734	459	147	126	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	84	Total	C	N	O	S	0	0	0
			674	430	126	116	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	C	N	O	0	0	0
			217	134	52	31			
21	XU	25	Total	C	N	O	0	0	0
			217	134	52	31			

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

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

- Molecule 23 is a RNA chain called E-site tRNA^{Ala}(GGC).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QW	76	Total	C	N	O	P	0	0	0
			1632	727	301	528	76			
23	XW	76	Total	C	N	O	P	0	0	0
			1632	727	301	528	76			

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QX	19	Total	C	N	O	P	0	0	0
			418	187	87	125	19			
24	XX	17	Total	C	N	O	P	0	0	0
			374	167	77	113	17			

- Molecule 25 is a RNA chain called A-site tRNA^{Ala}(GGC).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	QY	75	Total	C	N	O	P	0	0	0
			1603	714	288	526	75			
25	XY	76	Total	C	N	O	P	0	0	0
			1625	724	293	532	76			

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	R0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Y0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			

- Molecule 27 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	R1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
27	Y1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

- Molecule 28 is a protein called 50S ribosomal protein L29.

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

- Molecule 29 is a protein called 50S ribosomal protein L30.

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

- Molecule 30 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	R4	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			
30	Y4	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			

- Molecule 31 is a protein called 50S ribosomal protein L32.

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

- Molecule 32 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	R6	49	Total	C	N	O	S	0	0	0
			424	264	87	69	4			
32	Y6	49	Total	C	N	O	S	0	0	0
			424	264	87	69	4			

- Molecule 33 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	R7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			
33	Y7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 34 is a protein called 50S ribosomal protein L35.

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

- Molecule 35 is a protein called 50S ribosomal protein L36.

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

- Molecule 36 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	RA	2882	Total	C	N	O	P	0	0	0
			62071	27627	11611	19952	2881			
36	YA	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			

- Molecule 37 is a RNA chain called 5S rRNA.

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

- Molecule 38 is a protein called 50S ribosomal protein L2.

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

- Molecule 39 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	RE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
39	YE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 40 is a protein called 50S ribosomal protein L4.

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

- Molecule 41 is a protein called 50S ribosomal protein L5.

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

- Molecule 42 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	RH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	YH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

- Molecule 43 is a protein called 50S ribosomal protein L9.

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

- Molecule 44 is a protein called 50S ribosomal protein L13.

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

- Molecule 45 is a protein called 50S ribosomal protein L14.

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

- Molecule 46 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	RP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
46	YP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

- Molecule 47 is a protein called 50S ribosomal protein L16.

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

- Molecule 48 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	RR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
48	YR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 49 is a protein called 50S ribosomal protein L18.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L20.

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

- Molecule 52 is a protein called 50S ribosomal protein L21.

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

- Molecule 53 is a protein called 50S ribosomal protein L22.

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

- Molecule 54 is a protein called 50S ribosomal protein L23.

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

- Molecule 55 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	RY	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			
55	YY	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

- Molecule 56 is a protein called 50S ribosomal protein L25.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	85	Total	Mg	0	0
			85	85		
57	YV	1	Total	Mg	0	0
			1	1		
57	RP	2	Total	Mg	0	0
			2	2		
57	QX	1	Total	Mg	0	0
			1	1		
57	R7	1	Total	Mg	0	0
			1	1		

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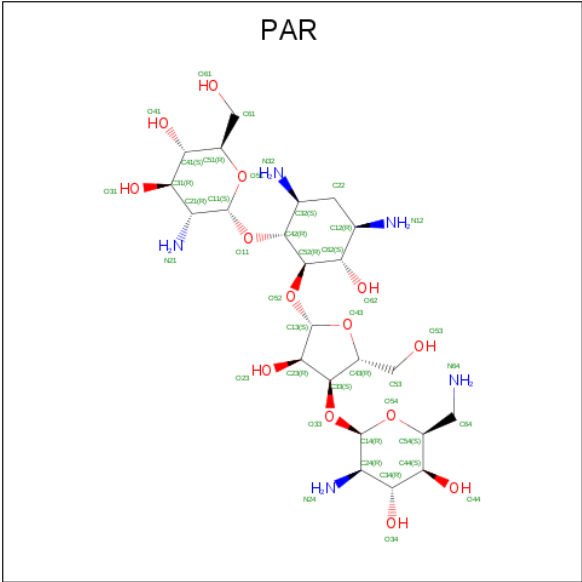
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	YA	379	Total 379	Mg 379	0	0
57	QM	2	Total 2	Mg 2	0	0
57	YH	1	Total 1	Mg 1	0	0
57	YR	2	Total 2	Mg 2	0	0
57	YD	3	Total 3	Mg 3	0	0
57	QV	4	Total 4	Mg 4	0	0
57	RX	1	Total 1	Mg 1	0	0
57	Y8	3	Total 3	Mg 3	0	0
57	XA	94	Total 94	Mg 94	0	0
57	RQ	1	Total 1	Mg 1	0	0
57	R0	1	Total 1	Mg 1	0	0
57	YU	2	Total 2	Mg 2	0	0
57	RU	1	Total 1	Mg 1	0	0
57	XJ	1	Total 1	Mg 1	0	0
57	QH	1	Total 1	Mg 1	0	0
57	XY	1	Total 1	Mg 1	0	0
57	YQ	1	Total 1	Mg 1	0	0
57	XF	1	Total 1	Mg 1	0	0
57	YX	3	Total 3	Mg 3	0	0
57	RD	1	Total 1	Mg 1	0	0
57	Y7	2	Total 2	Mg 2	0	0

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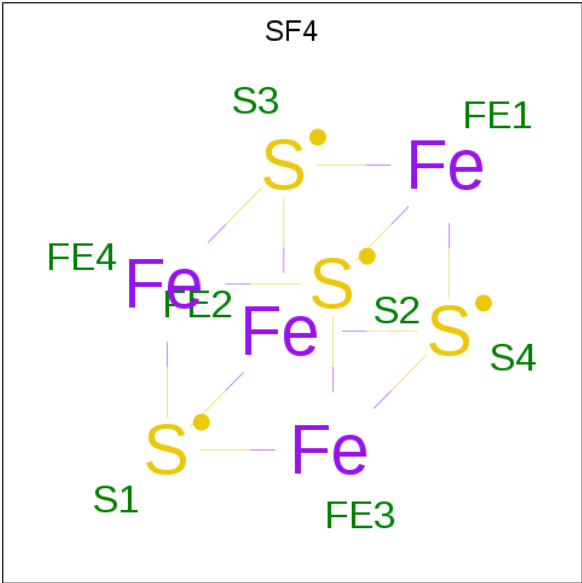
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QF	1	Total 1	Mg 1	0	0
57	R5	1	Total 1	Mg 1	0	0
57	Y0	1	Total 1	Mg 1	0	0
57	RA	321	Total 321	Mg 321	0	0
57	YP	3	Total 3	Mg 3	0	0
57	Y5	2	Total 2	Mg 2	0	0
57	RE	3	Total 3	Mg 3	0	0
57	YB	8	Total 8	Mg 8	0	0
57	XV	3	Total 3	Mg 3	0	0
57	RB	4	Total 4	Mg 4	0	0
57	Y2	1	Total 1	Mg 1	0	0
57	XD	1	Total 1	Mg 1	0	0
57	R8	1	Total 1	Mg 1	0	0
57	RF	1	Total 1	Mg 1	0	0
57	XM	1	Total 1	Mg 1	0	0
57	YE	3	Total 3	Mg 3	0	0

- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	QA	1	Total	C	N	O	0	0
			42	23	5	14		
58	XA	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	XN	1	Total	Zn	0	0
			1	1		

- Molecule 61 is water.

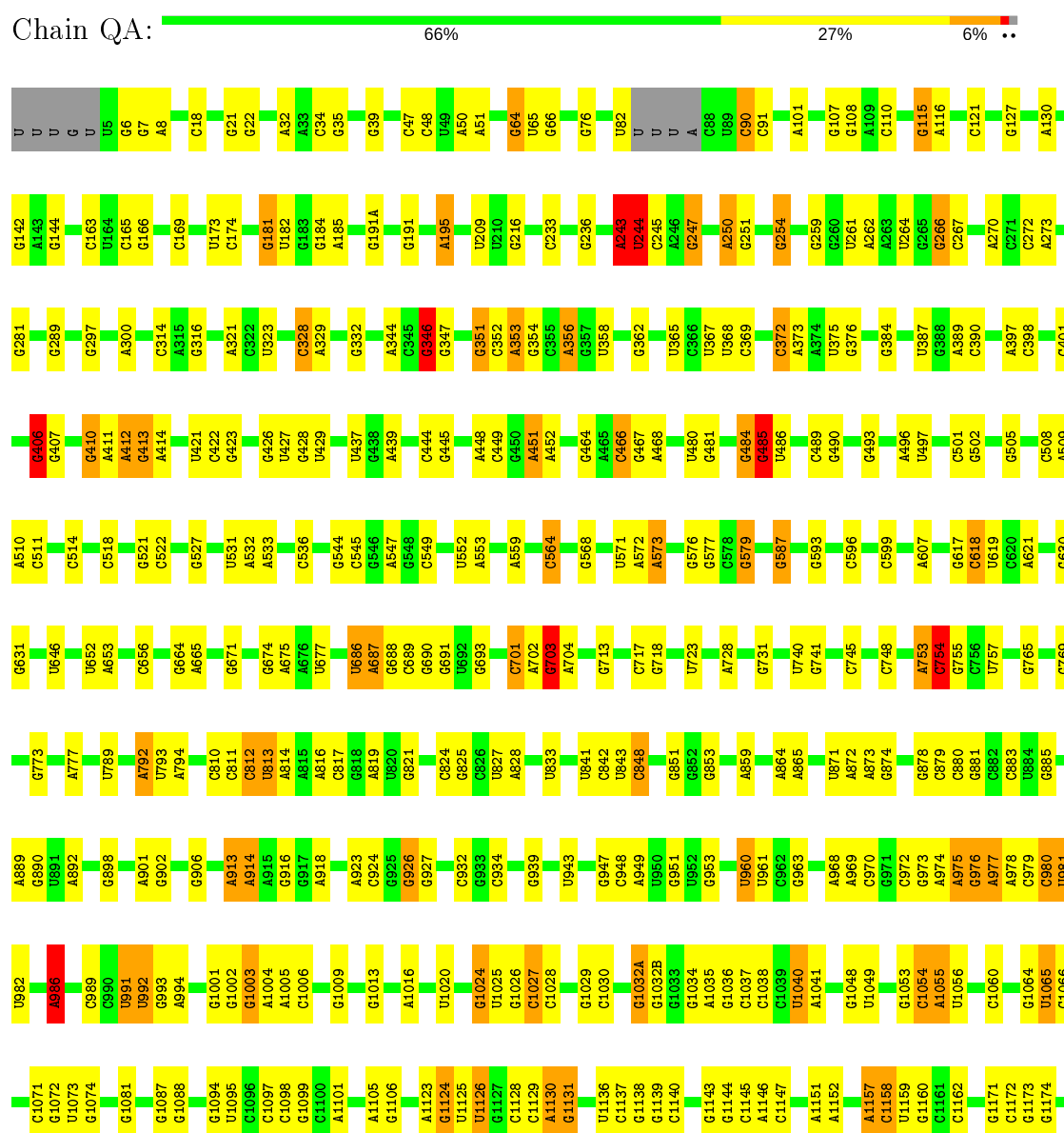
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	QA	1	Total	O	0	0
			1	1		
61	QX	1	Total	O	0	0
			1	1		

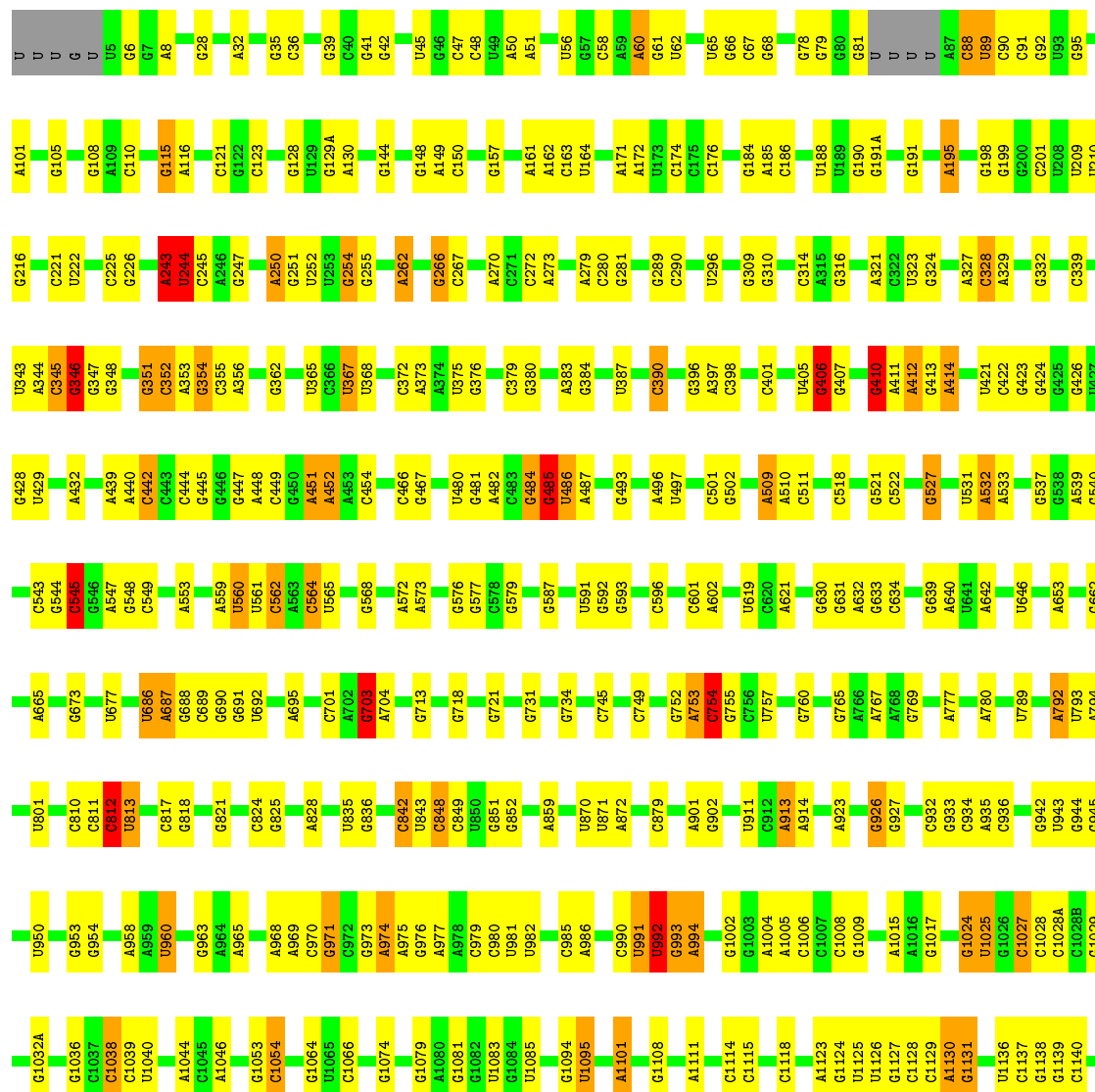
3 Residue-property plots

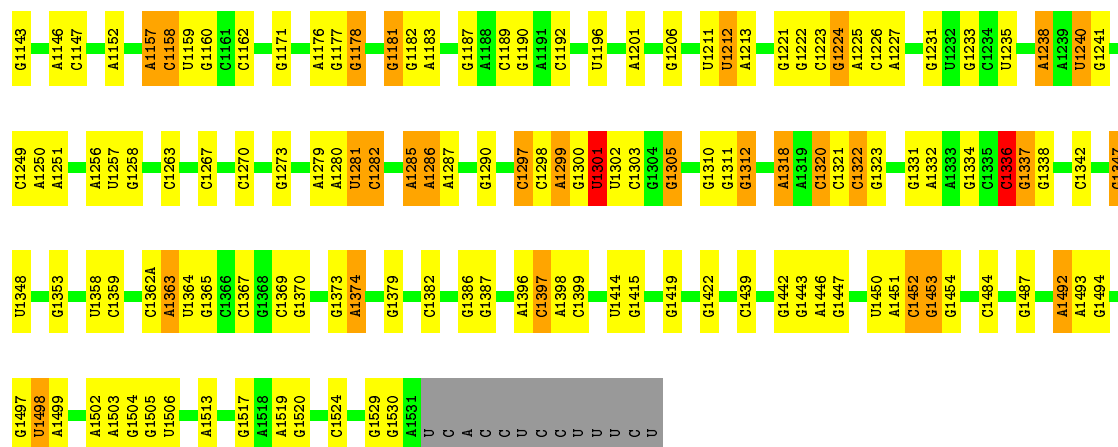
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS failed to run properly.

• Molecule 1: 16S rRNA

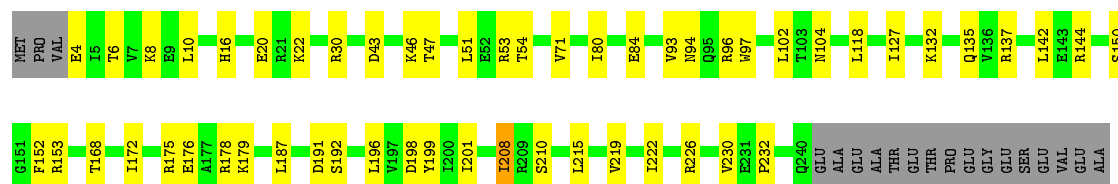






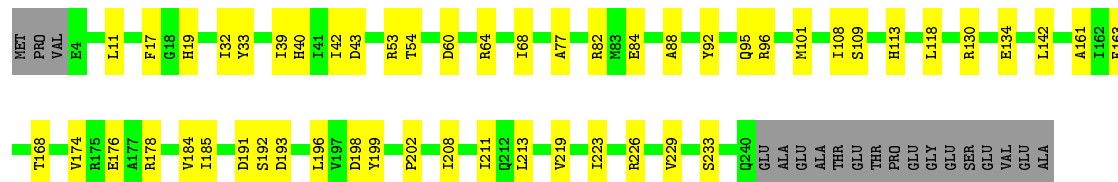
• Molecule 2: 30S ribosomal protein S2

Chain QB: 71% 21% 7%



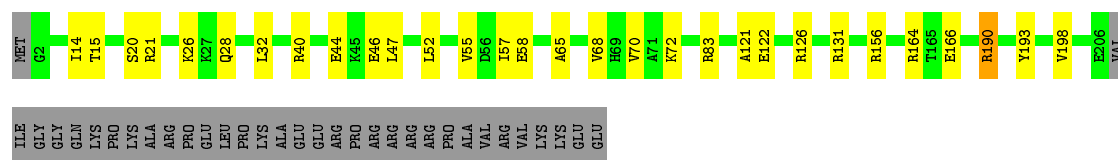
• Molecule 2: 30S ribosomal protein S2

Chain XB: 72% 20% 7%



• Molecule 3: 30S ribosomal protein S3

Chain QC: 73% 12% 14%



• Molecule 3: 30S ribosomal protein S3

Chain XC: 70% 16% 14%





- Molecule 7: 30S ribosomal protein S7

Chain QG: 85% 15%



- Molecule 7: 30S ribosomal protein S7

Chain XG: 85% 14%



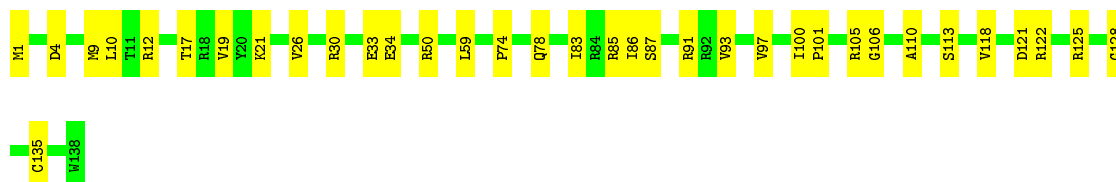
- Molecule 8: 30S ribosomal protein S8

Chain QH: 78% 22%



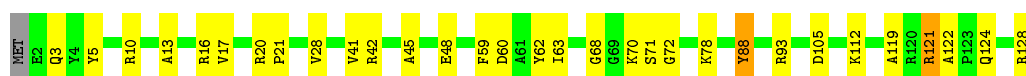
- Molecule 8: 30S ribosomal protein S8

Chain XH: 75% 25%



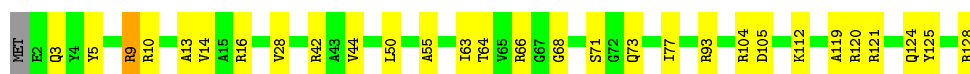
- Molecule 9: 30S ribosomal protein S9

Chain QI: 75% 23%




- Molecule 9: 30S ribosomal protein S9

Chain XI: 77% 22%



- 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: 



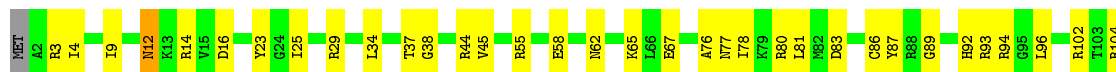
- Molecule 12: 30S ribosomal protein S12

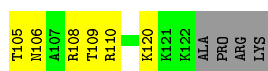
Chain XL: 



- Molecule 13: 30S ribosomal protein S13

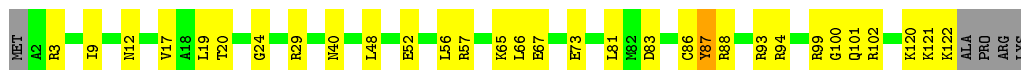
Chain QM: 





- Molecule 13: 30S ribosomal protein S13

Chain XM: 71% 24% ..



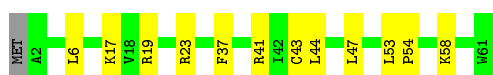
- Molecule 14: 30S ribosomal protein S14 type Z

Chain QN: 64% 31% ..



- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN: 79% 20% ..



- Molecule 15: 30S ribosomal protein S15

Chain QO: 87% 10% ..



- Molecule 15: 30S ribosomal protein S15

Chain XO: 98% ..



- Molecule 16: 30S ribosomal protein S16

Chain QP: 81% 14% 5%



- Molecule 16: 30S ribosomal protein S16

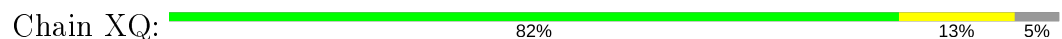
Chain XP: 82% 13% 5%



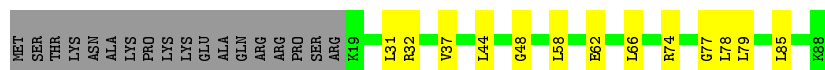
- Molecule 17: 30S ribosomal protein S17



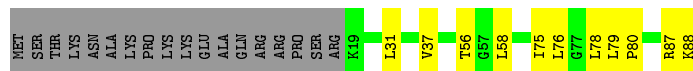
- Molecule 17: 30S ribosomal protein S17



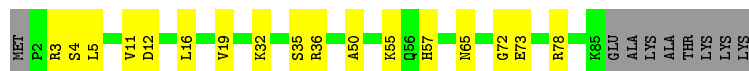
- Molecule 18: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S18



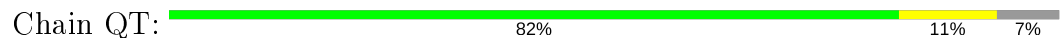
- Molecule 19: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S19



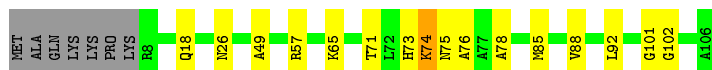
- Molecule 20: 30S ribosomal protein S20





- Molecule 20: 30S ribosomal protein S20

Chain XT: 78% 14% 7%



- Molecule 21: 30S ribosomal protein Thx

Chain QU: 70% 22% 7%



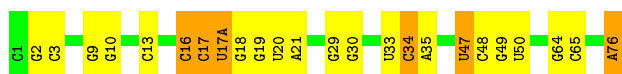
- Molecule 21: 30S ribosomal protein Thx

Chain XU: 74% 19% 7%



- Molecule 22: P-site tRNA^{fMet}

Chain QV: 69% 23% 8%



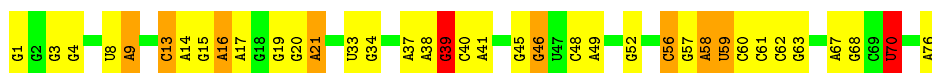
- Molecule 22: P-site tRNA^{fMet}

Chain XV: 74% 23% 3%



- Molecule 23: E-site tRNA^{Ala}(GGC)

Chain QW: 51% 36% 11% 2%

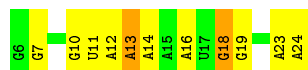


- Molecule 23: E-site tRNA^{Ala}(GGC)

Chain XW: 41% 42% 17%



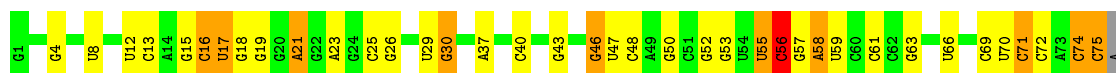
- Molecule 24: mRNA



- Molecule 24: mRNA



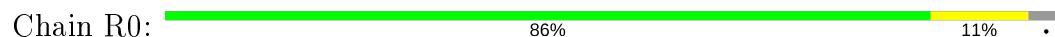
- Molecule 25: A-site tRNAAla(GGC)



- Molecule 25: A-site tRNAAla(GGC)



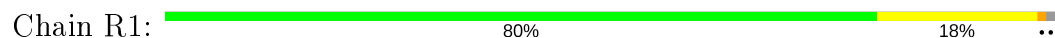
- Molecule 26: 50S ribosomal protein L27



- Molecule 26: 50S ribosomal protein L27



- Molecule 27: 50S ribosomal protein L28





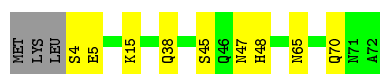
- Molecule 27: 50S ribosomal protein L28

Chain Y1: 86% 10% ..



- Molecule 28: 50S ribosomal protein L29

Chain R2: 83% 13% .



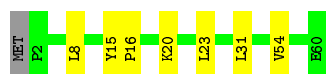
- Molecule 28: 50S ribosomal protein L29

Chain Y2: 79% 17% .



- Molecule 29: 50S ribosomal protein L30

Chain R3: 87% 12% .



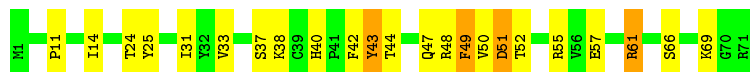
- Molecule 29: 50S ribosomal protein L30

Chain Y3: 87% 12% .



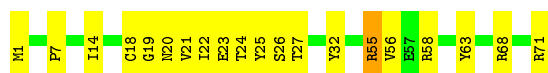
- Molecule 30: 50S ribosomal protein L31

Chain R4: 68% 27% 6%



- Molecule 30: 50S ribosomal protein L31

Chain Y4: 72% 27% .



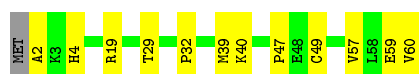
- Molecule 31: 50S ribosomal protein L32

Chain R5: 70% 27%



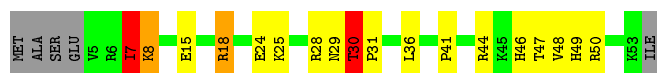
- Molecule 31: 50S ribosomal protein L32

Chain Y5: 78% 20%



- Molecule 32: 50S ribosomal protein L33

Chain R6: 57% 26% 9%



- Molecule 32: 50S ribosomal protein L33

Chain Y6: 63% 26% 9%



- Molecule 33: 50S ribosomal protein L34

Chain R7: 84% 16%



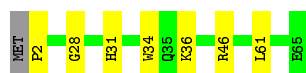
- Molecule 33: 50S ribosomal protein L34

Chain Y7: 90% 10%



- Molecule 34: 50S ribosomal protein L35

Chain R8: 88% 11%



- Molecule 34: 50S ribosomal protein L35



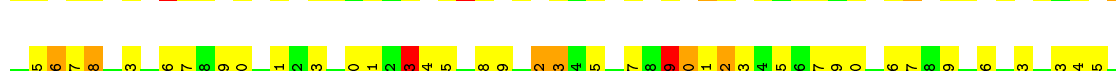
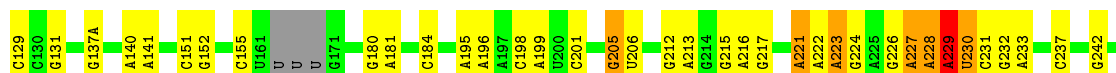
- Molecule 35: 50S ribosomal protein L36



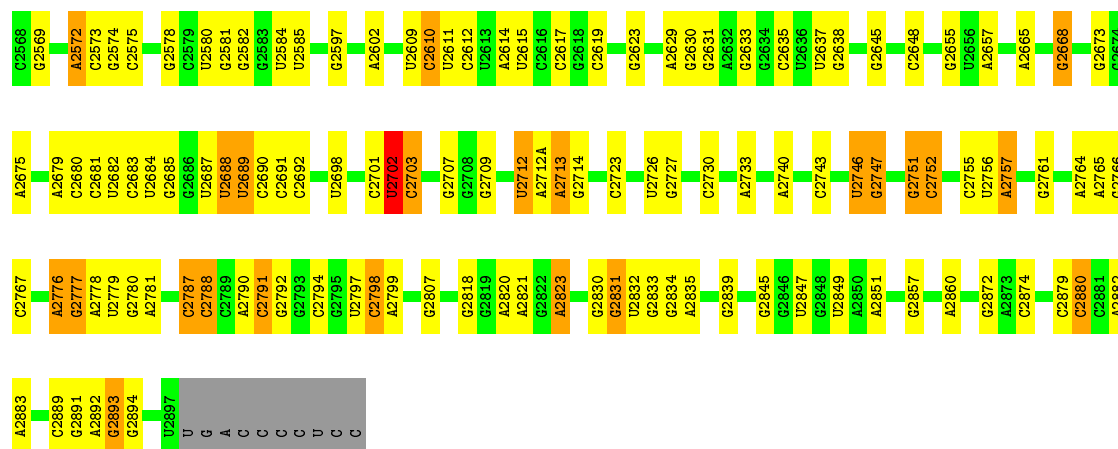
- Molecule 35: 50S ribosomal protein L36



- Molecule 36: 23S rRNA

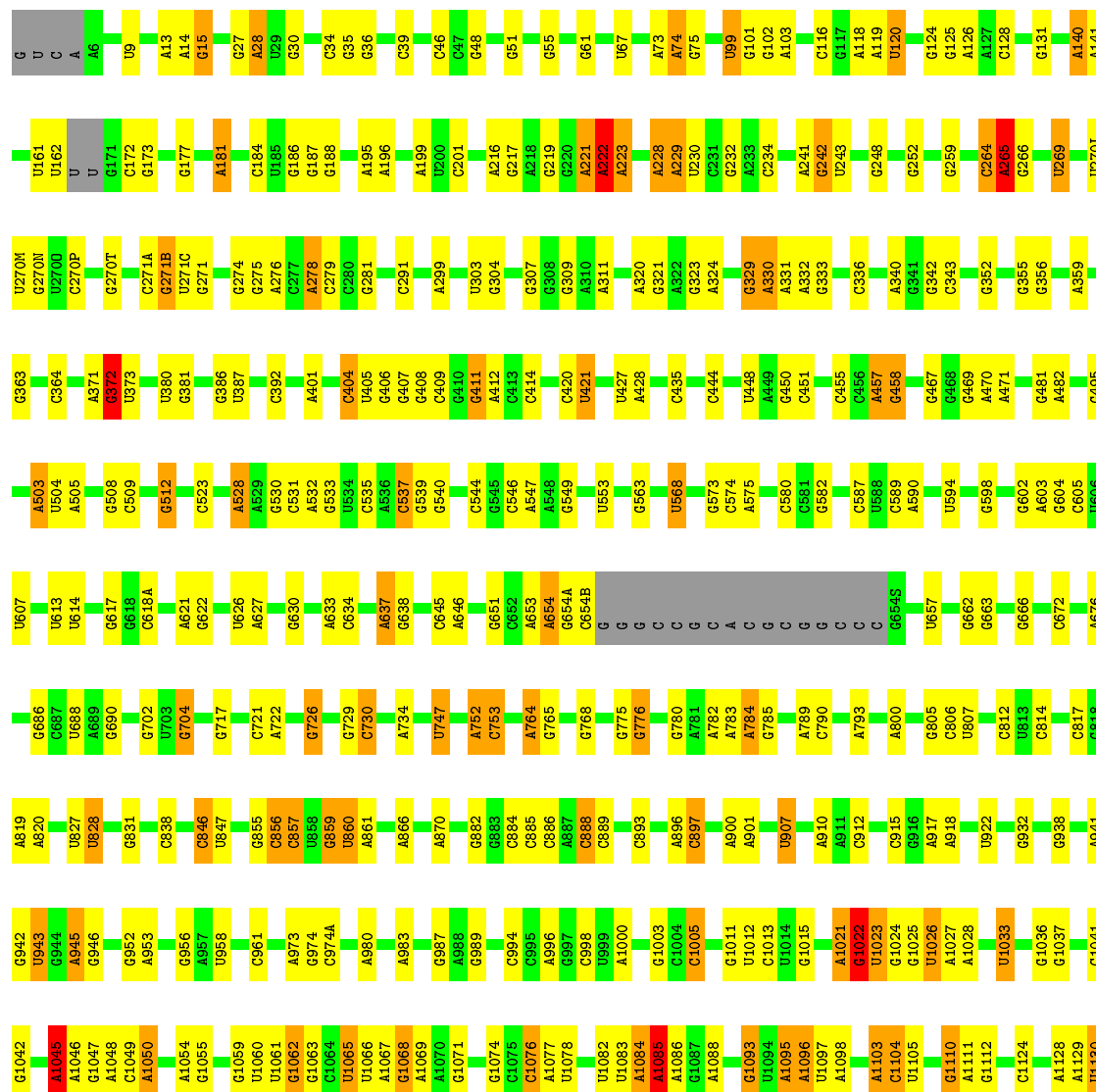


C2441	G2318	G2210	G2111	C1979	A1558	A1449	A1317	G1173	U1078	A1000	A901	A783
G2319	G2211	G2212	G2112	C1980	G1559	G1449A	A1321	A1174	C1079	A1003	C904	A784
A2320	U2213	U2214	U2113	A1981	C1565	U1454	G1327	U1175	U1082	G1008	C906	G785
G2445	G2215	G2216	A2114	G1689	A1567	G1455	A1328	A1177	A1084	C1013	C907	C790
G2325	G2115	G2116	G2116	C1684	A1568	C1458	U1329	C1178	A1085	G1011	A910	C791
A2333	A2217	A2218	A2117	G1695	A1569	G1460	C1330	C1179	A1086	U1012	A911	C792
G2334	U2118	U2119	A2119	A1698	A1570	G1461	A1331	C1180	G1087	U1014	C912	A793
A2335	G2120	G2121	G2121	U1576	U1576	C1462	G1332	G1184	A1088	G1015	A913	A800
C2342	G2238	G2239	A2126	G1703	U1577	C1467	U1341	A1189	G1091	C1016	C915	G805
A2346	G2243	U2244	G2127	G1725	U1578	A1467	A1342	A1190	C1092	G1019	C916	C806
C2347	U2245	U2246	G2128	A1853	A1579	A1471	A1349	G1191	G1093	A1020	A917	U807
C2350	G2249	G2250	C2129	G1728	A1581	G1479	U1352	G1192	U1094	A1021	A918	C812
G2484	U2130	G2131	U2130	A1729	A1586	G1480	A1353	G1195	A1095	G1022	A919	C812
G2354	G2131	G2132	G2131	G1731	U1595	U1482	U1353	A1204	A1096	U1023	U930	A819
C2355	U2132	G2133	U2132	C1742	G1595	G1483	A1365	U1205	A1098	G1025	G932	U827
G2494	G2133	A2134	A2134	G1743	C1598	A1486	G1368	U1206	C1104	G1026	G938	U828
G2495	A2135	A2136	A2135	G1756	C1599	A1490	A1378	A1210	U1105	A1027	A941	A829
C2498	G2136	G2137	G2137	G1762	G1600	G1491	A1379	U1211	G1110	U1033	A942	G831
G2502	A2019	A2020	C2138	A1762	A1603	G1492	A1384	G1217	G1112	G1036	A945	G832
A2503	C2021	C2022	C2138	G1763	C1607	G1493	G1385	A1220	U1113	G1039	A946	C838
U2504	G2023	G2023	C2146	G1764	A1608	A1494	A1388	G1236	G1114	U1044	U958	U830
U2506	G2147	G2148	G2147	A1773	A1609	U1497	G1388	A1237	G1115	C1043	A959	U860
G2383	G2148	G2149	G2148	G1776	A1610	C1506	U1391	G1238	G1116	A1045	A861	A861
G2384	G1906	G1907	G2154	G1776	C1617	A1507	U1391	G1238	G1117	A1046	A960	G862
C2385	C1909	C1910	G2155	G1779	A1618	A1508	U1394	G1238	G1122	A1047	A961	A863
A2392	C2039	C2043	G2156	A1780	C1637	A1509	A1395	G1252	C1123	G1048	A969	C856
C2402	C2043	C2043	A2158	C1781	G1622	A1510	C1403	A1284	C1124	U958	A969	C857
C2403	C2055	C2055	G2164	A1784	C1636	G1512	C1404	G1256	A1129	C1049	A969	U860
U2406	G2056	G2056	G2165	A1785	A1637	C1513	C1407	G1266	G1130	A1050	A969	A861
G2410	G2056	G2056	G2166	A1786	C1638	U1514	C1407	U1263	G1131	C1053	C961	G862
C2420	A2059	A2060	U2167	A1787	U1639	G1522	C1411	G1264	C1135	A1054	A969	A866
A2421	G2061	G2062	G2168	G1788	C1640	G1522	C1411	G1264	G1136	A1057	A973	G869
A2422	A2062	A2062	A2170	A1791	C1644	G1525	G1446	U1266	C1139	G1058	C974	G880
C2424	G2069	G2070	A2172	C1795	C1648	A1528	U1419	G1270	C1140	U1060	C974A	G881
C2425	G2070	G2071	A2173	G1799	G1651	A1533	U1420	G1271	U1141	U1061	A980	G882
A2426	A2071	A2071	A2176	G1800	A1652	G1534	G1421	U1273	U1142	U1065	A983	G883
C2427	A2077	A2077	G2176	G1801	G1653	U1535	G1423	A1287	A1143	U1066	A984	C884
G2428	U2086	U2086	G2187	A1802	A1654	C1537	A1427	G1296	G1151	A1067	C985	C885
G2429	C2309	C2309	C2188	G1811	C1662	G1538	C1428	U1300	G1154	G1068	C986	C886
A2430	A2310	A2311	U2189	A1815	C1667	G1542	G1441	A1301	G1155	A1070	A987	A887
U2431	A2311	A2312	G2190	A1816	A1668	A1543	G1442	U1301	A1156	G1071	A989	C888
U2432	U2089	U2089	G2191	G1817	A1668	A1544	G1442	A1301	A1156	A1072	A989	C889
C2433	G2093	G2093	G2192	G1818	A1668	A1544	G1442	A1301	A1156	A1073	A989	A896
A2434	C2314	C2314	G2192	A1819	A1668	A1544	G1442	A1301	A1156	G1074	A989	C897
A2435	G2315	G2315	A2198	A1970	A1668	A1544	G1442	A1301	A1156	C1075	C994	C898
A2564	A2316	A2316	A2199	A1971	G1674	A1545	C1445	A1315	G1170	A1077	C995	A899
A2565	C2317	C2317	A2199	A1972	C1675	A1545	C1445	A1316	G1171	A1077	A996	A900



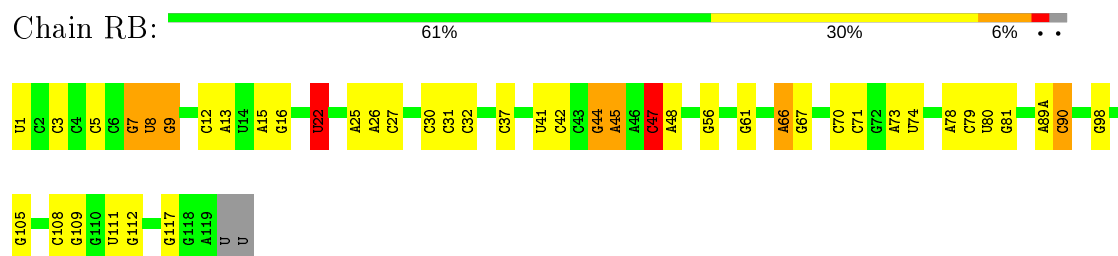
• Molecule 36: 23S rRNA

Chain YA: •

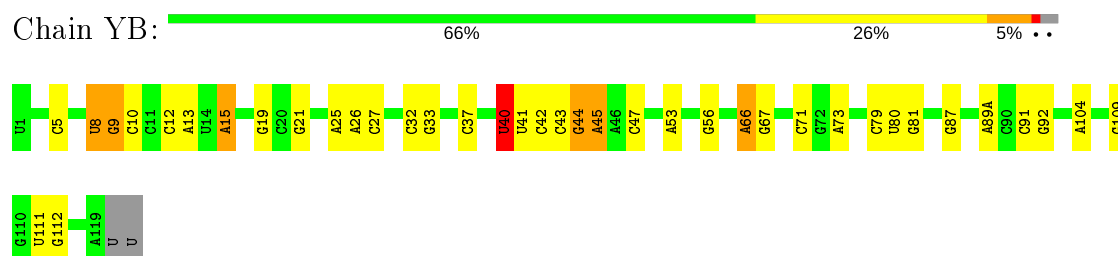




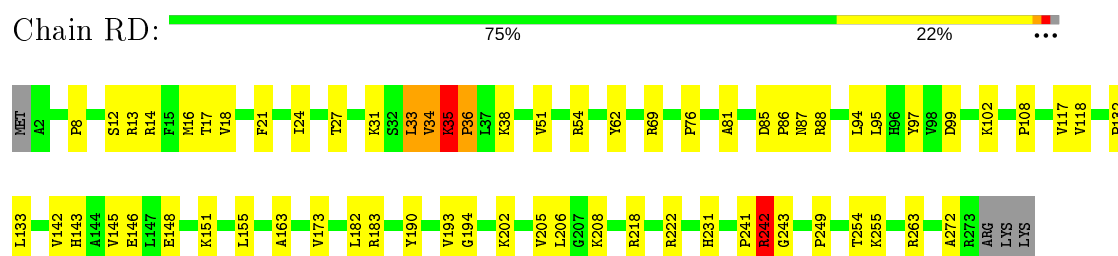
- Molecule 37: 5S rRNA



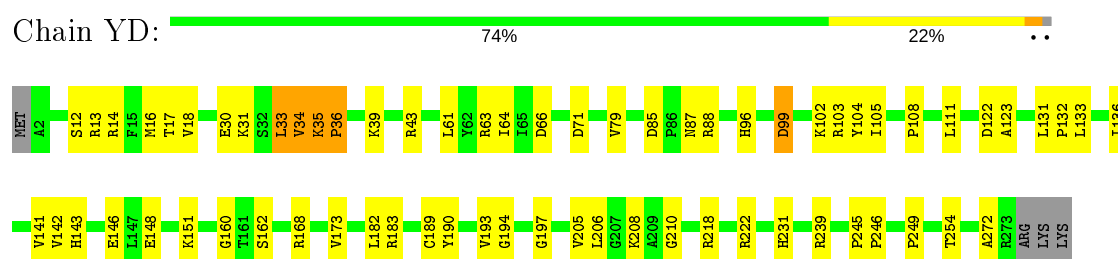
- Molecule 37: 5S rRNA



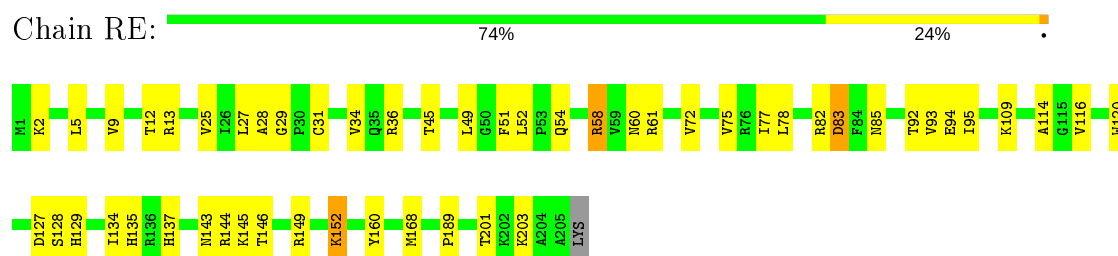
- Molecule 38: 50S ribosomal protein L2



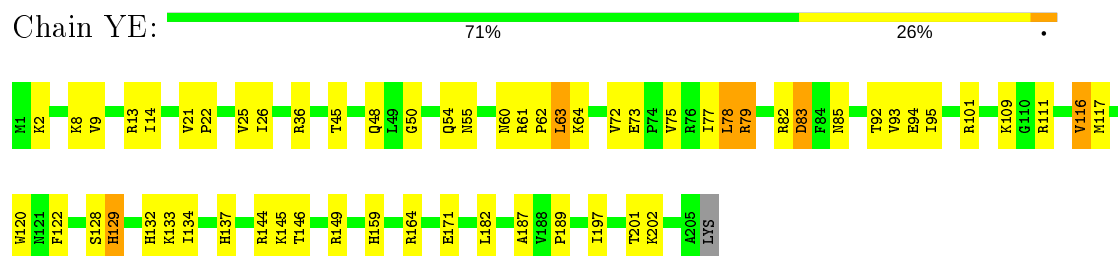
- Molecule 38: 50S ribosomal protein L2



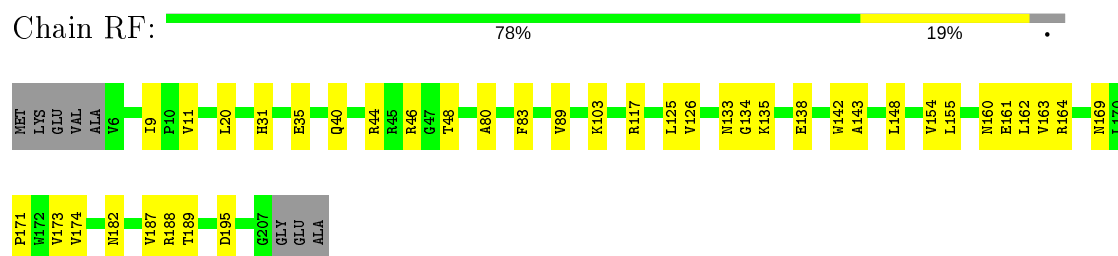
- Molecule 39: 50S ribosomal protein L3



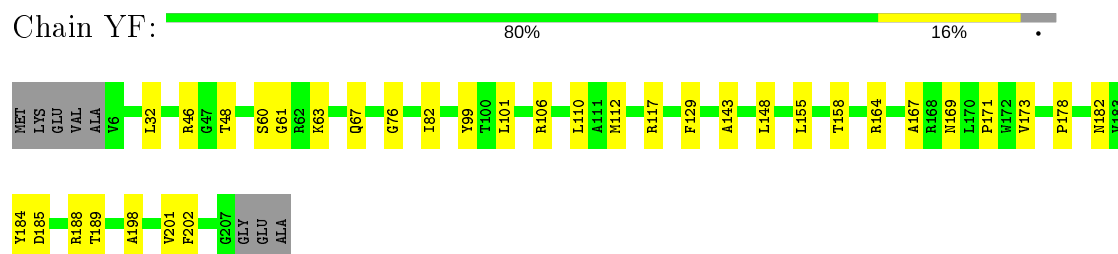
- Molecule 39: 50S ribosomal protein L3



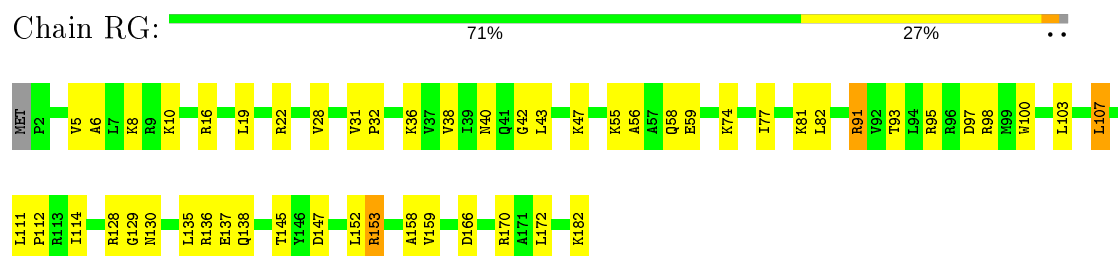
- Molecule 40: 50S ribosomal protein L4



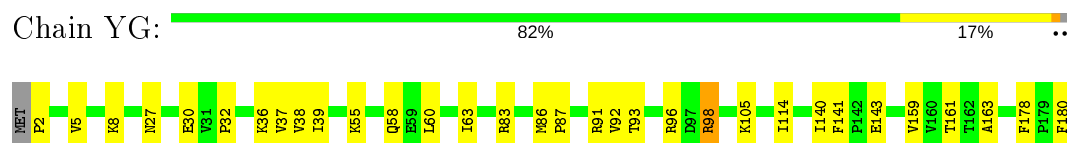
- Molecule 40: 50S ribosomal protein L4




- Molecule 41: 50S ribosomal protein L5



- Molecule 41: 50S ribosomal protein L5



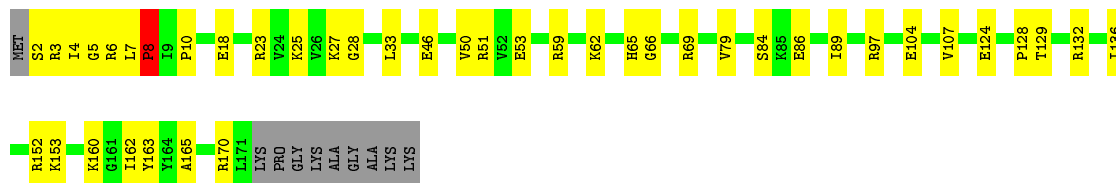
- Molecule 42: 50S ribosomal protein L6

Chain RH:  77% 17% • 6%




- Molecule 42: 50S ribosomal protein L6

Chain YH:  71% 23% • 6%




- Molecule 43: 50S ribosomal protein L9

Chain RI:  86% 13% •



- Molecule 43: 50S ribosomal protein L9

Chain YI:  79% 19% ••




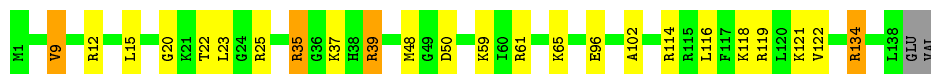
- Molecule 44: 50S ribosomal protein L13

Chain RN:  90% 9% •




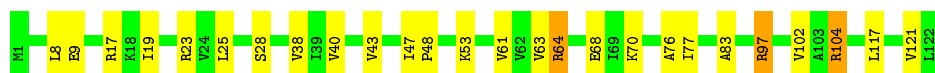
- Molecule 44: 50S ribosomal protein L13

Chain YN:  81% 14% ••



- Molecule 45: 50S ribosomal protein L14

Chain RO:  79% 19% •



- Molecule 45: 50S ribosomal protein L14

Chain YO: 76% 23%



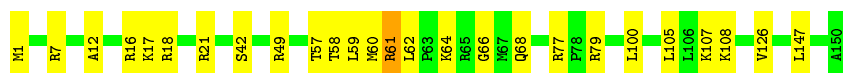
- Molecule 46: 50S ribosomal protein L15

Chain RP: 79% 21%



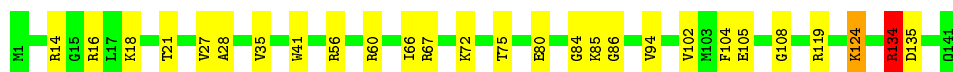
- Molecule 46: 50S ribosomal protein L15

Chain YP: 83% 17%



- Molecule 47: 50S ribosomal protein L16

Chain RQ: 81% 18%



- Molecule 47: 50S ribosomal protein L16

Chain YQ: 72% 27%

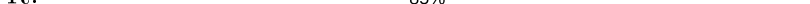


- Molecule 48: 50S ribosomal protein L17

Chain RR: 79% 19%



- Molecule 48: 50S ribosomal protein L17

Chain YR: 



- Molecule 49: 50S ribosomal protein L18

Chain RS: 79% 18% 3%



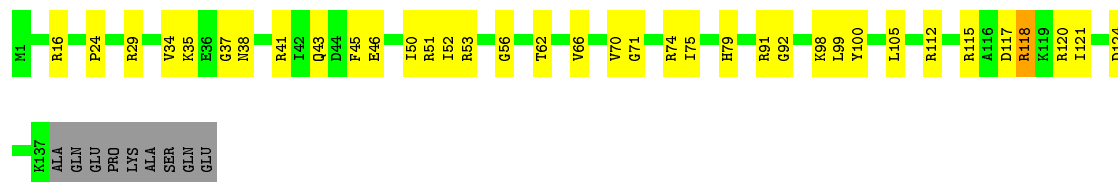
- Molecule 49: 50S ribosomal protein L18

Chain YS: 79% 20%



- Molecule 50: 50S ribosomal protein L19

Chain RT:  69% 24% • 6%



- Molecule 50: 50S ribosomal protein L19

Chain YT:  70% 24% 6%

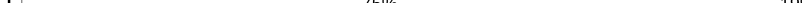


- Molecule 51: 50S ribosomal protein L20

Chain RU: 85% 13%



- Molecule 51: 50S ribosomal protein L20

Chain YU:  75% 19% ..



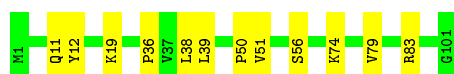
- Molecule 52: 50S ribosomal protein L21

Chain RV: 84% 16%



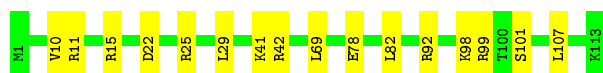
- Molecule 52: 50S ribosomal protein L21

Chain YV: 88% 12%



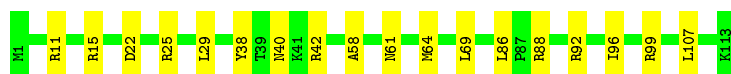
- Molecule 53: 50S ribosomal protein L22

Chain RW: 86% 14%



- Molecule 53: 50S ribosomal protein L22

Chain YW: 84% 16%



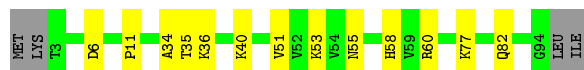
- Molecule 54: 50S ribosomal protein L23

Chain RX: 82% 14% .



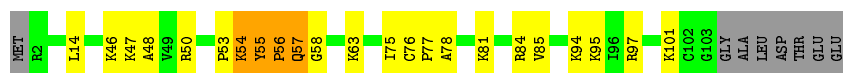
- Molecule 54: 50S ribosomal protein L23

Chain YX: 82% 14% .



- Molecule 55: 50S ribosomal protein L24

Chain RY: 72% 17% . 7%



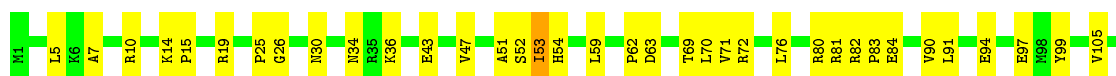
- Molecule 55: 50S ribosomal protein L24

Chain YY: 73% 18% 7%



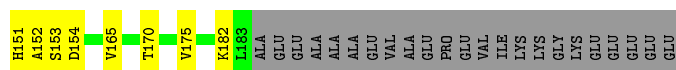
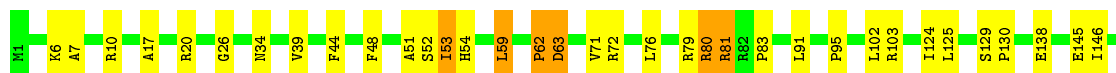
- Molecule 56: 50S ribosomal protein L25

Chain RZ: 62% 26% 11%



- Molecule 56: 50S ribosomal protein L25

Chain YZ: 68% 18% 11%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.00Å 453.48Å 625.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.99 – 3.20	Depositor
% Data completeness (in resolution range)	99.5 (49.99-3.20)	Depositor
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.237 , 0.270	Depositor
Wilson B-factor (Å ²)	99.1	Xtriage
Anisotropy	0.308	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	298371	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PAR, MG, SF4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	QA	0.54	0/36098	1.04	122/56341 (0.2%)
1	XA	0.55	0/36101	1.02	113/56346 (0.2%)
2	QB	0.38	0/1959	0.68	4/2642 (0.2%)
2	XB	0.34	0/1959	0.65	0/2642
3	QC	0.37	0/1629	0.67	0/2195
3	XC	0.32	0/1629	0.63	0/2195
4	QD	0.43	0/1704	0.61	1/2284 (0.0%)
4	XD	0.43	0/1704	0.64	0/2284
5	QE	0.33	0/1171	0.62	0/1576
5	XE	0.37	0/1171	0.66	1/1576 (0.1%)
6	QF	0.39	0/856	0.72	2/1154 (0.2%)
6	XF	0.37	0/856	0.66	0/1154
7	QG	0.33	0/1276	0.56	0/1709
7	XG	0.33	0/1276	0.60	0/1709
8	QH	0.34	0/1136	0.62	0/1527
8	XH	0.33	0/1136	0.61	0/1527
9	QI	0.36	0/1029	0.71	1/1379 (0.1%)
9	XI	0.36	0/1029	0.70	0/1379
10	QJ	0.34	0/814	0.62	0/1095
10	XJ	0.33	0/814	0.62	0/1095
11	QK	0.37	0/900	0.58	0/1213
11	XK	0.36	0/900	0.64	1/1213 (0.1%)
12	QL	0.38	0/991	0.70	1/1327 (0.1%)
12	XL	0.41	0/991	0.74	2/1327 (0.2%)
13	QM	0.37	0/974	0.80	0/1303
13	XM	0.35	0/974	0.77	1/1303 (0.1%)
14	QN	0.43	0/501	0.71	0/664
14	XN	0.50	0/501	0.81	1/664 (0.2%)
15	QO	0.32	0/745	0.56	0/992
15	XO	0.32	0/745	0.53	0/992
16	QP	0.44	0/721	0.74	1/970 (0.1%)
16	XP	0.37	0/721	0.75	1/970 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.45	1/847 (0.1%)	0.64	0/1131
17	XQ	0.33	0/847	0.61	0/1131
18	QR	0.31	0/579	0.59	0/768
18	XR	0.36	0/579	0.61	0/768
19	QS	0.34	0/689	0.66	0/926
19	XS	0.55	0/689	0.87	2/926 (0.2%)
20	QT	0.29	0/765	0.61	0/1007
20	XT	0.30	0/765	0.68	0/1007
21	QU	0.47	0/221	0.68	1/288 (0.3%)
21	XU	0.42	0/221	0.68	1/288 (0.3%)
22	QV	0.49	0/1832	1.04	6/2855 (0.2%)
22	XV	0.53	0/1832	1.02	4/2855 (0.1%)
23	QW	0.49	1/1826 (0.1%)	1.11	12/2845 (0.4%)
23	XW	0.51	1/1826 (0.1%)	1.14	10/2845 (0.4%)
24	QX	0.47	0/471	1.06	2/734 (0.3%)
24	XX	0.46	0/421	0.90	1/656 (0.2%)
25	QY	0.39	0/1791	1.09	8/2791 (0.3%)
25	XY	0.40	0/1816	1.11	14/2830 (0.5%)
26	R0	0.35	0/657	0.62	0/874
26	Y0	0.43	0/657	0.65	0/874
27	R1	0.40	0/770	0.70	1/1022 (0.1%)
27	Y1	0.49	0/770	0.70	0/1022
28	R2	0.33	0/583	0.64	0/771
28	Y2	0.34	0/583	0.69	0/771
29	R3	0.30	0/474	0.55	0/635
29	Y3	0.34	0/474	0.56	0/635
30	R4	0.51	1/594 (0.2%)	0.91	1/795 (0.1%)
30	Y4	0.48	0/594	0.81	1/795 (0.1%)
31	R5	0.39	0/473	0.82	1/639 (0.2%)
31	Y5	0.56	1/473 (0.2%)	0.80	0/639
32	R6	0.69	1/431 (0.2%)	1.10	2/575 (0.3%)
32	Y6	0.46	0/431	0.86	2/575 (0.3%)
33	R7	0.43	0/438	0.65	0/575
33	Y7	0.36	0/438	0.66	0/575
34	R8	0.42	0/525	0.72	0/691
34	Y8	0.43	0/525	0.72	0/691
35	R9	0.29	0/310	0.64	0/407
35	Y9	0.29	0/310	0.53	0/407
36	RA	0.60	0/69521	1.04	215/108529 (0.2%)
36	YA	0.64	1/69543 (0.0%)	1.04	216/108563 (0.2%)
37	RB	0.52	0/2878	1.07	14/4490 (0.3%)
37	YB	0.55	0/2878	1.04	5/4490 (0.1%)
38	RD	0.52	1/2165 (0.0%)	0.79	6/2919 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YD	0.48	0/2165	0.71	0/2919
39	RE	0.55	3/1601 (0.2%)	0.81	2/2160 (0.1%)
39	YE	0.49	0/1601	0.83	3/2160 (0.1%)
40	RF	0.42	0/1620	0.65	0/2194
40	YF	0.44	0/1620	0.68	1/2194 (0.0%)
41	RG	0.42	0/1499	0.74	1/2016 (0.0%)
41	YG	0.35	0/1499	0.70	3/2016 (0.1%)
42	RH	0.35	0/1332	0.76	0/1802
42	YH	0.43	0/1332	0.75	1/1802 (0.1%)
43	RI	0.49	0/1151	0.80	3/1558 (0.2%)
43	YI	0.43	0/1151	0.87	4/1558 (0.3%)
44	RN	0.37	0/1131	0.68	0/1525
44	YN	0.44	0/1131	0.76	4/1525 (0.3%)
45	RO	0.41	0/943	0.64	0/1269
45	YO	0.44	0/943	0.66	0/1269
46	RP	0.41	0/1162	0.77	0/1544
46	YP	0.43	0/1162	0.79	0/1544
47	RQ	0.43	0/1143	0.77	2/1527 (0.1%)
47	YQ	0.44	0/1143	0.76	0/1527
48	RR	0.34	0/982	0.67	0/1312
48	YR	0.35	0/982	0.70	0/1312
49	RS	0.45	0/892	0.80	2/1187 (0.2%)
49	YS	0.42	0/892	0.78	0/1187
50	RT	0.41	0/1155	0.73	0/1542
50	YT	0.37	0/1155	0.72	0/1542
51	RU	0.40	0/982	0.64	1/1306 (0.1%)
51	YU	0.47	1/982 (0.1%)	0.69	1/1306 (0.1%)
52	RV	0.38	0/790	0.70	2/1057 (0.2%)
52	YV	0.43	0/790	0.75	1/1057 (0.1%)
53	RW	0.40	0/911	0.65	0/1220
53	YW	0.36	0/911	0.62	0/1220
54	RX	0.38	0/739	0.62	0/993
54	YX	0.46	0/739	0.63	0/993
55	RY	0.43	0/798	0.82	1/1064 (0.1%)
55	YY	0.44	0/798	0.80	1/1064 (0.1%)
56	RZ	0.36	0/1493	0.79	3/2026 (0.1%)
56	YZ	0.40	0/1493	0.78	4/2026 (0.2%)
All	All	0.54	12/323336 (0.0%)	0.96	817/483880 (0.2%)

All (12) bond length outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	QW	1	G	OP3-P	-10.86	1.48	1.61
23	XW	1	G	OP3-P	-10.84	1.48	1.61
38	RD	35	LYS	C-N	7.52	1.48	1.34
39	RE	58	ARG	CZ-NH1	6.79	1.41	1.33
51	YU	69	CYS	CB-SG	-6.60	1.71	1.82
39	RE	58	ARG	CD-NE	6.23	1.57	1.46
17	QQ	49	GLU	CG-CD	5.99	1.60	1.51
32	R6	30	THR	C-N	5.85	1.45	1.34
31	Y5	60	VAL	CB-CG2	-5.71	1.40	1.52
39	RE	58	ARG	NE-CZ	5.48	1.40	1.33
36	YA	1095	A	N9-C4	5.29	1.41	1.37
30	R4	49	PHE	CB-CG	5.13	1.60	1.51

All (817) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	1317	C	O5'-P-OP1	-31.67	72.70	110.70
1	QA	1317	C	O5'-P-OP2	-24.74	81.02	110.70
1	QA	1317	C	OP1-P-OP2	13.74	140.21	119.60
1	QA	1301	U	N1-C2-O2	11.96	131.17	122.80
1	QA	1158	C	C2-N1-C1'	11.80	131.78	118.80
38	RD	242	ARG	CG-CD-NE	11.60	136.16	111.80
1	XA	1311	G	OP2-P-O3'	-11.37	80.19	105.20
1	QA	1301	U	C2-N1-C1'	11.31	131.27	117.70
1	QA	1301	U	N3-C2-O2	-11.30	114.29	122.20
1	QA	1316	G	OP2-P-O3'	-11.28	80.38	105.20
1	QA	328	C	N1-C2-O2	10.99	125.49	118.90
1	QA	1158	C	N1-C2-O2	10.80	125.38	118.90
1	XA	1054	C	N1-C2-O2	10.68	125.31	118.90
1	QA	328	C	C2-N1-C1'	10.53	130.38	118.80
1	QA	1316	G	OP1-P-O3'	-10.50	82.09	105.20
32	R6	29	ASN	C-N-CA	10.08	146.90	121.70
1	XA	1054	C	C2-N1-C1'	9.72	129.49	118.80
1	XA	1158	C	C2-N1-C1'	9.63	129.40	118.80
36	YA	2506	U	C2-N1-C1'	9.62	129.25	117.70
36	YA	1313	U	C2-N1-C1'	9.53	129.13	117.70
36	RA	2032	G	N3-C4-C5	-9.42	123.89	128.60
36	YA	860	U	N3-C2-O2	-9.42	115.61	122.20
1	QA	1322	C	N1-C2-O2	9.37	124.52	118.90
36	RA	856	C	C6-N1-C2	-9.29	116.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	R5	3	LYS	C-N-CA	9.26	144.86	121.70
36	RA	1914	C	N1-C2-O2	9.22	124.43	118.90
1	QA	1158	C	N3-C2-O2	-9.17	115.48	121.90
36	RA	120	U	N3-C2-O2	-9.14	115.80	122.20
25	QY	55	U	N1-C2-O2	9.02	129.11	122.80
25	XY	70	U	N1-C2-O2	9.01	129.11	122.80
36	YA	828	U	C2-N1-C1'	9.01	128.51	117.70
36	RA	120	U	N1-C2-O2	8.97	129.08	122.80
36	RA	1914	C	C2-N1-C1'	8.97	128.66	118.80
1	XA	1054	C	N3-C2-O2	-8.89	115.67	121.90
36	RA	1050	A	N9-C1'-C2'	-8.81	102.30	112.00
36	RA	613	U	N1-C2-O2	8.79	128.96	122.80
1	QA	328	C	N3-C2-O2	-8.63	115.86	121.90
51	YU	76	TYR	CA-CB-CG	8.62	129.78	113.40
36	YA	120	U	N3-C2-O2	-8.59	116.19	122.20
1	XA	1158	C	N1-C2-O2	8.51	124.01	118.90
36	YA	120	U	N1-C2-O2	8.48	128.74	122.80
36	YA	2506	U	N1-C2-O2	8.44	128.71	122.80
25	QY	55	U	N3-C2-O2	-8.40	116.32	122.20
1	QA	1322	C	N3-C2-O2	-8.36	116.05	121.90
36	RA	1313	U	N3-C2-O2	-8.33	116.37	122.20
1	QA	1158	C	C6-N1-C1'	-8.25	110.90	120.80
1	XA	812	C	P-O3'-C3'	8.24	129.59	119.70
1	QA	1322	C	C6-N1-C2	-8.22	117.01	120.30
25	XY	70	U	N3-C2-O2	-8.22	116.44	122.20
36	RA	120	U	C2-N1-C1'	8.22	127.56	117.70
25	XY	70	U	C2-N1-C1'	8.21	127.56	117.70
16	XP	38	TYR	CA-CB-CG	8.11	128.81	113.40
36	YA	1914	C	C2-N1-C1'	8.11	127.72	118.80
19	XS	44	MET	CG-SD-CE	8.10	113.16	100.20
36	RA	828	U	C2-N1-C1'	8.10	127.41	117.70
36	RA	2712	U	C2-N1-C1'	8.06	127.37	117.70
36	YA	120	U	C2-N1-C1'	8.05	127.36	117.70
36	RA	613	U	N3-C2-O2	-8.04	116.57	122.20
36	YA	1313	U	N3-C2-O2	-8.04	116.57	122.20
36	YA	1313	U	N1-C2-O2	8.03	128.42	122.80
36	YA	2506	U	N3-C2-O2	-8.00	116.60	122.20
36	RA	828	U	N3-C2-O2	-8.00	116.60	122.20
36	RA	828	U	N1-C2-O2	7.97	128.38	122.80
36	RA	1313	U	C2-N1-C1'	7.95	127.25	117.70
36	RA	2420	C	O5'-P-OP1	-7.91	98.58	105.70
36	RA	1313	U	N1-C2-O2	7.89	128.32	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	RA	227	A	P-O3'-C3'	7.87	129.14	119.70
36	YA	2210	G	C4-N9-C1'	7.79	136.62	126.50
36	RA	613	U	C2-N1-C1'	7.78	127.04	117.70
36	YA	828	U	N1-C2-O2	7.76	128.23	122.80
36	RA	1535	U	C2-N1-C1'	7.74	126.98	117.70
1	XA	1158	C	N3-C2-O2	-7.73	116.49	121.90
36	RA	2032	G	C6-C5-N7	-7.73	125.76	130.40
36	RA	1914	C	N3-C2-O2	-7.73	116.49	121.90
25	QY	55	U	C2-N1-C1'	7.67	126.91	117.70
36	RA	2712	U	N1-C2-O2	7.63	128.15	122.80
1	XA	792	A	O4'-C1'-N9	7.63	114.30	108.20
36	RA	860	U	N3-C2-O2	-7.62	116.86	122.20
36	RA	1543	A	O4'-C1'-N9	7.62	114.30	108.20
36	RA	2210	G	C4-N9-C1'	7.60	136.38	126.50
1	QA	1301	U	C6-N1-C1'	-7.58	110.58	121.20
1	QA	1158	C	C6-N1-C2	-7.51	117.30	120.30
36	YA	856	C	C6-N1-C2	-7.49	117.31	120.30
36	YA	2712	U	N3-C2-O2	-7.47	116.97	122.20
24	QX	18	G	OP2-P-O3'	7.47	121.63	105.20
36	YA	828	U	N3-C2-O2	-7.43	117.00	122.20
1	XA	346	G	N3-C4-N9	7.40	130.44	126.00
36	RA	2703	C	N1-C2-O2	7.39	123.33	118.90
1	QA	932	C	N1-C2-O2	7.37	123.32	118.90
1	QA	1024	G	O5'-P-OP1	7.37	119.55	110.70
40	YF	99	TYR	CA-CB-CG	7.37	127.41	113.40
36	RA	2168	G	C4-N9-C1'	7.37	136.08	126.50
1	QA	789	U	C2-N1-C1'	7.37	126.54	117.70
36	RA	856	C	C5-C6-N1	7.35	124.67	121.00
1	XA	1311	G	OP1-P-O3'	-7.33	89.07	105.20
1	XA	1312	G	O5'-P-OP2	7.31	119.47	110.70
1	QA	328	C	C6-N1-C1'	-7.31	112.03	120.80
1	XA	328	C	P-O3'-C3'	7.30	128.46	119.70
36	RA	1535	U	N1-C2-O2	7.28	127.89	122.80
36	YA	271(B)	G	P-O3'-C3'	7.27	128.42	119.70
1	XA	328	C	N1-C2-O2	7.26	123.25	118.90
36	RA	2702	U	N3-C2-O2	-7.25	117.13	122.20
36	YA	613	U	N3-C2-O2	-7.23	117.14	122.20
36	RA	1407	C	N1-C2-O2	7.22	123.23	118.90
22	XV	67	C	N1-C2-O2	7.22	123.23	118.90
36	YA	838	C	N1-C2-O2	7.20	123.22	118.90
36	YA	2688	U	N3-C2-O2	-7.18	117.17	122.20
1	QA	1065	U	P-O3'-C3'	7.18	128.32	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	RA	2889	C	N1-C2-O2	7.18	123.21	118.90
36	RA	2712	U	N3-C2-O2	-7.15	117.19	122.20
1	XA	812	C	OP2-P-O3'	7.14	120.91	105.20
1	XA	367	U	C2'-C3'-O3'	7.13	125.19	109.50
36	RA	2032	G	N3-C4-N9	7.11	130.26	126.00
1	XA	1158	C	C6-N1-C2	-7.10	117.46	120.30
1	XA	346	G	N3-C4-C5	-7.09	125.05	128.60
36	RA	1012	U	OP2-P-O3'	7.09	120.80	105.20
1	XA	254	G	O5'-P-OP1	-7.09	99.32	105.70
1	XA	1054	C	C6-N1-C1'	-7.08	112.30	120.80
1	XA	449	C	C2-N1-C1'	7.08	126.59	118.80
1	XA	328	C	C2-N1-C1'	7.07	126.58	118.80
32	R6	7	ILE	C-N-CA	7.06	139.36	121.70
36	RA	1558	A	P-O3'-C3'	7.06	128.17	119.70
1	QA	328	C	C6-N1-C2	-7.05	117.48	120.30
36	RA	1882	C	C6-N1-C2	-7.05	117.48	120.30
36	YA	1026	U	P-O3'-C3'	7.04	128.15	119.70
1	QA	328	C	P-O3'-C3'	7.03	128.14	119.70
36	YA	1558	A	P-O3'-C3'	7.03	128.14	119.70
36	RA	1535	U	N3-C2-O2	-7.02	117.29	122.20
1	QA	1297	C	P-O3'-C3'	7.01	128.11	119.70
36	YA	372	G	P-O3'-C3'	7.00	128.11	119.70
38	RD	242	ARG	CA-CB-CG	7.00	128.81	113.40
1	XA	1297	C	P-O3'-C3'	7.00	128.10	119.70
36	RA	285	C	N1-C2-O2	6.99	123.09	118.90
36	YA	2321	G	C4-N9-C1'	6.96	135.55	126.50
36	YA	860	U	N1-C2-O2	6.96	127.67	122.80
36	RA	2702	U	N1-C2-O2	6.95	127.67	122.80
1	XA	992	U	P-O3'-C3'	6.95	128.04	119.70
36	YA	404	C	P-O3'-C3'	6.93	128.02	119.70
36	YA	846	C	P-O3'-C3'	6.93	128.01	119.70
36	YA	1535	U	C2-N1-C1'	6.92	126.00	117.70
2	QB	137	ARG	CD-NE-CZ	6.91	133.28	123.60
1	QA	1498	U	P-O3'-C3'	6.90	127.98	119.70
1	QA	792	A	P-O3'-C3'	6.88	127.95	119.70
36	RA	229	A	OP2-P-O3'	6.87	120.32	105.20
1	XA	1027	C	P-O3'-C3'	6.86	127.94	119.70
36	YA	1914	C	N1-C2-O2	6.86	123.02	118.90
36	YA	618(A)	C	N1-C2-O2	6.86	123.02	118.90
23	QW	39	G	N3-C4-N9	6.86	130.12	126.00
6	QF	59	TYR	CA-CB-CG	6.86	126.43	113.40
1	QA	1322	C	C2-N1-C1'	6.85	126.33	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	1285	A	P-O3'-C3'	6.84	127.91	119.70
36	YA	2584	U	C2-N1-C1'	6.84	125.91	117.70
36	RA	2688	U	N3-C2-O2	-6.84	117.41	122.20
36	RA	846	C	P-O3'-C3'	6.83	127.90	119.70
25	XY	55	U	C2-N1-C1'	6.83	125.89	117.70
1	QA	181	G	P-O3'-C3'	6.82	127.88	119.70
1	XA	754	C	C2-N1-C1'	6.80	126.28	118.80
1	QA	789	U	N3-C2-O2	-6.80	117.44	122.20
36	RA	669	G	C4-N9-C1'	6.79	135.32	126.50
36	YA	2712	U	N1-C2-O2	6.79	127.55	122.80
36	RA	529	A	N7-C8-N9	6.78	117.19	113.80
1	XA	346	G	C4-N9-C1'	6.78	135.31	126.50
36	RA	1050	A	C4'-C3'-O3'	6.75	126.51	113.00
36	YA	2210	G	N3-C4-C5	-6.75	125.22	128.60
25	XY	70	U	OP1-P-O3'	6.73	120.01	105.20
36	RA	456	C	N1-C2-O2	6.73	122.94	118.90
36	RA	229	A	P-O3'-C3'	6.72	127.77	119.70
36	YA	2749	A	O5'-P-OP1	6.72	118.77	110.70
1	QA	1528	U	P-O3'-C3'	6.71	127.75	119.70
1	XA	449	C	N1-C2-O2	6.70	122.92	118.90
1	QA	1285	A	P-O3'-C3'	6.69	127.73	119.70
36	RA	404	C	P-O3'-C3'	6.69	127.73	119.70
1	QA	1202	G	O5'-P-OP1	-6.68	99.69	105.70
36	YA	1022	G	P-O3'-C3'	6.68	127.72	119.70
36	YA	893	C	N1-C2-O2	6.67	122.90	118.90
36	RA	1022	G	P-O3'-C3'	6.67	127.71	119.70
36	RA	205	G	P-O3'-C3'	6.67	127.70	119.70
36	YA	2210	G	N3-C4-N9	6.66	130.00	126.00
23	QW	39	G	C4-N9-C1'	6.66	135.16	126.50
36	YA	1095	A	C2-N3-C4	6.66	113.93	110.60
1	QA	992	U	P-O3'-C3'	6.64	127.67	119.70
37	RB	47	C	N1-C2-O2	6.64	122.88	118.90
36	YA	1314	C	N1-C2-O2	6.63	122.88	118.90
1	QA	1347	G	OP2-P-O3'	6.63	119.78	105.20
1	QA	812	C	P-O3'-C3'	6.63	127.66	119.70
1	QA	250	A	P-O3'-C3'	6.62	127.64	119.70
1	XA	1498	U	P-O3'-C3'	6.62	127.64	119.70
36	YA	140	A	N7-C8-N9	6.61	117.10	113.80
36	YA	2885	C	N1-C2-O2	6.61	122.86	118.90
36	YA	1535	U	N3-C2-O2	-6.61	117.57	122.20
36	RA	1786	A	N7-C8-N9	6.61	117.10	113.80
36	RA	1012	U	P-O3'-C3'	6.60	127.62	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	YA	752	A	P-O3'-C3'	6.60	127.62	119.70
36	YA	99	U	P-O3'-C3'	6.59	127.61	119.70
1	QA	687	A	P-O3'-C3'	6.59	127.61	119.70
36	RA	372	G	P-O3'-C3'	6.58	127.60	119.70
37	RB	31	C	N1-C2-O2	6.58	122.85	118.90
36	YA	99	U	OP2-P-O3'	6.58	119.68	105.20
36	YA	1653	G	P-O3'-C3'	6.56	127.57	119.70
36	RA	2889	C	C2-N1-C1'	6.54	126.00	118.80
43	YI	132	PRO	C-N-CA	6.54	138.05	121.70
49	RS	110	LEU	CA-CB-CG	6.53	130.33	115.30
36	YA	2210	G	C8-N9-C1'	-6.53	118.51	127.00
36	RA	856	C	N1-C2-O2	6.53	122.82	118.90
36	YA	1882	C	N1-C2-O2	6.53	122.82	118.90
1	QA	1027	C	P-O3'-C3'	6.52	127.53	119.70
36	RA	2787	C	C6-N1-C2	-6.51	117.69	120.30
22	QV	17	C	N1-C2-O2	6.51	122.81	118.90
36	RA	231	C	N1-C2-O2	6.51	122.81	118.90
1	XA	687	A	P-O3'-C3'	6.50	127.51	119.70
36	YA	1005	C	N1-C2-O2	6.50	122.80	118.90
36	YA	2321	G	N3-C4-C5	-6.50	125.35	128.60
1	QA	1346	A	P-O3'-C3'	6.47	127.47	119.70
1	XA	1267	C	C6-N1-C2	-6.47	117.71	120.30
1	QA	753	A	P-O3'-C3'	6.46	127.45	119.70
36	RA	530	G	O4'-C1'-N9	6.46	113.37	108.20
36	YA	503	A	P-O3'-C3'	6.46	127.45	119.70
1	XA	960	U	N1-C2-O2	6.44	127.31	122.80
36	YA	2681	C	P-O3'-C3'	6.44	127.42	119.70
36	YA	1445	C	N1-C2-O2	6.43	122.76	118.90
1	QA	369	C	N1-C2-O2	6.43	122.75	118.90
36	YA	1544	C	N1-C2-O2	6.42	122.75	118.90
36	RA	2889	C	N3-C2-O2	-6.42	117.41	121.90
1	QA	960	U	N1-C2-O2	6.41	127.29	122.80
36	YA	222	A	P-O3'-C3'	6.41	127.39	119.70
36	YA	637	A	P-O3'-C3'	6.41	127.39	119.70
1	QA	1336	C	N1-C2-O2	6.41	122.75	118.90
36	YA	1402	C	C6-N1-C2	-6.41	117.74	120.30
1	XA	545	C	C6-N1-C2	-6.40	117.74	120.30
1	XA	960	U	C2-N1-C1'	6.40	125.38	117.70
1	XA	1158	C	C6-N1-C1'	-6.40	113.12	120.80
23	XW	60	C	C6-N1-C2	-6.38	117.75	120.30
1	QA	1322	C	C5-C6-N1	6.38	124.19	121.00
36	RA	1045	A	P-O3'-C3'	6.38	127.35	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	RA	1686	C	N1-C2-O2	6.38	122.73	118.90
36	RA	2210	G	N3-C4-C5	-6.37	125.41	128.60
36	RA	1914	C	C6-N1-C1'	-6.37	113.16	120.80
23	QW	58	A	P-O3'-C3'	6.36	127.33	119.70
1	XA	60	A	P-O3'-C3'	6.36	127.33	119.70
36	YA	1445	C	N3-C2-O2	-6.36	117.45	121.90
1	XA	789	U	N3-C2-O2	-6.35	117.75	122.20
1	XA	484	G	P-O3'-C3'	6.35	127.32	119.70
1	QA	913	A	P-O3'-C3'	6.35	127.31	119.70
23	XW	58	A	P-O3'-C3'	6.33	127.30	119.70
36	YA	2015	A	C2-N3-C4	6.33	113.77	110.60
36	RA	2468	G	C4-N9-C1'	6.33	134.72	126.50
36	RA	265	A	O4'-C1'-N9	6.32	113.26	108.20
30	Y4	22	ILE	C-N-CA	6.32	137.51	121.70
36	YA	2321	G	N3-C4-N9	6.32	129.79	126.00
36	RA	2831	G	O5'-P-OP1	-6.32	100.02	105.70
36	RA	2126	A	P-O3'-C3'	6.31	127.27	119.70
1	XA	88	C	N1-C2-O2	6.31	122.69	118.90
36	RA	1882	C	N1-C2-O2	6.31	122.68	118.90
36	YA	2712	U	P-O3'-C3'	6.31	127.27	119.70
1	XA	754	C	N1-C2-O2	6.30	122.68	118.90
1	QA	484	G	P-O3'-C3'	6.30	127.26	119.70
36	RA	2032	G	C4-C5-C6	6.30	122.58	118.80
37	RB	71	C	N1-C2-O2	6.30	122.68	118.90
56	YZ	62	PRO	C-N-CA	6.29	137.44	121.70
1	QA	932	C	C2-N1-C1'	6.29	125.72	118.80
36	YA	343	C	C6-N1-C2	-6.28	117.79	120.30
24	QX	18	G	P-O3'-C3'	6.28	127.23	119.70
36	RA	2168	G	N3-C4-C5	-6.28	125.46	128.60
36	YA	2506	U	C6-N1-C1'	-6.27	112.42	121.20
39	YE	78	LEU	C-N-CA	6.27	137.37	121.70
43	YI	11	ASN	C-N-CA	6.27	137.37	121.70
1	QA	1260	C	C6-N1-C2	-6.26	117.80	120.30
1	QA	960	U	N3-C2-O2	-6.26	117.82	122.20
1	XA	410	G	OP1-P-O3'	6.25	118.96	105.20
36	RA	2787	C	C5-C6-N1	6.25	124.13	121.00
36	RA	1882	C	C5-C6-N1	6.25	124.12	121.00
36	YA	2610	C	P-O3'-C3'	6.24	127.18	119.70
36	RA	285	C	N3-C2-O2	-6.23	117.54	121.90
1	XA	913	A	P-O3'-C3'	6.23	127.18	119.70
36	RA	155	C	N1-C2-O2	6.23	122.64	118.90
12	XL	98	TYR	CA-CB-CG	6.23	125.23	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	1397	C	N1-C2-O2	6.22	122.64	118.90
1	XA	545	C	N1-C2-O2	6.21	122.63	118.90
36	RA	2210	G	C8-N9-C1'	-6.21	118.92	127.00
36	RA	637	A	P-O3'-C3'	6.20	127.14	119.70
36	RA	898	C	N1-C2-O2	6.20	122.62	118.90
36	YA	229	A	P-O3'-C3'	6.19	127.13	119.70
25	XY	16	C	C6-N1-C2	-6.19	117.83	120.30
36	RA	1653	G	P-O3'-C3'	6.18	127.12	119.70
39	RE	58	ARG	CD-NE-CZ	6.17	132.24	123.60
36	RA	1407	C	C2-N1-C1'	6.17	125.59	118.80
36	RA	1509	C	C6-N1-C2	-6.17	117.83	120.30
22	QV	34	C	N1-C2-O2	6.17	122.60	118.90
1	QA	90	C	N1-C2-O2	6.16	122.60	118.90
1	QA	485	G	P-O3'-C3'	6.16	127.09	119.70
36	YA	859	G	P-O3'-C3'	6.16	127.09	119.70
36	RA	271(B)	G	P-O3'-C3'	6.15	127.08	119.70
36	YA	1992	G	P-O3'-C3'	6.15	127.08	119.70
36	YA	1313	U	C6-N1-C1'	-6.15	112.59	121.20
23	QW	39	G	N3-C4-C5	-6.15	125.53	128.60
36	YA	1314	C	C2-N1-C1'	6.14	125.56	118.80
41	YG	83	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	XA	244	U	P-O3'-C3'	6.12	127.05	119.70
36	YA	912	C	N3-C2-O2	-6.12	117.61	121.90
1	XA	980	C	N1-C2-O2	6.12	122.57	118.90
1	QA	412	A	P-O3'-C3'	6.12	127.05	119.70
21	XU	18	TYR	CA-CB-CG	6.12	125.02	113.40
36	YA	1314	C	C6-N1-C2	-6.12	117.85	120.30
36	YA	1464	C	N1-C2-O2	6.12	122.57	118.90
36	YA	221	A	P-O3'-C3'	6.11	127.03	119.70
1	XA	412	A	P-O3'-C3'	6.11	127.03	119.70
36	YA	1535	U	N1-C2-O2	6.10	127.07	122.80
36	RA	2712	U	P-O3'-C3'	6.10	127.02	119.70
36	YA	1204	A	O4'-C1'-N9	6.10	113.08	108.20
36	YA	242	G	P-O3'-C3'	6.09	127.01	119.70
36	YA	1445	C	C6-N1-C2	-6.09	117.86	120.30
1	XA	690	G	O4'-C1'-N9	6.09	113.07	108.20
23	QW	70	U	N3-C2-O2	-6.07	117.95	122.20
36	RA	2060	A	P-O3'-C3'	6.07	126.98	119.70
22	XV	67	C	N3-C2-O2	-6.07	117.65	121.90
36	RA	205	G	OP2-P-O3'	6.05	118.52	105.20
43	RI	50	ARG	CD-NE-CZ	6.05	132.07	123.60
36	YA	1180	C	N1-C2-O2	6.05	122.53	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	346	G	N3-C4-N9	6.05	129.63	126.00
37	RB	31	C	N3-C2-O2	-6.05	117.67	121.90
36	RA	912	C	N1-C2-O2	6.04	122.53	118.90
36	YA	1914	C	N3-C2-O2	-6.03	117.68	121.90
1	XA	963	G	C6-C5-N7	-6.03	126.78	130.40
36	RA	2468	G	O4'-C1'-N9	6.03	113.02	108.20
1	XA	221	C	N1-C2-O2	6.02	122.51	118.90
1	QA	115	G	P-O3'-C3'	6.02	126.93	119.70
36	RA	2321	G	C4-N9-C1'	6.02	134.33	126.50
36	YA	856	C	P-O3'-C3'	6.02	126.92	119.70
16	QP	38	TYR	CA-CB-CG	6.01	124.83	113.40
36	RA	2210	G	N3-C4-N9	6.01	129.61	126.00
36	RA	838	C	N1-C2-O2	6.01	122.51	118.90
36	RA	1799	G	P-O3'-C3'	6.01	126.91	119.70
36	RA	1407	C	N3-C2-O2	-6.00	117.70	121.90
36	RA	1427	A	P-O3'-C3'	6.00	126.89	119.70
56	YZ	59	LEU	CA-CB-CG	6.00	129.09	115.30
36	YA	1446	C	N1-C2-O2	5.99	122.50	118.90
36	RA	1509	C	C5-C6-N1	5.99	124.00	121.00
36	YA	2688	U	C2-N1-C1'	5.99	124.89	117.70
36	YA	2787	C	N1-C2-O2	5.99	122.49	118.90
1	XA	345	C	P-O3'-C3'	5.99	126.88	119.70
1	QA	1097	C	N1-C2-O2	5.98	122.49	118.90
36	YA	613	U	C2-N1-C1'	5.98	124.88	117.70
1	QA	1347	G	P-O3'-C3'	5.98	126.87	119.70
36	RA	221	A	P-O3'-C3'	5.98	126.87	119.70
36	YA	1691	C	N1-C2-O2	5.97	122.48	118.90
1	XA	115	G	P-O3'-C3'	5.97	126.86	119.70
1	QA	449	C	C2-N1-C1'	5.97	125.36	118.80
1	QA	972	C	C6-N1-C2	-5.96	117.92	120.30
36	YA	1045	A	P-O3'-C3'	5.96	126.85	119.70
36	RA	856	C	N3-C2-O2	-5.95	117.73	121.90
1	QA	64	G	P-O3'-C3'	5.95	126.84	119.70
36	YA	1178	C	P-O3'-C3'	5.95	126.84	119.70
1	QA	789	U	N1-C2-O2	5.95	126.96	122.80
37	YB	40	U	N1-C2-O2	5.94	126.96	122.80
36	RA	99	U	P-O3'-C3'	5.94	126.82	119.70
36	YA	828	U	C6-N1-C1'	-5.94	112.89	121.20
1	XA	346	G	C8-N9-C1'	-5.93	119.29	127.00
22	QV	17	C	C2-N1-C1'	5.93	125.32	118.80
36	YA	2559	C	N1-C2-O2	5.93	122.46	118.90
36	RA	1513	C	C2-N1-C1'	5.92	125.32	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	YA	271(B)	G	OP2-P-O3'	5.92	118.22	105.20
1	XA	960	U	N3-C2-O2	-5.92	118.06	122.20
1	QA	328	C	C5-C6-N1	5.91	123.96	121.00
1	QA	1038	C	N1-C2-O2	5.91	122.45	118.90
1	XA	485	G	P-O3'-C3'	5.91	126.80	119.70
1	QA	410	G	OP1-P-O3'	5.91	118.21	105.20
1	XA	753	A	P-O3'-C3'	5.91	126.79	119.70
36	YA	1411	C	C6-N1-C2	-5.91	117.94	120.30
36	RA	372	G	OP2-P-O3'	5.91	118.20	105.20
36	RA	2168	G	C8-N9-C1'	-5.91	119.32	127.00
36	YA	2321	G	C8-N9-C1'	-5.91	119.32	127.00
56	RZ	63	ASP	CB-CG-OD1	5.90	123.61	118.30
24	XX	18	G	P-O3'-C3'	5.90	126.78	119.70
1	QA	1260	C	N3-C2-O2	-5.89	117.78	121.90
36	YA	2126	A	P-O3'-C3'	5.89	126.77	119.70
43	YI	12	LEU	CA-CB-CG	5.89	128.84	115.30
1	QA	1225	A	C4-N9-C1'	5.89	136.90	126.30
23	QW	60	C	C2-N1-C1'	5.89	125.28	118.80
36	RA	231	C	C2-N1-C1'	5.89	125.28	118.80
36	YA	195	A	P-O3'-C3'	5.88	126.76	119.70
36	YA	1402	C	C5-C6-N1	5.87	123.94	121.00
36	RA	1786	A	C4-N9-C1'	5.86	136.85	126.30
36	YA	1694	C	P-O3'-C3'	5.86	126.73	119.70
25	QY	16	C	C6-N1-C2	-5.86	117.96	120.30
36	YA	1021	A	C8-N9-C4	-5.85	103.46	105.80
1	XA	1038	C	N1-C2-O2	5.84	122.40	118.90
36	YA	264	C	N1-C2-O2	5.84	122.40	118.90
55	YY	4	LYS	C-N-CA	5.83	136.27	121.70
1	XA	89	U	P-O3'-C3'	5.82	126.69	119.70
36	YA	1640	C	C6-N1-C2	-5.82	117.97	120.30
36	RA	1992	G	P-O3'-C3'	5.82	126.69	119.70
1	QA	244	U	P-O3'-C3'	5.82	126.68	119.70
36	RA	1513	C	N1-C2-O2	5.82	122.39	118.90
36	YA	2439	A	P-O3'-C3'	5.81	126.68	119.70
23	QW	60	C	N1-C2-O2	5.81	122.39	118.90
36	YA	1914	C	C6-N1-C1'	-5.81	113.83	120.80
36	RA	2776	A	P-O3'-C3'	5.81	126.67	119.70
1	QA	266	G	P-O3'-C3'	5.81	126.67	119.70
1	XA	932	C	N1-C2-O2	5.80	122.38	118.90
36	RA	1204	A	O4'-C1'-N9	5.80	112.84	108.20
36	YA	912	C	N1-C2-O2	5.80	122.38	118.90
36	YA	229	A	OP2-P-O3'	5.79	117.95	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	YA	1950	G	O4'-C1'-N9	5.79	112.83	108.20
1	QA	754	C	N1-C2-O2	5.79	122.37	118.90
36	RA	2439	A	P-O3'-C3'	5.79	126.64	119.70
36	RA	1694	C	P-O3'-C3'	5.78	126.64	119.70
37	RB	31	C	C6-N1-C2	-5.78	117.99	120.30
36	RA	1078	U	P-O3'-C3'	5.77	126.63	119.70
36	YA	1950	G	C4-N9-C1'	5.77	134.00	126.50
36	RA	2648	C	N1-C2-O2	5.76	122.36	118.90
36	YA	1005	C	N3-C2-O2	-5.76	117.87	121.90
36	RA	1882	C	C2-N1-C1'	5.76	125.14	118.80
36	RA	1174	A	C4-N9-C1'	5.75	136.66	126.30
36	RA	512	G	P-O3'-C3'	5.75	126.60	119.70
36	RA	1314	C	C5-C6-N1	5.75	123.88	121.00
1	XA	250	A	P-O3'-C3'	5.75	126.60	119.70
36	RA	2314	C	N1-C2-O2	5.75	122.35	118.90
36	RA	752	A	P-O3'-C3'	5.74	126.59	119.70
36	RA	1407	C	C6-N1-C2	-5.74	118.00	120.30
36	YA	1085	A	P-O3'-C3'	5.74	126.59	119.70
23	QW	58	A	OP1-P-O3'	5.74	117.83	105.20
36	YA	1427	A	P-O3'-C3'	5.74	126.58	119.70
36	RA	503	A	P-O3'-C3'	5.73	126.58	119.70
56	RZ	111	VAL	C-N-CA	5.73	136.03	121.70
36	YA	1799	G	P-O3'-C3'	5.73	126.58	119.70
1	XA	1301	U	P-O3'-C3'	5.73	126.57	119.70
1	QA	1200	C	P-O3'-C3'	5.72	126.57	119.70
36	YA	1180	C	N3-C2-O2	-5.72	117.89	121.90
1	XA	754	C	N3-C2-O2	-5.72	117.90	121.90
36	RA	1742	C	N1-C2-O2	5.71	122.33	118.90
36	YA	2566	A	P-O3'-C3'	5.71	126.55	119.70
1	QA	1260	C	N1-C2-O2	5.71	122.32	118.90
36	YA	688	U	C5-C6-N1	5.71	125.55	122.70
36	YA	333	G	C4-N9-C1'	5.71	133.92	126.50
36	YA	859	G	OP2-P-O3'	5.70	117.74	105.20
1	QA	449	C	N1-C2-O2	5.70	122.32	118.90
36	RA	2688	U	N1-C2-O2	5.70	126.79	122.80
36	RA	2689	U	P-O3'-C3'	5.70	126.53	119.70
36	RA	2471	C	C6-N1-C2	-5.69	118.02	120.30
41	YG	83	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	QA	703	G	P-O3'-C3'	5.69	126.52	119.70
36	RA	269	U	N1-C2-O2	5.69	126.78	122.80
36	RA	74	A	P-O3'-C3'	5.68	126.52	119.70
39	RE	27	LEU	CA-CB-CG	5.68	128.37	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	RA	140	A	N7-C8-N9	5.68	116.64	113.80
36	YA	838	C	N3-C2-O2	-5.68	117.92	121.90
36	RA	1776	G	C4-N9-C1'	5.68	133.89	126.50
36	YA	1992	G	OP2-P-O3'	5.68	117.69	105.20
1	QA	314	C	C6-N1-C2	-5.67	118.03	120.30
36	RA	41	C	N1-C2-O2	5.67	122.30	118.90
36	YA	140	A	C8-N9-C4	-5.67	103.53	105.80
1	XA	266	G	P-O3'-C3'	5.67	126.51	119.70
1	XA	545	C	N3-C2-O2	-5.67	117.93	121.90
36	YA	2689	U	P-O3'-C3'	5.67	126.50	119.70
39	YE	54	GLN	C-N-CA	5.67	135.86	121.70
1	QA	1158	C	C5-C6-N1	5.66	123.83	121.00
1	QA	243	A	P-O3'-C3'	5.66	126.49	119.70
1	QA	1126	U	N3-C2-O2	-5.66	118.24	122.20
36	RA	2559	C	N1-C2-O2	5.66	122.29	118.90
36	RA	1513	C	C5-C6-N1	5.65	123.83	121.00
36	YA	265	A	O4'-C1'-N9	5.65	112.72	108.20
1	QA	932	C	N3-C2-O2	-5.65	117.94	121.90
23	XW	60	C	C2-N1-C1'	5.64	125.01	118.80
1	QA	514	C	N1-C2-O2	5.64	122.28	118.90
1	XA	1505	G	C8-N9-C1'	5.64	134.34	127.00
36	YA	752	A	OP2-P-O3'	5.64	117.61	105.20
1	QA	1439	C	N1-C2-O2	5.64	122.28	118.90
23	QW	70	U	N1-C2-O2	5.64	126.75	122.80
1	QA	353	A	OP2-P-O3'	5.63	117.60	105.20
38	RD	36	PRO	CA-N-CD	-5.63	103.61	111.50
36	YA	2832	U	OP2-P-O3'	5.63	117.59	105.20
36	YA	269	U	N3-C2-O2	-5.63	118.26	122.20
36	YA	856	C	N3-C2-O2	-5.63	117.96	121.90
36	YA	2776	A	P-O3'-C3'	5.63	126.45	119.70
37	YB	40	U	N3-C2-O2	-5.63	118.26	122.20
23	QW	39	G	C8-N9-C1'	-5.63	119.69	127.00
36	RA	1742	C	C6-N1-C2	-5.63	118.05	120.30
36	YA	269	U	N1-C2-O2	5.63	126.74	122.80
36	YA	2688	U	N1-C2-O2	5.62	126.74	122.80
36	RA	2889	C	C6-N1-C2	-5.62	118.05	120.30
36	YA	1786	A	C4-N9-C1'	5.62	136.41	126.30
36	YA	1882	C	N3-C2-O2	-5.62	117.97	121.90
36	RA	1026	U	P-O3'-C3'	5.61	126.43	119.70
1	QA	1203	C	N1-C2-O2	5.61	122.27	118.90
1	XA	634	C	N1-C2-O2	5.61	122.27	118.90
36	YA	1509	C	OP1-P-O3'	5.61	117.54	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	314	C	N1-C2-O2	5.60	122.26	118.90
32	Y6	15	GLU	C-N-CA	5.60	135.71	121.70
36	RA	2019	A	P-O3'-C3'	5.60	126.42	119.70
36	YA	2401	U	N1-C2-O2	5.60	126.72	122.80
36	YA	1411	C	N1-C2-O2	5.59	122.26	118.90
1	XA	1505	G	N3-C4-N9	-5.59	122.64	126.00
36	YA	2779	U	C2-N1-C1'	5.59	124.41	117.70
2	QB	137	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	XA	789	U	C2-N1-C1'	5.59	124.41	117.70
1	XA	1054	C	C6-N1-C2	-5.58	118.07	120.30
37	RB	70	C	C6-N1-C2	-5.57	118.07	120.30
36	YA	721	C	N1-C2-O2	5.57	122.24	118.90
38	RD	36	PRO	N-CA-C	5.57	126.58	112.10
36	RA	2831	G	C8-N9-C4	-5.56	104.17	106.40
36	RA	669	G	C8-N9-C1'	-5.56	119.77	127.00
36	RA	2566	A	P-O3'-C3'	5.56	126.37	119.70
36	RA	1544	C	N1-C2-O2	5.56	122.23	118.90
49	RS	112	PHE	N-CA-CB	5.56	120.60	110.60
36	YA	503	A	OP2-P-O3'	5.56	117.43	105.20
36	RA	2712	U	C6-N1-C1'	-5.55	113.43	121.20
1	XA	1439	C	N1-C2-O2	5.55	122.23	118.90
1	QA	254	G	O5'-P-OP1	-5.55	100.70	105.70
1	XA	328	C	N3-C2-O2	-5.55	118.02	121.90
22	XV	65	C	N1-C2-O2	5.55	122.23	118.90
36	RA	1881	C	N1-C2-O2	5.54	122.23	118.90
36	RA	2787	C	P-O3'-C3'	5.54	126.35	119.70
36	RA	345	A	P-O3'-C3'	5.54	126.35	119.70
1	XA	634	C	N3-C2-O2	-5.54	118.02	121.90
36	YA	2559	C	C6-N1-C2	-5.54	118.08	120.30
36	RA	1026	U	OP1-P-O3'	5.54	117.38	105.20
36	RA	155	C	N3-C2-O2	-5.53	118.03	121.90
36	YA	613	U	N1-C2-O2	5.53	126.67	122.80
36	YA	1819	A	P-O3'-C3'	5.53	126.34	119.70
25	XY	55	U	N3-C2-O2	-5.53	118.33	122.20
44	YN	9	VAL	C-N-CA	5.53	135.52	121.70
37	YB	66	A	P-O3'-C3'	5.53	126.33	119.70
51	RU	90	VAL	C-N-CA	5.52	135.50	121.70
1	QA	1477	C	N1-C2-O2	5.52	122.21	118.90
37	RB	30	C	N1-C2-O2	5.51	122.21	118.90
37	RB	66	A	P-O3'-C3'	5.51	126.31	119.70
23	XW	28	U	N3-C2-O2	-5.50	118.35	122.20
1	XA	88	C	N3-C2-O2	-5.50	118.05	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	88	C	C2-N1-C1'	5.50	124.85	118.80
1	QA	314	C	N3-C2-O2	-5.49	118.06	121.90
1	QA	564	C	N1-C2-O2	5.49	122.20	118.90
36	YA	1314	C	N3-C2-O2	-5.49	118.05	121.90
41	YG	83	ARG	CD-NE-CZ	5.49	131.29	123.60
36	YA	1640	C	C5-C6-N1	5.49	123.75	121.00
1	XA	849	C	N1-C2-O2	5.49	122.19	118.90
36	YA	2307	G	C4-N9-C1'	5.48	133.63	126.50
1	XA	89	U	C5-C6-N1	5.48	125.44	122.70
1	QA	960	U	P-O3'-C3'	5.47	126.27	119.70
37	RB	1	U	N1-C2-O2	5.47	126.63	122.80
36	RA	1023	U	N3-C2-O2	-5.47	118.37	122.20
12	XL	104	VAL	C-N-CA	5.47	135.38	121.70
14	XN	43	CYS	C-N-CA	5.47	135.37	121.70
36	RA	2682	U	N3-C2-O2	-5.46	118.38	122.20
1	QA	754	C	C2-N1-C1'	5.46	124.81	118.80
1	XA	1267	C	C5-C6-N1	5.46	123.73	121.00
1	XA	1397	C	C2-N1-C1'	5.46	124.81	118.80
23	XW	14	A	P-O3'-C3'	5.46	126.25	119.70
36	YA	1795	C	N1-C2-O2	5.46	122.17	118.90
1	XA	88	C	C6-N1-C2	-5.45	118.12	120.30
36	RA	635	C	C6-N1-C2	-5.45	118.12	120.30
1	XA	1505	G	C4-N9-C1'	-5.44	119.42	126.50
36	YA	2885	C	N3-C2-O2	-5.44	118.09	121.90
1	XA	980	C	C2-N1-C1'	5.44	124.78	118.80
1	XA	1025	U	C5-C6-N1	5.44	125.42	122.70
1	QA	1452	C	C2-N1-C1'	5.43	124.78	118.80
32	Y6	7	ILE	C-N-CA	5.43	135.29	121.70
37	RB	22	U	C5-C6-N1	5.43	125.42	122.70
1	XA	703	G	P-O3'-C3'	5.43	126.22	119.70
22	XV	17	C	N1-C2-O2	5.43	122.16	118.90
37	YB	15	A	OP1-P-O3'	5.43	117.14	105.20
21	QU	18	TYR	CA-CB-CG	5.42	123.70	113.40
36	RA	1332	G	C4-N9-C1'	5.42	133.55	126.50
36	RA	2703	C	C2-N1-C1'	5.42	124.76	118.80
1	QA	1203	C	C6-N1-C2	-5.42	118.13	120.30
36	YA	1464	C	N3-C2-O2	-5.42	118.11	121.90
1	QA	1126	U	N1-C2-O2	5.42	126.59	122.80
36	RA	856	C	P-O3'-C3'	5.42	126.20	119.70
37	RB	31	C	C2-N1-C1'	5.41	124.75	118.80
37	RB	71	C	N3-C2-O2	-5.41	118.11	121.90
11	XK	25	TYR	CA-CB-CG	5.41	123.69	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	485	G	OP2-P-O3'	5.41	117.10	105.20
36	YA	856	C	N1-C2-O2	5.40	122.14	118.90
56	RZ	62	PRO	C-N-CA	5.40	135.20	121.70
1	QA	369	C	N3-C2-O2	-5.40	118.12	121.90
36	RA	269	U	N3-C2-O2	-5.40	118.42	122.20
25	XY	55	U	O4'-C1'-N1	5.40	112.52	108.20
36	YA	1174	A	C4-N9-C1'	5.40	136.02	126.30
36	RA	1914	C	C6-N1-C2	-5.40	118.14	120.30
1	QA	346	G	N3-C4-C5	-5.39	125.90	128.60
36	RA	2314	C	N3-C2-O2	-5.39	118.12	121.90
36	YA	537	C	C6-N1-C2	-5.39	118.14	120.30
36	YA	1881	C	N1-C2-O2	5.39	122.13	118.90
1	XA	442	C	N1-C2-O2	5.39	122.13	118.90
1	XA	36	C	C6-N1-C2	-5.38	118.15	120.30
52	RV	35	LEU	CA-CB-CG	5.38	127.68	115.30
1	XA	243	A	P-O3'-C3'	5.38	126.16	119.70
1	XA	1374	A	O4'-C1'-N9	5.38	112.51	108.20
36	RA	2702	U	C2-N1-C1'	5.38	124.15	117.70
36	RA	1404	C	N1-C2-O2	5.38	122.13	118.90
36	RA	2032	G	C2-N3-C4	5.38	114.59	111.90
1	XA	58	C	N1-C2-O2	5.38	122.13	118.90
1	XA	1115	C	N1-C2-O2	5.38	122.13	118.90
23	XW	31	C	N1-C2-O2	5.38	122.13	118.90
36	RA	860	U	C6-N1-C2	-5.37	117.78	121.00
1	XA	560	U	P-O3'-C3'	5.37	126.15	119.70
1	QA	1097	C	N3-C2-O2	-5.37	118.14	121.90
36	RA	1979	C	C6-N1-C2	-5.37	118.15	120.30
36	RA	1992	G	OP2-P-O3'	5.37	117.01	105.20
36	YA	1509	C	P-O3'-C3'	5.36	126.13	119.70
36	YA	860	U	C6-N1-C2	-5.35	117.79	121.00
22	QV	17	C	N3-C2-O2	-5.35	118.16	121.90
1	XA	1336	C	OP2-P-O3'	5.35	116.96	105.20
13	XM	12	ASN	C-N-CA	5.34	135.06	121.70
1	XA	1225	A	C4-N9-C1'	5.34	135.91	126.30
36	RA	2746	U	P-O3'-C3'	5.34	126.11	119.70
1	XA	328	C	C6-N1-C2	-5.33	118.17	120.30
36	RA	420	C	C6-N1-C2	-5.33	118.17	120.30
36	RA	1819	A	P-O3'-C3'	5.33	126.10	119.70
36	RA	2471	C	C5-C6-N1	5.33	123.67	121.00
36	YA	1026	U	OP1-P-O3'	5.33	116.92	105.20
36	YA	1180	C	C2-N1-C1'	5.33	124.66	118.80
36	RA	2043	C	N1-C2-O2	5.33	122.10	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	410	G	P-O3'-C3'	5.33	126.09	119.70
36	YA	1956	U	N3-C2-O2	-5.33	118.47	122.20
1	XA	810	C	N1-C2-O2	5.33	122.09	118.90
1	QA	514	C	N3-C2-O2	-5.32	118.17	121.90
36	RA	1864	U	C5-C6-N1	5.32	125.36	122.70
25	QY	56	C	C6-N1-C2	-5.32	118.17	120.30
1	QA	986	A	O4'-C1'-N9	5.32	112.46	108.20
36	RA	2831	G	OP1-P-OP2	5.31	127.57	119.60
1	QA	1484	C	N1-C2-O2	5.31	122.09	118.90
36	RA	1513	C	C6-N1-C2	-5.31	118.17	120.30
36	RA	1742	C	N3-C2-O2	-5.31	118.18	121.90
36	YA	27	G	N3-C2-N2	-5.31	116.18	119.90
1	XA	963	G	N7-C8-N9	5.31	115.75	113.10
36	RA	898	C	N3-C2-O2	-5.30	118.19	121.90
1	QA	346	G	C4-N9-C1'	5.29	133.38	126.50
1	XA	990	C	C6-N1-C2	-5.29	118.18	120.30
36	RA	904	C	N1-C2-O2	5.28	122.07	118.90
36	YA	1882	C	C6-N1-C2	-5.28	118.19	120.30
36	RA	1909	C	N1-C2-O2	5.28	122.07	118.90
36	RA	269	U	C2-N1-C1'	5.28	124.03	117.70
36	YA	2350	C	N1-C2-O2	5.28	122.06	118.90
25	XY	52	G	C4-N9-C1'	5.27	133.36	126.50
1	QA	449	C	N3-C2-O2	-5.27	118.21	121.90
43	RI	131	LYS	N-CA-C	5.27	125.22	111.00
37	RB	70	C	N3-C2-O2	-5.26	118.22	121.90
36	RA	2874	C	N1-C2-O2	5.26	122.06	118.90
1	XA	932	C	N3-C2-O2	-5.26	118.22	121.90
36	RA	1142	U	N1-C2-O2	5.26	126.48	122.80
36	YA	1446	C	N3-C2-O2	-5.26	118.22	121.90
1	XA	1024	G	O5'-P-OP1	5.25	117.01	110.70
36	RA	1314	C	C6-N1-C2	-5.25	118.20	120.30
36	YA	1314	C	C5-C6-N1	5.25	123.63	121.00
36	RA	1528	A	N7-C8-N9	5.25	116.42	113.80
36	RA	529	A	C4-N9-C1'	5.25	135.75	126.30
36	YA	1076	C	N1-C2-O2	5.25	122.05	118.90
1	XA	689	C	N1-C2-O2	5.25	122.05	118.90
36	YA	1085	A	OP1-P-O3'	5.24	116.73	105.20
36	YA	1804	C	C6-N1-C2	-5.24	118.20	120.30
1	QA	1420	C	C6-N1-C2	-5.24	118.20	120.30
22	QV	34	C	N3-C2-O2	-5.24	118.23	121.90
1	QA	90	C	N3-C2-O2	-5.24	118.23	121.90
36	YA	278	A	P-O3'-C3'	5.24	125.98	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	YA	618(A)	C	N3-C2-O2	-5.24	118.23	121.90
36	YA	1691	C	N3-C2-O2	-5.23	118.24	121.90
36	YA	2307	G	O4'-C1'-N9	5.23	112.39	108.20
1	QA	406	G	C4-N9-C1'	5.23	133.30	126.50
36	YA	893	C	C2-N1-C1'	5.23	124.55	118.80
36	YA	1930	G	OP2-P-O3'	5.23	116.71	105.20
36	RA	420	C	N3-C2-O2	-5.23	118.24	121.90
36	RA	2617	C	N1-C2-O2	5.23	122.04	118.90
36	YA	2480	C	C6-N1-C2	-5.23	118.21	120.30
1	QA	1024	G	O5'-P-OP2	-5.22	101.00	105.70
27	R1	80	LEU	C-N-CA	5.22	134.76	121.70
36	RA	974(A)	C	C2-N1-C1'	5.22	124.55	118.80
36	RA	1141	U	O4'-C1'-N1	5.22	112.38	108.20
42	YH	163	TYR	CA-CB-CG	5.22	123.32	113.40
1	QA	410	G	P-O3'-C3'	5.22	125.96	119.70
25	XY	71	C	C6-N1-C2	-5.22	118.21	120.30
36	RA	613	U	C6-N1-C1'	-5.21	113.90	121.20
36	YA	856	C	C5-C6-N1	5.21	123.61	121.00
36	RA	1882	C	N3-C2-O2	-5.21	118.25	121.90
36	YA	2584	U	N1-C2-O2	5.21	126.45	122.80
30	R4	51	ASP	CB-CG-OD1	5.21	122.99	118.30
36	RA	930	U	C2-N1-C1'	5.21	123.95	117.70
36	RA	2350	C	N1-C2-O2	5.20	122.02	118.90
36	YA	654	A	C2-N3-C4	5.20	113.20	110.60
36	RA	828	U	C6-N1-C1'	-5.19	113.93	121.20
36	RA	1781	C	C2-N1-C1'	5.19	124.51	118.80
1	XA	412	A	OP2-P-O3'	5.19	116.62	105.20
36	YA	2787	C	C6-N1-C2	-5.19	118.22	120.30
43	RI	10	GLU	C-N-CA	5.19	134.67	121.70
38	RD	36	PRO	CA-C-N	-5.19	105.79	117.20
25	XY	54	U	C5-C6-N1	5.19	125.29	122.70
55	RY	55	TYR	CA-CB-CG	5.18	123.25	113.40
36	YA	2401	U	N3-C2-O2	-5.18	118.57	122.20
36	YA	1178	C	C6-N1-C2	-5.18	118.23	120.30
36	RA	838	C	N3-C2-O2	-5.18	118.28	121.90
25	XY	70	U	C5-C6-N1	5.18	125.29	122.70
37	YB	71	C	N1-C2-O2	5.18	122.00	118.90
39	YE	116	VAL	C-N-CA	5.18	134.64	121.70
6	QF	63	TYR	CA-CB-CG	5.17	123.23	113.40
41	RG	107	LEU	CA-CB-CG	5.17	127.20	115.30
36	YA	1930	G	P-O3'-C3'	5.17	125.91	119.70
23	XW	60	C	N3-C2-O2	-5.17	118.28	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	QV	3	C	N1-C2-O2	5.17	122.00	118.90
36	YA	753	C	C6-N1-C2	-5.17	118.23	120.30
36	YA	2318	G	O4'-C1'-N9	5.17	112.34	108.20
36	RA	2060	A	OP2-P-O3'	5.17	116.56	105.20
36	YA	747	U	C5-C4-O4	-5.17	122.80	125.90
36	YA	942	G	P-O3'-C3'	5.16	125.89	119.70
1	XA	963	G	N3-C4-N9	5.16	129.10	126.00
36	RA	2610	C	P-O3'-C3'	5.16	125.89	119.70
36	YA	1653	G	OP2-P-O3'	5.16	116.55	105.20
36	YA	1882	C	C2-N1-C1'	5.15	124.47	118.80
1	QA	1381	U	N1-C2-O2	5.15	126.41	122.80
36	YA	2779	U	N1-C2-O2	5.15	126.41	122.80
1	QA	1318	A	P-O3'-C3'	5.15	125.88	119.70
36	RA	1178	C	P-O3'-C3'	5.14	125.87	119.70
36	RA	1313	U	C6-N1-C1'	-5.14	114.00	121.20
9	QI	88	TYR	N-CA-C	-5.14	97.11	111.00
25	QY	71	C	C2-N1-C1'	5.14	124.46	118.80
36	YA	1669	A	C4-N9-C1'	5.14	135.56	126.30
52	YV	12	TYR	CA-CB-CG	5.14	123.17	113.40
36	RA	2039	C	N1-C2-O2	5.14	121.98	118.90
36	YA	1411	C	C5-C6-N1	5.14	123.57	121.00
36	YA	2681	C	OP2-P-O3'	5.14	116.50	105.20
56	YZ	81	ARG	C-N-CA	5.14	134.54	121.70
23	XW	16	A	C2-N3-C4	5.13	113.17	110.60
36	YA	2336	A	C5-C6-N6	-5.13	119.59	123.70
36	RA	231	C	N3-C2-O2	-5.13	118.31	121.90
36	RA	1023	U	N1-C2-O2	5.13	126.39	122.80
36	YA	2814	C	N1-C2-O2	5.13	121.98	118.90
36	YA	291	C	N1-C2-O2	5.12	121.97	118.90
1	QA	810	C	N1-C2-O2	5.12	121.97	118.90
56	YZ	63	ASP	CB-CG-OD1	5.12	122.91	118.30
1	QA	536	C	N1-C2-O2	5.12	121.97	118.90
36	RA	1819	A	OP2-P-O3'	5.11	116.45	105.20
1	XA	449	C	N3-C2-O2	-5.11	118.32	121.90
36	YA	333	G	C8-N9-C1'	-5.11	120.35	127.00
1	QA	244	U	OP2-P-O3'	5.11	116.45	105.20
23	QW	60	C	N3-C2-O2	-5.11	118.32	121.90
36	RA	221	A	OP2-P-O3'	5.11	116.44	105.20
36	RA	2307	G	C4-N9-C1'	5.11	133.14	126.50
36	RA	120	U	C6-N1-C1'	-5.11	114.05	121.20
36	YA	817	C	C6-N1-C2	-5.11	118.26	120.30
1	QA	980	C	N3-C2-O2	-5.11	118.33	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	XE	72	GLN	C-N-CA	5.11	134.47	121.70
36	YA	2342	C	C6-N1-C2	-5.10	118.26	120.30
25	XY	55	U	N1-C2-O2	5.10	126.37	122.80
36	YA	2114	A	C2-N3-C4	5.10	113.15	110.60
36	RA	1644	C	C6-N1-C2	-5.10	118.26	120.30
36	RA	2168	G	N3-C4-N9	5.10	129.06	126.00
36	RA	2138	C	C6-N1-C2	-5.10	118.26	120.30
25	XY	70	U	C6-N1-C1'	-5.10	114.06	121.20
36	YA	228	A	C2-N3-C4	5.10	113.15	110.60
36	RA	1686	C	N3-C2-O2	-5.09	118.33	121.90
1	XA	314	C	N1-C2-O2	5.09	121.96	118.90
1	XA	1157	A	C4-N9-C1'	5.09	135.47	126.30
23	QW	16	A	C2-N3-C4	5.09	113.14	110.60
1	XA	810	C	N3-C2-O2	-5.09	118.34	121.90
36	YA	1095	A	N3-C4-N9	5.09	131.47	127.40
36	YA	528	A	C6-N1-C2	5.09	121.65	118.60
36	YA	893	C	N3-C2-O2	-5.09	118.34	121.90
12	QL	104	VAL	C-N-CA	5.09	134.41	121.70
1	XA	789	U	N1-C2-O2	5.08	126.36	122.80
1	XA	176	C	N1-C2-O2	5.08	121.95	118.90
1	QA	932	C	C6-N1-C2	-5.08	118.27	120.30
1	QA	1301	U	C5-C6-N1	5.08	125.24	122.70
36	YA	2347	C	C6-N1-C2	-5.08	118.27	120.30
36	YA	537	C	N1-C2-O2	5.08	121.95	118.90
36	RA	2314	C	C6-N1-C2	-5.07	118.27	120.30
36	RA	702	G	C4-N9-C1'	5.07	133.09	126.50
23	XW	28	U	N1-C2-O2	5.07	126.35	122.80
36	YA	1604	C	C6-N1-C2	-5.07	118.27	120.30
36	YA	2584	U	O4'-C1'-N1	5.07	112.25	108.20
36	RA	1411	C	C6-N1-C2	-5.06	118.28	120.30
36	YA	1544	C	C2-N1-C1'	5.06	124.37	118.80
36	YA	1405	U	N3-C2-O2	-5.06	118.66	122.20
25	QY	71	C	C6-N1-C2	-5.06	118.28	120.30
36	RA	1180	C	N1-C2-O2	5.06	121.94	118.90
1	XA	406	G	C8-N9-C1'	-5.06	120.43	127.00
25	QY	71	C	N1-C2-O2	5.05	121.93	118.90
52	RV	12	TYR	CA-CB-CG	5.05	123.00	113.40
36	YA	544	C	N1-C2-O2	5.05	121.93	118.90
36	YA	1438	U	N3-C2-O2	-5.05	118.66	122.20
47	RQ	21	THR	N-CA-C	5.05	124.64	111.00
36	RA	1776	G	C8-N9-C1'	-5.05	120.43	127.00
37	RB	1	U	C2-N1-C1'	5.05	123.76	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	XS	9	VAL	C-N-CA	5.04	134.31	121.70
36	RA	456	C	C2-N1-C1'	5.04	124.35	118.80
1	XA	1114	C	N1-C2-O2	5.04	121.93	118.90
36	YA	1306	C	N1-C2-O2	5.04	121.93	118.90
36	YA	2559	C	N3-C2-O2	-5.04	118.37	121.90
1	XA	449	C	C6-N1-C1'	-5.04	114.75	120.80
36	YA	242	G	OP2-P-O3'	5.04	116.28	105.20
36	YA	1893	C	N1-C2-O2	5.04	121.92	118.90
44	YN	114	ARG	N-CA-C	-5.04	97.40	111.00
36	RA	1930	G	OP2-P-O3'	5.03	116.28	105.20
1	QA	1225	A	C8-N9-C1'	-5.03	118.64	127.70
36	RA	687	C	N1-C2-O2	5.03	121.92	118.90
38	RD	33	LEU	C-N-CA	5.03	134.28	121.70
36	YA	1095	A	C4-N9-C1'	5.03	135.35	126.30
1	QA	412	A	OP2-P-O3'	5.03	116.26	105.20
36	YA	1095	A	N3-C4-C5	-5.03	123.28	126.80
36	YA	2617	C	N1-C2-O2	5.03	121.92	118.90
1	QA	1336	C	N3-C2-O2	-5.03	118.38	121.90
47	RQ	134	ARG	N-CA-C	-5.03	97.43	111.00
36	YA	2757	A	O5'-P-OP1	-5.02	101.18	105.70
2	QB	137	ARG	NE-CZ-NH2	-5.02	117.79	120.30
36	YA	1899	G	N1-C2-N2	-5.02	111.68	116.20
36	YA	2844	G	C4-N9-C1'	5.02	133.03	126.50
1	QA	406	G	C8-N9-C1'	-5.02	120.48	127.00
44	YN	48	MET	CG-SD-CE	-5.02	92.17	100.20
1	QA	812	C	OP2-P-O3'	5.01	116.23	105.20
1	XA	375	U	N3-C2-O2	-5.01	118.69	122.20
23	XW	58	A	OP1-P-O3'	5.01	116.23	105.20
2	QB	230	VAL	C-N-CA	5.01	134.23	121.70
4	QD	38	TYR	CA-CB-CG	5.01	122.92	113.40
36	YA	241	A	OP1-P-O3'	5.01	116.22	105.20
43	YI	13	GLY	N-CA-C	5.01	125.63	113.10
36	RA	1881	C	N3-C2-O2	-5.01	118.39	121.90
44	YN	35	ARG	N-CA-C	-5.01	97.48	111.00
36	RA	420	C	N1-C2-O2	5.01	121.90	118.90
36	YA	27	G	N3-C4-N9	-5.01	123.00	126.00
36	RA	2043	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16273	201	0
1	XA	32249	0	16278	200	0
2	QB	1924	0	1975	27	0
2	XB	1924	0	1975	32	0
3	QC	1605	0	1668	17	0
3	XC	1605	0	1668	25	0
4	QD	1674	0	1718	27	0
4	XD	1674	0	1718	30	0
5	QE	1155	0	1213	19	0
5	XE	1155	0	1213	17	0
6	QF	843	0	857	7	0
6	XF	843	0	857	12	0
7	QG	1257	0	1296	15	0
7	XG	1257	0	1296	14	0
8	QH	1116	0	1177	20	0
8	XH	1116	0	1177	22	0
9	QI	1010	0	1037	25	0
9	XI	1010	0	1037	23	0
10	QJ	801	0	849	12	0
10	XJ	801	0	848	16	0
11	QK	885	0	904	11	0
11	XK	885	0	904	12	0
12	QL	975	0	1062	18	0
12	XL	975	0	1062	21	0
13	QM	964	0	1034	28	0
13	XM	964	0	1034	21	0
14	QN	492	0	533	18	0
14	XN	492	0	530	8	0
15	QO	734	0	771	7	0
15	XO	734	0	771	0	0
16	QP	705	0	725	10	0
16	XP	705	0	725	9	0
17	QQ	834	0	904	16	0
17	XQ	834	0	904	10	0
18	QR	574	0	644	10	0
18	XR	574	0	644	8	0
19	QS	674	0	699	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	XS	674	0	699	19	0
20	QT	763	0	861	10	0
20	XT	763	0	861	11	0
21	QU	217	0	234	5	0
21	XU	217	0	234	3	0
22	QV	1640	0	837	9	0
22	XV	1640	0	837	6	0
23	QW	1632	0	824	12	0
23	XW	1632	0	824	10	0
24	QX	418	0	207	4	0
24	XX	374	0	186	2	0
25	QY	1603	0	811	12	0
25	XY	1625	0	822	6	0
26	R0	648	0	672	6	0
26	Y0	648	0	672	21	0
27	R1	763	0	848	11	0
27	Y1	763	0	848	7	0
28	R2	581	0	629	7	0
28	Y2	581	0	628	7	0
29	R3	469	0	518	5	0
29	Y3	469	0	518	4	0
30	R4	581	0	577	23	0
30	Y4	581	0	577	13	0
31	R5	459	0	479	11	0
31	Y5	459	0	480	8	0
32	R6	424	0	450	16	0
32	Y6	424	0	450	10	0
33	R7	430	0	480	7	0
33	Y7	430	0	480	4	0
34	R8	517	0	582	6	0
34	Y8	517	0	582	13	0
35	R9	307	0	338	6	0
35	Y9	307	0	338	8	0
36	RA	62071	0	31280	311	0
36	YA	62091	0	31292	289	0
37	RB	2573	0	1306	19	0
37	YB	2573	0	1306	22	0
38	RD	2115	0	2195	53	0
38	YD	2115	0	2195	60	0
39	RE	1568	0	1634	36	0
39	YE	1568	0	1634	39	0
40	RF	1585	0	1632	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	YF	1585	0	1632	20	0
41	RG	1474	0	1535	38	0
41	YG	1474	0	1535	20	0
42	RH	1307	0	1382	25	0
42	YH	1307	0	1382	38	0
43	RI	1136	0	1223	16	0
43	YI	1136	0	1223	12	0
44	RN	1104	0	1180	7	0
44	YN	1104	0	1180	13	0
45	RO	933	0	996	22	0
45	YO	933	0	996	21	0
46	RP	1145	0	1226	24	0
46	YP	1145	0	1228	22	0
47	RQ	1122	0	1179	22	0
47	YQ	1122	0	1179	29	0
48	RR	968	0	1033	21	0
48	YR	968	0	1033	12	0
49	RS	882	0	943	17	0
49	YS	882	0	943	16	0
50	RT	1141	0	1202	25	0
50	YT	1141	0	1202	25	0
51	RU	964	0	1022	14	0
51	YU	964	0	1022	26	0
52	RV	779	0	852	9	0
52	YV	779	0	852	7	0
53	RW	900	0	964	10	0
53	YW	900	0	964	13	0
54	RX	725	0	777	10	0
54	YX	725	0	778	12	0
55	RY	785	0	878	13	0
55	YY	785	0	878	11	0
56	RZ	1461	0	1493	32	0
56	YZ	1461	0	1493	23	0
57	QA	85	0	0	0	0
57	QF	1	0	0	0	0
57	QH	1	0	0	0	0
57	QM	2	0	0	0	0
57	QV	4	0	0	0	0
57	QX	1	0	0	0	0
57	R0	1	0	0	0	0
57	R5	1	0	0	0	0
57	R7	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	R8	1	0	0	0	0
57	RA	321	0	0	0	0
57	RB	4	0	0	0	0
57	RD	1	0	0	0	0
57	RE	3	0	0	0	0
57	RF	1	0	0	0	0
57	RP	2	0	0	0	0
57	RQ	1	0	0	0	0
57	RU	1	0	0	0	0
57	RX	1	0	0	0	0
57	XA	94	0	0	0	0
57	XD	1	0	0	0	0
57	XF	1	0	0	0	0
57	XJ	1	0	0	0	0
57	XM	1	0	0	0	0
57	XV	3	0	0	0	0
57	XY	1	0	0	0	0
57	Y0	1	0	0	0	0
57	Y2	1	0	0	0	0
57	Y5	2	0	0	0	0
57	Y7	2	0	0	0	0
57	Y8	3	0	0	0	0
57	YA	379	0	0	0	0
57	YB	8	0	0	0	0
57	YD	3	0	0	0	0
57	YE	3	0	0	0	0
57	YH	1	0	0	0	0
57	YP	3	0	0	0	0
57	YQ	1	0	0	0	0
57	YR	2	0	0	0	0
57	YU	2	0	0	0	0
57	YV	1	0	0	0	0
57	YX	3	0	0	0	0
58	QA	42	0	45	2	0
58	XA	42	0	45	1	0
59	QD	8	0	0	0	0
59	XD	8	0	0	0	0
60	XN	1	0	0	0	0
61	QA	1	0	0	0	0
61	QX	1	0	0	0	0
All	All	298371	0	201332	2196	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 (2196) 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)
36:YA:1112:G:H5'	42:YH:3:ARG:HD3	1.20	1.19
36:YA:1112:G:H5'	42:YH:3:ARG:CD	1.79	1.12
43:RI:92:VAL:CG1	43:RI:120:ILE:HG23	1.82	1.09
42:RH:6:ARG:HD3	42:RH:6:ARG:H	1.19	1.07
38:YD:33:LEU:H	38:YD:33:LEU:HD23	1.19	1.06
32:R6:30:THR:HG22	32:R6:31:PRO:HD2	1.41	1.02
36:YA:1112:G:C5'	42:YH:3:ARG:HD3	1.93	0.99
38:YD:35:LYS:HB2	38:YD:36:PRO:HD2	1.46	0.95
36:RA:1113:U:OP1	42:RH:4:ILE:HD11	1.67	0.94
42:YH:8:PRO:HB2	42:YH:69:ARG:NH1	1.85	0.91
38:YD:35:LYS:CB	38:YD:36:PRO:CD	2.49	0.90
12:XL:24:VAL:HG13	12:XL:98:TYR:HE2	1.37	0.90
43:RI:92:VAL:HG13	43:RI:120:ILE:HG23	1.51	0.90
30:R4:49:PHE:CD2	30:R4:50:VAL:HG22	2.10	0.87
30:R4:49:PHE:CE2	30:R4:50:VAL:HG22	2.12	0.85
30:R4:49:PHE:CD2	30:R4:50:VAL:HG13	2.15	0.82
38:YD:35:LYS:CB	38:YD:36:PRO:HD2	2.09	0.82
43:RI:92:VAL:HG13	43:RI:120:ILE:CG2	2.09	0.82
19:XS:19:VAL:HG22	19:XS:44:MET:HG2	1.62	0.82
12:XL:24:VAL:HG13	12:XL:98:TYR:CE2	2.17	0.80
1:XA:691:G:N7	11:XK:26:ASN:ND2	2.31	0.78
38:YD:35:LYS:HB3	38:YD:36:PRO:HD3	1.66	0.78
1:QA:686:U:H1'	11:QK:42:TRP:HE1	1.48	0.77
38:YD:35:LYS:HB3	38:YD:36:PRO:CD	2.15	0.77
36:RA:2245:U:H5'	36:RA:2246:G:H5'	1.67	0.77
43:RI:92:VAL:CG2	43:RI:97:ILE:HD11	2.14	0.77
36:RA:2747:G:H21	36:RA:2757:A:H62	1.33	0.77
36:RA:1826:G:H4'	38:RD:242:ARG:HE	1.50	0.75
1:QA:1162:C:H42	1:QA:1174:G:H1	1.33	0.75
42:RH:6:ARG:HD3	42:RH:6:ARG:N	2.01	0.74
55:RY:50:ARG:HE	55:RY:54:LYS:HB2	1.51	0.74
1:XA:1318:A:H4'	19:XS:11:VAL:HG21	1.69	0.74
32:R6:30:THR:HG22	32:R6:31:PRO:CD	2.17	0.74
56:RZ:10:ARG:HE	56:RZ:36:LYS:HB3	1.52	0.73
5:QE:102:ALA:HB1	5:QE:106:PRO:HG2	1.71	0.73
43:YI:92:VAL:HG13	43:YI:120:ILE:HG23	1.70	0.73
42:YH:6:ARG:HH22	42:YH:62:LYS:HG2	1.55	0.72
36:YA:1243:G:H4'	46:YP:7:ARG:HH21	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:YA:1050:A:H5''	36:YA:1050:A:N3	2.05	0.72
39:YE:79:ARG:HG3	39:YE:197:ILE:HG21	1.71	0.72
35:Y9:13:LYS:HE2	35:Y9:28:GLU:HG3	1.72	0.71
37:RB:3:C:H42	37:RB:117:G:H1	1.38	0.71
1:QA:544:G:OP1	4:QD:59:ARG:NH2	2.24	0.71
43:RI:92:VAL:CG1	43:RI:120:ILE:CG2	2.63	0.71
1:XA:933:G:N7	7:XG:3:ARG:NH1	2.38	0.71
44:YN:15:LEU:HB2	44:YN:134:ARG:HB3	1.73	0.71
38:YD:33:LEU:N	38:YD:33:LEU:HD23	2.03	0.71
31:Y5:40:LYS:HD3	31:Y5:47:PRO:HD2	1.72	0.70
36:RA:2032:G:H21	39:RE:146:THR:HG23	1.56	0.70
42:RH:6:ARG:H	42:RH:6:ARG:CD	1.99	0.70
36:YA:2068:U:H3	36:YA:2430:A:H2	1.38	0.70
1:XA:1130:A:O2'	9:XI:3:GLN:NE2	2.25	0.70
3:QC:20:SER:HB2	3:QC:40:ARG:HH22	1.56	0.70
46:YP:58:THR:O	46:YP:61:ARG:NH2	2.24	0.70
36:RA:676:A:H8	36:RA:2069:G:H21	1.38	0.70
1:QA:1099:G:H5''	2:QB:96:ARG:HH12	1.56	0.70
28:R2:48:HIS:HD1	36:RA:95:G:HO2'	1.40	0.70
41:RG:38:VAL:HG11	41:RG:91:ARG:NH1	2.07	0.70
1:QA:664:G:H22	1:QA:741:G:H1	1.40	0.69
42:YH:8:PRO:HB2	42:YH:69:ARG:HH12	1.55	0.69
1:XA:8:A:N6	4:XD:205:GLU:O	2.26	0.69
2:XB:185:ILE:HG22	2:XB:199:TYR:HB2	1.75	0.69
43:RI:92:VAL:HG22	43:RI:97:ILE:HD11	1.72	0.69
22:QV:50:U:H3	22:QV:64:G:H1	1.41	0.69
36:RA:27:G:N2	36:RA:513:A:OP2	2.26	0.69
40:RF:143:ALA:HB1	40:RF:148:LEU:HB2	1.75	0.68
50:RT:118:ARG:HH21	50:RT:121:ILE:HG21	1.57	0.68
7:XG:111:ARG:HE	7:XG:123:GLU:HG2	1.59	0.68
1:QA:973:G:H5''	14:QN:31:ARG:HH21	1.57	0.68
46:RP:58:THR:O	46:RP:61:ARG:NH2	2.27	0.68
39:YE:36:ARG:NH1	39:YE:85:ASN:OD1	2.26	0.68
30:Y4:63:TYR:HE2	30:Y4:68:ARG:HG3	1.58	0.68
1:XA:686:U:H1'	11:XK:42:TRP:HE1	1.59	0.68
51:YU:76:TYR:CE2	51:YU:80:ILE:HD11	2.28	0.68
38:YD:36:PRO:HD3	38:YD:63:ARG:HG2	1.76	0.68
1:QA:501:C:OP1	12:QL:117:ARG:NH2	2.28	0.67
31:R5:4:HIS:O	36:RA:2056:G:N2	2.27	0.67
49:RS:34:HIS:NE2	49:RS:53:SER:OG	2.26	0.67
3:QC:58:GLU:HB2	3:QC:65:ALA:HB3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:RA:996:A:O2'	52:RV:11:GLN:NE2	2.28	0.67
42:RH:74:ASN:HD22	42:RH:138:LYS:HE2	1.57	0.67
3:XC:122:GLU:HG3	3:XC:126:ARG:HE	1.60	0.67
36:YA:2032:G:H21	39:YE:146:THR:HG23	1.60	0.67
45:YO:104:ARG:NH2	50:YT:43:GLN:OE1	2.27	0.67
14:QN:45:ARG:O	14:QN:49:HIS:ND1	2.27	0.66
30:R4:49:PHE:HD2	30:R4:50:VAL:N	1.93	0.66
30:R4:37:SER:HB2	41:RG:112:PRO:HB3	1.77	0.66
1:XA:105:G:OP2	20:XT:18:GLN:NE2	2.28	0.66
1:XA:1147:C:O2	9:XI:16:ARG:NH1	2.29	0.66
36:RA:2117:A:N7	36:RA:2172:U:N3	2.41	0.66
36:RA:322:A:H5''	40:RF:169:ASN:HD21	1.60	0.66
42:YH:6:ARG:HB3	42:YH:66:GLY:HA2	1.77	0.66
38:YD:35:LYS:HG2	38:YD:104:TYR:CE2	2.31	0.66
13:QM:87:TYR:H	19:QS:73:GLU:HB3	1.60	0.66
44:RN:54:VAL:HB	44:RN:122:VAL:HG12	1.77	0.66
1:XA:544:G:OP1	4:XD:59:ARG:NH2	2.28	0.66
5:XE:28:PHE:HD2	5:XE:51:VAL:HG13	1.61	0.66
42:YH:8:PRO:O	42:YH:69:ARG:CZ	2.44	0.66
36:YA:2701:C:H3'	36:YA:2702:U:H5''	1.78	0.65
1:QA:376:G:H1	1:QA:387:U:H3	1.43	0.65
5:XE:150:ARG:HA	5:XE:153:LYS:HE3	1.78	0.65
1:QA:1147:C:HO2'	9:QI:5:TYR:HH	1.41	0.65
1:QA:953:G:N7	13:QM:104:ARG:NH2	2.44	0.65
1:QA:689:C:H3'	1:QA:690:G:H21	1.61	0.65
1:QA:1130:A:O2'	9:QI:3:GLN:NE2	2.29	0.65
37:YB:9:G:OP1	49:YS:15:ARG:NH1	2.28	0.65
36:RA:1140:C:OP2	44:RN:66:LYS:NZ	2.30	0.65
3:XC:129:ALA:HB3	3:XC:132:ARG:HD2	1.78	0.65
31:Y5:4:HIS:O	36:YA:2056:G:N2	2.30	0.65
1:QA:553:A:H5''	12:QL:24:VAL:HG11	1.79	0.65
1:QA:236:G:H5''	17:QQ:42:TYR:OH	1.97	0.65
8:XH:110:ALA:HB3	8:XH:121:ASP:HB3	1.78	0.65
36:YA:2749:A:H8	36:YA:2749:A:OP2	1.80	0.65
23:XW:9:A:N6	23:XW:23:A:N7	2.45	0.65
36:YA:1112:G:C5'	42:YH:3:ARG:CD	2.62	0.65
36:RA:1049:C:H6	36:RA:1049:C:O5'	1.79	0.64
1:XA:186:C:H5'	20:XT:78:ALA:HB1	1.79	0.64
36:YA:1479:G:N7	36:YA:1510:A:N6	2.45	0.64
36:YA:2378:A:N1	49:YS:17:ARG:NH1	2.46	0.64
36:YA:1728:G:H8	36:YA:1732:A:H62	1.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:YZ:52:SER:O	56:YZ:54:HIS:N	2.31	0.64
13:QM:80:ARG:NH2	19:QS:65:ASN:O	2.30	0.64
1:XA:1123:A:H4'	10:XJ:36:GLY:HA3	1.80	0.64
38:YD:143:HIS:ND1	38:YD:194:GLY:O	2.30	0.64
31:Y5:29:THR:HG21	36:YA:2815:C:H5'	1.77	0.64
36:RA:2131:G:H4'	36:RA:2132:U:H4'	1.78	0.64
47:RQ:108:GLY:HA3	56:RZ:116:VAL:HG11	1.79	0.64
5:XE:102:ALA:HB1	5:XE:106:PRO:HG2	1.78	0.64
1:XA:501:C:OP1	12:XL:117:ARG:NH2	2.31	0.64
42:YH:6:ARG:HG3	42:YH:7:LEU:HD12	1.79	0.64
14:YN:6:LEU:HB3	14:YN:23:ARG:HH22	1.63	0.64
38:RD:27:THR:HG21	38:RD:81:ALA:HB1	1.79	0.64
42:RH:117:PRO:HB2	42:RH:121:ILE:HD13	1.80	0.64
36:YA:994:C:OP1	51:YU:53:ARG:NH2	2.31	0.64
43:YI:82:ARG:HE	43:YI:146:ALA:HB3	1.62	0.64
36:RA:2118:U:H3	36:RA:2148:G:H4'	1.63	0.63
30:Y4:18:CYS:SG	30:Y4:19:GLY:N	2.71	0.63
47:YQ:31:ASP:HA	47:YQ:134:ARG:HD2	1.80	0.63
36:RA:1019:U:H3	36:RA:1142(A):A:H62	1.46	0.63
36:RA:1043:C:H42	36:RA:1112:G:H1	1.45	0.63
36:RA:2747:G:OP1	42:RH:138:LYS:NZ	2.31	0.63
1:XA:970:C:N4	9:XI:128:ARG:OXT	2.31	0.63
1:XA:545:C:H5'	4:XD:72:GLU:HG3	1.78	0.63
30:Y4:55:ARG:HG2	30:Y4:56:VAL:HG23	1.81	0.63
36:YA:987:G:O2'	36:YA:1000:A:N3	2.30	0.63
36:YA:1112:G:H5'	42:YH:3:ARG:HD2	1.79	0.63
38:RD:8:PRO:HB3	38:RD:14:ARG:HB3	1.79	0.63
46:RP:46:LYS:HG2	46:RP:47:ASP:H	1.64	0.63
1:XA:157:G:H1	1:XA:164:U:H3	1.45	0.63
2:QB:118:LEU:HB3	2:QB:142:LEU:HD12	1.81	0.63
12:XL:58:VAL:HG11	12:XL:85:ILE:HD11	1.80	0.63
36:YA:690:G:O3'	38:YD:218:ARG:NH1	2.31	0.63
42:YH:153:LYS:HD2	42:YH:162:ILE:HD13	1.79	0.63
1:QA:593:G:H1	1:QA:646:U:H3	1.45	0.63
56:RZ:7:ALA:HB2	56:RZ:59:LEU:HB3	1.80	0.63
1:XA:339:C:OP2	45:YO:97:ARG:NH1	2.32	0.63
23:QW:16:A:N6	23:QW:59:U:O4	2.32	0.63
36:RA:1607:C:N4	36:RA:1622:G:OP2	2.32	0.63
55:RY:46:LYS:HG2	55:RY:63:LYS:HE3	1.80	0.63
36:YA:676:A:H8	36:YA:2069:G:H21	1.45	0.63
36:RA:2114:A:N6	36:RA:2119:A:N7	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:1450:U:O2'	1:XA:1451:A:N7	2.32	0.62
36:YA:2393:A:H5'	46:YP:62:LEU:HD12	1.80	0.62
45:RO:104:ARG:NH2	50:RT:43:GLN:OE1	2.31	0.62
19:QS:65:ASN:OD1	30:R4:55:ARG:NH1	2.32	0.62
21:QU:8:THR:HG23	21:QU:11:GLY:H	1.63	0.62
31:Y5:19:ARG:NH2	36:YA:1264:G:OP1	2.32	0.62
36:YA:820:A:N3	36:YA:943:U:O2'	2.32	0.62
45:YO:107:ARG:NH1	50:YT:36:GLU:OE1	2.33	0.62
13:QM:37:THR:O	13:QM:55:ARG:NH2	2.33	0.62
23:QW:9:A:OP2	23:QW:13:C:N4	2.32	0.62
36:RA:806:C:HO2'	36:RA:2445:G:HO2'	1.47	0.62
38:YD:31:LYS:HD2	38:YD:33:LEU:HD21	1.82	0.62
43:YI:64:GLU:OE1	43:YI:67:ARG:NH1	2.33	0.62
3:QC:47:LEU:HD22	3:QC:52:LEU:HB3	1.81	0.62
7:XG:15:ASP:HB3	7:XG:19:GLY:H	1.64	0.62
25:XY:56:C:H5''	36:YA:897:C:H5''	1.80	0.62
34:Y8:9:GLY:O	34:Y8:13:ARG:NH1	2.32	0.62
38:YD:30:GLU:HG3	38:YD:63:ARG:HH21	1.64	0.62
26:R0:77:ARG:NH2	36:RA:857:C:OP2	2.31	0.62
40:RF:135:LYS:HB2	40:RF:138:GLU:HG3	1.82	0.62
10:XJ:57:LYS:HE2	10:XJ:60:ARG:HH21	1.65	0.62
28:Y2:47:ASN:O	28:Y2:48:HIS:ND1	2.32	0.62
36:YA:67:U:H3	36:YA:74:A:H2	1.48	0.62
36:YA:1791:A:H5'	38:YD:206:LEU:HD12	1.82	0.62
51:YU:52:ARG:HD2	51:YU:55:ARG:HH21	1.63	0.62
35:R9:36:GLN:NE2	36:RA:1124:C:O2	2.32	0.62
42:YH:89:ILE:HB	42:YH:129:THR:HB	1.79	0.62
1:QA:691:G:N7	11:QK:26:ASN:ND2	2.47	0.62
1:XA:943:U:H1'	9:XI:124:GLN:HE22	1.64	0.62
35:Y9:30:PRO:HB2	36:YA:2527:C:H5''	1.82	0.61
36:RA:1791:A:N6	36:RA:1828:G:O2'	2.33	0.61
36:RA:768:G:O2'	36:RA:1379:A:N6	2.33	0.61
9:QI:42:ARG:NH1	9:QI:71:SER:OG	2.33	0.61
36:YA:2788:C:O2'	36:YA:2809:A:N3	2.32	0.61
36:RA:994:C:OP2	51:RU:54:LYS:NZ	2.32	0.61
19:XS:10:PHE:HZ	19:XS:16:LEU:HD13	1.65	0.61
9:XI:128:ARG:NH2	22:XV:33:U:OP2	2.33	0.61
36:YA:2404:C:O3'	46:YP:77:ARG:NH2	2.33	0.61
36:YA:265:A:N6	36:YA:427:U:O2'	2.34	0.61
44:YN:12:ARG:NH1	44:YN:50:ASP:OD2	2.33	0.61
32:R6:28:ARG:NH1	36:RA:2285:C:OP1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:YA:1652:A:OP1	48:YR:8:ARG:NH1	2.33	0.61
39:YE:14:ILE:HG22	39:YE:21:VAL:HB	1.82	0.61
36:YA:1194:A:N7	46:YP:16:ARG:NH1	2.48	0.61
13:XM:65:LYS:NZ	13:XM:73:GLU:OE1	2.31	0.61
28:R2:47:ASN:O	28:R2:48:HIS:ND1	2.34	0.61
36:RA:630:G:N2	36:RA:633:A:OP2	2.32	0.61
8:XH:106:GLY:O	8:XH:122:ARG:NH2	2.33	0.61
7:QG:94:ARG:NH1	7:QG:98:SER:OG	2.34	0.61
42:RH:35:VAL:HG13	42:RH:71:LEU:HD22	1.83	0.61
36:YA:2680:C:H5'	39:YE:189:PRO:HA	1.83	0.61
42:YH:86:GLU:OE2	42:YH:132:ARG:NH1	2.34	0.61
32:R6:24:GLU:OE2	36:RA:2286:A:N6	2.34	0.61
36:RA:39:C:O2	40:RF:46:ARG:NH2	2.34	0.61
8:QH:10:LEU:HD22	8:QH:83:ILE:HD11	1.83	0.60
9:QI:121:ARG:NH1	9:QI:122:ALA:O	2.33	0.60
1:XA:911:U:OP2	12:XL:97:ARG:NH2	2.33	0.60
8:XH:10:LEU:HD22	8:XH:83:ILE:HD11	1.82	0.60
36:YA:39:C:O2	40:YF:46:ARG:NH2	2.33	0.60
42:YH:7:LEU:HD12	42:YH:7:LEU:H	1.66	0.60
43:YI:86:THR:HA	43:YI:123:LEU:HB2	1.83	0.60
36:YA:1666:G:HO2'	45:YO:6:THR:HG1	1.49	0.60
1:QA:1328:C:O2'	13:QM:29:ARG:NH2	2.29	0.60
1:QA:619:U:N3	4:QD:134:ASP:OD1	2.32	0.60
3:QC:164:ARG:NH1	3:QC:166:GLU:OE1	2.33	0.60
2:QB:8:LYS:HG3	2:QB:10:LEU:H	1.65	0.60
2:QB:150:SER:O	2:QB:153:ARG:NH1	2.35	0.60
4:QD:62:GLN:HE22	4:QD:65:ARG:HH21	1.47	0.60
32:R6:36:LEU:HD13	32:R6:50:ARG:HD3	1.83	0.60
36:YA:1049:C:H6	36:YA:1049:C:O5'	1.83	0.60
17:QQ:66:SER:O	17:QQ:70:ARG:NH1	2.34	0.60
23:XW:6:U:H3	23:XW:67:A:H61	1.49	0.60
38:YD:108:PRO:HD2	38:YD:111:LEU:HD22	1.84	0.60
47:YQ:75:THR:HG21	47:YQ:85:LYS:HE3	1.83	0.60
40:YF:155:LEU:HB2	40:YF:189:THR:HG21	1.83	0.60
51:YU:92:ARG:O	51:YU:94:ASN:N	2.34	0.60
9:QI:112:LYS:HA	9:QI:119:ALA:HB2	1.83	0.60
12:XL:60:LEU:HD12	12:XL:62:SER:H	1.66	0.60
26:Y0:77:ARG:NH2	36:YA:857:C:OP2	2.34	0.60
36:YA:580:C:OP1	51:YU:33:ARG:NH2	2.35	0.60
1:QA:407:G:OP1	4:QD:115:ARG:NH2	2.35	0.60
36:RA:1093:G:H21	36:RA:1098:A:H62	1.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:936:C:O2	1:XA:1382:C:N4	2.34	0.60
26:Y0:21:LEU:HD21	26:Y0:41:ARG:HH11	1.67	0.60
1:QA:8:A:N6	4:QD:205:GLU:O	2.34	0.60
11:QK:18:ARG:HG2	11:QK:81:ASP:HB2	1.83	0.60
56:RZ:52:SER:O	56:RZ:54:HIS:N	2.33	0.60
1:XA:1131:G:H1	1:XA:1143:G:H21	1.50	0.60
27:Y1:18:ILE:HG12	27:Y1:37:ILE:HG12	1.84	0.60
36:YA:2141:G:H1	36:YA:2150:U:H3	1.48	0.60
1:QA:1286:A:H2'	1:QA:1287:A:H4'	1.84	0.60
36:RA:1800:C:OP2	38:RD:183:ARG:NH1	2.30	0.60
13:XM:3:ARG:HE	13:XM:9:ILE:HG21	1.67	0.60
38:YD:17:THR:HB	38:YD:205:VAL:H	1.67	0.60
54:YX:53:LYS:H	54:YX:82:GLN:HB3	1.67	0.60
14:QN:34:TYR:O	14:QN:38:GLY:N	2.31	0.60
36:RA:1061:U:H5'	36:RA:1070:A:H1'	1.84	0.60
1:XA:1128:C:OP1	9:XI:66:ARG:NH2	2.35	0.60
33:Y7:9:ARG:HE	33:Y7:47:ARG:HG3	1.67	0.60
14:QN:40:CYS:SG	14:QN:41:ARG:N	2.75	0.59
22:QV:9:G:O2'	22:QV:10:G:N7	2.35	0.59
38:YD:85:ASP:OD2	38:YD:88:ARG:NH1	2.34	0.59
51:YU:114:LYS:HA	51:YU:118:GLY:HA3	1.83	0.59
10:QJ:3:LYS:N	10:QJ:74:ILE:O	2.34	0.59
36:YA:2134:A:OP2	36:YA:2157:G:N2	2.35	0.59
36:YA:2646:C:OP2	36:YA:2732:G:O2'	2.20	0.59
37:YB:44:G:O2'	37:YB:47:C:N4	2.35	0.59
39:YE:2:LYS:HB3	39:YE:95:ILE:HD12	1.83	0.59
40:YF:185:ASP:OD1	40:YF:188:ARG:NH1	2.35	0.59
36:RA:530:G:O2'	36:RA:532:A:N7	2.36	0.59
2:XB:54:THR:HG22	2:XB:199:TYR:HB3	1.84	0.59
38:YD:96:HIS:CE1	38:YD:102:LYS:HE2	2.38	0.59
1:QA:323:U:OP1	20:QT:26:ASN:ND2	2.33	0.59
23:QW:21:A:N6	23:QW:46:G:O2'	2.35	0.59
7:XG:79:ARG:NH2	23:XW:33:U:O2'	2.32	0.59
26:Y0:27:GLU:HG2	26:Y0:68:GLU:HA	1.84	0.59
47:YQ:81:VAL:O	47:YQ:82:ARG:NE	2.34	0.59
36:RA:2683:C:OP1	50:RT:53:ARG:NH2	2.33	0.59
38:YD:35:LYS:HG2	38:YD:104:TYR:CD2	2.37	0.59
53:YW:88:ARG:HB2	53:YW:92:ARG:HB3	1.84	0.59
1:QA:1502:A:H2	1:QA:1505:G:H1	1.50	0.59
39:RE:34:VAL:HG21	39:RE:77:ILE:HD11	1.83	0.59
1:QA:401:C:OP2	4:QD:73:ARG:NH2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:QF:3:ARG:NH1	6:QF:38:GLU:OE1	2.36	0.59
36:RA:1570:A:H4'	38:RD:38:LYS:HE2	1.84	0.59
1:XA:448:A:OP2	1:XA:485:G:N2	2.33	0.59
19:XS:40:ILE:HD11	19:XS:62:ILE:HD12	1.84	0.59
36:YA:2632:A:HO2'	36:YA:2811:G:HO2'	1.46	0.59
5:QE:93:PRO:HG2	8:QH:105:ARG:HH21	1.67	0.59
1:QA:970:C:N4	9:QI:128:ARG:O	2.36	0.59
30:Y4:1:MET:SD	41:YG:98:ARG:NH1	2.72	0.59
36:YA:2130:U:HO2'	36:YA:2133:G:HO2'	1.51	0.59
42:YH:28:GLY:HA3	42:YH:79:VAL:HB	1.85	0.59
1:QA:765:G:N2	1:QA:813:U:OP2	2.33	0.59
1:XA:971:G:N2	1:XA:1363:A:OP2	2.36	0.59
5:XE:8:GLU:OE2	5:XE:63:ARG:NH2	2.35	0.59
1:QA:1381:U:H3	7:QG:79:ARG:HH21	1.51	0.59
13:QM:23:TYR:HB3	13:QM:67:GLU:HG2	1.84	0.59
36:RA:2547:U:O2	45:RO:23:ARG:NH1	2.35	0.59
36:RA:958:U:OP2	47:RQ:14:ARG:NH1	2.36	0.59
56:YZ:10:ARG:NH2	56:YZ:26:GLY:O	2.34	0.59
1:QA:924:C:O2'	1:QA:1502:A:N6	2.36	0.58
1:QA:259:G:OP1	20:QT:83:ARG:NE	2.33	0.58
1:XA:376:G:O3'	16:XP:5:ARG:NH1	2.36	0.58
1:XA:1493:A:OP2	36:YA:1913:A:N6	2.36	0.58
36:YA:1256:G:N2	40:YF:82:ILE:O	2.34	0.58
36:YA:952:G:OP1	47:YQ:16:ARG:NH1	2.36	0.58
49:YS:84:GLN:HA	49:YS:110:LEU:HA	1.85	0.58
36:RA:948:G:H1	36:RA:969:U:H3	1.51	0.58
2:XB:42:ILE:HD11	2:XB:202:PRO:HB2	1.83	0.58
36:RA:2584:U:H2'	36:RA:2585:U:H2'	1.85	0.58
36:RA:2743:C:OP2	36:RA:2755:C:N4	2.37	0.58
2:XB:68:ILE:HG12	2:XB:161:ALA:HB3	1.85	0.58
6:XF:87:ARG:NH1	18:XR:75:ILE:O	2.36	0.58
29:Y3:15:TYR:O	29:Y3:20:LYS:NZ	2.36	0.58
36:RA:372:G:N2	36:RA:401:A:OP2	2.36	0.58
1:XA:1321:C:H5''	1:XA:1322:C:H2'	1.86	0.58
3:XC:58:GLU:HB2	3:XC:65:ALA:HB3	1.85	0.58
4:XD:9:CYS:SG	4:XD:22:LYS:NZ	2.76	0.58
27:Y1:50:ARG:NH1	27:Y1:57:GLU:OE2	2.33	0.58
26:Y0:39:ARG:HH21	36:YA:2355:C:H1'	1.68	0.58
38:YD:34:VAL:HB	38:YD:35:LYS:HD3	1.85	0.58
44:YN:118:LYS:O	44:YN:121:LYS:NZ	2.35	0.58
1:QA:1013:G:N2	1:QA:1016:A:OP2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:827:U:O2	1:QA:874:G:N2	2.36	0.58
29:R3:15:TYR:O	29:R3:20:LYS:NZ	2.37	0.58
36:RA:2306:C:N4	41:RG:42:GLY:O	2.37	0.58
36:RA:270(E):G:H1	36:RA:270(U):C:H42	1.50	0.58
36:YA:2111:C:N3	36:YA:2118:U:O2'	2.36	0.58
1:QA:1228:C:OP1	13:QM:108:ARG:NH1	2.34	0.58
25:QY:74:C:H2'	25:QY:75:C:H5'	1.85	0.58
36:RA:223:A:O2'	36:RA:420:C:O2	2.21	0.58
50:RT:92:GLY:O	50:RT:120:ARG:NH2	2.36	0.58
2:XB:88:ALA:HB2	2:XB:219:VAL:HG13	1.84	0.58
10:XJ:3:LYS:N	10:XJ:74:ILE:O	2.36	0.58
36:YA:1130:U:O2	39:YE:149:ARG:NH2	2.35	0.58
38:YD:35:LYS:N	38:YD:35:LYS:HD3	2.19	0.58
42:YH:10:PRO:HD2	42:YH:50:VAL:H	1.66	0.58
30:R4:49:PHE:CE2	30:R4:50:VAL:CG2	2.86	0.58
36:RA:1791:A:H5'	38:RD:206:LEU:HD12	1.84	0.58
1:XA:765:G:N2	1:XA:813:U:OP2	2.36	0.58
7:XG:28:ASN:OD1	7:XG:36:LYS:NZ	2.37	0.58
8:XH:4:ASP:OD1	8:XH:85:ARG:NH1	2.36	0.58
1:QA:316:G:OP2	1:QA:351:G:O2'	2.21	0.58
36:RA:1652:A:OP1	48:RR:8:ARG:NH1	2.37	0.58
36:RA:414:C:O2	36:RA:1864:U:O2'	2.21	0.58
38:RD:148:GLU:HB2	38:RD:151:LYS:HD2	1.85	0.58
40:RF:11:VAL:HG21	40:RF:20:LEU:HD13	1.85	0.58
2:XB:84:GLU:HB3	2:XB:219:VAL:HG21	1.85	0.58
1:QA:943:U:H1'	9:QI:124:GLN:HE22	1.68	0.58
47:RQ:66:ILE:HA	47:RQ:104:PHE:HA	1.86	0.58
16:XP:20:VAL:HG23	16:XP:35:LYS:HA	1.86	0.58
40:YF:158:THR:O	40:YF:164:ARG:NH2	2.37	0.58
1:QA:1326:C:OP2	21:QU:6:ARG:NH1	2.36	0.58
1:QA:842:C:O2'	1:QA:848:C:N4	2.37	0.58
36:RA:2502:G:H5''	36:RA:2503:A:H5''	1.85	0.58
1:QA:1375:A:H4'	7:QG:29:LYS:HE3	1.86	0.57
1:XA:405:U:O4	4:XD:2:GLY:N	2.37	0.57
11:XK:87:THR:HA	11:XK:91:ARG:HD2	1.84	0.57
36:YA:2112:G:O6	36:YA:2169:A:N6	2.35	0.57
37:YB:8:U:O2'	49:YS:25:ARG:NH2	2.37	0.57
36:YA:958:U:OP2	47:YQ:14:ARG:NH1	2.37	0.57
3:QC:131:ARG:NH1	3:QC:166:GLU:OE2	2.36	0.57
47:RQ:14:ARG:O	47:RQ:72:LYS:NZ	2.29	0.57
47:RQ:75:THR:HG21	47:RQ:85:LYS:HE3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:XC:47:LEU:HD22	3:XC:52:LEU:HB3	1.86	0.57
51:YU:76:TYR:OH	51:YU:93:LYS:HE3	2.03	0.57
14:QN:31:ARG:HH11	14:QN:32:SER:HB2	1.69	0.57
31:R5:40:LYS:HZ3	31:R5:46:CYS:HB3	1.68	0.57
36:RA:1190:G:OP1	46:RP:34:GLY:N	2.37	0.57
37:RB:44:G:O2'	37:RB:47:C:N4	2.35	0.57
36:YA:1652:A:N6	48:YR:11:ASN:OD1	2.35	0.57
50:YT:110:ILE:HG23	50:YT:114:LEU:HD12	1.86	0.57
1:QA:1422:G:H5''	45:RO:48:PRO:HB3	1.86	0.57
8:QH:4:ASP:OD1	8:QH:85:ARG:NH1	2.37	0.57
15:QO:29:VAL:HG21	15:QO:81:LEU:HD21	1.85	0.57
19:XS:50:ALA:HB1	19:XS:57:HIS:HB3	1.86	0.57
30:R4:49:PHE:HD2	30:R4:50:VAL:HG13	1.65	0.57
36:RA:2298:A:H62	36:RA:2318:G:H8	1.51	0.57
17:XQ:66:SER:O	17:XQ:70:ARG:NH1	2.37	0.57
27:Y1:97:LEU:HD22	36:YA:270(T):G:H5''	1.87	0.57
36:YA:2483:C:N3	47:YQ:124:LYS:NZ	2.50	0.57
51:YU:90:VAL:HG13	52:YV:39:LEU:HB3	1.85	0.57
7:QG:143:ARG:NH1	23:QW:41:A:O2'	2.38	0.57
26:R0:27:GLU:HG3	26:R0:68:GLU:HA	1.85	0.57
36:RA:2010:G:H5''	53:RW:42:ARG:HB2	1.86	0.57
41:RG:38:VAL:O	41:RG:158:ALA:N	2.30	0.57
50:RT:35:LYS:HG3	50:RT:37:GLY:H	1.69	0.57
1:XA:343:U:O2	1:XA:346:G:N1	2.35	0.57
3:XC:20:SER:OG	3:XC:22:TRP:NE1	2.37	0.57
36:YA:918:A:N3	37:YB:80:U:O2'	2.36	0.57
38:YD:61:LEU:O	38:YD:63:ARG:NH1	2.38	0.57
36:YA:2495:G:H5''	47:YQ:81:VAL:HG12	1.87	0.57
1:QA:671:G:O2'	6:QF:80:ARG:NH2	2.38	0.57
36:RA:1130:U:O2	39:RE:149:ARG:NH2	2.37	0.57
1:XA:979:C:OP1	1:XA:1223:C:N4	2.38	0.57
36:YA:1196:C:HO2'	36:YA:1228:G:HO2'	1.52	0.57
36:YA:140:A:H8	36:YA:1408:C:HO2'	1.53	0.57
13:XM:93:ARG:NH1	36:YA:888:C:OP1	2.38	0.57
50:YT:62:THR:HG22	50:YT:75:ILE:HG12	1.86	0.57
1:QA:406:G:H21	4:QD:119:GLN:HE22	1.53	0.57
41:RG:59:GLU:OE1	41:RG:153:ARG:NH2	2.38	0.57
23:XW:3:G:H1	23:XW:70:U:H3	1.52	0.57
28:Y2:32:LEU:HD11	28:Y2:54:LYS:HG3	1.87	0.57
30:Y4:23:GLU:O	30:Y4:25:TYR:N	2.35	0.57
36:YA:2012:G:OP1	53:YW:11:ARG:NH2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1239:A:O2'	1:QA:1298:C:N4	2.33	0.57
1:QA:1495:U:O4	58:QA:1667:PAR:N12	2.38	0.57
1:QA:951:G:OP2	13:QM:102:ARG:NH1	2.38	0.57
28:R2:47:ASN:ND2	36:RA:94:G:N3	2.52	0.57
36:RA:639:U:H3	36:RA:649:G:H1	1.51	0.57
56:RZ:80:ARG:HE	56:RZ:82:ARG:HE	1.52	0.57
32:R6:41:PRO:HD2	32:R6:46:HIS:H	1.69	0.57
36:RA:987:G:O2'	36:RA:1000:A:N3	2.34	0.57
53:RW:78:GLU:OE2	53:RW:99:ARG:NH1	2.37	0.57
10:XJ:53:PRO:O	14:XN:41:ARG:NH2	2.37	0.57
39:YE:50:GLY:HA2	39:YE:77:ILE:HA	1.86	0.57
32:R6:28:ARG:HB3	32:R6:30:THR:OG1	2.05	0.56
34:R8:28:GLY:O	34:R8:36:LYS:NZ	2.37	0.56
36:RA:2312:U:OP2	41:RG:74:LYS:NZ	2.35	0.56
36:RA:1795:C:O2	38:RD:255:LYS:NZ	2.38	0.56
43:RI:92:VAL:HG11	43:RI:120:ILE:HG23	1.83	0.56
36:YA:336:C:O2'	55:YY:35:TYR:OH	2.22	0.56
39:YE:8:LYS:HA	39:YE:26:ILE:HG22	1.87	0.56
1:QA:142:G:O2'	1:QA:195:A:N6	2.38	0.56
1:XA:1379:G:O6	7:XG:2:ALA:N	2.38	0.56
32:Y6:18:ARG:NH2	36:YA:2401:U:OP1	2.37	0.56
52:YV:38:LEU:H	52:YV:51:VAL:HG23	1.71	0.56
1:QA:1321:C:H5''	1:QA:1322:C:H5''	1.86	0.56
26:R0:7:LEU:HD13	47:RQ:80:GLU:HG2	1.87	0.56
39:RE:31:CYS:HB3	39:RE:49:LEU:HB3	1.87	0.56
2:XB:223:ILE:HG13	2:XB:229:VAL:HG22	1.87	0.56
36:YA:1607:C:N4	36:YA:1622:G:OP2	2.31	0.56
36:YA:663:G:H5''	46:YP:18:ARG:HD3	1.86	0.56
2:QB:178:ARG:NH2	2:QB:196:LEU:O	2.38	0.56
54:RX:53:LYS:HE3	54:RX:55:ASN:HD21	1.71	0.56
1:XA:1002:G:H1	1:XA:1038:C:H42	1.53	0.56
36:YA:780:G:OP1	38:YD:218:ARG:NH2	2.38	0.56
44:YN:22:THR:OG1	44:YN:23:LEU:N	2.35	0.56
19:XS:23:ASN:ND2	19:XS:44:MET:SD	2.78	0.56
39:YE:63:LEU:O	39:YE:73:GLU:OE2	2.23	0.56
31:Y5:40:LYS:NZ	53:YW:38:TYR:OH	2.32	0.56
1:QA:439:A:OP2	1:QA:493:G:N1	2.36	0.56
15:QO:26:GLU:OE2	15:QO:77:ARG:NH1	2.39	0.56
47:RQ:135:ASP:OD2	56:RZ:81:ARG:NH2	2.39	0.56
36:RA:2882:A:OP1	48:RR:96:ARG:NH1	2.39	0.56
36:YA:1824:G:N3	38:YD:254:THR:OG1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:YE:116:VAL:HG23	39:YE:120:TRP:HD1	1.70	0.56
36:YA:2635:C:H5''	39:YE:78:LEU:HA	1.88	0.56
56:YZ:17:ALA:HA	56:YZ:20:ARG:HE	1.70	0.56
39:RE:128:SER:OG	39:RE:129:HIS:N	2.39	0.56
41:RG:170:ARG:NH2	41:RG:182:LYS:O	2.35	0.56
36:YA:2293:C:O2'	49:YS:93:LYS:NZ	2.33	0.56
50:YT:20:PRO:HD2	50:YT:86:ILE:HG23	1.87	0.56
1:XA:150:C:H42	1:XA:171:A:H62	1.54	0.56
36:YA:2392:A:H2	36:YA:2424:C:H42	1.54	0.56
2:QB:71:VAL:HA	2:QB:93:VAL:HB	1.87	0.56
36:RA:1048:A:H3'	36:RA:1049:C:C6	2.41	0.56
32:R6:46:HIS:HD1	36:RA:2371:G:HO2'	1.54	0.56
36:RA:2619:C:H5''	39:RE:152:LYS:HD3	1.87	0.56
10:XJ:31:GLY:HA2	10:XJ:78:ASN:HD22	1.70	0.56
36:YA:1689:A:H62	36:YA:1698:A:H2	1.54	0.56
36:RA:2115:G:N2	36:RA:2165:G:N7	2.51	0.56
36:RA:2685:G:OP1	50:RT:51:ARG:NH2	2.38	0.56
42:RH:137:ASP:HB3	42:RH:140:LYS:HG2	1.87	0.56
17:XQ:62:SER:OG	17:XQ:63:ARG:N	2.38	0.56
37:YB:5:C:O2'	37:YB:27:C:O2	2.24	0.56
42:YH:46:GLU:OE1	42:YH:51:ARG:NH1	2.38	0.56
1:QA:757:U:O2'	1:QA:879:C:O2	2.24	0.56
3:QC:47:LEU:HB3	3:QC:52:LEU:HD23	1.88	0.56
1:QA:437:U:O2	4:QD:119:GLN:NE2	2.39	0.56
11:QK:86:GLY:H	11:QK:112:THR:HG22	1.70	0.56
36:RA:2315:G:OP1	41:RG:36:LYS:NZ	2.39	0.56
1:XA:811:C:O2'	1:XA:901:A:N1	2.38	0.56
36:YA:309:G:N3	36:YA:329:G:O2'	2.39	0.56
42:YH:6:ARG:HB3	42:YH:66:GLY:CA	2.36	0.56
50:YT:51:ARG:HG3	50:YT:98:LYS:HE3	1.88	0.56
2:QB:54:THR:HG22	2:QB:199:TYR:HB3	1.88	0.55
36:RA:1681:G:HO2'	36:RA:1762:A:HO2'	1.54	0.55
36:RA:1980:G:O2'	36:RA:1982:C:OP2	2.20	0.55
13:XM:24:GLY:O	13:XM:29:ARG:NH1	2.39	0.55
25:QY:58:A:O2'	25:QY:61:C:N4	2.39	0.55
36:RA:2597:G:H5'	38:RD:243:GLY:HA3	1.89	0.55
36:RA:900:A:H3'	36:RA:901:A:H8	1.70	0.55
56:RZ:5:LEU:HD21	56:RZ:47:VAL:HG11	1.87	0.55
32:Y6:41:PRO:HD2	32:Y6:46:HIS:H	1.71	0.55
35:Y9:4:ARG:NH1	36:YA:2477:C:O2	2.34	0.55
36:YA:495:G:H21	53:YW:61:ASN:HD21	1.52	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:YF:117:ARG:NH2	46:YP:1:MET:O	2.39	0.55
56:YZ:39:VAL:HG21	56:YZ:44:PHE:HD1	1.71	0.55
3:QC:44:GLU:HA	3:QC:52:LEU:HD21	1.87	0.55
23:QW:3:G:H22	23:QW:70:U:H3	1.53	0.55
1:XA:481:G:O2'	1:XA:482:A:N7	2.36	0.55
37:YB:104:A:OP1	56:YZ:72:ARG:NH2	2.39	0.55
36:YA:2675:A:O2'	45:YO:29:ASN:ND2	2.40	0.55
1:QA:297:G:N2	1:QA:300:A:OP2	2.38	0.55
1:QA:587:G:N2	1:QA:754:C:OP2	2.37	0.55
32:R6:15:GLU:OE1	32:R6:18:ARG:NH2	2.38	0.55
36:RA:2751:G:OP2	42:RH:4:ILE:HG23	2.06	0.55
36:RA:642:G:H21	36:RA:646:A:H2	1.54	0.55
38:RD:143:HIS:ND1	38:RD:194:GLY:O	2.38	0.55
39:RE:2:LYS:HD3	39:RE:95:ILE:HG22	1.89	0.55
41:RG:47:LYS:HD3	41:RG:81:LYS:HB2	1.89	0.55
43:RI:92:VAL:HG13	43:RI:92:VAL:O	2.07	0.55
1:XA:522:C:H41	12:XL:53:ARG:HH22	1.53	0.55
5:XE:75:THR:OG1	5:XE:76:ILE:N	2.39	0.55
36:YA:807:U:O2'	36:YA:2060:A:N1	2.38	0.55
38:YD:33:LEU:H	38:YD:33:LEU:CD2	1.95	0.55
9:QI:10:ARG:HE	9:QI:105:ASP:HB2	1.72	0.55
38:RD:85:ASP:OD2	38:RD:88:ARG:NH1	2.35	0.55
42:RH:54:ARG:NH1	42:RH:57:ASP:OD1	2.40	0.55
3:XC:88:ARG:NH2	3:XC:101:LEU:O	2.39	0.55
1:XA:954:G:H5'	13:XM:121:LYS:HG2	1.89	0.55
36:YA:1093:G:H21	36:YA:1098:A:H62	1.54	0.55
36:YA:259:G:H21	36:YA:621:A:H8	1.53	0.55
8:QH:42:GLU:HG3	8:QH:109:ILE:HD12	1.88	0.55
17:QQ:9:VAL:HG22	17:QQ:56:VAL:HG22	1.87	0.55
36:RA:832:G:OP1	46:RP:36:LYS:NZ	2.40	0.55
45:RO:25:LEU:HB2	45:RO:38:VAL:HG23	1.89	0.55
1:XA:971:G:OP2	1:XA:1231:G:N2	2.37	0.55
5:XE:12:LEU:HB3	5:XE:31:LEU:HB3	1.87	0.55
1:QA:1055:A:N3	3:QC:156:ARG:NH1	2.55	0.55
1:QA:1172:C:H2'	1:QA:1173:G:H8	1.71	0.55
38:RD:182:LEU:H	38:RD:272:ALA:HB3	1.71	0.55
52:RV:24:LYS:HA	52:RV:92:THR:HG23	1.89	0.55
25:QY:53:G:H2'	56:RZ:183:LEU:HB2	1.88	0.55
36:YA:605:C:O2	36:YA:657:U:O2'	2.24	0.55
40:YF:143:ALA:HB1	40:YF:148:LEU:HB2	1.88	0.55
9:QI:128:ARG:NH2	22:QV:34:C:OP2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:R1:4:VAL:HG23	27:R1:11:ARG:HB3	1.89	0.55
43:YI:79:ILE:HB	43:YI:142:VAL:HG12	1.89	0.55
32:R6:15:GLU:HA	32:R6:49:HIS:HA	1.88	0.55
36:RA:1265:A:H61	36:RA:2013:A:H5''	1.72	0.55
42:RH:5:GLY:O	42:RH:8:PRO:HD3	2.07	0.55
53:RW:69:LEU:HD13	53:RW:107:LEU:HD13	1.88	0.55
38:YD:96:HIS:ND1	38:YD:102:LYS:HG2	2.21	0.55
1:QA:18:C:H5''	5:QE:127:ASN:HD21	1.72	0.55
1:QA:674:G:N2	1:QA:717:C:O2	2.39	0.55
9:QI:128:ARG:HH22	22:QV:33:U:H3'	1.72	0.55
31:R5:45:VAL:HA	31:R5:51:TYR:HE2	1.72	0.55
36:RA:2680:C:H5'	39:RE:189:PRO:HA	1.88	0.55
36:RA:2788:C:OP1	39:RE:61:ARG:NH2	2.40	0.55
39:RE:92:THR:HG23	39:RE:94:GLU:H	1.72	0.55
40:RF:40:GLN:HE22	40:RF:182:ASN:HB2	1.72	0.55
1:XA:1178:G:N2	1:XA:1181:G:N7	2.55	0.55
23:XW:66:U:H2'	23:XW:67:A:H8	1.71	0.55
32:Y6:26:ASN:ND2	32:Y6:35:GLU:OE2	2.40	0.55
36:YA:1728:G:N1	36:YA:1730:U:OP2	2.40	0.55
56:YZ:52:SER:O	56:YZ:54:HIS:ND1	2.40	0.55
1:QA:406:G:H5'	4:QD:5:ILE:HD11	1.88	0.54
36:RA:1779:U:OP2	36:RA:1784:A:N6	2.33	0.54
8:XH:101:PRO:O	8:XH:125:ARG:NH2	2.40	0.54
36:RA:2392:A:OP2	36:RA:2422:A:N6	2.40	0.54
48:RR:103:ARG:NH1	48:RR:108:GLY:O	2.39	0.54
10:XJ:45:ARG:HB3	10:XJ:65:LEU:HB3	1.89	0.54
29:Y3:8:LEU:HB2	29:Y3:28:LEU:HD13	1.88	0.54
36:YA:28:A:N6	36:YA:512:G:O2'	2.40	0.54
41:YG:37:VAL:HG22	41:YG:159:VAL:HG12	1.89	0.54
1:QA:1372:U:OP1	9:QI:72:GLY:N	2.40	0.54
33:R7:49:ARG:NH1	36:RA:128:C:O2'	2.34	0.54
1:XA:1178:G:OP2	9:XI:93:ARG:NH2	2.39	0.54
2:XB:192:SER:OG	2:XB:193:ASP:N	2.40	0.54
22:XV:63:G:H4'	26:Y0:11:ARG:HH22	1.72	0.54
36:YA:1600:C:OP1	54:YX:58:HIS:NE2	2.35	0.54
36:YA:2657:A:O2'	42:YH:160:LYS:NZ	2.39	0.54
36:YA:372:G:N2	36:YA:401:A:OP2	2.39	0.54
36:YA:2683:C:OP1	50:YT:53:ARG:NH2	2.40	0.54
25:QY:21:A:N6	25:QY:46:G:O2'	2.40	0.54
38:RD:35:LYS:HB3	38:RD:36:PRO:HD3	1.89	0.54
36:RA:2296:U:OP2	49:RS:9:ARG:NH1	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:1322:C:H5'	13:XM:100:GLY:HA2	1.88	0.54
1:XA:945:G:N2	1:XA:1334:G:O2'	2.41	0.54
3:XC:14:ILE:HG12	3:XC:15:THR:HG23	1.89	0.54
13:XM:99:ARG:HB2	13:XM:101:GLN:HE22	1.72	0.54
41:YG:161:THR:HG22	41:YG:163:ALA:H	1.72	0.54
9:QI:128:ARG:NH1	22:QV:35:A:OP2	2.40	0.54
33:R7:10:ARG:HH12	36:RA:1378:A:H5''	1.73	0.54
36:RA:1667:G:O2'	36:RA:1991:U:O4	2.25	0.54
38:RD:12:SER:HB2	38:RD:208:LYS:HB3	1.88	0.54
56:RZ:10:ARG:NH2	56:RZ:26:GLY:O	2.41	0.54
2:XB:82:ARG:NH1	2:XB:92:TYR:OH	2.40	0.54
13:XM:83:ASP:OD1	13:XM:93:ARG:NH2	2.41	0.54
36:YA:855:G:H1	36:YA:922:U:H3	1.56	0.54
51:YU:52:ARG:HD2	51:YU:55:ARG:NH2	2.21	0.54
6:QF:95:GLU:O	18:QR:32:ARG:NH1	2.40	0.54
36:RA:1342:A:OP1	54:RX:36:LYS:NZ	2.35	0.54
38:RD:33:LEU:O	38:RD:35:LYS:N	2.39	0.54
36:YA:1598:C:O3'	54:YX:35:THR:OG1	2.26	0.54
1:QA:468:A:OP1	16:QP:75:ARG:NH2	2.40	0.54
4:QD:38:TYR:CE2	4:QD:45:GLN:HG3	2.42	0.54
1:QA:1123:A:H4'	10:QJ:36:GLY:HA3	1.88	0.54
47:RQ:27:VAL:HG21	47:RQ:134:ARG:HA	1.90	0.54
1:XA:1129:C:O2'	1:XA:1131:G:N7	2.40	0.54
1:XA:950:U:H3'	13:XM:102:ARG:HH21	1.72	0.54
13:XM:93:ARG:HG2	13:XM:94:ARG:HH21	1.73	0.54
36:YA:1021:A:OP2	44:YN:65:LYS:NZ	2.37	0.54
36:RA:1638:C:O2	36:RA:2698:U:O2'	2.26	0.54
36:RA:861:A:N3	37:RB:79:C:O2'	2.41	0.54
36:RA:2575:C:H5'	39:RE:144:ARG:HG2	1.90	0.54
1:XA:1305:G:O2'	1:XA:1332:A:N6	2.40	0.54
1:XA:380:G:N2	1:XA:383:A:OP2	2.40	0.54
2:XB:33:TYR:HB2	2:XB:43:ASP:HB2	1.89	0.54
9:XI:42:ARG:NH1	9:XI:71:SER:OG	2.41	0.54
26:Y0:68:GLU:HG3	26:Y0:80:HIS:HB2	1.90	0.54
37:YB:40:U:H3	37:YB:43:C:H5''	1.73	0.54
28:R2:4:SER:OG	28:R2:5:GLU:N	2.39	0.54
36:RA:1065:U:H3	36:RA:1073:A:H61	1.54	0.54
40:RF:195:ASP:OD1	40:RF:195:ASP:N	2.38	0.54
1:XA:401:C:O2'	1:XA:621:A:N3	2.37	0.54
12:XL:39:VAL:HB	12:XL:57:LYS:HB2	1.90	0.54
36:YA:1800:C:OP2	38:YD:183:ARG:NH1	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:XW:76:A:N6	36:YA:2422:A:O4'	2.41	0.54
36:YA:36:G:N3	36:YA:450:G:O2'	2.41	0.54
56:YZ:102:LEU:HD11	56:YZ:124:ILE:HG12	1.90	0.54
1:QA:191:G:O2'	20:QT:101:GLY:O	2.25	0.54
4:XD:23:GLY:N	4:XD:26:CYS:SG	2.78	0.54
36:YA:814:C:O2'	36:YA:1225:C:N3	2.41	0.54
36:YA:2033:A:O2'	36:YA:2035:G:OP2	2.23	0.54
1:QA:1098:C:OP1	2:QB:144:ARG:NH2	2.42	0.53
2:QB:84:GLU:HG3	2:QB:215:LEU:HB3	1.89	0.53
10:QJ:48:THR:HA	10:QJ:62:HIS:HB3	1.88	0.53
36:RA:1817:G:OP1	38:RD:88:ARG:NH2	2.42	0.53
37:YB:87:G:N2	37:YB:89(A):A:OP2	2.35	0.53
45:YO:64:ARG:HB2	45:YO:83:ALA:HB3	1.90	0.53
1:QA:948:C:H2'	1:QA:949:A:H8	1.72	0.53
1:QA:1073:U:O2	2:QB:104:ASN:ND2	2.42	0.53
7:QG:78:ARG:NH1	7:QG:154:TYR:O	2.40	0.53
18:QR:58:LEU:HD23	18:QR:62:GLU:HB3	1.90	0.53
37:RB:89(A):A:O3'	47:RQ:16:ARG:NH2	2.41	0.53
36:YA:1441:G:H2'	36:YA:1442:G:H8	1.73	0.53
36:YA:2882:A:OP1	48:YR:96:ARG:NH1	2.40	0.53
36:YA:414:C:O2	36:YA:1864:U:O2'	2.23	0.53
47:YQ:41:TRP:HB3	47:YQ:94:VAL:HG21	1.90	0.53
1:QA:107:G:N7	20:QT:15:ARG:NH2	2.56	0.53
1:QA:414:A:OP2	1:QA:428:G:N2	2.36	0.53
36:RA:781:A:OP1	38:RD:218:ARG:NH2	2.41	0.53
41:RG:55:LYS:HA	41:RG:58:GLN:HE22	1.74	0.53
37:RB:7:G:H21	49:RS:38:GLN:HE22	1.56	0.53
3:XC:55:VAL:HG12	3:XC:68:VAL:HG12	1.89	0.53
1:XA:537:G:OP1	12:XL:113:ARG:NH2	2.41	0.53
36:YA:861:A:N3	37:YB:79:C:O2'	2.41	0.53
41:YG:60:LEU:HD12	41:YG:63:ILE:HD11	1.90	0.53
36:RA:1022:G:N2	36:RA:1023:U:O4	2.36	0.53
36:RA:1815:A:OP2	38:RD:54:ARG:NH2	2.41	0.53
36:RA:2258:C:O2'	36:RA:2427:C:OP2	2.26	0.53
8:QH:20:TYR:HE2	8:QH:75:ARG:HD2	1.74	0.53
13:QM:65:LYS:HD3	30:R4:52:THR:HG21	1.91	0.53
37:RB:8:U:H3	37:RB:112:G:H1	1.55	0.53
52:RV:62:LEU:HD11	52:RV:95:LEU:HB2	1.90	0.53
5:XE:137:GLU:OE1	5:XE:140:ARG:NH1	2.40	0.53
36:YA:1791:A:N6	36:YA:1828:G:O2'	2.36	0.53
39:YE:134:ILE:HA	39:YE:137:HIS:HD2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:QD:201:GLN:HE21	5:QE:99:GLY:HA2	1.74	0.53
36:RA:2134:A:OP2	36:RA:2157:G:N2	2.42	0.53
46:RP:59:LEU:HA	46:RP:61:ARG:HH21	1.74	0.53
32:Y6:28:ARG:HG3	32:Y6:30:THR:H	1.74	0.53
50:YT:36:GLU:HG3	50:YT:41:ARG:HE	1.73	0.53
13:QM:93:ARG:HH11	36:RA:887:A:H5'	1.74	0.53
34:R8:61:LEU:HD13	36:RA:593:G:H4'	1.90	0.53
36:RA:942:G:O2'	36:RA:1189:A:N3	2.38	0.53
1:XA:195:A:OP1	20:XT:65:LYS:NZ	2.40	0.53
56:YZ:53:ILE:HG22	56:YZ:71:VAL:HG13	1.90	0.53
4:QD:53:ASP:HB3	4:QD:57:ARG:HH12	1.74	0.53
11:QK:58:PRO:HB2	11:QK:93:GLN:HG3	1.91	0.53
36:RA:2572:A:OP1	36:RA:2574:G:O2'	2.26	0.53
38:RD:76:PRO:HB3	38:RD:118:VAL:HG22	1.91	0.53
39:RE:114:ALA:HB3	39:RE:160:TYR:HB3	1.91	0.53
43:RI:92:VAL:CG2	43:RI:97:ILE:CD1	2.87	0.53
1:XA:1305:G:N2	1:XA:1332:A:OP2	2.42	0.53
13:XM:19:LEU:HD21	13:XM:56:LEU:HD21	1.90	0.53
34:Y8:28:GLY:O	34:Y8:36:LYS:NZ	2.42	0.53
50:YT:24:PRO:HD3	50:YT:52:ILE:HD12	1.90	0.53
12:QL:58:VAL:HG11	12:QL:85:ILE:HD11	1.91	0.53
27:R1:51:VAL:HG21	27:R1:74:VAL:HG21	1.91	0.53
36:RA:184:C:O2'	36:RA:217:G:N3	2.37	0.53
36:RA:2635:C:H5''	39:RE:78:LEU:HA	1.90	0.53
36:RA:1252:G:N2	51:RU:37:GLU:OE2	2.42	0.53
4:XD:38:TYR:CE2	4:XD:45:GLN:HG3	2.44	0.53
6:XF:30:LEU:HD23	6:XF:75:LEU:HD11	1.91	0.53
11:XK:86:GLY:O	11:XK:91:ARG:NH1	2.42	0.53
25:XY:4:G:H1	25:XY:69:C:H42	1.54	0.53
39:YE:117:MET:HA	39:YE:122:PHE:H	1.73	0.53
47:YQ:66:ILE:HA	47:YQ:104:PHE:HA	1.89	0.53
18:QR:48:GLY:O	18:QR:74:ARG:NH2	2.42	0.53
19:QS:16:LEU:HA	19:QS:19:VAL:HG12	1.90	0.53
30:R4:42:PHE:O	30:R4:44:THR:N	2.42	0.53
46:RP:36:LYS:HD3	46:RP:39:LYS:HB3	1.89	0.53
1:XA:587:G:N2	1:XA:754:C:OP2	2.42	0.53
11:XK:22:HIS:HB3	11:XK:29:ILE:HG23	1.91	0.53
1:XA:1321:C:H4'	13:XM:87:TYR:HE1	1.74	0.53
36:YA:1022:G:N2	36:YA:1023:U:O4	2.42	0.53
36:YA:2816:C:O2	36:YA:2883:A:O2'	2.24	0.53
30:R4:49:PHE:CD2	30:R4:50:VAL:N	2.76	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:RA:180:G:N2	36:RA:215:G:O6	2.42	0.52
36:RA:2637:U:OP1	39:RE:82:ARG:NH1	2.43	0.52
38:RD:145:VAL:HB	38:RD:155:LEU:HB2	1.91	0.52
36:RA:1327:C:O2'	48:RR:105:ARG:NH2	2.41	0.52
1:XA:1281:U:H5''	1:XA:1282:C:H5	1.74	0.52
38:YD:123:ALA:HB3	38:YD:131:LEU:HG	1.91	0.52
42:YH:153:LYS:HB3	42:YH:162:ILE:H	1.74	0.52
53:YW:69:LEU:HD13	53:YW:107:LEU:HD13	1.90	0.52
36:RA:2791:C:OP1	36:RA:2893:G:N2	2.43	0.52
36:RA:605:C:O2	36:RA:657:U:O2'	2.28	0.52
2:XB:178:ARG:HH22	8:XH:74:PRO:HB3	1.74	0.52
34:Y8:58:ILE:HG22	46:YP:49:ARG:HH11	1.74	0.52
27:R1:83:GLU:HG2	27:R1:85:LEU:H	1.74	0.52
36:RA:2668:G:O2'	42:RH:111:HIS:NE2	2.38	0.52
55:RY:46:LYS:NZ	55:RY:47:LYS:O	2.42	0.52
4:XD:150:GLU:OE2	4:XD:153:ARG:NH1	2.43	0.52
6:XF:3:ARG:NH1	6:XF:38:GLU:OE2	2.42	0.52
48:YR:104:ARG:NH2	48:YR:107:ASP:OD2	2.38	0.52
2:QB:127:ILE:O	2:QB:135:GLN:NE2	2.32	0.52
5:QE:35:GLY:HA3	5:QE:112:LEU:HB3	1.92	0.52
36:RA:2198:A:OP1	43:RI:33:ARG:NH2	2.40	0.52
37:RB:22:U:H3	37:RB:61:G:H1	1.57	0.52
46:RP:98:GLU:O	46:RP:102:ARG:NH2	2.42	0.52
36:RA:662:G:OP1	46:RP:15:ARG:NH1	2.43	0.52
48:RR:51:LEU:HD22	48:RR:66:VAL:HG13	1.91	0.52
12:XL:70:ILE:HG13	12:XL:100:ILE:HD12	1.90	0.52
19:XS:32:LYS:HA	19:XS:50:ALA:HB3	1.90	0.52
19:XS:63:THR:OG1	19:XS:65:ASN:OD1	2.23	0.52
1:QA:989:C:H1'	1:QA:1016:A:H2	1.75	0.52
1:QA:1328:C:HO2'	13:QM:29:ARG:HH21	1.55	0.52
36:RA:2130:U:HO2'	36:RA:2133:G:HO2'	1.58	0.52
36:RA:2468:G:OP1	47:RQ:119:ARG:NH2	2.40	0.52
42:RH:6:ARG:HG3	42:RH:54:ARG:HH21	1.73	0.52
56:RZ:136:PHE:HE2	56:RZ:138:GLU:HB2	1.74	0.52
56:RZ:5:LEU:H	56:RZ:59:LEU:HA	1.73	0.52
35:Y9:2:LYS:O	35:Y9:35:ARG:N	2.43	0.52
36:YA:1899:G:H21	36:YA:1902:C:H41	1.57	0.52
36:YA:2291:U:O2'	36:YA:2374:C:O2	2.27	0.52
38:YD:168:ARG:HG2	38:YD:173:VAL:HG12	1.92	0.52
39:YE:9:VAL:HB	39:YE:25:VAL:HG23	1.92	0.52
1:QA:1288:A:N3	1:QA:1352:C:O2'	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:1221:G:OP1	1:XA:1321:C:N4	2.40	0.52
1:XA:1279:A:OP1	10:XJ:7:LYS:NZ	2.39	0.52
1:XA:501:C:H1'	1:XA:549:C:H1'	1.92	0.52
1:XA:254:G:O2'	17:XQ:16:GLN:O	2.27	0.52
36:YA:793:A:OP2	36:YA:2071:A:O2'	2.28	0.52
51:YU:52:ARG:CD	51:YU:55:ARG:HH21	2.22	0.52
36:RA:2847:U:OP1	50:RT:98:LYS:NZ	2.38	0.52
1:XA:1494:G:N7	58:XA:1679:PAR:N32	2.58	0.52
1:XA:272:C:H2'	1:XA:273:A:H8	1.73	0.52
36:YA:141:A:H8	36:YA:1595:G:H21	1.56	0.52
36:RA:1788:C:OP1	38:RD:222:ARG:NH2	2.43	0.52
36:RA:300:A:OP1	55:RY:84:ARG:NH2	2.41	0.52
56:RZ:53:ILE:HG22	56:RZ:71:VAL:HG13	1.91	0.52
7:QG:116:ALA:HA	7:QG:119:ARG:HE	1.75	0.52
36:RA:1394:U:O2	54:RX:16:LYS:NZ	2.39	0.52
41:RG:103:LEU:O	41:RG:107:LEU:HD22	2.10	0.52
36:RA:1652:A:N6	48:RR:11:ASN:OD1	2.34	0.52
19:XS:19:VAL:HG11	19:XS:41:VAL:HG11	1.92	0.52
1:QA:1192:C:O2	5:QE:25:ARG:NH2	2.42	0.52
1:QA:165:C:H2'	1:QA:166:G:H8	1.75	0.52
36:RA:2119:A:N6	36:RA:2170:A:N7	2.48	0.52
37:RB:5:C:O2'	37:RB:27:C:O2	2.28	0.52
40:RF:161:GLU:HG2	40:RF:164:ARG:HH21	1.74	0.52
48:RR:38:VAL:HG22	48:RR:112:ALA:HB2	1.91	0.52
56:RZ:19:ARG:NH1	56:RZ:84:GLU:O	2.43	0.52
1:XA:376:G:H1	1:XA:387:U:H3	1.57	0.52
36:YA:1093:G:OP1	42:YH:170:ARG:NH1	2.43	0.52
36:YA:998:C:OP2	51:YU:58:ARG:NH1	2.39	0.52
37:YB:44:G:H1'	37:YB:47:C:H42	1.75	0.52
40:YF:101:LEU:O	40:YF:106:ARG:NH1	2.43	0.52
49:YS:67:ARG:NH2	49:YS:103:GLU:OE1	2.41	0.52
3:QC:14:ILE:HG22	3:QC:15:THR:HG23	1.92	0.51
19:QS:3:ARG:HH22	19:QS:11:VAL:HB	1.74	0.51
45:RO:97:ARG:H	45:RO:117:LEU:HD23	1.74	0.51
37:RB:8:U:O3'	49:RS:25:ARG:NH2	2.41	0.51
4:XD:98:GLU:HA	4:XD:103:ASN:HD22	1.75	0.51
36:YA:1288:U:O3'	36:YA:1647:G:N2	2.43	0.51
1:XA:410:G:H21	1:XA:432:A:H62	1.58	0.51
2:QB:80:ILE:HD11	2:QB:208:ILE:HG23	1.92	0.51
12:QL:60:LEU:HD21	12:QL:64:TYR:HB2	1.91	0.51
14:QN:59:ALA:HB1	14:QN:61:TRP:HZ3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:QT:26:ASN:HB2	20:QT:71:THR:HG23	1.91	0.51
36:RA:793:A:OP2	36:RA:2071:A:O2'	2.27	0.51
41:RG:97:ASP:H	41:RG:100:TRP:HD1	1.56	0.51
25:XY:53:G:H1	25:XY:61:C:H42	1.59	0.51
1:QA:824:C:O2'	8:QH:1:MET:N	2.43	0.51
25:QY:50:G:H21	25:QY:66:U:H3	1.59	0.51
38:RD:254:THR:HG23	38:RD:255:LYS:HG3	1.93	0.51
41:RG:16:ARG:HE	41:RG:31:VAL:HG11	1.75	0.51
47:RQ:35:VAL:HB	47:RQ:102:VAL:HG12	1.93	0.51
1:XA:1414:U:H2'	1:XA:1415:G:H8	1.74	0.51
3:XC:46:GLU:HG3	3:XC:83:ARG:HH22	1.75	0.51
10:QJ:49:VAL:HG13	14:QN:41:ARG:HB2	1.93	0.51
1:QA:376:G:H5''	16:QP:5:ARG:HB2	1.93	0.51
30:R4:49:PHE:HD2	30:R4:50:VAL:HG22	1.68	0.51
36:RA:2688:U:OP1	36:RA:2713:A:N6	2.43	0.51
36:RA:2540:C:O2'	36:RA:2740:A:N3	2.38	0.51
36:RA:2777:G:OP2	36:RA:2781:A:O2'	2.29	0.51
33:R7:35:ARG:NH1	36:RA:54:G:O2'	2.43	0.51
44:RN:42:TRP:O	51:RU:64:ARG:NE	2.43	0.51
2:XB:77:ALA:HB2	2:XB:211:ILE:HD13	1.91	0.51
36:RA:500:G:N1	36:RA:503:A:OP2	2.42	0.51
1:XA:352:C:O2	1:XA:355:C:N4	2.41	0.51
10:XJ:84:GLN:HG3	10:XJ:85:LEU:HD12	1.91	0.51
36:YA:1859:A:N6	36:YA:1883:G:O2'	2.44	0.51
1:QA:979:C:OP1	1:QA:1223:C:N4	2.44	0.51
6:QF:50:TYR:HE1	18:QR:77:GLY:HA2	1.75	0.51
29:R3:8:LEU:HA	29:R3:54:VAL:HG12	1.92	0.51
36:RA:392:C:H5''	36:RA:409:C:H5''	1.93	0.51
39:RE:201:THR:HG22	39:RE:203:LYS:H	1.75	0.51
1:XA:619:U:N3	4:XD:134:ASP:OD1	2.34	0.51
6:XF:36:ARG:NH2	6:XF:38:GLU:OE2	2.44	0.51
28:Y2:29:LYS:HD2	28:Y2:57:ILE:HD13	1.93	0.51
38:YD:148:GLU:HB2	38:YD:151:LYS:HD2	1.92	0.51
2:QB:187:LEU:HA	2:QB:201:ILE:HG13	1.93	0.51
36:RA:1662:C:O2'	36:RA:2687:U:OP1	2.29	0.51
1:XA:527:G:O6	12:XL:49:ASN:ND2	2.44	0.51
1:XA:701:C:O2	1:XA:703:G:N1	2.44	0.51
9:XI:13:ALA:HB2	9:XI:68:GLY:HA3	1.93	0.51
20:XT:49:ALA:HB2	20:XT:92:LEU:HD11	1.92	0.51
1:QA:1224:G:O2'	1:QA:1322:C:OP2	2.29	0.51
2:QB:198:ASP:OD1	8:QH:68:ARG:NH1	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:QC:122:GLU:OE2	3:QC:126:ARG:NH2	2.40	0.51
20:QT:53:LEU:HD12	20:QT:100:ILE:HG23	1.93	0.51
23:QW:37:A:N6	23:QW:39:G:N7	2.58	0.51
31:R5:13:LYS:HG2	31:R5:16:ARG:HH21	1.75	0.51
36:RA:1479:G:OP2	36:RA:1510:A:N6	2.38	0.51
36:RA:442:G:H1'	40:RF:48:THR:HG21	1.93	0.51
56:RZ:132:ASN:HD21	56:RZ:160:GLY:HA3	1.74	0.51
1:XA:406:G:H5'	4:XD:5:ILE:HD11	1.92	0.51
5:XE:105:VAL:HG21	5:XE:128:PRO:HB3	1.92	0.51
13:XM:86:CYS:SG	13:XM:87:TYR:N	2.84	0.51
31:Y5:49:CYS:H	31:Y5:57:VAL:HG12	1.76	0.51
36:YA:956:G:OP2	47:YQ:14:ARG:NH2	2.44	0.51
4:QD:53:ASP:O	4:QD:57:ARG:NH1	2.44	0.51
36:RA:2008:C:H2'	36:RA:2009:G:H8	1.75	0.51
36:RA:2115:G:N1	36:RA:2164:C:OP2	2.44	0.51
36:RA:2508:G:H1	36:RA:2580:U:H3	1.59	0.51
45:RO:47:ILE:O	45:RO:53:LYS:NZ	2.41	0.51
34:Y8:29:LYS:NZ	36:YA:2418:A:OP2	2.36	0.51
36:YA:2788:C:OP1	39:YE:61:ARG:NH1	2.44	0.51
2:QB:168:THR:HB	2:QB:192:SER:HB2	1.94	0.50
36:RA:2006:C:O2'	36:RA:2823:A:N3	2.42	0.50
45:RO:17:ARG:HE	45:RO:47:ILE:HD13	1.75	0.50
3:XC:11:ARG:NH2	3:XC:177:THR:O	2.44	0.50
20:XT:26:ASN:HB2	20:XT:71:THR:HG23	1.94	0.50
1:XA:1286:A:H5''	21:XU:26:LYS:HD3	1.93	0.50
50:YT:3:ARG:HB2	50:YT:6:LEU:HB2	1.92	0.50
1:QA:247:G:OP2	17:QQ:101:ARG:NE	2.43	0.50
1:QA:573:A:N3	1:QA:883:C:O2'	2.42	0.50
2:QB:97:TRP:HZ3	2:QB:172:ILE:HG12	1.76	0.50
55:RY:85:VAL:HG12	55:RY:94:LYS:HA	1.93	0.50
1:XA:1347:G:O2'	1:XA:1373:G:N1	2.40	0.50
6:XF:30:LEU:HB3	6:XF:35:ALA:HB3	1.93	0.50
32:Y6:7:ILE:HG13	32:Y6:8:LYS:H	1.76	0.50
36:YA:1899:G:H21	36:YA:1902:C:N4	2.08	0.50
36:YA:2777:G:OP2	36:YA:2781:A:O2'	2.28	0.50
1:QA:1032(A):G:H2'	1:QA:1032(B):G:H8	1.76	0.50
58:QA:1667:PAR:N24	58:QA:1667:PAR:O44	2.44	0.50
1:QA:362:G:N2	1:QA:365:U:OP2	2.44	0.50
1:QA:452:A:H62	1:QA:480:U:H3	1.59	0.50
1:QA:878:G:H5'	8:QH:89:PRO:HG2	1.93	0.50
23:QW:3:G:H2'	23:QW:4:G:H8	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:RA:693:C:O2'	36:RA:1353:A:N3	2.37	0.50
22:QV:76:A:H3'	36:RA:2585:U:H5	1.77	0.50
36:RA:2723:C:OP1	48:RR:3:HIS:ND1	2.38	0.50
23:XW:19:G:N2	23:XW:56:C:N3	2.60	0.50
41:YG:5:VAL:HG13	41:YG:8:LYS:HB3	1.93	0.50
11:QK:93:GLN:OE1	11:QK:96:ARG:NH2	2.37	0.50
33:R7:22:MET:HA	33:R7:28:ARG:HG2	1.93	0.50
36:RA:805:G:N2	36:RA:829:A:OP1	2.40	0.50
39:RE:29:GLY:H	39:RE:51:PHE:HE1	1.58	0.50
46:RP:89:ALA:O	46:RP:121:LYS:NZ	2.41	0.50
1:XA:1336:C:O2	1:XA:1337:G:N1	2.44	0.50
1:XA:1492:A:OP1	12:XL:47:LYS:N	2.45	0.50
2:XB:178:ARG:NH1	2:XB:196:LEU:O	2.45	0.50
1:XA:1249:C:O2'	9:XI:73:GLN:NE2	2.44	0.50
33:Y7:49:ARG:NH1	36:YA:128:C:O2'	2.45	0.50
33:Y7:7:PRO:HB2	36:YA:1309:G:H4'	1.92	0.50
36:YA:523:C:O2	36:YA:553:U:O2'	2.29	0.50
36:YA:730:C:OP1	36:YA:1775:U:O2'	2.29	0.50
42:YH:6:ARG:HH22	42:YH:62:LYS:CG	2.23	0.50
56:YZ:125:LEU:HB3	56:YZ:165:VAL:HG23	1.92	0.50
5:QE:18:ARG:HH21	5:QE:25:ARG:HB3	1.76	0.50
14:QN:40:CYS:HB3	14:QN:43:CYS:HB2	1.94	0.50
36:RA:1600:C:OP1	54:RX:58:HIS:NE2	2.32	0.50
36:RA:2727:G:O2'	45:RO:70:LYS:NZ	2.44	0.50
8:XH:86:ILE:HG12	8:XH:135:CYS:HA	1.93	0.50
12:XL:25:PRO:HD2	12:XL:98:TYR:OH	2.12	0.50
36:YA:764:A:H5'	38:YD:210:GLY:HA2	1.94	0.50
49:YS:87:PHE:HE1	49:YS:102:ALA:HB2	1.76	0.50
52:YV:74:LYS:HB2	52:YV:83:ARG:HB2	1.91	0.50
56:YZ:91:LEU:HD23	56:YZ:130:PRO:HB3	1.93	0.50
13:QM:92:HIS:HA	13:QM:110:ARG:HH21	1.77	0.50
35:R9:4:ARG:NE	35:R9:6:SER:O	2.44	0.50
38:RD:132:PRO:HG3	38:RD:190:TYR:CE1	2.46	0.50
41:RG:145:THR:HG23	41:RG:147:ASP:H	1.77	0.50
41:RG:5:VAL:H	41:RG:8:LYS:HE3	1.76	0.50
3:XC:59:ARG:HG2	3:XC:64:VAL:HG12	1.94	0.50
31:Y5:32:PRO:HA	31:Y5:39:MET:HA	1.93	0.50
36:YA:1490:A:O2'	38:YD:99:ASP:OD2	2.30	0.50
2:QB:47:THR:O	2:QB:51:LEU:N	2.45	0.50
11:QK:34:ASP:OD1	11:QK:38:ASN:N	2.45	0.50
13:QM:58:GLU:O	13:QM:62:ASN:ND2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1223:C:OP2	19:QS:78:ARG:NH2	2.45	0.50
36:RA:1217:C:OP1	51:RU:15:LYS:NZ	2.39	0.50
36:RA:2681:C:OP2	39:RE:109:LYS:NZ	2.39	0.50
52:RV:66:ARG:HA	52:RV:90:PRO:HA	1.93	0.50
1:XA:452:A:H62	1:XA:480:U:H3	1.58	0.50
38:YD:182:LEU:H	38:YD:272:ALA:HB3	1.76	0.50
1:QA:1128:C:H42	1:QA:1143:G:H1	1.59	0.50
1:QA:833:U:H3	1:QA:853:G:H1	1.60	0.50
9:QI:48:GLU:HB2	9:QI:78:LYS:HZ1	1.75	0.50
27:RI:68:PRO:HG3	43:RI:27:ARG:HH22	1.76	0.50
2:XB:168:THR:OG1	2:XB:191:ASP:OD2	2.21	0.50
4:XD:62:GLN:HE22	4:XD:65:ARG:HH21	1.60	0.50
5:XE:35:GLY:HA3	5:XE:112:LEU:HB3	1.94	0.50
23:XW:3:G:H22	23:XW:70:U:H3	1.60	0.50
36:YA:783:A:H8	36:YA:784:A:H4'	1.77	0.50
52:YV:36:PRO:HA	52:YV:56:SER:HB3	1.94	0.50
16:QP:13:HIS:O	16:QP:42:ARG:NH1	2.45	0.50
36:RA:141:A:H8	36:RA:1595:G:H21	1.60	0.50
47:RQ:28:ALA:N	47:RQ:105:GLU:OE2	2.43	0.50
53:RW:29:LEU:HD22	53:RW:69:LEU:HD11	1.94	0.50
4:XD:59:ARG:HE	4:XD:59:ARG:HA	1.77	0.50
1:XA:1015:A:OP1	19:XS:14:HIS:NE2	2.45	0.50
36:YA:574:C:N3	39:YE:145:LYS:NZ	2.60	0.50
38:YD:133:LEU:HD23	38:YD:136:ILE:HD12	1.94	0.50
36:YA:2032:G:N2	39:YE:146:THR:HG23	2.24	0.50
44:YN:35:ARG:HG3	44:YN:37:LYS:HG3	1.94	0.50
12:QL:57:LYS:HG2	12:QL:67:THR:HG22	1.94	0.49
1:QA:947:G:O3'	13:QM:109:THR:OG1	2.30	0.49
26:R0:32:ARG:H	26:R0:35:ASN:ND2	2.10	0.49
30:R4:57:GLU:HA	30:R4:61:ARG:HG3	1.95	0.49
36:RA:2645:G:N2	36:RA:2767:C:OP2	2.45	0.49
36:RA:320:A:O2'	36:RA:322:A:OP2	2.22	0.49
5:XE:60:TYR:OH	5:XE:64:ARG:NH2	2.43	0.49
50:YT:24:PRO:HA	50:YT:49:VAL:HG13	1.93	0.49
56:YZ:151:HIS:HA	56:YZ:170:THR:HA	1.93	0.49
1:QA:811:C:O2'	1:QA:901:A:N1	2.45	0.49
2:QB:132:LYS:HA	2:QB:135:GLN:HB2	1.93	0.49
4:QD:19:LEU:HD11	4:QD:63:LYS:HG3	1.94	0.49
38:RD:95:LEU:HD13	38:RD:97:TYR:CE1	2.46	0.49
45:RO:77:ILE:HB	50:RT:74:ARG:HD2	1.94	0.49
7:XG:16:LEU:HD23	9:XI:44:VAL:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:YD:122:ASP:OD1	38:YD:122:ASP:N	2.45	0.49
26:Y0:7:LEU:HD23	47:YQ:83:MET:HG2	1.94	0.49
51:YU:27:LEU:HD12	51:YU:31:SER:HB2	1.93	0.49
1:QA:451:A:OP1	1:QA:481:G:N2	2.43	0.49
43:RI:130:TYR:HB3	43:RI:136:VAL:HG13	1.93	0.49
46:RP:92:GLU:OE1	46:RP:121:LYS:NZ	2.41	0.49
45:RO:64:ARG:HH12	50:RT:70:VAL:HG21	1.77	0.49
3:XC:189:ALA:HB3	3:XC:196:LEU:HB2	1.95	0.49
9:XI:112:LYS:HA	9:XI:119:ALA:HB2	1.94	0.49
27:Y1:87:PRO:HA	27:Y1:90:ILE:HB	1.94	0.49
36:YA:116:C:O2'	36:YA:126:A:N3	2.41	0.49
36:YA:1667:G:O2'	36:YA:1991:U:O4	2.29	0.49
51:YU:50:ARG:O	51:YU:54:LYS:NZ	2.45	0.49
53:YW:86:LEU:HD22	53:YW:96:ILE:HD11	1.94	0.49
54:YX:53:LYS:O	54:YX:82:GLN:N	2.43	0.49
1:QA:1230:C:H5'	22:QV:30:G:H5"	1.94	0.49
8:QH:119:LEU:HB3	8:QH:123:GLU:HG3	1.94	0.49
16:QP:14:ASN:HA	16:QP:42:ARG:HH11	1.77	0.49
36:RA:2857:G:N2	36:RA:2860:A:OP2	2.33	0.49
46:RP:122:PRO:HB3	46:RP:141:ALA:HB1	1.94	0.49
12:XL:77:LEU:HD21	12:XL:107:ALA:HB2	1.95	0.49
36:YA:598:G:H1'	46:YP:12:ALA:HB2	1.94	0.49
36:YA:690:G:H4'	38:YD:218:ARG:HH22	1.76	0.49
42:YH:7:LEU:N	42:YH:8:PRO:HD2	2.28	0.49
50:YT:66:VAL:HA	50:YT:71:GLY:HA2	1.93	0.49
36:RA:463:G:N2	36:RA:466:A:OP2	2.39	0.49
39:RE:9:VAL:HB	39:RE:25:VAL:HG13	1.93	0.49
1:XA:502:G:OP1	12:XL:118:SER:N	2.37	0.49
1:XA:745:C:OP1	1:XA:851:G:O2'	2.30	0.49
6:XF:37:VAL:HA	6:XF:65:VAL:HG12	1.94	0.49
8:XH:91:ARG:NE	17:XQ:32:TYR:O	2.46	0.49
36:YA:482:A:H4'	55:YY:47:LYS:HD2	1.95	0.49
38:YD:66:ASP:OD2	38:YD:103:ARG:NH1	2.43	0.49
50:YT:16:ARG:HH21	50:YT:19:LEU:HD21	1.78	0.49
1:QA:1261:A:H62	1:QA:1274:G:H21	1.60	0.49
36:RA:2111:C:N3	36:RA:2118:U:O2'	2.44	0.49
36:RA:631:A:OP1	46:RP:64:LYS:NZ	2.42	0.49
50:RT:51:ARG:NH1	50:RT:100:TYR:OH	2.45	0.49
36:YA:380:U:H2'	36:YA:381:G:H8	1.78	0.49
37:YB:33:G:H5'	41:YG:2:PRO:HG3	1.93	0.49
38:YD:64:ILE:HG23	38:YD:64:ILE:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:YQ:28:ALA:HB3	47:YQ:67:ARG:HH12	1.76	0.49
48:YR:96:ARG:HG2	48:YR:115:GLU:HG2	1.95	0.49
56:YZ:151:HIS:HB3	56:YZ:170:THR:HG22	1.94	0.49
1:QA:1304:G:N2	1:QA:1332:A:OP2	2.46	0.49
36:RA:1824:G:N3	38:RD:254:THR:OG1	2.45	0.49
44:RN:115:ARG:HA	44:RN:118:LYS:HD2	1.95	0.49
53:RW:22:ASP:OD1	53:RW:25:ARG:NH1	2.39	0.49
37:RB:74:U:H1'	56:RZ:34:ASN:HD21	1.78	0.49
1:XA:1348:U:H4'	9:XI:120:ARG:HG3	1.93	0.49
3:XC:47:LEU:HB3	3:XC:52:LEU:HD23	1.95	0.49
6:XF:7:ASN:HB3	18:XR:76:LEU:HD11	1.95	0.49
26:Y0:45:PHE:CE2	26:Y0:69:PHE:HE2	2.31	0.49
8:QH:82:HIS:N	8:QH:138:TRP:OXT	2.45	0.49
25:QY:25:C:H2'	25:QY:26:G:H8	1.78	0.49
36:RA:2313:C:H4'	41:RG:91:ARG:HD2	1.94	0.49
1:XA:401:C:OP2	4:XD:73:ARG:NH2	2.45	0.49
1:XA:532:A:H2	1:XA:1206:G:H21	1.60	0.49
3:XC:29:TYR:OH	14:XN:54:PRO:O	2.29	0.49
26:Y0:32:ARG:H	26:Y0:35:ASN:ND2	2.11	0.49
36:YA:2010:G:H5''	53:YW:42:ARG:HB2	1.95	0.49
39:YE:48:GLN:OE1	39:YE:64:LYS:NZ	2.46	0.49
40:YF:63:LYS:HG3	40:YF:76:GLY:HA2	1.95	0.49
54:YX:53:LYS:NZ	54:YX:55:ASN:OD1	2.46	0.49
1:QA:452:A:OP1	16:QP:43:LYS:NZ	2.45	0.49
36:RA:1538:G:H2'	36:RA:1539:G:H8	1.78	0.49
41:RG:19:LEU:HD23	41:RG:22:ARG:HD2	1.95	0.49
1:XA:835:U:H3	1:XA:851:G:H1	1.59	0.49
7:XG:111:ARG:NH2	7:XG:126:ASP:OD2	2.46	0.49
13:XM:17:VAL:O	13:XM:20:THR:OG1	2.26	0.49
36:YA:2115:G:O2'	36:YA:2166:G:OP1	2.27	0.49
36:YA:1693:U:O2'	38:YD:14:ARG:NH2	2.45	0.49
49:YS:39:ILE:HD11	49:YS:73:LEU:HD21	1.95	0.49
1:QA:356:A:N3	1:QA:368:U:O2'	2.36	0.49
13:QM:3:ARG:HD2	13:QM:9:ILE:HG12	1.95	0.49
50:RT:35:LYS:HE3	50:RT:38:ASN:H	1.78	0.49
1:XA:1347:G:N2	1:XA:1374:A:OP2	2.33	0.49
1:XA:28:G:O2'	1:XA:296:U:OP1	2.27	0.49
36:YA:1266:G:O5'	53:YW:15:ARG:NH2	2.46	0.49
38:YD:160:GLY:N	38:YD:197:GLY:O	2.46	0.49
43:YI:60:GLU:OE1	43:YI:61:ARG:NH2	2.42	0.49
48:YR:38:VAL:HG22	48:YR:112:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:184:G:H2'	1:QA:185:A:H8	1.76	0.48
36:RA:1441:G:H2'	36:RA:1442:G:H8	1.78	0.48
36:RA:2295:C:OP1	49:RS:10:ARG:NH1	2.46	0.48
36:YA:1055:G:O2'	36:YA:1085:A:N1	2.35	0.48
36:YA:2751:G:C8	36:YA:2751:G:C3'	2.95	0.48
26:Y0:72:ARG:NH2	37:YB:10:C:OP1	2.45	0.48
1:QA:1503:A:O2'	24:QX:12:A:N6	2.46	0.48
1:QA:745:C:OP1	1:QA:851:G:O2'	2.29	0.48
19:QS:4:SER:O	19:QS:4:SER:OG	2.31	0.48
36:RA:137(A):G:H21	54:RX:41:ASN:HD21	1.61	0.48
47:RQ:16:ARG:HG2	47:RQ:18:LYS:HZ2	1.78	0.48
56:RZ:30:ASN:HB3	56:RZ:90:VAL:HB	1.95	0.48
2:XB:223:ILE:HA	2:XB:226:ARG:HB3	1.94	0.48
11:XK:34:ASP:OD1	11:XK:38:ASN:N	2.46	0.48
28:Y2:4:SER:OG	28:Y2:5:GLU:N	2.46	0.48
42:YH:2:SER:HA	42:YH:7:LEU:HD22	1.95	0.48
43:YI:72:LEU:HD23	43:YI:138:ILE:HD12	1.94	0.48
40:RF:133:ASN:HA	40:RF:162:LEU:HD23	1.93	0.48
36:RA:535:C:O3'	51:RU:53:ARG:NH1	2.46	0.48
4:XD:128:VAL:HG11	4:XD:138:TYR:HE2	1.78	0.48
20:XT:85:MET:HA	20:XT:88:VAL:HG12	1.95	0.48
23:XW:26:G:H1	23:XW:44:A:H61	1.61	0.48
36:YA:2502:G:H5''	36:YA:2503:A:H5''	1.94	0.48
2:QB:4:GLU:HG3	2:QB:6:THR:H	1.78	0.48
3:QC:70:VAL:HG12	3:QC:72:LYS:H	1.79	0.48
20:XT:57:ARG:NH1	20:XT:102:GLY:O	2.39	0.48
22:XV:16:C:O2'	22:XV:17(A):U:OP2	2.26	0.48
43:YI:12:LEU:HB2	43:YI:19:VAL:HG21	1.94	0.48
1:QA:508:C:OP1	4:QD:209:ARG:NH2	2.45	0.48
1:QA:865:A:N3	1:QA:918:A:O2'	2.40	0.48
1:QA:890:G:O2'	1:QA:906:G:O6	2.27	0.48
18:QR:31:LEU:HD12	18:QR:66:LEU:HB2	1.96	0.48
19:QS:5:LEU:HD11	30:R4:66:SER:HA	1.96	0.48
36:RA:1388:G:O2'	36:RA:1525:G:O2'	2.25	0.48
36:RA:2469:A:H5''	36:RA:2470:G:C8	2.49	0.48
38:RD:35:LYS:HB3	38:RD:36:PRO:CD	2.44	0.48
41:RG:129:GLY:HA2	41:RG:166:ASP:HA	1.95	0.48
2:XB:168:THR:HG23	2:XB:192:SER:HB2	1.94	0.48
36:YA:1084:A:N1	36:YA:1085:A:N6	2.58	0.48
44:YN:59:LYS:HE3	44:YN:61:ARG:HH12	1.79	0.48
45:YO:19:ILE:HG22	45:YO:43:VAL:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:YQ:103:MET:HB3	47:YQ:104:PHE:HD1	1.78	0.48
55:YY:76:CYS:O	55:YY:78:ALA:N	2.43	0.48
56:YZ:48:PHE:HA	56:YZ:51:ALA:HB3	1.95	0.48
36:RA:1651:G:H4'	48:RR:39:PRO:HG2	1.96	0.48
36:RA:629:G:N3	36:RA:639:U:O2'	2.46	0.48
55:RY:14:LEU:HB2	55:RY:75:ILE:HD11	1.95	0.48
1:XA:1279:A:O2'	1:XA:1281:U:OP2	2.29	0.48
5:XE:51:VAL:HG23	5:XE:52:PRO:HD3	1.94	0.48
13:XM:87:TYR:H	19:XS:73:GLU:HB3	1.79	0.48
36:YA:392:C:H5''	36:YA:409:C:H5''	1.96	0.48
37:YB:111:U:H2'	37:YB:112:G:H8	1.78	0.48
39:YE:128:SER:OG	39:YE:129:HIS:N	2.45	0.48
40:YF:60:SER:OG	40:YF:61:GLY:N	2.46	0.48
2:QB:102:LEU:HB2	2:QB:176:GLU:HG2	1.96	0.48
1:QA:1060:C:OP1	14:QN:45:ARG:NH2	2.47	0.48
25:QY:4:G:H1	25:QY:69:C:H42	1.61	0.48
36:RA:2379:G:OP1	49:RS:23:ARG:NH2	2.47	0.48
48:RR:53:HIS:HA	48:RR:56:LYS:HD3	1.94	0.48
1:XA:757:U:O2'	1:XA:879:C:O2	2.30	0.48
36:YA:13:A:O2'	36:YA:15:G:N7	2.45	0.48
36:YA:2375:G:N2	36:YA:2378:A:OP2	2.43	0.48
49:RS:40:ILE:HG22	49:RS:47:THR:HG23	1.96	0.48
56:RZ:170:THR:O	56:RZ:170:THR:OG1	2.31	0.48
3:XC:150:LYS:HD2	3:XC:173:VAL:HG11	1.96	0.48
4:XD:116:GLN:HE21	4:XD:157:LEU:HD21	1.79	0.48
8:XH:100:ILE:HG22	8:XH:125:ARG:HH21	1.78	0.48
17:XQ:24:GLU:OE2	17:XQ:37:LYS:NZ	2.46	0.48
36:YA:1065:U:O2'	36:YA:1074:G:N2	2.47	0.48
36:YA:1068:G:O2'	36:YA:1096:A:N3	2.37	0.48
36:YA:1138:G:O2'	44:YN:102:ALA:O	2.29	0.48
1:QA:1129:C:O2'	1:QA:1131:G:N7	2.46	0.48
13:QM:3:ARG:HA	13:QM:9:ILE:HD13	1.95	0.48
36:RA:2215:G:H2'	36:RA:2216:G:H8	1.79	0.48
36:RA:919:G:N2	36:RA:2269:A:OP2	2.46	0.48
36:RA:2291:U:O2'	36:RA:2374:C:O2	2.29	0.48
36:RA:2798:C:N3	36:RA:2799:A:N6	2.62	0.48
40:RF:187:VAL:HG11	46:RP:6:LEU:HD11	1.94	0.48
1:XA:451:A:OP1	1:XA:481:G:N2	2.46	0.48
4:XD:15:GLU:OE2	4:XD:66:ARG:NH1	2.47	0.48
9:XI:50:LEU:O	9:XI:55:ALA:N	2.46	0.48
36:YA:1203:G:O6	36:YA:1204:A:N6	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:YA:2590:A:H5''	38:YD:239:ARG:HG3	1.95	0.48
1:QA:1329:A:OP1	13:QM:29:ARG:N	2.36	0.48
1:QA:986:A:H4'	19:QS:55:LYS:HD3	1.95	0.48
19:QS:32:LYS:HA	19:QS:50:ALA:HB3	1.94	0.48
1:QA:1320:C:H1'	19:QS:73:GLU:HG3	1.96	0.48
27:R1:87:PRO:O	27:R1:91:LYS:N	2.38	0.48
32:R6:41:PRO:HG2	32:R6:44:ARG:H	1.78	0.48
36:RA:1266:G:O5'	53:RW:15:ARG:NH2	2.46	0.48
39:RE:36:ARG:NH1	39:RE:85:ASN:OD1	2.40	0.48
37:RB:45:A:O4'	41:RG:95:ARG:NH1	2.47	0.48
36:RA:2657:A:O3'	42:RH:160:LYS:NZ	2.44	0.48
1:XA:642:A:N3	8:XH:113:SER:OG	2.41	0.48
36:YA:1697:G:OP2	36:YA:1698:A:O2'	2.28	0.48
34:Y8:2:PRO:O	36:YA:666:G:N2	2.47	0.48
36:YA:729:G:P	38:YD:13:ARG:HD3	2.54	0.48
36:YA:958:U:O2	37:YB:89(A):A:O2'	2.26	0.48
42:YH:86:GLU:HB2	42:YH:165:ALA:HB2	1.96	0.48
55:YY:93:GLY:O	55:YY:95:LYS:NZ	2.47	0.48
1:QA:769:G:H4'	1:QA:1513:A:H4'	1.95	0.47
1:QA:489:C:H2'	1:QA:490:G:H8	1.78	0.47
4:QD:119:GLN:HE21	4:QD:123:HIS:CE1	2.32	0.47
19:QS:36:ARG:NH2	19:QS:72:GLY:O	2.47	0.47
36:RA:2851:A:O2'	48:RR:64:ARG:NH2	2.47	0.47
36:RA:578:A:OP1	36:RA:1255:U:O2'	2.29	0.47
38:RD:108:PRO:HB3	38:RD:143:HIS:CE1	2.48	0.47
46:RP:88:LEU:HD12	46:RP:95:VAL:HG11	1.96	0.47
56:RZ:99:TYR:HB3	56:RZ:123:ASP:HB2	1.96	0.47
56:RZ:126:VAL:HG11	56:RZ:161:VAL:HG13	1.96	0.47
1:XA:486:U:H2'	1:XA:487:A:H8	1.79	0.47
21:XU:8:THR:HG22	21:XU:10:ARG:H	1.79	0.47
36:YA:1041:C:H2'	36:YA:1042:G:H8	1.78	0.47
1:QA:923:A:N6	1:QA:1392:G:O6	2.47	0.47
36:RA:2701:C:H3'	36:RA:2702:U:H5''	1.96	0.47
29:R3:16:PRO:HA	36:RA:969:U:H5'	1.96	0.47
45:RO:23:ARG:NH2	45:RO:28:SER:O	2.47	0.47
36:RA:2845:G:OP1	50:RT:56:GLY:N	2.48	0.47
1:XA:923:A:O2'	1:XA:1399:C:OP2	2.25	0.47
1:XA:323:U:OP1	20:XT:26:ASN:ND2	2.46	0.47
1:XA:553:A:O2'	12:XL:29:GLY:O	2.31	0.47
1:XA:824:C:O2'	8:XH:1:MET:N	2.47	0.47
8:XH:97:VAL:HG21	8:XH:128:GLY:HA2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:YH:5:GLY:C	42:YH:8:PRO:HD2	2.34	0.47
47:YQ:28:ALA:N	47:YQ:105:GLU:OE2	2.47	0.47
47:YQ:77:LYS:NZ	47:YQ:83:MET:O	2.47	0.47
1:QA:571:U:O4	1:QA:864:A:N6	2.46	0.47
2:QB:43:ASP:HB3	2:QB:46:LYS:HB2	1.96	0.47
13:QM:14:ARG:NH2	13:QM:16:ASP:OD2	2.40	0.47
18:QR:37:VAL:HG11	18:QR:78:LEU:HB3	1.95	0.47
36:RA:1048:A:H3'	36:RA:1049:C:C5	2.49	0.47
38:RD:231:HIS:CD2	38:RD:249:PRO:HG3	2.49	0.47
42:RH:149:ARG:HG2	42:RH:154:PRO:HB3	1.95	0.47
1:XA:1320:C:H5'	19:XS:70:LYS:HD3	1.95	0.47
1:XA:362:G:N2	1:XA:365:U:OP2	2.41	0.47
1:XA:390:C:H4'	16:XP:28:ARG:HH21	1.79	0.47
1:XA:406:G:H21	4:XD:119:GLN:HE22	1.61	0.47
1:XA:953:G:H5'	1:XA:965:A:H61	1.79	0.47
8:XH:87:SER:HB2	8:XH:93:VAL:HG22	1.96	0.47
26:Y0:7:LEU:HG	47:YQ:80:GLU:HG3	1.96	0.47
36:YA:1598:C:H5'	54:YX:36:LYS:HB2	1.97	0.47
36:YA:28:A:HO2'	36:YA:582:G:HO2'	1.61	0.47
49:YS:94:TYR:CE2	49:YS:99:LYS:HA	2.49	0.47
54:YX:40:LYS:HG3	54:YX:51:VAL:HB	1.95	0.47
56:YZ:153:SER:OG	56:YZ:154:ASP:N	2.47	0.47
1:QA:1034:G:N2	1:QA:1035:A:N7	2.61	0.47
1:QA:1223:C:H5''	1:QA:1224:G:H5''	1.95	0.47
1:QA:522:C:OP2	12:QL:69:TYR:OH	2.30	0.47
1:QA:618:C:H5'	1:QA:619:U:H5''	1.97	0.47
1:QA:814:A:OP2	1:QA:816:A:N6	2.45	0.47
36:RA:1012:U:OP1	51:RU:75:ASN:ND2	2.40	0.47
36:RA:2513:G:N2	39:RE:143:ASN:OD1	2.48	0.47
36:RA:2630:G:H2'	36:RA:2631:G:C8	2.49	0.47
37:RB:37:C:N3	37:RB:48:A:O2'	2.46	0.47
38:RD:21:PHE:HD1	38:RD:24:ILE:HD12	1.79	0.47
48:RR:12:ARG:HB2	48:RR:17:ARG:HG3	1.97	0.47
36:RA:2012:G:OP1	53:RW:11:ARG:NH2	2.46	0.47
1:XA:1074:G:H1	1:XA:1083:U:H3	1.62	0.47
5:XE:100:VAL:HG23	5:XE:118:ILE:HG22	1.96	0.47
18:XR:37:VAL:HG22	18:XR:78:LEU:HB3	1.95	0.47
36:YA:1654:A:OP2	48:YR:2:ARG:NH1	2.44	0.47
34:Y8:25:MET:HG3	46:YP:64:LYS:HB2	1.96	0.47
12:QL:33:ARG:HG2	12:QL:60:LEU:HD12	1.96	0.47
30:R4:49:PHE:HE2	30:R4:50:VAL:CG2	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:RA:265:A:N6	36:RA:427:U:O2'	2.47	0.47
38:RD:13:ARG:NH1	38:RD:16:MET:SD	2.88	0.47
40:RF:117:ARG:NH2	40:RF:189:THR:O	2.37	0.47
1:XA:1348:U:H3	1:XA:1374:A:H2	1.63	0.47
1:XA:1422:G:H5''	45:YO:48:PRO:HB3	1.95	0.47
5:XE:93:PRO:HG2	8:XH:105:ARG:HH21	1.78	0.47
1:XA:110:C:O2'	16:XP:25:ARG:O	2.30	0.47
24:XX:12:A:O2'	24:XX:13:A:O3'	2.31	0.47
38:YD:71:ASP:HB2	38:YD:103:ARG:HH12	1.79	0.47
39:YE:92:THR:OG1	39:YE:93:VAL:N	2.46	0.47
36:YA:2292:C:OP1	49:YS:17:ARG:NH2	2.47	0.47
50:YT:19:LEU:HD22	50:YT:86:ILE:HG22	1.95	0.47
55:YY:50:ARG:HH12	55:YY:55:TYR:HD2	1.63	0.47
36:RA:2880:C:O2'	48:RR:90:ARG:NH1	2.44	0.47
36:RA:807:U:OP2	46:RP:41:ARG:NH1	2.47	0.47
36:RA:832:G:H4'	46:RP:45:LEU:HD11	1.95	0.47
1:XA:280:C:N3	17:XQ:39:SER:N	2.61	0.47
13:XM:57:ARG:NH1	30:Y4:32:TYR:OH	2.47	0.47
42:YH:107:VAL:HG11	42:YH:153:LYS:HG2	1.95	0.47
42:YH:84:SER:OG	42:YH:132:ARG:NH2	2.48	0.47
48:YR:63:ARG:HG2	48:YR:80:PHE:CE2	2.49	0.47
1:QA:413:G:O2'	1:QA:428:G:N2	2.47	0.47
4:QD:98:GLU:HA	4:QD:103:ASN:HD22	1.80	0.47
7:QG:16:LEU:HD12	9:QI:41:VAL:HG12	1.96	0.47
33:R7:49:ARG:HH22	36:RA:129:C:H5'	1.80	0.47
36:RA:2120:G:H2'	36:RA:2121:G:H8	1.80	0.47
41:RG:130:ASN:HB3	41:RG:159:VAL:HG13	1.96	0.47
56:RZ:76:LEU:HA	56:RZ:83:PRO:HA	1.95	0.47
1:XA:692:U:OP1	11:XK:124:LYS:NZ	2.34	0.47
17:XQ:88:TYR:HE1	17:XQ:92:ARG:HH21	1.63	0.47
32:Y6:14:THR:HG23	32:Y6:16:CYS:H	1.80	0.47
36:YA:2531:A:H61	36:YA:2662:A:H61	1.61	0.47
37:YB:37:C:O2	49:YS:95:HIS:NE2	2.41	0.47
1:QA:1352:C:OP1	21:QU:3:LYS:NZ	2.39	0.47
2:QB:20:GLU:HG3	2:QB:191:ASP:HB2	1.96	0.47
1:QA:674:G:H5'	6:QF:50:TYR:HE2	1.79	0.47
32:R6:7:ILE:HG13	32:R6:8:LYS:H	1.79	0.47
42:RH:4:ILE:HB	42:RH:6:ARG:NH1	2.30	0.47
36:RA:1190:G:H5'	46:RP:32:THR:HA	1.96	0.47
53:RW:82:LEU:HB2	53:RW:98:LYS:HB2	1.97	0.47
1:XA:447:G:H21	1:XA:487:A:H62	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:YA:1780:A:O2'	36:YA:1781:C:O2	2.28	0.47
36:YA:2503:A:O2'	36:YA:2505:G:OP2	2.25	0.47
36:YA:223:A:O2'	36:YA:420:C:O2	2.25	0.47
39:YE:45:THR:OG1	39:YE:83:ASP:OD1	2.32	0.47
40:YF:167:ALA:HB1	40:YF:173:VAL:HG11	1.97	0.47
56:YZ:7:ALA:HA	56:YZ:39:VAL:HG12	1.97	0.47
2:QB:219:VAL:HA	2:QB:222:ILE:HD13	1.97	0.47
5:QE:144:THR:N	5:QE:147:ASP:OD1	2.48	0.47
10:QJ:78:ASN:HB2	10:QJ:81:THR:HG23	1.95	0.47
13:QM:4:ILE:H	13:QM:9:ILE:HG21	1.80	0.47
27:R1:78:LYS:HE2	36:RA:270(R):G:H21	1.78	0.47
39:RE:134:ILE:HA	39:RE:137:HIS:HD2	1.79	0.47
36:RA:2730:C:O2'	39:RE:168:MET:O	2.27	0.47
41:RG:5:VAL:HB	41:RG:8:LYS:HG2	1.96	0.47
45:RO:102:VAL:HG23	45:RO:121:VAL:HG23	1.97	0.47
47:RQ:75:THR:OG1	47:RQ:86:GLY:O	2.32	0.47
37:RB:7:G:H21	49:RS:38:GLN:NE2	2.12	0.47
1:XA:1250:A:N3	1:XA:1370:G:O2'	2.42	0.47
23:QW:67:A:H2'	23:QW:68:G:H8	1.78	0.47
41:RG:38:VAL:HB	41:RG:158:ALA:HB3	1.97	0.47
1:XA:1111:A:N1	3:XC:177:THR:HG22	2.30	0.47
36:YA:1398:C:OP1	54:YX:53:LYS:NZ	2.43	0.47
36:YA:2729:G:H1'	39:YE:187:ALA:HB2	1.97	0.47
1:QA:375:U:O2	16:QP:28:ARG:NH1	2.47	0.47
6:QF:50:TYR:CE1	18:QR:77:GLY:HA2	2.50	0.47
36:RA:2692:C:O2	36:RA:2847:U:O2'	2.27	0.47
43:RI:31:LEU:HD21	43:RI:38:LEU:HG	1.97	0.47
47:RQ:41:TRP:HB3	47:RQ:94:VAL:HG21	1.96	0.47
2:XB:84:GLU:OE2	2:XB:233:SER:OG	2.28	0.47
36:YA:1939:U:OP1	36:YA:2604:U:O2'	2.32	0.47
36:YA:2291:U:H3	36:YA:2341:G:H1	1.63	0.47
36:YA:535:C:O3'	51:YU:53:ARG:NH1	2.48	0.47
36:YA:2633:G:O2'	39:YE:60:ASN:ND2	2.48	0.47
1:QA:976:G:OP2	1:QA:1358:U:O2'	2.32	0.46
36:RA:288:C:H2'	36:RA:289:A:H8	1.80	0.46
43:RI:76:THR:HG21	43:RI:141:LYS:HE3	1.96	0.46
46:RP:115:LEU:HB2	46:RP:131:SER:HB2	1.96	0.46
1:XA:486:U:H2'	1:XA:487:A:C8	2.50	0.46
2:XB:60:ASP:HB3	2:XB:64:ARG:HH12	1.81	0.46
18:XR:56:THR:HB	18:XR:58:LEU:HD13	1.97	0.46
26:Y0:45:PHE:HE2	26:Y0:69:PHE:CE2	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:YA:2786:U:O2'	39:YE:62:PRO:O	2.33	0.46
41:YG:178:PHE:HB3	41:YG:180:PHE:HE1	1.79	0.46
37:YB:45:A:OP2	41:YG:96:ARG:NH2	2.48	0.46
47:YQ:32:TYR:CE1	47:YQ:133:ARG:HG3	2.50	0.46
47:YQ:63:LYS:HD2	56:YZ:175:VAL:HG21	1.97	0.46
48:YR:87:TYR:HD1	48:YR:90:ARG:HD2	1.80	0.46
8:QH:36:LEU:HD23	8:QH:39:LEU:HD12	1.97	0.46
37:RB:111:U:H2'	37:RB:112:G:H8	1.79	0.46
1:XA:426:G:OP1	4:XD:38:TYR:OH	2.30	0.46
7:XG:70:LYS:HE2	7:XG:97:GLN:HG2	1.96	0.46
8:XH:26:VAL:O	8:XH:59:LEU:N	2.44	0.46
26:Y0:10:THR:HG22	26:Y0:12:ASN:H	1.79	0.46
34:Y8:46:ARG:NH1	36:YA:630:G:OP1	2.49	0.46
36:YA:2751:G:H3'	36:YA:2751:G:H8	1.79	0.46
45:YO:77:ILE:HB	50:YT:74:ARG:HD2	1.98	0.46
1:QA:1336:C:O2'	1:QA:1337:G:O4'	2.33	0.46
1:QA:545:C:O2'	1:QA:549:C:OP1	2.33	0.46
12:QL:60:LEU:HG	12:QL:62:SER:H	1.80	0.46
14:QN:24:CYS:HB2	14:QN:28:GLY:H	1.81	0.46
36:RA:1853:A:N3	36:RA:2233:U:O2'	2.42	0.46
36:RA:345:A:O2'	36:RA:347:A:N7	2.44	0.46
34:R8:46:ARG:NH2	36:RA:631:A:OP1	2.49	0.46
39:RE:45:THR:OG1	39:RE:83:ASP:OD1	2.34	0.46
56:RZ:130:PRO:HA	56:RZ:133:ILE:HD11	1.98	0.46
1:XA:129(A):G:N2	1:XA:188:U:O2'	2.48	0.46
36:YA:1327:C:O2'	48:YR:105:ARG:NH2	2.49	0.46
36:YA:2295:C:H5	49:YS:13:ARG:HH12	1.62	0.46
5:QE:98:THR:HB	5:QE:117:ASP:HB3	1.97	0.46
13:QM:78:ILE:HA	13:QM:81:LEU:HG	1.97	0.46
36:RA:1116:C:H2'	36:RA:1117:G:H8	1.80	0.46
36:RA:2077:A:OP1	36:RA:2238:G:N2	2.39	0.46
1:XA:62:U:O2'	1:XA:379:C:O2	2.29	0.46
32:Y6:10:LEU:HD13	36:YA:2420:C:H5''	1.97	0.46
36:YA:2416:C:O3'	46:YP:64:LYS:NZ	2.49	0.46
41:YG:55:LYS:HD3	41:YG:58:GLN:HE21	1.81	0.46
46:YP:57:THR:HG23	46:YP:59:LEU:HB2	1.96	0.46
1:QA:34:C:H2'	1:QA:35:G:H8	1.81	0.46
1:QA:975:A:H4'	1:QA:976:G:H5''	1.97	0.46
1:QA:979:C:O2	14:QN:19:ARG:NE	2.45	0.46
23:QW:76:A:N1	34:R8:31:HIS:NE2	2.64	0.46
36:RA:1462:C:H4'	36:RA:2703:C:H5'	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:RA:906:G:O2'	47:RQ:67:ARG:NH2	2.40	0.46
43:RI:92:VAL:HG21	43:RI:97:ILE:HD11	1.94	0.46
36:RA:2561:A:H4'	45:RO:40:VAL:HG11	1.96	0.46
3:XC:188:LEU:HD23	3:XC:190:ARG:HE	1.80	0.46
31:Y5:2:ALA:HA	36:YA:2015:A:N3	2.31	0.46
36:YA:2125:G:N1	36:YA:2172:U:OP1	2.43	0.46
36:YA:2474:C:H5''	36:YA:2475:C:H5	1.79	0.46
44:YN:116:LEU:HD23	44:YN:119:ARG:HD2	1.97	0.46
47:YQ:24:GLY:H	47:YQ:101:ARG:HD2	1.80	0.46
36:YA:2250:G:C4	47:YQ:82:ARG:HG3	2.51	0.46
1:QA:243:A:H4'	1:QA:244:U:H3'	1.97	0.46
29:R3:8:LEU:HD13	29:R3:23:LEU:HD11	1.98	0.46
30:R4:14:ILE:HD11	30:R4:33:VAL:HG12	1.98	0.46
32:R6:25:LYS:HE3	34:R8:34:TRP:HE3	1.80	0.46
2:XB:118:LEU:HB3	2:XB:142:LEU:HD12	1.97	0.46
25:XY:75:C:O2	36:YA:2507:C:O2'	2.29	0.46
26:Y0:20:ARG:HG2	36:YA:2271:G:H5'	1.96	0.46
36:YA:806:C:O2	36:YA:2444:G:O2'	2.30	0.46
47:YQ:39:PRO:HB3	47:YQ:99:PRO:HD3	1.96	0.46
33:R7:8:ASN:HB3	33:R7:11:LYS:HB3	1.98	0.46
36:RA:1999:C:O2	36:RA:2687:U:O2'	2.31	0.46
36:RA:2313:C:O4'	41:RG:40:ASN:ND2	2.49	0.46
36:RA:2633:G:O2'	39:RE:60:ASN:ND2	2.47	0.46
36:RA:2751:G:H5''	36:RA:2752:C:H5	1.81	0.46
36:RA:259:G:H21	36:RA:621:A:H8	1.64	0.46
38:RD:51:VAL:HG11	38:RD:54:ARG:HE	1.81	0.46
1:XA:444:C:H2'	1:XA:445:G:H8	1.81	0.46
1:XA:780:A:N6	1:XA:801:U:OP2	2.38	0.46
3:XC:47:LEU:CD2	3:XC:52:LEU:HB3	2.45	0.46
6:XF:45:LEU:HD12	6:XF:59:TYR:HD1	1.80	0.46
9:XI:28:VAL:HG12	9:XI:63:ILE:HB	1.97	0.46
14:YN:44:LEU:HA	14:YN:47:LEU:HB2	1.98	0.46
36:YA:1103:A:H5'	36:YA:1104:C:H5	1.81	0.46
36:YA:1441:G:H2'	36:YA:1442:G:C8	2.51	0.46
55:YY:50:ARG:HB2	55:YY:53:PRO:HD2	1.97	0.46
1:QA:1326:C:OP1	21:QU:17:THR:OG1	2.30	0.46
1:QA:939:G:H5''	7:QG:102:ARG:NH1	2.31	0.46
26:R0:39:ARG:HH21	36:RA:2355:C:H1'	1.81	0.46
36:RA:242:G:O2'	36:RA:254:G:O6	2.27	0.46
36:RA:458:G:O2'	36:RA:469:G:O6	2.26	0.46
36:RA:955:C:OP1	47:RQ:85:LYS:NZ	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:RE:127:ASP:HA	39:RE:135:HIS:HD2	1.81	0.46
54:RX:53:LYS:HB3	54:RX:82:GLN:HB3	1.98	0.46
29:Y3:8:LEU:HA	29:Y3:54:VAL:HG12	1.97	0.46
36:YA:2734:A:H62	36:YA:2770:G:H21	1.62	0.46
51:YU:75:ASN:O	51:YU:78:THR:OG1	2.32	0.46
3:QC:26:LYS:HD2	14:QN:35:ARG:HH12	1.80	0.46
36:RA:1266:G:O2'	36:RA:2012:G:O6	2.23	0.46
37:RB:9:G:P	49:RS:25:ARG:HH22	2.39	0.46
41:RG:56:ALA:HA	41:RG:153:ARG:HH21	1.81	0.46
1:XA:1233:G:O2'	1:XA:1365:G:OP1	2.31	0.46
1:XA:673:G:O3'	6:XF:87:ARG:NH2	2.49	0.46
36:YA:2212:A:H1'	36:YA:2215:G:C4	2.51	0.46
39:YE:92:THR:HG23	39:YE:94:GLU:H	1.80	0.46
45:YO:2:ILE:HB	45:YO:33:ALA:HB3	1.97	0.46
55:YY:29:GLU:HB3	55:YY:38:ILE:HG12	1.98	0.46
56:YZ:76:LEU:HA	56:YZ:83:PRO:HA	1.96	0.46
1:QA:426:G:OP1	4:QD:38:TYR:OH	2.28	0.46
3:QC:121:ALA:HB2	3:QC:198:VAL:HG11	1.97	0.46
13:QM:12:ASN:N	13:QM:45:VAL:HG23	2.30	0.46
36:RA:2276:G:OP2	47:RQ:84:GLY:N	2.49	0.46
30:R4:38:LYS:HZ1	41:RG:111:LEU:HD22	1.81	0.46
41:RG:43:LEU:HD21	41:RG:153:ARG:HG3	1.98	0.46
50:RT:50:ILE:HD11	50:RT:100:TYR:HA	1.97	0.46
52:RV:7:THR:HG23	52:RV:22:VAL:HG21	1.97	0.46
1:XA:1222:G:OP1	19:XS:78:ARG:NH1	2.49	0.46
2:XB:101:MET:HA	2:XB:108:ILE:HG13	1.98	0.46
11:XK:21:ILE:HG13	11:XK:30:VAL:HG12	1.98	0.46
22:XV:9:G:O2'	22:XV:10:G:N7	2.48	0.46
36:YA:181:A:H1'	36:YA:435:C:H5'	1.98	0.46
1:QA:1151:A:H1'	10:QJ:39:PRO:HB2	1.97	0.45
1:QA:1372:U:H5"	9:QI:71:SER:HB3	1.96	0.45
1:QA:401:C:O2'	1:QA:621:A:N3	2.43	0.45
9:QI:13:ALA:HB2	9:QI:68:GLY:HA3	1.97	0.45
36:RA:1542:G:O6	36:RA:1543:A:N6	2.49	0.45
48:RR:54:LEU:HG	48:RR:62:ALA:HB1	1.98	0.45
49:RS:15:ARG:HD2	49:RS:25:ARG:NH2	2.30	0.45
56:RZ:72:ARG:NH2	56:RZ:97:GLU:O	2.49	0.45
1:XA:243:A:H4'	1:XA:244:U:H3'	1.98	0.45
1:XA:439:A:OP2	1:XA:493:G:N1	2.38	0.45
10:XJ:84:GLN:HB2	10:XJ:88:LEU:HD12	1.98	0.45
28:Y2:28:LYS:HD3	28:Y2:53:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:YA:568:U:O5'	36:YA:945:A:N6	2.48	0.45
1:QA:1422:G:H2'	1:QA:1423:G:H8	1.80	0.45
17:QQ:28:PRO:HA	17:QQ:35:VAL:HA	1.98	0.45
37:RB:78:A:H62	37:RB:98:G:H21	1.64	0.45
36:YA:1638:C:O2	36:YA:2698:U:O2'	2.33	0.45
36:YA:184:C:O2'	36:YA:217:G:N3	2.46	0.45
36:YA:2666:C:O2	42:YH:152:ARG:NH1	2.49	0.45
36:YA:1033:U:O4	36:YA:2750:A:C2	2.69	0.45
36:YA:602:G:HO2'	36:YA:604:G:HO2'	1.46	0.45
39:YE:117:MET:HA	39:YE:122:PHE:N	2.31	0.45
41:YG:32:PRO:HB3	41:YG:163:ALA:HB2	1.98	0.45
44:YN:9:VAL:HG21	44:YN:39:ARG:HH22	1.81	0.45
3:QC:46:GLU:O	3:QC:83:ARG:NH2	2.49	0.45
1:QA:617:G:H4'	16:QP:44:THR:HB	1.97	0.45
36:RA:2118:U:O2	36:RA:2148:G:O2'	2.26	0.45
36:RA:281:G:H21	36:RA:359:A:H62	1.63	0.45
42:RH:31:GLY:H	42:RH:79:VAL:HG13	1.81	0.45
2:XB:32:ILE:HD11	2:XB:40:HIS:HB3	1.98	0.45
9:XI:9:ARG:HB3	9:XI:14:VAL:HG23	1.99	0.45
1:XA:562:C:H1'	12:XL:15:ARG:HD2	1.98	0.45
36:YA:1143:A:OP1	44:YN:25:ARG:NH1	2.39	0.45
36:YA:124:G:N2	36:YA:126:A:O2'	2.48	0.45
36:YA:768:G:O2'	36:YA:1379:A:N6	2.43	0.45
41:YG:140:ILE:HG13	41:YG:141:PHE:HD1	1.81	0.45
36:YA:1151:G:O2'	51:YU:77:SER:O	2.29	0.45
5:QE:105:VAL:HG21	5:QE:128:PRO:HB3	1.98	0.45
5:QE:78:HIS:CG	8:QH:104:ARG:HD2	2.51	0.45
1:XA:639:G:H2'	1:XA:640:A:H8	1.81	0.45
34:Y8:22:VAL:HB	34:Y8:53:PRO:HB3	1.98	0.45
18:QR:44:LEU:HD11	18:QR:79:LEU:HD23	1.98	0.45
30:R4:14:ILE:HD13	30:R4:31:ILE:HG23	1.98	0.45
31:R5:15:ARG:NH2	36:RA:2022:U:OP2	2.47	0.45
36:RA:65:C:O2'	36:RA:456:C:N3	2.34	0.45
36:RA:1567:A:H3'	38:RD:86:PRO:HG3	1.98	0.45
36:RA:2684:U:O2'	45:RO:68:GLU:OE2	2.31	0.45
56:RZ:47:VAL:O	56:RZ:51:ALA:N	2.48	0.45
1:XA:128:G:O2'	17:XQ:3:LYS:NZ	2.39	0.45
1:XA:509:A:N3	1:XA:543:C:O2'	2.42	0.45
1:XA:979:C:O2	14:YN:19:ARG:NE	2.49	0.45
8:XH:34:GLU:HB3	8:XH:118:VAL:HG11	1.99	0.45
23:XW:66:U:H2'	23:XW:67:A:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:YA:30:G:O2'	36:YA:1214:A:N3	2.39	0.45
36:YA:2468:G:OP1	47:YQ:119:ARG:NH2	2.40	0.45
43:YI:81:VAL:HG11	43:YI:88:ILE:HD12	1.97	0.45
45:YO:24:VAL:HG13	45:YO:30:ALA:HB3	1.98	0.45
45:YO:17:ARG:HH21	45:YO:47:ILE:HD12	1.81	0.45
46:YP:64:LYS:O	46:YP:66:GLY:N	2.49	0.45
1:QA:1048:G:H5'	14:QN:3:ARG:HE	1.80	0.45
1:QA:825:G:O2'	8:QH:12:ARG:NH1	2.49	0.45
1:QA:977:A:H1'	1:QA:981:U:H3	1.81	0.45
2:QB:168:THR:HG21	2:QB:191:ASP:HB3	1.98	0.45
26:R0:70:GLN:OE1	26:R0:80:HIS:NE2	2.49	0.45
36:RA:1565:C:H5''	38:RD:18:VAL:HG21	1.99	0.45
39:RE:52:LEU:O	39:RE:75:VAL:N	2.44	0.45
40:RF:174:VAL:HG21	40:RF:188:ARG:HH21	1.81	0.45
1:XA:184:G:H2'	1:XA:185:A:H8	1.82	0.45
36:YA:1028:A:N3	36:YA:2486:G:O2'	2.41	0.45
36:YA:1033:U:C4	36:YA:2750:A:C2	3.04	0.45
36:YA:2751:G:C8	36:YA:2751:G:O5'	2.70	0.45
36:YA:321:G:O2'	36:YA:340:A:N3	2.46	0.45
36:YA:602:G:O2'	36:YA:604:G:O2'	2.26	0.45
36:YA:776:G:N7	36:YA:793:A:O2'	2.49	0.45
48:YR:3:HIS:O	48:YR:5:LYS:N	2.50	0.45
1:QA:977:A:O2'	1:QA:981:U:N3	2.50	0.45
30:R4:48:ARG:HH21	30:R4:51:ASP:HB2	1.82	0.45
38:RD:132:PRO:HA	38:RD:190:TYR:HA	1.99	0.45
36:RA:2377:A:O2'	49:RS:111:GLU:O	2.24	0.45
1:XA:1192:C:O2	5:XE:25:ARG:NH2	2.50	0.45
38:YD:231:HIS:CD2	38:YD:249:PRO:HG3	2.51	0.45
50:YT:118:ARG:HA	50:YT:121:ILE:HB	1.99	0.45
55:YY:19:LYS:HG3	55:YY:20:TYR:CD1	2.51	0.45
55:YY:42:VAL:O	55:YY:65:ALA:N	2.47	0.45
4:QD:194:LEU:HD23	4:QD:196:LEU:HD23	1.99	0.45
1:QA:264:U:O2'	17:QQ:64:PRO:O	2.26	0.45
32:R6:18:ARG:HH22	32:R6:47:THR:HG21	1.81	0.45
35:R9:1:MET:HG3	36:RA:2477:C:H2'	1.99	0.45
41:RG:114:ILE:HD11	41:RG:135:LEU:HD23	1.99	0.45
44:RN:35:ARG:HG3	44:RN:37:LYS:HG3	1.99	0.45
36:RA:2294:C:OP2	49:RS:13:ARG:NH2	2.49	0.45
1:XA:992:U:H3	1:XA:1044:A:H62	1.63	0.45
54:YX:34:ALA:O	54:YX:77:LYS:NZ	2.36	0.45
1:QA:1512:U:H2'	1:QA:1513:A:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:448:A:OP2	1:QA:485:G:N2	2.38	0.45
36:RA:918:A:N3	37:RB:80:U:O2'	2.49	0.45
36:RA:984:A:H5''	36:RA:985:C:H5	1.82	0.45
41:RG:32:PRO:HB2	41:RG:172:LEU:HD13	1.98	0.45
4:XD:119:GLN:HE21	4:XD:123:HIS:CE1	2.34	0.45
10:XJ:38:ILE:HD11	10:XJ:71:LEU:HD23	1.98	0.45
30:Y4:7:PRO:HB2	30:Y4:27:THR:HG21	1.97	0.45
36:YA:2441:C:OP2	36:YA:2586:C:O2'	2.32	0.45
36:YA:320:A:N3	40:YF:169:ASN:ND2	2.64	0.45
25:XY:54:U:O5'	47:YQ:51:ARG:NH1	2.49	0.45
50:YT:92:GLY:HA2	50:YT:116:ALA:HA	1.99	0.45
1:QA:254:G:O2'	17:QQ:16:GLN:O	2.34	0.45
13:QM:14:ARG:H	13:QM:44:ARG:HA	1.80	0.45
30:R4:49:PHE:CD2	30:R4:50:VAL:CG2	2.92	0.45
38:RD:8:PRO:HB3	38:RD:14:ARG:HE	1.82	0.45
50:RT:62:THR:HG22	50:RT:75:ILE:HG12	1.99	0.45
1:XA:1320:C:OP1	19:XS:70:LYS:NZ	2.37	0.45
2:XB:130:ARG:HB3	2:XB:134:GLU:HB2	1.99	0.45
22:XV:16:C:H4'	22:XV:17(A):U:H5''	1.99	0.45
36:YA:1045:A:N3	36:YA:1047:G:N2	2.65	0.45
36:YA:1171:G:O6	36:YA:1174:A:N6	2.49	0.45
2:QB:16:HIS:HD2	2:QB:210:SER:HA	1.82	0.44
7:QG:104:LEU:HD12	7:QG:124:LEU:HD22	1.99	0.44
9:QI:20:ARG:O	9:QI:60:ASP:N	2.49	0.44
20:QT:100:ILE:HG13	20:QT:102:GLY:H	1.82	0.44
36:RA:2212:A:H1'	36:RA:2215:G:C4	2.52	0.44
46:RP:95:VAL:HG13	46:RP:100:LEU:HD11	1.98	0.44
1:XA:767:A:O2'	1:XA:1524:C:O2	2.29	0.44
14:YN:37:PHE:HE2	14:YN:53:LEU:HD22	1.80	0.44
35:Y9:19:ARG:HB3	36:YA:2756:U:H5''	1.99	0.44
36:YA:1033:U:C4	36:YA:2750:A:N1	2.85	0.44
36:YA:2773:C:OP1	39:YE:164:ARG:NE	2.49	0.44
50:YT:64:ARG:NH1	50:YT:106:SER:OG	2.49	0.44
51:YU:69:CYS:O	51:YU:73:GLY:N	2.50	0.44
10:QJ:50:ILE:HA	10:QJ:60:ARG:HB2	1.99	0.44
27:R1:18:ILE:HG12	27:R1:37:ILE:HG12	1.99	0.44
36:RA:2102:U:H3	36:RA:2187:G:H1	1.65	0.44
36:RA:237:C:O2	36:RA:609:A:O2'	2.31	0.44
36:RA:2484:G:H1'	47:RQ:124:LYS:HG3	2.00	0.44
38:RD:146:GLU:OE2	38:RD:151:LYS:N	2.43	0.44
38:RD:142:VAL:N	38:RD:163:ALA:O	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:RD:133:LEU:HB3	38:RD:173:VAL:HG11	1.99	0.44
1:XA:316:G:OP2	1:XA:351:G:O2'	2.29	0.44
1:XA:407:G:H5''	4:XD:115:ARG:HB3	1.99	0.44
1:XA:812:C:H4'	1:XA:813:U:H5'	1.98	0.44
16:XP:6:LEU:HB3	16:XP:17:TYR:HB3	2.00	0.44
36:YA:48:G:N1	36:YA:177:G:OP2	2.48	0.44
36:YA:411:G:OP2	36:YA:2406:U:O2'	2.32	0.44
1:QA:1202:G:O4'	14:QN:29:ARG:NH2	2.46	0.44
8:QH:21:LYS:O	8:QH:65:TYR:OH	2.28	0.44
1:QA:1147:C:O2	9:QI:16:ARG:NH2	2.50	0.44
19:QS:12:ASP:OD2	19:QS:35:SER:OG	2.32	0.44
38:RD:142:VAL:HG23	38:RD:193:VAL:HA	1.99	0.44
53:RW:10:VAL:HG13	53:RW:101:SER:HB2	1.98	0.44
55:RY:56:PRO:HB2	55:RY:57:GLN:H	1.60	0.44
1:XA:1079:G:O2'	5:XE:14:ARG:NH2	2.48	0.44
3:XC:48:TYR:OH	3:XC:122:GLU:OE1	2.31	0.44
7:XG:113:GLU:HB2	7:XG:119:ARG:HG2	1.98	0.44
7:XG:5:ARG:HH21	7:XG:6:ARG:HG3	1.81	0.44
47:YQ:52:VAL:HA	47:YQ:55:VAL:HG22	2.00	0.44
16:QP:38:TYR:HE1	16:QP:47:ASP:O	1.99	0.44
36:RA:1165:U:H3	36:RA:1184:G:H1	1.64	0.44
36:RA:1403:C:H5''	36:RA:1471:A:H1'	1.99	0.44
36:RA:2679:A:OP2	39:RE:160:TYR:OH	2.34	0.44
36:RA:181:A:H1'	36:RA:435:C:H5'	2.00	0.44
48:RR:98:LEU:N	48:RR:113:LEU:O	2.45	0.44
1:XA:1101:A:N6	2:XB:176:GLU:OE2	2.50	0.44
1:XA:376:G:H5''	16:XP:5:ARG:HB2	1.97	0.44
26:Y0:23:VAL:HG21	36:YA:857:C:H4'	1.98	0.44
36:YA:303:U:H2'	36:YA:304:G:H8	1.82	0.44
36:YA:582:G:OP1	51:YU:14:HIS:ND1	2.40	0.44
39:YE:26:ILE:HD11	39:YE:182:LEU:HD23	1.99	0.44
42:YH:33:LEU:HD11	42:YH:136:ILE:HG22	1.99	0.44
49:RS:30:ARG:HD2	49:RS:97:ARG:HD3	1.98	0.44
50:RT:16:ARG:H	50:RT:79:HIS:HD2	1.66	0.44
1:XA:825:G:O2'	8:XH:12:ARG:NH1	2.51	0.44
4:XD:105:VAL:HG13	4:XD:110:PHE:HB2	1.98	0.44
8:XH:19:VAL:HG13	8:XH:21:LYS:HG3	1.99	0.44
32:Y6:24:GLU:OE2	36:YA:2346:A:O2'	2.35	0.44
36:YA:1568:G:H5''	38:YD:61:LEU:HG	2.00	0.44
42:YH:8:PRO:O	42:YH:69:ARG:NH2	2.49	0.44
5:QE:88:LYS:HB3	5:QE:123:LEU:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:RA:1316:U:H2'	36:RA:1317:A:H8	1.83	0.44
43:RI:128:LEU:HB2	43:RI:138:ILE:HG23	1.99	0.44
36:RA:390:A:C6	46:RP:71:VAL:HG21	2.53	0.44
55:RY:95:LYS:HA	55:RY:101:LYS:HB3	2.00	0.44
3:XC:65:ALA:HA	3:XC:100:ALA:HB3	1.98	0.44
11:XK:108:ILE:HB	18:XR:87:ARG:HA	2.00	0.44
19:XS:36:ARG:NH2	19:XS:72:GLY:O	2.50	0.44
36:YA:1128:A:N7	36:YA:2489:G:O2'	2.49	0.44
51:YU:52:ARG:NE	51:YU:55:ARG:HH21	2.16	0.44
1:QA:677:U:H3	1:QA:713:G:H22	1.65	0.44
2:QB:43:ASP:OD2	2:QB:46:LYS:N	2.43	0.44
8:QH:104:ARG:HG3	8:QH:107:LEU:HB2	1.99	0.44
9:QI:21:PRO:HA	9:QI:59:PHE:HA	1.99	0.44
10:QJ:12:ASP:HB3	10:QJ:15:THR:HG22	1.99	0.44
36:RA:1454:U:O2'	36:RA:1455:G:N7	2.44	0.44
36:RA:2851:A:O3'	48:RR:64:ARG:NH2	2.51	0.44
1:XA:1118:C:OP1	9:XI:104:ARG:NH1	2.46	0.44
1:XA:1240:U:OP2	7:XG:116:ALA:N	2.49	0.44
1:XA:414:A:OP2	1:XA:428:G:N2	2.42	0.44
1:XA:593:G:H1	1:XA:646:U:H3	1.66	0.44
8:XH:17:THR:O	8:XH:78:GLN:NE2	2.48	0.44
36:YA:1171:G:H1	36:YA:1178:C:H42	1.66	0.44
37:YB:91:C:H2'	37:YB:92:G:C8	2.52	0.44
36:YA:1657:C:H4'	39:YE:133:LYS:HB3	2.00	0.44
42:YH:124:GLU:HB3	42:YH:132:ARG:HB3	1.99	0.44
1:QA:1289:A:N1	1:QA:1371:G:O2'	2.41	0.44
3:QC:40:ARG:NH2	3:QC:57:ILE:HD13	2.33	0.44
4:QD:140:VAL:HG11	4:QD:146:ILE:HD11	1.99	0.44
22:QV:47:U:N3	25:QY:17:U:OP1	2.50	0.44
36:RA:2086:U:OP2	38:RD:263:ARG:NE	2.40	0.44
1:XA:454:C:OP1	16:XP:75:ARG:NH2	2.50	0.44
4:XD:175:SER:HB3	4:XD:186:LEU:HD11	1.99	0.44
4:XD:173:TRP:CD1	4:XD:189:PRO:HG3	2.52	0.44
26:Y0:45:PHE:CE2	26:Y0:69:PHE:CE2	3.05	0.44
36:YA:672:C:OP2	46:YP:42:SER:OG	2.34	0.44
36:YA:1205:U:C4	40:YF:171:PRO:HA	2.52	0.44
53:YW:22:ASP:OD1	53:YW:25:ARG:NH1	2.41	0.44
1:QA:1040:U:H2'	1:QA:1041:A:H8	1.83	0.44
4:QD:105:VAL:HG13	4:QD:110:PHE:HB2	2.00	0.44
17:QQ:18:THR:OG1	17:QQ:69:LYS:NZ	2.40	0.44
25:QY:25:C:H2'	25:QY:26:G:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:RA:1510:A:O2'	36:RA:1511:A:N7	2.46	0.44
36:RA:2392:A:H2	36:RA:2424:C:H42	1.65	0.44
42:RH:87:LEU:HD12	42:RH:162:ILE:HG22	2.00	0.44
45:RO:63:VAL:HG23	45:RO:64:ARG:HD3	1.98	0.44
36:RA:483:A:O2'	55:RY:48:ALA:O	2.31	0.44
4:XD:6:GLY:H	4:XD:115:ARG:HH12	1.65	0.44
8:XH:33:GLU:OE2	8:XH:50:ARG:NE	2.41	0.44
30:Y4:58:ARG:HE	30:Y4:63:TYR:HA	1.83	0.44
38:YD:141:VAL:HG13	38:YD:162:SER:HB2	2.00	0.44
44:YN:96:GLU:HB2	44:YN:122:VAL:HG12	2.00	0.44
45:YO:8:LEU:HB2	45:YO:19:ILE:HG13	2.00	0.44
51:YU:52:ARG:HE	51:YU:55:ARG:HH21	1.66	0.44
56:YZ:103:ARG:HB3	56:YZ:138:GLU:HA	1.99	0.44
36:RA:2305:A:H1'	41:RG:136:ARG:HB3	2.00	0.43
39:RE:134:ILE:HA	39:RE:137:HIS:CD2	2.52	0.43
41:RG:38:VAL:HA	41:RG:93:THR:HA	2.00	0.43
52:RV:62:LEU:HB2	52:RV:93:GLU:HB2	2.00	0.43
55:RY:76:CYS:O	55:RY:78:ALA:N	2.46	0.43
1:XA:1251:A:N3	1:XA:1369:C:O2'	2.43	0.43
1:XA:324:G:N2	1:XA:327:A:OP2	2.49	0.43
36:YA:2258:C:O2'	36:YA:2427:C:OP2	2.31	0.43
35:Y9:24:TYR:OH	36:YA:2742:C:OP2	2.30	0.43
38:YD:142:VAL:HG23	38:YD:193:VAL:HA	2.00	0.43
40:YF:184:TYR:CZ	40:YF:188:ARG:HD2	2.53	0.43
1:QA:368:U:OP1	43:YI:91:SER:OG	2.36	0.43
1:QA:880:C:H2'	1:QA:881:G:H8	1.82	0.43
4:QD:79:PHE:HZ	4:QD:204:ILE:HA	1.82	0.43
4:QD:205:GLU:OE2	5:QE:107:ARG:NH1	2.51	0.43
36:RA:1113:U:H2'	36:RA:1114:G:H8	1.82	0.43
36:RA:1394:U:H4'	36:RA:1603:A:H4'	1.99	0.43
36:RA:259:G:H2'	36:RA:260:G:H8	1.82	0.43
13:XM:81:LEU:HD12	13:XM:88:ARG:HB2	2.00	0.43
30:Y4:58:ARG:O	30:Y4:71:ARG:NH1	2.51	0.43
30:Y4:26:SER:OG	41:YG:143:GLU:OE2	2.28	0.43
50:YT:33:LYS:HB3	50:YT:82:LEU:HD12	1.99	0.43
48:YR:103:ARG:HH11	53:YW:40:ASN:HD22	1.66	0.43
56:YZ:145:GLU:HG3	56:YZ:146:ILE:H	1.82	0.43
4:QD:59:ARG:HH21	4:QD:62:GLN:HG3	1.83	0.43
5:QE:99:GLY:H	5:QE:117:ASP:CG	2.21	0.43
10:QJ:44:VAL:HG22	10:QJ:66:ARG:HD2	2.00	0.43
23:QW:56:C:C2	36:RA:2169:A:H8	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:QW:62:C:H2'	23:QW:63:G:H8	1.82	0.43
36:RA:993:G:OP1	51:RU:50:ARG:NH2	2.45	0.43
38:RD:31:LYS:HE3	38:RD:102:LYS:HD3	1.98	0.43
44:RN:22:THR:OG1	44:RN:23:LEU:N	2.51	0.43
37:RB:90:C:OP2	47:RQ:16:ARG:NE	2.52	0.43
48:RR:98:LEU:HB2	48:RR:113:LEU:HB3	2.00	0.43
13:XM:120:LYS:HG3	13:XM:121:LYS:H	1.82	0.43
16:XP:43:LYS:HG2	16:XP:48:TRP:CD2	2.53	0.43
36:YA:1666:G:N3	45:YO:3:GLN:NE2	2.66	0.43
36:YA:219:G:N3	36:YA:234:C:O2'	2.49	0.43
36:YA:994:C:H3'	51:YU:54:LYS:HE3	2.00	0.43
40:YF:182:ASN:OD1	40:YF:185:ASP:N	2.45	0.43
36:YA:1093:G:H5'	42:YH:170:ARG:HH12	1.83	0.43
1:QA:1124:G:H3'	1:QA:1145:C:N4	2.33	0.43
1:QA:21:G:H21	1:QA:914:A:H62	1.64	0.43
1:QA:406:G:N2	4:QD:119:GLN:HE22	2.15	0.43
10:QJ:49:VAL:HG21	14:QN:44:LEU:HD22	2.01	0.43
1:QA:110:C:O2'	16:QP:25:ARG:O	2.29	0.43
30:R4:43:TYR:HA	30:R4:47:GLN:HG3	1.99	0.43
36:RA:1428:C:N4	36:RA:1570:A:OP2	2.44	0.43
36:RA:579:G:O2'	36:RA:2019:A:OP1	2.27	0.43
40:RF:155:LEU:HB2	40:RF:189:THR:HG21	2.01	0.43
1:XA:501:C:H2'	1:XA:502:G:H8	1.82	0.43
1:XA:954:G:H21	1:XA:1227:A:H62	1.66	0.43
1:XA:985:C:H2'	1:XA:986:A:C8	2.53	0.43
3:XC:84:ILE:HG12	3:XC:88:ARG:HE	1.83	0.43
9:XI:5:TYR:HE1	9:XI:16:ARG:HB2	1.83	0.43
1:XA:926:G:H22	24:XX:16:A:P	2.41	0.43
36:YA:1062:G:H2'	36:YA:1063:G:C8	2.53	0.43
36:YA:1394:U:H4'	36:YA:1603:A:H4'	1.99	0.43
36:YA:994:C:OP2	51:YU:54:LYS:NZ	2.49	0.43
38:YD:108:PRO:HB3	38:YD:143:HIS:CE1	2.53	0.43
36:YA:2314:C:OP1	41:YG:91:ARG:NH1	2.52	0.43
1:QA:1073:U:H2'	1:QA:1074:G:H8	1.83	0.43
7:QG:58:PRO:HA	7:QG:61:VAL:HG22	2.01	0.43
1:QA:1178:G:OP2	9:QI:93:ARG:NH2	2.52	0.43
35:R9:9:ARG:HH21	35:R9:16:VAL:HG12	1.82	0.43
35:R9:25:VAL:HB	35:R9:34:GLN:HB2	2.00	0.43
36:RA:1113:U:H2'	36:RA:1114:G:C8	2.53	0.43
36:RA:151:C:H2'	36:RA:152:G:H8	1.84	0.43
36:RA:2120:G:H2'	36:RA:2121:G:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:RG:16:ARG:NH2	41:RG:28:VAL:HG22	2.34	0.43
54:RX:30:VAL:HG21	54:RX:39:ILE:HD11	2.01	0.43
1:XA:45:U:H3	1:XA:396:G:H1	1.66	0.43
1:XA:851:G:H2'	1:XA:852:G:C8	2.54	0.43
7:XG:123:GLU:O	7:XG:127:ALA:N	2.50	0.43
1:XA:35:G:N2	12:XL:118:SER:OG	2.46	0.43
36:YA:2688:U:OP1	36:YA:2713:A:N6	2.51	0.43
38:YD:12:SER:O	38:YD:16:MET:HB2	2.19	0.43
42:YH:5:GLY:O	42:YH:8:PRO:HD2	2.18	0.43
55:YY:6:HIS:NE2	55:YY:69:ALA:O	2.37	0.43
32:R6:36:LEU:HD11	32:R6:48:VAL:HG22	2.00	0.43
36:RA:597:U:H2'	36:RA:598:G:C8	2.53	0.43
45:RO:38:VAL:HG12	45:RO:61:VAL:HB	2.01	0.43
1:XA:501:C:H2'	1:XA:502:G:C8	2.53	0.43
1:XA:591:U:OP1	8:XH:30:ARG:NH1	2.52	0.43
1:XA:67:C:H2'	1:XA:68:G:C8	2.53	0.43
2:XB:174:VAL:HG13	2:XB:184:VAL:HG11	2.01	0.43
2:XB:19:HIS:HA	2:XB:39:ILE:HD11	2.00	0.43
1:XA:407:G:H5''	4:XD:115:ARG:HD3	1.99	0.43
12:XL:105:TYR:HA	12:XL:105:TYR:HD1	1.72	0.43
36:YA:1434:A:H61	36:YA:1558:A:N6	2.15	0.43
36:YA:2392:A:H8	46:YP:60:MET:HG2	1.83	0.43
55:YY:50:ARG:H	55:YY:50:ARG:HD3	1.82	0.43
1:QA:1157:A:H62	1:QA:1178:G:N2	2.15	0.43
1:QA:1294:G:H2'	1:QA:1295:G:H8	1.83	0.43
4:QD:64:LEU:HB2	4:QD:198:VAL:HG11	2.01	0.43
8:QH:106:GLY:O	8:QH:122:ARG:NH2	2.52	0.43
1:QA:599:C:O2'	8:QH:129:VAL:O	2.26	0.43
13:QM:86:CYS:SG	13:QM:89:GLY:N	2.91	0.43
24:QX:12:A:O2'	24:QX:13:A:O3'	2.37	0.43
30:R4:11:PRO:HG3	30:R4:25:TYR:CZ	2.54	0.43
41:RG:138:GLN:HE22	41:RG:152:LEU:HA	1.83	0.43
45:RO:104:ARG:NH1	50:RT:34:VAL:HG11	2.34	0.43
36:RA:1155:A:O3'	51:RU:55:ARG:NH1	2.51	0.43
54:RX:58:HIS:CE1	54:RX:77:LYS:HD3	2.54	0.43
1:XA:1386:G:H2'	1:XA:1387:G:H8	1.84	0.43
1:XA:677:U:H3	1:XA:713:G:H22	1.66	0.43
1:XA:406:G:N2	4:XD:119:GLN:HE22	2.17	0.43
10:XJ:61:GLU:OE2	14:YN:58:LYS:NZ	2.50	0.43
14:YN:37:PHE:CE2	14:YN:53:LEU:HD22	2.53	0.43
28:Y2:37:PHE:CD1	54:YX:11:PRO:HD3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:YA:1788:C:OP1	38:YD:222:ARG:NH2	2.52	0.43
38:YD:146:GLU:HB2	38:YD:189:CYS:HB3	2.01	0.43
39:YE:109:LYS:O	39:YE:111:ARG:NH1	2.52	0.43
40:YF:198:ALA:HA	40:YF:201:VAL:HG22	2.00	0.43
42:YH:53:GLU:HA	42:YH:65:HIS:CE1	2.54	0.43
1:QA:1087:G:H2'	1:QA:1088:G:H8	1.84	0.43
1:QA:579:G:H5'	1:QA:728:A:H1'	2.00	0.43
1:QA:553:A:O2'	12:QL:29:GLY:O	2.29	0.43
13:QM:25:ILE:HA	13:QM:29:ARG:HD2	2.01	0.43
31:R5:11:THR:OG1	36:RA:1263:U:O3'	2.36	0.43
36:RA:1422:G:H1	36:RA:1576:U:H3	1.67	0.43
36:RA:224:G:O6	36:RA:419:C:O2'	2.31	0.43
36:RA:229:A:H4'	36:RA:230:U:H5'	2.00	0.43
1:XA:973:G:H3'	1:XA:974:A:H5''	2.01	0.43
41:YG:114:ILE:HD11	41:YG:140:ILE:HD13	2.00	0.43
45:YO:8:LEU:HD13	45:YO:82:ASN:HB3	2.00	0.43
56:YZ:95:PRO:HA	56:YZ:129:SER:HA	2.01	0.43
1:QA:1105:A:H2'	1:QA:1106:G:H8	1.84	0.43
3:QC:55:VAL:HG12	3:QC:68:VAL:HG22	2.01	0.43
5:QE:33:VAL:HG13	5:QE:112:LEU:HD12	2.00	0.43
28:R2:38:GLN:HB3	28:R2:45:SER:HB2	2.01	0.43
36:RA:1508:A:O2'	36:RA:1509:C:O4'	2.32	0.43
36:RA:1827:C:OP2	38:RD:222:ARG:NH1	2.52	0.43
31:R5:12:SER:OG	36:RA:2021:C:OP1	2.29	0.43
40:RF:154:VAL:HG12	40:RF:173:VAL:HG22	2.00	0.43
56:RZ:5:LEU:HD12	56:RZ:43:GLU:HG3	2.01	0.43
56:RZ:19:ARG:HD3	56:RZ:84:GLU:HA	2.00	0.43
1:XA:1224:G:O2'	1:XA:1322:C:OP2	2.37	0.43
1:XA:1484:C:O2'	36:YA:1960:A:O2'	2.28	0.43
1:XA:123:C:O2'	1:XA:290:C:O2	2.33	0.43
8:XH:9:MET:HG3	8:XH:26:VAL:HG21	1.99	0.43
36:YA:1827:C:O2'	36:YA:1970:A:N3	2.44	0.43
36:YA:2151:G:H2'	36:YA:2152:G:H8	1.83	0.43
36:YA:2287:A:N6	36:YA:2344:U:H3	2.16	0.43
36:YA:587:C:OP2	46:YP:21:ARG:NH1	2.52	0.43
36:YA:907:U:O2'	47:YQ:101:ARG:NH2	2.50	0.43
37:YB:111:U:H2'	37:YB:112:G:C8	2.54	0.43
38:YD:79:VAL:HG21	38:YD:111:LEU:HD11	2.01	0.43
46:YP:100:LEU:HD12	46:YP:105:LEU:HD12	2.00	0.43
1:QA:1510:U:H2'	1:QA:1511:G:C8	2.54	0.43
1:QA:656:C:O2	15:QO:28:GLN:NE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:824:C:H2'	1:QA:825:G:H8	1.84	0.43
1:QA:1249:C:H1'	9:QL:70:LYS:HE3	2.01	0.43
13:QM:105:THR:HG22	13:QM:106:ASN:H	1.84	0.43
38:RD:35:LYS:HA	38:RD:35:LYS:HD3	1.66	0.43
46:RP:57:THR:OG1	46:RP:58:THR:N	2.52	0.43
1:XA:1414:U:H2'	1:XA:1415:G:C8	2.52	0.43
4:XD:163:GLU:HA	4:XD:166:LYS:HE3	2.01	0.43
10:XJ:8:LEU:HB3	10:XJ:16:LEU:HD21	2.01	0.43
36:YA:222:A:H3'	36:YA:421:U:H5'	2.01	0.43
41:YG:27:ASN:HB3	41:YG:30:GLU:HG3	2.01	0.43
49:YS:7:TYR:HA	49:YS:10:ARG:HH21	1.83	0.43
5:QE:102:ALA:O	5:QE:107:ARG:NH2	2.51	0.42
12:QL:54:LYS:HB3	12:QL:70:ILE:HD12	2.01	0.42
36:RA:13:A:O2'	36:RA:15:G:N7	2.51	0.42
39:RE:144:ARG:HB3	39:RE:145:LYS:H	1.53	0.42
46:RP:65:ARG:O	46:RP:68:GLN:NE2	2.31	0.42
50:RT:91:ARG:NE	50:RT:124:ASP:OD2	2.37	0.42
50:RT:24:PRO:HD3	50:RT:52:ILE:HD12	2.01	0.42
50:RT:66:VAL:HA	50:RT:71:GLY:HA2	1.99	0.42
45:RO:76:ALA:HB3	50:RT:75:ILE:HD12	2.01	0.42
1:XA:993:G:O2'	1:XA:994:A:N7	2.52	0.42
20:XT:73:HIS:HB3	20:XT:74:LYS:H	1.58	0.42
36:YA:1174:A:H2	36:YA:1176:G:H4'	1.84	0.42
38:YD:108:PRO:HG2	38:YD:111:LEU:HB2	2.00	0.42
49:YS:87:PHE:CE1	49:YS:102:ALA:HB2	2.54	0.42
49:YS:12:PHE:O	49:YS:16:ASN:ND2	2.52	0.42
1:QA:1151:A:H2'	1:QA:1152:A:H8	1.84	0.42
1:QA:740:U:H2'	1:QA:741:G:H8	1.84	0.42
36:RA:270(F):U:H3	36:RA:270(T):G:H1	1.66	0.42
36:RA:783:A:H8	36:RA:784:A:H4'	1.83	0.42
37:RB:48:A:OP2	49:RS:30:ARG:NH2	2.52	0.42
39:RE:116:VAL:HG23	39:RE:120:TRP:HD1	1.84	0.42
48:RR:3:HIS:HB3	48:RR:4:LEU:H	1.65	0.42
1:XA:1358:U:OP2	1:XA:1359:C:N4	2.43	0.42
1:XA:1452:C:H4'	1:XA:1453:G:H5'	2.00	0.42
3:XC:17:ASP:O	3:XC:54:ARG:NH2	2.52	0.42
5:XE:98:THR:OG1	5:XE:99:GLY:N	2.52	0.42
9:XI:63:ILE:HG21	9:XI:77:ILE:HD12	2.00	0.42
19:XS:18:LYS:HE2	19:XS:22:LEU:HD11	2.01	0.42
36:YA:630:G:N2	36:YA:633:A:OP2	2.33	0.42
36:YA:780:G:H21	36:YA:783:A:H62	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:YG:39:ILE:HB	41:YG:92:VAL:HG13	2.01	0.42
47:YQ:16:ARG:HG2	47:YQ:17:LEU:H	1.85	0.42
1:QA:1151:A:H2'	1:QA:1152:A:C8	2.54	0.42
1:QA:130:A:N6	1:QA:233:C:O2	2.52	0.42
1:QA:272:C:H2'	1:QA:273:A:C8	2.54	0.42
1:QA:7:G:O2'	5:QE:120:THR:O	2.37	0.42
1:QA:898:G:N2	1:QA:901:A:OP2	2.48	0.42
8:QH:109:ILE:HG23	8:QH:137:VAL:HB	2.01	0.42
14:QN:26:ARG:NH1	14:QN:43:CYS:SG	2.85	0.42
15:QO:79:ARG:HD3	15:QO:79:ARG:H	1.84	0.42
1:QA:127:G:O2'	17:QQ:2:PRO:O	2.37	0.42
31:R5:51:TYR:HB2	31:R5:56:LYS:HB3	2.01	0.42
34:R8:2:PRO:HA	36:RA:591:C:H1'	2.01	0.42
36:RA:117:G:OP2	36:RA:119:A:O2'	2.29	0.42
36:RA:212:G:H2'	36:RA:213:A:C8	2.54	0.42
42:RH:85:LYS:HD2	42:RH:85:LYS:HA	1.86	0.42
2:XB:163:PHE:HA	2:XB:185:ILE:HG13	2.00	0.42
36:YA:589:C:H2'	36:YA:590:A:C8	2.55	0.42
53:YW:29:LEU:HD22	53:YW:69:LEU:HD11	2.00	0.42
28:Y2:29:LYS:NZ	54:YX:6:ASP:OD2	2.51	0.42
1:QA:1172:C:H2'	1:QA:1173:G:C8	2.53	0.42
1:QA:346:G:OP1	50:RT:41:ARG:NH2	2.52	0.42
36:RA:1441:G:H2'	36:RA:1442:G:C8	2.55	0.42
36:RA:1509:C:H3'	36:RA:1510:A:H5''	2.01	0.42
38:RD:81:ALA:HB3	38:RD:94:LEU:HB3	2.02	0.42
39:RE:28:ALA:HB3	39:RE:93:VAL:HG23	2.02	0.42
41:RG:77:ILE:H	41:RG:82:LEU:HD11	1.84	0.42
1:XA:1131:G:H1	1:XA:1143:G:N2	2.16	0.42
9:XI:10:ARG:HE	9:XI:105:ASP:HB3	1.83	0.42
36:YA:2296:U:OP2	49:YS:9:ARG:NH1	2.52	0.42
36:YA:457:A:N6	36:YA:471:A:OP2	2.51	0.42
37:YB:40:U:N3	37:YB:43:C:H5''	2.34	0.42
51:YU:92:ARG:NE	52:YV:11:GLN:HB2	2.34	0.42
31:R5:41:PRO:O	31:R5:44:THR:OG1	2.36	0.42
36:RA:1636:C:H2'	36:RA:1637:A:C8	2.55	0.42
36:RA:2315:G:O2'	41:RG:128:ARG:NH2	2.42	0.42
36:RA:529:A:H8	36:RA:530:G:C5	2.37	0.42
36:RA:659:C:H2'	36:RA:660:G:H8	1.84	0.42
45:RO:8:LEU:HB2	45:RO:19:ILE:HG13	2.01	0.42
1:XA:262:A:H5''	20:XT:76:ALA:HB2	2.02	0.42
10:XJ:4:ILE:HG22	10:XJ:100:THR:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:YA:1262:A:OP1	53:YW:99:ARG:NH1	2.47	0.42
36:YA:407:G:H2'	36:YA:408:G:H8	1.84	0.42
39:YE:201:THR:OG1	39:YE:202:LYS:N	2.51	0.42
33:Y7:47:ARG:HH22	54:YX:60:ARG:NH1	2.17	0.42
9:QI:45:ALA:O	9:QI:78:LYS:NZ	2.40	0.42
12:QL:102:ARG:HB3	12:QL:109:GLY:HA2	2.02	0.42
29:R3:8:LEU:HG	29:R3:31:LEU:HD12	2.02	0.42
36:RA:1971:A:C4	38:RD:241:PRO:HB3	2.55	0.42
41:RG:136:ARG:HG3	41:RG:137:GLU:HG3	2.01	0.42
45:RO:64:ARG:HE	45:RO:83:ALA:HB3	1.83	0.42
51:RU:61:TRP:CE2	51:RU:94:ASN:HB2	2.54	0.42
10:XJ:44:VAL:HG22	10:XJ:66:ARG:HD3	2.01	0.42
26:Y0:73:GLY:HA3	37:YB:12:C:H2'	2.01	0.42
27:Y1:3:LYS:HD2	27:Y1:43:TYR:HD2	1.85	0.42
30:Y4:14:ILE:HG12	30:Y4:21:VAL:HB	2.02	0.42
30:Y4:20:ASN:OD1	30:Y4:21:VAL:N	2.53	0.42
34:Y8:14:VAL:HG13	34:Y8:22:VAL:HG13	2.00	0.42
36:YA:1270:C:H5''	36:YA:1271:G:H5'	2.02	0.42
37:YB:91:C:H2'	37:YB:92:G:H8	1.84	0.42
43:YI:3:VAL:HG12	43:YI:38:LEU:HA	2.02	0.42
1:QA:1005:A:H4'	1:QA:1037:C:H1'	2.01	0.42
1:QA:1355:G:H2'	1:QA:1356:G:H8	1.84	0.42
1:QA:464:G:C6	1:QA:466:C:H5'	2.54	0.42
5:QE:51:VAL:HG13	5:QE:52:PRO:HD3	2.02	0.42
36:RA:953:A:OP2	47:RQ:18:LYS:NZ	2.41	0.42
49:RS:49:VAL:HG21	49:RS:77:ALA:HA	2.02	0.42
1:XA:1299:A:C8	1:XA:1301:U:H1'	2.54	0.42
26:Y0:33:ALA:N	26:Y0:64:ASP:OD1	2.52	0.42
7:QG:65:ALA:HB1	7:QG:127:ALA:HB3	2.01	0.42
13:QM:76:ALA:O	13:QM:80:ARG:N	2.52	0.42
1:QA:1187:G:O2'	14:QN:61:TRP:OXT	2.32	0.42
15:QO:39:LEU:HG	15:QO:56:LEU:HD12	2.02	0.42
20:QT:71:THR:O	20:QT:73:HIS:N	2.52	0.42
22:QV:16:C:H4'	22:QV:17(A):U:H5''	2.01	0.42
23:QW:3:G:H2'	23:QW:4:G:C8	2.53	0.42
27:R1:60:PHE:HB3	27:R1:62:VAL:HG13	2.00	0.42
30:R4:11:PRO:HA	30:R4:25:TYR:HA	2.00	0.42
38:RD:17:THR:HG1	38:RD:205:VAL:H	1.67	0.42
38:RD:62:TYR:HA	38:RD:87:ASN:ND2	2.35	0.42
40:RF:160:ASN:HB3	40:RF:163:VAL:HG12	2.02	0.42
41:RG:38:VAL:HG13	41:RG:93:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:RX:55:ASN:HB2	54:RX:80:ILE:HG12	2.00	0.42
1:XA:1367:C:OP2	9:XI:112:LYS:NZ	2.53	0.42
1:XA:255:G:OP1	17:XQ:69:LYS:NZ	2.47	0.42
2:XB:11:LEU:HD13	2:XB:213:LEU:HD11	2.01	0.42
2:XB:95:GLN:OE1	2:XB:96:ARG:NH1	2.53	0.42
9:XI:16:ARG:HG3	9:XI:64:THR:HB	2.02	0.42
36:YA:2145:C:H2'	36:YA:2147:G:C2	2.55	0.42
36:YA:2469:A:H5''	36:YA:2470:G:C8	2.55	0.42
39:YE:2:LYS:HD2	39:YE:95:ILE:HB	2.01	0.42
1:XA:344:A:H4'	50:YT:39:ARG:HH12	1.85	0.42
1:QA:675:A:H1'	11:QK:116:HIS:ND1	2.34	0.42
27:R1:87:PRO:HA	27:R1:90:ILE:HB	2.02	0.42
36:RA:1826:G:H4'	38:RD:242:ARG:NE	2.25	0.42
49:RS:14:VAL:HG11	49:RS:89:ARG:NH2	2.34	0.42
50:RT:50:ILE:HG13	50:RT:99:LEU:HD12	2.01	0.42
1:XA:41:G:H2'	1:XA:42:G:H8	1.85	0.42
36:YA:2789:C:H1'	36:YA:2892:A:H2	1.85	0.42
36:YA:307:G:H21	36:YA:330:A:N6	2.18	0.42
39:YE:13:ARG:HA	39:YE:22:PRO:HA	2.02	0.42
39:YE:78:LEU:O	39:YE:79:ARG:HG2	2.20	0.42
42:YH:97:ARG:NH2	42:YH:104:GLU:OE1	2.52	0.42
51:YU:108:GLU:O	51:YU:112:ARG:HG2	2.20	0.42
51:YU:24:TYR:HB2	51:YU:29:SER:HB3	2.02	0.42
51:YU:90:VAL:HG22	52:YV:39:LEU:HD12	2.01	0.42
11:QK:91:ARG:NH2	11:QK:110:ASP:OD2	2.53	0.42
12:QL:93:LEU:HD23	12:QL:96:VAL:HG21	2.01	0.42
17:QQ:45:HIS:CD2	17:QQ:47:PRO:HG3	2.54	0.42
36:RA:807:U:O2'	36:RA:2060:A:N1	2.48	0.42
36:RA:226:G:O2'	36:RA:228:A:N6	2.53	0.42
42:RH:106:THR:HG22	42:RH:108:GLY:H	1.85	0.42
49:RS:21:THR:HG22	49:RS:23:ARG:HH11	1.85	0.42
1:XA:225:C:H2'	1:XA:226:G:H8	1.84	0.42
1:XA:309:G:H2'	1:XA:310:G:H8	1.84	0.42
2:XB:184:VAL:HG23	2:XB:198:ASP:H	1.85	0.42
1:XA:1235:U:H5''	21:XU:3:LYS:HD2	2.01	0.42
45:YO:1:MET:HB2	45:YO:32:TYR:HB3	2.02	0.42
46:YP:57:THR:O	46:YP:59:LEU:N	2.51	0.42
1:QA:1498:U:OP2	24:QX:16:A:O2'	2.36	0.41
3:QC:28:GLN:HG3	3:QC:32:LEU:HD13	2.02	0.41
9:QI:28:VAL:HG12	9:QI:63:ILE:HB	2.01	0.41
10:QJ:30:SER:HB2	10:QJ:80:LYS:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:QK:44:SER:H	11:QK:47:VAL:HG22	1.85	0.41
12:QL:117:ARG:HH22	12:QL:124:LYS:HD3	1.85	0.41
17:QQ:26:GLN:HB3	17:QQ:37:LYS:HG2	2.02	0.41
36:RA:1205:U:C4	40:RF:171:PRO:HA	2.55	0.41
1:XA:1095:U:P	1:XA:1108:G:H1	2.43	0.41
1:XA:161:A:H2'	1:XA:162:A:C8	2.55	0.41
1:XA:352:C:O2'	1:XA:354:G:OP1	2.31	0.41
27:Y1:2:SER:N	36:YA:1364:G:N7	2.68	0.41
32:Y6:24:GLU:HG3	32:Y6:25:LYS:H	1.85	0.41
36:YA:2074:U:HO2'	36:YA:2597:G:HO2'	1.63	0.41
38:YD:13:ARG:NH1	38:YD:16:MET:SD	2.93	0.41
36:YA:1188:U:H4'	52:YV:79:VAL:HG22	2.02	0.41
1:QA:501:C:H2'	1:QA:502:G:H8	1.85	0.41
7:QG:24:THR:O	7:QG:28:ASN:ND2	2.53	0.41
15:QO:87:ILE:HG22	15:QO:88:ARG:H	1.84	0.41
25:QY:29:U:H2'	25:QY:30:G:H8	1.85	0.41
27:R1:23:LYS:HB3	27:R1:29:GLY:HA3	2.01	0.41
31:R5:25:LEU:HD11	53:RW:41:LYS:HE3	2.01	0.41
32:R6:41:PRO:HD2	32:R6:46:HIS:N	2.34	0.41
36:RA:1950:G:N2	36:RA:1950:G:OP2	2.37	0.41
36:RA:2630:G:H2'	36:RA:2631:G:H8	1.85	0.41
40:RF:9:ILE:HD11	40:RF:125:LEU:HD23	2.02	0.41
42:RH:45:VAL:HG22	42:RH:50:VAL:HG23	2.02	0.41
1:XA:564:C:OP2	12:XL:15:ARG:NH2	2.51	0.41
1:XA:601:C:H2'	1:XA:602:A:C8	2.55	0.41
1:XA:662:G:O2'	1:XA:836:G:OP1	2.38	0.41
1:XA:1189:C:H4'	3:XC:10:PHE:CE1	2.55	0.41
1:XA:191:G:O2'	20:XT:101:GLY:O	2.37	0.41
22:XV:50:U:H3	22:XV:64:G:H1	1.68	0.41
36:YA:1799:G:H8	36:YA:1799:G:H2'	1.77	0.41
36:YA:2751:G:C8	36:YA:2751:G:H3'	2.55	0.41
40:YF:32:LEU:HB3	40:YF:112:MET:HE1	2.01	0.41
1:QA:261:U:OP2	20:QT:79:ARG:NH2	2.53	0.41
1:QA:444:C:H2'	1:QA:445:G:H8	1.86	0.41
1:QA:892:A:H62	1:QA:906:G:H21	1.68	0.41
31:R5:20:ARG:HA	31:R5:23:HIS:ND1	2.34	0.41
36:RA:1287:A:C8	48:RR:104:ARG:HD3	2.56	0.41
36:RA:2100:G:H1	36:RA:2189:U:H3	1.67	0.41
36:RA:2581:G:N2	36:RA:2581:G:OP2	2.42	0.41
42:RH:24:VAL:N	42:RH:35:VAL:O	2.44	0.41
50:RT:118:ARG:HA	50:RT:121:ILE:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:539:A:H2'	1:XA:540:G:C8	2.55	0.41
1:XA:769:G:H4'	1:XA:1513:A:H4'	2.02	0.41
11:XK:28:THR:HG21	11:XK:90:GLY:HA3	2.01	0.41
36:YA:1972:A:H2'	36:YA:1973:G:H8	1.85	0.41
36:YA:2443:C:H2'	36:YA:2444:G:C8	2.55	0.41
38:YD:12:SER:HB2	38:YD:208:LYS:HB3	2.02	0.41
38:YD:132:PRO:HG3	38:YD:190:TYR:CE1	2.55	0.41
40:YF:178:PRO:HB3	40:YF:198:ALA:HB2	2.01	0.41
1:QA:1087:G:H2'	1:QA:1088:G:C8	2.55	0.41
1:QA:1352:C:H2'	1:QA:1353:G:C8	2.56	0.41
6:QF:48:LEU:HD22	18:QR:77:GLY:HA3	2.02	0.41
11:QK:110:ASP:HB3	18:QR:85:LEU:HB3	2.03	0.41
15:QO:85:LEU:HB2	15:QO:87:ILE:HD11	2.02	0.41
16:QP:6:LEU:HD23	16:QP:17:TYR:CG	2.55	0.41
36:RA:1140:C:O3'	44:RN:25:ARG:NH2	2.49	0.41
36:RA:2431:U:N3	36:RA:2434:A:OP2	2.48	0.41
36:RA:2638:G:OP1	39:RE:82:ARG:NH2	2.45	0.41
36:RA:363(B):G:H2'	36:RA:363(C):G:H8	1.85	0.41
36:RA:448:U:N3	36:RA:583:G:N3	2.67	0.41
28:R2:48:HIS:CE1	36:RA:95:G:HO2'	2.38	0.41
36:RA:2830:G:H5'	39:RE:58:ARG:NH2	2.35	0.41
40:RF:126:VAL:HG11	40:RF:142:TRP:HH2	1.85	0.41
50:RT:29:ARG:HA	50:RT:46:GLU:HA	2.03	0.41
1:XA:673:G:H4'	6:XF:87:ARG:NH1	2.35	0.41
1:XA:991:U:O4	1:XA:1212:U:O2'	2.29	0.41
2:XB:109:SER:O	2:XB:113:HIS:ND1	2.48	0.41
7:XG:54:THR:HG23	7:XG:56:GLN:H	1.85	0.41
45:YO:76:ALA:HB3	50:YT:75:ILE:HD12	2.02	0.41
1:QA:1071:C:H2'	1:QA:1072:G:H8	1.85	0.41
1:QA:948:C:H2'	1:QA:949:A:C8	2.53	0.41
12:QL:39:VAL:HG22	12:QL:57:LYS:HB2	2.02	0.41
17:QQ:6:LEU:HD12	17:QQ:71:PHE:HE2	1.86	0.41
25:QY:52:G:O2'	47:RQ:56:ARG:NH2	2.44	0.41
36:RA:345:A:H2'	36:RA:347:A:H62	1.86	0.41
36:RA:607:U:H5''	40:RF:103:LYS:NZ	2.35	0.41
36:RA:1454:U:H5'	48:RR:63:ARG:NH1	2.36	0.41
51:RU:90:VAL:HG12	51:RU:91:ASP:H	1.84	0.41
52:RV:75:PHE:HD1	52:RV:82:ARG:HG3	1.85	0.41
55:RY:76:CYS:SG	55:RY:77:PRO:HD2	2.60	0.41
56:RZ:14:LYS:HA	56:RZ:15:PRO:HD3	1.95	0.41
13:XM:87:TYR:N	19:XS:73:GLU:HB3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y1:91:LYS:HB3	27:Y1:92:LYS:H	1.63	0.41
29:Y3:39:ASP:OD1	29:Y3:44:ARG:NH2	2.48	0.41
35:Y9:4:ARG:O	35:Y9:37:GLY:N	2.52	0.41
36:YA:172:C:H2'	36:YA:173:G:H8	1.85	0.41
36:YA:2092:U:OP1	36:YA:2199:A:O2'	2.38	0.41
36:YA:2298:A:H62	36:YA:2318:G:H8	1.69	0.41
38:YD:245:PRO:HA	38:YD:246:PRO:HD3	1.95	0.41
56:YZ:6:LYS:O	56:YZ:62:PRO:HD3	2.20	0.41
56:YZ:79:ARG:HD2	56:YZ:80:ARG:HH11	1.85	0.41
7:QG:93:PRO:HA	7:QG:96:GLN:HB2	2.03	0.41
12:QL:111:LYS:HD3	12:QL:111:LYS:HA	1.96	0.41
36:RA:2043:C:OP1	36:RA:2777:G:O2'	2.31	0.41
36:RA:363(B):G:H2'	36:RA:363(C):G:C8	2.56	0.41
40:RF:48:THR:OG1	40:RF:48:THR:O	2.37	0.41
41:RG:6:ALA:O	41:RG:10:LYS:N	2.51	0.41
51:RU:58:ARG:O	51:RU:62:ILE:HG12	2.21	0.41
56:RZ:105:VAL:N	56:RZ:138:GLU:OE2	2.46	0.41
2:XB:17:PHE:HB2	2:XB:42:ILE:HG23	2.03	0.41
3:XC:88:ARG:NH1	3:XC:101:LEU:H	2.19	0.41
11:XK:33:THR:OG1	11:XK:34:ASP:N	2.53	0.41
13:XM:66:LEU:HB3	13:XM:67:GLU:H	1.66	0.41
32:Y6:25:LYS:HG2	34:Y8:34:TRP:NE1	2.36	0.41
36:YA:186:G:H2'	36:YA:187:G:H8	1.84	0.41
36:YA:281:G:H21	36:YA:359:A:H62	1.69	0.41
36:YA:594:U:H3	36:YA:663:G:H1	1.69	0.41
36:YA:870:A:OP1	47:YQ:6:ARG:NH2	2.54	0.41
50:YT:73:GLU:OE2	50:YT:103:ARG:NE	2.52	0.41
1:QA:963:G:H21	10:QJ:55:LYS:HE2	1.85	0.41
12:QL:117:ARG:HB2	12:QL:117:ARG:HE	1.58	0.41
13:QM:94:ARG:HB3	13:QM:96:LEU:HD13	2.02	0.41
17:QQ:22:LEU:HD11	17:QQ:39:SER:HB2	2.02	0.41
33:R7:47:ARG:HH22	54:RX:60:ARG:NH2	2.18	0.41
35:R9:10:ILE:HD13	36:RA:2477:C:H41	1.85	0.41
36:RA:1423:G:OP1	36:RA:1492:G:O2'	2.37	0.41
36:RA:2154:G:H2'	36:RA:2155:G:C8	2.56	0.41
39:RE:5:LEU:HD12	39:RE:51:PHE:HB2	2.03	0.41
45:RO:19:ILE:HG22	45:RO:43:VAL:HA	2.03	0.41
56:RZ:10:ARG:HH12	56:RZ:25:PRO:HB3	1.86	0.41
1:XA:279:A:OP1	1:XA:280:C:O2'	2.26	0.41
34:Y8:31:HIS:CD2	34:Y8:32:LEU:HG	2.56	0.41
36:YA:1196:C:O2'	36:YA:1228:G:O2'	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:YE:55:ASN:ND2	39:YE:75:VAL:HG22	2.36	0.41
8:QH:23:SER:OG	8:QH:24:THR:N	2.54	0.41
13:QM:34:LEU:O	13:QM:38:GLY:N	2.53	0.41
36:RA:586:A:H4'	40:RF:89:VAL:HG11	2.02	0.41
25:XY:18:G:O6	56:YZ:182:LYS:NZ	2.50	0.41
36:YA:1048:A:OP2	36:YA:1110:G:N2	2.47	0.41
36:YA:1309:G:O2'	36:YA:1611:C:O2'	2.26	0.41
1:QA:1143:G:H2'	1:QA:1144:G:C8	2.56	0.41
1:QA:991:U:O4	1:QA:1212:U:O2'	2.26	0.41
4:QD:18:LYS:HB3	4:QD:20:TYR:HE1	1.85	0.41
28:R2:48:HIS:ND1	36:RA:95:G:O2'	2.45	0.41
36:RA:1270:C:H5''	36:RA:1271:G:H5'	2.03	0.41
36:RA:78:A:H2'	36:RA:79:G:H8	1.85	0.41
38:RD:34:VAL:HG12	38:RD:34:VAL:O	2.21	0.41
40:RF:80:ALA:HB3	40:RF:83:PHE:HD2	1.86	0.41
45:RO:9:GLU:H	45:RO:83:ALA:HA	1.86	0.41
46:RP:84:ASN:HA	46:RP:115:LEU:O	2.20	0.41
48:RR:98:LEU:O	48:RR:113:LEU:N	2.39	0.41
55:RY:84:ARG:O	55:RY:95:LYS:N	2.46	0.41
1:XA:444:C:H2'	1:XA:445:G:C8	2.56	0.41
1:XA:452:A:O2'	16:XP:72:ARG:NE	2.54	0.41
6:XF:60:PHE:HE2	18:XR:78:LEU:HD21	1.85	0.41
19:XS:10:PHE:CB	19:XS:39:THR:H	2.34	0.41
30:Y4:26:SER:HB2	41:YG:105:LYS:HD3	2.02	0.41
38:YD:39:LYS:NZ	38:YD:87:ASN:OD1	2.37	0.41
40:YF:48:THR:OG1	40:YF:48:THR:O	2.38	0.41
45:YO:63:VAL:HA	45:YO:106:LEU:HD21	2.02	0.41
1:QA:926:G:H22	24:QX:16:A:P	2.43	0.41
7:QG:17:VAL:HG23	7:QG:18:TYR:CD2	2.56	0.41
19:QS:50:ALA:HB1	19:QS:57:HIS:HB3	2.03	0.41
36:RA:1316:U:H2'	36:RA:1317:A:C8	2.56	0.41
36:RA:1689:A:H62	36:RA:1698:A:H2	1.69	0.41
36:RA:2316:C:O5'	41:RG:128:ARG:NH2	2.54	0.41
36:RA:65:C:H1'	36:RA:456:C:H42	1.86	0.41
36:RA:581:C:OP1	51:RU:31:SER:OG	2.39	0.41
1:XA:944:G:N1	1:XA:1338:G:OP2	2.42	0.41
1:XA:198:G:H2'	1:XA:199:G:H8	1.85	0.41
1:XA:591:U:H2'	1:XA:592:G:C8	2.56	0.41
2:XB:95:GLN:HB3	2:XB:96:ARG:H	1.77	0.41
36:YA:1417:C:O2'	36:YA:1587:A:N3	2.46	0.41
36:YA:1918:A:O2'	36:YA:1920:C:N4	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:YA:2656:U:H3	36:YA:2665:A:H2	1.69	0.41
36:YA:458:G:O2'	36:YA:469:G:O6	2.32	0.41
36:YA:1565:C:H5''	38:YD:18:VAL:HG21	2.02	0.41
40:YF:110:LEU:HG	40:YF:202:PHE:HE1	1.86	0.41
41:YG:86:MET:HA	41:YG:87:PRO:HD2	1.94	0.41
1:QA:1054:C:O2'	1:QA:1056:U:OP2	2.38	0.41
1:QA:1129:C:OP1	9:QI:62:TYR:OH	2.30	0.41
1:QA:1412:C:H2'	1:QA:1413:A:C8	2.56	0.41
1:QA:701:C:O2	1:QA:703:G:N1	2.54	0.41
12:QL:105:TYR:HD1	12:QL:105:TYR:HA	1.76	0.41
1:QA:552:U:O2'	12:QL:86:ARG:O	2.38	0.41
14:QN:31:ARG:NH1	14:QN:32:SER:HB2	2.35	0.41
17:QQ:59:ILE:HD12	17:QQ:71:PHE:HD2	1.85	0.41
1:QA:262:A:H5''	20:QT:76:ALA:HB2	2.03	0.41
36:RA:270(V):G:H2'	36:RA:270(W):G:H8	1.86	0.41
50:RT:117:ASP:OD2	50:RT:120:ARG:NE	2.51	0.41
1:XA:501:C:O2	1:XA:549:C:O2'	2.32	0.41
1:XA:842:C:O2'	1:XA:848:C:N4	2.54	0.41
18:XR:79:LEU:HA	18:XR:80:PRO:HD3	1.97	0.41
19:XS:44:MET:N	19:XS:44:MET:SD	2.94	0.41
26:Y0:46:LYS:HD2	26:Y0:78:TYR:CE1	2.56	0.41
26:Y0:70:GLN:OE1	26:Y0:80:HIS:NE2	2.35	0.41
36:YA:2723:C:OP2	39:YE:109:LYS:NZ	2.54	0.41
36:YA:2822:G:OP1	39:YE:159:HIS:NE2	2.54	0.41
36:YA:704:G:H2'	36:YA:726:G:N2	2.36	0.41
36:YA:729:G:H5'	36:YA:730:C:H5''	2.03	0.41
39:YE:101:ARG:NH1	39:YE:171:GLU:HB2	2.36	0.41
47:YQ:116:GLU:O	47:YQ:120:ILE:HG12	2.21	0.41
1:QA:372:C:H42	1:QA:389:A:H62	1.69	0.40
2:QB:175:ARG:O	2:QB:179:LYS:HG2	2.21	0.40
17:QQ:100:LYS:O	17:QQ:101:ARG:NE	2.54	0.40
27:R1:11:ARG:NH2	36:RA:1365:A:O2'	2.54	0.40
36:RA:26:G:H1'	36:RA:515:A:H61	1.86	0.40
36:RA:2723:C:OP1	39:RE:109:LYS:HD3	2.21	0.40
42:RH:71:LEU:O	42:RH:71:LEU:HD23	2.21	0.40
56:RZ:153:SER:H	56:RZ:167:PRO:HB3	1.87	0.40
3:XC:141:VAL:HG11	3:XC:202:ILE:HD12	2.02	0.40
4:XD:82:ALA:HB1	4:XD:92:VAL:HG23	2.04	0.40
13:XM:48:LEU:HD12	13:XM:52:GLU:HG3	2.04	0.40
35:Y9:36:GLN:NE2	36:YA:1124:C:O2	2.53	0.40
36:YA:2572:A:OP1	36:YA:2574:G:O2'	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:YA:307:G:H21	36:YA:330:A:H62	1.68	0.40
45:YO:87:ILE:HD12	45:YO:91:LEU:HA	2.02	0.40
34:Y8:12:LYS:HG2	46:YP:68:GLN:HG2	2.03	0.40
45:YO:78:ARG:NE	50:YT:73:GLU:OE1	2.54	0.40
53:YW:58:ALA:HB1	53:YW:64:MET:HB2	2.03	0.40
8:QH:120:THR:OG1	8:QH:121:ASP:N	2.54	0.40
36:RA:2494:G:H2'	36:RA:2495:G:H8	1.85	0.40
42:RH:109:PHE:CE2	42:RH:152:ARG:HG3	2.55	0.40
1:XA:1342:C:H4'	9:XI:125:TYR:HB3	2.01	0.40
17:XQ:22:LEU:HD11	17:XQ:39:SER:HB2	2.02	0.40
36:YA:2123:G:H2'	36:YA:2124:G:C8	2.57	0.40
36:YA:2315:G:OP1	41:YG:36:LYS:NZ	2.45	0.40
41:YG:38:VAL:HG22	41:YG:93:THR:HG22	2.03	0.40
43:YI:83:ALA:H	43:YI:144:VAL:HG23	1.86	0.40
46:YP:126:VAL:HG22	46:YP:147:LEU:HD22	2.03	0.40
36:YA:662:G:H5''	46:YP:17:LYS:HG2	2.02	0.40
1:QA:939:G:OP1	7:QG:102:ARG:NH1	2.44	0.40
9:QI:17:VAL:HG12	9:QI:63:ILE:HD12	2.02	0.40
36:RA:322:A:H5''	40:RF:169:ASN:ND2	2.33	0.40
36:RA:1820:U:C2	38:RD:202:LYS:HB2	2.57	0.40
36:RA:1490:A:O2'	38:RD:99:ASP:OD1	2.38	0.40
40:RF:11:VAL:HG22	40:RF:125:LEU:HB2	2.02	0.40
40:RF:31:HIS:NE2	40:RF:35:GLU:OE2	2.54	0.40
56:RZ:69:THR:OG1	56:RZ:70:LEU:N	2.55	0.40
56:RZ:70:LEU:HB2	56:RZ:91:LEU:HD11	2.04	0.40
1:XA:1074:G:O2'	1:XA:1101:A:N1	2.48	0.40
1:XA:1238:A:H62	1:XA:1301:U:H3	1.69	0.40
6:XF:97:PHE:HD2	18:XR:31:LEU:HD21	1.86	0.40
12:XL:115:LYS:O	12:XL:117:ARG:N	2.55	0.40
36:YA:1048:A:P	36:YA:1110:G:H22	2.44	0.40
37:YB:91:C:OP1	47:YQ:19:GLY:HA2	2.21	0.40
38:YD:105:ILE:HA	38:YD:105:ILE:HD12	1.92	0.40
44:YN:20:GLY:HA2	44:YN:61:ARG:HD3	2.02	0.40
46:YP:59:LEU:HA	46:YP:61:ARG:HH21	1.85	0.40
50:YT:116:ALA:HB3	50:YT:118:ARG:NH1	2.36	0.40
1:QA:1002:G:H2'	1:QA:1003:G:C8	2.57	0.40
1:QA:1325:C:H4'	21:QU:17:THR:HG21	2.03	0.40
1:QA:489:C:H2'	1:QA:490:G:C8	2.56	0.40
17:QQ:53:LEU:HD23	17:QQ:85:VAL:HG11	2.04	0.40
36:RA:1296:G:OP1	36:RA:2709:G:O2'	2.26	0.40
36:RA:195:A:H61	36:RA:198:C:H3'	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:RD:69:ARG:HH22	38:RD:117:VAL:HG12	1.87	0.40
39:RE:12:THR:OG1	39:RE:13:ARG:N	2.53	0.40
46:RP:95:VAL:HB	46:RP:125:VAL:HG12	2.03	0.40
55:RY:54:LYS:HB3	55:RY:55:TYR:H	1.57	0.40
56:RZ:110:GLY:O	56:RZ:114:GLY:N	2.54	0.40
1:XA:148:G:H2'	1:XA:149:A:H8	1.86	0.40
1:XA:973:G:O4'	10:XJ:55:LYS:HG2	2.21	0.40
10:XJ:23:ILE:HG23	10:XJ:85:LEU:HD21	2.02	0.40
11:XK:82:VAL:HB	11:XK:108:ILE:HD13	2.03	0.40
36:YA:2308:G:H22	36:YA:2311:A:H2	1.70	0.40
36:YA:355:G:H2'	36:YA:356:G:H8	1.87	0.40
42:YH:18:GLU:HB3	42:YH:25:LYS:HB2	2.03	0.40
1:QA:7:G:H21	5:QE:121:LYS:HG2	1.87	0.40
36:RA:270(I):G:H1	36:RA:270(Q):C:H42	1.68	0.40
25:QY:56:C:N4	36:RA:881:G:H21	2.20	0.40
38:RD:31:LYS:HA	38:RD:31:LYS:HD2	1.94	0.40
51:RU:58:ARG:HA	51:RU:61:TRP:HB2	2.04	0.40
51:RU:92:ARG:HB3	52:RV:11:GLN:NE2	2.37	0.40
52:RV:32:THR:OG1	52:RV:59:ALA:O	2.34	0.40
1:XA:1396:A:H2	5:XE:19:MET:HG3	1.87	0.40
1:XA:198:G:H2'	1:XA:199:G:C8	2.56	0.40
4:XD:59:ARG:O	4:XD:63:LYS:N	2.52	0.40
34:Y8:26:LYS:HD2	34:Y8:47:LYS:HD3	2.02	0.40
36:YA:1382:G:O3'	36:YA:1573:G:N2	2.54	0.40
26:Y0:75:LEU:HD21	36:YA:2334:G:C6	2.56	0.40
45:Y0:120:GLU:OE1	50:YT:67:SER:OG	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	235/256 (92%)	206 (88%)	26 (11%)	3 (1%)	12	47
2	XB	235/256 (92%)	205 (87%)	29 (12%)	1 (0%)	34	69
3	QC	203/239 (85%)	182 (90%)	20 (10%)	1 (0%)	29	67
3	XC	203/239 (85%)	187 (92%)	15 (7%)	1 (0%)	29	67
4	QD	206/209 (99%)	201 (98%)	4 (2%)	1 (0%)	29	67
4	XD	206/209 (99%)	200 (97%)	5 (2%)	1 (0%)	29	67
5	QE	149/162 (92%)	141 (95%)	8 (5%)	0	100	100
5	XE	149/162 (92%)	139 (93%)	8 (5%)	2 (1%)	12	47
6	QF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
6	XF	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
7	QG	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
7	XG	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
8	QH	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
8	XH	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
9	QI	125/128 (98%)	115 (92%)	10 (8%)	0	100	100
9	XI	125/128 (98%)	112 (90%)	13 (10%)	0	100	100
10	QJ	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
10	XJ	97/105 (92%)	82 (84%)	15 (16%)	0	100	100
11	QK	117/129 (91%)	106 (91%)	11 (9%)	0	100	100
11	XK	117/129 (91%)	105 (90%)	12 (10%)	0	100	100
12	QL	123/131 (94%)	109 (89%)	13 (11%)	1 (1%)	19	58
12	XL	123/131 (94%)	107 (87%)	13 (11%)	3 (2%)	6	34
13	QM	119/126 (94%)	100 (84%)	16 (13%)	3 (2%)	5	32
13	XM	119/126 (94%)	98 (82%)	21 (18%)	0	100	100
14	QN	58/61 (95%)	52 (90%)	5 (9%)	1 (2%)	9	42
14	XN	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	9	42
15	QO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
15	XO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	QP	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
16	XP	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
17	QQ	98/105 (93%)	94 (96%)	4 (4%)	0	100	100
17	XQ	98/105 (93%)	95 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	QR	68/88 (77%)	67 (98%)	1 (2%)	0	100	100
18	XR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
19	QS	82/93 (88%)	69 (84%)	13 (16%)	0	100	100
19	XS	82/93 (88%)	69 (84%)	12 (15%)	1 (1%)	13	49
20	QT	97/106 (92%)	87 (90%)	10 (10%)	0	100	100
20	XT	97/106 (92%)	89 (92%)	6 (6%)	2 (2%)	7	37
21	QU	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
21	XU	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
26	R0	80/85 (94%)	74 (92%)	6 (8%)	0	100	100
26	Y0	80/85 (94%)	76 (95%)	4 (5%)	0	100	100
27	R1	95/98 (97%)	84 (88%)	9 (10%)	2 (2%)	7	37
27	Y1	95/98 (97%)	83 (87%)	10 (10%)	2 (2%)	7	37
28	R2	67/72 (93%)	62 (92%)	4 (6%)	1 (2%)	10	44
28	Y2	67/72 (93%)	61 (91%)	5 (8%)	1 (2%)	10	44
29	R3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
29	Y3	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
30	R4	69/71 (97%)	45 (65%)	21 (30%)	3 (4%)	2	20
30	Y4	69/71 (97%)	47 (68%)	21 (30%)	1 (1%)	11	46
31	R5	57/60 (95%)	49 (86%)	8 (14%)	0	100	100
31	Y5	57/60 (95%)	49 (86%)	8 (14%)	0	100	100
32	R6	47/54 (87%)	24 (51%)	20 (43%)	3 (6%)	1	10
32	Y6	47/54 (87%)	31 (66%)	16 (34%)	0	100	100
33	R7	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
33	Y7	47/49 (96%)	44 (94%)	2 (4%)	1 (2%)	7	37
34	R8	62/65 (95%)	51 (82%)	11 (18%)	0	100	100
34	Y8	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	4	26
35	R9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
35	Y9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
38	RD	270/276 (98%)	248 (92%)	20 (7%)	2 (1%)	22	61
38	YD	270/276 (98%)	244 (90%)	24 (9%)	2 (1%)	22	61
39	RE	203/206 (98%)	172 (85%)	28 (14%)	3 (2%)	10	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	YE	203/206 (98%)	174 (86%)	21 (10%)	8 (4%)	3	22
40	RF	200/210 (95%)	188 (94%)	11 (6%)	1 (0%)	29	67
40	YF	200/210 (95%)	184 (92%)	14 (7%)	2 (1%)	15	54
41	RG	179/182 (98%)	159 (89%)	20 (11%)	0	100	100
41	YG	179/182 (98%)	165 (92%)	14 (8%)	0	100	100
42	RH	168/180 (93%)	141 (84%)	26 (16%)	1 (1%)	25	64
42	YH	168/180 (93%)	141 (84%)	25 (15%)	2 (1%)	13	49
43	RI	144/148 (97%)	126 (88%)	16 (11%)	2 (1%)	11	46
43	YI	144/148 (97%)	125 (87%)	15 (10%)	4 (3%)	5	29
44	RN	136/140 (97%)	121 (89%)	15 (11%)	0	100	100
44	YN	136/140 (97%)	121 (89%)	15 (11%)	0	100	100
45	RO	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
45	YO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
46	RP	148/150 (99%)	125 (84%)	23 (16%)	0	100	100
46	YP	148/150 (99%)	126 (85%)	20 (14%)	2 (1%)	11	46
47	RQ	139/141 (99%)	117 (84%)	22 (16%)	0	100	100
47	YQ	139/141 (99%)	118 (85%)	19 (14%)	2 (1%)	11	46
48	RR	116/118 (98%)	107 (92%)	7 (6%)	2 (2%)	9	42
48	YR	116/118 (98%)	109 (94%)	5 (4%)	2 (2%)	9	42
49	RS	109/112 (97%)	94 (86%)	15 (14%)	0	100	100
49	YS	109/112 (97%)	91 (84%)	17 (16%)	1 (1%)	17	56
50	RT	135/146 (92%)	118 (87%)	17 (13%)	0	100	100
50	YT	135/146 (92%)	120 (89%)	15 (11%)	0	100	100
51	RU	115/118 (98%)	108 (94%)	6 (5%)	1 (1%)	17	56
51	YU	115/118 (98%)	107 (93%)	6 (5%)	2 (2%)	9	42
52	RV	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
52	YV	99/101 (98%)	84 (85%)	14 (14%)	1 (1%)	15	54
53	RW	111/113 (98%)	102 (92%)	9 (8%)	0	100	100
53	YW	111/113 (98%)	104 (94%)	7 (6%)	0	100	100
54	RX	90/96 (94%)	84 (93%)	6 (7%)	0	100	100
54	YX	90/96 (94%)	89 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	RY	100/110 (91%)	71 (71%)	24 (24%)	5 (5%)	2	16
55	YY	100/110 (91%)	73 (73%)	22 (22%)	5 (5%)	2	16
56	RZ	181/206 (88%)	150 (83%)	29 (16%)	2 (1%)	14	51
56	YZ	181/206 (88%)	154 (85%)	23 (13%)	4 (2%)	6	35
All	All	11470/12126 (95%)	10262 (90%)	1114 (10%)	94 (1%)	19	58

All (94) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	QD	5	ILE
30	R4	24	THR
30	R4	43	TYR
32	R6	8	LYS
32	R6	30	THR
38	RD	34	VAL
38	RD	35	LYS
39	RE	72	VAL
48	RR	4	LEU
55	RY	54	LYS
56	RZ	53	ILE
4	XD	5	ILE
20	XT	74	LYS
30	Y4	24	THR
38	YD	35	LYS
43	YI	133	HIS
46	YP	108	LYS
48	YR	4	LEU
51	YU	93	LYS
55	YY	5	MET
55	YY	57	GLN
56	YZ	53	ILE
13	QM	83	ASP
27	R1	92	LYS
48	RR	3	HIS
51	RU	92	ARG
55	RY	57	GLN
3	XC	12	LEU
12	XL	105	TYR
12	XL	116	SER
20	XT	75	ASN
27	Y1	92	LYS

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Mol	Chain	Res	Type
34	Y8	63	PRO
39	YE	83	ASP
42	YH	128	PRO
43	YI	12	LEU
48	YR	3	HIS
49	YS	62	LYS
2	QB	208	ILE
12	QL	105	TYR
14	QN	17	LYS
39	RE	54	GLN
42	RH	128	PRO
55	RY	53	PRO
55	RY	56	PRO
12	XL	115	LYS
14	XN	17	LYS
38	YD	36	PRO
39	YE	79	ARG
39	YE	129	HIS
39	YE	132	HIS
47	YQ	78	PRO
55	YY	56	PRO
56	YZ	59	LEU
56	YZ	63	ASP
56	YZ	152	ALA
2	QB	22	LYS
3	QC	190	ARG
13	QM	12	ASN
43	RI	119	PRO
5	XE	73	ASN
19	XS	10	PHE
27	Y1	91	LYS
28	Y2	71	ASN
39	YE	63	LEU
40	YF	67	GLN
43	YI	134	PRO
46	YP	107	LYS
51	YU	92	ARG
13	QM	120	LYS
27	R1	91	LYS
28	R2	70	GLN
39	RE	83	ASP
33	Y7	48	LYS

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Mol	Chain	Res	Type
39	YE	72	VAL
39	YE	82	ARG
39	YE	144	ARG
42	YH	8	PRO
43	RI	132	PRO
5	XE	74	GLY
40	YF	129	PHE
43	YI	10	GLU
30	R4	40	HIS
55	RY	58	GLY
2	XB	208	ILE
55	YY	55	TYR
34	Y8	62	LEU
52	YV	50	PRO
55	YY	58	GLY
2	QB	232	PRO
32	R6	7	ILE
40	RF	134	GLY
56	RZ	94	GLU
47	YQ	19	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	205/220 (93%)	200 (98%)	5 (2%)	49	77
2	XB	205/220 (93%)	204 (100%)	1 (0%)	88	95
3	QC	159/188 (85%)	156 (98%)	3 (2%)	57	81
3	XC	159/188 (85%)	159 (100%)	0	100	100
4	QD	173/181 (96%)	173 (100%)	0	100	100
4	XD	173/181 (96%)	170 (98%)	3 (2%)	60	83
5	QE	116/123 (94%)	116 (100%)	0	100	100
5	XE	116/123 (94%)	116 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	QF	90/90 (100%)	89 (99%)	1 (1%)	73	88
6	XF	90/90 (100%)	90 (100%)	0	100	100
7	QG	126/127 (99%)	126 (100%)	0	100	100
7	XG	126/127 (99%)	125 (99%)	1 (1%)	81	93
8	QH	119/119 (100%)	119 (100%)	0	100	100
8	XH	119/119 (100%)	119 (100%)	0	100	100
9	QI	98/99 (99%)	96 (98%)	2 (2%)	55	80
9	XI	98/99 (99%)	96 (98%)	2 (2%)	55	80
10	QJ	89/92 (97%)	88 (99%)	1 (1%)	73	88
10	XJ	89/92 (97%)	89 (100%)	0	100	100
11	QK	90/99 (91%)	90 (100%)	0	100	100
11	XK	90/99 (91%)	88 (98%)	2 (2%)	52	79
12	QL	104/108 (96%)	104 (100%)	0	100	100
12	XL	104/108 (96%)	103 (99%)	1 (1%)	76	90
13	QM	97/101 (96%)	96 (99%)	1 (1%)	76	90
13	XM	97/101 (96%)	94 (97%)	3 (3%)	40	72
14	QN	49/50 (98%)	46 (94%)	3 (6%)	18	54
14	XN	49/50 (98%)	49 (100%)	0	100	100
15	QO	79/80 (99%)	77 (98%)	2 (2%)	47	77
15	XO	79/80 (99%)	78 (99%)	1 (1%)	69	87
16	QP	72/74 (97%)	72 (100%)	0	100	100
16	XP	72/74 (97%)	71 (99%)	1 (1%)	67	86
17	QQ	95/97 (98%)	93 (98%)	2 (2%)	53	79
17	XQ	95/97 (98%)	95 (100%)	0	100	100
18	QR	61/77 (79%)	61 (100%)	0	100	100
18	XR	61/77 (79%)	60 (98%)	1 (2%)	62	84
19	QS	73/80 (91%)	73 (100%)	0	100	100
19	XS	73/80 (91%)	73 (100%)	0	100	100
20	QT	76/82 (93%)	75 (99%)	1 (1%)	69	87
20	XT	76/82 (93%)	76 (100%)	0	100	100
21	QU	20/22 (91%)	20 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	XU	20/22 (91%)	20 (100%)	0	100	100
26	R0	65/67 (97%)	65 (100%)	0	100	100
26	Y0	65/67 (97%)	62 (95%)	3 (5%)	27	63
27	R1	82/83 (99%)	82 (100%)	0	100	100
27	Y1	82/83 (99%)	80 (98%)	2 (2%)	49	77
28	R2	64/67 (96%)	62 (97%)	2 (3%)	40	72
28	Y2	64/67 (96%)	64 (100%)	0	100	100
29	R3	51/52 (98%)	51 (100%)	0	100	100
29	Y3	51/52 (98%)	51 (100%)	0	100	100
30	R4	63/63 (100%)	61 (97%)	2 (3%)	39	71
30	Y4	63/63 (100%)	62 (98%)	1 (2%)	62	84
31	R5	51/52 (98%)	50 (98%)	1 (2%)	55	80
31	Y5	51/52 (98%)	50 (98%)	1 (2%)	55	80
32	R6	48/52 (92%)	47 (98%)	1 (2%)	53	79
32	Y6	48/52 (92%)	48 (100%)	0	100	100
33	R7	42/42 (100%)	42 (100%)	0	100	100
33	Y7	42/42 (100%)	42 (100%)	0	100	100
34	R8	54/55 (98%)	54 (100%)	0	100	100
34	Y8	54/55 (98%)	54 (100%)	0	100	100
35	R9	34/34 (100%)	32 (94%)	2 (6%)	19	54
35	Y9	34/34 (100%)	34 (100%)	0	100	100
38	RD	214/218 (98%)	213 (100%)	1 (0%)	88	95
38	YD	214/218 (98%)	210 (98%)	4 (2%)	57	81
39	RE	165/166 (99%)	164 (99%)	1 (1%)	86	94
39	YE	165/166 (99%)	165 (100%)	0	100	100
40	RF	161/166 (97%)	160 (99%)	1 (1%)	86	94
40	YF	161/166 (97%)	161 (100%)	0	100	100
41	RG	155/156 (99%)	152 (98%)	3 (2%)	57	81
41	YG	155/156 (99%)	154 (99%)	1 (1%)	86	94
42	RH	142/148 (96%)	140 (99%)	2 (1%)	67	86
42	YH	142/148 (96%)	137 (96%)	5 (4%)	36	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	RI	122/124 (98%)	121 (99%)	1 (1%)	81	93
43	YI	122/124 (98%)	122 (100%)	0	100	100
44	RN	117/119 (98%)	116 (99%)	1 (1%)	78	91
44	YN	117/119 (98%)	115 (98%)	2 (2%)	60	83
45	RO	100/100 (100%)	97 (97%)	3 (3%)	41	73
45	YO	100/100 (100%)	99 (99%)	1 (1%)	76	90
46	RP	116/116 (100%)	115 (99%)	1 (1%)	78	91
46	YP	116/116 (100%)	114 (98%)	2 (2%)	60	83
47	RQ	111/111 (100%)	108 (97%)	3 (3%)	44	75
47	YQ	111/111 (100%)	109 (98%)	2 (2%)	59	82
48	RR	101/101 (100%)	101 (100%)	0	100	100
48	YR	101/101 (100%)	101 (100%)	0	100	100
49	RS	87/88 (99%)	84 (97%)	3 (3%)	37	70
49	YS	87/88 (99%)	85 (98%)	2 (2%)	50	78
50	RT	120/127 (94%)	115 (96%)	5 (4%)	30	65
50	YT	120/127 (94%)	119 (99%)	1 (1%)	81	93
51	RU	93/94 (99%)	92 (99%)	1 (1%)	73	88
51	YU	93/94 (99%)	89 (96%)	4 (4%)	29	64
52	RV	82/82 (100%)	82 (100%)	0	100	100
52	YV	82/82 (100%)	81 (99%)	1 (1%)	71	88
53	RW	92/92 (100%)	91 (99%)	1 (1%)	73	88
53	YW	92/92 (100%)	92 (100%)	0	100	100
54	RX	74/78 (95%)	73 (99%)	1 (1%)	67	86
54	YX	74/78 (95%)	74 (100%)	0	100	100
55	RY	85/91 (93%)	83 (98%)	2 (2%)	49	77
55	YY	85/91 (93%)	84 (99%)	1 (1%)	71	88
56	RZ	162/179 (90%)	160 (99%)	2 (1%)	71	88
56	YZ	162/179 (90%)	159 (98%)	3 (2%)	57	81
All	All	9688/10064 (96%)	9575 (99%)	113 (1%)	71	88

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	QB	30	ARG
2	QB	53	ARG
2	QB	94	ASN
2	QB	152	PHE
2	QB	226	ARG
3	QC	21	ARG
3	QC	190	ARG
3	QC	193	TYR
6	QF	59	TYR
9	QI	88	TYR
9	QI	121	ARG
10	QJ	54	PHE
13	QM	77	ASN
14	QN	4	LYS
14	QN	31	ARG
14	QN	41	ARG
15	QO	77	ARG
15	QO	79	ARG
17	QQ	87	LYS
17	QQ	91	ARG
20	QT	86	ARG
28	R2	15	LYS
28	R2	65	ASN
30	R4	61	ARG
30	R4	69	LYS
31	R5	56	LYS
32	R6	18	ARG
35	R9	29	ASN
35	R9	35	ARG
38	RD	242	ARG
39	RE	152	LYS
40	RF	44	ARG
41	RG	91	ARG
41	RG	98	ARG
41	RG	153	ARG
42	RH	6	ARG
42	RH	23	ARG
43	RI	77	LEU
44	RN	39	ARG
45	RO	64	ARG
45	RO	97	ARG
45	RO	104	ARG
46	RP	61	ARG

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Mol	Chain	Res	Type
47	RQ	60	ARG
47	RQ	124	LYS
47	RQ	134	ARG
49	RS	3	ARG
49	RS	25	ARG
49	RS	112	PHE
50	RT	45	PHE
50	RT	105	LEU
50	RT	112	ARG
50	RT	115	ARG
50	RT	118	ARG
51	RU	79	PHE
53	RW	92	ARG
54	RX	65	ARG
55	RY	81	LYS
55	RY	97	ARG
56	RZ	122	ARG
56	RZ	131	ARG
2	XB	53	ARG
4	XD	31	CYS
4	XD	59	ARG
4	XD	209	ARG
7	XG	94	ARG
9	XI	9	ARG
9	XI	121	ARG
11	XK	51	LYS
11	XK	126	ARG
12	XL	98	TYR
13	XM	40	ASN
13	XM	87	TYR
13	XM	122	LYS
15	XO	65	ARG
16	XP	5	ARG
18	XR	88	LYS
26	Y0	14	ARG
26	Y0	24	LYS
26	Y0	74	ARG
27	Y1	3	LYS
27	Y1	80	LEU
30	Y4	55	ARG
31	Y5	59	GLU
38	YD	33	LEU

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Mol	Chain	Res	Type
38	YD	34	VAL
38	YD	43	ARG
38	YD	99	ASP
41	YG	98	ARG
42	YH	4	ILE
42	YH	8	PRO
42	YH	23	ARG
42	YH	27	LYS
42	YH	59	ARG
44	YN	39	ARG
44	YN	134	ARG
45	YO	78	ARG
46	YP	61	ARG
46	YP	79	ARG
47	YQ	5	ARG
47	YQ	59	ARG
49	YS	87	PHE
49	YS	112	PHE
50	YT	99	LEU
51	YU	52	ARG
51	YU	76	TYR
51	YU	79	PHE
51	YU	94	ASN
52	YV	19	LYS
55	YY	50	ARG
56	YZ	34	ASN
56	YZ	80	ARG
56	YZ	81	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
2	QB	76	GLN
4	QD	119	GLN
4	QD	201	GLN
7	QG	28	ASN
7	QG	68	ASN
9	QI	124	GLN
35	R9	29	ASN
39	RE	135	HIS
39	RE	137	HIS
39	RE	180	ASN

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Mol	Chain	Res	Type
40	RF	40	GLN
40	RF	169	ASN
50	RT	79	HIS
52	RV	11	GLN
52	RV	87	HIS
54	RX	41	ASN
54	RX	55	ASN
4	XD	119	GLN
6	XF	7	ASN
7	XG	68	ASN
9	XI	3	GLN
9	XI	73	GLN
9	XI	124	GLN
10	XJ	78	ASN
10	XJ	84	GLN
11	XK	26	ASN
13	XM	40	ASN
15	XO	37	ASN
34	Y8	31	HIS
38	YD	227	ASN
39	YE	55	ASN
39	YE	137	HIS
41	YG	58	GLN
42	YH	147	ASN
45	YO	3	GLN
45	YO	29	ASN
49	YS	34	HIS
53	YW	34	ASN
53	YW	61	ASN
56	YZ	55	HIS
56	YZ	121	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1522 (98%)	274 (18%)	34 (2%)
1	XA	1498/1522 (98%)	285 (19%)	30 (2%)
22	QV	76/77 (98%)	15 (19%)	0
22	XV	76/77 (98%)	11 (14%)	0
23	QW	75/76 (98%)	24 (32%)	1 (1%)
23	XW	75/76 (98%)	38 (50%)	2 (2%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	QX	18/19 (94%)	8 (44%)	1 (5%)
24	XX	16/19 (84%)	7 (43%)	1 (6%)
25	QY	74/76 (97%)	28 (37%)	0
25	XY	75/76 (98%)	31 (41%)	0
36	RA	2879/2915 (98%)	607 (21%)	47 (1%)
36	YA	2880/2915 (98%)	578 (20%)	44 (1%)
37	RB	119/122 (97%)	24 (20%)	1 (0%)
37	YB	119/122 (97%)	20 (16%)	1 (0%)
All	All	9478/9614 (98%)	1950 (20%)	162 (1%)

All (1950) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	22	G
1	QA	32	A
1	QA	39	G
1	QA	47	C
1	QA	48	C
1	QA	50	A
1	QA	51	A
1	QA	64	G
1	QA	65	U
1	QA	66	G
1	QA	76	G
1	QA	82	U
1	QA	90	C
1	QA	91	C
1	QA	101	A
1	QA	108	G
1	QA	116	A
1	QA	121	C
1	QA	144	G
1	QA	163	C
1	QA	169	C
1	QA	173	U
1	QA	174	C
1	QA	182	U
1	QA	191(A)	G
1	QA	195	A
1	QA	209	U
1	QA	216	G

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Mol	Chain	Res	Type
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	321	A
1	QA	328	C
1	QA	329	A
1	QA	332	G
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	358	U
1	QA	367	U
1	QA	372	C
1	QA	373	A
1	QA	384	G
1	QA	390	C
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	421	U
1	QA	422	C
1	QA	423	G
1	QA	427	U
1	QA	429	U
1	QA	451	A
1	QA	466	C
1	QA	467	G
1	QA	485	G

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Mol	Chain	Res	Type
1	QA	486	U
1	QA	496	A
1	QA	497	U
1	QA	505	G
1	QA	509	A
1	QA	510	A
1	QA	511	C
1	QA	518	C
1	QA	521	G
1	QA	527	G
1	QA	531	U
1	QA	532	A
1	QA	533	A
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	576	G
1	QA	577	G
1	QA	579	G
1	QA	587	G
1	QA	596	C
1	QA	607	A
1	QA	618	C
1	QA	630	G
1	QA	631	G
1	QA	652	U
1	QA	653	A
1	QA	665	A
1	QA	686	U
1	QA	688	G
1	QA	693	G
1	QA	701	C
1	QA	702	A
1	QA	703	G
1	QA	704	A
1	QA	718	G
1	QA	723	U
1	QA	731	G
1	QA	748	C

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Mol	Chain	Res	Type
1	QA	754	C
1	QA	755	G
1	QA	773	G
1	QA	777	A
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
1	QA	841	U
1	QA	843	U
1	QA	848	C
1	QA	859	A
1	QA	871	U
1	QA	872	A
1	QA	873	A
1	QA	885	G
1	QA	889	A
1	QA	902	G
1	QA	914	A
1	QA	916	G
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	974	A
1	QA	975	A
1	QA	976	G
1	QA	977	A
1	QA	978	A
1	QA	980	C
1	QA	981	U
1	QA	982	U
1	QA	986	A
1	QA	991	U
1	QA	992	U

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Mol	Chain	Res	Type
1	QA	993	G
1	QA	994	A
1	QA	1001	G
1	QA	1003	G
1	QA	1004	A
1	QA	1006	C
1	QA	1009	G
1	QA	1020	U
1	QA	1024	G
1	QA	1025	U
1	QA	1026	G
1	QA	1028	C
1	QA	1029	G
1	QA	1030	C
1	QA	1032(A)	G
1	QA	1036	G
1	QA	1040	U
1	QA	1049	U
1	QA	1053	G
1	QA	1054	C
1	QA	1055	A
1	QA	1064	G
1	QA	1065	U
1	QA	1066	C
1	QA	1081	G
1	QA	1094	G
1	QA	1095	U
1	QA	1101	A
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

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Mol	Chain	Res	Type
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	1214	C
1	QA	1224	G
1	QA	1225	A
1	QA	1238	A
1	QA	1240	U
1	QA	1241	G
1	QA	1256	A
1	QA	1257	U
1	QA	1258	G
1	QA	1260	C
1	QA	1270	C
1	QA	1280	A
1	QA	1281	U
1	QA	1285	A
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	1301	U
1	QA	1302	U
1	QA	1303	C
1	QA	1305	G
1	QA	1317	C
1	QA	1318	A
1	QA	1319	A
1	QA	1321	C
1	QA	1322	C

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Mol	Chain	Res	Type
1	QA	1323	G
1	QA	1326	C
1	QA	1329	A
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	1364	U
1	QA	1370	G
1	QA	1397	C
1	QA	1398	A
1	QA	1402	C
1	QA	1419	G
1	QA	1442	G
1	QA	1443	G
1	QA	1452	C
1	QA	1453	G
1	QA	1454	G
1	QA	1487	G
1	QA	1492	A
1	QA	1499	A
1	QA	1503	A
1	QA	1504	G
1	QA	1505	G
1	QA	1506	U
1	QA	1517	G
1	QA	1519	A
1	QA	1520	G
1	QA	1529	G
1	QA	1530	G
22	QV	2	G
22	QV	13	C
22	QV	16	C
22	QV	17	C
22	QV	17(A)	U
22	QV	18	G
22	QV	19	G

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Mol	Chain	Res	Type
22	QV	20	U
22	QV	21	A
22	QV	29	G
22	QV	47	U
22	QV	48	C
22	QV	49	G
22	QV	65	C
22	QV	76	A
23	QW	8	U
23	QW	9	A
23	QW	13	C
23	QW	14	A
23	QW	15	G
23	QW	17	A
23	QW	19	G
23	QW	20	G
23	QW	21	A
23	QW	33	U
23	QW	34	G
23	QW	38	A
23	QW	39	G
23	QW	40	C
23	QW	45	G
23	QW	46	G
23	QW	48	C
23	QW	49	A
23	QW	52	G
23	QW	56	C
23	QW	57	G
23	QW	59	U
23	QW	61	C
23	QW	70	U
24	QX	7	G
24	QX	10	G
24	QX	11	U
24	QX	13	A
24	QX	14	A
24	QX	19	G
24	QX	23	A
24	QX	24	A
25	QY	8	U
25	QY	12	U

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Mol	Chain	Res	Type
25	QY	13	C
25	QY	15	G
25	QY	16	C
25	QY	17	U
25	QY	18	G
25	QY	19	G
25	QY	21	A
25	QY	23	A
25	QY	30	G
25	QY	37	A
25	QY	40	C
25	QY	43	G
25	QY	46	G
25	QY	47	U
25	QY	48	C
25	QY	55	U
25	QY	56	C
25	QY	57	G
25	QY	58	A
25	QY	59	U
25	QY	63	G
25	QY	70	U
25	QY	71	C
25	QY	72	C
25	QY	74	C
25	QY	75	C
36	RA	14	A
36	RA	15	G
36	RA	27	G
36	RA	34	C
36	RA	35	G
36	RA	46	C
36	RA	51	G
36	RA	55	G
36	RA	61	G
36	RA	71	A
36	RA	74	A
36	RA	75	G
36	RA	82	G
36	RA	83	G
36	RA	101	G
36	RA	102	G

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Mol	Chain	Res	Type
36	RA	103	A
36	RA	114	U
36	RA	118	A
36	RA	120	U
36	RA	125	G
36	RA	131	G
36	RA	196	A
36	RA	199	A
36	RA	201	C
36	RA	206	U
36	RA	216	A
36	RA	221	A
36	RA	222	A
36	RA	223	A
36	RA	228	A
36	RA	229	A
36	RA	230	U
36	RA	232	G
36	RA	233	A
36	RA	248	G
36	RA	249	C
36	RA	252	G
36	RA	265	A
36	RA	266	G
36	RA	269	U
36	RA	270(L)	U
36	RA	270(M)	U
36	RA	270(N)	G
36	RA	270(P)	C
36	RA	271(C)	U
36	RA	271	G
36	RA	273(F)	C
36	RA	275	G
36	RA	276	A
36	RA	277	C
36	RA	285	C
36	RA	299	A
36	RA	306	U
36	RA	311	A
36	RA	322	A
36	RA	323	G
36	RA	324	A

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Mol	Chain	Res	Type
36	RA	329	G
36	RA	330	A
36	RA	338	G
36	RA	346	A
36	RA	352	G
36	RA	363(E)	U
36	RA	364	C
36	RA	371	A
36	RA	372	G
36	RA	373	U
36	RA	386	G
36	RA	395	U
36	RA	405	U
36	RA	411	G
36	RA	412	A
36	RA	428	A
36	RA	444	C
36	RA	448	U
36	RA	455	C
36	RA	457	A
36	RA	458	G
36	RA	467	G
36	RA	470	A
36	RA	481	G
36	RA	501	A
36	RA	504	U
36	RA	505	A
36	RA	508	G
36	RA	509	C
36	RA	512	G
36	RA	513	A
36	RA	527	C
36	RA	529	A
36	RA	531	C
36	RA	532	A
36	RA	533	G
36	RA	537	C
36	RA	539	G
36	RA	540	G
36	RA	546	C
36	RA	547	A
36	RA	549	G

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Mol	Chain	Res	Type
36	RA	556	G
36	RA	563	G
36	RA	573	G
36	RA	574	C
36	RA	575	A
36	RA	583	G
36	RA	587	C
36	RA	603	A
36	RA	606	U
36	RA	607	U
36	RA	614	U
36	RA	615	G
36	RA	617	G
36	RA	621	A
36	RA	622	G
36	RA	626	U
36	RA	627	A
36	RA	631	A
36	RA	634	C
36	RA	637	A
36	RA	638	G
36	RA	645	C
36	RA	646	A
36	RA	651	G
36	RA	652	C
36	RA	654	A
36	RA	654(A)	G
36	RA	669	G
36	RA	686	G
36	RA	702	G
36	RA	705	A
36	RA	717	G
36	RA	722	A
36	RA	730	C
36	RA	753	C
36	RA	762	U
36	RA	764	A
36	RA	765	G
36	RA	776	G
36	RA	782	A
36	RA	784	A
36	RA	785	G

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Mol	Chain	Res	Type
36	RA	790	C
36	RA	792	G
36	RA	800	A
36	RA	805	G
36	RA	812	C
36	RA	819	A
36	RA	827	U
36	RA	828	U
36	RA	831	G
36	RA	847	U
36	RA	856	C
36	RA	857	C
36	RA	859	G
36	RA	860	U
36	RA	863	A
36	RA	866	A
36	RA	869	G
36	RA	880	G
36	RA	881	G
36	RA	882	G
36	RA	884	C
36	RA	885	C
36	RA	886	C
36	RA	888	C
36	RA	889	C
36	RA	896	A
36	RA	898	C
36	RA	900	A
36	RA	901	A
36	RA	906	G
36	RA	907	U
36	RA	910	A
36	RA	915	C
36	RA	917	A
36	RA	918	A
36	RA	932	G
36	RA	938	G
36	RA	941	A
36	RA	945	A
36	RA	946	G
36	RA	953	A
36	RA	958	U

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Mol	Chain	Res	Type
36	RA	959	A
36	RA	961	C
36	RA	973	A
36	RA	974	G
36	RA	974(A)	C
36	RA	980	A
36	RA	983	A
36	RA	989	G
36	RA	996	A
36	RA	1003	G
36	RA	1008	C
36	RA	1011	G
36	RA	1012	U
36	RA	1013	C
36	RA	1015	G
36	RA	1020	A
36	RA	1022	G
36	RA	1023	U
36	RA	1024	G
36	RA	1026	U
36	RA	1027	A
36	RA	1033	U
36	RA	1036	G
36	RA	1039	G
36	RA	1044	G
36	RA	1045	A
36	RA	1046	A
36	RA	1047	G
36	RA	1049	C
36	RA	1050	A
36	RA	1053	C
36	RA	1054	A
36	RA	1057	A
36	RA	1059	G
36	RA	1060	U
36	RA	1061	U
36	RA	1065	U
36	RA	1066	U
36	RA	1067	A
36	RA	1068	G
36	RA	1069	A
36	RA	1071	G

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Mol	Chain	Res	Type
36	RA	1074	G
36	RA	1076	C
36	RA	1077	A
36	RA	1078	U
36	RA	1079	C
36	RA	1082	U
36	RA	1083	U
36	RA	1084	A
36	RA	1085	A
36	RA	1086	A
36	RA	1088	A
36	RA	1091	G
36	RA	1093	G
36	RA	1095	A
36	RA	1096	A
36	RA	1097	U
36	RA	1104	C
36	RA	1105	U
36	RA	1110	G
36	RA	1111	A
36	RA	1122	G
36	RA	1129	A
36	RA	1130	U
36	RA	1131	G
36	RA	1135	C
36	RA	1136	G
36	RA	1139	G
36	RA	1140	C
36	RA	1141	U
36	RA	1142	U
36	RA	1142(A)	A
36	RA	1143	A
36	RA	1151	G
36	RA	1154	G
36	RA	1155	A
36	RA	1156	A
36	RA	1170	G
36	RA	1173	G
36	RA	1174	A
36	RA	1175	U
36	RA	1176	G
36	RA	1179	C

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Mol	Chain	Res	Type
36	RA	1192	G
36	RA	1195	G
36	RA	1204	A
36	RA	1205	U
36	RA	1206	G
36	RA	1210	A
36	RA	1211	U
36	RA	1220	A
36	RA	1236	G
36	RA	1238	G
36	RA	1252	G
36	RA	1253	A
36	RA	1256	G
36	RA	1265	A
36	RA	1271	G
36	RA	1272	A
36	RA	1273	U
36	RA	1300	U
36	RA	1301	A
36	RA	1313	U
36	RA	1314	C
36	RA	1321	A
36	RA	1329	U
36	RA	1330	C
36	RA	1341	U
36	RA	1349	A
36	RA	1352	U
36	RA	1365	A
36	RA	1368	G
36	RA	1378	A
36	RA	1379	A
36	RA	1384	A
36	RA	1385	G
36	RA	1391	U
36	RA	1395	A
36	RA	1407	C
36	RA	1411	C
36	RA	1416	G
36	RA	1419	A
36	RA	1420	U
36	RA	1421	G
36	RA	1427	A

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Mol	Chain	Res	Type
36	RA	1428	C
36	RA	1444(A)	A
36	RA	1445	C
36	RA	1449	A
36	RA	1449(A)	G
36	RA	1455	G
36	RA	1458	C
36	RA	1460	A
36	RA	1461	G
36	RA	1467	C
36	RA	1471	A
36	RA	1482	U
36	RA	1483	G
36	RA	1486	A
36	RA	1490	A
36	RA	1491	G
36	RA	1493	C
36	RA	1494	A
36	RA	1497	U
36	RA	1506	C
36	RA	1507	A
36	RA	1508	A
36	RA	1510	A
36	RA	1511	A
36	RA	1514	U
36	RA	1522	G
36	RA	1533	C
36	RA	1535	U
36	RA	1536	A
36	RA	1537	C
36	RA	1538	G
36	RA	1543	A
36	RA	1544	C
36	RA	1545	A
36	RA	1558	A
36	RA	1559	G
36	RA	1566	A
36	RA	1569	A
36	RA	1578	U
36	RA	1579	A
36	RA	1581	G
36	RA	1586	A

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Mol	Chain	Res	Type
36	RA	1598	C
36	RA	1608	A
36	RA	1610	A
36	RA	1617	C
36	RA	1618	A
36	RA	1640	C
36	RA	1648	C
36	RA	1654	A
36	RA	1667	G
36	RA	1668	A
36	RA	1674	G
36	RA	1675	C
36	RA	1695	G
36	RA	1698	A
36	RA	1703	G
36	RA	1725	G
36	RA	1728	G
36	RA	1729	A
36	RA	1731	G
36	RA	1742	C
36	RA	1743	G
36	RA	1756	G
36	RA	1762	A
36	RA	1763	G
36	RA	1764	G
36	RA	1773	A
36	RA	1780	A
36	RA	1781	C
36	RA	1791	A
36	RA	1799	G
36	RA	1800	C
36	RA	1802	A
36	RA	1811	G
36	RA	1816	G
36	RA	1820	U
36	RA	1828	G
36	RA	1829	A
36	RA	1833	U
36	RA	1835	G
36	RA	1847	A
36	RA	1858	G
36	RA	1864	U

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Mol	Chain	Res	Type
36	RA	1870	C
36	RA	1872	A
36	RA	1878	G
36	RA	1882	C
36	RA	1888	G
36	RA	1889	A
36	RA	1906	G
36	RA	1913	A
36	RA	1929	G
36	RA	1930	G
36	RA	1931	U
36	RA	1936	A
36	RA	1938	A
36	RA	1955	U
36	RA	1963	U
36	RA	1965	C
36	RA	1967	C
36	RA	1969	A
36	RA	1970	A
36	RA	1971	A
36	RA	1972	A
36	RA	1982	C
36	RA	1991	U
36	RA	1992	G
36	RA	1993	U
36	RA	2004	G
36	RA	2019	A
36	RA	2020	A
36	RA	2023	G
36	RA	2031	A
36	RA	2032	G
36	RA	2033	A
36	RA	2039	C
36	RA	2043	C
36	RA	2055	C
36	RA	2056	G
36	RA	2059	A
36	RA	2060	A
36	RA	2061	G
36	RA	2062	A
36	RA	2069	G
36	RA	2089	U

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Mol	Chain	Res	Type
36	RA	2093	G
36	RA	2111	C
36	RA	2112	G
36	RA	2113	U
36	RA	2114	A
36	RA	2115	G
36	RA	2117	A
36	RA	2126	A
36	RA	2127	G
36	RA	2128	C
36	RA	2131	G
36	RA	2132	U
36	RA	2133	G
36	RA	2136	C
36	RA	2146	C
36	RA	2148	G
36	RA	2158	A
36	RA	2165	G
36	RA	2166	G
36	RA	2168	G
36	RA	2169	A
36	RA	2170	A
36	RA	2173	A
36	RA	2176	A
36	RA	2190	G
36	RA	2192	G
36	RA	2198	A
36	RA	2199	A
36	RA	2210	G
36	RA	2211	G
36	RA	2212	A
36	RA	2213	U
36	RA	2215	G
36	RA	2225	A
36	RA	2238	G
36	RA	2239	G
36	RA	2243	U
36	RA	2249	U
36	RA	2266	A
36	RA	2275	C
36	RA	2280	G
36	RA	2283	C

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Mol	Chain	Res	Type
36	RA	2287	A
36	RA	2288	A
36	RA	2305	A
36	RA	2307	G
36	RA	2308	G
36	RA	2310	A
36	RA	2311	A
36	RA	2312	U
36	RA	2315	G
36	RA	2319	G
36	RA	2320	A
36	RA	2321	G
36	RA	2325	G
36	RA	2333	A
36	RA	2334	G
36	RA	2335	A
36	RA	2342	C
36	RA	2346	A
36	RA	2347	C
36	RA	2350	C
36	RA	2354	G
36	RA	2383	G
36	RA	2385	C
36	RA	2402	C
36	RA	2403	C
36	RA	2406	U
36	RA	2410	G
36	RA	2423	U
36	RA	2425	A
36	RA	2429	G
36	RA	2430	A
36	RA	2435	A
36	RA	2439	A
36	RA	2440	C
36	RA	2441	C
36	RA	2444	G
36	RA	2445	G
36	RA	2448	A
36	RA	2467	C
36	RA	2469	A
36	RA	2470	G
36	RA	2475	C

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Mol	Chain	Res	Type
36	RA	2498	C
36	RA	2502	G
36	RA	2505	G
36	RA	2506	U
36	RA	2513	G
36	RA	2514	U
36	RA	2519	U
36	RA	2520	C
36	RA	2529	G
36	RA	2530	A
36	RA	2542	A
36	RA	2543	G
36	RA	2554	U
36	RA	2562	U
36	RA	2564	A
36	RA	2567	G
36	RA	2569	G
36	RA	2572	A
36	RA	2573	C
36	RA	2578	G
36	RA	2582	G
36	RA	2602	A
36	RA	2609	U
36	RA	2611	U
36	RA	2612	C
36	RA	2614	A
36	RA	2615	U
36	RA	2623	G
36	RA	2629	A
36	RA	2655	G
36	RA	2665	A
36	RA	2668	G
36	RA	2673	G
36	RA	2675	A
36	RA	2689	U
36	RA	2690	C
36	RA	2691	C
36	RA	2702	U
36	RA	2707	G
36	RA	2712	U
36	RA	2712(A)	A
36	RA	2713	A

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Mol	Chain	Res	Type
36	RA	2714	G
36	RA	2726	U
36	RA	2733	A
36	RA	2746	U
36	RA	2747	G
36	RA	2751	G
36	RA	2752	C
36	RA	2756	U
36	RA	2757	A
36	RA	2761	G
36	RA	2764	A
36	RA	2765	A
36	RA	2766	G
36	RA	2777	G
36	RA	2778	A
36	RA	2779	U
36	RA	2780	G
36	RA	2787	C
36	RA	2788	C
36	RA	2790	A
36	RA	2791	C
36	RA	2792	G
36	RA	2794	C
36	RA	2797	U
36	RA	2798	C
36	RA	2807	G
36	RA	2818	G
36	RA	2820	A
36	RA	2821	A
36	RA	2823	A
36	RA	2831	G
36	RA	2832	U
36	RA	2833	G
36	RA	2834	G
36	RA	2835	A
36	RA	2839	G
36	RA	2849	U
36	RA	2872	G
36	RA	2879	C
36	RA	2880	C
36	RA	2883	A
36	RA	2891	G

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Mol	Chain	Res	Type
36	RA	2892	A
36	RA	2893	G
36	RA	2894	G
37	RB	7	G
37	RB	8	U
37	RB	9	G
37	RB	12	C
37	RB	13	A
37	RB	15	A
37	RB	16	G
37	RB	22	U
37	RB	25	A
37	RB	26	A
37	RB	32	C
37	RB	41	U
37	RB	42	C
37	RB	44	G
37	RB	45	A
37	RB	47	C
37	RB	56	G
37	RB	67	G
37	RB	73	A
37	RB	81	G
37	RB	90	C
37	RB	105	G
37	RB	108	C
37	RB	109	G
1	XA	6	G
1	XA	32	A
1	XA	39	G
1	XA	47	C
1	XA	48	C
1	XA	50	A
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	81	G
1	XA	88	C
1	XA	89	U

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Mol	Chain	Res	Type
1	XA	90	C
1	XA	91	C
1	XA	92	G
1	XA	95	G
1	XA	101	A
1	XA	108	G
1	XA	116	A
1	XA	121	C
1	XA	130	A
1	XA	144	G
1	XA	163	C
1	XA	172	A
1	XA	174	C
1	XA	190	G
1	XA	191(A)	G
1	XA	195	A
1	XA	201	C
1	XA	209	U
1	XA	210	U
1	XA	216	G
1	XA	222	U
1	XA	244	U
1	XA	245	C
1	XA	247	G
1	XA	251	G
1	XA	252	U
1	XA	262	A
1	XA	267	C
1	XA	270	A
1	XA	281	G
1	XA	289	G
1	XA	321	A
1	XA	328	C
1	XA	329	A
1	XA	332	G
1	XA	345	C
1	XA	346	G
1	XA	347	G
1	XA	348	G
1	XA	351	G
1	XA	352	C
1	XA	353	A

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Mol	Chain	Res	Type
1	XA	354	G
1	XA	356	A
1	XA	367	U
1	XA	368	U
1	XA	372	C
1	XA	373	A
1	XA	384	G
1	XA	390	C
1	XA	397	A
1	XA	398	C
1	XA	406	G
1	XA	411	A
1	XA	412	A
1	XA	413	G
1	XA	414	A
1	XA	421	U
1	XA	422	C
1	XA	423	G
1	XA	424	G
1	XA	429	U
1	XA	440	A
1	XA	442	C
1	XA	451	A
1	XA	452	A
1	XA	466	C
1	XA	467	G
1	XA	485	G
1	XA	486	U
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	521	G
1	XA	527	G
1	XA	531	U
1	XA	532	A
1	XA	533	A
1	XA	545	C
1	XA	547	A
1	XA	548	G

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Mol	Chain	Res	Type
1	XA	559	A
1	XA	561	U
1	XA	562	C
1	XA	564	C
1	XA	565	U
1	XA	568	G
1	XA	572	A
1	XA	573	A
1	XA	576	G
1	XA	577	G
1	XA	579	G
1	XA	596	C
1	XA	630	G
1	XA	631	G
1	XA	632	A
1	XA	633	G
1	XA	653	A
1	XA	665	A
1	XA	686	U
1	XA	688	G
1	XA	695	A
1	XA	704	A
1	XA	718	G
1	XA	721	G
1	XA	731	G
1	XA	734	G
1	XA	749	C
1	XA	752	G
1	XA	753	A
1	XA	754	C
1	XA	755	G
1	XA	760	G
1	XA	777	A
1	XA	792	A
1	XA	793	U
1	XA	794	A
1	XA	813	U
1	XA	817	C
1	XA	818	G
1	XA	821	G
1	XA	828	A
1	XA	842	C

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Mol	Chain	Res	Type
1	XA	843	U
1	XA	848	C
1	XA	859	A
1	XA	870	U
1	XA	871	U
1	XA	872	A
1	XA	902	G
1	XA	914	A
1	XA	926	G
1	XA	927	G
1	XA	934	C
1	XA	935	A
1	XA	942	G
1	XA	958	A
1	XA	960	U
1	XA	968	A
1	XA	969	A
1	XA	971	G
1	XA	974	A
1	XA	975	A
1	XA	976	G
1	XA	977	A
1	XA	981	U
1	XA	982	U
1	XA	991	U
1	XA	992	U
1	XA	993	G
1	XA	994	A
1	XA	1004	A
1	XA	1005	A
1	XA	1006	C
1	XA	1008	C
1	XA	1009	G
1	XA	1017	G
1	XA	1024	G
1	XA	1025	U
1	XA	1028	C
1	XA	1028(A)	C
1	XA	1029	G
1	XA	1032(A)	G
1	XA	1036	G
1	XA	1039	C

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Mol	Chain	Res	Type
1	XA	1040	U
1	XA	1046	A
1	XA	1053	G
1	XA	1054	C
1	XA	1064	G
1	XA	1066	C
1	XA	1081	G
1	XA	1085	U
1	XA	1094	G
1	XA	1095	U
1	XA	1101	A
1	XA	1124	G
1	XA	1125	U
1	XA	1126	U
1	XA	1127	G
1	XA	1130	A
1	XA	1131	G
1	XA	1136	U
1	XA	1137	C
1	XA	1138	G
1	XA	1139	G
1	XA	1140	C
1	XA	1146	A
1	XA	1152	A
1	XA	1157	A
1	XA	1158	C
1	XA	1159	U
1	XA	1160	G
1	XA	1162	C
1	XA	1171	G
1	XA	1176	A
1	XA	1177	G
1	XA	1178	G
1	XA	1181	G
1	XA	1182	G
1	XA	1183	A
1	XA	1187	G
1	XA	1190	G
1	XA	1196	U
1	XA	1201	A
1	XA	1211	U
1	XA	1212	U

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Mol	Chain	Res	Type
1	XA	1213	A
1	XA	1224	G
1	XA	1226	C
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	1263	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	1298	C
1	XA	1299	A
1	XA	1300	G
1	XA	1302	U
1	XA	1303	C
1	XA	1305	G
1	XA	1310	G
1	XA	1312	G
1	XA	1318	A
1	XA	1320	C
1	XA	1322	C
1	XA	1323	G
1	XA	1331	G
1	XA	1336	C
1	XA	1337	G
1	XA	1347	G
1	XA	1353	G
1	XA	1362(A)	C
1	XA	1363	A
1	XA	1364	U
1	XA	1398	A
1	XA	1419	G
1	XA	1442	G
1	XA	1443	G

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Mol	Chain	Res	Type
1	XA	1446	A
1	XA	1447	G
1	XA	1452	C
1	XA	1453	G
1	XA	1454	G
1	XA	1487	G
1	XA	1492	A
1	XA	1497	G
1	XA	1499	A
1	XA	1502	A
1	XA	1503	A
1	XA	1504	G
1	XA	1506	U
1	XA	1517	G
1	XA	1519	A
1	XA	1520	G
1	XA	1529	G
1	XA	1530	G
22	XV	13	C
22	XV	16	C
22	XV	17(A)	U
22	XV	18	G
22	XV	19	G
22	XV	20	U
22	XV	21	A
22	XV	47	U
22	XV	48	C
22	XV	49	G
22	XV	76	A
23	XW	8	U
23	XW	13	C
23	XW	14	A
23	XW	15	G
23	XW	16	A
23	XW	17	A
23	XW	18	G
23	XW	19	G
23	XW	20	G
23	XW	21	A
23	XW	26	G
23	XW	28	U
23	XW	31	C

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Mol	Chain	Res	Type
23	XW	32	A
23	XW	33	U
23	XW	34	G
23	XW	35	G
23	XW	36	C
23	XW	38	A
23	XW	39	G
23	XW	40	C
23	XW	41	A
23	XW	43	G
23	XW	44	A
23	XW	45	G
23	XW	46	G
23	XW	47	U
23	XW	48	C
23	XW	49	A
23	XW	52	G
23	XW	56	C
23	XW	57	G
23	XW	58	A
23	XW	59	U
23	XW	61	C
23	XW	66	U
23	XW	70	U
23	XW	76	A
24	XX	7	G
24	XX	9	G
24	XX	10	G
24	XX	11	U
24	XX	12	A
24	XX	13	A
24	XX	19	G
25	XY	2	G
25	XY	7	A
25	XY	12	U
25	XY	15	G
25	XY	16	C
25	XY	17	U
25	XY	18	G
25	XY	19	G
25	XY	21	A
25	XY	29	U

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Mol	Chain	Res	Type
25	XY	30	G
25	XY	36	C
25	XY	37	A
25	XY	42	A
25	XY	46	G
25	XY	47	U
25	XY	48	C
25	XY	50	G
25	XY	51	C
25	XY	52	G
25	XY	53	G
25	XY	54	U
25	XY	55	U
25	XY	56	C
25	XY	57	G
25	XY	58	A
25	XY	59	U
25	XY	61	C
25	XY	69	C
25	XY	71	C
25	XY	74	C
36	YA	9	U
36	YA	14	A
36	YA	15	G
36	YA	28	A
36	YA	34	C
36	YA	35	G
36	YA	46	C
36	YA	51	G
36	YA	55	G
36	YA	61	G
36	YA	73	A
36	YA	74	A
36	YA	75	G
36	YA	99	U
36	YA	101	G
36	YA	102	G
36	YA	103	A
36	YA	118	A
36	YA	119	A
36	YA	120	U
36	YA	125	G

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Mol	Chain	Res	Type
36	YA	131	G
36	YA	161	U
36	YA	162	U
36	YA	181	A
36	YA	188	G
36	YA	196	A
36	YA	199	A
36	YA	201	C
36	YA	216	A
36	YA	221	A
36	YA	222	A
36	YA	223	A
36	YA	228	A
36	YA	229	A
36	YA	230	U
36	YA	232	G
36	YA	242	G
36	YA	243	U
36	YA	248	G
36	YA	252	G
36	YA	264	C
36	YA	265	A
36	YA	266	G
36	YA	269	U
36	YA	270(L)	U
36	YA	270(M)	U
36	YA	270(N)	G
36	YA	270(P)	C
36	YA	271(A)	C
36	YA	271(B)	G
36	YA	271(C)	U
36	YA	271	G
36	YA	274	G
36	YA	275	G
36	YA	276	A
36	YA	278	A
36	YA	279	C
36	YA	299	A
36	YA	311	A
36	YA	323	G
36	YA	324	A
36	YA	329	G

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Mol	Chain	Res	Type
36	YA	330	A
36	YA	331	A
36	YA	332	A
36	YA	342	G
36	YA	352	G
36	YA	363	G
36	YA	364	C
36	YA	371	A
36	YA	372	G
36	YA	373	U
36	YA	386	G
36	YA	387	U
36	YA	405	U
36	YA	406	G
36	YA	411	G
36	YA	412	A
36	YA	421	U
36	YA	428	A
36	YA	444	C
36	YA	448	U
36	YA	451	C
36	YA	455	C
36	YA	457	A
36	YA	458	G
36	YA	467	G
36	YA	470	A
36	YA	481	G
36	YA	504	U
36	YA	505	A
36	YA	508	G
36	YA	509	C
36	YA	512	G
36	YA	528	A
36	YA	530	G
36	YA	531	C
36	YA	532	A
36	YA	533	G
36	YA	537	C
36	YA	539	G
36	YA	540	G
36	YA	546	C
36	YA	547	A

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Mol	Chain	Res	Type
36	YA	549	G
36	YA	563	G
36	YA	568	U
36	YA	573	G
36	YA	575	A
36	YA	603	A
36	YA	607	U
36	YA	614	U
36	YA	617	G
36	YA	622	G
36	YA	626	U
36	YA	627	A
36	YA	634	C
36	YA	637	A
36	YA	638	G
36	YA	645	C
36	YA	646	A
36	YA	651	G
36	YA	654	A
36	YA	654(A)	G
36	YA	654(B)	C
36	YA	686	G
36	YA	702	G
36	YA	704	G
36	YA	717	G
36	YA	722	A
36	YA	726	G
36	YA	730	C
36	YA	734	A
36	YA	747	U
36	YA	753	C
36	YA	764	A
36	YA	765	G
36	YA	775	G
36	YA	776	G
36	YA	782	A
36	YA	784	A
36	YA	785	G
36	YA	789	A
36	YA	790	C
36	YA	800	A
36	YA	805	G

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Mol	Chain	Res	Type
36	YA	812	C
36	YA	819	A
36	YA	827	U
36	YA	828	U
36	YA	831	G
36	YA	847	U
36	YA	856	C
36	YA	857	C
36	YA	860	U
36	YA	866	A
36	YA	882	G
36	YA	884	C
36	YA	885	C
36	YA	886	C
36	YA	888	C
36	YA	889	C
36	YA	896	A
36	YA	897	C
36	YA	900	A
36	YA	901	A
36	YA	907	U
36	YA	910	A
36	YA	915	C
36	YA	917	A
36	YA	932	G
36	YA	938	G
36	YA	941	A
36	YA	943	U
36	YA	945	A
36	YA	946	G
36	YA	953	A
36	YA	961	C
36	YA	973	A
36	YA	974	G
36	YA	974(A)	C
36	YA	980	A
36	YA	983	A
36	YA	989	G
36	YA	996	A
36	YA	1003	G
36	YA	1005	C
36	YA	1011	G

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Mol	Chain	Res	Type
36	YA	1012	U
36	YA	1013	C
36	YA	1015	G
36	YA	1022	G
36	YA	1023	U
36	YA	1024	G
36	YA	1025	G
36	YA	1026	U
36	YA	1027	A
36	YA	1033	U
36	YA	1036	G
36	YA	1037	G
36	YA	1045	A
36	YA	1046	A
36	YA	1050	A
36	YA	1054	A
36	YA	1059	G
36	YA	1060	U
36	YA	1061	U
36	YA	1062	G
36	YA	1065	U
36	YA	1066	U
36	YA	1067	A
36	YA	1068	G
36	YA	1069	A
36	YA	1071	G
36	YA	1076	C
36	YA	1077	A
36	YA	1078	U
36	YA	1082	U
36	YA	1083	U
36	YA	1084	A
36	YA	1086	A
36	YA	1088	A
36	YA	1093	G
36	YA	1095	A
36	YA	1096	A
36	YA	1097	U
36	YA	1103	A
36	YA	1104	C
36	YA	1105	U
36	YA	1110	G

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Mol	Chain	Res	Type
36	YA	1111	A
36	YA	1129	A
36	YA	1130	U
36	YA	1135	C
36	YA	1136	G
36	YA	1139	G
36	YA	1141	U
36	YA	1142	U
36	YA	1142(A)	A
36	YA	1173	G
36	YA	1174	A
36	YA	1175	U
36	YA	1176	G
36	YA	1178	C
36	YA	1179	C
36	YA	1195	G
36	YA	1204	A
36	YA	1205	U
36	YA	1210	A
36	YA	1211	U
36	YA	1218	C
36	YA	1220	A
36	YA	1236	G
36	YA	1238	G
36	YA	1240	U
36	YA	1244	G
36	YA	1253	A
36	YA	1256	G
36	YA	1265	A
36	YA	1272	A
36	YA	1273	U
36	YA	1300	U
36	YA	1301	A
36	YA	1306	C
36	YA	1325	G
36	YA	1329	U
36	YA	1332	G
36	YA	1341	U
36	YA	1349	A
36	YA	1352	U
36	YA	1365	A
36	YA	1368	G

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Mol	Chain	Res	Type
36	YA	1378	A
36	YA	1379	A
36	YA	1384	A
36	YA	1385	G
36	YA	1391	U
36	YA	1395	A
36	YA	1406	U
36	YA	1407	C
36	YA	1411	C
36	YA	1416	G
36	YA	1419	A
36	YA	1420	U
36	YA	1421	G
36	YA	1428	C
36	YA	1444(A)	A
36	YA	1449	A
36	YA	1449(A)	G
36	YA	1455	G
36	YA	1458	C
36	YA	1459	G
36	YA	1460	A
36	YA	1461	G
36	YA	1467	C
36	YA	1471	A
36	YA	1482	U
36	YA	1483	G
36	YA	1493	C
36	YA	1497	U
36	YA	1507	A
36	YA	1508	A
36	YA	1510	A
36	YA	1511	A
36	YA	1514	U
36	YA	1523	U
36	YA	1533	C
36	YA	1534	G
36	YA	1535	U
36	YA	1536	A
36	YA	1537	C
36	YA	1538	G
36	YA	1540	G
36	YA	1543	A

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Mol	Chain	Res	Type
36	YA	1544	C
36	YA	1545	A
36	YA	1554	A
36	YA	1558	A
36	YA	1559	G
36	YA	1566	A
36	YA	1569	A
36	YA	1578	U
36	YA	1579	A
36	YA	1585	C
36	YA	1586	A
36	YA	1591	G
36	YA	1598	C
36	YA	1607	C
36	YA	1608	A
36	YA	1610	A
36	YA	1616	A
36	YA	1617	C
36	YA	1618	A
36	YA	1640	C
36	YA	1648	C
36	YA	1654	A
36	YA	1668	A
36	YA	1674	G
36	YA	1695	G
36	YA	1699	G
36	YA	1700	A
36	YA	1725	G
36	YA	1728	G
36	YA	1729	A
36	YA	1730	U
36	YA	1731	G
36	YA	1732	A
36	YA	1733	G
36	YA	1742	C
36	YA	1743	G
36	YA	1750	G
36	YA	1754	C
36	YA	1756	G
36	YA	1762	A
36	YA	1763	G
36	YA	1764	G

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Mol	Chain	Res	Type
36	YA	1773	A
36	YA	1780	A
36	YA	1791	A
36	YA	1799	G
36	YA	1800	C
36	YA	1802	A
36	YA	1811	G
36	YA	1815	A
36	YA	1816	G
36	YA	1820	U
36	YA	1828	G
36	YA	1829	A
36	YA	1835	G
36	YA	1847	A
36	YA	1858	G
36	YA	1869	G
36	YA	1870	C
36	YA	1872	A
36	YA	1878	G
36	YA	1882	C
36	YA	1888	G
36	YA	1889	A
36	YA	1913	A
36	YA	1914	C
36	YA	1919	A
36	YA	1929	G
36	YA	1930	G
36	YA	1931	U
36	YA	1936	A
36	YA	1938	A
36	YA	1939	U
36	YA	1955	U
36	YA	1963	U
36	YA	1965	C
36	YA	1967	C
36	YA	1969	A
36	YA	1970	A
36	YA	1971	A
36	YA	1972	A
36	YA	1981	A
36	YA	1982	C
36	YA	1991	U

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Mol	Chain	Res	Type
36	YA	1992	G
36	YA	1993	U
36	YA	2004	G
36	YA	2020	A
36	YA	2021	C
36	YA	2023	G
36	YA	2031	A
36	YA	2032	G
36	YA	2033	A
36	YA	2043	C
36	YA	2055	C
36	YA	2056	G
36	YA	2059	A
36	YA	2060	A
36	YA	2061	G
36	YA	2062	A
36	YA	2069	G
36	YA	2093	G
36	YA	2111	C
36	YA	2113	U
36	YA	2114	A
36	YA	2115	G
36	YA	2116	G
36	YA	2118	U
36	YA	2119	A
36	YA	2120	G
36	YA	2126	A
36	YA	2127	G
36	YA	2128	C
36	YA	2132	U
36	YA	2133	G
36	YA	2136	C
36	YA	2147	G
36	YA	2148	G
36	YA	2158	A
36	YA	2159	G
36	YA	2166	G
36	YA	2168	G
36	YA	2169	A
36	YA	2171	A
36	YA	2173	A
36	YA	2176	A

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Mol	Chain	Res	Type
36	YA	2189	U
36	YA	2190	G
36	YA	2192	G
36	YA	2198	A
36	YA	2210	G
36	YA	2211	G
36	YA	2212	A
36	YA	2213	U
36	YA	2215	G
36	YA	2225	A
36	YA	2238	G
36	YA	2239	G
36	YA	2243	U
36	YA	2275	C
36	YA	2278	A
36	YA	2283	C
36	YA	2287	A
36	YA	2288	A
36	YA	2307	G
36	YA	2308	G
36	YA	2311	A
36	YA	2318	G
36	YA	2319	G
36	YA	2320	A
36	YA	2325	G
36	YA	2334	G
36	YA	2336	A
36	YA	2342	C
36	YA	2345	G
36	YA	2346	A
36	YA	2347	C
36	YA	2350	C
36	YA	2358	G
36	YA	2383	G
36	YA	2385	C
36	YA	2392	A
36	YA	2402	C
36	YA	2403	C
36	YA	2406	U
36	YA	2410	G
36	YA	2421	G
36	YA	2422	A

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Mol	Chain	Res	Type
36	YA	2423	U
36	YA	2425	A
36	YA	2429	G
36	YA	2430	A
36	YA	2435	A
36	YA	2439	A
36	YA	2440	C
36	YA	2441	C
36	YA	2447	G
36	YA	2448	A
36	YA	2450	A
36	YA	2469	A
36	YA	2470	G
36	YA	2475	C
36	YA	2476	A
36	YA	2478	A
36	YA	2494	G
36	YA	2502	G
36	YA	2505	G
36	YA	2506	U
36	YA	2513	G
36	YA	2518	A
36	YA	2520	C
36	YA	2529	G
36	YA	2542	A
36	YA	2543	G
36	YA	2554	U
36	YA	2562	U
36	YA	2567	G
36	YA	2572	A
36	YA	2578	G
36	YA	2582	G
36	YA	2602	A
36	YA	2609	U
36	YA	2611	U
36	YA	2612	C
36	YA	2615	U
36	YA	2629	A
36	YA	2632	A
36	YA	2637	U
36	YA	2646	C
36	YA	2665	A

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Mol	Chain	Res	Type
36	YA	2673	G
36	YA	2682	U
36	YA	2689	U
36	YA	2690	C
36	YA	2702	U
36	YA	2703	C
36	YA	2707	G
36	YA	2712	U
36	YA	2712(A)	A
36	YA	2713	A
36	YA	2714	G
36	YA	2718	G
36	YA	2726	U
36	YA	2733	A
36	YA	2744	G
36	YA	2749	A
36	YA	2751	G
36	YA	2752	C
36	YA	2756	U
36	YA	2757	A
36	YA	2759	G
36	YA	2761	G
36	YA	2764	A
36	YA	2765	A
36	YA	2777	G
36	YA	2778	A
36	YA	2779	U
36	YA	2780	G
36	YA	2787	C
36	YA	2788	C
36	YA	2789	C
36	YA	2790	A
36	YA	2791	C
36	YA	2792	G
36	YA	2797	U
36	YA	2807	G
36	YA	2808	U
36	YA	2813	A
36	YA	2818	G
36	YA	2820	A
36	YA	2821	A
36	YA	2823	A

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Mol	Chain	Res	Type
36	YA	2830	G
36	YA	2833	G
36	YA	2834	G
36	YA	2835	A
36	YA	2872	G
36	YA	2879	C
36	YA	2880	C
36	YA	2891	G
36	YA	2892	A
36	YA	2893	G
36	YA	2894	G
37	YB	8	U
37	YB	9	G
37	YB	13	A
37	YB	15	A
37	YB	19	G
37	YB	21	G
37	YB	25	A
37	YB	26	A
37	YB	32	C
37	YB	40	U
37	YB	41	U
37	YB	42	C
37	YB	44	G
37	YB	45	A
37	YB	53	A
37	YB	56	G
37	YB	67	G
37	YB	73	A
37	YB	81	G
37	YB	109	G

All (162) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	QA	64	G
1	QA	115	G
1	QA	181	G
1	QA	243	A
1	QA	244	U
1	QA	250	A
1	QA	266	G

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Mol	Chain	Res	Type
1	QA	328	C
1	QA	410	G
1	QA	412	A
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	960	U
1	QA	992	U
1	QA	1025	U
1	QA	1027	C
1	QA	1065	U
1	QA	1200	C
1	QA	1201	A
1	QA	1285	A
1	QA	1297	C
1	QA	1318	A
1	QA	1336	C
1	QA	1346	A
1	QA	1347	G
1	QA	1498	U
1	QA	1528	U
23	QW	58	A
24	QX	18	G
36	RA	74	A
36	RA	99	U
36	RA	102	G
36	RA	205	G
36	RA	221	A
36	RA	227	A
36	RA	229	A
36	RA	271(B)	G
36	RA	345	A
36	RA	372	G
36	RA	404	C
36	RA	503	A
36	RA	512	G

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Mol	Chain	Res	Type
36	RA	637	A
36	RA	752	A
36	RA	846	C
36	RA	856	C
36	RA	1012	U
36	RA	1022	G
36	RA	1026	U
36	RA	1045	A
36	RA	1049	C
36	RA	1078	U
36	RA	1085	A
36	RA	1178	C
36	RA	1427	A
36	RA	1558	A
36	RA	1653	G
36	RA	1694	C
36	RA	1799	G
36	RA	1819	A
36	RA	1930	G
36	RA	1992	G
36	RA	2019	A
36	RA	2060	A
36	RA	2126	A
36	RA	2320	A
36	RA	2439	A
36	RA	2518	A
36	RA	2566	A
36	RA	2602	A
36	RA	2610	C
36	RA	2689	U
36	RA	2712	U
36	RA	2746	U
36	RA	2776	A
36	RA	2787	C
37	RB	66	A
1	XA	60	A
1	XA	78	G
1	XA	89	U
1	XA	115	G
1	XA	243	A
1	XA	244	U
1	XA	250	A

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Mol	Chain	Res	Type
1	XA	266	G
1	XA	328	C
1	XA	345	C
1	XA	367	U
1	XA	410	G
1	XA	412	A
1	XA	484	G
1	XA	485	G
1	XA	509	A
1	XA	560	U
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	1301	U
1	XA	1336	C
1	XA	1397	C
1	XA	1498	U
23	XW	14	A
23	XW	58	A
24	XX	18	G
36	YA	99	U
36	YA	221	A
36	YA	222	A
36	YA	229	A
36	YA	242	G
36	YA	271(B)	G
36	YA	278	A
36	YA	372	G
36	YA	404	C
36	YA	503	A
36	YA	637	A
36	YA	653	A
36	YA	752	A
36	YA	827	U
36	YA	846	C
36	YA	856	C

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Mol	Chain	Res	Type
36	YA	859	G
36	YA	1022	G
36	YA	1026	U
36	YA	1045	A
36	YA	1085	A
36	YA	1178	C
36	YA	1204	A
36	YA	1210	A
36	YA	1332	G
36	YA	1427	A
36	YA	1558	A
36	YA	1653	G
36	YA	1694	C
36	YA	1698	A
36	YA	1799	G
36	YA	1819	A
36	YA	1930	G
36	YA	1980	G
36	YA	1992	G
36	YA	2126	A
36	YA	2439	A
36	YA	2566	A
36	YA	2610	C
36	YA	2681	C
36	YA	2689	U
36	YA	2712	U
36	YA	2751	G
36	YA	2776	A
37	YB	66	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 955 ligands modelled in this entry, 951 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
59	SF4	XD	501	4	0,12,12	0.00	-	-		
59	SF4	QD	501	4	0,12,12	0.00	-	-		
58	PAR	QA	1667	-	45,45,45	0.69	0	64,67,67	1.20	6 (9%)
58	PAR	XA	1679	-	45,45,45	0.65	0	64,67,67	1.41	6 (9%)

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
59	SF4	XD	501	4	-	-	0/6/5/5
59	SF4	QD	501	4	-	-	0/6/5/5
58	PAR	QA	1667	-	-	4/18/94/94	0/4/4/4
58	PAR	XA	1679	-	-	7/18/94/94	0/4/4/4

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	XA	1679	PAR	C14-O33-C33	-4.13	107.75	117.96
58	QA	1667	PAR	C13-O52-C52	-3.60	109.04	117.96
58	XA	1679	PAR	C13-O52-C52	-3.48	109.35	117.96
58	XA	1679	PAR	O33-C14-C24	3.38	114.03	108.22
58	XA	1679	PAR	C44-C34-C24	3.23	116.63	111.07
58	XA	1679	PAR	O54-C54-C44	2.49	114.22	109.69
58	QA	1667	PAR	O62-C62-C12	-2.43	105.37	109.81
58	XA	1679	PAR	O54-C14-C24	-2.41	104.63	110.06
58	QA	1667	PAR	O11-C42-C32	-2.35	103.57	109.18
58	QA	1667	PAR	O33-C33-C23	-2.28	103.98	111.32
58	QA	1667	PAR	O52-C13-C23	2.27	112.67	107.96
58	QA	1667	PAR	C14-O33-C33	-2.08	112.81	117.96

There are no chirality outliers.

All (11) torsion outliers are listed below:

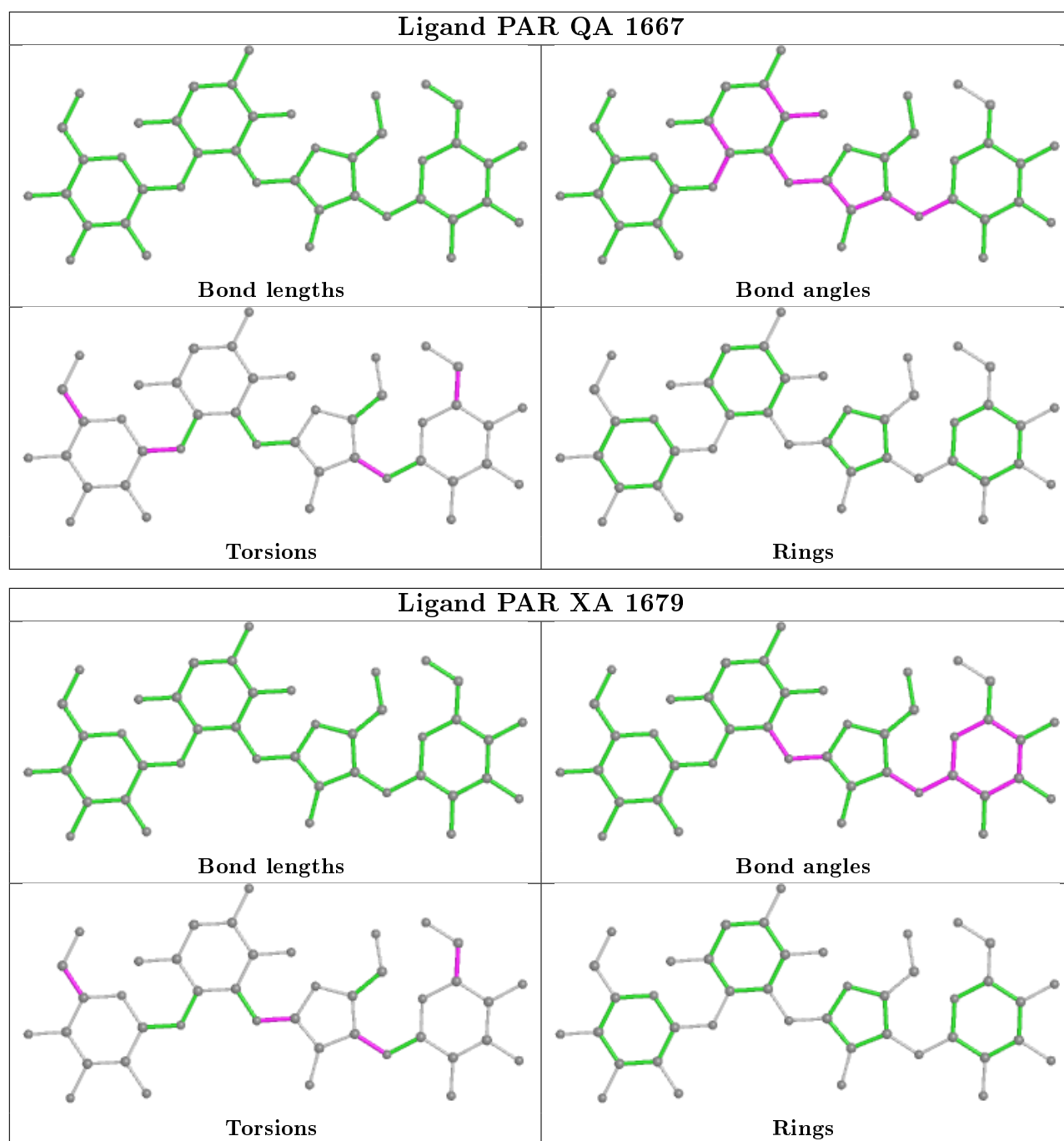
Mol	Chain	Res	Type	Atoms
58	XA	1679	PAR	C44-C54-C64-N64
58	XA	1679	PAR	O54-C54-C64-N64
58	QA	1667	PAR	O54-C54-C64-N64
58	XA	1679	PAR	O51-C51-C61-O61
58	QA	1667	PAR	O51-C51-C61-O61
58	XA	1679	PAR	C43-C33-O33-C14
58	QA	1667	PAR	O51-C11-O11-C42
58	XA	1679	PAR	C23-C13-O52-C52
58	XA	1679	PAR	C23-C33-O33-C14
58	QA	1667	PAR	C23-C33-O33-C14
58	XA	1679	PAR	C41-C51-C61-O61

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	QA	1667	PAR	2	0
58	XA	1679	PAR	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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.