



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2020 – 08:42 AM BST

PDB ID : 6OPE
Title : Crystal structure of tRNA^{Ala}(GGC) U32-A38 bound to near-cognate 70S A site
Authors : Nguyen, H.A.; Sunita, S.; Dunham, C.M.
Deposited on : 2019-04-24
Resolution : 3.10 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

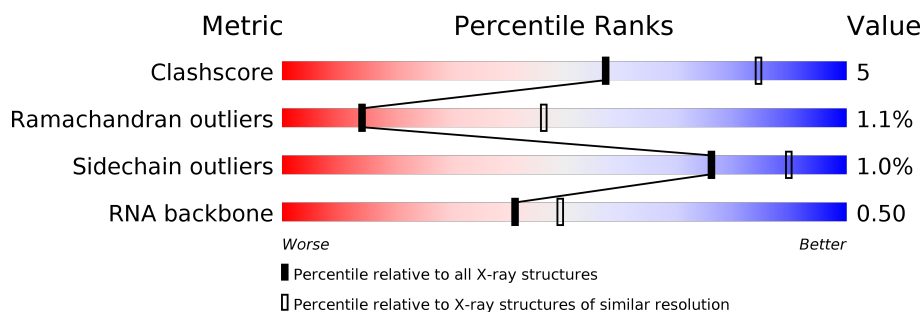
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

















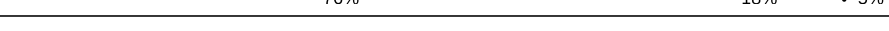

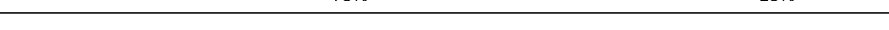
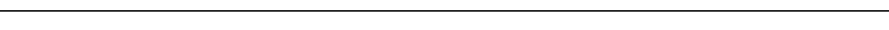
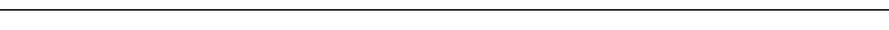
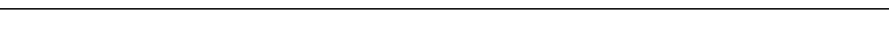
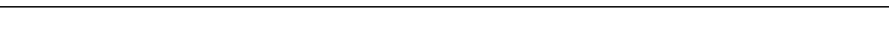
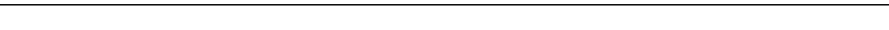

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	63% 29% 6% ..
1	XA	1522	64% 28% 6% ..
2	QB	256	74% 18% 7%
2	XB	256	74% 19% 7%
3	QC	239	67% 17% • 14%
3	XC	239	74% 12% 14%
4	QD	209	81% 17% •

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Mol	Chain	Length	Quality of chain
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	131	
12	XL	131	
13	QM	126	
13	XM	126	
14	QN	61	
14	XN	61	
15	QO	89	
15	XO	89	
16	QP	88	
16	XP	88	









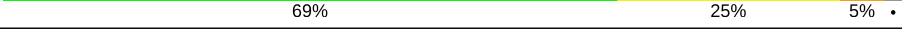


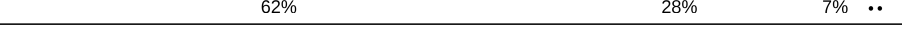

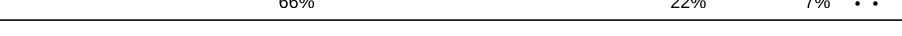


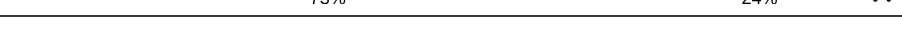

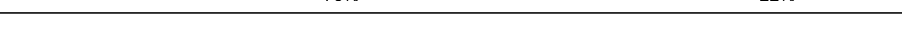
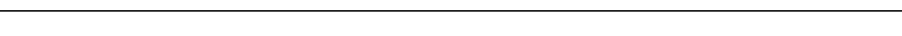

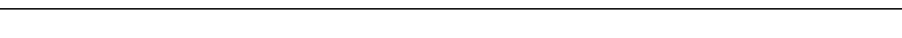
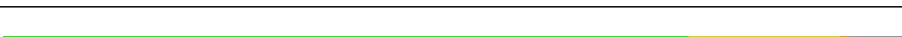


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Mol	Chain	Length	Quality of chain
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QX	19	
23	XX	19	
24	QY	76	
24	XY	76	
25	R0	85	
25	Y0	85	
26	R1	98	
26	Y1	98	
27	R2	72	
27	Y2	72	
28	R3	60	
28	Y3	60	
29	R4	71	


























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Mol	Chain	Length	Quality of chain
29	Y4	71	
30	R5	60	
30	Y5	60	
31	R6	54	
31	Y6	54	
32	R7	49	
32	Y7	49	
33	R8	65	
33	Y8	65	
34	R9	37	
34	Y9	37	
35	RA	2915	
35	YA	2915	
36	RB	122	
36	YB	122	
37	RD	276	
37	YD	276	
38	RE	206	
38	YE	206	
39	RF	210	
39	YF	210	
40	RG	182	
40	YG	182	
41	RH	180	
41	YH	180	




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Mol	Chain	Length	Quality of chain
42	RI	148	 76% 20% ...
42	YI	148	 81% 17% ..
43	RN	140	 83% 14% ..
43	YN	140	 87% 11% ..
44	RO	122	 77% 21% .
44	YO	122	 80% 18% .
45	RP	150	 75% 23% ..
45	YP	150	 78% 21% .
46	RQ	141	 82% 16% .
46	YQ	141	 79% 18% .
47	RR	118	 80% 19% .
47	YR	118	 81% 19% .
48	RS	112	 85% 11%
48	YS	112	 79% 17% ...
49	RT	146	 70% 23% . 6%
49	YT	146	 67% 25% . 6%
50	RU	118	 81% 16% ...
50	YU	118	 84% 12%
51	RV	101	 74% 25% .
51	YV	101	 86% 12% ..
52	RW	113	 81% 19%
52	YW	113	 81% 19%
53	RX	96	 80% 16% .
53	YX	96	 82% 13% . .
54	RY	110	 76% 15% . 7%

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Mol	Chain	Length	Quality of chain
54	YY	110	 81% 12% 7%
55	RZ	206	 65% 22% • 11%
55	YZ	206	 67% 20% • 11%

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 294981 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 mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	18	Total	C	N	O	P	0	0	0
			396	177	82	119	18			
23	XX	18	Total	C	N	O	P	0	0	0
			396	177	82	119	18			

- Molecule 24 is a RNA chain called A-site tRNA^{Ala}(GGC) U32-A38.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	75	Total	C	N	O	P	0	0	0
			1602	714	288	525	75			
24	XY	75	Total	C	N	O	P	0	0	0
			1602	714	288	525	75			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QA	73	Total	Mg	0	0
			73	73		
56	RP	3	Total	Mg	0	0
			3	3		
56	QX	2	Total	Mg	0	0
			2	2		
56	YA	347	Total	Mg	0	0
			347	347		
56	QM	1	Total	Mg	0	0
			1	1		
56	YR	1	Total	Mg	0	0
			1	1		
56	Y9	1	Total	Mg	0	0
			1	1		
56	Y1	1	Total	Mg	0	0
			1	1		
56	XX	1	Total	Mg	0	0
			1	1		

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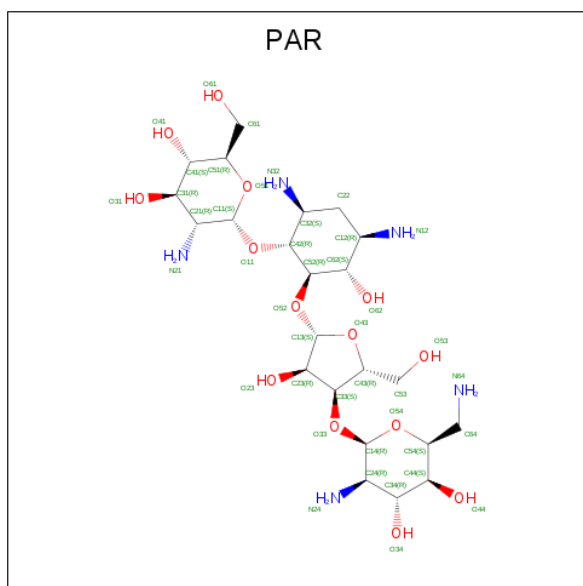
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QV	1	Total 1	Mg 1	0	0
56	Y8	1	Total 1	Mg 1	0	0
56	XA	91	Total 91	Mg 91	0	0
56	R0	1	Total 1	Mg 1	0	0
56	RU	1	Total 1	Mg 1	0	0
56	Y0	1	Total 1	Mg 1	0	0
56	YQ	3	Total 3	Mg 3	0	0
56	YN	1	Total 1	Mg 1	0	0
56	XF	1	Total 1	Mg 1	0	0
56	YX	1	Total 1	Mg 1	0	0
56	RR	1	Total 1	Mg 1	0	0
56	RD	1	Total 1	Mg 1	0	0
56	QF	1	Total 1	Mg 1	0	0
56	R5	1	Total 1	Mg 1	0	0
56	RA	281	Total 281	Mg 281	0	0
56	YP	3	Total 3	Mg 3	0	0
56	Y5	1	Total 1	Mg 1	0	0
56	R9	1	Total 1	Mg 1	0	0
56	RE	4	Total 4	Mg 4	0	0
56	YB	6	Total 6	Mg 6	0	0
56	Y6	2	Total 2	Mg 2	0	0

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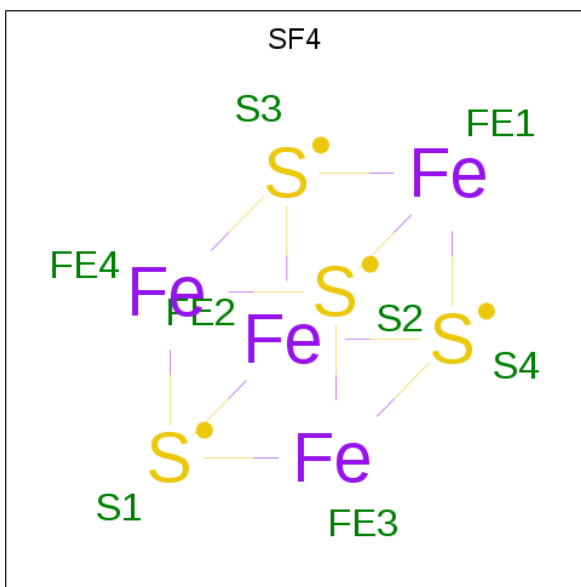
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	XV	2	Total	Mg	0	0
			2	2		
56	RB	4	Total	Mg	0	0
			4	4		
56	Y2	1	Total	Mg	0	0
			1	1		
56	R8	1	Total	Mg	0	0
			1	1		
56	RF	1	Total	Mg	0	0
			1	1		
56	XM	1	Total	Mg	0	0
			1	1		
56	YE	3	Total	Mg	0	0
			3	3		

- Molecule 57 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



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

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



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

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

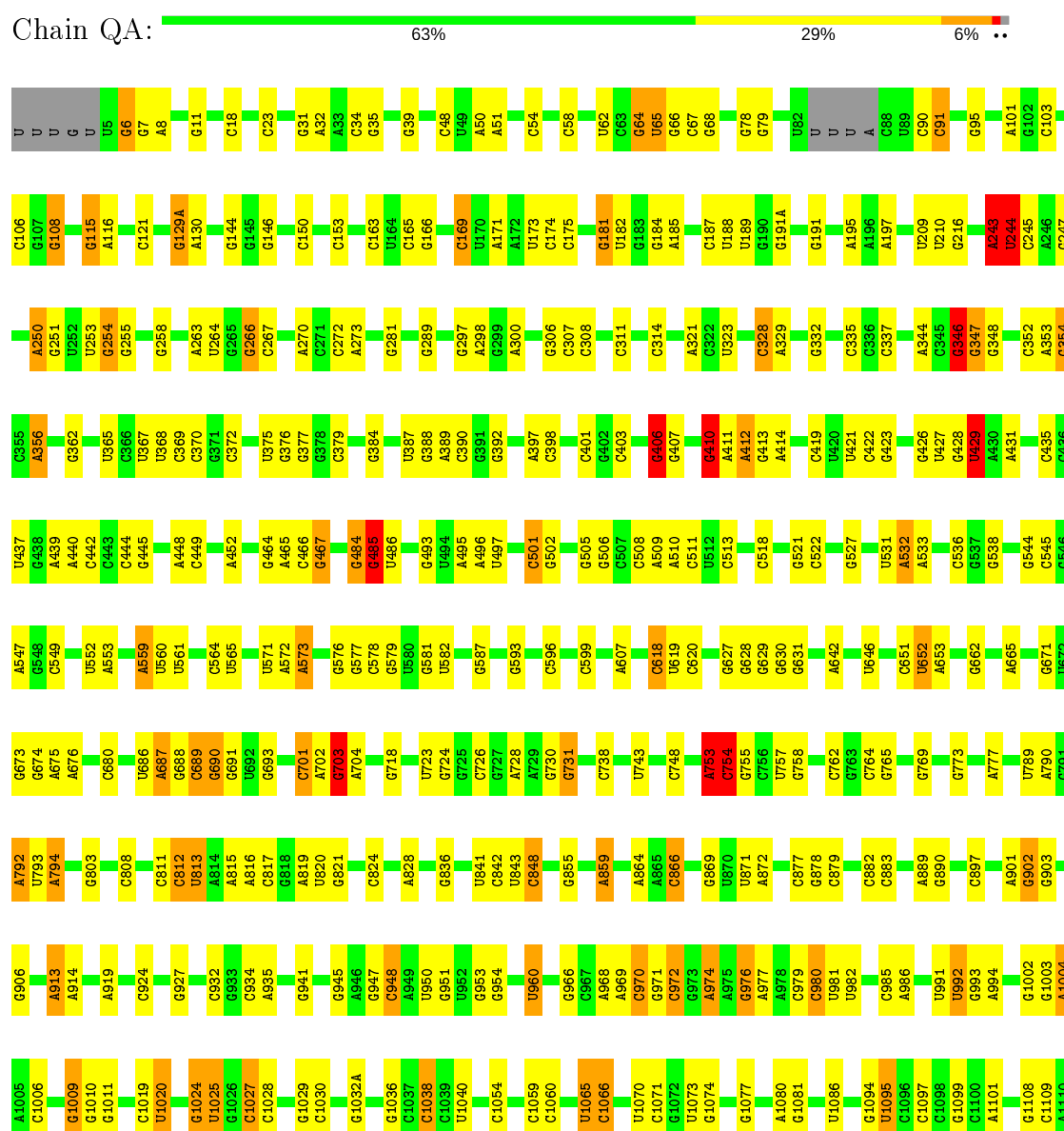
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	Y9	1	Total	Zn	0	0
			1	1		
59	R9	1	Total	Zn	0	0
			1	1		
59	QN	1	Total	Zn	0	0
			1	1		
59	XN	1	Total	Zn	0	0
			1	1		

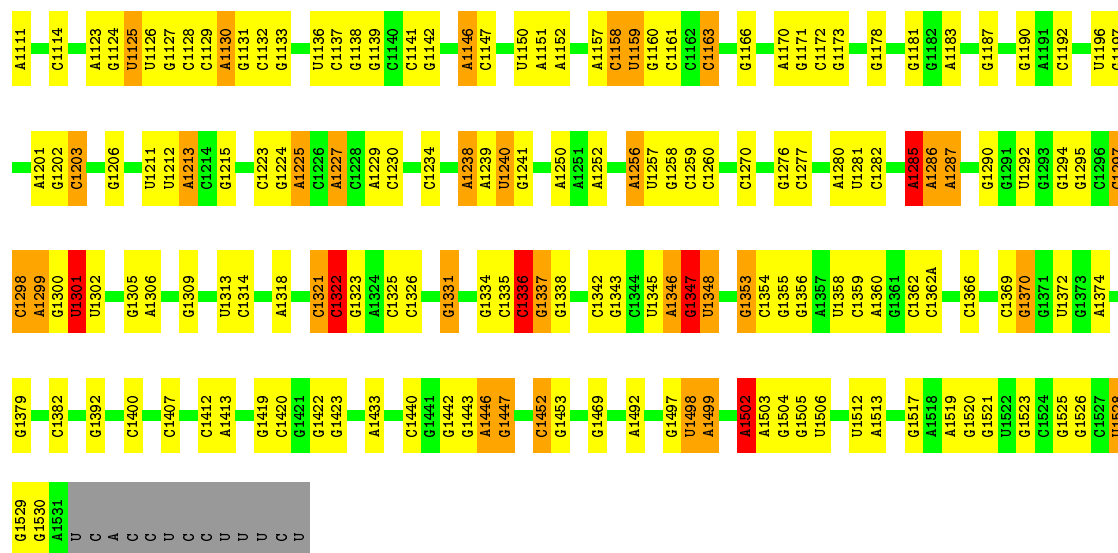
3 Residue-property plots

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.

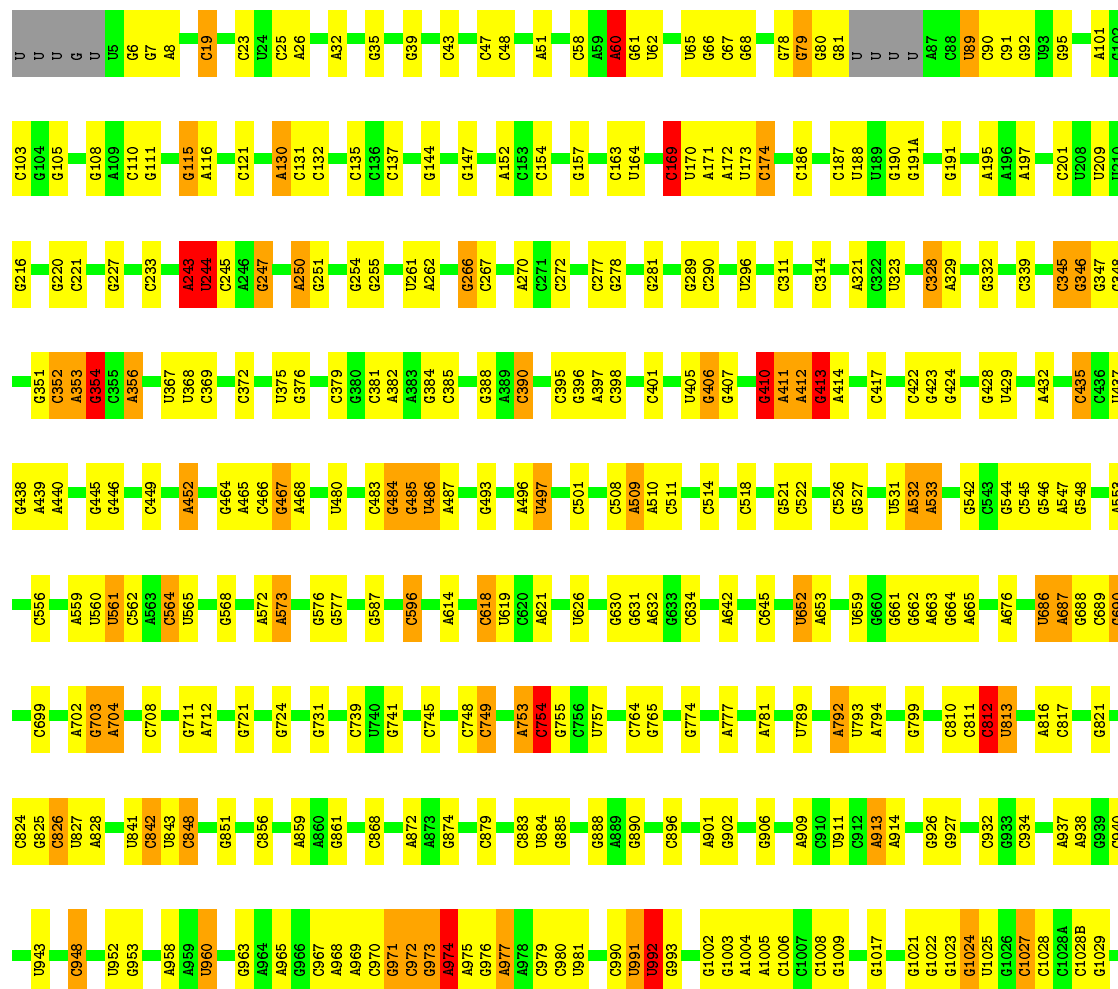
• Molecule 1: 16S rRNA

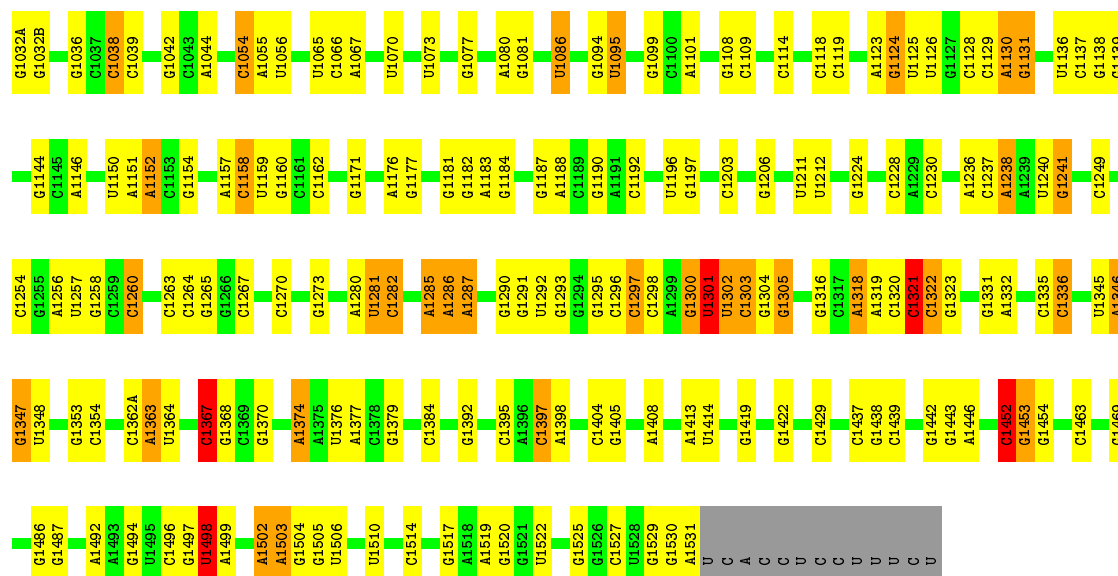




• Molecule 1: 16S rRNA

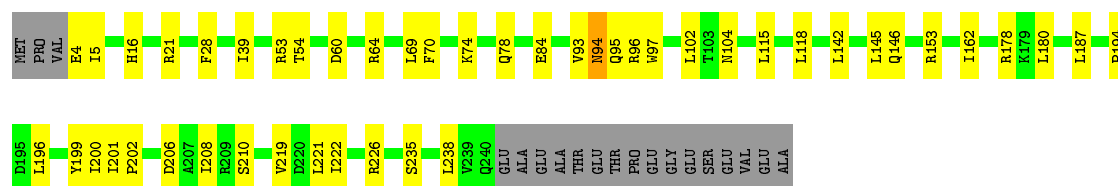
Chain XA: 64% 28% 6% ..





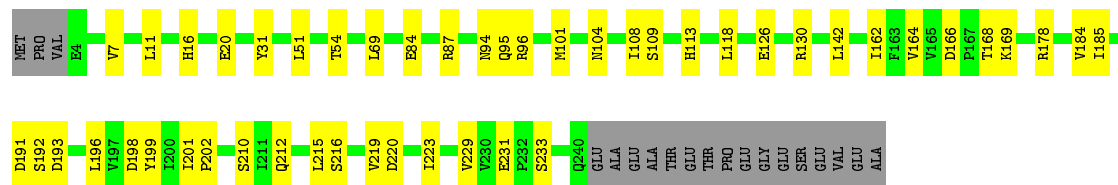
• Molecule 2: 30S ribosomal protein S2

Chain QB: 74% 18% 7%



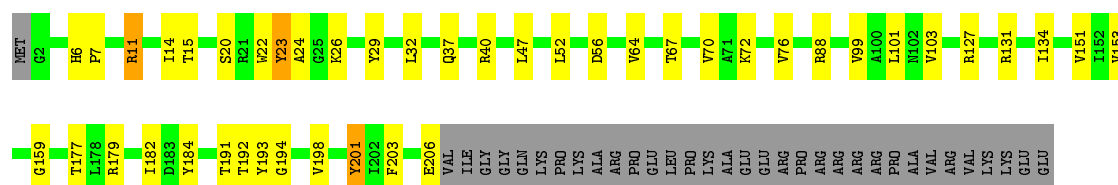
• Molecule 2: 30S ribosomal protein S2

Chain XB: 74% 19% 7%




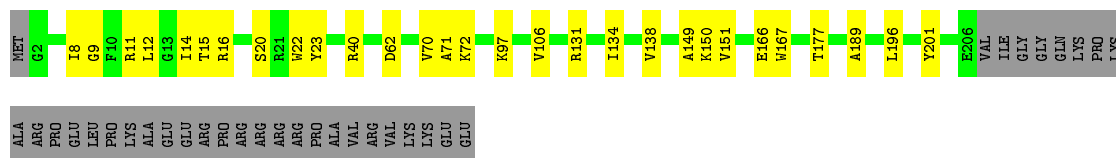
• Molecule 3: 30S ribosomal protein S3

Chain QC: 67% 17% 14%




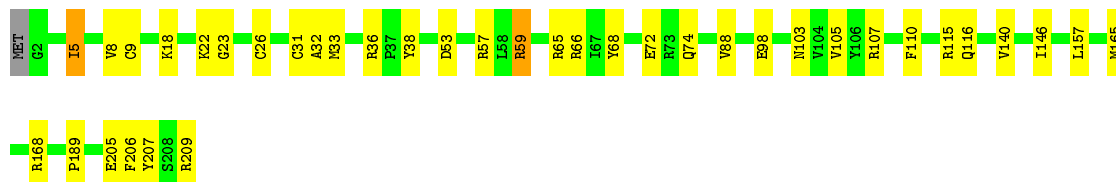
• Molecule 3: 30S ribosomal protein S3

Chain XC:  74% 12% 14%




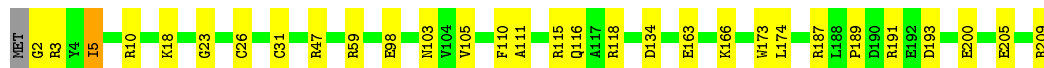
- Molecule 4: 30S ribosomal protein S4

Chain QD:  81% 17%




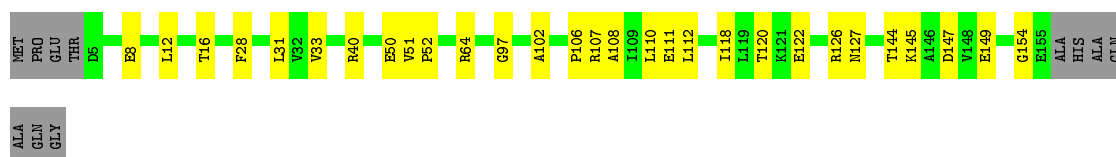
- Molecule 4: 30S ribosomal protein S4

Chain XD:  85% 14%




- Molecule 5: 30S ribosomal protein S5

Chain QE:  75% 18% 7%



- Molecule 5: 30S ribosomal protein S5

Chain XE:  83% 10% 7%




- Molecule 6: 30S ribosomal protein S6

Chain QF:  87% 13%




- Molecule 6: 30S ribosomal protein S6

Chain XF:  87% 13%



- Molecule 7: 30S ribosomal protein S7

Chain QG:  88% 12%




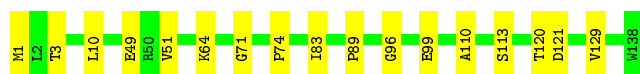
- Molecule 7: 30S ribosomal protein S7

Chain XG:  91% 8%




- Molecule 8: 30S ribosomal protein S8

Chain QH:  88% 12%



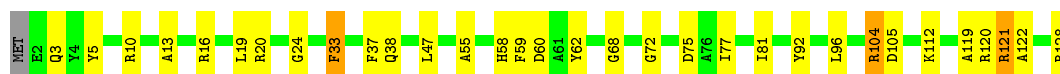
- Molecule 8: 30S ribosomal protein S8

Chain XH:  77% 23%



- Molecule 9: 30S ribosomal protein S9

Chain QI:  74% 23%



- Molecule 9: 30S ribosomal protein S9

Chain XI:  73% 27%




- Molecule 10: 30S ribosomal protein S10

Chain QJ: 



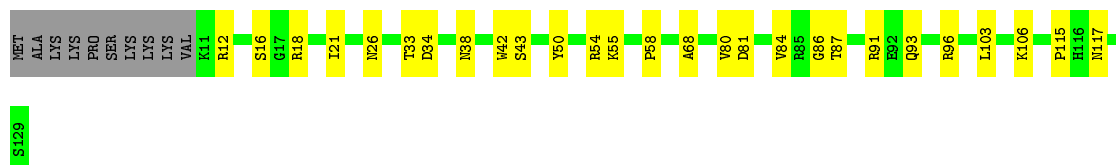
- Molecule 10: 30S ribosomal protein S10

Chain XJ: 




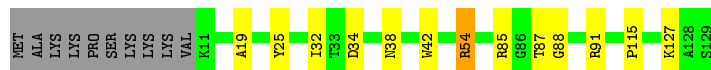
- Molecule 11: 30S ribosomal protein S11

Chain QK: 




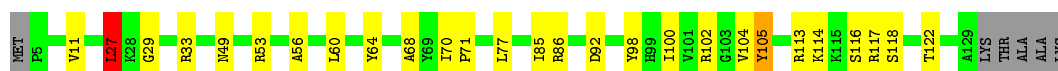
- Molecule 11: 30S ribosomal protein S11

Chain XK: 




- Molecule 12: 30S ribosomal protein S12

Chain QL: 



- Molecule 12: 30S ribosomal protein S12

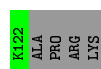
Chain XL: 



- Molecule 13: 30S ribosomal protein S13

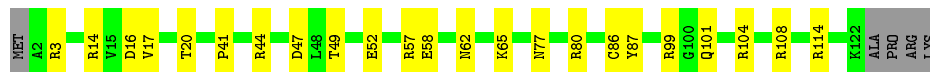
Chain QM: 





- Molecule 13: 30S ribosomal protein S13

Chain XM: 78% 18% .



- Molecule 14: 30S ribosomal protein S14 type Z

Chain QN: 75% 23% .



- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN: 85% 13% .



- Molecule 15: 30S ribosomal protein S15

Chain QO: 84% 13% ..



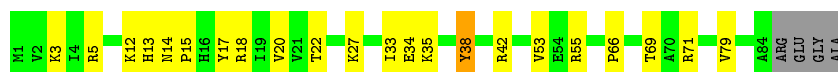
- Molecule 15: 30S ribosomal protein S15

Chain XO: 92% 7% .



- Molecule 16: 30S ribosomal protein S16

Chain QP: 70% 24% . 5%

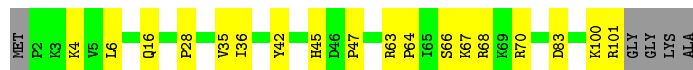
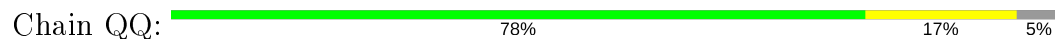


- Molecule 16: 30S ribosomal protein S16

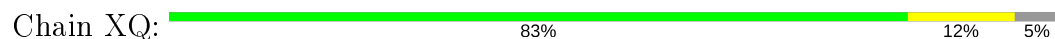
Chain XP: 80% 15% . 5%



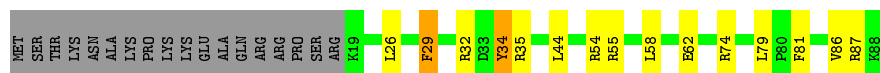
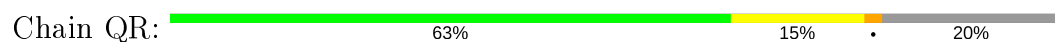
- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S18



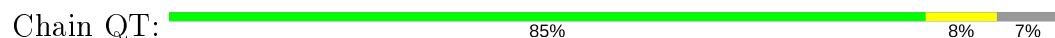
- Molecule 19: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20





- Molecule 20: 30S ribosomal protein S20

Chain XT: 75% 15% 7%



- Molecule 21: 30S ribosomal protein Thx

Chain QU: 70% 22% 7%



- Molecule 21: 30S ribosomal protein Thx

Chain XU: 78% 15% 7%



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

Chain QV: 70% 26% 1%



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

Chain XV: 74% 22% 1%



- Molecule 23: mRNA

Chain QX: 26% 63% 5% 5%

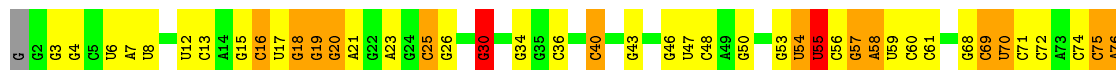


- Molecule 23: mRNA

Chain XX: 42% 42% 11% 5%



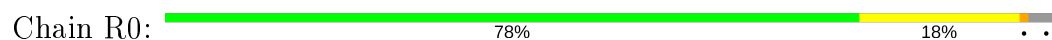
- Molecule 24: A-site tRNAAla(GGC) U32-A38



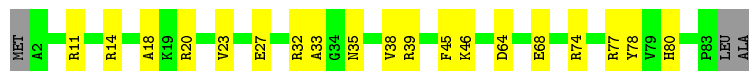
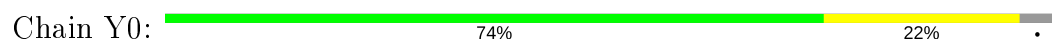
- Molecule 24: A-site tRNAAla(GGC) U32-A38



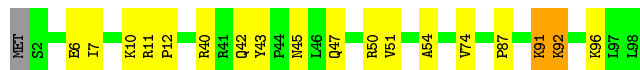
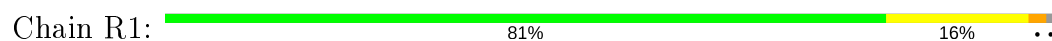
- Molecule 25: 50S ribosomal protein L27



- Molecule 25: 50S ribosomal protein L27



- Molecule 26: 50S ribosomal protein L28



- Molecule 26: 50S ribosomal protein L28



- Molecule 27: 50S ribosomal protein L29

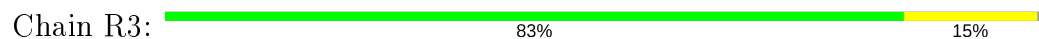




- Molecule 27: 50S ribosomal protein L29



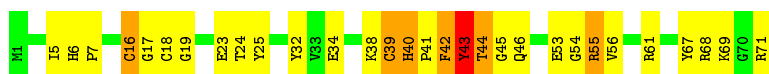
- Molecule 28: 50S ribosomal protein L30



- Molecule 28: 50S ribosomal protein L30



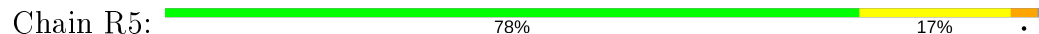
- Molecule 29: 50S ribosomal protein L31



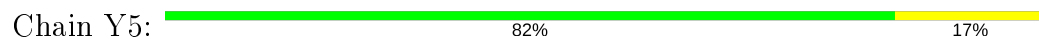
- Molecule 29: 50S ribosomal protein L31



- Molecule 30: 50S ribosomal protein L32



- Molecule 30: 50S ribosomal protein L32

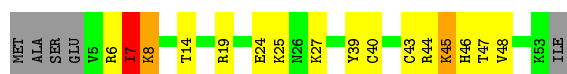




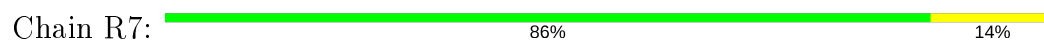
- Molecule 31: 50S ribosomal protein L33



- Molecule 31: 50S ribosomal protein L33



- Molecule 32: 50S ribosomal protein L34



- Molecule 32: 50S ribosomal protein L34



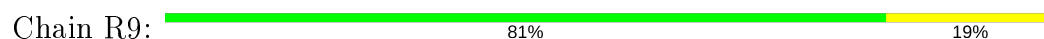
- Molecule 33: 50S ribosomal protein L35



- Molecule 33: 50S ribosomal protein L35

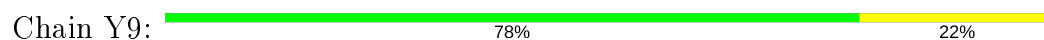


- Molecule 34: 50S ribosomal protein L36

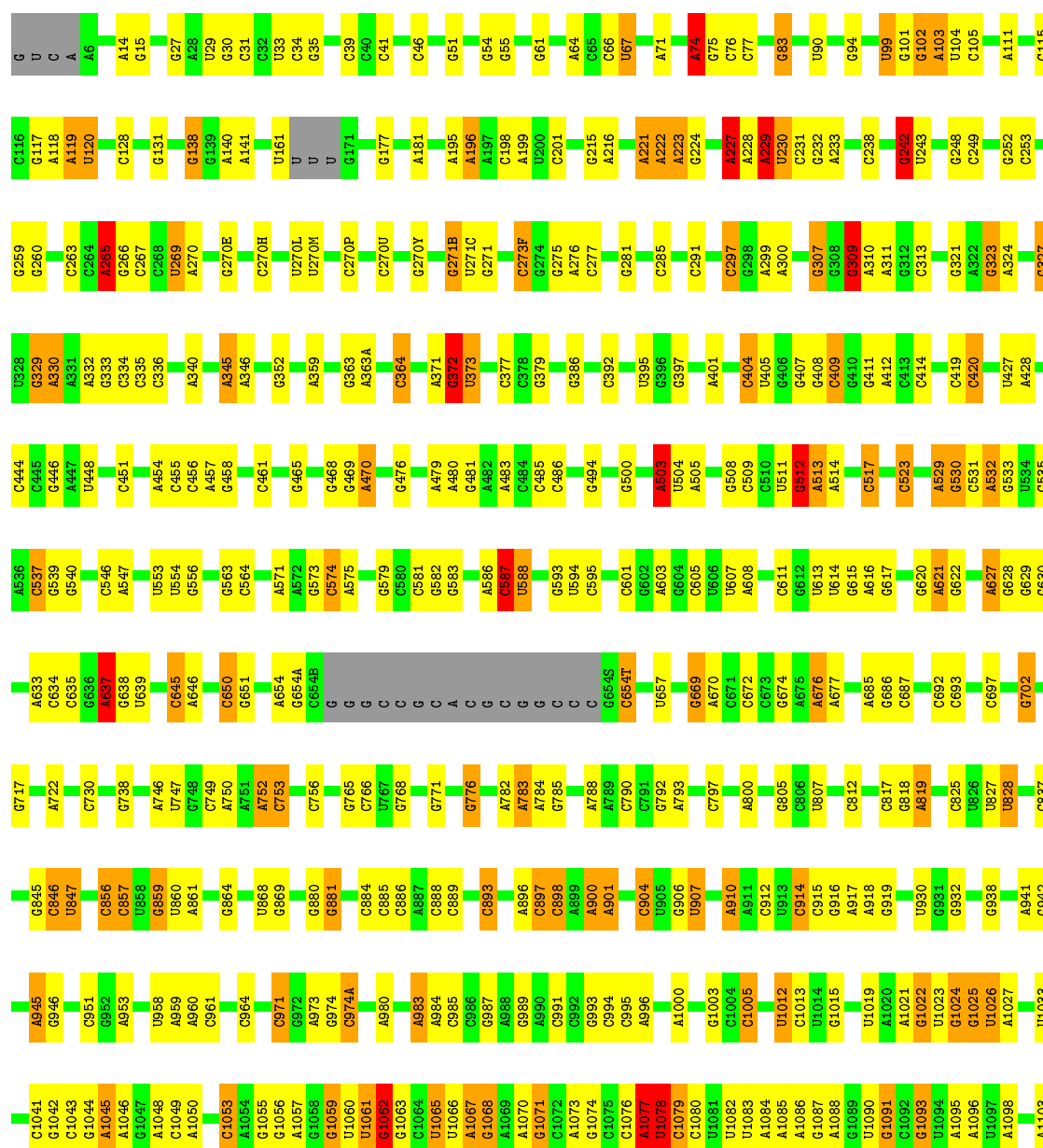




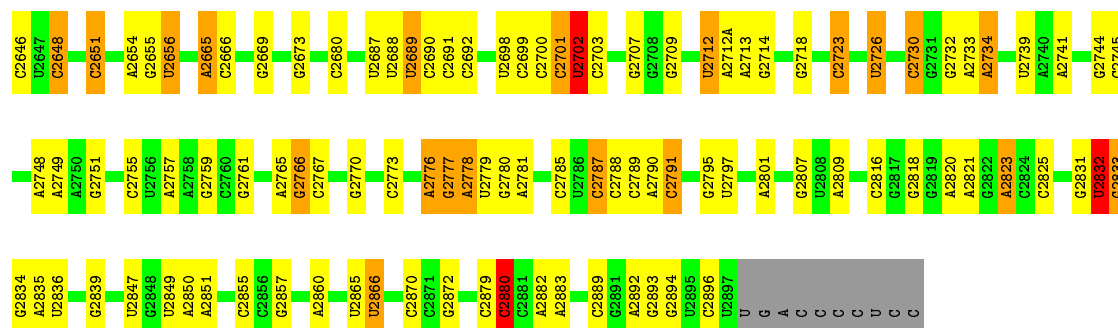
- Molecule 34: 50S ribosomal protein L36



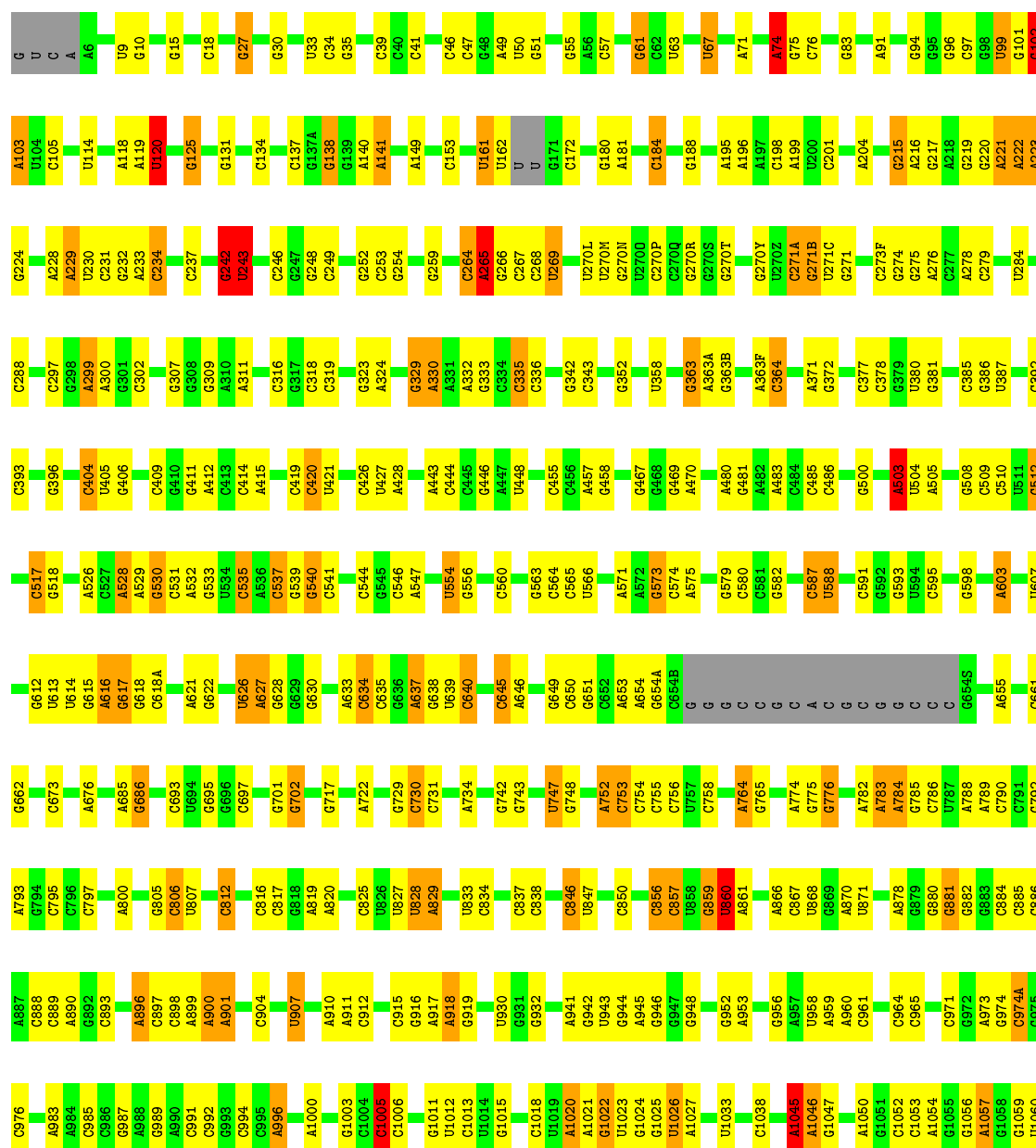
- Molecule 35: 23S rRNA



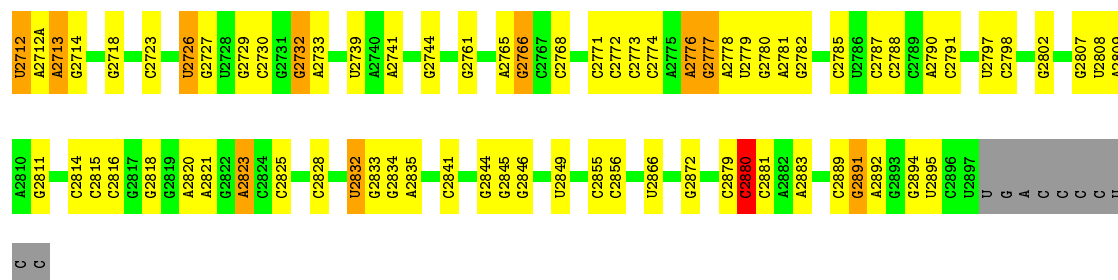
G2554	G2415	C2313	G2210	G1786	G1666	A1558	C1458	G1332	C1217	C1104
G2555	G2416	G2318	G2211	A1787	G1667	G1559	G1459	G1333	A1460	U1105
C2559	G2417	G2319	U2212	A1791	A1668	A1566	A1461	U1341	A1220	G1110
G2420	G2420	A2019	A2020	G1792	A1669	A1567	C1467	A1342	G1228	G1111
G2421	G2023	A2021	G2023	C1793	G1674	G1568	C1468	A1349	G1228	G1112
A2422	A2031	G2032	G2032	U1794	C1675	A1569	C1468	U1352	C1233	U1113
U2423	G2032	G2032	G2032	C1795	G1681	C1574	A1471	A1353	C1233	G1122
G2424	G2033	G2033	G2033	U1796	C1686	C1575	C1474	A1365	G1236	C1123
G2425	G2036	G2036	G2036	C1797	U1688	U1578	G1479	G1368	G1237	C1124
A2426	G2037	G2037	G2037	U1798	A1689	A1586	G1479	G1369	G1238	U1130
G2427	G2038	G2038	G2038	C1800	A1690	A1587	G1480	G1370	G1239	G1131
G2428	G2039	G2039	G2039	C1804	C1691	C1588	U1482	C1376	U1240	C1135
G2429	G2040	G2040	G2040	G1811	C1694	C1589	G1484	C1377	G1244	G1136
A2430	G2041	G2041	G2041	A1815	G1695	G1595	G1485	C1378	G1252	G1137
A2435	G2042	G2042	G2042	G1816	A1698	C1598	A1490	A1378	A1253	G1138
G2439	G2043	G2043	G2043	U1817	C1703	C1599	C1493	U1255	U1254	G1139
G2440	G2044	G2044	G2044	A1818	G1708	C1600	A1494	G1256	C1257	C1140
C2441	G2045	G2045	G2045	U1820	C1708	A1603	A1495	A1384	C1258	A142A
G2445	G2046	G2046	G2046	G1827	C1711	C1607	A1496	G1385	A1155	A1155
A2448	G2047	G2047	G2047	A1829	G1725	A1608	U1497	A1262	A1262	G1168
G2468	G2048	G2048	G2048	C1832	G1728	A1609	C1502	U1263	U1263	G1169
A2469	G2049	G2049	G2049	U1833	A1729	C1611	U1503	G1264	A1265	G1170
G2470	G2050	G2050	G2050	G1834	U1730	C1615	C1504	C1403	G1266	G1171
C2471	G2051	G2051	G2051	U1835	G1731	A1616	C1506	C1404	C1404	G1172
G2475	G2052	G2052	G2052	C1844	C1734	C1617	C1509	U1405	G1271	A1174
A2478	G2053	G2053	G2053	A1847	C1742	A1618	A1510	U1406	A1272	U1175
G2483	G2054	G2054	G2054	A1848	G1743	G1622	A1511	C1407	U1273	G1176
G2484	G2055	G2055	G2055	G1858	G1756	C1630A	G1512	C1411	A1278	A1177
G2494	G2056	G2056	G2056	A1859	C1762	C1636	G1514	G1416	A1284	C1178
G2495	G2057	G2057	G2057	G1860	G1763	A1637	G1525	A1419	C1290	G1183
C2498	G2058	G2058	G2058	G1863	G1764	C1638	G1533	U1420	C1295	G1187
C2499	G2059	G2059	G2059	U1864	C1765	U1639	G1534	G1421	G1296	U1188
G2502	G2060	G2060	G2060	G1869	U1766	C1640	U1535	C1428	U1300	A1189
A2503	G2061	G2061	G2061	A1872	C1773	C1644	C1536	C1437	A1301	G1190
G2504	G2062	G2062	G2062	G1878	C1774	G1648	G1537	G1441	G1306	G1191
C2505	G2063	G2063	G2063	C1880	U1775	G1649	C1538	G1442	C1305	G1192
G2506	G2064	G2064	G2064	C1881	G1776	G1650	G1543	A1444A	G1309	A1194
A2518	G2065	G2065	G2065	C1882	U1777	G1651	C1544	C1445	C1306	G1195
U2519	G2066	G2066	G2066	G1883	U1778	G1652	A1545	U1312	U1312	A1204
G2527	G2067	G2067	G2067	A1884	U1779	G1653	C1546	U1313	U1313	G1206
U2528	G2068	G2068	G2068	A1885	A1780	G1654	C1547	A1449	C1314	A1210
G2529	G2069	G2069	G2069	C1888	C1782	C1657	C1548	G1454	G1319	U1211
A2542	G2070	G2070	G2070	A1889	A1783	C1658	A1554	U1454	U1329	G1212
G2543	G2071	G2071	G2071	U2011	A1784	C1658	A1554	G1455	U1329	A1214



- Molecule 35: 23S rRNA

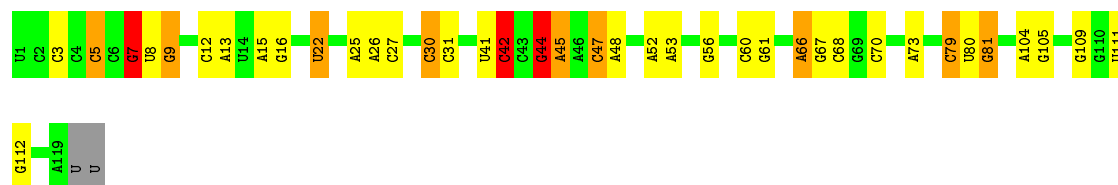


C2480	A2602	G2383	C2275	G2061	U1963	G1835	A1732	A1608		U1391	G1266	G1140	U1061
G2481	U2609	C2384	C2283	A2062	G1964	C1836	G1733	A1609	A1496	U1394	G1266	U1141	G1062
G2483	C2610	C2385		C2065	C1965	A1847	C1742	C1617	U1497	A1395	A1272	U1142	G1063
G2490	U2611	G2391	A2287	C2066	C1967	A1853	G1743	A1618	C1504	U1396	C1290	C1153	U1065
U2491	C2612	A2392	G2185	U2068	A1969	G1858	C1764	G1622	C1506		C1291		U1066
G2494	U2615	C2393	G2186	G2069	A1970	A1859	A1765	A1631	A1507		C1295	C1158	A1067
C2498	C2616	U2291	G2187	G2070	A1971	G1869	A1766		A1508		G1296		A1068
	G2617	A2169	A2071	G2072	A1972		A1767	C1638	C1509	C1402		G1173	A1069
G2502	G2618	A2170	C2403	C2073	G1979	A1872	G1763	U1639	A1510	C1407	U1300	A1174	A1070
A2503	C2619	A2171	C2404	U2074	G1980	G1878	G1764	C1640	A1511	C1408	A1301	G1176	G1071
U2504		U2172	G2075	U2076	A1981	G1879	C1765		U1514			A1177	G1074
G2506	A2632	A2173	U2077		C1982	C1880		C1644	U1514	C1411	C1306	C1178	C1075
		A2176	U2079	U2080	G1988	C1881	G1769	C1648	U1523	G1416		C1179	C1076
A2518		C2177			U1981	C1882	A1773				G1309		U1077
	C2646	C2178		G2090	G1982	G1883	G1776	G1651	A1528	A1419	G1310	G1187	U1078
G2524	U2653	C2185	G2307		U1991	A1884		A1652	A1529	U1420	U1188	U1188	U1082
G2525	A2654	G2186	C2308	G2093	G1994		G1779	G1653	G1530	G1421	U1313	U1190	A1084
G2529	U2655	G2187	U1995	U2096	C1996	A1889	A1780	A1654	U1535	A1427	C1314	G1195	A1085
	U2656	C2188	U1995	C2097	G1996		C1781	C1656	A1536	C1428	C1315		A1086
A2542		U2189	C2006	U2098	C2006	C1892	A1784	C1657	C1537	U1433	G1327	C1200	A1087
G2543	G2659	G2190	G2009	U2099		C1893			G1539	A1434	U1329		A1088
G2544	A2660	G2191	U2100	U2101	G2010	G1896	A1785	C1662	G1540	C1437	G1332	G1203	G1089
G2545	U2661	U2102	G2101	G2102	U2011		A1787	G1667	U1541	U1438	C1333	A1204	U1093
U2547	A2662	A2198	U2102	A2013	A2013	G1899	C1788	A1668	G1542	A1444	G1338	U1206	U1094
				A2014	A2014	A1900	A1789	A1669	A1543	C1445			A1095
U2554		G2210	C2111	U2016	U2016	C1902	C1790	C1670	C1544		U1341	A1210	A1096
C2559	C2667	G2211	G2112	A2015	A2015	C1905	A1791		A1545	A1449	U1342	U1211	U1097
U2562		U2212	U2113			G1906	C1797	G1675	C1549	G1449	A1343	A1214	A1103
A2561	G2673	G2215	G2116	A2019	A2019	G1906	U1798			A1454	G1344		C1104
U2563		A2225	G2117	C2021	C2021	C1914	C1800	G1682	G1559	U1454		G1218	U1105
G2444		U2233	U2118	U2022	U2022		G1801	C1686		G1465	A1349	G1219	G1106
A2564	A2679	G2234	A2119	G2023	G2023	A1919	C1804		C1565	C1468	U1352	A1220	G1110
A2566	U2682	G2235	G2125	A2031	A2031	C1920	U1805	A1689	A1566	G1469	A1353	C1222	A1111
G2567	C2683	C2236	A2126	C2032	C2032	G1929	U1806	C1690	A1567	A1460	G1363	C1223	G1112
		G2237	G2127	A2033	A2033	U1931	U1808	C1691	G1568	G1461	G1364		U1113
U2572	U2687	C2238	C2128	U2034	U2034		G1811	U1692	A1569	C1462	C1365	G1233	C1121
C2573	U2688	G2239	C2129	G2035	G2035	A1937	G1816	G1695	A1570	C1467	G1366	G1238	G1122
G2574	U2689	U2243	U2130	C2039	C2039	A1938	G1817		A1571		A1366	G1239	G1123
C2575	C2690	G2246	G2131	G2043	G2043	U1939	U1818	A1698	U1578	A1471	G1367	U1240	G1124
G2576	C2691		U2132	C2044	C2044	U1940	U1819	G1699	A1579		G1368	G1125	G1125
A2577	C2692	G2246	G2133			C1947	U1820	A1700	A1581	G1478	C1370	A1246	A1126
G2578	U2698	U2249	C2138	G2053	G2053		G1824		C1585	G1479	C1376		A1129
C2579		G2253	G2146	A2054	A2054	G1950	A1825	G1725	A1586	U1479		G1250	U1130
U2580	C2701	C2258	C2147	C2055	C2055	U1955	G1826		G1484	G1483	A1379	C1251	G1131
U2584	U2702	G2259	G2148	G2056	G2056	U1956	G1827	G1728	G1595	G1485	A1384	G1256	C1135
C2585		C2268	G2149	A2057	A2057	U1957	C1827		C1598	A1490	G1385	G1256	G1136
U2586	G2707	C2268	G2150	A2058	A2058	C1958	A1829	U1729	C1598		C1386	G1264	G1137
C2587	U2708		G2151	A2059	A2059			U1730			C1387		G1138
G2592	C2710												G1139
G2597	A2711												



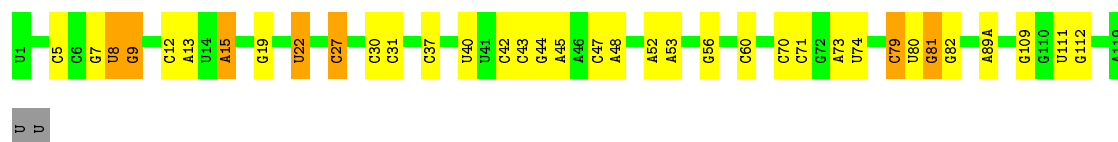
• Molecule 36: 5S rRNA

Chain RB: 66% 22% 7% . .



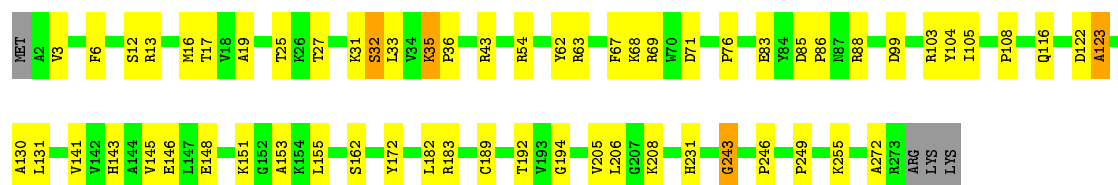
• Molecule 36: 5S rRNA

Chain YB: 69% 24% 6% .



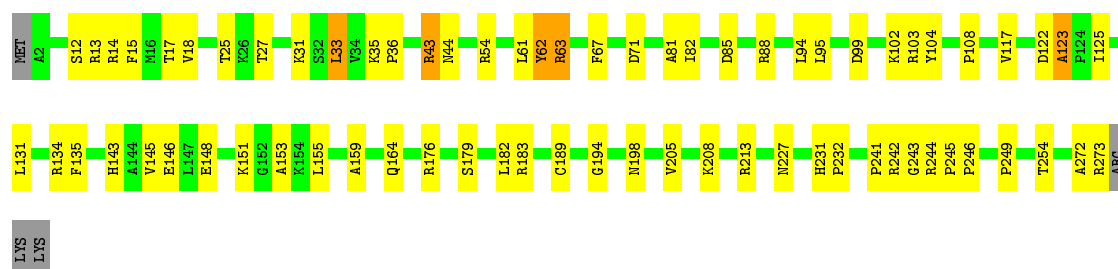
• Molecule 37: 50S ribosomal protein L2

Chain RD: 76% 21% . .

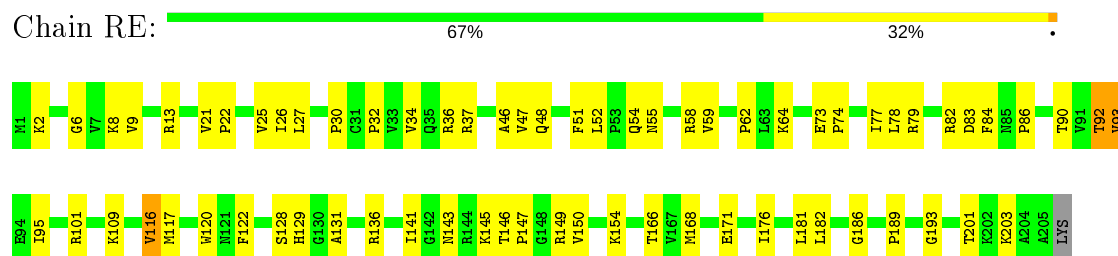


• Molecule 37: 50S ribosomal protein L2

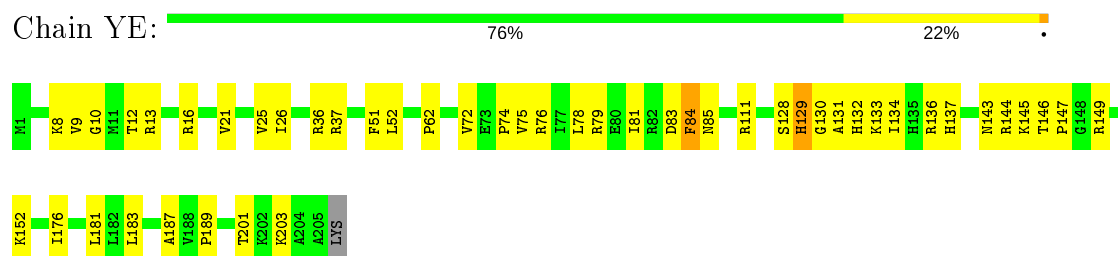
Chain YD: 73% 24% . .



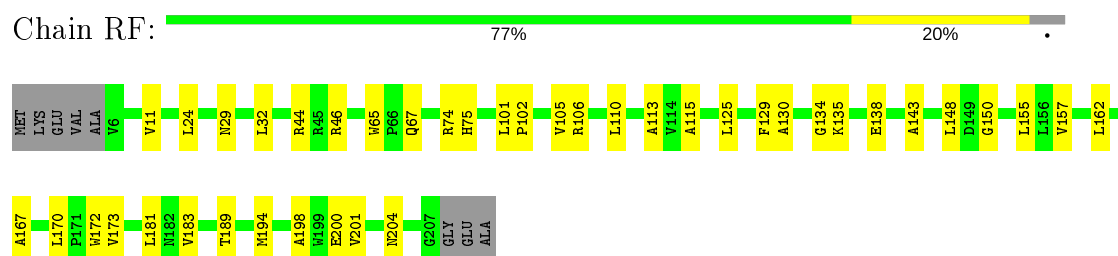
- Molecule 38: 50S ribosomal protein L3



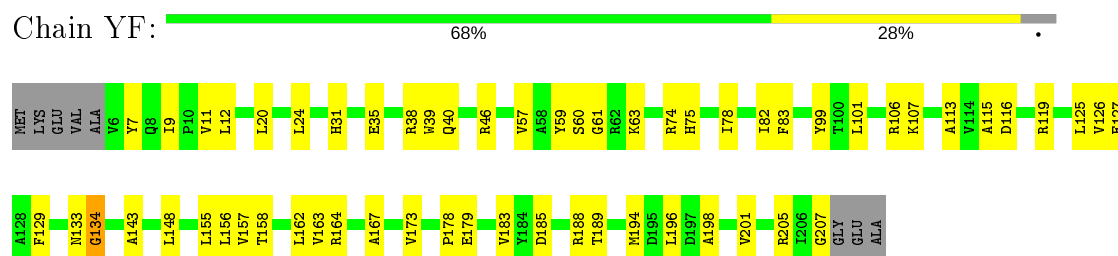
- Molecule 38: 50S ribosomal protein L3



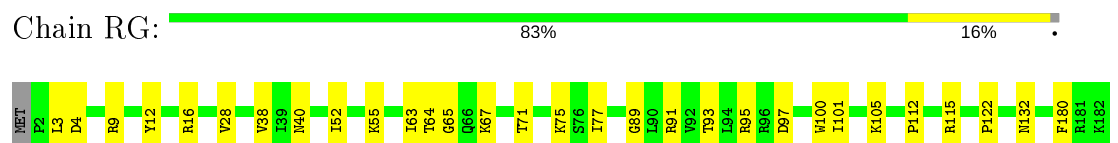
- Molecule 39: 50S ribosomal protein L4




- Molecule 39: 50S ribosomal protein L4

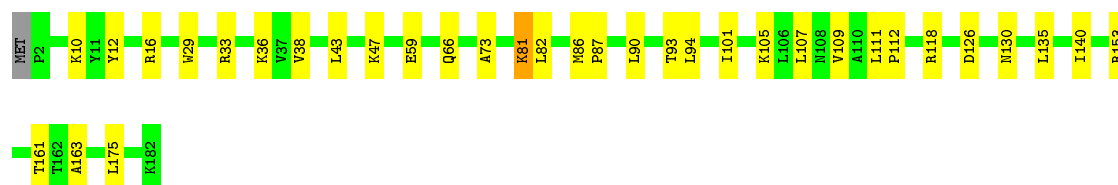


- Molecule 40: 50S ribosomal protein L5




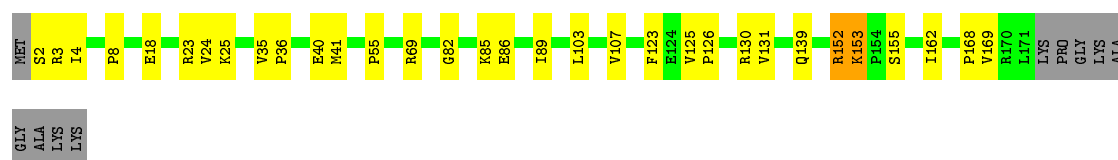
- Molecule 40: 50S ribosomal protein L5

Chain YG:  81% 18% ..




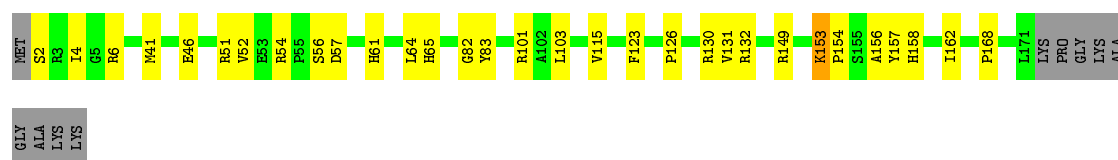
- Molecule 41: 50S ribosomal protein L6

Chain RH:  77% 17% • 6%



- Molecule 41: 50S ribosomal protein L6

Chain YH:  77% 17% • 6%




- Molecule 42: 50S ribosomal protein L9

Chain RI:  76% 20% ..




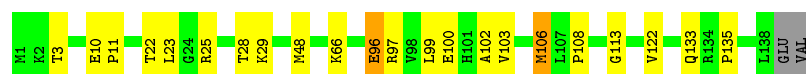
- Molecule 42: 50S ribosomal protein L9

Chain YI:  81% 17% ..




- Molecule 43: 50S ribosomal protein L13

Chain RN:  83% 14% ..




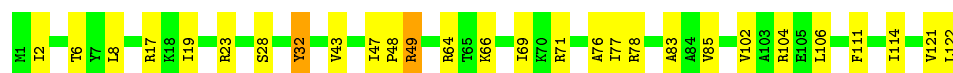
- Molecule 43: 50S ribosomal protein L13

Chain YN:  87% 11% ..




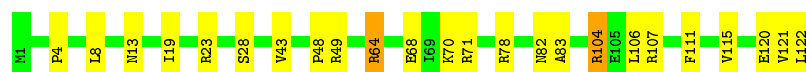
- Molecule 44: 50S ribosomal protein L14

Chain RO:  77% 21% .



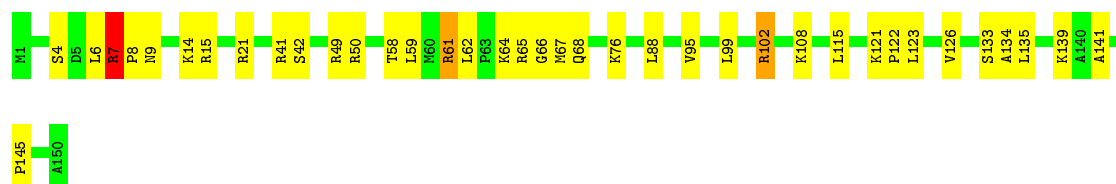
- Molecule 44: 50S ribosomal protein L14

Chain YO:  80% 18% .




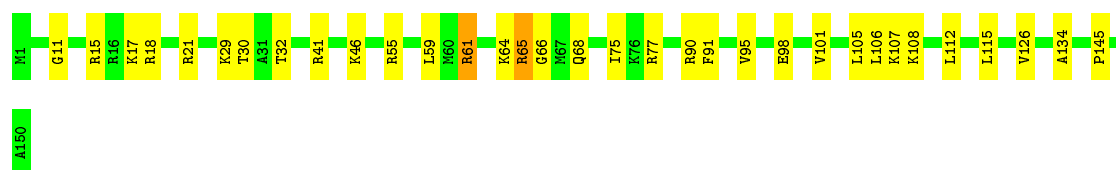
- Molecule 45: 50S ribosomal protein L15

Chain RP:  75% 23% ..




- Molecule 45: 50S ribosomal protein L15

Chain YP:  78% 21% .




- Molecule 46: 50S ribosomal protein L16

Chain RQ:  82% 16% .



- Molecule 46: 50S ribosomal protein L16

Chain YQ:  79% 18% .



- Molecule 47: 50S ribosomal protein L17

Chain RR: 80% 19%



- Molecule 47: 50S ribosomal protein L17

Chain YR: 81% 19%



- Molecule 48: 50S ribosomal protein L18

Chain RS: 85% 11%



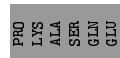
- Molecule 48: 50S ribosomal protein L18

Chain YS: 79% 17%



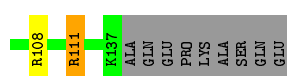
- Molecule 49: 50S ribosomal protein L19

Chain RT: 70% 23% 6%




- Molecule 49: 50S ribosomal protein L19

Chain YT: 67% 25% 6%




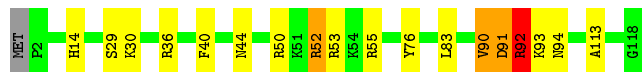
- Molecule 50: 50S ribosomal protein L20

Chain RU:  81% 16% ...




- Molecule 50: 50S ribosomal protein L20

Chain YU:  84% 12% ..




- Molecule 51: 50S ribosomal protein L21

Chain RV:  74% 25% .




- Molecule 51: 50S ribosomal protein L21

Chain YV:  86% 12% ..




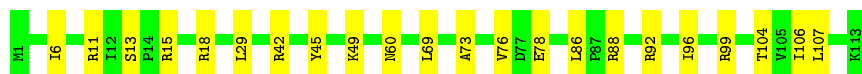
- Molecule 52: 50S ribosomal protein L22

Chain RW:  81% 19%



- Molecule 52: 50S ribosomal protein L22

Chain YW:  81% 19%




- Molecule 53: 50S ribosomal protein L23

Chain RX:  80% 16% .




- Molecule 53: 50S ribosomal protein L23

Chain YX:  82% 13% • •




- Molecule 54: 50S ribosomal protein L24

Chain RY:  76% 15% • 7%



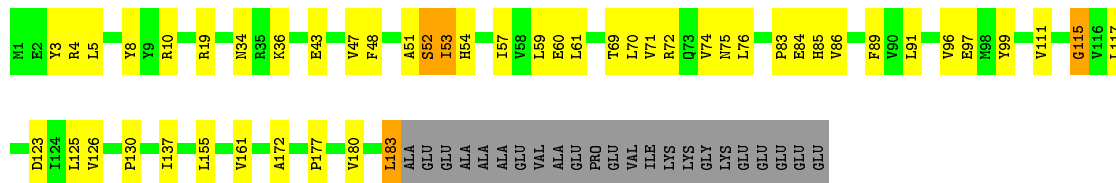
- Molecule 54: 50S ribosomal protein L24

Chain YY:  81% 12% 7%



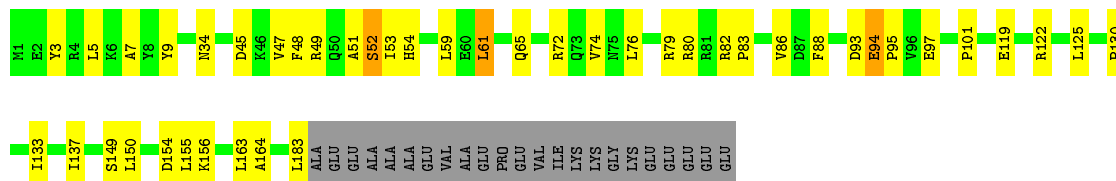
- Molecule 55: 50S ribosomal protein L25

Chain RZ:  65% 22% • 11%



- Molecule 55: 50S ribosomal protein L25

Chain YZ:  67% 20% • 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	209.38Å 449.76Å 619.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.74 – 3.10	Depositor
% Data completeness (in resolution range)	97.2 (49.74-3.10)	Depositor
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.225 , 0.266	Depositor
Wilson B-factor (Å ²)	68.8	Xtriage
Anisotropy	0.328	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	294981	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% 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	1.05	0/36098	1.14	177/56341 (0.3%)
1	XA	1.14	0/36101	1.18	234/56346 (0.4%)
2	QB	0.48	0/1959	0.68	0/2642
2	XB	0.55	0/1959	0.68	0/2642
3	QC	0.50	0/1629	0.69	2/2195 (0.1%)
3	XC	0.52	0/1629	0.66	0/2195
4	QD	0.58	0/1704	0.63	0/2284
4	XD	0.58	0/1704	0.65	0/2284
5	QE	0.55	1/1171 (0.1%)	0.67	0/1576
5	XE	0.54	0/1171	0.65	1/1576 (0.1%)
6	QF	0.60	0/856	0.62	0/1154
6	XF	0.58	0/856	0.66	0/1154
7	QG	0.51	0/1276	0.65	1/1709 (0.1%)
7	XG	0.52	0/1276	0.65	0/1709
8	QH	0.51	0/1136	0.66	0/1527
8	XH	0.59	0/1136	0.66	0/1527
9	QI	0.53	0/1029	0.77	0/1379
9	XI	0.53	0/1029	0.72	0/1379
10	QJ	0.46	0/814	0.64	0/1095
10	XJ	0.53	0/814	0.63	0/1095
11	QK	0.55	0/900	0.64	0/1213
11	XK	0.53	0/900	0.63	0/1213
12	QL	0.56	0/991	0.76	3/1327 (0.2%)
12	XL	0.63	0/991	0.75	1/1327 (0.1%)
13	QM	0.52	0/974	0.79	1/1303 (0.1%)
13	XM	0.50	0/974	0.72	0/1303
14	QN	0.55	0/501	0.67	0/664
14	XN	0.62	0/501	0.75	0/664
15	QO	0.50	0/745	0.59	0/992
15	XO	0.48	0/745	0.59	0/992
16	QP	0.58	0/721	0.75	2/970 (0.2%)
16	XP	0.55	0/721	0.76	1/970 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.60	0/847	0.65	1/1131 (0.1%)
17	XQ	0.59	0/847	0.64	1/1131 (0.1%)
18	QR	0.59	0/579	0.73	0/768
18	XR	0.57	0/579	0.65	0/768
19	QS	0.47	0/689	0.70	0/926
19	XS	0.62	0/689	0.97	2/926 (0.2%)
20	QT	0.48	0/765	0.66	0/1007
20	XT	0.44	0/765	0.71	1/1007 (0.1%)
21	QU	0.59	0/221	0.73	0/288
21	XU	0.67	0/221	0.81	1/288 (0.3%)
22	QV	0.91	0/1832	1.23	17/2855 (0.6%)
22	XV	1.07	0/1832	1.13	7/2855 (0.2%)
23	QX	0.77	0/446	1.06	2/695 (0.3%)
23	XX	0.87	0/446	1.17	1/695 (0.1%)
24	QY	0.74	0/1790	1.20	15/2789 (0.5%)
24	XY	0.78	0/1790	1.20	10/2789 (0.4%)
25	R0	0.59	0/657	0.68	1/874 (0.1%)
25	Y0	0.69	0/657	0.69	0/874
26	R1	0.63	0/770	0.79	2/1022 (0.2%)
26	Y1	0.64	0/770	0.76	1/1022 (0.1%)
27	R2	0.52	0/583	0.68	0/771
27	Y2	0.56	0/583	0.75	0/771
28	R3	0.50	0/474	0.57	0/635
28	Y3	0.57	0/474	0.58	0/635
29	R4	0.61	0/594	1.05	2/795 (0.3%)
29	Y4	0.56	0/594	1.05	3/795 (0.4%)
30	R5	0.60	0/473	0.92	2/639 (0.3%)
30	Y5	0.68	0/473	0.74	0/639
31	R6	0.70	0/431	1.14	2/575 (0.3%)
31	Y6	0.73	0/431	1.04	2/575 (0.3%)
32	R7	0.66	0/438	0.66	0/575
32	Y7	0.71	0/438	0.71	0/575
33	R8	0.64	0/525	0.86	1/691 (0.1%)
33	Y8	0.78	1/525 (0.2%)	0.84	0/691
34	R9	0.61	0/310	0.54	0/407
34	Y9	0.67	0/310	0.60	0/407
35	RA	1.23	8/69521 (0.0%)	1.22	496/108529 (0.5%)
35	YA	1.38	19/69543 (0.0%)	1.26	627/108563 (0.6%)
36	RB	0.99	0/2878	1.19	16/4490 (0.4%)
36	YB	1.23	0/2878	1.22	17/4490 (0.4%)
37	RD	0.71	0/2165	0.76	1/2919 (0.0%)
37	YD	0.75	0/2165	0.78	2/2919 (0.1%)
38	RE	0.63	0/1601	0.82	4/2160 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YE	0.71	0/1601	0.85	1/2160 (0.0%)
39	RF	0.65	0/1620	0.67	0/2194
39	YF	0.72	1/1620 (0.1%)	0.71	1/2194 (0.0%)
40	RG	0.51	0/1499	0.72	0/2016
40	YG	0.55	0/1499	0.70	1/2016 (0.0%)
41	RH	0.50	0/1332	0.81	2/1802 (0.1%)
41	YH	0.63	0/1332	0.84	3/1802 (0.2%)
42	RI	0.59	2/1151 (0.2%)	0.90	7/1558 (0.4%)
42	YI	0.52	0/1151	0.83	2/1558 (0.1%)
43	RN	0.57	0/1131	0.71	1/1525 (0.1%)
43	YN	0.63	0/1131	0.74	2/1525 (0.1%)
44	RO	0.62	0/943	0.66	1/1269 (0.1%)
44	YO	0.72	0/943	0.76	2/1269 (0.2%)
45	RP	0.59	0/1162	0.89	0/1544
45	YP	0.61	0/1162	0.85	1/1544 (0.1%)
46	RQ	0.63	0/1143	0.83	2/1527 (0.1%)
46	YQ	0.71	0/1143	0.87	3/1527 (0.2%)
47	RR	0.62	0/982	0.69	0/1312
47	YR	0.64	0/982	0.72	0/1312
48	RS	0.55	0/892	0.92	5/1187 (0.4%)
48	YS	0.59	0/892	0.78	1/1187 (0.1%)
49	RT	0.61	0/1155	0.78	3/1542 (0.2%)
49	YT	0.66	0/1155	0.82	4/1542 (0.3%)
50	RU	0.61	0/982	0.67	1/1306 (0.1%)
50	YU	0.70	0/982	0.69	1/1306 (0.1%)
51	RV	0.58	0/790	0.82	2/1057 (0.2%)
51	YV	0.76	0/790	0.88	2/1057 (0.2%)
52	RW	0.66	0/911	0.70	0/1220
52	YW	0.64	0/911	0.66	0/1220
53	RX	0.66	0/739	0.70	0/993
53	YX	0.71	0/739	0.67	0/993
54	RY	0.59	0/798	0.69	0/1064
54	YY	0.70	0/798	0.76	0/1064
55	RZ	0.52	0/1493	0.81	4/2026 (0.2%)
55	YZ	0.56	0/1493	0.78	2/2026 (0.1%)
All	All	1.08	32/319657 (0.0%)	1.11	1714/478147 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
48	RS	0	1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	Y8	23	VAL	CB-CG1	-8.00	1.36	1.52
35	YA	528	A	N9-C4	-7.92	1.33	1.37
35	YA	1021	A	N9-C4	-7.85	1.33	1.37
35	YA	1142(A)	A	N9-C4	-7.78	1.33	1.37
35	YA	2287	A	N9-C4	-7.34	1.33	1.37
35	YA	27	G	N9-C4	-6.99	1.32	1.38
42	RI	133	HIS	C-N	6.98	1.47	1.34
35	RA	2448	A	N9-C4	-6.50	1.33	1.37
35	RA	1204	A	N9-C4	-6.20	1.34	1.37
35	YA	27	G	N3-C4	-6.14	1.31	1.35
35	RA	586	A	N9-C4	-6.03	1.34	1.37
5	QE	8	GLU	CG-CD	6.02	1.60	1.51
35	YA	1095	A	N9-C4	5.91	1.41	1.37
35	YA	2058	A	N9-C4	-5.69	1.34	1.37
35	YA	1020	A	N9-C4	-5.62	1.34	1.37
35	YA	783	A	N7-C5	-5.57	1.35	1.39
35	RA	1786	A	N7-C5	-5.48	1.35	1.39
35	YA	774	A	N9-C4	-5.43	1.34	1.37
35	YA	2561	A	N9-C4	-5.43	1.34	1.37
35	YA	829	A	N9-C4	-5.40	1.34	1.37
35	YA	1021	A	N3-C4	-5.39	1.31	1.34
35	RA	783	A	N9-C4	-5.37	1.34	1.37
35	YA	74	A	N9-C4	-5.35	1.34	1.37
35	YA	71	A	N9-C4	-5.27	1.34	1.37
35	YA	627	A	N9-C4	-5.24	1.34	1.37
35	YA	2452	C	N1-C6	-5.21	1.34	1.37
42	RI	134	PRO	N-CD	-5.19	1.40	1.47
35	RA	1142(A)	A	N9-C4	-5.13	1.34	1.37
35	RA	2378	A	N9-C4	-5.12	1.34	1.37
35	YA	1571	A	N9-C4	-5.10	1.34	1.37
35	RA	685	A	N9-C4	-5.06	1.34	1.37
39	YF	57	VAL	CB-CG1	-5.03	1.42	1.52

All (1714) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	XS	10	PHE	CB-CG-CD1	12.46	129.52	120.80
1	QA	1301	U	N1-C2-O2	11.86	131.10	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	2506	U	C2-N1-C1'	11.85	131.92	117.70
1	QA	1301	U	C2-N1-C1'	11.78	131.83	117.70
35	YA	2506	U	C2-N1-C1'	11.73	131.77	117.70
35	RA	2506	U	N3-C2-O2	-11.66	114.04	122.20
1	QA	328	C	N1-C2-O2	11.60	125.86	118.90
19	XS	10	PHE	CB-CG-CD2	-11.54	112.72	120.80
35	RA	2506	U	N1-C2-O2	11.50	130.85	122.80
1	XA	1336	C	N1-C2-O2	11.40	125.74	118.90
22	QV	17	C	N1-C2-O2	11.36	125.72	118.90
35	YA	2506	U	N1-C2-O2	11.16	130.61	122.80
35	YA	2506	U	N3-C2-O2	-11.13	114.41	122.20
35	YA	2688	U	N3-C2-O2	-11.00	114.50	122.20
35	RA	613	U	N3-C2-O2	-10.78	114.65	122.20
29	R4	43	TYR	CA-CB-CG	10.64	133.61	113.40
1	QA	1301	U	N3-C2-O2	-10.56	114.81	122.20
35	YA	856	C	C6-N1-C2	-10.56	116.08	120.30
35	RA	828	U	N3-C2-O2	-10.55	114.81	122.20
35	YA	2474	C	N1-C2-O2	10.52	125.21	118.90
22	QV	17	C	C2-N1-C1'	10.45	130.30	118.80
46	YQ	5	ARG	CG-CD-NE	-10.41	89.94	111.80
35	YA	860	U	N3-C2-O2	-10.23	115.04	122.20
35	YA	27	G	N3-C4-N9	-10.13	119.92	126.00
1	XA	1336	C	C2-N1-C1'	10.02	129.82	118.80
35	YA	1313	U	C2-N1-C1'	10.01	129.72	117.70
35	RA	1914	C	N1-C2-O2	9.99	124.89	118.90
1	XA	1336	C	N3-C2-O2	-9.98	114.91	121.90
22	QV	17(A)	U	N3-C2-O2	-9.82	115.33	122.20
1	XA	1054	C	N1-C2-O2	9.81	124.78	118.90
29	Y4	39	CYS	C-N-CA	9.74	146.06	121.70
22	QV	17	C	C6-N1-C2	-9.62	116.45	120.30
22	QV	17	C	N3-C2-O2	-9.59	115.19	121.90
35	RA	613	U	N1-C2-O2	9.59	129.51	122.80
35	YA	1396	U	N1-C2-O2	9.57	129.50	122.80
35	YA	265	A	O4'-C1'-N9	9.46	115.77	108.20
35	RA	1914	C	N3-C2-O2	-9.35	115.36	121.90
1	QA	1158	C	C2-N1-C1'	9.32	129.06	118.80
35	YA	1396	U	C2-N1-C1'	9.28	128.84	117.70
35	RA	2712	U	N3-C2-O2	-9.23	115.74	122.20
1	XA	792	A	O4'-C1'-N9	9.21	115.57	108.20
35	RA	828	U	C2-N1-C1'	9.18	128.71	117.70
48	RS	17	ARG	CG-CD-NE	9.14	130.99	111.80
1	XA	963	G	C6-C5-N7	-9.13	124.92	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	1396	U	N3-C2-O2	-9.03	115.88	122.20
35	RA	2755	C	C5-C6-N1	8.99	125.50	121.00
35	YA	2712	U	N3-C2-O2	-8.96	115.93	122.20
35	RA	1313	U	N3-C2-O2	-8.94	115.94	122.20
35	RA	1882	C	C6-N1-C2	-8.94	116.72	120.30
36	YB	31	C	C6-N1-C2	-8.91	116.73	120.30
35	YA	2584	U	N3-C2-O2	-8.88	115.98	122.20
35	RA	1914	C	C2-N1-C1'	8.87	128.55	118.80
35	YA	1314	C	N1-C2-O2	8.86	124.22	118.90
24	XY	59	U	N1-C2-O2	8.82	128.98	122.80
35	YA	650	C	C6-N1-C2	-8.80	116.78	120.30
35	YA	271(A)	C	N1-C2-O2	8.77	124.16	118.90
30	R5	3	LYS	C-N-CA	8.75	143.58	121.70
1	XA	1336	C	C6-N1-C2	-8.72	116.81	120.30
35	RA	837	C	C6-N1-C2	-8.71	116.82	120.30
35	RA	1313	U	C2-N1-C1'	8.70	128.14	117.70
24	QY	54	U	C5-C6-N1	8.69	127.05	122.70
35	RA	860	U	N3-C2-O2	-8.69	116.12	122.20
44	YO	71	ARG	CG-CD-NE	8.68	130.03	111.80
35	RA	856	C	C5-C6-N1	8.68	125.34	121.00
35	YA	2474	C	N3-C2-O2	-8.67	115.83	121.90
1	XA	1054	C	N3-C2-O2	-8.64	115.85	121.90
35	RA	856	C	C6-N1-C2	-8.64	116.84	120.30
1	XA	812	C	P-O3'-C3'	8.63	130.06	119.70
26	R1	10	LYS	C-N-CA	8.63	143.27	121.70
35	RA	828	U	N1-C2-O2	8.62	128.84	122.80
35	YA	1204	A	O4'-C1'-N9	8.58	115.07	108.20
35	YA	1121	C	C6-N1-C2	-8.56	116.87	120.30
35	YA	120	U	C2-N1-C1'	8.53	127.94	117.70
1	QA	1158	C	N1-C2-O2	8.52	124.01	118.90
1	XA	827	U	N3-C2-O2	-8.52	116.24	122.20
35	RA	1543	A	O4'-C1'-N9	8.51	115.01	108.20
1	QA	328	C	N3-C2-O2	-8.50	115.95	121.90
35	RA	2712	U	N1-C2-O2	8.46	128.72	122.80
35	RA	1332	G	N7-C8-N9	8.46	117.33	113.10
1	XA	1301	U	N1-C2-O2	8.44	128.70	122.80
1	QA	1301	U	C6-N1-C1'	-8.43	109.40	121.20
35	RA	2286	A	N9-C4-C5	-8.40	102.44	105.80
51	YV	81	TYR	CA-CB-CG	8.38	129.33	113.40
35	YA	753	C	C6-N1-C2	-8.38	116.95	120.30
35	RA	1204	A	O4'-C1'-N9	8.37	114.90	108.20
1	XA	739	C	C6-N1-C2	-8.35	116.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	1163	C	C6-N1-C2	-8.27	116.99	120.30
22	QV	17(A)	U	N1-C2-O2	8.27	128.59	122.80
35	RA	1407	C	N1-C2-O2	8.24	123.84	118.90
35	RA	2205	C	C6-N1-C2	-8.21	117.01	120.30
1	XA	827	U	C2-N1-C1'	8.19	127.53	117.70
35	YA	856	C	C5-C6-N1	8.17	125.08	121.00
35	YA	120	U	N1-C2-O2	8.15	128.50	122.80
1	XA	346	G	N3-C4-N9	8.14	130.89	126.00
35	YA	860	U	C2-N1-C1'	8.12	127.45	117.70
35	YA	271(A)	C	N3-C2-O2	-8.12	116.22	121.90
35	YA	1931	U	N3-C2-O2	-8.11	116.52	122.20
35	RA	1407	C	C6-N1-C2	-8.10	117.06	120.30
35	YA	1914	C	C2-N1-C1'	8.09	127.69	118.80
35	YA	120	U	N3-C2-O2	-8.08	116.54	122.20
35	YA	860	U	N1-C2-O2	8.08	128.46	122.80
35	RA	915	C	C6-N1-C2	-8.07	117.07	120.30
35	YA	2856	C	C6-N1-C2	-8.07	117.07	120.30
12	QL	105	TYR	CA-CB-CG	8.07	128.73	113.40
35	RA	1404	C	N1-C2-O2	8.06	123.74	118.90
1	QA	254	G	O5'-P-OP1	-8.06	98.45	105.70
35	YA	1402	C	C6-N1-C2	-8.03	117.09	120.30
35	RA	2712	U	C2-N1-C1'	8.03	127.33	117.70
35	RA	1654	A	O5'-P-OP1	-8.02	98.49	105.70
35	YA	912	C	C6-N1-C2	-8.01	117.10	120.30
1	QA	328	C	C2-N1-C1'	8.00	127.60	118.80
35	YA	2688	U	N1-C2-O2	7.99	128.39	122.80
35	YA	1881	C	C6-N1-C2	-7.98	117.11	120.30
1	XA	1301	U	N3-C2-O2	-7.97	116.62	122.20
35	YA	560	C	N1-C2-O2	7.95	123.67	118.90
35	RA	2702	U	N1-C2-O2	7.94	128.36	122.80
1	XA	1158	C	C2-N1-C1'	7.92	127.51	118.80
35	RA	2506	U	C6-N1-C1'	-7.91	110.12	121.20
35	RA	595	C	C5-C6-N1	7.89	124.94	121.00
24	QY	70	U	N1-C2-O2	7.84	128.28	122.80
1	QA	960	U	N1-C2-O2	7.83	128.28	122.80
22	QV	17(A)	U	C2-N1-C1'	7.81	127.07	117.70
35	RA	2210	G	C4-N9-C1'	7.80	136.63	126.50
35	RA	2755	C	C6-N1-C2	-7.79	117.19	120.30
22	XV	17(A)	U	N3-C2-O2	-7.78	116.76	122.20
35	YA	1314	C	C6-N1-C2	-7.77	117.19	120.30
35	YA	2584	U	C2-N1-C1'	7.77	127.02	117.70
35	YA	528	A	C2-N3-C4	-7.75	106.72	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	1956	U	N3-C2-O2	-7.75	116.77	122.20
1	QA	1336	C	N1-C2-O2	7.74	123.55	118.90
35	YA	1178	C	C6-N1-C2	-7.74	117.20	120.30
35	YA	1313	U	N3-C2-O2	-7.73	116.79	122.20
35	YA	1879	C	C6-N1-C2	-7.73	117.21	120.30
35	RA	1804	C	C6-N1-C2	-7.73	117.21	120.30
35	RA	2584	U	N3-C2-O2	-7.69	116.81	122.20
35	RA	2591	C	C6-N1-C2	-7.69	117.22	120.30
35	YA	2832	U	P-O3'-C3'	7.69	128.93	119.70
35	YA	385	C	N3-C2-O2	-7.69	116.52	121.90
35	RA	650	C	C6-N1-C2	-7.68	117.23	120.30
22	QV	17(A)	U	C6-N1-C2	-7.68	116.39	121.00
35	YA	1376	C	N1-C2-O2	7.68	123.51	118.90
48	RS	17	ARG	CD-NE-CZ	7.67	134.34	123.60
1	QA	1322	C	N1-C2-O2	7.67	123.50	118.90
35	RA	1314	C	C5-C6-N1	7.66	124.83	121.00
35	YA	898	C	N1-C2-O2	7.66	123.50	118.90
1	XA	328	C	N1-C2-O2	7.65	123.49	118.90
35	YA	2506	U	C6-N1-C1'	-7.65	110.48	121.20
35	RA	2702	U	N3-C2-O2	-7.65	116.84	122.20
35	YA	1899	G	C4-N9-C1'	7.65	136.44	126.50
35	RA	1786	A	N7-C8-N9	7.65	117.62	113.80
35	YA	1306	C	C6-N1-C2	-7.65	117.24	120.30
35	YA	817	C	C6-N1-C2	-7.64	117.24	120.30
35	YA	1914	C	N1-C2-O2	7.64	123.48	118.90
35	RA	2703	C	N1-C2-O2	7.63	123.48	118.90
35	YA	1314	C	C2-N1-C1'	7.63	127.19	118.80
35	RA	650	C	C5-C6-N1	7.63	124.81	121.00
24	XY	59	U	N3-C2-O2	-7.63	116.86	122.20
36	YB	22	U	C5-C6-N1	7.62	126.51	122.70
35	RA	1899	G	C4-N9-C1'	7.62	136.40	126.50
35	YA	837	C	C6-N1-C2	-7.61	117.25	120.30
35	YA	1437	C	N1-C2-O2	7.61	123.46	118.90
35	RA	1992	G	C2'-C3'-O3'	7.60	126.23	109.50
35	RA	1882	C	C5-C6-N1	7.60	124.80	121.00
35	YA	930	U	C2-N1-C1'	7.59	126.81	117.70
35	YA	1950	G	C4-N9-C1'	7.59	136.36	126.50
31	Y6	7	ILE	C-N-CA	7.58	140.66	121.70
31	R6	7	ILE	C-N-CA	7.58	140.65	121.70
35	YA	2712	U	N1-C2-O2	7.58	128.11	122.80
35	YA	1021	A	C8-N9-C4	-7.58	102.77	105.80
1	XA	328	C	C2-N1-C1'	7.58	127.13	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	RB	70	C	C6-N1-C2	-7.55	117.28	120.30
1	XA	963	G	N3-C4-N9	7.55	130.53	126.00
35	YA	758	C	C6-N1-C2	-7.55	117.28	120.30
35	YA	97	C	C6-N1-C2	-7.53	117.29	120.30
35	YA	243	U	C5-C6-N1	7.53	126.47	122.70
35	RA	669	G	C4-N9-C1'	7.52	136.27	126.50
35	YA	1578	U	N3-C2-O2	-7.51	116.94	122.20
35	RA	613	U	C2-N1-C1'	7.51	126.71	117.70
24	XY	72	C	N1-C2-O2	7.51	123.40	118.90
35	YA	2210	G	C4-N9-C1'	7.51	136.26	126.50
1	XA	826	C	C6-N1-C2	-7.50	117.30	120.30
35	RA	912	C	C6-N1-C2	-7.49	117.30	120.30
35	YA	378	C	C6-N1-C2	-7.48	117.31	120.30
35	RA	2350	C	N1-C2-O2	7.48	123.39	118.90
35	RA	1407	C	C2-N1-C1'	7.47	127.02	118.80
35	RA	1332	G	C4-N9-C1'	7.47	136.21	126.50
35	YA	2559	C	C5-C6-N1	7.47	124.73	121.00
1	XA	1024	G	O5'-P-OP1	7.47	119.66	110.70
1	QA	1158	C	N3-C2-O2	-7.46	116.68	121.90
1	XA	749	C	C6-N1-C2	-7.46	117.31	120.30
35	RA	1644	C	C6-N1-C2	-7.45	117.32	120.30
35	RA	2210	G	C8-N9-C1'	-7.44	117.33	127.00
33	R8	61	LEU	C-N-CA	7.42	140.26	121.70
35	YA	2712	U	C2-N1-C1'	7.42	126.60	117.70
35	YA	1313	U	N1-C2-O2	7.41	127.99	122.80
1	QA	1066	C	N1-C2-O2	7.39	123.33	118.90
1	QA	1407	C	C5-C6-N1	7.38	124.69	121.00
1	QA	1297	C	P-O3'-C3'	7.38	128.56	119.70
35	YA	1955	U	N3-C2-O2	-7.38	117.03	122.20
35	RA	1558	A	P-O3'-C3'	7.35	128.52	119.70
1	XA	328	C	P-O3'-C3'	7.35	128.52	119.70
35	RA	227	A	P-O3'-C3'	7.34	128.51	119.70
1	XA	699	C	C6-N1-C2	-7.34	117.36	120.30
35	YA	2474	C	C2-N1-C1'	7.33	126.87	118.80
1	QA	960	U	C2-N1-C1'	7.33	126.50	117.70
35	YA	1332	G	N7-C8-N9	7.31	116.75	113.10
35	YA	2559	C	C6-N1-C2	-7.31	117.38	120.30
35	YA	1332	G	C6-C5-N7	-7.30	126.02	130.40
35	YA	2044	C	C6-N1-C2	-7.30	117.38	120.30
1	QA	1161	C	N1-C2-O2	7.30	123.28	118.90
1	XA	346	G	N3-C4-C5	-7.29	124.95	128.60
35	YA	783	A	N7-C8-N9	7.29	117.45	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	2712	U	P-O3'-C3'	7.29	128.45	119.70
35	YA	1314	C	N3-C2-O2	-7.27	116.81	121.90
35	YA	634	C	C6-N1-C2	-7.27	117.39	120.30
1	XA	972	C	C6-N1-C2	-7.26	117.39	120.30
35	YA	783	A	C5-N7-C8	-7.26	100.27	103.90
35	YA	385	C	C2-N1-C1'	7.25	126.77	118.80
35	RA	2044	C	C6-N1-C2	-7.25	117.40	120.30
3	QC	23	TYR	CA-CB-CG	7.23	127.14	113.40
35	RA	420	C	C6-N1-C2	-7.23	117.41	120.30
35	RA	898	C	N1-C2-O2	7.23	123.24	118.90
35	YA	1026	U	P-O3'-C3'	7.23	128.38	119.70
35	RA	140	A	N7-C8-N9	7.23	117.42	113.80
24	XY	59	U	C2-N1-C1'	7.22	126.37	117.70
35	YA	560	C	N3-C2-O2	-7.22	116.84	121.90
35	YA	2646	C	N1-C2-O2	7.22	123.23	118.90
1	XA	254	G	O5'-P-OP1	-7.22	99.20	105.70
35	YA	161	U	N3-C2-O2	-7.22	117.15	122.20
1	XA	314	C	C6-N1-C2	-7.21	117.42	120.30
1	QA	789	U	N3-C2-O2	-7.21	117.16	122.20
35	RA	1313	U	N1-C2-O2	7.20	127.84	122.80
35	RA	2286	A	C8-N9-C4	7.19	108.68	105.80
35	YA	333	G	C4-N9-C1'	7.19	135.85	126.50
35	YA	1174	A	C2-N3-C4	7.19	114.20	110.60
1	QA	1407	C	C6-N1-C2	-7.19	117.42	120.30
1	XA	749	C	C5-C6-N1	7.19	124.59	121.00
35	YA	2403	C	N1-C2-O2	7.19	123.22	118.90
35	YA	2880	C	C6-N1-C2	-7.19	117.42	120.30
35	RA	2591	C	C5-C6-N1	7.18	124.59	121.00
35	RA	2787	C	N1-C2-O2	7.18	123.21	118.90
35	YA	385	C	N1-C2-O2	7.18	123.21	118.90
35	YA	846	C	O5'-P-OP1	-7.18	99.24	105.70
35	RA	1305	C	N1-C2-O2	7.17	123.20	118.90
1	QA	1440	C	N1-C2-O2	7.17	123.20	118.90
35	YA	2044	C	C5-C6-N1	7.16	124.58	121.00
35	YA	1914	C	N3-C2-O2	-7.15	116.89	121.90
1	XA	435	C	C6-N1-C2	-7.14	117.44	120.30
35	YA	2681	C	P-O3'-C3'	7.14	128.26	119.70
1	QA	328	C	P-O3'-C3'	7.13	128.26	119.70
35	RA	120	U	N1-C2-O2	7.12	127.79	122.80
35	RA	140	A	C8-N9-C4	-7.12	102.95	105.80
35	RA	1881	C	C6-N1-C2	-7.11	117.46	120.30
35	RA	1022	G	P-O3'-C3'	7.11	128.23	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	2584	U	C2-N1-C1'	7.11	126.23	117.70
35	RA	1314	C	C6-N1-C2	-7.10	117.46	120.30
35	YA	1640	C	C5-C6-N1	7.10	124.55	121.00
35	RA	120	U	C2-N1-C1'	7.10	126.22	117.70
35	YA	27	G	N3-C2-N2	-7.08	114.94	119.90
55	RZ	183	LEU	CA-CB-CG	7.08	131.58	115.30
35	YA	537	C	C6-N1-C2	-7.07	117.47	120.30
35	YA	1535	U	C2-N1-C1'	7.07	126.18	117.70
35	RA	229	A	OP2-P-O3'	7.07	120.75	105.20
48	RS	36	TYR	CA-CB-CG	7.07	126.83	113.40
1	QA	346	G	N3-C4-N9	7.06	130.24	126.00
24	QY	70	U	C5-C6-N1	7.06	126.23	122.70
36	YB	31	C	C2-N1-C1'	7.06	126.56	118.80
36	YB	70	C	C6-N1-C2	-7.06	117.48	120.30
35	YA	1021	A	C2-N3-C4	-7.06	107.07	110.60
35	RA	1314	C	N1-C2-O2	7.05	123.13	118.90
35	RA	229	A	P-O3'-C3'	7.05	128.16	119.70
35	RA	1332	G	C8-N9-C4	-7.05	103.58	106.40
35	RA	1407	C	C5-C6-N1	7.05	124.52	121.00
1	QA	311	C	C6-N1-C2	-7.05	117.48	120.30
1	QA	1322	C	N3-C2-O2	-7.03	116.98	121.90
35	YA	528	A	N3-C4-N9	-7.03	121.78	127.40
35	RA	66	C	C6-N1-C2	-7.02	117.49	120.30
1	QA	337	C	C6-N1-C2	-7.02	117.49	120.30
1	XA	1109	C	C6-N1-C2	-7.02	117.49	120.30
35	RA	1658	C	C6-N1-C2	-7.00	117.50	120.30
1	XA	827	U	N1-C2-O2	7.00	127.70	122.80
35	YA	2403	C	C6-N1-C2	-7.00	117.50	120.30
35	RA	1332	G	C6-C5-N7	-7.00	126.20	130.40
35	RA	2559	C	N1-C2-O2	7.00	123.10	118.90
1	QA	1285	A	P-O3'-C3'	7.00	128.10	119.70
22	XV	17(A)	U	N1-C2-O2	6.99	127.69	122.80
22	QV	17	C	C5-C6-N1	6.98	124.49	121.00
35	RA	1407	C	N3-C2-O2	-6.98	117.01	121.90
35	YA	2688	U	C2-N1-C1'	6.98	126.07	117.70
1	QA	1203	C	C6-N1-C2	-6.98	117.51	120.30
35	YA	385	C	C6-N1-C2	-6.97	117.51	120.30
16	XP	38	TYR	CA-CB-CG	6.97	126.64	113.40
35	RA	1598	C	C6-N1-C2	-6.96	117.52	120.30
35	RA	2210	G	N3-C4-N9	6.96	130.18	126.00
35	YA	1095	A	C2-N3-C4	6.94	114.07	110.60
35	YA	528	A	N3-C4-C5	6.94	131.66	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	792	A	P-O3'-C3'	6.94	128.03	119.70
35	YA	930	U	N1-C2-O2	6.94	127.66	122.80
36	YB	31	C	N3-C2-O2	-6.93	117.05	121.90
35	YA	1314	C	C5-C6-N1	6.92	124.46	121.00
1	XA	812	C	OP2-P-O3'	6.92	120.41	105.20
35	YA	1407	C	C5-C6-N1	6.91	124.45	121.00
35	YA	1558	A	P-O3'-C3'	6.90	127.98	119.70
35	RA	2044	C	C5-C6-N1	6.89	124.44	121.00
35	YA	828	U	C2-N1-C1'	6.88	125.96	117.70
35	YA	1899	G	N3-C4-N9	6.88	130.13	126.00
1	XA	449	C	C2-N1-C1'	6.87	126.36	118.80
1	XA	963	G	N1-C2-N2	-6.87	110.02	116.20
1	QA	1065	U	P-O3'-C3'	6.87	127.94	119.70
39	YF	7	TYR	CA-CB-CG	6.87	126.45	113.40
1	XA	789	U	C2-N1-C1'	6.87	125.94	117.70
35	RA	1882	C	C2-N1-C1'	6.86	126.34	118.80
1	XA	789	U	N3-C2-O2	-6.85	117.40	122.20
35	YA	613	U	N3-C2-O2	-6.85	117.40	122.20
35	YA	1496	A	N7-C8-N9	6.85	117.22	113.80
35	YA	2889	C	C6-N1-C2	-6.85	117.56	120.30
35	YA	2321	G	C4-N9-C1'	6.85	135.40	126.50
1	XA	980	C	C6-N1-C2	-6.83	117.57	120.30
35	RA	753	C	C6-N1-C2	-6.83	117.57	120.30
35	YA	1686	C	C6-N1-C2	-6.83	117.57	120.30
35	YA	1022	G	P-O3'-C3'	6.82	127.89	119.70
35	RA	1793	C	C6-N1-C2	-6.82	117.57	120.30
35	RA	1124	C	C6-N1-C2	-6.82	117.57	120.30
1	QA	1066	C	C2-N1-C1'	6.81	126.30	118.80
35	RA	817	C	C6-N1-C2	-6.81	117.58	120.30
35	YA	2895	U	C5-C6-N1	6.81	126.10	122.70
1	QA	1024	G	O5'-P-OP1	6.80	118.86	110.70
43	YN	48	MET	CG-SD-CE	-6.80	89.32	100.20
22	QV	17(A)	U	C5-C6-N1	6.79	126.10	122.70
1	XA	58	C	C6-N1-C2	-6.79	117.58	120.30
35	RA	2688	U	N3-C2-O2	-6.79	117.45	122.20
35	YA	404	C	P-O3'-C3'	6.79	127.84	119.70
35	RA	1908	C	C6-N1-C2	-6.78	117.59	120.30
35	YA	661	C	C6-N1-C2	-6.77	117.59	120.30
1	QA	812	C	P-O3'-C3'	6.77	127.83	119.70
21	XU	18	TYR	CA-CB-CG	6.77	126.27	113.40
35	YA	846	C	P-O3'-C3'	6.77	127.82	119.70
35	RA	1233	C	C6-N1-C2	-6.76	117.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	828	U	N3-C2-O2	-6.76	117.46	122.20
35	RA	1437	C	C6-N1-C2	-6.76	117.59	120.30
1	XA	1297	C	P-O3'-C3'	6.76	127.81	119.70
35	YA	27	G	N3-C4-C5	6.76	131.98	128.60
35	RA	313	C	C6-N1-C2	-6.75	117.60	120.30
1	XA	1027	C	P-O3'-C3'	6.75	127.80	119.70
35	YA	930	U	N3-C2-O2	-6.75	117.47	122.20
35	RA	1404	C	N3-C2-O2	-6.74	117.18	121.90
1	XA	328	C	C6-N1-C2	-6.73	117.61	120.30
35	YA	1899	G	N3-C4-C5	-6.73	125.24	128.60
35	YA	27	G	N9-C4-C5	6.72	108.09	105.40
35	RA	263	C	C6-N1-C2	-6.72	117.61	120.30
35	RA	1045	A	P-O3'-C3'	6.72	127.77	119.70
1	QA	328	C	C6-N1-C2	-6.72	117.61	120.30
1	XA	1367	C	C6-N1-C2	-6.72	117.61	120.30
35	YA	1899	G	C8-N9-C1'	-6.72	118.26	127.00
1	QA	789	U	C2-N1-C1'	6.72	125.76	117.70
22	QV	62	C	N1-C2-O2	6.72	122.93	118.90
35	RA	846	C	P-O3'-C3'	6.71	127.76	119.70
35	RA	1804	C	C5-C6-N1	6.71	124.36	121.00
35	YA	222	A	P-O3'-C3'	6.70	127.74	119.70
35	YA	268	C	N1-C2-O2	6.70	122.92	118.90
35	RA	120	U	N3-C2-O2	-6.70	117.51	122.20
20	XT	73	HIS	C-N-CA	6.69	138.44	121.70
1	XA	1354	C	C6-N1-C2	-6.69	117.62	120.30
16	QP	38	TYR	CA-CB-CG	6.69	126.11	113.40
35	YA	1788	C	C6-N1-C2	-6.69	117.62	120.30
35	YA	753	C	C5-C6-N1	6.69	124.34	121.00
35	RA	635	C	C6-N1-C2	-6.68	117.63	120.30
35	RA	1914	C	C6-N1-C2	-6.68	117.63	120.30
1	XA	992	U	P-O3'-C3'	6.67	127.71	119.70
35	YA	1982	C	C6-N1-C2	-6.67	117.63	120.30
35	YA	1021	A	C5-N7-C8	-6.66	100.57	103.90
35	YA	1797	C	C5-C6-N1	6.66	124.33	121.00
35	RA	242	G	P-O3'-C3'	6.66	127.69	119.70
35	YA	1528	A	N7-C8-N9	6.66	117.13	113.80
35	YA	2667	C	C6-N1-C2	-6.65	117.64	120.30
35	YA	1005	C	N1-C2-O2	6.65	122.89	118.90
1	QA	1161	C	N3-C2-O2	-6.65	117.25	121.90
1	XA	449	C	N1-C2-O2	6.65	122.89	118.90
35	RA	2576	G	C4-N9-C1'	6.64	135.14	126.50
35	YA	1881	C	N1-C2-O2	6.64	122.89	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	1544	C	N1-C2-O2	6.64	122.88	118.90
1	QA	1347	G	P-O3'-C3'	6.64	127.67	119.70
35	YA	2350	C	N1-C2-O2	6.64	122.88	118.90
1	QA	1528	U	P-O3'-C3'	6.63	127.66	119.70
1	XA	1498	U	P-O3'-C3'	6.63	127.66	119.70
35	YA	1955	U	P-O3'-C3'	6.63	127.66	119.70
1	XA	687	A	P-O3'-C3'	6.63	127.66	119.70
1	XA	314	C	N1-C2-O2	6.63	122.88	118.90
1	XA	60	A	P-O3'-C3'	6.63	127.66	119.70
1	QA	992	U	P-O3'-C3'	6.63	127.66	119.70
35	RA	307	G	O5'-P-OP1	-6.63	99.74	105.70
35	YA	613	U	C2-N1-C1'	6.63	125.65	117.70
35	YA	114	U	C2-N1-C1'	6.62	125.65	117.70
1	QA	410	G	P-O3'-C3'	6.62	127.65	119.70
35	YA	783	A	C8-N9-C4	-6.62	103.15	105.80
35	YA	2702	U	O5'-P-OP2	-6.62	99.74	105.70
48	RS	88	ASP	C-N-CA	6.62	138.25	121.70
1	XA	963	G	N3-C2-N2	6.62	124.53	119.90
1	QA	250	A	P-O3'-C3'	6.62	127.64	119.70
1	QA	1038	C	N1-C2-O2	6.62	122.87	118.90
1	XA	1285	A	P-O3'-C3'	6.62	127.64	119.70
1	XA	1301	U	C2-N1-C1'	6.62	125.64	117.70
35	RA	2403	C	C5-C6-N1	6.61	124.31	121.00
35	YA	420	C	N1-C2-O2	6.61	122.87	118.90
35	RA	2688	U	C2-N1-C1'	6.61	125.63	117.70
1	XA	1439	C	C6-N1-C2	-6.61	117.66	120.30
35	YA	1332	G	C4-N9-C1'	6.60	135.08	126.50
35	RA	1053	C	C6-N1-C2	-6.60	117.66	120.30
36	RB	31	C	N1-C2-O2	6.60	122.86	118.90
35	YA	1021	A	N7-C8-N9	6.60	117.10	113.80
36	YB	79	C	C6-N1-C2	-6.60	117.66	120.30
1	QA	1158	C	C6-N1-C2	-6.59	117.66	120.30
1	XA	913	A	P-O3'-C3'	6.59	127.61	119.70
48	YS	110	LEU	CA-CB-CG	6.59	130.46	115.30
35	RA	1078	U	P-O3'-C3'	6.59	127.61	119.70
1	XA	1114	C	N1-C2-O2	6.59	122.85	118.90
35	YA	912	C	N3-C2-O2	-6.59	117.29	121.90
35	RA	2712	U	P-O3'-C3'	6.59	127.60	119.70
1	QA	687	A	P-O3'-C3'	6.58	127.60	119.70
35	RA	1496	A	N7-C8-N9	6.58	117.09	113.80
35	YA	97	C	N1-C2-O2	6.58	122.85	118.90
35	YA	1712	C	C6-N1-C2	-6.58	117.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	404	C	P-O3'-C3'	6.57	127.59	119.70
1	QA	1027	C	P-O3'-C3'	6.57	127.58	119.70
1	XA	1367	C	C5-C6-N1	6.57	124.28	121.00
35	YA	2403	C	N3-C2-O2	-6.56	117.31	121.90
35	RA	2043	C	N1-C2-O2	6.56	122.84	118.90
1	XA	509	A	C8-N9-C4	-6.56	103.17	105.80
1	QA	1498	U	P-O3'-C3'	6.56	127.57	119.70
35	YA	2210	G	C8-N9-C1'	-6.56	118.47	127.00
35	YA	269	U	N3-C2-O2	-6.56	117.61	122.20
35	YA	335	C	C6-N1-C2	-6.56	117.68	120.30
1	XA	1024	G	O5'-P-OP2	-6.55	99.80	105.70
1	QA	484	G	P-O3'-C3'	6.55	127.56	119.70
35	YA	806	C	C6-N1-C2	-6.55	117.68	120.30
1	QA	106	C	C6-N1-C2	-6.55	117.68	120.30
35	RA	1549	C	C6-N1-C2	-6.55	117.68	120.30
48	RS	17	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	QA	346	G	N3-C4-C5	-6.55	125.33	128.60
35	RA	115	C	C6-N1-C2	-6.55	117.68	120.30
1	XA	1158	C	C6-N1-C2	-6.55	117.68	120.30
35	YA	1363	C	N1-C2-O2	6.54	122.82	118.90
35	RA	1411	C	C6-N1-C2	-6.54	117.69	120.30
36	RB	42	C	C6-N1-C2	-6.53	117.69	120.30
35	RA	837	C	C5-C6-N1	6.52	124.26	121.00
1	XA	545	C	N3-C2-O2	-6.52	117.34	121.90
35	YA	1950	G	O4'-C1'-N9	6.52	113.42	108.20
46	RQ	9	TYR	CA-CB-CG	6.52	125.79	113.40
35	RA	2112	G	N3-C4-C5	-6.52	125.34	128.60
35	RA	1295	C	C6-N1-C2	-6.51	117.69	120.30
1	XA	1367	C	C2-N1-C1'	6.51	125.96	118.80
35	YA	2785	C	C6-N1-C2	-6.51	117.70	120.30
35	RA	537	C	N1-C2-O2	6.51	122.81	118.90
35	RA	2060	A	P-O3'-C3'	6.51	127.51	119.70
35	RA	2073	C	C6-N1-C2	-6.51	117.70	120.30
1	QA	1346	A	P-O3'-C3'	6.51	127.51	119.70
35	RA	2321	G	C4-N9-C1'	6.50	134.96	126.50
35	RA	2832	U	OP2-P-O3'	6.50	119.51	105.20
1	XA	1260	C	C6-N1-C2	-6.50	117.70	120.30
35	RA	1795	C	C6-N1-C2	-6.50	117.70	120.30
35	YA	1578	U	N1-C2-O2	6.50	127.35	122.80
1	QA	314	C	C6-N1-C2	-6.49	117.70	120.30
35	YA	2210	G	N3-C4-N9	6.49	129.89	126.00
35	RA	1376	C	N1-C2-O2	6.49	122.79	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	1514	C	C6-N1-C2	-6.49	117.70	120.30
35	RA	1204	A	C2-N3-C4	-6.48	107.36	110.60
1	XA	545	C	N1-C2-O2	6.48	122.79	118.90
35	YA	1827	C	C6-N1-C2	-6.48	117.71	120.30
1	XA	1038	C	N1-C2-O2	6.48	122.79	118.90
35	YA	67	U	C5-C6-N1	6.48	125.94	122.70
24	XY	72	C	N3-C2-O2	-6.47	117.37	121.90
35	RA	1786	A	C8-N9-C4	-6.47	103.21	105.80
1	XA	221	C	C5-C6-N1	6.47	124.23	121.00
35	YA	271(B)	G	P-O3'-C3'	6.47	127.46	119.70
1	XA	1158	C	N3-C2-O2	-6.47	117.37	121.90
35	RA	1686	C	N1-C2-O2	6.46	122.78	118.90
35	YA	1799	G	P-O3'-C3'	6.46	127.46	119.70
1	XA	137	C	N1-C2-O2	6.46	122.78	118.90
35	RA	530	G	O4'-C1'-N9	6.46	113.37	108.20
35	YA	1463	C	C6-N1-C2	-6.46	117.72	120.30
1	XA	328	C	N3-C2-O2	-6.46	117.38	121.90
1	QA	328	C	C5-C6-N1	6.46	124.23	121.00
35	YA	2701	C	C6-N1-C2	-6.45	117.72	120.30
24	QY	36	C	C6-N1-C2	-6.45	117.72	120.30
35	YA	1445	C	C6-N1-C2	-6.45	117.72	120.30
1	XA	1384	C	N1-C2-O2	6.45	122.77	118.90
1	XA	972	C	N3-C2-O2	-6.45	117.39	121.90
35	YA	2342	C	C6-N1-C2	-6.44	117.72	120.30
35	YA	974(A)	C	N1-C2-O2	6.44	122.76	118.90
35	YA	2584	U	N1-C2-O2	6.44	127.31	122.80
35	YA	859	G	P-O3'-C3'	6.43	127.42	119.70
35	RA	637	A	P-O3'-C3'	6.43	127.42	119.70
35	RA	669	G	C8-N9-C1'	-6.43	118.64	127.00
1	XA	484	G	P-O3'-C3'	6.43	127.42	119.70
12	XL	120	TYR	CA-CB-CG	6.43	125.62	113.40
1	QA	1336	C	C2-N1-C1'	6.43	125.87	118.80
35	YA	1218	C	C6-N1-C2	-6.43	117.73	120.30
1	QA	401	C	C6-N1-C2	-6.43	117.73	120.30
35	RA	41	C	N1-C2-O2	6.43	122.76	118.90
35	RA	1178	C	C6-N1-C2	-6.43	117.73	120.30
24	QY	25	C	C6-N1-C2	-6.43	117.73	120.30
35	YA	1988	C	C6-N1-C2	-6.43	117.73	120.30
22	QV	17	C	C6-N1-C1'	-6.42	113.09	120.80
22	XV	71	C	C6-N1-C2	-6.42	117.73	120.30
35	YA	1549	C	N1-C2-O2	6.42	122.75	118.90
35	YA	915	C	N1-C2-O2	6.42	122.75	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	76	C	N1-C2-O2	6.42	122.75	118.90
35	YA	2416	C	C5-C6-N1	6.41	124.21	121.00
35	YA	637	A	P-O3'-C3'	6.41	127.39	119.70
49	YT	100	TYR	CA-CB-CG	6.41	125.57	113.40
1	XA	960	U	C2-N1-C1'	6.40	125.39	117.70
35	YA	2236	C	C5-C6-N1	6.40	124.20	121.00
35	YA	41	C	C5-C6-N1	6.40	124.20	121.00
35	RA	2723	C	C6-N1-C2	-6.40	117.74	120.30
1	XA	135	C	C6-N1-C2	-6.39	117.74	120.30
1	QA	687	A	N1-C6-N6	-6.38	114.77	118.60
35	YA	1694	C	P-O3'-C3'	6.38	127.36	119.70
35	YA	1363	C	N3-C2-O2	-6.38	117.43	121.90
35	YA	1882	C	N1-C2-O2	6.38	122.73	118.90
35	YA	834	C	C6-N1-C2	-6.38	117.75	120.30
35	RA	860	U	C2-N1-C1'	6.37	125.35	117.70
35	RA	1352	U	N3-C2-O2	-6.37	117.74	122.20
1	QA	1163	C	C5-C6-N1	6.37	124.19	121.00
35	YA	1797	C	C6-N1-C2	-6.37	117.75	120.30
1	QA	1066	C	N3-C2-O2	-6.37	117.44	121.90
35	YA	755	C	C6-N1-C2	-6.36	117.75	120.30
35	YA	161	U	N1-C2-O2	6.36	127.25	122.80
35	YA	269	U	N1-C2-O2	6.36	127.25	122.80
35	YA	2129	C	N1-C2-O2	6.36	122.71	118.90
35	RA	2137	C	N1-C2-O2	6.35	122.71	118.90
1	QA	410	G	OP1-P-O3'	6.34	119.15	105.20
1	XA	1336	C	C6-N1-C1'	-6.34	113.19	120.80
35	RA	1314	C	C2-N1-C1'	6.33	125.77	118.80
1	XA	410	G	OP1-P-O3'	6.33	119.12	105.20
35	RA	2870	C	C6-N1-C2	-6.33	117.77	120.30
35	YA	1534	G	N3-C4-N9	6.33	129.80	126.00
1	QA	932	C	N1-C2-O2	6.32	122.69	118.90
35	RA	752	A	P-O3'-C3'	6.32	127.28	119.70
35	RA	253	C	N1-C2-O2	6.32	122.69	118.90
35	RA	1233	C	C5-C6-N1	6.32	124.16	121.00
35	RA	1306	C	N1-C2-O2	6.32	122.69	118.90
35	YA	2662	A	C8-N9-C4	-6.32	103.27	105.80
35	YA	1656	C	C6-N1-C2	-6.31	117.78	120.30
35	YA	1827	C	N3-C2-O2	-6.31	117.48	121.90
35	YA	2825	C	C6-N1-C2	-6.31	117.78	120.30
35	YA	816	C	N1-C2-O2	6.31	122.68	118.90
36	RB	47	C	N3-C4-C5	6.30	124.42	121.90
42	RI	134	PRO	C-N-CA	6.30	137.46	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	1158	C	C6-N1-C1'	-6.30	113.24	120.80
1	QA	1097	C	C6-N1-C2	-6.30	117.78	120.30
1	QA	948	C	N1-C2-O2	6.30	122.68	118.90
1	XA	826	C	C5-C6-N1	6.29	124.14	121.00
38	RE	27	LEU	CA-CB-CG	6.29	129.76	115.30
1	QA	913	A	P-O3'-C3'	6.29	127.25	119.70
35	YA	1076	C	N1-C2-O2	6.28	122.67	118.90
35	YA	1411	C	C6-N1-C2	-6.28	117.79	120.30
35	YA	1892	C	C6-N1-C2	-6.28	117.79	120.30
35	YA	1881	C	C5-C6-N1	6.28	124.14	121.00
1	XA	754	C	C2-N1-C1'	6.28	125.70	118.80
35	RA	828	U	C6-N1-C2	-6.28	117.23	121.00
35	YA	229	A	P-O3'-C3'	6.27	127.23	119.70
35	YA	1534	G	N3-C4-C5	-6.27	125.46	128.60
35	YA	1905	C	C6-N1-C2	-6.27	117.79	120.30
1	XA	345	C	P-O3'-C3'	6.27	127.22	119.70
24	XY	36	C	C6-N1-C2	-6.27	117.79	120.30
35	RA	1077	A	C2-N3-C4	6.27	113.73	110.60
35	YA	114	U	N1-C2-O2	6.27	127.19	122.80
35	YA	2889	C	N1-C2-O2	6.27	122.66	118.90
35	RA	1899	G	C8-N9-C4	-6.26	103.89	106.40
35	RA	1786	A	C5-N7-C8	-6.26	100.77	103.90
1	XA	89	U	P-O3'-C3'	6.26	127.21	119.70
35	YA	242	G	P-O3'-C3'	6.26	127.21	119.70
35	YA	2774	C	N1-C2-O2	6.26	122.66	118.90
1	QA	449	C	C2-N1-C1'	6.26	125.68	118.80
1	XA	1158	C	N1-C2-O2	6.26	122.65	118.90
35	YA	1437	C	N3-C2-O2	-6.25	117.53	121.90
1	QA	753	A	P-O3'-C3'	6.25	127.19	119.70
35	RA	1312	U	P-O3'-C3'	6.25	127.19	119.70
35	YA	1956	U	N1-C2-O2	6.24	127.17	122.80
35	RA	1653	G	P-O3'-C3'	6.24	127.19	119.70
35	RA	2350	C	N3-C2-O2	-6.24	117.53	121.90
35	RA	222	A	P-O3'-C3'	6.24	127.19	119.70
35	RA	1799	G	P-O3'-C3'	6.24	127.19	119.70
1	QA	1440	C	N3-C2-O2	-6.23	117.54	121.90
35	YA	1955	U	N1-C2-O2	6.23	127.16	122.80
1	XA	990	C	C6-N1-C2	-6.23	117.81	120.30
35	YA	1776	G	C4-N9-C1'	6.23	134.60	126.50
1	XA	963	G	N7-C8-N9	6.23	116.21	113.10
1	XA	1336	C	C5-C6-N1	6.23	124.11	121.00
35	RA	1711	C	C6-N1-C2	-6.22	117.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	1399	C	C6-N1-C2	-6.22	117.81	120.30
35	RA	2726	U	N3-C2-O2	-6.22	117.84	122.20
35	YA	2881	C	C6-N1-C2	-6.22	117.81	120.30
35	YA	1662	C	C6-N1-C2	-6.22	117.81	120.30
35	YA	2726	U	N3-C2-O2	-6.21	117.85	122.20
35	YA	1882	C	C5-C6-N1	6.21	124.11	121.00
35	YA	2416	C	C6-N1-C2	-6.21	117.82	120.30
35	RA	1892	C	C6-N1-C2	-6.21	117.82	120.30
35	RA	912	C	N1-C2-O2	6.20	122.62	118.90
35	YA	1535	U	N1-C2-O2	6.20	127.14	122.80
35	RA	1781	C	C2-N1-C1'	6.20	125.62	118.80
35	RA	2832	U	P-O3'-C3'	6.20	127.14	119.70
35	YA	618(A)	C	N1-C2-O2	6.19	122.61	118.90
35	YA	1950	G	C8-N9-C1'	-6.19	118.95	127.00
35	YA	1218	C	C5-C6-N1	6.19	124.09	121.00
35	RA	2417	C	C6-N1-C2	-6.19	117.83	120.30
35	YA	1804	C	N1-C2-O2	6.19	122.61	118.90
35	YA	634	C	N3-C2-O2	-6.18	117.57	121.90
35	RA	1999	C	C6-N1-C2	-6.18	117.83	120.30
22	XV	34	C	N1-C2-O2	6.18	122.61	118.90
35	RA	766	C	C6-N1-C2	-6.18	117.83	120.30
35	YA	510	C	N1-C2-O2	6.18	122.61	118.90
35	YA	2039	C	C6-N1-C2	-6.18	117.83	120.30
35	YA	838	C	C6-N1-C2	-6.17	117.83	120.30
43	YN	114	ARG	N-CA-C	-6.17	94.33	111.00
1	XA	412	A	P-O3'-C3'	6.17	127.11	119.70
35	YA	1712	C	C5-C6-N1	6.17	124.09	121.00
55	YZ	9	TYR	CA-CB-CG	6.17	125.13	113.40
1	QA	485	G	P-O3'-C3'	6.16	127.10	119.70
35	YA	2295	C	C6-N1-C2	-6.16	117.84	120.30
1	XA	58	C	C5-C6-N1	6.16	124.08	121.00
23	XX	18	G	P-O3'-C3'	6.16	127.09	119.70
1	QA	1059	C	C6-N1-C2	-6.16	117.84	120.30
35	RA	2478	A	O5'-P-OP2	-6.16	100.16	105.70
35	YA	1427	A	P-O3'-C3'	6.16	127.09	119.70
35	RA	31	C	C6-N1-C2	-6.15	117.84	120.30
35	YA	2681	C	OP2-P-O3'	6.15	118.73	105.20
35	RA	2439	A	P-O3'-C3'	6.15	127.08	119.70
35	YA	2844	G	C4-N9-C1'	6.15	134.49	126.50
35	RA	645	C	C5-C6-N1	6.15	124.07	121.00
24	XY	59	U	C5-C6-N1	6.14	125.77	122.70
35	RA	372	G	P-O3'-C3'	6.13	127.06	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	1694	C	P-O3'-C3'	6.13	127.06	119.70
41	YH	82	GLY	N-CA-C	6.13	128.43	113.10
24	QY	72	C	N1-C2-O2	6.12	122.57	118.90
35	RA	2691	C	C5-C6-N1	6.12	124.06	121.00
1	XA	244	U	P-O3'-C3'	6.12	127.04	119.70
23	QX	18	G	P-O3'-C3'	6.12	127.04	119.70
35	RA	231	C	N1-C2-O2	6.12	122.57	118.90
35	RA	2471	C	N1-C2-O2	6.12	122.57	118.90
1	XA	1260	C	N1-C2-O2	6.12	122.57	118.90
35	YA	1313	U	C6-N1-C1'	-6.12	112.63	121.20
35	YA	1765	C	N1-C2-O2	6.12	122.57	118.90
35	YA	2402	C	P-O3'-C3'	6.12	127.04	119.70
35	RA	99	U	P-O3'-C3'	6.12	127.04	119.70
35	YA	1881	C	C2-N1-C1'	6.12	125.53	118.80
35	YA	2610	C	P-O3'-C3'	6.12	127.04	119.70
35	RA	2880	C	N3-C2-O2	-6.11	117.62	121.90
35	RA	2043	C	C5-C6-N1	6.11	124.06	121.00
35	YA	1306	C	C5-C6-N1	6.11	124.06	121.00
35	RA	2073	C	C5-C6-N1	6.11	124.05	121.00
35	RA	2084	C	C6-N1-C2	-6.11	117.86	120.30
35	YA	134	C	N3-C2-O2	-6.11	117.63	121.90
35	RA	1427	A	P-O3'-C3'	6.10	127.02	119.70
35	RA	503	A	P-O3'-C3'	6.10	127.02	119.70
35	YA	2662	A	N7-C8-N9	6.10	116.85	113.80
35	RA	273(F)	C	C6-N1-C2	-6.10	117.86	120.30
22	QV	75	C	C6-N1-C2	-6.09	117.86	120.30
35	YA	795	C	C6-N1-C2	-6.09	117.86	120.30
1	XA	137	C	N3-C2-O2	-6.09	117.64	121.90
35	YA	1021	A	N3-C4-N9	-6.09	122.53	127.40
35	RA	231	C	C5-C6-N1	6.09	124.04	121.00
35	YA	268	C	N3-C2-O2	-6.09	117.64	121.90
35	RA	273(F)	C	N1-C2-O2	6.08	122.55	118.90
1	XA	533	A	O5'-P-OP1	-6.08	100.23	105.70
35	RA	1598	C	C5-C6-N1	6.08	124.04	121.00
35	RA	2126	A	P-O3'-C3'	6.08	126.99	119.70
1	XA	1267	C	C5-C6-N1	6.08	124.04	121.00
35	YA	2471	C	N1-C2-O2	6.08	122.55	118.90
35	YA	2814	C	N3-C2-O2	-6.07	117.65	121.90
35	YA	2889	C	N3-C2-O2	-6.07	117.65	121.90
1	QA	442	C	C6-N1-C2	-6.07	117.87	120.30
43	RN	48	MET	CG-SD-CE	-6.07	90.49	100.20
36	YB	70	C	C5-C6-N1	6.07	124.03	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	752	A	P-O3'-C3'	6.07	126.98	119.70
35	YA	57	C	C6-N1-C2	-6.07	117.87	120.30
24	QY	16	C	C6-N1-C2	-6.06	117.88	120.30
35	YA	2889	C	C2-N1-C1'	6.06	125.47	118.80
35	RA	221	A	P-O3'-C3'	6.06	126.97	119.70
35	RA	523	C	C6-N1-C2	-6.06	117.88	120.30
1	XA	1367	C	N1-C2-O2	6.06	122.53	118.90
35	YA	2855	C	N1-C2-O2	6.05	122.53	118.90
35	RA	2703	C	C2-N1-C1'	6.05	125.45	118.80
35	YA	1881	C	N3-C2-O2	-6.05	117.67	121.90
35	YA	1893	C	N1-C2-O2	6.05	122.53	118.90
35	YA	2856	C	C5-C6-N1	6.05	124.03	121.00
35	RA	912	C	C5-C6-N1	6.04	124.02	121.00
1	XA	1384	C	N3-C2-O2	-6.04	117.67	121.90
35	RA	2889	C	N1-C2-O2	6.03	122.52	118.90
35	RA	1474	C	C6-N1-C2	-6.02	117.89	120.30
1	XA	686	U	N3-C2-O2	-6.02	117.98	122.20
1	QA	244	U	P-O3'-C3'	6.02	126.93	119.70
35	YA	1640	C	C6-N1-C2	-6.02	117.89	120.30
23	QX	18	G	OP2-P-O3'	6.02	118.44	105.20
35	RA	1589	C	N1-C2-O2	6.02	122.51	118.90
35	RA	2889	C	N3-C2-O2	-6.02	117.69	121.90
35	YA	2766	G	C4-N9-C1'	6.01	134.32	126.50
35	YA	2441	C	N3-C2-O2	-6.01	117.69	121.90
1	XA	764	C	C6-N1-C2	-6.01	117.90	120.30
35	RA	2785	C	C6-N1-C2	-6.01	117.90	120.30
1	QA	960	U	N3-C2-O2	-6.01	118.00	122.20
1	XA	137	C	C6-N1-C2	-6.01	117.90	120.30
35	YA	333	G	C8-N9-C1'	-6.00	119.19	127.00
35	YA	580	C	C6-N1-C2	-6.00	117.90	120.30
35	RA	291	C	C6-N1-C2	-6.00	117.90	120.30
35	YA	1396	U	C5-C6-N1	6.00	125.70	122.70
35	RA	2855	C	C6-N1-C2	-5.99	117.90	120.30
1	QA	501	C	C6-N1-C2	-5.99	117.90	120.30
1	XA	346	G	C4-N9-C1'	5.99	134.29	126.50
35	RA	2260	C	N3-C2-O2	-5.99	117.71	121.90
35	YA	2566	A	P-O3'-C3'	5.99	126.88	119.70
35	RA	1178	C	C5-C6-N1	5.98	123.99	121.00
35	YA	517	C	C6-N1-C2	-5.98	117.91	120.30
35	YA	2739	U	N3-C2-O2	-5.98	118.01	122.20
1	QA	1502	A	C5-N7-C8	-5.98	100.91	103.90
35	YA	2776	A	P-O3'-C3'	5.98	126.87	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	YH	153	LYS	N-CA-C	5.98	127.14	111.00
35	RA	797	C	C6-N1-C2	-5.97	117.91	120.30
35	RA	1725	G	C4-N9-C1'	5.97	134.27	126.50
35	YA	2468	G	C4-N9-C1'	5.97	134.27	126.50
1	QA	369	C	N1-C2-O2	5.97	122.48	118.90
35	RA	2403	C	C6-N1-C2	-5.97	117.91	120.30
35	RA	2648	C	N1-C2-O2	5.97	122.48	118.90
35	RA	2691	C	C6-N1-C2	-5.97	117.91	120.30
1	XA	963	G	C4-N9-C1'	5.97	134.26	126.50
35	RA	783	A	C5-N7-C8	-5.97	100.92	103.90
35	YA	867	C	C5-C6-N1	5.97	123.98	121.00
35	RA	860	U	C6-N1-C2	-5.97	117.42	121.00
42	YI	11	ASN	C-N-CA	5.96	136.61	121.70
35	YA	2439	A	P-O3'-C3'	5.96	126.86	119.70
24	QY	54	U	C2-N3-C4	5.96	130.58	127.00
35	RA	951	C	C6-N1-C2	-5.96	117.92	120.30
35	RA	2880	C	C6-N1-C2	-5.96	117.92	120.30
35	RA	76	C	N3-C2-O2	-5.96	117.73	121.90
35	YA	976	C	C6-N1-C2	-5.96	117.92	120.30
35	YA	1313	U	C5-C6-N1	5.96	125.68	122.70
35	RA	601	C	C6-N1-C2	-5.95	117.92	120.30
35	YA	1549	C	N3-C2-O2	-5.95	117.74	121.90
1	QA	1369	C	N3-C2-O2	-5.94	117.74	121.90
36	RB	66	A	P-O3'-C3'	5.94	126.83	119.70
35	YA	2768	C	C6-N1-C2	-5.94	117.92	120.30
35	YA	485	C	C6-N1-C2	-5.94	117.92	120.30
35	YA	2321	G	C8-N9-C1'	-5.94	119.28	127.00
1	XA	266	G	P-O3'-C3'	5.93	126.82	119.70
35	YA	912	C	N1-C2-O2	5.93	122.46	118.90
35	YA	1535	U	N3-C2-O2	-5.93	118.05	122.20
35	YA	1788	C	C5-C6-N1	5.93	123.97	121.00
1	QA	1163	C	C2-N1-C1'	5.93	125.32	118.80
35	YA	535	C	C6-N1-C2	-5.93	117.93	120.30
35	YA	1675	C	N3-C2-O2	-5.93	117.75	121.90
35	YA	2441	C	N1-C2-O2	5.93	122.46	118.90
24	QY	54	U	N1-C2-O2	5.93	126.95	122.80
1	QA	346	G	C4-N9-C1'	5.93	134.20	126.50
35	RA	1786	A	C4-N9-C1'	5.93	136.97	126.30
35	YA	47	C	C6-N1-C2	-5.93	117.93	120.30
35	YA	1018	C	C6-N1-C2	-5.92	117.93	120.30
3	QC	201	TYR	CA-CB-CG	5.92	124.64	113.40
35	RA	1026	U	P-O3'-C3'	5.92	126.80	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	1827	C	N3-C2-O2	-5.91	117.76	121.90
49	RT	105	LEU	CA-CB-CG	5.91	128.90	115.30
35	RA	517	C	C6-N1-C2	-5.91	117.94	120.30
35	RA	1062	G	C4-N9-C1'	5.91	134.18	126.50
1	QA	435	C	C6-N1-C2	-5.91	117.94	120.30
35	RA	1062	G	N3-C4-N9	5.91	129.54	126.00
1	QA	1066	C	C6-N1-C2	-5.91	117.94	120.30
35	YA	237	C	C6-N1-C2	-5.91	117.94	120.30
1	QA	1024	G	O5'-P-OP2	-5.91	100.39	105.70
35	RA	1899	G	N3-C4-C5	-5.90	125.65	128.60
1	QA	980	C	N1-C2-O2	5.90	122.44	118.90
35	YA	991	C	C6-N1-C2	-5.90	117.94	120.30
1	XA	115	G	P-O3'-C3'	5.90	126.78	119.70
35	RA	1574	C	C6-N1-C2	-5.89	117.94	120.30
35	RA	2656	U	N1-C2-O2	5.89	126.93	122.80
41	RH	82	GLY	N-CA-C	5.89	127.84	113.10
1	XA	963	G	C4-C5-N7	5.89	113.16	110.80
1	QA	412	A	P-O3'-C3'	5.89	126.77	119.70
35	RA	2178	C	C6-N1-C2	-5.89	117.94	120.30
35	YA	1882	C	C6-N1-C2	-5.89	117.94	120.30
35	RA	297	C	C6-N1-C2	-5.89	117.94	120.30
35	YA	1052	C	C6-N1-C2	-5.89	117.94	120.30
35	YA	1549	C	C6-N1-C2	-5.89	117.94	120.30
24	QY	70	U	C2-N1-C1'	5.89	124.77	117.70
35	RA	2610	C	P-O3'-C3'	5.89	126.77	119.70
35	YA	2096	U	C5-C6-N1	5.89	125.64	122.70
35	YA	2773	C	C6-N1-C2	-5.89	117.94	120.30
35	RA	1644	C	N1-C2-O2	5.89	122.43	118.90
1	XA	314	C	C5-C6-N1	5.88	123.94	121.00
35	YA	99	U	P-O3'-C3'	5.88	126.76	119.70
35	YA	544	C	N1-C2-O2	5.88	122.43	118.90
35	RA	898	C	N3-C2-O2	-5.88	117.79	121.90
1	XA	485	G	P-O3'-C3'	5.88	126.75	119.70
1	XA	169	C	N1-C2-O2	5.87	122.42	118.90
1	XA	753	A	P-O3'-C3'	5.87	126.75	119.70
35	YA	1200	C	C6-N1-C2	-5.87	117.95	120.30
1	QA	442	C	C5-C6-N1	5.87	123.94	121.00
1	QA	689	C	N1-C2-O2	5.87	122.42	118.90
35	RA	974(A)	C	C2-N1-C1'	5.87	125.26	118.80
35	RA	1375	C	C6-N1-C2	-5.87	117.95	120.30
29	Y4	40	HIS	N-CA-C	5.87	126.84	111.00
35	YA	1914	C	C6-N1-C1'	-5.87	113.76	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	2205	C	C5-C6-N1	5.87	123.93	121.00
1	QA	115	G	P-O3'-C3'	5.86	126.73	119.70
42	RI	11	ASN	C-N-CA	5.86	136.36	121.70
35	YA	915	C	N3-C2-O2	-5.86	117.80	121.90
35	YA	2420	C	C6-N1-C2	-5.86	117.95	120.30
35	RA	265	A	O4'-C1'-N9	5.86	112.89	108.20
35	RA	523	C	C5-C6-N1	5.86	123.93	121.00
35	YA	1882	C	C2-N1-C1'	5.86	125.25	118.80
35	YA	1931	U	C6-N1-C2	-5.86	117.48	121.00
35	RA	530	G	N1-C6-O6	-5.86	116.39	119.90
35	RA	2063	C	C6-N1-C2	-5.85	117.96	120.30
1	XA	1254	C	C6-N1-C2	-5.85	117.96	120.30
35	RA	1644	C	C5-C6-N1	5.85	123.92	121.00
35	YA	1804	C	N3-C2-O2	-5.85	117.81	121.90
35	RA	1506	C	C6-N1-C2	-5.85	117.96	120.30
35	RA	1567	A	N1-C6-N6	-5.85	115.09	118.60
35	YA	650	C	C5-C6-N1	5.85	123.92	121.00
35	RA	485	C	N1-C2-O2	5.84	122.41	118.90
35	RA	2776	A	P-O3'-C3'	5.84	126.71	119.70
35	YA	812	C	C6-N1-C2	-5.84	117.96	120.30
35	YA	393	C	C6-N1-C2	-5.84	117.96	120.30
1	QA	442	C	N1-C2-O2	5.84	122.40	118.90
35	RA	898	C	C2-N1-C1'	5.84	125.22	118.80
35	RA	2889	C	C2-N1-C1'	5.84	125.22	118.80
1	XA	314	C	N3-C2-O2	-5.84	117.81	121.90
35	RA	1305	C	N3-C2-O2	-5.83	117.82	121.90
35	RA	930	U	N1-C2-O2	5.83	126.88	122.80
35	YA	508	G	N3-C4-N9	5.83	129.50	126.00
35	YA	1653	G	P-O3'-C3'	5.83	126.70	119.70
35	YA	1992	G	P-O3'-C3'	5.83	126.70	119.70
35	YA	97	C	N3-C2-O2	-5.83	117.82	121.90
1	XA	896	C	C5-C6-N1	5.83	123.91	121.00
35	RA	1914	C	C6-N1-C1'	-5.83	113.81	120.80
1	QA	429	U	C5-C6-N1	5.82	125.61	122.70
35	RA	2405	G	P-O3'-C3'	5.82	126.69	119.70
35	RA	2755	C	C2-N1-C1'	5.82	125.20	118.80
55	RZ	3	TYR	CA-CB-CG	5.82	124.46	113.40
35	YA	426	C	N1-C2-O2	5.82	122.39	118.90
35	YA	512	G	O4'-C1'-N9	5.82	112.86	108.20
35	YA	2043	C	C5-C6-N1	5.82	123.91	121.00
35	YA	2723	C	C6-N1-C2	-5.82	117.97	120.30
35	RA	1636	C	C6-N1-C2	-5.82	117.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	2575	C	C6-N1-C2	-5.82	117.97	120.30
35	RA	1930	G	OP2-P-O3'	5.81	117.98	105.20
35	YA	67	U	N3-C4-O4	5.81	123.47	119.40
35	YA	2350	C	N3-C2-O2	-5.81	117.83	121.90
35	YA	898	C	N3-C2-O2	-5.80	117.84	121.90
35	YA	1931	U	N1-C2-O2	5.80	126.86	122.80
35	YA	2841	C	C6-N1-C2	-5.80	117.98	120.30
1	QA	1502	A	N7-C8-N9	5.80	116.70	113.80
35	RA	1616	A	C4-C5-N7	5.80	113.60	110.70
35	YA	613	U	N1-C2-O2	5.80	126.86	122.80
35	YA	1095	A	N3-C4-N9	5.80	132.04	127.40
35	YA	2424	C	N1-C2-O2	5.80	122.38	118.90
36	YB	30	C	N1-C2-O2	5.80	122.38	118.90
1	XA	369	C	C5-C6-N1	5.79	123.90	121.00
1	XA	1203	C	C6-N1-C2	-5.79	117.98	120.30
35	YA	2126	A	P-O3'-C3'	5.79	126.65	119.70
35	RA	1882	C	N1-C2-O2	5.79	122.37	118.90
35	YA	618(A)	C	N3-C2-O2	-5.79	117.85	121.90
1	XA	354	G	C4-N9-C1'	5.79	134.02	126.50
35	YA	1407	C	N1-C2-O2	5.79	122.37	118.90
1	XA	980	C	C5-C6-N1	5.78	123.89	121.00
1	XA	1070	U	N1-C2-O2	5.78	126.85	122.80
1	QA	1192	C	C6-N1-C2	-5.78	117.99	120.30
35	RA	2789	C	N1-C2-O2	5.78	122.37	118.90
1	XA	1070	U	N3-C2-O2	-5.78	118.16	122.20
35	YA	1979	C	C6-N1-C2	-5.78	117.99	120.30
1	XA	1374	A	O4'-C1'-N9	5.77	112.82	108.20
51	YV	91	TYR	CA-CB-CG	5.77	124.37	113.40
35	RA	77	C	C5-C6-N1	5.77	123.89	121.00
35	YA	965	C	C5-C6-N1	5.77	123.89	121.00
35	YA	1396	U	C6-N1-C1'	-5.77	113.12	121.20
35	YA	2321	G	N3-C4-N9	5.77	129.46	126.00
35	YA	2772	C	C6-N1-C2	-5.77	117.99	120.30
35	YA	754	C	C6-N1-C2	-5.77	117.99	120.30
46	YQ	25	ASP	CB-CG-OD1	5.77	123.49	118.30
1	QA	266	G	P-O3'-C3'	5.77	126.62	119.70
35	YA	529	A	N7-C8-N9	5.77	116.68	113.80
1	QA	536	C	N1-C2-O2	5.76	122.36	118.90
55	RZ	8	TYR	CA-CB-CG	5.76	124.35	113.40
1	QA	1230	C	C6-N1-C2	-5.76	118.00	120.30
1	XA	991	U	C2-N1-C1'	5.76	124.61	117.70
35	YA	273(F)	C	N1-C2-O2	5.76	122.36	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	808	C	C6-N1-C2	-5.75	118.00	120.30
35	YA	120	U	C6-N1-C1'	-5.75	113.14	121.20
35	YA	2701	C	P-O3'-C3'	5.75	126.61	119.70
36	RB	31	C	N3-C2-O2	-5.75	117.87	121.90
35	RA	512	G	P-O3'-C3'	5.75	126.60	119.70
1	XA	369	C	C6-N1-C2	-5.75	118.00	120.30
35	YA	76	C	C5-C6-N1	5.75	123.88	121.00
1	QA	596	C	N1-C2-O2	5.75	122.35	118.90
26	R1	43	TYR	CA-CB-CG	5.75	124.32	113.40
35	RA	2294	C	N1-C2-O2	5.75	122.35	118.90
35	YA	731	C	C6-N1-C2	-5.74	118.00	120.30
35	RA	1306	C	N3-C2-O2	-5.74	117.88	121.90
35	YA	273(F)	C	C6-N1-C2	-5.74	118.00	120.30
1	QA	1114	C	C6-N1-C2	-5.74	118.00	120.30
35	RA	2321	G	C8-N9-C1'	-5.74	119.54	127.00
35	YA	102	G	P-O3'-C3'	5.74	126.59	119.70
35	YA	1467	C	C6-N1-C2	-5.74	118.00	120.30
35	YA	1686	C	C2-N1-C1'	5.74	125.11	118.80
35	YA	2666	C	N3-C2-O2	-5.74	117.89	121.90
35	YA	1045	A	P-O3'-C3'	5.73	126.58	119.70
1	QA	1225	A	C4-N9-C1'	5.73	136.62	126.30
35	RA	702	G	C4-N9-C1'	5.73	133.95	126.50
35	YA	377	C	C6-N1-C2	-5.73	118.01	120.30
1	QA	754	C	N1-C2-O2	5.73	122.34	118.90
35	RA	749	C	C6-N1-C2	-5.73	118.01	120.30
35	RA	1688	U	N3-C2-O2	-5.73	118.19	122.20
35	YA	1407	C	C6-N1-C2	-5.72	118.01	120.30
17	XQ	42	TYR	CA-CB-CG	5.72	124.27	113.40
35	RA	930	U	N3-C2-O2	-5.72	118.20	122.20
51	RV	35	LEU	CA-CB-CG	5.72	128.45	115.30
1	XA	169	C	C2-N1-C1'	5.72	125.09	118.80
35	YA	1095	A	N3-C4-C5	-5.72	122.80	126.80
35	YA	1222	C	C6-N1-C2	-5.72	118.01	120.30
12	QL	27	LEU	C-N-CA	5.71	135.98	121.70
35	YA	2138	C	C5-C6-N1	5.71	123.86	121.00
36	YB	71	C	N1-C2-O2	5.71	122.33	118.90
35	RA	372	G	OP2-P-O3'	5.71	117.77	105.20
35	RA	587	C	P-O3'-C3'	5.71	126.55	119.70
35	RA	1688	U	C6-N1-C2	-5.71	117.57	121.00
35	RA	1504	C	C6-N1-C2	-5.71	118.02	120.30
35	RA	420	C	N3-C2-O2	-5.71	117.91	121.90
1	XA	932	C	N1-C2-O2	5.71	122.32	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	911	A	C8-N9-C4	-5.70	103.52	105.80
35	YA	1528	A	C8-N9-C4	-5.70	103.52	105.80
35	YA	1332	G	C5-N7-C8	-5.70	101.45	104.30
1	QA	762	C	C6-N1-C2	-5.70	118.02	120.30
35	RA	2703	C	N3-C2-O2	-5.70	117.91	121.90
35	YA	1905	C	C2-N1-C1'	5.69	125.06	118.80
35	RA	611	C	C6-N1-C2	-5.69	118.02	120.30
1	XA	974	A	O4'-C1'-N9	5.69	112.75	108.20
1	QA	1109	C	N3-C2-O2	-5.69	117.92	121.90
35	RA	2112	G	C4-N9-C1'	5.69	133.89	126.50
35	YA	964	C	C6-N1-C2	-5.69	118.03	120.30
35	RA	271(B)	G	P-O3'-C3'	5.68	126.52	119.70
37	YD	63	ARG	N-CA-C	-5.68	95.65	111.00
35	RA	2378	A	N9-C4-C5	-5.68	103.53	105.80
35	YA	1920	C	C5-C6-N1	5.68	123.84	121.00
35	RA	267	C	C6-N1-C2	-5.68	118.03	120.30
35	RA	2363	C	C6-N1-C2	-5.68	118.03	120.30
35	YA	2559	C	N1-C2-O2	5.68	122.31	118.90
35	RA	253	C	C6-N1-C2	-5.68	118.03	120.30
1	XA	186	C	C6-N1-C2	-5.68	118.03	120.30
35	RA	1544	C	N1-C2-O2	5.67	122.31	118.90
35	RA	74	A	P-O3'-C3'	5.67	126.51	119.70
1	QA	243	A	P-O3'-C3'	5.67	126.50	119.70
35	YA	540	G	C4-N9-C1'	5.67	133.87	126.50
35	YA	1691	C	C6-N1-C2	-5.67	118.03	120.30
35	RA	1899	G	C8-N9-C1'	-5.67	119.63	127.00
35	RA	2566	A	P-O3'-C3'	5.67	126.50	119.70
22	QV	32	C	N1-C2-O2	5.67	122.30	118.90
35	YA	992	C	N1-C2-O2	5.67	122.30	118.90
35	RA	1844	C	C6-N1-C2	-5.67	118.03	120.30
24	QY	70	U	N3-C2-O2	-5.66	118.23	122.20
1	QA	175	C	C6-N1-C2	-5.66	118.04	120.30
1	XA	1056	U	N3-C2-O2	-5.66	118.24	122.20
35	RA	1816	G	N7-C8-N9	5.66	115.93	113.10
1	QA	346	G	C2-N3-C4	5.66	114.73	111.90
1	XA	1228	C	N3-C2-O2	-5.66	117.94	121.90
1	QA	1336	C	N3-C2-O2	-5.66	117.94	121.90
35	RA	2211	G	C4-N9-C1'	5.66	133.85	126.50
35	RA	1313	U	C6-N1-C2	-5.65	117.61	121.00
35	YA	184	C	N1-C2-O2	5.65	122.29	118.90
35	YA	1142(A)	A	N3-C4-C5	5.65	130.76	126.80
35	RA	2730	C	C6-N1-C2	-5.65	118.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	288	C	N1-C2-O2	5.65	122.29	118.90
35	YA	828	U	N1-C2-O2	5.65	126.75	122.80
1	XA	754	C	C6-N1-C2	-5.65	118.04	120.30
35	YA	2646	C	N3-C2-O2	-5.65	117.95	121.90
35	YA	2828	C	C6-N1-C2	-5.65	118.04	120.30
1	XA	1056	U	N1-C2-O2	5.65	126.75	122.80
35	YA	912	C	C2-N1-C1'	5.64	125.00	118.80
1	XA	132	C	N1-C2-O2	5.64	122.28	118.90
35	RA	2836	U	C5-C6-N1	5.63	125.52	122.70
1	XA	266	G	C4-C5-N7	5.63	113.05	110.80
35	YA	2506	U	C6-N1-C2	-5.63	117.62	121.00
1	XA	314	C	C2-N1-C1'	5.63	125.00	118.80
35	YA	1790	C	N1-C2-O2	5.63	122.28	118.90
35	YA	587	C	P-O3'-C3'	5.63	126.45	119.70
35	RA	2320	A	C2-N3-C4	5.63	113.41	110.60
36	RB	3	C	C5-C6-N1	5.63	123.81	121.00
1	XA	754	C	N3-C2-O2	-5.63	117.96	121.90
1	XA	1109	C	N3-C2-O2	-5.62	117.96	121.90
35	YA	2307	G	C4-N9-C1'	5.62	133.81	126.50
35	YA	1528	A	C5-N7-C8	-5.62	101.09	103.90
1	XA	250	A	P-O3'-C3'	5.62	126.44	119.70
35	RA	2896	C	C6-N1-C2	-5.62	118.05	120.30
35	RA	1658	C	C5-C6-N1	5.62	123.81	121.00
35	RA	537	C	N3-C2-O2	-5.61	117.97	121.90
35	YA	2739	U	N1-C2-O2	5.61	126.73	122.80
35	RA	1599	C	C6-N1-C2	-5.61	118.06	120.30
1	XA	1505	G	N9-C4-C5	5.61	107.64	105.40
35	RA	1496	A	C5-N7-C8	-5.61	101.10	103.90
35	YA	898	C	C2-N1-C1'	5.61	124.97	118.80
35	YA	1332	G	C4-C5-N7	5.61	113.04	110.80
35	RA	564	C	C6-N1-C2	-5.60	118.06	120.30
35	YA	1352	U	C6-N1-C2	-5.60	117.64	121.00
1	XA	221	C	N1-C2-O2	5.60	122.26	118.90
1	XA	764	C	C5-C6-N1	5.60	123.80	121.00
35	YA	1376	C	C5-C6-N1	5.60	123.80	121.00
24	QY	55	U	C2-N1-C1'	5.60	124.42	117.70
35	RA	1971	A	C2-N3-C4	5.60	113.40	110.60
1	QA	1038	C	N3-C2-O2	-5.60	117.98	121.90
35	RA	67	U	C5-C6-N1	5.60	125.50	122.70
35	RA	2584	U	N1-C2-O2	5.60	126.72	122.80
35	YA	560	C	C6-N1-C2	-5.59	118.06	120.30
46	YQ	9	TYR	CA-CB-CG	5.59	124.03	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	Y4	39	CYS	N-CA-C	-5.59	95.90	111.00
1	XA	1439	C	N1-C2-O2	5.59	122.25	118.90
35	YA	2043	C	C6-N1-C2	-5.59	118.06	120.30
35	RA	1644	C	N3-C2-O2	-5.59	117.99	121.90
35	RA	1793	C	N3-C2-O2	-5.59	117.99	121.90
35	YA	1174	A	C4-N9-C1'	5.59	136.36	126.30
35	YA	1174	A	N3-C4-C5	-5.59	122.89	126.80
40	YG	94	LEU	CB-CG-CD2	-5.59	101.50	111.00
37	YD	33	LEU	CA-CB-CG	5.59	128.15	115.30
24	QY	40	C	N1-C2-O2	5.59	122.25	118.90
35	RA	2699	C	C6-N1-C2	-5.59	118.06	120.30
35	YA	860	U	C6-N1-C1'	-5.59	113.38	121.20
35	YA	1506	C	C6-N1-C2	-5.59	118.07	120.30
1	XA	1496	C	C6-N1-C2	-5.58	118.07	120.30
35	YA	697	C	C6-N1-C2	-5.58	118.07	120.30
35	RA	2702	U	C2-N1-C1'	5.58	124.40	117.70
35	YA	1313	U	C6-N1-C2	-5.58	117.65	121.00
1	XA	749	C	C2-N1-C1'	5.58	124.94	118.80
35	RA	2471	C	C6-N1-C2	-5.58	118.07	120.30
35	YA	635	C	C6-N1-C2	-5.58	118.07	120.30
35	YA	74	A	C2-N3-C4	-5.58	107.81	110.60
35	YA	2287	A	N3-C4-C5	5.58	130.70	126.80
35	RA	2112	G	N3-C4-N9	5.57	129.34	126.00
1	XA	435	C	C5-C6-N1	5.57	123.79	121.00
1	XA	971	G	C4-N9-C1'	-5.57	119.25	126.50
35	YA	2814	C	C6-N1-C2	-5.57	118.07	120.30
35	RA	1920	C	C6-N1-C2	-5.57	118.07	120.30
35	YA	783	A	C4-C5-N7	5.57	113.49	110.70
35	YA	2328	A	N7-C8-N9	5.57	116.59	113.80
35	YA	1893	C	N3-C2-O2	-5.57	118.00	121.90
35	YA	2394	C	C6-N1-C2	-5.57	118.07	120.30
35	YA	2321	G	N3-C4-C5	-5.57	125.82	128.60
35	RA	529	A	C2-N3-C4	5.57	113.38	110.60
35	RA	1902	C	C6-N1-C2	-5.57	118.07	120.30
35	RA	2767	C	C6-N1-C2	-5.57	118.07	120.30
36	YB	15	A	OP1-P-O3'	5.57	117.45	105.20
35	RA	1174	A	C4-N9-C1'	5.57	136.32	126.30
35	YA	2689	U	P-O3'-C3'	5.57	126.38	119.70
35	RA	856	C	P-O3'-C3'	5.56	126.38	119.70
35	YA	97	C	C5-C6-N1	5.56	123.78	121.00
35	RA	1686	C	C5-C6-N1	5.56	123.78	121.00
1	XA	1114	C	N3-C2-O2	-5.56	118.01	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	2392	A	N7-C8-N9	5.55	116.58	113.80
35	YA	2855	C	N3-C2-O2	-5.55	118.01	121.90
35	RA	2576	G	N3-C4-C5	-5.55	125.82	128.60
35	YA	134	C	N1-C2-O2	5.55	122.23	118.90
35	RA	1600	C	N3-C2-O2	-5.55	118.02	121.90
1	XA	1321	C	C6-N1-C2	-5.55	118.08	120.30
35	YA	828	U	C6-N1-C2	-5.55	117.67	121.00
35	YA	1135	C	N1-C2-O2	5.55	122.23	118.90
35	YA	242	G	OP2-P-O3'	5.55	117.41	105.20
35	RA	1375	C	C5-C6-N1	5.55	123.77	121.00
35	RA	1686	C	C6-N1-C2	-5.54	118.08	120.30
1	XA	991	U	N1-C2-O2	5.54	126.68	122.80
35	YA	992	C	N3-C2-O2	-5.54	118.02	121.90
36	YB	31	C	N1-C2-O2	5.54	122.23	118.90
35	RA	2468	G	C4-N9-C1'	5.54	133.70	126.50
1	XA	686	U	N1-C2-O2	5.54	126.68	122.80
1	XA	1505	G	N3-C4-N9	-5.54	122.67	126.00
35	YA	172	C	C6-N1-C2	-5.54	118.08	120.30
1	XA	896	C	C6-N1-C2	-5.54	118.08	120.30
1	QA	449	C	N1-C2-O2	5.54	122.22	118.90
35	RA	825	C	C6-N1-C2	-5.54	118.08	120.30
35	RA	915	C	N3-C2-O2	-5.54	118.02	121.90
1	QA	764	C	N1-C2-O2	5.54	122.22	118.90
35	YA	1607	C	C5-C6-N1	5.54	123.77	121.00
35	RA	860	U	N1-C2-O2	5.54	126.67	122.80
35	YA	243	U	C2-N1-C1'	5.54	124.34	117.70
35	YA	302	C	C6-N1-C2	-5.54	118.08	120.30
35	YA	1781	C	N1-C2-O2	5.54	122.22	118.90
35	RA	105	C	C6-N1-C2	-5.53	118.09	120.30
1	XA	449	C	N3-C2-O2	-5.53	118.03	121.90
1	XA	1439	C	C5-C6-N1	5.53	123.77	121.00
1	XA	704	A	O5'-P-OP1	-5.53	100.72	105.70
35	RA	77	C	C6-N1-C2	-5.53	118.09	120.30
35	YA	1786	A	N7-C8-N9	5.53	116.56	113.80
35	YA	2236	C	C6-N1-C2	-5.53	118.09	120.30
35	RA	817	C	C5-C6-N1	5.53	123.76	121.00
35	RA	1510	A	C2-N3-C4	5.53	113.36	110.60
35	RA	1544	C	N3-C2-O2	-5.53	118.03	121.90
35	YA	420	C	N3-C2-O2	-5.53	118.03	121.90
31	R6	34	LEU	CA-CB-CG	5.52	128.00	115.30
35	RA	530	G	C5-C6-O6	5.52	131.91	128.60
35	YA	246	C	N1-C2-O2	5.52	122.21	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	1445	C	N3-C2-O2	-5.52	118.03	121.90
1	XA	856	C	C6-N1-C2	-5.52	118.09	120.30
1	XA	1038	C	N3-C2-O2	-5.52	118.04	121.90
35	RA	1786	A	C4-C5-N7	5.52	113.46	110.70
22	XV	34	C	C2-N1-C1'	5.52	124.87	118.80
35	YA	1905	C	N3-C2-O2	-5.52	118.04	121.90
35	YA	2772	C	C5-C6-N1	5.52	123.76	121.00
1	QA	103	C	N3-C2-O2	-5.51	118.04	121.90
35	RA	1394	U	C5-C6-N1	5.51	125.46	122.70
36	RB	7	G	C4-C5-N7	5.51	113.00	110.80
1	XA	634	C	C6-N1-C2	-5.51	118.09	120.30
1	QA	1369	C	N1-C2-O2	5.51	122.21	118.90
35	RA	309	G	O5'-P-OP1	5.51	117.31	110.70
1	QA	1097	C	N3-C2-O2	-5.51	118.04	121.90
35	RA	465	G	C8-N9-C4	-5.51	104.20	106.40
35	RA	1549	C	C5-C6-N1	5.51	123.75	121.00
35	YA	817	C	C5-C6-N1	5.51	123.75	121.00
35	YA	2730	C	C6-N1-C2	-5.51	118.10	120.30
1	XA	810	C	C6-N1-C2	-5.51	118.10	120.30
35	RA	2688	U	N1-C2-O2	5.50	126.65	122.80
35	RA	912	C	C2-N1-C1'	5.50	124.85	118.80
35	RA	1881	C	C5-C6-N1	5.50	123.75	121.00
35	YA	645	C	C6-N1-C2	-5.50	118.10	120.30
35	YA	2524	G	C8-N9-C4	-5.50	104.20	106.40
38	RE	116	VAL	C-N-CA	5.50	135.44	121.70
35	YA	1386	C	C6-N1-C2	-5.50	118.10	120.30
35	YA	2138	C	C6-N1-C2	-5.50	118.10	120.30
1	QA	1277	C	C6-N1-C2	-5.50	118.10	120.30
22	QV	62	C	N3-C2-O2	-5.49	118.06	121.90
35	RA	2161	C	N1-C2-O2	5.49	122.20	118.90
1	XA	255	G	N1-C6-O6	-5.49	116.60	119.90
45	YP	59	LEU	N-CA-C	-5.49	96.17	111.00
1	XA	514	C	C6-N1-C2	-5.49	118.10	120.30
1	XA	826	C	C2-N1-C1'	5.49	124.84	118.80
1	XA	169	C	C5-C6-N1	5.49	123.74	121.00
35	YA	1670	C	C5-C6-N1	5.48	123.74	121.00
35	YA	2506	U	C5-C6-N1	5.48	125.44	122.70
35	RA	2116	G	C8-N9-C4	-5.48	104.21	106.40
37	RD	35	LYS	N-CA-C	5.48	125.80	111.00
1	XA	703	G	P-O3'-C3'	5.48	126.28	119.70
1	XA	346	G	C8-N9-C1'	-5.48	119.88	127.00
35	YA	2771	C	C6-N1-C2	-5.48	118.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	354	G	C4-N9-C1'	5.47	133.62	126.50
1	QA	882	C	N1-C2-O2	5.47	122.18	118.90
35	YA	27	G	C8-N9-C1'	5.47	134.12	127.00
35	YA	1233	C	C6-N1-C2	-5.47	118.11	120.30
35	RA	530	G	N3-C4-N9	-5.47	122.72	126.00
35	RA	1403	C	N1-C2-O2	5.47	122.18	118.90
35	YA	2210	G	N3-C4-C5	-5.47	125.87	128.60
35	RA	2076	U	C5-C6-N1	5.47	125.43	122.70
35	YA	105	C	C5-C6-N1	5.47	123.73	121.00
35	YA	1333	C	N1-C2-O2	5.47	122.18	118.90
35	RA	971	C	C6-N1-C2	-5.46	118.11	120.30
35	YA	1095	A	C4-N9-C1'	5.46	136.14	126.30
55	YZ	3	TYR	CA-CB-CG	5.46	123.78	113.40
1	QA	764	C	N3-C2-O2	-5.46	118.08	121.90
41	RH	153	LYS	N-CA-C	5.46	125.75	111.00
36	YB	30	C	C6-N1-C2	-5.46	118.11	120.30
1	XA	948	C	C6-N1-C2	-5.46	118.12	120.30
1	QA	882	C	N3-C2-O2	-5.46	118.08	121.90
35	YA	2185	C	C6-N1-C2	-5.46	118.12	120.30
1	QA	58	C	C6-N1-C2	-5.46	118.12	120.30
1	XA	272	C	N3-C2-O2	-5.46	118.08	121.90
35	RA	253	C	C5-C6-N1	5.45	123.73	121.00
35	RA	1899	G	N7-C8-N9	5.45	115.83	113.10
35	YA	74	A	O4'-C1'-N9	-5.45	103.84	108.20
1	XA	169	C	C6-N1-C2	-5.45	118.12	120.30
35	YA	2468	G	O4'-C1'-N9	5.45	112.56	108.20
1	QA	1230	C	C5-C6-N1	5.45	123.72	121.00
35	RA	2787	C	N3-C2-O2	-5.45	118.08	121.90
35	YA	1178	C	P-O3'-C3'	5.45	126.24	119.70
35	RA	914	C	C6-N1-C2	-5.45	118.12	120.30
35	RA	1983	C	C6-N1-C2	-5.45	118.12	120.30
35	YA	871	U	O5'-P-OP1	-5.45	100.80	105.70
1	XA	385	C	C6-N1-C2	-5.44	118.12	120.30
35	YA	284	U	C6-N1-C2	-5.44	117.73	121.00
35	YA	1376	C	C2-N1-C1'	5.44	124.79	118.80
35	RA	1178	C	P-O3'-C3'	5.44	126.23	119.70
35	RA	140	A	C5-N7-C8	-5.44	101.18	103.90
35	RA	692	C	C5-C6-N1	5.44	123.72	121.00
26	Y1	43	TYR	CA-CB-CG	5.44	123.74	113.40
35	YA	1598	C	C6-N1-C2	-5.44	118.12	120.30
35	YA	1295	C	C6-N1-C2	-5.44	118.12	120.30
24	QY	30	G	N3-C4-N9	5.44	129.26	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	120	U	C6-N1-C1'	-5.44	113.59	121.20
35	RA	904	C	N1-C2-O2	5.44	122.16	118.90
1	QA	789	U	N1-C2-O2	5.44	126.61	122.80
35	RA	2321	G	N3-C4-N9	5.44	129.26	126.00
35	YA	2403	C	C2-N1-C1'	5.43	124.78	118.80
35	YA	1804	C	C6-N1-C2	-5.43	118.13	120.30
1	XA	1039	C	N1-C2-O2	5.43	122.16	118.90
35	RA	2321	G	N3-C4-C5	-5.43	125.89	128.60
35	YA	944	G	C4-N9-C1'	5.43	133.56	126.50
35	RA	1827	C	N1-C2-O2	5.43	122.16	118.90
1	QA	1071	C	C6-N1-C2	-5.43	118.13	120.30
17	QQ	42	TYR	CA-CB-CG	5.42	123.70	113.40
35	YA	634	C	N1-C2-O2	5.42	122.15	118.90
35	RA	1578	U	N3-C2-O2	-5.42	118.41	122.20
35	RA	2036	C	N3-C2-O2	-5.42	118.11	121.90
1	XA	827	U	C6-N1-C1'	-5.42	113.62	121.20
35	YA	1433	U	C5-C6-N1	5.42	125.41	122.70
1	XA	991	U	C5-C6-N1	5.42	125.41	122.70
35	YA	1786	A	C5-N7-C8	-5.42	101.19	103.90
35	RA	231	C	C6-N1-C2	-5.41	118.14	120.30
35	RA	1534	G	N3-C4-N9	5.41	129.25	126.00
35	YA	2688	U	C5-C4-O4	5.41	129.15	125.90
1	QA	1502	A	C4-C5-N7	5.41	113.40	110.70
35	RA	1600	C	C6-N1-C2	-5.41	118.14	120.30
35	YA	264	C	N1-C2-O2	5.41	122.14	118.90
35	RA	2210	G	N3-C4-C5	-5.40	125.90	128.60
35	RA	2559	C	C6-N1-C2	-5.40	118.14	120.30
1	XA	652	U	N1-C2-O2	5.40	126.58	122.80
1	QA	181	G	P-O3'-C3'	5.40	126.18	119.70
1	QA	690	G	O4'-C1'-N9	5.40	112.52	108.20
1	QA	960	U	C6-N1-C1'	-5.40	113.64	121.20
35	RA	2689	U	P-O3'-C3'	5.40	126.18	119.70
1	XA	233	C	C6-N1-C2	-5.40	118.14	120.30
35	YA	640	C	C6-N1-C2	-5.40	118.14	120.30
35	YA	1387	C	C6-N1-C2	-5.40	118.14	120.30
35	YA	1879	C	C5-C6-N1	5.39	123.70	121.00
1	XA	1290	G	C4-N9-C1'	5.39	133.51	126.50
35	RA	2471	C	C2-N1-C1'	5.39	124.73	118.80
35	RA	1062	G	C8-N9-C1'	-5.39	120.00	127.00
1	XA	417	C	C6-N1-C2	-5.39	118.15	120.30
1	XA	699	C	C5-C6-N1	5.38	123.69	121.00
35	YA	595	C	C5-C6-N1	5.38	123.69	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	2575	C	C5-C6-N1	5.38	123.69	121.00
35	RA	595	C	C6-N1-C2	-5.38	118.15	120.30
1	XA	739	C	C5-C6-N1	5.38	123.69	121.00
1	XA	810	C	N3-C2-O2	-5.38	118.13	121.90
1	XA	1527	C	C6-N1-C2	-5.38	118.15	120.30
42	RI	126	TYR	CA-CB-CG	5.38	123.61	113.40
49	RT	100	TYR	CA-CB-CG	5.38	123.61	113.40
35	YA	1994	C	C6-N1-C2	-5.37	118.15	120.30
35	RA	702	G	C8-N9-C1'	-5.37	120.02	127.00
35	RA	2559	C	N3-C2-O2	-5.37	118.14	121.90
35	YA	2056	G	N3-C2-N2	-5.37	116.14	119.90
35	RA	196	A	C2-N3-C4	5.37	113.28	110.60
36	RB	60	C	C6-N1-C2	-5.37	118.15	120.30
35	YA	343	C	C6-N1-C2	-5.37	118.15	120.30
35	YA	1506	C	N1-C2-O2	5.37	122.12	118.90
35	YA	1988	C	C5-C6-N1	5.37	123.68	121.00
35	RA	1314	C	N3-C2-O2	-5.37	118.14	121.90
35	YA	503	A	P-O3'-C3'	5.37	126.14	119.70
35	YA	529	A	C2-N3-C4	5.37	113.28	110.60
35	YA	1496	A	C8-N9-C4	-5.36	103.66	105.80
16	QP	17	TYR	CA-CB-CG	5.36	123.59	113.40
35	YA	1411	C	N1-C2-O2	5.36	122.12	118.90
35	YA	595	C	C6-N1-C2	-5.36	118.16	120.30
35	RA	1376	C	N3-C2-O2	-5.36	118.15	121.90
35	RA	1879	C	C6-N1-C2	-5.36	118.16	120.30
35	YA	893	C	C6-N1-C2	-5.36	118.16	120.30
35	YA	1920	C	C6-N1-C2	-5.36	118.16	120.30
36	RB	22	U	C5-C6-N1	5.36	125.38	122.70
1	XA	1505	G	C8-N9-C1'	5.36	133.96	127.00
35	RA	364	C	C5-C6-N1	5.35	123.68	121.00
1	XA	311	C	C6-N1-C2	-5.35	118.16	120.30
1	XA	353	A	OP2-P-O3'	5.35	116.98	105.20
35	YA	1686	C	N1-C2-O2	5.35	122.11	118.90
35	RA	912	C	N3-C2-O2	-5.35	118.15	121.90
1	XA	1384	C	C6-N1-C2	-5.35	118.16	120.30
1	QA	1322	C	C6-N1-C2	-5.35	118.16	120.30
35	YA	2097	C	N1-C2-O2	5.35	122.11	118.90
1	XA	1008	C	N1-C2-O2	5.35	122.11	118.90
35	YA	1535	U	O4'-C1'-N1	5.35	112.48	108.20
49	YT	111	ARG	N-CA-C	-5.35	96.56	111.00
42	RI	133	HIS	N-CA-C	-5.35	96.56	111.00
1	XA	1346	A	C8-N9-C4	5.35	107.94	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	271(B)	G	OP2-P-O3'	5.35	116.97	105.20
35	YA	904	C	C6-N1-C2	-5.35	118.16	120.30
35	RA	273(F)	C	N3-C2-O2	-5.35	118.16	121.90
35	YA	1376	C	N3-C2-O2	-5.34	118.16	121.90
35	YA	234	C	C6-N1-C2	-5.34	118.16	120.30
35	YA	1686	C	C5-C6-N1	5.34	123.67	121.00
1	QA	1203	C	C5-C6-N1	5.34	123.67	121.00
35	YA	816	C	N3-C2-O2	-5.34	118.16	121.90
1	QA	369	C	C6-N1-C2	-5.34	118.16	120.30
35	RA	1026	U	OP1-P-O3'	5.34	116.95	105.20
35	RA	1535	U	N3-C2-O2	-5.34	118.46	122.20
1	QA	1336	C	P-O3'-C3'	5.34	126.11	119.70
1	XA	1230	C	C5-C6-N1	5.34	123.67	121.00
35	YA	971	C	C6-N1-C2	-5.34	118.17	120.30
35	YA	140	A	N7-C8-N9	5.33	116.47	113.80
35	YA	1765	C	N3-C2-O2	-5.33	118.17	121.90
35	RA	2559	C	C5-C6-N1	5.33	123.67	121.00
35	YA	2097	C	C6-N1-C2	-5.33	118.17	120.30
35	YA	1496	A	C5-N7-C8	-5.33	101.24	103.90
35	YA	201	C	C6-N1-C2	-5.33	118.17	120.30
35	YA	99	U	C2-N1-C1'	5.32	124.09	117.70
35	YA	1402	C	C5-C6-N1	5.32	123.66	121.00
35	YA	2832	U	OP2-P-O3'	5.32	116.91	105.20
1	QA	1097	C	N1-C2-O2	5.32	122.09	118.90
35	RA	2378	A	C8-N9-C4	5.32	107.93	105.80
1	XA	131	C	N1-C2-O2	5.32	122.09	118.90
35	YA	267	C	C6-N1-C2	-5.32	118.17	120.30
35	YA	269	U	C2-N1-C1'	5.32	124.08	117.70
35	YA	1982	C	C5-C6-N1	5.32	123.66	121.00
35	RA	1332	G	C5-N7-C8	-5.32	101.64	104.30
35	YA	537	C	N3-C2-O2	-5.32	118.18	121.90
35	YA	1105	U	N3-C2-O2	-5.32	118.48	122.20
31	Y6	46	HIS	N-CA-C	5.31	125.34	111.00
35	RA	461	C	N1-C2-O2	5.31	122.09	118.90
1	QA	866	C	C5-C6-N1	5.31	123.65	121.00
35	YA	911	A	N7-C8-N9	5.31	116.45	113.80
1	QA	972	C	C6-N1-C2	-5.31	118.18	120.30
1	XA	596	C	N1-C2-O2	5.31	122.08	118.90
35	YA	253	C	C6-N1-C2	-5.31	118.18	120.30
46	RQ	27	VAL	N-CA-C	-5.31	96.67	111.00
1	QA	970	C	N1-C2-O2	5.30	122.08	118.90
35	RA	1786	A	C6-C5-N7	-5.30	128.59	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	1881	C	N3-C2-O2	-5.30	118.19	121.90
1	XA	290	C	N1-C2-O2	5.30	122.08	118.90
35	RA	856	C	C2'-C3'-O3'	5.30	122.19	113.70
35	YA	1087	G	C8-N9-C4	-5.30	104.28	106.40
1	XA	328	C	C5-C6-N1	5.30	123.65	121.00
1	XA	1452	C	N1-C2-O2	5.30	122.08	118.90
35	RA	1180	C	N1-C2-O2	5.30	122.08	118.90
35	RA	776	G	C4-N9-C1'	5.30	133.39	126.50
1	QA	307	C	N1-C2-O2	5.30	122.08	118.90
35	RA	1437	C	C5-C6-N1	5.30	123.65	121.00
35	RA	1691	C	N1-C2-O2	5.30	122.08	118.90
35	RA	271(B)	G	OP2-P-O3'	5.29	116.85	105.20
35	RA	687	C	C2-N1-C1'	5.29	124.62	118.80
35	YA	535	C	C5-C6-N1	5.29	123.65	121.00
1	QA	412	A	OP2-P-O3'	5.29	116.85	105.20
35	RA	269	U	N1-C2-O2	5.29	126.50	122.80
1	XA	243	A	P-O3'-C3'	5.29	126.05	119.70
1	XA	1439	C	N3-C2-O2	-5.29	118.19	121.90
35	RA	914	C	C5-C6-N1	5.29	123.64	121.00
35	YA	114	U	C5-C6-N1	5.29	125.34	122.70
35	RA	2576	G	C8-N9-C1'	-5.29	120.12	127.00
35	YA	1781	C	N3-C2-O2	-5.29	118.20	121.90
12	QL	104	VAL	C-N-CA	5.29	134.92	121.70
36	RB	31	C	C2-N1-C1'	5.29	124.62	118.80
35	YA	702	G	C4-N9-C1'	5.29	133.38	126.50
35	YA	2617	C	N1-C2-O2	5.29	122.07	118.90
35	YA	1438	U	C5-C6-N1	5.29	125.34	122.70
1	XA	792	A	N7-C8-N9	5.28	116.44	113.80
35	YA	856	C	P-O3'-C3'	5.28	126.04	119.70
35	YA	2562	U	N3-C2-O2	-5.28	118.50	122.20
35	RA	409	C	N1-C2-O2	5.28	122.07	118.90
1	XA	221	C	C6-N1-C2	-5.28	118.19	120.30
35	YA	1956	U	C6-N1-C2	-5.28	117.83	121.00
35	RA	588	U	O5'-P-OP1	-5.28	100.95	105.70
1	XA	1429	C	N1-C2-O2	5.28	122.07	118.90
35	YA	1686	C	N3-C2-O2	-5.28	118.20	121.90
35	RA	242	G	OP2-P-O3'	5.28	116.81	105.20
55	RZ	115	GLY	N-CA-C	5.28	126.29	113.10
35	RA	1468	C	C6-N1-C2	-5.28	118.19	120.30
35	RA	2766	G	C4-N9-C1'	5.28	133.36	126.50
35	YA	2441	C	C6-N1-C2	-5.28	118.19	120.30
35	YA	2443	C	N3-C2-O2	-5.28	118.21	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	YB	22	U	C6-N1-C2	-5.28	117.83	121.00
35	YA	41	C	C6-N1-C2	-5.27	118.19	120.30
35	YA	529	A	C4-N9-C1'	5.27	135.79	126.30
35	YA	974(A)	C	C2-N1-C1'	5.27	124.60	118.80
1	QA	370	C	N1-C2-O2	5.27	122.06	118.90
35	RA	1708	C	C6-N1-C2	-5.27	118.19	120.30
35	RA	2307	G	C4-N9-C1'	5.27	133.35	126.50
35	RA	530	G	C6-C5-N7	5.27	133.56	130.40
35	YA	2559	C	C2-N1-C1'	5.27	124.60	118.80
35	RA	1502	C	N3-C4-N4	5.27	121.69	118.00
35	RA	1774	C	C5-C6-N1	5.27	123.64	121.00
1	XA	1395	C	N1-C2-O2	5.27	122.06	118.90
5	XE	72	GLN	C-N-CA	5.27	134.88	121.70
35	YA	2490	G	C4-C5-N7	5.27	112.91	110.80
35	YA	1053	C	C6-N1-C2	-5.27	118.19	120.30
35	YA	1656	C	C5-C6-N1	5.27	123.63	121.00
1	QA	1234	C	N3-C2-O2	-5.26	118.21	121.90
35	RA	2471	C	C5-C6-N1	5.26	123.63	121.00
42	RI	14	ASP	C-N-CA	5.26	134.86	121.70
30	R5	51	TYR	C-N-CA	5.26	134.85	121.70
35	YA	316	C	C6-N1-C2	-5.26	118.20	120.30
1	QA	792	A	C4-N9-C1'	5.26	135.77	126.30
35	YA	141	A	N7-C8-N9	5.26	116.43	113.80
35	YA	544	C	C6-N1-C2	-5.26	118.20	120.30
41	YH	83	TYR	N-CA-C	5.26	125.20	111.00
35	RA	676	A	O4'-C1'-N9	5.26	112.41	108.20
35	YA	1598	C	C2-N1-C1'	5.26	124.58	118.80
35	YA	2666	C	N1-C2-O2	5.25	122.05	118.90
24	QY	69	C	N1-C2-O2	5.25	122.05	118.90
35	YA	1174	A	N3-C4-N9	5.25	131.60	127.40
35	YA	850	C	C6-N1-C2	-5.25	118.20	120.30
1	QA	1163	C	N1-C2-O2	5.25	122.05	118.90
35	RA	1781	C	N1-C2-O2	5.25	122.05	118.90
35	YA	1315	C	N3-C2-O2	-5.25	118.23	121.90
1	QA	1336	C	C6-N1-C2	-5.25	118.20	120.30
1	QA	1447	G	C4-N9-C1'	5.25	133.32	126.50
35	YA	528	A	C5-N7-C8	-5.25	101.28	103.90
36	YB	27	C	C6-N1-C2	-5.25	118.20	120.30
35	RA	1766	U	C5-C6-N1	5.25	125.32	122.70
35	YA	1223	C	C6-N1-C2	-5.25	118.20	120.30
35	RA	1021	A	C8-N9-C4	-5.24	103.70	105.80
35	RA	1982	C	C5-C4-N4	-5.24	116.53	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	358	U	C5-C6-N1	5.24	125.32	122.70
35	RA	738	G	N3-C4-C5	-5.24	125.98	128.60
1	XA	381	C	N1-C2-O2	5.24	122.04	118.90
35	YA	2238	G	N3-C4-N9	5.24	129.14	126.00
35	YA	1085	A	P-O3'-C3'	5.24	125.99	119.70
35	RA	692	C	C6-N1-C2	-5.24	118.20	120.30
35	RA	2701	C	C6-N1-C2	-5.24	118.20	120.30
35	RA	654(T)	C	N1-C2-O2	5.24	122.04	118.90
35	YA	1992	G	OP2-P-O3'	5.24	116.72	105.20
35	YA	2474	C	C6-N1-C1'	-5.24	114.52	120.80
35	RA	333	G	C4-N9-C1'	5.23	133.30	126.50
35	YA	2391	G	O4'-C1'-N9	5.23	112.39	108.20
35	RA	2506	U	C6-N1-C2	-5.23	117.86	121.00
35	YA	1544	C	N3-C2-O2	-5.23	118.24	121.90
35	RA	2559	C	C2-N1-C1'	5.23	124.55	118.80
35	YA	221	A	P-O3'-C3'	5.23	125.97	119.70
38	YE	37	ARG	C-N-CA	5.23	134.77	121.70
1	QA	449	C	N3-C2-O2	-5.23	118.24	121.90
35	RA	1332	G	C8-N9-C1'	-5.23	120.20	127.00
35	RA	991	C	C6-N1-C2	-5.22	118.21	120.30
35	YA	1568	G	C8-N9-C1'	5.22	133.79	127.00
35	YA	2307	G	C8-N9-C4	-5.22	104.31	106.40
1	QA	1452	C	N1-C2-O2	5.22	122.03	118.90
35	YA	1352	U	N3-C2-O2	-5.22	118.54	122.20
35	RA	1290	C	C6-N1-C2	-5.22	118.21	120.30
35	RA	1920	C	C5-C6-N1	5.22	123.61	121.00
1	QA	565	U	C5-C4-O4	-5.22	122.77	125.90
35	YA	1315	C	C6-N1-C2	-5.22	118.21	120.30
35	YA	2766	G	C8-N9-C1'	-5.22	120.22	127.00
35	YA	1786	A	C4-N9-C1'	5.22	135.69	126.30
35	YA	974(A)	C	N3-C2-O2	-5.22	118.25	121.90
35	YA	2774	C	N3-C2-O2	-5.22	118.25	121.90
1	XA	973	G	C8-N9-C4	-5.21	104.31	106.40
35	RA	1589	C	N3-C2-O2	-5.21	118.25	121.90
35	YA	2403	C	C5-C6-N1	5.21	123.61	121.00
1	QA	726	C	C6-N1-C2	-5.21	118.22	120.30
35	RA	1376	C	C6-N1-C2	-5.21	118.22	120.30
35	RA	893	C	N1-C2-O2	5.21	122.02	118.90
35	RA	1461	G	C4-N9-C1'	5.21	133.27	126.50
35	YA	2443	C	C6-N1-C2	-5.21	118.22	120.30
1	XA	1395	C	C2-N1-C1'	5.21	124.53	118.80
35	YA	1950	G	C6-C5-N7	-5.21	127.28	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	1982	C	N3-C4-N4	5.20	121.64	118.00
35	RA	74	A	O4'-C1'-N9	-5.20	104.04	108.20
35	RA	1797	C	C5-C6-N1	5.20	123.60	121.00
35	RA	2616	C	C6-N1-C2	-5.20	118.22	120.30
35	YA	1644	C	C6-N1-C2	-5.20	118.22	120.30
1	QA	932	C	C2-N1-C1'	5.20	124.52	118.80
1	XA	43	C	C6-N1-C2	-5.20	118.22	120.30
1	QA	1070	U	N3-C2-O2	-5.20	118.56	122.20
1	XA	963	G	C4-C5-C6	5.20	121.92	118.80
22	XV	34	C	N3-C2-O2	-5.20	118.26	121.90
35	YA	1437	C	C2-N1-C1'	5.20	124.52	118.80
35	YA	393	C	C5-C6-N1	5.19	123.60	121.00
35	YA	141	A	C5-N7-C8	-5.19	101.30	103.90
35	YA	318	C	C6-N1-C2	-5.19	118.22	120.30
35	YA	1827	C	N1-C2-O2	5.19	122.02	118.90
35	RA	1819	A	P-O3'-C3'	5.19	125.93	119.70
35	YA	650	C	N3-C2-O2	-5.19	118.27	121.90
35	YA	2504	U	N1-C2-O2	5.19	126.43	122.80
35	YA	2814	C	N1-C2-O2	5.19	122.01	118.90
1	XA	328	C	OP2-P-O3'	5.19	116.61	105.20
36	RB	30	C	N1-C2-O2	5.18	122.01	118.90
1	XA	174	C	C6-N1-C2	-5.18	118.23	120.30
1	XA	645	C	N3-C2-O2	-5.18	118.27	121.90
1	QA	91	C	N3-C2-O2	-5.18	118.27	121.90
1	QA	680	C	C6-N1-C2	-5.18	118.23	120.30
35	RA	102	G	P-O3'-C3'	5.18	125.92	119.70
35	RA	1187	G	N7-C8-N9	5.18	115.69	113.10
35	RA	1404	C	C6-N1-C2	-5.18	118.23	120.30
35	YA	1005	C	N3-C2-O2	-5.18	118.27	121.90
35	YA	564	C	C6-N1-C2	-5.18	118.23	120.30
35	YA	797	C	C6-N1-C2	-5.18	118.23	120.30
35	YA	2328	A	C8-N9-C4	-5.18	103.73	105.80
35	RA	273(F)	C	C5-C6-N1	5.18	123.59	121.00
35	RA	2616	C	N3-C2-O2	-5.18	118.27	121.90
35	YA	965	C	C6-N1-C2	-5.18	118.23	120.30
42	YI	131	LYS	N-CA-C	5.18	124.97	111.00
1	QA	1163	C	N3-C2-O2	-5.17	118.28	121.90
35	RA	2311	A	C8-N9-C4	-5.17	103.73	105.80
13	QM	13	LYS	N-CA-C	5.17	124.96	111.00
35	RA	409	C	N3-C2-O2	-5.17	118.28	121.90
1	XA	977	A	N7-C8-N9	5.17	116.39	113.80
35	YA	786	C	C6-N1-C2	-5.17	118.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	2611	U	C5-C6-N1	5.17	125.29	122.70
36	RB	44	G	C4-N9-C1'	-5.17	119.78	126.50
1	QA	1313	U	C5-C6-N1	5.17	125.28	122.70
1	XA	960	U	N1-C2-O2	5.17	126.42	122.80
35	YA	2726	U	C2-N1-C1'	5.17	123.90	117.70
35	RA	456	C	N3-C2-O2	-5.17	118.28	121.90
35	YA	138	G	O4'-C1'-N9	5.17	112.33	108.20
1	QA	1301	U	C5-C6-N1	5.17	125.28	122.70
35	RA	307	G	N7-C8-N9	5.17	115.68	113.10
1	XA	645	C	N1-C2-O2	5.17	122.00	118.90
35	RA	1930	G	P-O3'-C3'	5.16	125.90	119.70
35	YA	41	C	N1-C2-O2	5.16	122.00	118.90
35	RA	1502	C	C6-N1-C2	-5.16	118.24	120.30
35	RA	1941	C	C5-C6-N1	5.16	123.58	121.00
35	YA	673	C	C6-N1-C2	-5.16	118.24	120.30
1	QA	308	C	C6-N1-C2	-5.16	118.24	120.30
35	RA	2656	U	N3-C2-O2	-5.16	118.59	122.20
35	YA	270(Y)	G	C8-N9-C4	-5.16	104.34	106.40
1	QA	980	C	N3-C2-O2	-5.16	118.29	121.90
1	QA	1158	C	C5-C6-N1	5.16	123.58	121.00
22	QV	34	C	N1-C2-O2	5.16	121.99	118.90
35	RA	2394	C	C6-N1-C2	-5.16	118.24	120.30
44	YO	4	PRO	C-N-CA	5.16	134.59	121.70
35	RA	313	C	C5-C6-N1	5.15	123.58	121.00
1	XA	19	C	N3-C2-O2	-5.15	118.29	121.90
35	RA	480	A	OP1-P-O3'	5.15	116.53	105.20
35	RA	1534	G	C4-N9-C1'	5.15	133.20	126.50
35	RA	1795	C	C5-C6-N1	5.15	123.58	121.00
35	RA	1931	U	N3-C2-O2	-5.15	118.59	122.20
1	XA	413	G	O4'-C1'-N9	5.15	112.32	108.20
35	YA	1836	C	N3-C2-O2	-5.15	118.29	121.90
1	XA	948	C	C5-C6-N1	5.15	123.58	121.00
35	YA	153	C	C6-N1-C2	-5.15	118.24	120.30
35	YA	2667	C	C5-C6-N1	5.15	123.58	121.00
1	XA	1263	C	N1-C2-O2	5.15	121.99	118.90
1	QA	328	C	C2-N3-C4	5.15	122.47	119.90
35	RA	66	C	C5-C6-N1	5.15	123.57	121.00
35	YA	228	A	C8-N9-C4	-5.14	103.74	105.80
35	RA	537	C	C6-N1-C2	-5.14	118.24	120.30
51	RV	45	THR	N-CA-C	5.14	124.89	111.00
1	XA	690	G	C4-N9-C1'	5.14	133.18	126.50
35	YA	1038	C	N1-C2-O2	5.14	121.98	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	1833	U	N3-C2-O2	-5.14	118.60	122.20
35	YA	268	C	C6-N1-C2	-5.14	118.24	120.30
35	YA	588	U	O5'-P-OP1	-5.14	101.07	105.70
35	YA	2066	C	N1-C2-O2	5.14	121.98	118.90
35	YA	2056	G	C4-N9-C1'	5.14	133.18	126.50
35	YA	591	C	C6-N1-C2	-5.13	118.25	120.30
35	RA	2097	C	C6-N1-C2	-5.13	118.25	120.30
1	QA	369	C	C2-N1-C1'	5.13	124.44	118.80
1	XA	290	C	N3-C2-O2	-5.13	118.31	121.90
35	YA	541	C	C6-N1-C2	-5.13	118.25	120.30
35	YA	1947	C	C6-N1-C2	-5.13	118.25	120.30
35	RA	1514	U	C2-N1-C1'	5.13	123.86	117.70
35	YA	2079	U	C5-C6-N1	5.13	125.27	122.70
1	QA	346	G	C8-N9-C1'	-5.13	120.33	127.00
1	QA	703	G	P-O3'-C3'	5.13	125.85	119.70
35	RA	1502	C	C5-C6-N1	5.13	123.56	121.00
1	XA	991	U	N3-C2-O2	-5.13	118.61	122.20
24	XY	56	C	N1-C2-O2	5.13	121.98	118.90
35	RA	530	G	N9-C4-C5	5.13	107.45	105.40
1	XA	1114	C	C2-N1-C1'	5.13	124.44	118.80
35	YA	316	C	N1-C2-O2	5.13	121.98	118.90
35	YA	1888	G	N3-C4-N9	5.13	129.08	126.00
38	RE	186	GLY	N-CA-C	5.12	125.91	113.10
1	XA	526	C	C5-C6-N1	5.12	123.56	121.00
35	YA	1669	A	C4-N9-C1'	5.12	135.52	126.30
35	YA	1411	C	N3-C2-O2	-5.12	118.32	121.90
35	YA	1779	U	C2-N1-C1'	5.12	123.84	117.70
35	RA	2699	C	C5-C6-N1	5.12	123.56	121.00
1	XA	1260	C	N3-C2-O2	-5.12	118.32	121.90
35	YA	1005	C	C2-N1-C1'	5.12	124.43	118.80
35	YA	1437	C	C6-N1-C2	-5.12	118.25	120.30
1	XA	1086	U	C5-C6-N1	5.12	125.26	122.70
35	YA	18	C	C6-N1-C2	-5.12	118.25	120.30
35	YA	137	C	C6-N1-C2	-5.12	118.25	120.30
35	YA	2039	C	C5-C6-N1	5.12	123.56	121.00
35	YA	2096	U	C6-N1-C2	-5.12	117.93	121.00
35	RA	529	A	C4-N9-C1'	5.11	135.50	126.30
35	RA	1574	C	C5-C6-N1	5.11	123.56	121.00
35	YA	859	G	OP2-P-O3'	5.11	116.45	105.20
35	YA	1509	C	OP1-P-O3'	5.11	116.45	105.20
35	YA	2666	C	C6-N1-C2	-5.11	118.25	120.30
1	QA	1420	C	C6-N1-C2	-5.11	118.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	269	U	N3-C2-O2	-5.11	118.62	122.20
35	RA	752	A	OP2-P-O3'	5.11	116.44	105.20
35	RA	1258	C	C6-N1-C2	-5.11	118.25	120.30
35	RA	1062	G	N3-C4-C5	-5.11	126.05	128.60
35	RA	1406	U	N3-C2-O2	-5.11	118.62	122.20
25	R0	26	TYR	CA-CB-CG	5.11	123.10	113.40
35	RA	828	U	C6-N1-C1'	-5.11	114.05	121.20
1	QA	449	C	C6-N1-C2	-5.11	118.26	120.30
1	QA	1070	U	C6-N1-C2	-5.11	117.94	121.00
35	RA	2702	U	O4'-C1'-N1	5.11	112.28	108.20
35	YA	335	C	C5-C6-N1	5.11	123.55	121.00
35	RA	345	A	P-O3'-C3'	5.10	125.82	119.70
1	XA	1505	G	N3-C2-N2	-5.10	116.33	119.90
35	YA	838	C	C5-C6-N1	5.10	123.55	121.00
35	YA	1979	C	N1-C2-O2	5.10	121.96	118.90
35	YA	2880	C	C5-C6-N1	5.10	123.55	121.00
35	RA	756	C	N3-C2-O2	-5.10	118.33	121.90
35	RA	1776	G	C4-N9-C1'	5.10	133.13	126.50
36	RB	5	C	N1-C2-O2	5.10	121.96	118.90
44	RO	32	TYR	CA-CB-CG	5.10	123.08	113.40
1	XA	792	A	C4-N9-C1'	5.10	135.48	126.30
35	YA	2692	C	N3-C2-O2	-5.10	118.33	121.90
35	YA	404	C	OP2-P-O3'	5.10	116.41	105.20
50	RU	90	VAL	C-N-CA	5.09	134.44	121.70
35	YA	1786	A	C4-C5-N7	5.09	113.25	110.70
35	YA	2473	U	N3-C2-O2	-5.09	118.63	122.20
35	YA	1411	C	C5-C6-N1	5.09	123.55	121.00
36	YB	43	C	C6-N1-C2	-5.09	118.26	120.30
35	RA	2129	C	N1-C2-O2	5.09	121.95	118.90
1	XA	868	C	N3-C2-O2	-5.09	118.34	121.90
35	YA	2317	C	C6-N1-C2	-5.09	118.26	120.30
1	QA	687	A	C2-N3-C4	5.09	113.14	110.60
24	XY	72	C	C6-N1-C2	-5.09	118.26	120.30
35	YA	2726	U	N1-C2-O2	5.09	126.36	122.80
35	RA	1963	U	C5-C6-N1	5.09	125.24	122.70
35	RA	2626	C	C6-N1-C2	-5.09	118.27	120.30
1	XA	932	C	C2-N1-C1'	5.09	124.39	118.80
35	YA	1178	C	N3-C2-O2	-5.09	118.34	121.90
35	YA	1956	U	C2-N1-C1'	5.08	123.80	117.70
1	QA	328	C	C6-N1-C1'	-5.08	114.70	120.80
35	RA	253	C	N3-C2-O2	-5.08	118.34	121.90
35	RA	1691	C	N3-C2-O2	-5.08	118.34	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	410	G	P-O3'-C3'	5.08	125.80	119.70
1	QA	652	U	N3-C2-O2	-5.08	118.64	122.20
35	RA	1765	C	C6-N1-C2	-5.08	118.27	120.30
42	RI	132	PRO	C-N-CA	5.08	134.40	121.70
35	YA	1534	G	C4-N9-C1'	5.08	133.10	126.50
1	XA	1114	C	C6-N1-C2	-5.08	118.27	120.30
35	RA	2620	C	C5-C6-N1	5.08	123.54	121.00
1	XA	354	G	C8-N9-C1'	-5.08	120.40	127.00
1	XA	963	G	N3-C4-C5	-5.08	126.06	128.60
35	YA	626	U	C6-N1-C2	-5.08	117.95	121.00
1	QA	689	C	C6-N1-C2	-5.08	118.27	120.30
35	RA	1404	C	C2-N1-C1'	5.08	124.38	118.80
35	RA	1575	C	N1-C2-O2	5.08	121.94	118.90
42	RI	13	GLY	N-CA-C	5.08	125.79	113.10
35	YA	756	C	C6-N1-C2	-5.08	118.27	120.30
35	YA	1158	C	C6-N1-C2	-5.08	118.27	120.30
1	XA	497	U	N1-C2-O2	5.07	126.35	122.80
35	RA	964	C	C6-N1-C2	-5.07	118.27	120.30
35	YA	1332	G	C8-N9-C1'	-5.07	120.41	127.00
35	YA	265	A	C5-C6-N1	5.07	120.23	117.70
24	XY	16	C	C6-N1-C2	-5.07	118.27	120.30
35	YA	529	A	C8-N9-C4	-5.07	103.77	105.80
35	YA	661	C	C5-C6-N1	5.07	123.53	121.00
1	QA	812	C	OP2-P-O3'	5.07	116.34	105.20
35	RA	2226	C	N1-C2-O2	5.07	121.94	118.90
1	XA	154	C	N3-C2-O2	-5.07	118.35	121.90
35	YA	565	C	N1-C2-O2	5.07	121.94	118.90
35	RA	945	A	C4-C5-N7	5.06	113.23	110.70
1	QA	103	C	N1-C2-O2	5.06	121.94	118.90
35	YA	838	C	N1-C2-O2	5.06	121.94	118.90
35	YA	1053	C	N1-C2-O2	5.06	121.94	118.90
35	YA	2439	A	N7-C8-N9	5.06	116.33	113.80
1	XA	1297	C	OP2-P-O3'	5.06	116.33	105.20
35	YA	228	A	C2-N3-C4	5.06	113.13	110.60
35	YA	2066	C	C5-C6-N1	5.06	123.53	121.00
1	QA	897	C	N1-C2-O2	5.06	121.94	118.90
1	QA	1019	C	C6-N1-C2	-5.06	118.28	120.30
35	RA	1832	C	C6-N1-C2	-5.06	118.28	120.30
38	RE	82	ARG	C-N-CA	5.06	134.34	121.70
35	YA	537	C	N1-C2-O2	5.06	121.93	118.90
1	QA	1499	A	O5'-P-OP1	-5.06	101.15	105.70
35	RA	29	U	C5-C6-N1	5.05	125.23	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	YT	99	LEU	CA-CB-CG	5.05	126.92	115.30
35	RA	2060	A	OP2-P-O3'	5.05	116.31	105.20
35	YA	930	U	C6-N1-C1'	-5.05	114.13	121.20
1	XA	789	U	N1-C2-O2	5.05	126.33	122.80
35	RA	613	U	C6-N1-C2	-5.04	117.97	121.00
1	QA	465	A	N1-C6-N6	-5.04	115.57	118.60
1	QA	1238	A	O5'-P-OP1	-5.04	101.16	105.70
35	RA	307	G	C8-N9-C4	-5.04	104.38	106.40
35	RA	373	U	N3-C2-O2	-5.04	118.67	122.20
35	YA	825	C	C6-N1-C2	-5.04	118.28	120.30
36	YB	60	C	C6-N1-C2	-5.04	118.28	120.30
49	RT	99	LEU	CA-CB-CG	5.04	126.90	115.30
22	XV	69	C	N3-C2-O2	-5.04	118.37	121.90
35	RA	2318	G	C4-N9-C1'	5.04	133.05	126.50
36	RB	68	C	C6-N1-C2	-5.04	118.28	120.30
1	XA	754	C	N1-C2-O2	5.04	121.92	118.90
1	XA	1397	C	C6-N1-C2	-5.04	118.28	120.30
1	QA	108	G	C4-N9-C1'	5.04	133.05	126.50
35	RA	104	U	N1-C2-O2	5.04	126.33	122.80
35	YA	1142(A)	A	N3-C4-N9	-5.04	123.37	127.40
35	YA	1514	U	C2-N1-C1'	5.04	123.75	117.70
35	YA	1264	G	N7-C8-N9	5.04	115.62	113.10
35	RA	2651	C	N1-C2-O2	5.04	121.92	118.90
35	YA	1819	A	P-O3'-C3'	5.04	125.74	119.70
29	R4	39	CYS	N-CA-C	-5.03	97.41	111.00
35	RA	1411	C	C5-C6-N1	5.03	123.52	121.00
35	RA	1657	C	C6-N1-C2	-5.03	118.29	120.30
35	RA	270(H)	C	C6-N1-C2	-5.03	118.29	120.30
1	XA	1303	C	C6-N1-C2	-5.03	118.29	120.30
1	XA	1397	C	C2-N1-C1'	5.03	124.33	118.80
35	YA	540	G	C8-N9-C4	-5.03	104.39	106.40
35	YA	1142(A)	A	C2-N3-C4	-5.03	108.08	110.60
35	YA	1343	G	C4-N9-C1'	5.03	133.04	126.50
35	YA	2053	G	O5'-P-OP1	-5.03	101.17	105.70
35	YA	1006	C	C6-N1-C2	-5.03	118.29	120.30
1	QA	406	G	C4-N9-C1'	5.03	133.03	126.50
35	YA	140	A	C8-N9-C4	-5.03	103.79	105.80
35	YA	231	C	C2-N1-C1'	5.03	124.33	118.80
22	QV	1	C	C6-N1-C2	-5.03	118.29	120.30
35	RA	1882	C	N3-C2-O2	-5.03	118.38	121.90
35	RA	2044	C	N1-C2-O2	5.02	121.92	118.90
35	RA	2107	C	C6-N1-C2	-5.02	118.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	1336	C	OP2-P-O3'	5.02	116.25	105.20
35	RA	588	U	C5-C6-N1	5.02	125.21	122.70
35	RA	2036	C	N1-C2-O2	5.02	121.91	118.90
35	YA	364	C	N3-C2-O2	-5.02	118.39	121.90
35	YA	2368	C	C6-N1-C2	-5.02	118.29	120.30
1	QA	753	A	OP2-P-O3'	5.02	116.24	105.20
35	RA	1474	C	N3-C2-O2	-5.02	118.39	121.90
35	YA	1433	U	C6-N1-C2	-5.02	117.99	121.00
35	YA	2261	C	C6-N1-C2	-5.02	118.29	120.30
50	YU	92	ARG	C-N-CA	5.02	134.24	121.70
1	QA	1336	C	C5-C6-N1	5.02	123.51	121.00
35	RA	697	C	C5-C6-N1	5.01	123.51	121.00
1	XA	545	C	C6-N1-C2	-5.01	118.29	120.30
35	YA	2592	G	N3-C4-N9	5.01	129.01	126.00
1	XA	963	G	N9-C4-C5	-5.01	103.39	105.40
35	YA	2074	U	C6-N1-C2	-5.01	117.99	121.00
35	YA	2891	G	C4-N9-C1'	5.01	133.01	126.50
35	YA	1836	C	N1-C2-O2	5.01	121.91	118.90
35	YA	2768	C	C5-C6-N1	5.01	123.50	121.00
1	QA	435	C	N3-C2-O2	-5.01	118.39	121.90
35	RA	377	C	C6-N1-C2	-5.01	118.30	120.30
35	RA	1461	G	N7-C8-N9	5.01	115.60	113.10
1	XA	1260	C	C5-C6-N1	5.01	123.50	121.00
36	YB	30	C	N3-C2-O2	-5.01	118.40	121.90
7	QG	56	GLN	C-N-CA	5.00	134.21	121.70
35	RA	404	C	OP2-P-O3'	5.00	116.21	105.20
35	YA	1504	C	N1-C2-O2	5.00	121.90	118.90
35	RA	1513	C	C5-C6-N1	5.00	123.50	121.00
35	RA	2238	G	C4-N9-C1'	5.00	133.00	126.50
36	RB	79	C	C6-N1-C2	-5.00	118.30	120.30
35	YA	1805	U	N1-C2-N3	5.00	117.90	114.90
49	YT	105	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
48	RS	17	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16277	208	0
1	XA	32249	0	16279	169	0
2	QB	1924	0	1975	27	0
2	XB	1924	0	1975	28	0
3	QC	1605	0	1668	37	0
3	XC	1605	0	1668	16	0
4	QD	1674	0	1718	30	0
4	XD	1674	0	1718	21	0
5	QE	1155	0	1213	20	0
5	XE	1155	0	1213	8	0
6	QF	843	0	857	10	0
6	XF	843	0	857	8	0
7	QG	1257	0	1296	11	0
7	XG	1257	0	1296	8	0
8	QH	1116	0	1177	13	0
8	XH	1116	0	1177	19	0
9	QI	1010	0	1037	23	0
9	XI	1010	0	1037	24	0
10	QJ	801	0	849	18	0
10	XJ	801	0	849	15	0
11	QK	885	0	904	17	0
11	XK	885	0	904	9	0
12	QL	975	0	1062	17	0
12	XL	975	0	1062	15	0
13	QM	964	0	1034	35	0
13	XM	964	0	1034	17	0
14	QN	492	0	529	14	0
14	XN	492	0	529	5	0
15	QO	734	0	771	7	0
15	XO	734	0	771	4	0
16	QP	705	0	725	14	0
16	XP	705	0	725	12	0
17	QQ	834	0	904	11	0
17	XQ	834	0	904	9	0
18	QR	574	0	644	13	0
18	XR	574	0	644	8	0
19	QS	674	0	699	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	XS	674	0	699	13	0
20	QT	763	0	860	6	0
20	XT	763	0	861	17	0
21	QU	217	0	234	5	0
21	XU	217	0	234	1	0
22	QV	1640	0	837	4	0
22	XV	1640	0	837	3	0
23	QX	396	0	197	2	0
23	XX	396	0	197	3	0
24	QY	1602	0	811	23	0
24	XY	1602	0	811	10	0
25	R0	648	0	672	15	0
25	Y0	648	0	672	10	0
26	R1	763	0	847	13	0
26	Y1	763	0	848	12	0
27	R2	581	0	629	15	0
27	Y2	581	0	629	11	0
28	R3	469	0	518	5	0
28	Y3	469	0	518	4	0
29	R4	581	0	577	17	0
29	Y4	581	0	577	16	0
30	R5	459	0	480	9	0
30	Y5	459	0	480	10	0
31	R6	424	0	450	11	0
31	Y6	424	0	450	11	0
32	R7	430	0	480	7	0
32	Y7	430	0	480	6	0
33	R8	517	0	582	17	0
33	Y8	517	0	582	30	0
34	R9	307	0	335	5	0
34	Y9	307	0	335	6	0
35	RA	62071	0	31280	341	0
35	YA	62091	0	31290	289	0
36	RB	2573	0	1306	15	0
36	YB	2573	0	1306	13	0
37	RD	2115	0	2195	43	0
37	YD	2115	0	2195	51	0
38	RE	1568	0	1633	45	0
38	YE	1568	0	1634	31	0
39	RF	1585	0	1632	22	0
39	YF	1585	0	1632	32	0
40	RG	1474	0	1535	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	YG	1474	0	1535	18	0
41	RH	1307	0	1382	20	0
41	YH	1307	0	1382	20	0
42	RI	1136	0	1223	12	0
42	YI	1136	0	1223	11	0
43	RN	1104	0	1180	23	0
43	YN	1104	0	1180	8	0
44	RO	933	0	996	23	0
44	YO	933	0	996	19	0
45	RP	1145	0	1227	30	0
45	YP	1145	0	1227	27	0
46	RQ	1122	0	1179	23	0
46	YQ	1122	0	1177	20	0
47	RR	968	0	1033	17	0
47	YR	968	0	1033	16	0
48	RS	882	0	943	9	0
48	YS	882	0	943	16	0
49	RT	1141	0	1202	29	0
49	YT	1141	0	1202	23	0
50	RU	964	0	1022	22	0
50	YU	964	0	1022	19	0
51	RV	779	0	852	17	0
51	YV	779	0	852	12	0
52	RW	900	0	964	15	0
52	YW	900	0	964	17	0
53	RX	725	0	778	9	0
53	YX	725	0	778	9	0
54	RY	785	0	878	14	0
54	YY	785	0	878	9	0
55	RZ	1461	0	1493	27	0
55	YZ	1461	0	1493	32	0
56	QA	73	0	0	0	0
56	QF	1	0	0	0	0
56	QM	1	0	0	0	0
56	QV	1	0	0	0	0
56	QX	2	0	0	0	0
56	R0	1	0	0	0	0
56	R5	1	0	0	0	0
56	R8	1	0	0	0	0
56	R9	1	0	0	0	0
56	RA	281	0	0	0	0
56	RB	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	RD	1	0	0	0	0
56	RE	4	0	0	0	0
56	RF	1	0	0	0	0
56	RP	3	0	0	0	0
56	RR	1	0	0	0	0
56	RU	1	0	0	0	0
56	XA	91	0	0	0	0
56	XF	1	0	0	0	0
56	XM	1	0	0	0	0
56	XV	2	0	0	0	0
56	XX	1	0	0	0	0
56	Y0	1	0	0	0	0
56	Y1	1	0	0	0	0
56	Y2	1	0	0	0	0
56	Y5	1	0	0	0	0
56	Y6	2	0	0	0	0
56	Y8	1	0	0	0	0
56	Y9	1	0	0	0	0
56	YA	347	0	0	0	0
56	YB	6	0	0	0	0
56	YE	3	0	0	0	0
56	YN	1	0	0	0	0
56	YP	3	0	0	0	0
56	YQ	3	0	0	0	0
56	YR	1	0	0	0	0
56	YX	1	0	0	0	0
57	QA	42	0	45	0	0
57	XA	42	0	45	4	0
58	QD	8	0	0	0	0
58	XD	8	0	0	0	0
59	QN	1	0	0	0	0
59	R9	1	0	0	0	0
59	XN	1	0	0	0	0
59	Y9	1	0	0	0	0
All	All	294981	0	199665	2182	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 (2182) 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)
55:YZ:94:GLU:CG	55:YZ:95:PRO:HD3	1.74	1.18
35:RA:1138:G:H21	43:RN:106:MET:HE1	1.13	1.11
35:RA:2055:C:H5'	35:RA:2056:G:H5''	1.35	1.07
55:YZ:94:GLU:HB3	55:YZ:95:PRO:CD	1.85	1.07
19:QS:10:PHE:HB2	19:QS:16:LEU:HD11	1.34	1.06
35:RA:1138:G:H21	43:RN:106:MET:CE	1.72	1.02
26:Y1:4:VAL:HG12	26:Y1:11:ARG:HD3	1.41	1.01
55:YZ:94:GLU:HG3	55:YZ:95:PRO:HD3	1.42	1.00
55:YZ:94:GLU:CB	55:YZ:95:PRO:HD3	1.90	1.00
25:R0:69:PHE:CE2	25:R0:79:VAL:HG22	1.98	0.96
25:R0:69:PHE:CD2	25:R0:79:VAL:HG22	2.00	0.96
3:QC:159:GLY:CA	3:QC:193:TYR:HE2	1.78	0.96
3:QC:159:GLY:CA	3:QC:193:TYR:CE2	2.50	0.95
55:YZ:94:GLU:CB	55:YZ:95:PRO:CD	2.45	0.94
49:RT:54:ARG:HA	49:RT:59:THR:HG23	1.52	0.90
4:QD:68:TYR:HE1	4:QD:103:ASN:ND2	1.70	0.90
24:QY:76:A:H2	35:RA:2583:G:H21	1.17	0.89
38:RE:13:ARG:HH21	49:RT:58:ASN:HB2	1.39	0.88
3:QC:159:GLY:HA2	3:QC:193:TYR:CE2	2.10	0.86
3:QC:159:GLY:HA2	3:QC:193:TYR:CD2	2.12	0.85
3:QC:159:GLY:N	3:QC:193:TYR:HE2	1.75	0.84
33:Y8:4:MET:CE	33:Y8:61:LEU:CD1	2.55	0.84
35:RA:1138:G:N3	43:RN:106:MET:CE	2.42	0.83
35:RA:1138:G:N2	43:RN:106:MET:CE	2.42	0.82
10:XJ:57:LYS:HD2	10:XJ:60:ARG:HH21	1.44	0.82
35:RA:1138:G:N2	43:RN:106:MET:HE1	1.93	0.82
41:YH:103:LEU:HD22	41:YH:123:PHE:CE2	2.16	0.81
55:YZ:94:GLU:HB3	55:YZ:95:PRO:HD3	1.56	0.80
55:YZ:94:GLU:HB3	55:YZ:95:PRO:HD2	1.63	0.80
41:YH:103:LEU:HD22	41:YH:123:PHE:HE2	1.47	0.79
24:QY:76:A:C2	35:RA:2583:G:N2	2.48	0.79
33:Y8:4:MET:SD	33:Y8:61:LEU:HD12	2.23	0.78
3:XC:9:GLY:HA2	3:XC:12:LEU:HD23	1.65	0.78
35:RA:1043:C:H42	35:RA:1112:G:H1	1.30	0.77
18:QR:26:LEU:HD11	18:QR:29:PHE:CE2	2.20	0.77
38:RE:13:ARG:NH2	49:RT:58:ASN:HB2	2.00	0.76
26:Y1:11:ARG:HG3	26:Y1:12:PRO:HD2	1.69	0.75
35:YA:2102:U:H3	35:YA:2187:G:H1	1.35	0.75
26:Y1:4:VAL:CG1	26:Y1:11:ARG:HD3	2.15	0.75
1:XA:659:U:H5''	15:XO:5:LYS:HE3	1.67	0.75
35:RA:676:A:H8	35:RA:2069:G:H21	1.35	0.74
24:XY:5:C:H42	24:XY:68:G:H1	1.36	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:QR:26:LEU:HD11	18:QR:29:PHE:HE2	1.53	0.73
33:Y8:4:MET:HE3	33:Y8:61:LEU:CD1	2.18	0.73
3:QC:20:SER:HB2	3:QC:40:ARG:HH22	1.54	0.72
38:YE:143:ASN:HD22	38:YE:147:PRO:HG2	1.54	0.72
13:QM:84:ILE:HD11	13:QM:86:CYS:HB2	1.72	0.72
32:Y7:9:ARG:NH1	35:YA:1310:G:OP2	2.22	0.72
35:RA:2056:G:N3	35:RA:2056:G:H2'	2.02	0.72
2:QB:178:ARG:HH22	8:QH:74:PRO:HB3	1.54	0.71
13:QM:80:ARG:O	13:QM:84:ILE:HG21	1.90	0.71
30:Y5:4:HIS:O	35:YA:2056:G:N2	2.23	0.71
5:QE:51:VAL:HG23	5:QE:52:PRO:HD3	1.71	0.71
30:Y5:38:ALA:HB3	30:Y5:40:LYS:HZ3	1.54	0.71
33:Y8:62:LEU:HD13	35:YA:242:G:H5''	1.73	0.71
39:YF:107:LYS:HD2	39:YF:207:GLY:H	1.56	0.71
18:QR:54:ARG:HH21	18:QR:55:ARG:HH22	1.38	0.71
35:YA:1693:U:H1'	37:YD:14:ARG:HH22	1.56	0.71
19:XS:10:PHE:HZ	19:XS:16:LEU:HB2	1.58	0.69
37:RD:35:LYS:NZ	37:RD:83:GLU:OE1	2.24	0.69
1:QA:1360:A:OP2	14:QN:35:ARG:NH2	2.26	0.69
31:Y6:14:THR:HG21	31:Y6:19:ARG:HH21	1.58	0.69
50:YU:92:ARG:NH1	51:YV:11:GLN:O	2.25	0.69
1:XA:544:G:OP1	4:XD:59:ARG:NH2	2.26	0.69
37:YD:182:LEU:H	37:YD:272:ALA:HB3	1.58	0.69
35:YA:1728:G:H8	35:YA:1732:A:H62	1.41	0.69
41:YH:130:ARG:HH12	41:YH:132:ARG:HH21	1.40	0.69
5:QE:154:GLY:HA2	8:QH:64:LYS:HD2	1.74	0.69
35:RA:1061:U:H5'	35:RA:1070:A:H1'	1.75	0.69
45:RP:58:THR:O	45:RP:61:ARG:NH2	2.26	0.69
54:RY:73:ARG:HD2	54:RY:82:PRO:HB2	1.75	0.69
30:R5:16:ARG:NH2	35:RA:517:C:OP1	2.26	0.68
35:RA:2055:C:H5'	35:RA:2056:G:C5'	2.19	0.68
35:RA:2100:G:H1	35:RA:2189:U:H3	1.39	0.68
36:YB:74:U:H1'	55:YZ:34:ASN:HD21	1.57	0.68
1:XA:1295:G:N2	1:XA:1302:U:O4	2.27	0.68
25:R0:69:PHE:CE2	25:R0:79:VAL:CG2	2.76	0.68
50:RU:44:ASN:HD21	51:RV:75:PHE:HB3	1.58	0.68
51:YV:76:LYS:HG3	51:YV:81:TYR:CD1	2.28	0.68
9:QI:10:ARG:HE	9:QI:105:ASP:HB2	1.58	0.68
7:XG:15:ASP:HB3	7:XG:19:GLY:H	1.57	0.68
35:RA:1138:G:N3	43:RN:106:MET:HE3	2.07	0.68
33:Y8:4:MET:HE3	33:Y8:61:LEU:HD13	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Y9:27:CYS:SG	34:Y9:28:GLU:N	2.67	0.68
35:RA:1607:C:N4	35:RA:1622:G:OP2	2.27	0.68
35:RA:2055:C:C5'	35:RA:2056:G:H5''	2.19	0.68
44:YO:104:ARG:NH2	49:YT:43:GLN:OE1	2.26	0.68
29:Y4:14:ILE:HG22	29:Y4:31:ILE:HB	1.75	0.68
10:QJ:61:GLU:OE1	14:QN:45:ARG:NH1	2.27	0.67
35:RA:2313:C:H4'	40:RG:91:ARG:HG3	1.76	0.67
35:YA:2068:U:H3	35:YA:2430:A:H2	1.42	0.67
39:RF:143:ALA:HB1	39:RF:148:LEU:HB2	1.75	0.67
36:RB:7:G:H21	48:RS:38:GLN:HE22	1.40	0.67
35:YA:39:C:O2	39:YF:46:ARG:NH2	2.26	0.67
49:YT:51:ARG:HG2	49:YT:98:LYS:HD2	1.75	0.67
30:Y5:29:THR:HG21	35:YA:2815:C:H5'	1.76	0.67
1:QA:1009:G:H1	1:QA:1020:U:H3	1.43	0.67
13:XM:99:ARG:HB2	13:XM:101:GLN:HE22	1.59	0.67
33:Y8:65:GLU:HB2	35:YA:628:G:OP1	1.94	0.67
37:RD:35:LYS:HD2	37:RD:63:ARG:HG3	1.77	0.66
10:XJ:50:ILE:HA	10:XJ:60:ARG:HB3	1.76	0.66
35:RA:1138:G:C2	43:RN:106:MET:CE	2.79	0.66
35:YA:1902:C:OP1	37:YD:242:ARG:NH1	2.28	0.66
54:YY:39:VAL:HG13	54:YY:42:VAL:HB	1.77	0.66
35:RA:1138:G:N3	43:RN:106:MET:HE2	2.11	0.66
1:XA:1316:G:N7	19:XS:7:LYS:NZ	2.43	0.66
35:YA:2483:C:N3	46:YQ:124:LYS:NZ	2.40	0.66
50:YU:92:ARG:HD2	51:YV:11:GLN:HB2	1.78	0.66
37:RD:182:LEU:H	37:RD:272:ALA:HB3	1.59	0.66
1:QA:407:G:H5''	4:QD:115:ARG:HG2	1.77	0.66
35:RA:2115:G:N2	35:RA:2165:G:N7	2.41	0.66
35:RA:958:U:OP2	46:RQ:14:ARG:NH1	2.28	0.66
1:XA:664:G:H22	1:XA:741:G:H1	1.42	0.66
1:XA:8:A:N6	4:XD:205:GLU:O	2.29	0.66
34:R9:27:CYS:SG	34:R9:28:GLU:N	2.69	0.66
35:RA:2032:G:N2	38:RE:146:THR:OG1	2.29	0.66
27:Y2:47:ASN:ND2	35:YA:94:G:N3	2.44	0.66
1:QA:1073:U:O2	2:QB:104:ASN:ND2	2.29	0.65
10:QJ:3:LYS:N	10:QJ:74:ILE:O	2.30	0.65
35:RA:1112:G:HO2'	41:RH:2:SER:N	1.95	0.65
49:RT:53:ARG:O	49:RT:59:THR:HG23	1.96	0.65
35:YA:2013:A:N3	52:YW:88:ARG:NH2	2.43	0.65
1:QA:1252:A:H61	1:QA:1285:A:H61	1.43	0.65
2:XB:168:THR:HB	2:XB:192:SER:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:QC:159:GLY:N	3:QC:193:TYR:CE2	2.63	0.65
17:QQ:66:SER:O	17:QQ:70:ARG:NH1	2.29	0.65
19:XS:50:ALA:HB1	19:XS:57:HIS:HB3	1.77	0.65
35:YA:265:A:N6	35:YA:427:U:O2'	2.30	0.65
50:RU:90:VAL:HG22	51:RV:39:LEU:HD12	1.78	0.65
10:XJ:57:LYS:HD2	10:XJ:60:ARG:NH2	2.10	0.65
1:XA:686:U:H1'	11:XK:42:TRP:HE1	1.62	0.65
35:YA:919:G:N2	35:YA:2269:A:OP2	2.29	0.65
1:QA:8:A:N6	4:QD:205:GLU:O	2.29	0.65
4:QD:68:TYR:CE1	4:QD:103:ASN:ND2	2.59	0.65
55:YZ:52:SER:O	55:YZ:54:HIS:N	2.30	0.65
15:QO:26:GLU:OE2	15:QO:77:ARG:NH1	2.30	0.65
38:RE:143:ASN:HD22	38:RE:147:PRO:HG2	1.61	0.65
18:XR:86:VAL:HG12	18:XR:87:ARG:HG2	1.78	0.65
33:Y8:65:GLU:CD	33:Y8:65:GLU:H	2.00	0.65
38:YE:78:LEU:HG	38:YE:79:ARG:HG3	1.79	0.65
35:YA:960:A:H61	46:YQ:82:ARG:HH21	1.43	0.64
3:QC:47:LEU:HD11	3:QC:76:VAL:HG12	1.79	0.64
35:RA:27:G:N2	35:RA:513:A:OP2	2.30	0.64
2:XB:212:GLN:NE2	2:XB:216:SER:OG	2.30	0.64
38:RE:176:ILE:HB	38:RE:181:LEU:HB2	1.79	0.64
38:YE:36:ARG:NH1	38:YE:85:ASN:OD1	2.30	0.64
37:RD:13:ARG:NH1	37:RD:16:MET:SD	2.70	0.64
55:RZ:52:SER:O	55:RZ:54:HIS:N	2.31	0.64
5:XE:102:ALA:HB1	5:XE:106:PRO:HG2	1.80	0.64
3:QC:56:ASP:HB2	3:QC:67:THR:HB	1.79	0.64
35:RA:2751:G:N7	41:RH:2:SER:OG	2.28	0.64
29:R4:16:CYS:SG	29:R4:17:GLY:N	2.69	0.64
55:RZ:99:TYR:HB3	55:RZ:123:ASP:HB2	1.79	0.64
15:XO:7:GLU:OE2	15:XO:38:ARG:NH2	2.27	0.64
35:YA:1113:U:H5'	41:YH:2:SER:HB3	1.79	0.64
35:RA:2651:C:H42	35:RA:2669:G:H1	1.42	0.64
41:RH:89:ILE:HG22	41:RH:162:ILE:HG12	1.78	0.64
54:YY:55:TYR:HE2	54:YY:61:ILE:HG21	1.61	0.64
39:RF:29:ASN:HD22	39:RF:32:LEU:HD23	1.63	0.64
2:XB:223:ILE:HG23	2:XB:229:VAL:HG22	1.78	0.64
12:XL:71:PRO:O	12:XL:102:ARG:NH1	2.30	0.64
19:QS:9:VAL:CG1	19:QS:39:THR:HB	2.28	0.64
37:YD:85:ASP:OD2	37:YD:88:ARG:NH1	2.31	0.64
35:YA:1693:U:O2	37:YD:14:ARG:NH1	2.30	0.63
19:QS:3:ARG:HH12	19:QS:11:VAL:HG11	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:XB:231:GLU:HG3	2:XB:233:SER:H	1.61	0.63
36:YB:9:G:OP1	48:YS:15:ARG:NH1	2.28	0.63
35:RA:2303:G:N3	40:RG:132:ASN:ND2	2.47	0.63
8:XH:18:ARG:NH2	8:XH:81:HIS:O	2.32	0.63
35:YA:1068:G:O2'	35:YA:1096:A:N3	2.31	0.63
45:YP:65:ARG:O	45:YP:68:GLN:NE2	2.32	0.63
16:XP:45:THR:HG22	16:XP:47:ASP:H	1.63	0.63
3:QC:7:PRO:O	3:QC:11:ARG:NE	2.31	0.63
4:QD:18:LYS:NZ	4:QD:31:CYS:SG	2.71	0.63
35:RA:321:G:O2'	35:RA:340:A:N3	2.32	0.63
35:RA:67:U:H3	35:RA:74:A:H2	1.45	0.63
37:YD:17:THR:HB	37:YD:205:VAL:H	1.63	0.63
52:RW:11:ARG:HH21	52:RW:98:LYS:HD2	1.64	0.63
1:QA:406:G:H5'	4:QD:5:ILE:HD11	1.80	0.63
35:RA:2701:C:H3'	35:RA:2702:U:H5''	1.79	0.63
35:RA:300:A:OP1	54:RY:86:ARG:NH2	2.32	0.63
44:RO:2:ILE:HG23	44:RO:6:THR:HG21	1.79	0.63
4:XD:18:LYS:NZ	4:XD:31:CYS:SG	2.71	0.63
30:Y5:19:ARG:NH2	35:YA:1264:G:OP1	2.28	0.63
1:QA:1086:U:H3	1:QA:1099:G:H22	1.47	0.62
1:QA:878:G:H5'	8:QH:89:PRO:HG2	1.81	0.62
3:QC:64:VAL:HG22	3:QC:99:VAL:HA	1.81	0.62
35:RA:1667:G:OP2	35:RA:1667:G:H8	1.82	0.62
35:YA:2130:U:HO2'	35:YA:2133:G:HO2'	1.47	0.62
45:RP:65:ARG:O	45:RP:68:GLN:NE2	2.28	0.62
35:YA:2392:A:H2	35:YA:2424:C:H42	1.47	0.62
42:RI:90:GLY:O	42:RI:121:LYS:NZ	2.32	0.62
11:QK:86:GLY:O	11:QK:91:ARG:NH1	2.32	0.62
1:XA:992:U:H3	1:XA:1044:A:H62	1.46	0.62
35:YA:67:U:H3	35:YA:74:A:H2	1.48	0.62
55:YZ:7:ALA:HB2	55:YZ:59:LEU:HB3	1.80	0.62
3:QC:76:VAL:HG21	3:QC:103:VAL:HG21	1.81	0.62
49:RT:51:ARG:HG2	49:RT:98:LYS:HD2	1.81	0.62
17:XQ:66:SER:O	17:XQ:70:ARG:NH1	2.33	0.62
13:QM:2:ALA:HA	13:QM:11:ARG:HG2	1.82	0.62
29:R4:39:CYS:SG	29:R4:40:HIS:N	2.72	0.62
34:R9:36:GLN:NE2	35:RA:1124:C:O2	2.32	0.62
35:RA:1991:U:H6	35:RA:1991:U:O5'	1.82	0.62
35:YA:2292:C:OP1	48:YS:17:ARG:NH2	2.32	0.62
41:RH:107:VAL:O	41:RH:153:LYS:NZ	2.33	0.62
35:RA:1056:G:H21	35:RA:1103:A:H62	1.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:765:G:N2	1:XA:813:U:OP2	2.33	0.62
37:YD:27:THR:HG21	37:YD:81:ALA:HB1	1.80	0.62
1:QA:979:C:OP1	1:QA:1223:C:N4	2.33	0.62
46:RQ:27:VAL:HG21	46:RQ:134:ARG:HA	1.82	0.62
1:XA:406:G:H5'	4:XD:5:ILE:HD11	1.79	0.62
1:XA:501:C:OP1	12:XL:117:ARG:NH2	2.33	0.62
42:YI:40:THR:HG23	42:YI:43:ASN:H	1.65	0.62
2:QB:178:ARG:NH1	2:QB:196:LEU:O	2.33	0.61
1:XA:1073:U:O2	2:XB:104:ASN:ND2	2.33	0.61
25:Y0:27:GLU:HG3	25:Y0:68:GLU:HA	1.82	0.61
39:YF:116:ASP:OD1	39:YF:119:ARG:NH2	2.32	0.61
42:RI:30:LEU:HB3	42:RI:36:ALA:HB3	1.83	0.61
37:YD:148:GLU:HB2	37:YD:151:LYS:HD2	1.82	0.61
1:QA:544:G:OP1	4:QD:59:ARG:NH2	2.33	0.61
35:YA:987:G:O2'	35:YA:1000:A:N3	2.33	0.61
1:QA:1306:A:N6	1:QA:1331:G:O2'	2.33	0.61
25:Y0:77:ARG:NH2	35:YA:857:C:OP2	2.32	0.61
1:QA:686:U:H1'	11:QK:42:TRP:HE1	1.65	0.61
46:RQ:66:ILE:HA	46:RQ:104:PHE:HA	1.83	0.61
1:XA:1130:A:O2'	9:XI:3:GLN:NE2	2.34	0.61
29:Y4:68:ARG:HG2	29:Y4:69:LYS:HG2	1.82	0.61
38:YE:201:THR:HG22	38:YE:203:LYS:H	1.65	0.61
50:YU:44:ASN:HD21	51:YV:75:PHE:HB3	1.65	0.61
37:RD:143:HIS:ND1	37:RD:194:GLY:O	2.32	0.61
51:YV:7:THR:HG23	51:YV:22:VAL:HG11	1.83	0.61
8:QH:10:LEU:HD22	8:QH:83:ILE:HD11	1.82	0.61
19:QS:10:PHE:HB2	19:QS:16:LEU:CD1	2.22	0.61
30:Y5:2:ALA:N	35:YA:2015:A:N3	2.48	0.61
35:YA:573:G:N1	35:YA:2031:A:OP2	2.24	0.61
35:YA:807:U:O2	39:YF:74:ARG:NH2	2.34	0.61
5:QE:102:ALA:HB1	5:QE:106:PRO:HG2	1.83	0.60
9:QI:10:ARG:NH1	9:QI:75:ASP:OD2	2.34	0.60
11:QK:58:PRO:HB2	11:QK:93:GLN:HG3	1.82	0.60
35:RA:1059:G:O6	35:RA:1079:C:N4	2.34	0.60
35:RA:994:C:OP1	50:RU:53:ARG:NH2	2.33	0.60
52:YW:18:ARG:HD2	52:YW:76:VAL:HG13	1.82	0.60
11:QK:18:ARG:HG2	11:QK:81:ASP:HB2	1.83	0.60
27:R2:47:ASN:ND2	35:RA:94:G:N3	2.48	0.60
33:R8:58:ILE:HG13	45:RP:49:ARG:HD2	1.83	0.60
9:XI:31:GLN:HE21	9:XI:35:GLU:HG2	1.66	0.60
35:YA:948:G:N2	35:YA:985:C:OP2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:RB:52:A:O2'	36:RB:53:A:N7	2.34	0.60
35:RA:1800:C:OP2	37:RD:183:ARG:NH1	2.33	0.60
35:RA:1130:U:O2	38:RE:149:ARG:NH2	2.34	0.60
1:XA:1123:A:H4'	10:XJ:36:GLY:HA3	1.83	0.60
3:XC:20:SER:HB2	3:XC:40:ARG:HH22	1.66	0.60
8:XH:34:GLU:OE1	8:XH:37:ARG:NH2	2.35	0.60
35:YA:2575:C:H5'	38:YE:144:ARG:HG2	1.82	0.60
39:YF:143:ALA:HB1	39:YF:148:LEU:HB2	1.84	0.60
35:YA:996:A:OP2	50:YU:92:ARG:NH2	2.33	0.60
26:R1:51:VAL:HG21	26:R1:74:VAL:HG11	1.84	0.60
33:Y8:62:LEU:N	33:Y8:63:PRO:HD3	2.15	0.60
35:YA:571:A:O2'	51:YV:78:LYS:NZ	2.35	0.60
55:YZ:94:GLU:HG3	55:YZ:95:PRO:CD	2.26	0.60
1:QA:1147:C:HO2'	9:QI:5:TYR:HH	1.48	0.60
35:RA:1980:G:O2'	35:RA:1982:C:OP2	2.20	0.60
38:RE:26:ILE:HG23	38:RE:182:LEU:HB3	1.81	0.60
32:R7:39:ARG:NH2	35:RA:468:G:N7	2.49	0.60
38:RE:117:MET:HA	38:RE:122:PHE:H	1.67	0.60
1:XA:1348:U:H3	1:XA:1374:A:H2	1.48	0.60
21:XU:8:THR:HG23	21:XU:11:GLY:H	1.66	0.60
33:Y8:4:MET:SD	33:Y8:61:LEU:CD1	2.89	0.60
6:QF:3:ARG:NH1	6:QF:38:GLU:OE2	2.34	0.60
39:YF:185:ASP:OD1	39:YF:188:ARG:NH1	2.35	0.60
35:YA:2727:G:O2'	44:YO:70:LYS:NZ	2.34	0.60
1:QA:842:C:O2'	1:QA:848:C:N4	2.34	0.60
35:RA:693:C:O2'	35:RA:1353:A:N3	2.31	0.60
37:RD:85:ASP:OD2	37:RD:88:ARG:NH1	2.32	0.60
1:XA:1118:C:OP1	9:XI:104:ARG:NH1	2.35	0.60
35:RA:864:G:H1'	35:RA:914:C:H42	1.65	0.60
51:RV:52:VAL:HG21	51:RV:55:ALA:HB3	1.84	0.60
1:XA:1124:G:H1'	10:XJ:38:ILE:HD13	1.84	0.60
27:Y2:7:ARG:NH2	35:YA:102:G:OP1	2.35	0.60
1:XA:842:C:O2'	1:XA:848:C:N4	2.35	0.60
1:XA:970:C:N4	9:XI:128:ARG:OXT	2.35	0.60
35:YA:662:G:OP1	45:YP:15:ARG:NH1	2.35	0.60
35:YA:820:A:N3	35:YA:943:U:O2'	2.33	0.60
55:YZ:119:GLU:HG3	55:YZ:122:ARG:HB3	1.83	0.60
35:RA:309:G:N3	35:RA:329:G:O2'	2.34	0.59
38:RE:128:SER:OG	38:RE:129:HIS:N	2.35	0.59
55:RZ:69:THR:OG1	55:RZ:70:LEU:N	2.35	0.59
33:Y8:14:VAL:HG23	45:YP:61:ARG:HH21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Y8:46:ARG:NH1	35:YA:630:G:OP1	2.35	0.59
35:RA:2759:G:N2	41:RH:139:GLN:OE1	2.35	0.59
1:XA:375:U:H5''	16:XP:69:THR:HG21	1.83	0.59
6:XF:35:ALA:HB1	6:XF:65:VAL:HG11	1.84	0.59
35:YA:1689:A:H62	35:YA:1698:A:H2	1.50	0.59
52:YW:78:GLU:OE2	52:YW:99:ARG:NH1	2.34	0.59
1:QA:587:G:N2	1:QA:754:C:OP2	2.35	0.59
25:R0:77:ARG:NH2	35:RA:857:C:OP2	2.35	0.59
35:RA:910:A:H62	46:RQ:12:GLN:HA	1.68	0.59
1:QA:1347:G:N2	1:QA:1374:A:OP2	2.36	0.59
28:R3:6:VAL:HG12	28:R3:56:VAL:HG12	1.85	0.59
35:RA:141:A:H8	35:RA:1595:G:H21	1.50	0.59
37:RD:31:LYS:NZ	37:RD:32:SER:OG	2.36	0.59
46:RQ:75:THR:HG21	46:RQ:85:LYS:HE3	1.84	0.59
27:Y2:29:LYS:HE3	27:Y2:57:ILE:HG21	1.84	0.59
33:Y8:13:ARG:HG3	45:YP:61:ARG:NH2	2.16	0.59
1:QA:1002:G:H1	1:QA:1038:C:H42	1.49	0.59
1:QA:945:G:N2	1:QA:1334:G:O2'	2.36	0.59
1:QA:439:A:OP2	1:QA:493:G:N1	2.34	0.59
1:QA:582:U:OP1	15:QO:68:ARG:NH2	2.33	0.59
27:R2:66:GLU:OE2	27:R2:70:GLN:NE2	2.35	0.59
36:RB:44:G:O2'	36:RB:47:C:N4	2.36	0.59
1:XA:587:G:N2	1:XA:754:C:OP2	2.35	0.59
35:YA:2291:U:O2'	35:YA:2374:C:O2	2.20	0.59
35:YA:309:G:N3	35:YA:329:G:O2'	2.34	0.59
35:YA:2680:C:OP2	38:YE:111:ARG:NH2	2.35	0.59
35:YA:662:G:H5''	45:YP:17:LYS:HG2	1.85	0.59
48:YS:106:ARG:NH1	48:YS:107:GLU:OE2	2.35	0.59
34:R9:22:ARG:HH12	35:RA:2741:A:H5''	1.66	0.59
35:RA:750:A:OP1	35:RA:1615:C:N4	2.35	0.59
46:RQ:12:GLN:HE21	46:RQ:72:LYS:HG3	1.68	0.59
49:RT:16:ARG:NH1	49:RT:80:SER:O	2.35	0.59
2:XB:118:LEU:HB3	2:XB:142:LEU:HD12	1.84	0.59
35:YA:2032:G:N2	38:YE:146:THR:OG1	2.33	0.59
35:YA:2680:C:H5'	38:YE:189:PRO:HA	1.85	0.59
49:YT:16:ARG:HH21	49:YT:19:LEU:HD21	1.66	0.59
24:QY:53:G:O2'	46:RQ:51:ARG:NH2	2.36	0.59
35:YA:184:C:O2'	35:YA:217:G:N3	2.34	0.59
35:YA:2343:C:HO2'	35:YA:2373:G:HO2'	1.48	0.59
35:YA:517:C:O2'	52:YW:18:ARG:NH2	2.36	0.59
1:QA:1259:C:H42	1:QA:1276:G:H1	1.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:414:C:O2	35:RA:1864:U:O2'	2.21	0.59
40:RG:4:ASP:OD1	40:RG:9:ARG:NH1	2.36	0.59
35:YA:729:G:OP2	37:YD:13:ARG:NH1	2.35	0.59
52:YW:88:ARG:HB2	52:YW:92:ARG:HB3	1.84	0.59
7:QG:152:ALA:O	7:QG:155:ARG:HD2	2.03	0.59
16:QP:15:PRO:HD2	16:QP:42:ARG:HD2	1.85	0.59
1:XA:1510:U:H3	1:XA:1525:G:H1	1.50	0.59
9:XI:25:LYS:N	9:XI:60:ASP:OD1	2.36	0.59
35:YA:2701:C:H3'	35:YA:2702:U:H5''	1.84	0.59
27:R2:51:ARG:HH21	27:R2:55:ARG:HH22	1.51	0.59
1:XA:405:U:O4	4:XD:2:GLY:N	2.36	0.59
35:YA:1364:G:N2	35:YA:1367:A:OP2	2.29	0.59
35:YA:952:G:OP1	46:YQ:16:ARG:NH1	2.36	0.59
1:QA:410:G:N2	1:QA:431:A:N7	2.51	0.58
14:QN:27:CYS:SG	14:QN:28:GLY:N	2.75	0.58
28:R3:12:PRO:O	28:R3:20:LYS:NZ	2.35	0.58
35:RA:1309:G:HO2'	35:RA:1611:C:HO2'	1.46	0.58
44:RO:17:ARG:HE	44:RO:47:ILE:HD13	1.68	0.58
35:RA:960:A:H61	46:RQ:82:ARG:HH21	1.50	0.58
1:XA:1296:C:OP1	13:XM:44:ARG:NH2	2.36	0.58
35:YA:336:C:HO2'	54:YY:35:TYR:HH	1.49	0.58
10:QJ:78:ASN:HB2	10:QJ:81:THR:HG23	1.84	0.58
27:R2:47:ASN:O	27:R2:48:HIS:ND1	2.36	0.58
49:RT:62:THR:HG22	49:RT:75:ILE:HG12	1.85	0.58
1:XA:1241:G:OP1	7:XG:35:LYS:NZ	2.36	0.58
33:Y8:14:VAL:HG23	45:YP:61:ARG:NH2	2.18	0.58
46:YQ:20:ALA:HB3	55:YZ:79:ARG:HE	1.68	0.58
19:QS:50:ALA:HB1	19:QS:57:HIS:HB3	1.84	0.58
27:R2:4:SER:OG	27:R2:5:GLU:N	2.34	0.58
1:XA:407:G:H5''	4:XD:115:ARG:HB3	1.83	0.58
38:RE:116:VAL:HG23	38:RE:120:TRP:HD1	1.68	0.58
1:XA:1503:A:O2'	23:XX:12:A:N6	2.36	0.58
35:YA:2304:G:H22	35:YA:2312:U:H3	1.51	0.58
35:YA:2787:C:H1'	38:YE:62:PRO:HG3	1.86	0.58
42:YI:12:LEU:HG	42:YI:19:VAL:HG11	1.85	0.58
9:QI:121:ARG:NH1	9:QI:122:ALA:O	2.36	0.58
9:QI:33:PHE:CE1	9:QI:37:PHE:HD2	2.21	0.58
6:XF:94:GLN:OE1	18:XR:32:ARG:NH1	2.37	0.58
39:YF:101:LEU:O	39:YF:106:ARG:NH1	2.36	0.58
6:XF:36:ARG:NH2	6:XF:38:GLU:OE2	2.36	0.58
13:XM:77:ASN:OD1	29:Y4:71:ARG:NH1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:QC:47:LEU:HB3	3:QC:52:LEU:HD23	1.85	0.58
46:RQ:81:VAL:O	46:RQ:82:ARG:NH1	2.36	0.58
35:YA:10:G:N2	35:YA:2802:G:OP1	2.35	0.58
2:XB:185:ILE:HG22	2:XB:199:TYR:HB2	1.85	0.58
2:XB:20:GLU:HG3	2:XB:191:ASP:OD1	2.04	0.58
35:YA:1454:U:O2'	35:YA:1455:G:N7	2.35	0.58
35:YA:2118:U:H3	35:YA:2147:G:HO2'	1.51	0.58
39:YF:11:VAL:HG22	39:YF:125:LEU:HB2	1.86	0.58
55:YZ:5:LEU:H	55:YZ:59:LEU:HA	1.67	0.58
43:RN:99:LEU:O	43:RN:103:VAL:HG23	2.03	0.58
35:YA:2111:C:N3	35:YA:2118:U:O2'	2.35	0.58
1:QA:189:U:O2	17:QQ:63:ARG:NH2	2.37	0.58
1:QA:593:G:H1	1:QA:646:U:H3	1.51	0.58
1:QA:811:C:O2'	1:QA:901:A:N1	2.37	0.58
35:RA:223:A:O2'	35:RA:420:C:O2	2.20	0.58
31:R6:46:HIS:HD1	35:RA:2371:G:HO2'	1.41	0.58
45:RP:135:LEU:HB3	45:RP:139:LYS:HE2	1.84	0.58
42:YI:68:LEU:HD13	42:YI:71:ILE:HD11	1.85	0.58
1:QA:437:U:H3	1:QA:495:A:H62	1.51	0.57
13:QM:99:ARG:HB2	13:QM:101:GLN:HE22	1.69	0.57
35:RA:486:C:O2'	52:RW:60:ASN:ND2	2.35	0.57
37:RD:17:THR:HB	37:RD:205:VAL:H	1.68	0.57
38:RE:141:ILE:O	38:RE:154:LYS:NZ	2.36	0.57
1:XA:1494:G:N7	57:XA:1670:PAR:N32	2.52	0.57
35:YA:1057:A:N6	35:YA:1087:G:OP2	2.37	0.57
1:QA:1004:A:H1'	1:QA:1036:G:H22	1.70	0.57
35:RA:1791:A:H5'	37:RD:206:LEU:HD12	1.86	0.57
35:RA:807:U:OP2	45:RP:41:ARG:NH1	2.37	0.57
9:XI:42:ARG:NH1	9:XI:71:SER:OG	2.37	0.57
35:YA:1266:G:O5'	52:YW:15:ARG:NH2	2.37	0.57
27:R2:66:GLU:OE1	27:R2:69:ARG:NH1	2.37	0.57
35:RA:1140:C:OP2	43:RN:66:LYS:NZ	2.34	0.57
35:RA:1266:G:O5'	52:RW:15:ARG:NH2	2.36	0.57
35:RA:605:C:O2	35:RA:657:U:O2'	2.21	0.57
37:RD:76:PRO:HB2	37:RD:116:GLN:HE21	1.69	0.57
39:RF:101:LEU:O	39:RF:106:ARG:NH1	2.37	0.57
39:RF:200:GLU:O	39:RF:204:ASN:ND2	2.37	0.57
6:XF:80:ARG:NH2	6:XF:88:VAL:O	2.37	0.57
27:Y2:23:LYS:NZ	27:Y2:27:GLU:OE2	2.35	0.57
1:QA:538:G:H5''	12:QL:114:LYS:HB2	1.86	0.57
26:R1:6:GLU:O	26:R1:91:LYS:NZ	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:2258:C:O2'	35:RA:2427:C:OP2	2.21	0.57
1:XA:486:U:H2'	1:XA:487:A:H8	1.68	0.57
35:YA:1859:A:N6	35:YA:1883:G:O2'	2.38	0.57
39:YF:31:HIS:NE2	39:YF:35:GLU:OE2	2.37	0.57
35:YA:138:G:N2	53:YX:44:GLU:OE1	2.32	0.57
1:QA:1074:G:OP1	5:QE:64:ARG:NH2	2.37	0.57
35:RA:2055:C:OP1	35:RA:2056:G:H5''	2.04	0.57
35:RA:900:A:H3'	35:RA:901:A:H8	1.70	0.57
2:XB:54:THR:HG22	2:XB:199:TYR:HB3	1.86	0.57
25:Y0:39:ARG:HH21	35:YA:2355:C:H1'	1.68	0.57
35:YA:2777:G:OP2	35:YA:2781:A:O2'	2.23	0.57
13:QM:80:ARG:O	13:QM:84:ILE:CG2	2.52	0.57
15:QO:29:VAL:HG21	15:QO:81:LEU:HD21	1.86	0.57
1:XA:532:A:H2	1:XA:1206:G:H21	1.52	0.57
35:YA:918:A:N3	36:YB:80:U:O2'	2.35	0.57
2:QB:118:LEU:HB3	2:QB:142:LEU:HD12	1.86	0.57
1:QA:1309:G:O2'	13:QM:77:ASN:ND2	2.37	0.57
33:R8:28:GLY:O	33:R8:36:LYS:NZ	2.38	0.57
55:RZ:53:ILE:HG22	55:RZ:71:VAL:HG13	1.87	0.57
3:XC:138:VAL:HG13	3:XC:149:ALA:HB3	1.87	0.57
22:XV:50:U:H3	22:XV:64:G:H1	1.53	0.57
3:QC:179:ARG:HD2	3:QC:206:GLU:HG2	1.86	0.57
38:RE:78:LEU:HG	38:RE:79:ARG:HG2	1.85	0.57
4:QD:72:GLU:OE2	4:QD:207:TYR:OH	2.23	0.57
9:QI:13:ALA:HB2	9:QI:68:GLY:HA3	1.85	0.57
24:QY:18:G:N2	24:QY:57:G:N7	2.51	0.57
35:YA:1853:A:N3	35:YA:2233:U:O2'	2.33	0.57
35:YA:2287:A:H62	35:YA:2344:U:H3	1.49	0.57
47:YR:96:ARG:HE	47:YR:117:VAL:HG12	1.70	0.57
35:RA:2396:G:H1	35:RA:2420:C:H42	1.53	0.57
35:YA:612:G:N2	35:YA:616:A:O2'	2.37	0.57
29:R4:56:VAL:HG12	29:R4:61:ARG:HG2	1.87	0.56
55:RZ:97:GLU:HB3	55:RZ:125:LEU:HD11	1.87	0.56
33:Y8:28:GLY:O	33:Y8:44:LYS:NZ	2.29	0.56
43:YN:12:ARG:NH1	43:YN:50:ASP:OD2	2.38	0.56
4:QD:98:GLU:OE2	4:QD:107:ARG:HG3	2.04	0.56
35:RA:2010:G:H5''	52:RW:42:ARG:HB2	1.86	0.56
10:XJ:3:LYS:N	10:XJ:74:ILE:O	2.38	0.56
24:XY:4:G:H1	24:XY:69:C:H42	1.52	0.56
48:YS:106:ARG:HA	48:YS:110:LEU:HD11	1.87	0.56
49:YT:20:PRO:HD2	49:YT:86:ILE:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:QB:74:LYS:NZ	2:QB:206:ASP:OD1	2.36	0.56
36:RB:104:A:OP1	55:RZ:72:ARG:NH2	2.38	0.56
38:YE:128:SER:OG	38:YE:129:HIS:N	2.38	0.56
11:QK:50:TYR:HD2	11:QK:54:ARG:HB3	1.70	0.56
1:QA:376:G:H5''	16:QP:5:ARG:HB2	1.86	0.56
43:RN:108:PRO:HG2	43:RN:113:GLY:HA2	1.87	0.56
20:XT:100:ILE:HG12	20:XT:102:GLY:H	1.68	0.56
24:XY:56:C:H5''	35:YA:896:A:H2'	1.87	0.56
7:QG:94:ARG:NH1	7:QG:98:SER:OG	2.38	0.56
35:RA:868:U:O2	46:RQ:8:LYS:NZ	2.38	0.56
26:R1:47:GLN:OE1	35:RA:2228:G:N2	2.39	0.56
55:RZ:126:VAL:HG11	55:RZ:161:VAL:HG13	1.87	0.56
1:XA:937:A:O2'	7:XG:76:ARG:NH2	2.38	0.56
38:YE:8:LYS:HA	38:YE:26:ILE:HG22	1.88	0.56
20:QT:100:ILE:HG22	20:QT:102:GLY:H	1.69	0.56
30:Y5:53:ALA:O	47:YR:96:ARG:NH1	2.34	0.56
39:YF:12:LEU:HB3	39:YF:126:VAL:HG12	1.87	0.56
42:YI:26:ALA:HA	42:YI:30:LEU:HB2	1.87	0.56
55:YZ:72:ARG:NH1	55:YZ:97:GLU:O	2.38	0.56
17:QQ:100:LYS:O	17:QQ:101:ARG:NH2	2.38	0.56
35:RA:1138:G:C2	43:RN:106:MET:HE3	2.41	0.56
57:XA:1670:PAR:O44	57:XA:1670:PAR:N64	2.39	0.56
35:YA:861:A:N3	36:YB:79:C:O2'	2.36	0.56
38:RE:2:LYS:HB2	38:RE:95:ILE:HD12	1.88	0.56
1:XA:971:G:N2	1:XA:1363:A:OP2	2.39	0.56
1:XA:811:C:O2'	1:XA:901:A:N1	2.38	0.56
11:XK:87:THR:HA	11:XK:91:ARG:HD2	1.86	0.56
30:Y5:7:PRO:O	35:YA:2016:U:O2'	2.22	0.56
29:R4:18:CYS:SG	29:R4:19:GLY:N	2.78	0.56
35:RA:2832:U:H4'	35:RA:2833:G:H5''	1.88	0.56
49:RT:50:ILE:HD11	49:RT:100:TYR:HA	1.88	0.56
4:XD:187:ARG:NH2	4:XD:193:ASP:OD2	2.37	0.56
9:XI:19:LEU:HB3	9:XI:59:PHE:HD2	1.71	0.56
35:YA:956:G:OP2	46:YQ:14:ARG:NH2	2.38	0.56
1:QA:1422:G:H5''	44:RO:48:PRO:HB3	1.87	0.56
1:QA:689:C:OP2	11:QK:55:LYS:NZ	2.39	0.56
3:QC:159:GLY:CA	3:QC:193:TYR:CD2	2.83	0.56
31:R6:43:CYS:SG	31:R6:44:ARG:NH1	2.78	0.56
35:RA:1138:G:N2	43:RN:106:MET:HE3	2.21	0.56
39:RF:155:LEU:HB2	39:RF:189:THR:HG21	1.88	0.56
1:XA:1305:G:O2'	1:XA:1332:A:N6	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:2127:G:H22	35:YA:2162:G:H1'	1.71	0.56
37:YD:134:ARG:HG3	37:YD:135:PHE:HD1	1.71	0.56
35:YA:1754:C:H5	49:YT:96:ARG:HH21	1.52	0.56
13:QM:23:TYR:HB3	13:QM:67:GLU:HG2	1.88	0.55
35:RA:1019:U:H3	35:RA:1142(A):A:H62	1.53	0.55
35:RA:1490:A:O2'	37:RD:99:ASP:OD1	2.24	0.55
35:YA:1327:C:O2'	47:YR:105:ARG:NH2	2.37	0.55
1:QA:1224:G:O2'	1:QA:1322:C:OP2	2.24	0.55
1:QA:1338:G:N3	22:QV:41:C:O2'	2.39	0.55
43:RN:25:ARG:O	43:RN:29:LYS:NZ	2.39	0.55
49:RT:27:THR:HG22	49:RT:48:ILE:HG12	1.88	0.55
1:QA:757:U:O2'	1:QA:879:C:O2	2.24	0.55
9:QI:3:GLN:OE1	9:QI:20:ARG:NH2	2.38	0.55
1:XA:708:C:OP1	11:XK:85:ARG:NH2	2.38	0.55
26:R1:87:PRO:O	26:R1:91:LYS:N	2.37	0.55
35:RA:138:G:N2	53:RX:44:GLU:OE2	2.39	0.55
40:RG:63:ILE:HG13	40:RG:64:THR:HG23	1.88	0.55
14:XN:29:ARG:HD3	14:XN:40:CYS:HB2	1.89	0.55
18:XR:48:GLY:O	18:XR:74:ARG:NH2	2.39	0.55
41:YH:156:ALA:O	41:YH:158:HIS:N	2.39	0.55
42:YI:79:ILE:HB	42:YI:142:VAL:HA	1.88	0.55
3:QC:131:ARG:HE	5:QE:50:GLU:HG2	1.71	0.55
35:RA:910:A:N3	35:RA:2264:C:O2'	2.38	0.55
39:YF:155:LEU:HB2	39:YF:189:THR:HG21	1.87	0.55
16:QP:66:PRO:HG2	16:QP:71:ARG:HE	1.71	0.55
47:RR:53:HIS:HA	47:RR:56:LYS:HD3	1.89	0.55
1:XA:1086:U:H3	1:XA:1099:G:H22	1.54	0.55
1:QA:1422:G:O3'	44:RO:49:ARG:NH1	2.40	0.55
1:QA:1129:C:OP1	9:QI:62:TYR:OH	2.24	0.55
13:QM:80:ARG:HH12	19:QS:69:HIS:HE1	1.55	0.55
35:RA:942:G:O2'	35:RA:1189:A:N3	2.38	0.55
35:RA:2096:U:H3	35:RA:2193:G:H1	1.55	0.55
35:RA:2406:U:OP1	35:RA:2411:A:N6	2.39	0.55
35:RA:1638:C:O2	35:RA:2698:U:O2'	2.23	0.55
1:XA:105:G:OP2	20:XT:18:GLN:NE2	2.39	0.55
35:YA:2033:A:O2'	35:YA:2035:G:OP2	2.22	0.55
35:YA:574:C:N3	38:YE:145:LYS:NZ	2.54	0.55
40:YG:161:THR:HG22	40:YG:163:ALA:H	1.71	0.55
50:YU:90:VAL:O	50:YU:92:ARG:N	2.34	0.55
49:RT:30:VAL:HG12	49:RT:86:ILE:HG12	1.89	0.55
3:XC:11:ARG:NH2	3:XC:177:THR:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:1498:U:OP2	23:XX:16:A:O2'	2.25	0.55
35:YA:776:G:N7	35:YA:793:A:O2'	2.40	0.55
49:YT:24:PRO:HA	49:YT:49:VAL:HG23	1.89	0.55
1:QA:376:G:H1	1:QA:387:U:H3	1.55	0.55
33:R8:48:PHE:HE2	35:RA:650:C:OP1	1.89	0.55
35:RA:297:C:OP1	54:RY:87:LYS:NZ	2.40	0.55
35:RA:307:G:H21	35:RA:330:A:H62	1.53	0.55
36:RB:48:A:OP2	48:RS:30:ARG:NH2	2.40	0.55
38:RE:6:GLY:HA3	38:RE:26:ILE:HD11	1.89	0.55
4:XD:98:GLU:HA	4:XD:103:ASN:HD22	1.70	0.55
7:XG:151:TYR:HE1	11:XK:54:ARG:HG2	1.71	0.55
8:XH:73:ASP:OD1	8:XH:75:ARG:NH1	2.40	0.55
37:YD:71:ASP:HB2	37:YD:103:ARG:HH12	1.71	0.55
6:XF:81:ILE:HD11	37:YD:125:ILE:HB	1.89	0.55
43:YN:96:GLU:HB2	43:YN:122:VAL:HG12	1.89	0.55
1:QA:642:A:N3	8:QH:113:SER:OG	2.37	0.55
24:QY:30:G:H1	24:QY:40:C:H42	1.55	0.55
33:R8:7:HIS:HD2	45:RP:50:ARG:HH11	1.55	0.55
35:RA:768:G:O2'	35:RA:1379:A:N6	2.40	0.55
42:RI:73:GLU:HG3	42:RI:136:VAL:HG23	1.89	0.55
35:YA:27:G:N2	35:YA:512:G:O2'	2.40	0.55
1:QA:129(A):G:N2	1:QA:188:U:HO2'	2.05	0.54
4:QD:98:GLU:HG2	4:QD:189:PRO:HG2	1.88	0.54
1:QA:1372:U:OP1	9:QI:72:GLY:N	2.41	0.54
35:RA:2291:U:O2'	35:RA:2374:C:O2	2.25	0.54
1:XA:1152:A:OP1	10:XJ:70:ARG:NH2	2.36	0.54
27:Y2:14:ARG:NH1	27:Y2:66:GLU:OE1	2.40	0.54
47:YR:38:VAL:HG22	47:YR:112:ALA:HB2	1.89	0.54
1:QA:356:A:N3	1:QA:368:U:O2'	2.34	0.54
1:QA:448:A:OP2	1:QA:485:G:N2	2.35	0.54
3:QC:159:GLY:HA3	3:QC:193:TYR:CE2	2.42	0.54
44:RO:23:ARG:NH2	44:RO:28:SER:O	2.40	0.54
1:XA:152:A:H62	1:XA:169:C:H42	1.54	0.54
1:XA:278:G:OP2	17:XQ:92:ARG:NH2	2.40	0.54
4:XD:23:GLY:N	4:XD:26:CYS:SG	2.79	0.54
40:YG:29:TRP:O	40:YG:33:ARG:NH1	2.40	0.54
45:YP:64:LYS:O	45:YP:66:GLY:N	2.39	0.54
1:QA:1240:U:OP1	7:QG:119:ARG:NH2	2.40	0.54
35:RA:2119:A:N6	35:RA:2170:A:N7	2.53	0.54
35:YA:1791:A:N6	35:YA:1828:G:O2'	2.35	0.54
35:YA:2683:C:O2	44:YO:70:LYS:NZ	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:YB:5:C:O2'	36:YB:27:C:O2	2.25	0.54
49:YT:27:THR:HA	49:YT:48:ILE:HA	1.87	0.54
16:QP:13:HIS:O	16:QP:42:ARG:NH1	2.40	0.54
35:RA:1093:G:H21	35:RA:1098:A:H62	1.53	0.54
13:XM:80:ARG:NH1	19:XS:65:ASN:O	2.40	0.54
1:XA:1316:G:H4'	14:XN:18:VAL:HG11	1.90	0.54
18:XR:51:LEU:HD22	18:XR:55:ARG:HD2	1.90	0.54
52:YW:69:LEU:HD13	52:YW:107:LEU:HD13	1.89	0.54
1:QA:1321:C:H5''	1:QA:1322:C:H5''	1.89	0.54
10:QJ:33:GLN:HE21	10:QJ:75:ILE:HD13	1.72	0.54
13:QM:37:THR:O	13:QM:55:ARG:NH1	2.40	0.54
35:RA:83:G:N2	35:RA:103:A:OP2	2.41	0.54
35:RA:2692:C:O2	35:RA:2847:U:O2'	2.21	0.54
36:RB:9:G:OP1	48:RS:15:ARG:NH1	2.41	0.54
28:Y3:8:LEU:HB2	28:Y3:28:LEU:HD13	1.89	0.54
35:YA:1800:C:OP2	37:YD:183:ARG:NH1	2.38	0.54
35:YA:1651:G:N7	47:YR:11:ASN:ND2	2.55	0.54
1:QA:377:G:OP1	16:QP:3:LYS:NZ	2.38	0.54
24:QY:76:A:H2'	35:RA:2585:U:H5	1.72	0.54
20:XT:89:ARG:HD2	20:XT:104:LEU:HD11	1.90	0.54
55:YZ:74:VAL:HG22	55:YZ:86:VAL:HG23	1.87	0.54
25:R0:23:VAL:HG13	25:R0:38:VAL:HG22	1.89	0.54
35:RA:2857:G:N2	35:RA:2860:A:OP2	2.35	0.54
35:RA:637:A:OP1	45:RP:133:SER:OG	2.22	0.54
1:XA:508:C:OP1	4:XD:209:ARG:NH2	2.39	0.54
1:XA:943:U:H1'	9:XI:124:GLN:HE22	1.72	0.54
3:XC:20:SER:OG	3:XC:22:TRP:NE1	2.39	0.54
29:Y4:23:GLU:O	29:Y4:25:TYR:N	2.39	0.54
35:YA:1728:G:N1	35:YA:1730:U:OP2	2.41	0.54
35:YA:2010:G:H5''	52:YW:42:ARG:HB2	1.90	0.54
43:YN:22:THR:OG1	43:YN:23:LEU:N	2.41	0.54
2:QB:69:LEU:HB3	2:QB:162:ILE:HG22	1.90	0.54
6:QF:94:GLN:OE1	18:QR:32:ARG:NH1	2.41	0.54
26:R1:40:ARG:NH2	35:RA:2232:U:OP2	2.41	0.54
29:R4:42:PHE:O	29:R4:44:THR:N	2.41	0.54
35:RA:1815:A:OP2	37:RD:54:ARG:NH2	2.40	0.54
35:RA:2111:C:N3	35:RA:2118:U:O2'	2.40	0.54
37:YD:146:GLU:HB3	37:YD:189:CYS:HB3	1.90	0.54
41:YH:46:GLU:OE1	41:YH:51:ARG:NH1	2.41	0.54
1:QA:11:G:O2'	1:QA:506:G:N2	2.40	0.54
1:QA:573:A:N3	1:QA:883:C:O2'	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:QG:26:PHE:HD2	7:QG:43:PHE:CE2	2.26	0.54
10:QJ:38:ILE:HD11	10:QJ:71:LEU:HD23	1.89	0.54
35:RA:372:G:N2	35:RA:401:A:OP2	2.33	0.54
49:RT:52:ILE:HG12	49:RT:61:PHE:HB3	1.90	0.54
1:XA:1119:C:OP2	9:XI:9:ARG:NH2	2.41	0.54
35:YA:2065:C:O2	35:YA:2449:U:N3	2.34	0.54
38:YE:81:ILE:HG21	38:YE:84:PHE:HD2	1.73	0.54
45:YP:18:ARG:HH21	45:YP:32:THR:HG21	1.73	0.54
1:QA:1166:G:N2	1:QA:1170:A:OP2	2.40	0.54
1:QA:444:C:H2'	1:QA:445:G:H8	1.73	0.54
3:QC:88:ARG:HE	3:QC:101:LEU:HB2	1.72	0.54
29:R4:5:ILE:HB	40:RG:67:LYS:HD2	1.89	0.54
35:RA:1689:A:H62	35:RA:1698:A:H2	1.56	0.54
1:XA:439:A:OP2	1:XA:493:G:N1	2.37	0.54
2:XB:16:HIS:HD2	2:XB:210:SER:HA	1.72	0.54
3:XC:14:ILE:HG12	3:XC:15:THR:HG23	1.90	0.54
33:R8:34:TRP:O	33:R8:35:GLN:NE2	2.41	0.53
35:RA:1065:U:O2'	35:RA:1074:G:N2	2.41	0.53
35:RA:1342:A:OP1	53:RX:36:LYS:NZ	2.35	0.53
40:YG:38:VAL:HG22	40:YG:93:THR:HG23	1.89	0.53
5:QE:108:ALA:HA	5:QE:111:GLU:HG2	1.89	0.53
7:QG:75:VAL:HA	7:QG:88:PRO:HA	1.89	0.53
1:XA:339:C:OP1	44:YO:13:ASN:ND2	2.41	0.53
1:XA:103:C:OP2	20:XT:17:ARG:NH2	2.39	0.53
13:XM:65:LYS:HB3	29:Y4:50:VAL:HG11	1.90	0.53
1:QA:23:C:OP2	1:QA:561:U:N3	2.40	0.53
1:QA:414:A:OP2	1:QA:428:G:N2	2.41	0.53
2:QB:115:LEU:HD12	2:QB:145:LEU:HG	1.89	0.53
31:R6:7:ILE:HG13	31:R6:8:LYS:H	1.72	0.53
35:RA:1652:A:OP1	47:RR:8:ARG:NH1	2.36	0.53
35:RA:2207:C:O2	37:RD:151:LYS:NZ	2.35	0.53
35:RA:2777:G:OP2	35:RA:2781:A:O2'	2.25	0.53
20:XT:73:HIS:HB3	20:XT:74:LYS:HD3	1.90	0.53
35:YA:1065:U:O2'	35:YA:1074:G:N2	2.41	0.53
35:YA:307:G:H21	35:YA:330:A:H62	1.57	0.53
46:YQ:66:ILE:HA	46:YQ:104:PHE:HA	1.90	0.53
35:RA:1901:A:OP2	37:RD:255:LYS:NZ	2.34	0.53
2:XB:126:GLU:OE2	2:XB:130:ARG:NH1	2.41	0.53
8:XH:4:ASP:OD2	8:XH:85:ARG:NE	2.39	0.53
1:QA:582:U:OP2	1:QA:758:G:N1	2.33	0.53
1:QA:689:C:H3'	1:QA:690:G:H21	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:QE:50:GLU:HG3	5:QE:52:PRO:HD2	1.89	0.53
8:QH:110:ALA:HB3	8:QH:121:ASP:HB3	1.90	0.53
24:QY:76:A:H2	35:RA:2583:G:N2	1.96	0.53
8:XH:91:ARG:NE	17:XQ:32:TYR:O	2.41	0.53
1:XA:953:G:N7	13:XM:104:ARG:NH2	2.57	0.53
35:YA:2469:A:H2	35:YA:2481:G:H21	1.56	0.53
1:QA:544:G:OP2	4:QD:66:ARG:NH2	2.42	0.53
11:QK:33:THR:OG1	11:QK:34:ASP:N	2.41	0.53
35:RA:530:G:O2'	35:RA:532:A:N7	2.41	0.53
1:XA:953:G:H5'	1:XA:965:A:H61	1.73	0.53
10:XJ:26:ALA:O	10:XJ:84:GLN:NE2	2.41	0.53
37:YD:179:SER:O	37:YD:273:ARG:NH2	2.41	0.53
1:QA:769:G:H4'	1:QA:1513:A:H4'	1.91	0.53
10:QJ:45:ARG:HB2	10:QJ:65:LEU:HB3	1.91	0.53
35:RA:918:A:N3	36:RB:80:U:O2'	2.41	0.53
35:YA:486:C:O2'	52:YW:60:ASN:ND2	2.41	0.53
1:QA:571:U:O4	1:QA:864:A:N6	2.42	0.53
24:QY:75:C:O5'	24:QY:75:C:H6	1.92	0.53
40:RG:16:ARG:HH21	40:RG:28:VAL:HG22	1.74	0.53
1:XA:564:C:OP2	12:XL:15:ARG:NH2	2.37	0.53
1:XA:618:C:H5'	1:XA:619:U:H5''	1.89	0.53
35:YA:1087:G:O4'	35:YA:1103:A:N6	2.42	0.53
35:YA:806:C:O2	35:YA:2444:G:O2'	2.25	0.53
1:QA:662:G:H1	1:QA:743:U:H3	1.56	0.53
2:QB:78:GLN:O	2:QB:94:ASN:ND2	2.36	0.53
35:RA:458:G:O2'	35:RA:469:G:O6	2.23	0.53
39:RF:134:GLY:H	39:RF:162:LEU:HD12	1.73	0.53
45:RP:59:LEU:HA	45:RP:61:ARG:HH21	1.73	0.53
1:XA:1316:G:N1	1:XA:1319:A:OP2	2.41	0.53
13:XM:3:ARG:O	13:XM:57:ARG:NH1	2.40	0.53
33:Y8:14:VAL:CG2	45:YP:61:ARG:NH2	2.72	0.53
35:YA:526:A:O2'	35:YA:2043:C:O2	2.23	0.53
37:YD:134:ARG:HG3	37:YD:135:PHE:CD1	2.44	0.53
45:YP:115:LEU:HA	45:YP:134:ALA:HB2	1.90	0.53
1:QA:1348:U:H4'	9:QI:120:ARG:HG3	1.92	0.53
11:QK:87:THR:HA	11:QK:91:ARG:HD2	1.91	0.53
55:RZ:57:ILE:HG23	55:RZ:69:THR:HG23	1.91	0.53
1:XA:573:A:N3	1:XA:883:C:O2'	2.41	0.53
2:XB:87:ARG:NH2	2:XB:220:ASP:OD1	2.38	0.53
48:YS:26:LEU:HB3	48:YS:87:PHE:HA	1.90	0.53
3:QC:191:THR:OG1	3:QC:194:GLY:O	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:2680:C:H5'	38:RE:189:PRO:HA	1.90	0.52
35:RA:819:A:OP2	35:RA:1187:G:N2	2.29	0.52
40:RG:75:LYS:HE3	40:RG:77:ILE:HD11	1.91	0.52
53:RX:11:PRO:HA	53:RX:28:PHE:HA	1.91	0.52
40:YG:47:LYS:HD3	40:YG:81:LYS:HB2	1.91	0.52
1:QA:673:G:O3'	6:QF:87:ARG:NH2	2.43	0.52
3:QC:182:ILE:HG12	3:QC:203:PHE:HA	1.92	0.52
9:QI:104:ARG:NH1	9:QI:105:ASP:O	2.43	0.52
12:QL:33:ARG:HG2	12:QL:60:LEU:HD12	1.90	0.52
26:R1:92:LYS:HE2	26:R1:96:LYS:HD3	1.91	0.52
35:RA:2787:C:H1'	38:RE:62:PRO:HG3	1.90	0.52
39:RF:113:ALA:HB2	39:RF:183:VAL:HG23	1.92	0.52
1:XA:62:U:O2'	1:XA:379:C:O2	2.25	0.52
1:XA:60:A:OP1	1:XA:111:G:N2	2.42	0.52
13:XM:58:GLU:O	13:XM:62:ASN:ND2	2.42	0.52
35:YA:942:G:O2'	35:YA:1189:A:N3	2.38	0.52
37:RD:146:GLU:HB3	37:RD:189:CYS:HB3	1.90	0.52
1:XA:401:C:O2'	1:XA:621:A:N3	2.38	0.52
31:Y6:43:CYS:SG	31:Y6:44:ARG:N	2.82	0.52
35:YA:1769:G:O2'	35:YA:1958:C:OP1	2.21	0.52
35:YA:2547:U:O2	44:YO:23:ARG:NH1	2.41	0.52
52:YW:18:ARG:NH1	52:YW:76:VAL:O	2.42	0.52
1:QA:866:C:O2'	1:QA:919:A:OP1	2.27	0.52
35:RA:1394:U:H4'	35:RA:1603:A:H4'	1.92	0.52
35:RA:1791:A:N6	35:RA:1828:G:O2'	2.43	0.52
1:XA:1150:U:O4	1:XA:1151:A:N6	2.43	0.52
1:XA:1422:G:H5''	44:YO:48:PRO:HB3	1.92	0.52
1:XA:67:C:H2'	1:XA:68:G:C8	2.45	0.52
2:XB:7:VAL:HG22	2:XB:11:LEU:HD21	1.91	0.52
9:XI:121:ARG:NH1	9:XI:122:ALA:O	2.43	0.52
24:XY:9:A:O2'	24:XY:10:G:N7	2.41	0.52
35:YA:1113:U:OP1	41:YH:2:SER:N	2.42	0.52
44:YO:68:GLU:OE2	44:YO:78:ARG:NH1	2.42	0.52
35:YA:958:U:OP2	46:YQ:14:ARG:NH1	2.42	0.52
7:QG:116:ALA:HA	7:QG:119:ARG:HE	1.75	0.52
22:QV:1:C:O3'	46:RQ:87:LYS:NZ	2.42	0.52
35:RA:1999:C:O2	35:RA:2687:U:O2'	2.27	0.52
38:RE:34:VAL:HG21	38:RE:77:ILE:HD11	1.91	0.52
13:XM:14:ARG:NH2	13:XM:41:PRO:O	2.41	0.52
1:QA:1239:A:O2'	1:QA:1298:C:N4	2.43	0.52
35:YA:2115:G:N2	35:YA:2165:G:O6	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:YE:176:ILE:HB	38:YE:181:LEU:HB2	1.92	0.52
49:YT:19:LEU:HD22	49:YT:86:ILE:HG22	1.92	0.52
50:YU:50:ARG:HG2	50:YU:53:ARG:HH22	1.74	0.52
52:YW:29:LEU:HD22	52:YW:69:LEU:HD11	1.91	0.52
1:QA:824:C:O2'	8:QH:1:MET:N	2.42	0.52
35:RA:2308:G:H22	35:RA:2311:A:H2	1.58	0.52
35:RA:906:G:O2'	46:RQ:67:ARG:NH2	2.39	0.52
35:RA:2635:C:H5''	38:RE:78:LEU:HA	1.92	0.52
1:XA:191:G:O2'	20:XT:101:GLY:O	2.27	0.52
7:XG:5:ARG:HE	7:XG:6:ARG:H	1.58	0.52
40:YG:59:GLU:OE1	40:YG:153:ARG:NH2	2.35	0.52
31:R6:36:LEU:HD13	31:R6:50:ARG:HE	1.75	0.52
35:RA:2666:C:O2	41:RH:152:ARG:NH1	2.42	0.52
41:RH:3:ARG:NH1	41:RH:4:ILE:O	2.43	0.52
35:RA:1138:G:O2'	43:RN:102:ALA:O	2.27	0.52
1:XA:745:C:OP1	1:XA:851:G:O2'	2.27	0.52
9:XI:17:VAL:HA	9:XI:63:ILE:HG22	1.91	0.52
48:YS:39:ILE:HD12	48:YS:85:VAL:HG11	1.91	0.52
35:YA:1252:G:N7	50:YU:36:ARG:NH1	2.57	0.52
36:RB:44:G:H1'	36:RB:47:C:H42	1.74	0.52
42:RI:92:VAL:HG23	42:RI:120:ILE:HG23	1.91	0.52
46:RQ:67:ARG:NH1	46:RQ:105:GLU:OE2	2.42	0.52
1:QA:1446:A:O2'	49:RT:125:ARG:NH1	2.43	0.52
1:XA:262:A:H5''	20:XT:76:ALA:HB2	1.92	0.52
15:XO:24:SER:OG	15:XO:25:THR:N	2.42	0.52
1:XA:227:G:N2	16:XP:62:VAL:O	2.38	0.52
19:XS:19:VAL:HG21	19:XS:44:MET:HB3	1.92	0.52
35:YA:1291:C:H5'	35:YA:1536:A:H5'	1.92	0.52
41:YH:153:LYS:HB3	41:YH:162:ILE:H	1.74	0.52
1:QA:1382:C:O2'	7:QG:79:ARG:NH1	2.43	0.52
13:QM:57:ARG:NH1	29:R4:34:GLU:O	2.43	0.52
54:RY:39:VAL:HG13	54:RY:42:VAL:HB	1.91	0.52
10:XJ:38:ILE:HD12	10:XJ:39:PRO:HD2	1.92	0.52
12:XL:24:VAL:HG13	12:XL:98:TYR:HE1	1.75	0.52
35:YA:1296:G:OP1	35:YA:2709:G:O2'	2.22	0.52
35:YA:1478:G:H2'	35:YA:1479:G:H8	1.74	0.52
35:YA:259:G:H21	35:YA:621:A:H8	1.58	0.52
35:YA:1824:G:N3	37:YD:254:THR:OG1	2.42	0.52
44:YO:106:LEU:HB3	44:YO:111:PHE:HB2	1.92	0.52
1:QA:1159:U:O2'	1:QA:1160:G:N7	2.40	0.51
30:R5:36:CYS:SG	30:R5:37:LYS:N	2.83	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:180:G:N2	35:YA:215:G:O6	2.43	0.51
35:YA:2597:G:H5'	37:YD:243:GLY:HA3	1.92	0.51
35:YA:598:G:H5'	45:YP:11:GLY:HA3	1.92	0.51
7:QG:20:ASP:HB3	7:QG:23:VAL:HG23	1.92	0.51
16:QP:34:GLU:OE1	16:QP:55:ARG:NH2	2.37	0.51
29:R4:54:GLY:HA3	29:R4:71:ARG:HG2	1.93	0.51
41:RH:153:LYS:HB3	41:RH:162:ILE:H	1.75	0.51
53:RX:34:ALA:O	53:RX:77:LYS:NZ	2.39	0.51
55:RZ:137:ILE:HG21	55:RZ:155:LEU:HD23	1.92	0.51
1:XA:410:G:H21	1:XA:432:A:H62	1.58	0.51
1:XA:464:G:N2	1:XA:467:G:N7	2.59	0.51
35:YA:2295:C:OP1	48:YS:10:ARG:NH1	2.43	0.51
1:QA:1359:C:O2'	1:QA:1362:C:N4	2.42	0.51
1:QA:676:A:H1'	11:QK:115:PRO:HB3	1.92	0.51
1:QA:986:A:N3	19:QS:52:TYR:OH	2.32	0.51
1:QA:1130:A:O2'	9:QL:3:GLN:NE2	2.42	0.51
7:XG:27:ILE:HA	7:XG:30:ILE:HD12	1.91	0.51
15:XO:4:THR:HG23	15:XO:7:GLU:H	1.75	0.51
35:YA:958:U:O2	36:YB:89(A):A:O2'	2.26	0.51
36:YB:8:U:O2'	48:YS:25:ARG:NH2	2.43	0.51
49:YT:62:THR:HG22	49:YT:75:ILE:HG12	1.93	0.51
3:QC:127:ARG:HH22	3:QC:192:THR:H	1.58	0.51
35:RA:523:C:O2	35:RA:553:U:O2'	2.29	0.51
1:XA:1392:G:H21	1:XA:1502:A:H8	1.58	0.51
1:XA:375:U:O2	16:XP:28:ARG:NH1	2.43	0.51
1:XA:1367:C:H5''	9:XI:114:TYR:HA	1.93	0.51
33:Y8:62:LEU:CD1	35:YA:242:G:H5''	2.41	0.51
48:YS:15:ARG:NE	48:YS:88:ASP:OD1	2.43	0.51
53:YX:57:LEU:HG	53:YX:78:LYS:HB2	1.91	0.51
1:QA:375:U:H5''	16:QP:69:THR:HG21	1.92	0.51
1:QA:64:G:H4'	1:QA:65:U:H5'	1.93	0.51
2:QB:54:THR:HG22	2:QB:199:TYR:HB3	1.91	0.51
16:QP:18:ARG:HA	16:QP:38:TYR:HA	1.93	0.51
1:XA:405:U:OP2	4:XD:3:ARG:NH2	2.38	0.51
4:XD:105:VAL:HG13	4:XD:110:PHE:HB2	1.92	0.51
1:QA:1287:A:H2	1:QA:1353:G:H1'	1.76	0.51
1:QA:130:A:N3	1:QA:263:A:O2'	2.41	0.51
1:QA:794:A:HO2'	1:QA:1521:G:HO2'	1.57	0.51
1:QA:559:A:H4'	1:QA:560:U:H3'	1.91	0.51
1:QA:1123:A:H4'	10:QJ:36:GLY:HA3	1.92	0.51
47:RR:70:LEU:HD12	47:RR:76:VAL:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:XC:62:ASP:HA	3:XC:97:LYS:HD3	1.93	0.51
33:Y8:14:VAL:HG13	33:Y8:22:VAL:HG13	1.92	0.51
34:Y9:36:GLN:NE2	35:YA:1124:C:O2	2.43	0.51
41:YH:52:VAL:O	41:YH:65:HIS:NE2	2.36	0.51
42:YI:114:LEU:HD13	42:YI:130:TYR:HD1	1.76	0.51
1:QA:7:G:O2'	5:QE:120:THR:O	2.29	0.51
3:QC:14:ILE:HG12	3:QC:15:THR:HG23	1.93	0.51
37:RD:141:VAL:HG13	37:RD:162:SER:HB2	1.91	0.51
19:XS:36:ARG:NH2	19:XS:72:GLY:O	2.44	0.51
27:Y2:41:ILE:HG13	27:Y2:44:LEU:HD13	1.92	0.51
35:YA:701:G:O2'	35:YA:1631:A:N1	2.44	0.51
49:YT:54:ARG:HA	49:YT:59:THR:HG23	1.93	0.51
3:QC:184:TYR:CE1	3:QC:201:TYR:HE1	2.29	0.51
11:QK:21:ILE:HB	11:QK:84:VAL:HG12	1.91	0.51
13:QM:66:LEU:HD12	13:QM:68:GLY:H	1.74	0.51
28:R3:9:VAL:HG11	28:R3:55:ARG:HD3	1.93	0.51
28:R3:29:ARG:NH1	35:RA:1183:G:O3'	2.44	0.51
35:RA:1817:G:OP1	37:RD:88:ARG:NH2	2.44	0.51
35:RA:1962:C:O2'	35:RA:1964:G:OP2	2.29	0.51
35:RA:336:C:O2'	54:RY:35:TYR:OH	2.27	0.51
35:RA:259:G:H21	35:RA:621:A:H8	1.58	0.51
41:RH:18:GLU:HB3	41:RH:25:LYS:HB3	1.93	0.51
44:RO:8:LEU:HB2	44:RO:19:ILE:HG13	1.92	0.51
6:XF:9:VAL:HB	6:XF:87:ARG:HB2	1.92	0.51
35:YA:535:C:O3'	50:YU:53:ARG:NH1	2.44	0.51
35:YA:878:A:N6	35:YA:899:A:O2'	2.38	0.51
36:YB:48:A:OP2	48:YS:30:ARG:NH2	2.44	0.51
39:YF:59:TYR:HD2	39:YF:78:ILE:HG13	1.76	0.51
18:QR:58:LEU:HB3	18:QR:62:GLU:HG3	1.93	0.51
24:QY:55:U:H3	55:RZ:183:LEU:HB3	1.76	0.51
31:R6:6:ARG:HD2	31:R6:7:ILE:H	1.75	0.51
37:RD:108:PRO:HB3	37:RD:143:HIS:CE1	2.46	0.51
10:XJ:3:LYS:NZ	10:XJ:75:ILE:O	2.41	0.51
35:YA:220:G:O2'	35:YA:233:A:N3	2.41	0.51
35:YA:2287:A:N6	35:YA:2344:U:H3	2.08	0.51
38:YE:10:GLY:HA3	49:YT:8:LYS:HD3	1.92	0.51
52:YW:86:LEU:HD22	52:YW:96:ILE:HD11	1.92	0.51
1:QA:335:C:O2'	1:QA:1433:A:N3	2.38	0.51
13:QM:84:ILE:CD1	13:QM:86:CYS:HB2	2.39	0.51
35:RA:1681:G:HO2'	35:RA:1762:A:HO2'	1.54	0.51
39:RF:198:ALA:HA	39:RF:201:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:RH:23:ARG:HA	41:RH:36:PRO:HA	1.91	0.51
3:XC:70:VAL:HG12	3:XC:72:LYS:H	1.76	0.51
5:XE:12:LEU:HB3	5:XE:31:LEU:HB3	1.93	0.51
38:YE:52:LEU:HB2	38:YE:75:VAL:HG22	1.93	0.51
1:QA:165:C:H2'	1:QA:166:G:H8	1.77	0.50
24:QY:58:A:N7	55:RZ:183:LEU:HB2	2.26	0.50
25:R0:32:ARG:H	25:R0:35:ASN:ND2	2.09	0.50
35:RA:2055:C:O2	35:RA:2572:A:N6	2.44	0.50
9:XI:10:ARG:NH1	9:XI:75:ASP:OD2	2.45	0.50
17:XQ:28:PRO:HA	17:XQ:35:VAL:HA	1.92	0.50
35:YA:793:A:N6	35:YA:2073:C:OP1	2.43	0.50
50:YU:29:SER:OG	50:YU:30:LYS:NZ	2.40	0.50
50:YU:52:ARG:HD2	50:YU:55:ARG:NH2	2.26	0.50
35:RA:579:G:O2'	35:RA:2019:A:OP1	2.27	0.50
1:XA:1002:G:H2'	1:XA:1003:G:H8	1.76	0.50
8:XH:13:ILE:HG23	8:XH:63:LEU:HD11	1.92	0.50
49:YT:39:ARG:HH22	49:YT:41:ARG:HD3	1.77	0.50
55:YZ:45:ASP:OD1	55:YZ:49:ARG:NE	2.43	0.50
14:QN:45:ARG:O	14:QN:49:HIS:ND1	2.30	0.50
19:QS:32:LYS:HA	19:QS:50:ALA:HB3	1.93	0.50
29:R4:6:HIS:CE1	40:RG:67:LYS:H	2.30	0.50
38:RE:92:THR:OG1	38:RE:93:VAL:N	2.44	0.50
47:RR:3:HIS:O	47:RR:5:LYS:N	2.45	0.50
50:RU:91:ASP:HA	50:RU:95:LEU:HD12	1.94	0.50
14:XN:4:LYS:HA	14:XN:7:ILE:HG12	1.94	0.50
20:XT:26:ASN:HB2	20:XT:71:THR:HG23	1.93	0.50
35:YA:907:U:O2'	46:YQ:101:ARG:NH2	2.44	0.50
1:QA:651:C:N4	1:QA:753:A:OP2	2.44	0.50
38:RE:48:GLN:OE1	38:RE:64:LYS:NZ	2.44	0.50
49:RT:54:ARG:HA	49:RT:59:THR:CG2	2.33	0.50
26:Y1:5:CYS:SG	26:Y1:8:SER:OG	2.69	0.50
35:YA:1203:G:O6	35:YA:1204:A:N6	2.44	0.50
35:YA:1980:G:O2'	35:YA:1982:C:OP2	2.29	0.50
35:YA:363(A):A:H2'	35:YA:363(B):G:H8	1.76	0.50
51:YV:52:VAL:HG21	51:YV:55:ALA:HB3	1.93	0.50
1:QA:1422:G:H2'	1:QA:1423:G:H8	1.77	0.50
12:QL:70:ILE:HG13	12:QL:100:ILE:HD12	1.92	0.50
35:RA:2120:G:H2'	35:RA:2121:G:H8	1.76	0.50
35:RA:458:G:N2	35:RA:470:A:OP2	2.36	0.50
51:RV:24:LYS:HA	51:RV:92:THR:HG23	1.92	0.50
52:RW:86:LEU:HD22	52:RW:96:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:XB:84:GLU:HG3	2:XB:215:LEU:HB3	1.94	0.50
1:QA:1060:C:OP1	14:QN:45:ARG:NH2	2.44	0.50
1:QA:264:U:O2'	17:QQ:64:PRO:O	2.26	0.50
31:R6:14:THR:HG1	31:R6:19:ARG:HE	1.56	0.50
35:RA:1213:A:N3	35:RA:1238:G:O2'	2.41	0.50
35:RA:265:A:N6	35:RA:427:U:O2'	2.45	0.50
35:RA:2730:C:O2'	38:RE:168:MET:O	2.23	0.50
44:RO:106:LEU:HB3	44:RO:111:PHE:HB2	1.93	0.50
2:XB:192:SER:OG	2:XB:193:ASP:N	2.45	0.50
1:XA:1249:C:O2'	9:XI:73:GLN:NE2	2.45	0.50
37:YD:164:GLN:OE1	37:YD:176:ARG:NH2	2.37	0.50
39:YF:60:SER:OG	39:YF:61:GLY:N	2.43	0.50
1:QA:618:C:H5'	1:QA:619:U:H5''	1.94	0.50
2:QB:21:ARG:HB3	2:QB:39:ILE:HG13	1.93	0.50
19:QS:3:ARG:HH12	19:QS:11:VAL:CG1	2.25	0.50
32:R7:7:PRO:HB2	35:RA:1309:G:H4'	1.93	0.50
35:RA:1990:C:H2'	35:RA:1991:U:C6	2.47	0.50
35:RA:2130:U:O2'	35:RA:2133:G:O2'	2.26	0.50
55:RZ:47:VAL:O	55:RZ:51:ALA:N	2.39	0.50
1:XA:1452:C:H4'	1:XA:1453:G:H5'	1.93	0.50
35:YA:2688:U:OP1	35:YA:2713:A:N6	2.45	0.50
44:YO:120:GLU:OE1	49:YT:67:SER:OG	2.27	0.50
1:QA:1128:C:H1'	1:QA:1146:A:H61	1.76	0.50
35:RA:224:G:O6	35:RA:419:C:O2'	2.27	0.50
35:RA:270(E):G:H1	35:RA:270(U):C:H42	1.59	0.50
52:RW:59:VAL:HG21	52:RW:66:GLU:HB2	1.94	0.50
1:XA:1077:G:N2	1:XA:1080:A:OP2	2.37	0.50
35:YA:2646:C:OP2	35:YA:2732:G:O2'	2.25	0.50
39:YF:179:GLU:HA	39:YF:205:ARG:HH22	1.74	0.50
50:YU:40:PHE:HB3	51:YV:75:PHE:CD2	2.47	0.50
1:QA:1336:C:H1'	1:QA:1337:G:C2	2.47	0.50
19:QS:33:THR:OG1	19:QS:34:TRP:N	2.45	0.50
25:R0:39:ARG:HH21	35:RA:2355:C:H1'	1.77	0.50
35:RA:677:A:O2'	35:RA:2070:G:O2'	2.29	0.50
49:RT:49:VAL:HG12	49:RT:63:VAL:HG22	1.92	0.50
1:XA:1318:A:H4'	19:XS:11:VAL:HG11	1.94	0.50
1:XA:352:C:O2'	1:XA:354:G:OP1	2.22	0.50
29:Y4:33:VAL:HG21	40:YG:109:VAL:HG13	1.94	0.50
1:QA:1366:C:O2'	10:QJ:60:ARG:NH2	2.39	0.49
1:QA:429:U:OP2	4:QD:36:ARG:NH2	2.43	0.49
20:QT:71:THR:HG22	20:QT:72:LEU:HG	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:2064:C:O2'	35:RA:2251:G:N2	2.41	0.49
35:RA:2773:C:OP1	38:RE:166:THR:OG1	2.26	0.49
39:RF:135:LYS:HB3	39:RF:138:GLU:HG3	1.94	0.49
44:RO:2:ILE:HG23	44:RO:6:THR:CG2	2.42	0.49
1:QA:974:A:OP2	14:QN:29:ARG:NH2	2.35	0.49
2:QB:84:GLU:OE2	2:QB:235:SER:OG	2.30	0.49
27:R2:32:LEU:O	27:R2:36:ARG:N	2.43	0.49
25:R0:19:LYS:NZ	35:RA:2387:U:O2'	2.44	0.49
35:RA:2839:G:H5'	47:RR:46:GLY:HA2	1.94	0.49
1:XA:390:C:O3'	16:XP:28:ARG:NH2	2.41	0.49
3:XC:150:LYS:HG3	3:XC:167:TRP:HE1	1.77	0.49
3:XC:150:LYS:HB3	3:XC:201:TYR:HB2	1.94	0.49
33:Y8:62:LEU:HD13	35:YA:242:G:C5'	2.41	0.49
41:YH:56:SER:OG	41:YH:61:HIS:ND1	2.35	0.49
8:QH:96:GLY:H	8:QH:99:GLU:HG3	1.77	0.49
1:XA:1028(B):C:N4	1:XA:1032(B):G:O6	2.45	0.49
1:XA:757:U:O2'	1:XA:879:C:O2	2.30	0.49
35:YA:1479:G:OP2	35:YA:1510:A:N6	2.38	0.49
35:YA:2502:G:H5''	35:YA:2503:A:H5''	1.93	0.49
1:QA:578:C:O2'	1:QA:728:A:N3	2.37	0.49
35:RA:1112:G:O3'	41:RH:2:SER:N	2.45	0.49
35:RA:1669:A:H2'	35:RA:1669:A:N3	2.27	0.49
51:RV:23:GLU:OE2	51:RV:89:GLN:NE2	2.45	0.49
31:Y6:47:THR:HG22	31:Y6:48:VAL:H	1.76	0.49
35:YA:1020:A:N6	35:YA:1141:U:O2'	2.45	0.49
44:YO:107:ARG:HG3	44:YO:115:VAL:HG11	1.94	0.49
2:QB:28:PHE:HD1	2:QB:194:PRO:HD3	1.78	0.49
25:R0:27:GLU:HG3	25:R0:68:GLU:HA	1.95	0.49
35:RA:327:G:N2	54:RY:70:SER:OG	2.46	0.49
38:RE:36:ARG:HH12	38:RE:86:PRO:HD2	1.77	0.49
44:RO:64:ARG:HB2	44:RO:83:ALA:HB3	1.94	0.49
50:RU:90:VAL:HG11	51:RV:40:LEU:HG	1.93	0.49
1:XA:1002:G:H1	1:XA:1038:C:H42	1.60	0.49
1:XA:676:A:H1'	11:XK:115:PRO:HB3	1.94	0.49
1:XA:110:C:O2'	16:XP:25:ARG:O	2.29	0.49
2:QB:70:PHE:O	2:QB:93:VAL:N	2.44	0.49
1:QA:1147:C:O2	9:QI:16:ARG:NH1	2.46	0.49
18:QR:34:TYR:CD1	18:QR:35:ARG:HG3	2.48	0.49
26:R1:11:ARG:HD3	26:R1:12:PRO:HD2	1.93	0.49
27:R2:22:GLU:OE2	27:R2:68:ARG:NH2	2.45	0.49
35:RA:1403:C:H5'	35:RA:1471:A:H1'	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:1638:C:O3'	35:RA:2709:G:N2	2.46	0.49
35:RA:2115:G:N1	35:RA:2164:C:OP2	2.45	0.49
37:RD:12:SER:HB2	37:RD:208:LYS:HB3	1.93	0.49
45:RP:9:ASN:N	45:RP:9:ASN:OD1	2.44	0.49
2:XB:84:GLU:HB3	2:XB:219:VAL:HG21	1.92	0.49
8:XH:7:ALA:HB2	8:XH:85:ARG:HD3	1.95	0.49
31:Y6:25:LYS:HE2	31:Y6:27:LYS:NZ	2.28	0.49
35:YA:380:U:H2'	35:YA:381:G:H8	1.77	0.49
1:QA:1325:C:H4'	21:QU:17:THR:HG21	1.95	0.49
35:RA:2392:A:OP2	35:RA:2422:A:N6	2.46	0.49
48:RS:15:ARG:HD2	48:RS:25:ARG:HH11	1.78	0.49
1:XA:452:A:H62	1:XA:480:U:H3	1.59	0.49
9:XI:9:ARG:HG2	9:XI:14:VAL:HG22	1.94	0.49
31:Y6:25:LYS:HE2	31:Y6:27:LYS:HZ3	1.78	0.49
35:YA:833:U:O2	45:YP:55:ARG:NH1	2.46	0.49
18:QR:44:LEU:HD11	18:QR:79:LEU:HD23	1.95	0.49
35:RA:1190:G:H2'	35:RA:1191:G:H8	1.77	0.49
35:RA:807:U:O2'	35:RA:2060:A:N1	2.40	0.49
35:RA:238:C:O2'	35:RA:608:A:N3	2.43	0.49
1:XA:1128:C:N3	1:XA:1144:G:N2	2.60	0.49
35:YA:243:U:OP2	35:YA:254:G:N1	2.44	0.49
35:YA:2656:U:H3	35:YA:2665:A:H2	1.61	0.49
35:YA:900:A:H3'	35:YA:901:A:H8	1.77	0.49
26:R1:42:GLN:OE1	35:RA:379:G:N2	2.39	0.49
26:R1:45:ASN:HB2	35:RA:397:G:H5''	1.94	0.49
2:XB:184:VAL:HG13	2:XB:198:ASP:H	1.78	0.49
26:Y1:65:SER:HG	26:Y1:66:HIS:HD1	1.60	0.49
28:Y3:15:TYR:O	28:Y3:20:LYS:NZ	2.46	0.49
35:YA:1490:A:O2'	37:YD:99:ASP:OD1	2.31	0.49
49:YT:64:ARG:HG3	49:YT:73:GLU:HG2	1.94	0.49
1:QA:953:G:N7	13:QM:104:ARG:NH2	2.56	0.49
13:QM:37:THR:OG1	13:QM:55:ARG:NH1	2.46	0.49
31:R6:27:LYS:HE2	35:RA:2284:C:H3'	1.94	0.49
35:RA:2470:G:OP1	46:RQ:56:ARG:NH2	2.46	0.49
49:RT:24:PRO:HD3	49:RT:52:ILE:HD12	1.94	0.49
54:RY:83:THR:OG1	54:RY:84:ARG:N	2.46	0.49
55:RZ:5:LEU:HD22	55:RZ:43:GLU:HB3	1.95	0.49
4:XD:98:GLU:HG2	4:XD:189:PRO:HG2	1.95	0.49
35:YA:1530:G:O6	35:YA:1542:G:N2	2.45	0.49
51:YV:76:LYS:HG3	51:YV:81:TYR:HD1	1.75	0.49
55:YZ:61:LEU:HB3	55:YZ:65:GLN:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:2865:U:OP2	49:RT:119:LYS:NZ	2.39	0.48
42:RI:64:GLU:HG3	42:RI:67:ARG:HH21	1.78	0.48
1:XA:642:A:N3	8:XH:113:SER:OG	2.38	0.48
2:XB:164:VAL:HG12	2:XB:166:ASP:H	1.77	0.48
5:XE:75:THR:OG1	5:XE:76:ILE:N	2.46	0.48
24:XY:75:C:H2'	24:XY:76:A:C8	2.48	0.48
35:YA:868:U:O2	46:YQ:8:LYS:NZ	2.45	0.48
35:YA:996:A:H4'	50:YU:92:ARG:HE	1.77	0.48
1:QA:545:C:OP2	4:QD:65:ARG:NH2	2.41	0.48
11:QK:34:ASP:OD1	11:QK:38:ASN:N	2.46	0.48
35:RA:984:A:H5''	35:RA:985:C:H5	1.77	0.48
46:RQ:24:GLY:H	46:RQ:101:ARG:HD2	1.79	0.48
35:RA:2295:C:H5	48:RS:13:ARG:HH12	1.59	0.48
35:YA:1342:A:O2'	35:YA:1344:G:OP2	2.27	0.48
35:YA:2125:G:N1	35:YA:2172:U:OP1	2.43	0.48
35:YA:807:U:OP2	45:YP:41:ARG:NH1	2.46	0.48
51:YV:60:GLU:OE1	51:YV:97:LYS:NZ	2.38	0.48
4:QD:23:GLY:N	4:QD:26:CYS:SG	2.72	0.48
6:QF:36:ARG:NH1	6:QF:66:GLU:OE1	2.46	0.48
7:QG:105:VAL:O	7:QG:109:ASN:ND2	2.46	0.48
50:RU:92:ARG:HE	50:RU:94:ASN:HB3	1.77	0.48
35:RA:335:C:H4'	54:RY:73:ARG:HE	1.78	0.48
35:YA:1246:A:OP1	45:YP:15:ARG:NH2	2.37	0.48
35:YA:335:C:H4'	54:YY:73:ARG:HE	1.76	0.48
35:YA:300:A:OP2	54:YY:84:ARG:NH1	2.47	0.48
1:QA:1392:G:H21	1:QA:1502:A:H8	1.60	0.48
1:QA:403:C:OP2	4:QD:74:GLN:NE2	2.46	0.48
1:QA:662:G:O2'	1:QA:836:G:OP1	2.32	0.48
2:QB:178:ARG:NH2	8:QH:71:GLY:O	2.46	0.48
13:QM:82:MET:CE	13:QM:92:HIS:HB3	2.42	0.48
37:RD:25:THR:O	37:RD:27:THR:N	2.46	0.48
43:RN:22:THR:OG1	43:RN:23:LEU:N	2.45	0.48
35:RA:1666:G:O2'	44:RO:6:THR:OG1	2.28	0.48
55:RZ:5:LEU:H	55:RZ:59:LEU:HA	1.79	0.48
25:Y0:18:ALA:O	25:Y0:20:ARG:NH1	2.46	0.48
35:YA:1338:G:N7	53:YX:62:LYS:NZ	2.54	0.48
40:YG:12:TYR:HA	40:YG:16:ARG:HD3	1.94	0.48
1:QA:1213:A:N6	1:QA:1215:G:N3	2.61	0.48
1:QA:129(A):G:N2	1:QA:188:U:O2'	2.46	0.48
35:RA:1651:G:H4'	47:RR:39:PRO:HG2	1.96	0.48
35:RA:363:G:H2'	35:RA:363(A):A:H8	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:476:G:N1	35:RA:479:A:OP2	2.43	0.48
37:RD:31:LYS:HB3	37:RD:35:LYS:HG2	1.94	0.48
1:XA:1236:A:H4'	1:XA:1304:G:H4'	1.95	0.48
1:XA:413:G:O2'	1:XA:428:G:N2	2.46	0.48
8:XH:10:LEU:HD22	8:XH:83:ILE:HD11	1.95	0.48
22:XV:63:G:H4'	25:Y0:11:ARG:HH22	1.79	0.48
37:YD:108:PRO:HB3	37:YD:143:HIS:CE1	2.49	0.48
1:QA:297:G:N2	1:QA:300:A:OP2	2.45	0.48
1:QA:976:G:P	14:QN:32:SER:H	2.36	0.48
4:QD:59:ARG:HA	4:QD:59:ARG:HE	1.78	0.48
35:RA:1568:G:OP2	37:RD:63:ARG:NH2	2.42	0.48
35:RA:281:G:H21	35:RA:359:A:H62	1.61	0.48
37:RD:231:HIS:CD2	37:RD:249:PRO:HG3	2.48	0.48
55:RZ:48:PHE:HA	55:RZ:51:ALA:HB3	1.95	0.48
9:XI:26:VAL:HG22	9:XI:61:ALA:HB3	1.96	0.48
1:QA:532:A:H2	1:QA:1206:G:H21	1.61	0.48
28:R3:8:LEU:HA	28:R3:54:VAL:HG12	1.96	0.48
35:RA:1296:G:OP1	35:RA:2709:G:O2'	2.22	0.48
52:RW:29:LEU:HD22	52:RW:69:LEU:HD11	1.95	0.48
10:XJ:44:VAL:HG22	10:XJ:66:ARG:HG2	1.96	0.48
19:XS:68:GLY:HA2	29:Y4:68:ARG:HB2	1.95	0.48
35:YA:2470:G:H5'	46:YQ:56:ARG:HH21	1.79	0.48
55:YZ:130:PRO:HA	55:YZ:133:ILE:HD11	1.95	0.48
1:QA:1080:A:H5''	5:QE:16:THR:HG21	1.94	0.48
6:QF:9:VAL:HB	6:QF:87:ARG:HB2	1.94	0.48
35:RA:1479:G:OP2	35:RA:1510:A:N6	2.39	0.48
35:RA:2245:U:H5'	35:RA:2246:G:H5'	1.95	0.48
48:RS:26:LEU:HB3	48:RS:87:PHE:HA	1.95	0.48
19:XS:32:LYS:HA	19:XS:50:ALA:HB3	1.96	0.48
27:Y2:41:ILE:HD11	27:Y2:44:LEU:HD22	1.95	0.48
35:YA:1780:A:O2'	35:YA:1781:C:O2	2.27	0.48
35:YA:1858:G:H2'	35:YA:1883:G:H22	1.78	0.48
41:YH:41:MET:HE1	41:YH:64:LEU:HB3	1.95	0.48
35:RA:2415:G:H4'	45:RP:67:MET:H	1.79	0.48
47:RR:42:LYS:HG2	47:RR:45:ARG:HH12	1.79	0.48
25:Y0:23:VAL:HG22	25:Y0:38:VAL:HG22	1.96	0.48
37:YD:35:LYS:NZ	37:YD:102:LYS:O	2.47	0.48
37:YD:95:LEU:HD22	37:YD:117:VAL:HG21	1.96	0.48
1:QA:970:C:N4	9:QI:128:ARG:OXT	2.46	0.48
27:R2:31:GLU:O	27:R2:35:LEU:N	2.45	0.48
35:RA:2816:C:O2	35:RA:2883:A:O2'	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:RO:19:ILE:HG22	44:RO:43:VAL:HA	1.94	0.48
49:RT:73:GLU:OE2	49:RT:103:ARG:NE	2.41	0.48
12:XL:60:LEU:HD12	12:XL:62:SER:H	1.78	0.48
29:Y4:55:ARG:HG3	29:Y4:56:VAL:HG23	1.95	0.48
32:Y7:7:PRO:HB2	35:YA:1309:G:H4'	1.96	0.48
35:YA:1638:C:O2	35:YA:2698:U:O2'	2.31	0.48
35:YA:1682:G:OP1	35:YA:1699:G:N1	2.45	0.48
35:YA:2258:C:O2'	35:YA:2427:C:OP2	2.32	0.48
35:YA:2446:G:N2	35:YA:2449:U:O2	2.38	0.48
35:YA:414:C:H2'	35:YA:415:A:C8	2.48	0.48
38:YE:25:VAL:HG12	38:YE:183:LEU:HG	1.96	0.48
41:YH:103:LEU:HD13	41:YH:131:VAL:HG21	1.96	0.48
1:QA:924:C:O2'	1:QA:1502:A:N6	2.47	0.47
12:QL:117:ARG:HB2	12:QL:122:THR:HB	1.96	0.47
42:RI:128:LEU:O	42:RI:138:ILE:N	2.40	0.47
33:R8:30:ARG:HH21	45:RP:62:LEU:HD13	1.79	0.47
1:XA:79:G:H2'	1:XA:80:G:H8	1.78	0.47
31:Y6:24:GLU:HG3	31:Y6:25:LYS:H	1.79	0.47
35:YA:1568:G:H5''	37:YD:61:LEU:HG	1.97	0.47
51:YV:76:LYS:HG3	51:YV:81:TYR:CE1	2.48	0.47
54:YY:14:LEU:HB2	54:YY:75:ILE:HD11	1.96	0.47
1:QA:323:U:OP1	20:QT:26:ASN:ND2	2.47	0.47
1:QA:980:C:O2'	14:QN:9:LYS:NZ	2.46	0.47
35:RA:1779:U:OP2	35:RA:1784:A:N6	2.39	0.47
35:RA:995:C:O2	43:RN:3:THR:OG1	2.32	0.47
35:RA:2012:G:OP1	52:RW:11:ARG:NH2	2.47	0.47
1:XA:1065:U:O2	1:XA:1067:A:N6	2.43	0.47
1:XA:826:C:H5'	8:XH:12:ARG:HH21	1.79	0.47
16:XP:14:ASN:HA	16:XP:42:ARG:HH11	1.79	0.47
20:XT:74:LYS:H	20:XT:74:LYS:HD3	1.80	0.47
35:YA:807:U:O2'	35:YA:2060:A:N1	2.41	0.47
35:YA:2632:A:HO2'	35:YA:2811:G:HO2'	1.52	0.47
35:YA:223:A:O2'	35:YA:420:C:O2	2.27	0.47
55:YZ:125:LEU:HG	55:YZ:164:ALA:HB3	1.95	0.47
1:QA:346:G:OP1	49:RT:41:ARG:NH2	2.40	0.47
24:QY:4:G:H1	24:QY:69:C:H42	1.62	0.47
35:RA:2393:A:H5'	45:RP:62:LEU:HB3	1.96	0.47
35:RA:2734:A:H62	35:RA:2770:G:H21	1.61	0.47
35:RA:2791:C:OP1	35:RA:2893:G:N2	2.47	0.47
42:RI:1:MET:N	42:RI:21:VAL:O	2.40	0.47
35:RA:2495:G:H5''	46:RQ:81:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:1321:C:H5''	1:XA:1322:C:H5''	1.97	0.47
1:XA:1347:G:N2	1:XA:1374:A:OP2	2.38	0.47
1:XA:689:C:H3'	1:XA:690:G:H21	1.79	0.47
2:XB:109:SER:O	2:XB:113:HIS:ND1	2.46	0.47
24:XY:55:U:O2'	24:XY:57:G:OP2	2.24	0.47
34:Y9:25:VAL:HB	34:Y9:34:GLN:HB2	1.96	0.47
1:QA:191:G:O2'	20:QT:101:GLY:O	2.32	0.47
1:QA:559:A:OP1	5:QE:126:ARG:NH2	2.48	0.47
1:QA:718:G:H5'	11:QK:117:ASN:HB2	1.96	0.47
1:QA:890:G:O2'	1:QA:906:G:O6	2.27	0.47
4:XD:59:ARG:HE	4:XD:59:ARG:HA	1.79	0.47
24:XY:58:A:O2'	24:XY:61:C:N4	2.46	0.47
25:Y0:32:ARG:H	25:Y0:35:ASN:ND2	2.12	0.47
35:YA:2402:C:H1'	35:YA:2403:C:H5	1.79	0.47
38:YE:75:VAL:HG23	38:YE:76:ARG:HG2	1.96	0.47
35:YA:1250:G:OP2	45:YP:21:ARG:NH1	2.47	0.47
45:YP:90:ARG:NH2	45:YP:105:LEU:HD11	2.29	0.47
1:QA:153:C:N3	1:QA:169:C:N4	2.63	0.47
1:QA:254:G:O2'	17:QQ:16:GLN:O	2.32	0.47
13:QM:84:ILE:HG13	13:QM:84:ILE:O	2.15	0.47
33:R8:16:ILE:HD12	33:R8:57:ARG:HG2	1.95	0.47
35:RA:994:C:OP2	50:RU:54:LYS:NZ	2.34	0.47
41:RH:24:VAL:N	41:RH:35:VAL:O	2.44	0.47
45:RP:4:SER:O	45:RP:7:ARG:NH1	2.48	0.47
47:RR:103:ARG:NH1	47:RR:108:GLY:O	2.47	0.47
35:YA:1568:G:OP2	37:YD:63:ARG:NH2	2.42	0.47
35:YA:2543:G:H2'	35:YA:2544:G:C8	2.49	0.47
35:YA:603:A:H5''	35:YA:655:A:H61	1.78	0.47
55:YZ:97:GLU:HG2	55:YZ:125:LEU:HD11	1.96	0.47
1:QA:1294:G:H2'	1:QA:1295:G:C8	2.50	0.47
1:QA:1321:C:OP1	13:QM:88:ARG:NH2	2.48	0.47
5:QE:145:LYS:NZ	5:QE:149:GLU:OE2	2.43	0.47
35:RA:2068:U:H3	35:RA:2430:A:H2	1.62	0.47
38:RE:9:VAL:HB	38:RE:25:VAL:HG23	1.97	0.47
1:XA:1281:U:H5''	1:XA:1282:C:H5	1.79	0.47
7:XG:20:ASP:HB3	7:XG:23:VAL:HG12	1.95	0.47
26:Y1:78:LYS:HG2	35:YA:270(R):G:H21	1.80	0.47
33:Y8:4:MET:CE	33:Y8:61:LEU:HD12	2.35	0.47
37:YD:43:ARG:HB2	37:YD:54:ARG:HB2	1.95	0.47
39:YF:134:GLY:H	39:YF:162:LEU:HD22	1.80	0.47
50:YU:91:ASP:O	50:YU:93:LYS:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:YX:61:GLY:N	53:YX:75:ASP:OD1	2.39	0.47
9:QI:112:LYS:HA	9:QI:119:ALA:HB2	1.97	0.47
30:R5:3:LYS:HB3	30:R5:4:HIS:H	1.41	0.47
35:RA:1860:G:H1	35:RA:1882:C:H42	1.63	0.47
48:RS:38:GLN:HE21	48:RS:47:THR:HG21	1.80	0.47
48:RS:10:ARG:NE	48:RS:91:PRO:O	2.40	0.47
35:YA:1130:U:O2	38:YE:149:ARG:NH2	2.42	0.47
39:YF:157:VAL:HB	39:YF:194:MET:HB3	1.97	0.47
46:YQ:50:ALA:HB1	46:YQ:121:ALA:HB1	1.96	0.47
1:QA:1286:A:N6	1:QA:1354:C:O3'	2.47	0.47
3:QC:20:SER:OG	3:QC:22:TRP:NE1	2.48	0.47
12:QL:49:ASN:ND2	12:QL:92:ASP:OD2	2.39	0.47
24:QY:19:G:C6	35:RA:881:G:H4'	2.50	0.47
35:RA:2635:C:H5'	38:RE:77:ILE:HG23	1.97	0.47
35:RA:859:G:O2'	35:RA:916:G:O6	2.23	0.47
29:R4:38:LYS:HE3	40:RG:112:PRO:HG3	1.97	0.47
54:RY:99:CYS:SG	54:RY:100:ALA:N	2.87	0.47
1:XA:1316:G:N2	1:XA:1318:A:H3'	2.29	0.47
26:Y1:80:LEU:HG	26:Y1:81:LYS:HG3	1.97	0.47
26:Y1:8:SER:HB3	26:Y1:66:HIS:CE1	2.50	0.47
35:YA:1826:G:H4'	37:YD:242:ARG:HH21	1.79	0.47
1:QA:1294:G:H2'	1:QA:1295:G:H8	1.79	0.47
1:QA:426:G:OP1	4:QD:38:TYR:OH	2.27	0.47
3:QC:184:TYR:HE1	3:QC:201:TYR:HE1	1.63	0.47
29:R4:43:TYR:O	29:R4:45:GLY:N	2.47	0.47
35:RA:2043:C:OP1	35:RA:2777:G:O2'	2.29	0.47
35:RA:2056:G:C2'	35:RA:2056:G:N3	2.77	0.47
44:RO:71:ARG:NH2	44:RO:122:LEU:O	2.48	0.47
46:RQ:29:PHE:N	46:RQ:105:GLU:OE1	2.41	0.47
35:RA:1217:C:OP1	50:RU:15:LYS:NZ	2.43	0.47
1:XA:938:A:N3	1:XA:1376:U:O2'	2.44	0.47
34:Y9:22:ARG:HH12	35:YA:2741:A:H5''	1.79	0.47
39:YF:63:LYS:NZ	39:YF:75:HIS:O	2.37	0.47
39:YF:9:ILE:HD11	39:YF:20:LEU:HD22	1.96	0.47
15:QO:24:SER:HB3	15:QO:27:VAL:HG23	1.97	0.47
6:QF:97:PHE:HB2	18:QR:32:ARG:HH21	1.80	0.47
29:R4:25:TYR:HE2	40:RG:3:LEU:HD12	1.80	0.47
35:RA:2133:G:H1'	35:RA:2158:A:H61	1.79	0.47
35:RA:392:C:H5''	35:RA:409:C:H5''	1.96	0.47
32:R7:35:ARG:NH1	35:RA:54:G:O2'	2.46	0.47
35:RA:535:C:O3'	50:RU:53:ARG:NH1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:RW:68:ARG:HH21	52:RW:112:GLY:HA3	1.79	0.47
1:XA:356:A:N3	1:XA:368:U:O2'	2.34	0.47
35:YA:1607:C:N4	35:YA:1622:G:OP2	2.33	0.47
1:QA:941:G:OP1	7:QG:32:ARG:NH1	2.48	0.47
12:QL:71:PRO:O	12:QL:102:ARG:NH1	2.47	0.47
24:QY:56:C:H5''	35:RA:897:C:H5'	1.96	0.47
35:RA:1228:G:OP2	50:RU:16:LYS:NZ	2.41	0.47
36:RB:42:C:N4	40:RG:91:ARG:HH12	2.12	0.47
43:RN:133:GLN:HG2	43:RN:135:PRO:HD3	1.97	0.47
1:XA:1129:C:O2'	1:XA:1131:G:N7	2.48	0.47
8:XH:110:ALA:HB3	8:XH:121:ASP:HB3	1.97	0.47
35:YA:2126:A:N6	35:YA:2163:C:O2'	2.47	0.47
35:YA:2788:C:O2'	35:YA:2809:A:N3	2.40	0.47
44:YO:64:ARG:HH12	49:YT:70:VAL:HG21	1.80	0.47
45:YP:29:LYS:HD3	45:YP:30:THR:HG23	1.97	0.47
1:QA:1150:U:O4	1:QA:1151:A:N6	2.48	0.46
13:QM:13:LYS:HG3	13:QM:44:ARG:HD2	1.97	0.46
35:RA:30:G:O2'	35:RA:1214:A:N3	2.47	0.46
35:RA:2377:A:H2'	35:RA:2378:A:C8	2.50	0.46
35:RA:2749:A:H5''	41:RH:4:ILE:HD11	1.97	0.46
37:RD:122:ASP:N	37:RD:122:ASP:OD1	2.42	0.46
35:RA:674:G:H21	39:RF:74:ARG:HH12	1.62	0.46
1:XA:1463:C:OP1	49:YT:111:ARG:NH1	2.48	0.46
2:XB:101:MET:HA	2:XB:108:ILE:HG13	1.96	0.46
39:YF:133:ASN:H	39:YF:162:LEU:HD13	1.80	0.46
35:YA:2012:G:OP1	52:YW:11:ARG:NH2	2.48	0.46
3:QC:184:TYR:CE1	3:QC:201:TYR:CE1	3.03	0.46
11:QK:93:GLN:OE1	11:QK:96:ARG:NH2	2.43	0.46
13:QM:80:ARG:HH12	19:QS:69:HIS:CE1	2.34	0.46
24:QY:54:U:O4	55:RZ:183:LEU:N	2.48	0.46
35:RA:987:G:O2'	35:RA:1000:A:N3	2.43	0.46
35:RA:2008:C:H2'	35:RA:2009:G:H8	1.80	0.46
35:RA:2055:C:OP1	35:RA:2056:G:H4'	2.15	0.46
35:RA:2597:G:H5'	37:RD:243:GLY:HA3	1.97	0.46
36:RB:5:C:OP1	36:RB:61:G:O2'	2.24	0.46
38:RE:52:LEU:O	38:RE:74:PRO:HA	2.15	0.46
55:RZ:115:GLY:H	55:RZ:177:PRO:HD3	1.80	0.46
4:XD:3:ARG:HD3	4:XD:118:ARG:NE	2.30	0.46
35:YA:1077:A:H5'	35:YA:1078:U:H5''	1.96	0.46
37:YD:122:ASP:OD1	37:YD:122:ASP:N	2.48	0.46
29:R4:53:GLU:OE2	29:R4:55:ARG:NE	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:1921:G:H2'	35:RA:1922:G:H8	1.80	0.46
35:RA:2219:G:OP1	37:RD:172:TYR:OH	2.27	0.46
36:RB:5:C:O2'	36:RB:27:C:O2	2.34	0.46
35:RA:1649:G:O2'	47:RR:107:ASP:OD2	2.23	0.46
50:RU:102:GLU:OE2	51:RV:13:ARG:NH2	2.48	0.46
54:RY:46:LYS:HG2	54:RY:60:PHE:HD2	1.80	0.46
35:YA:693:C:O2'	35:YA:1353:A:N3	2.43	0.46
35:YA:1858:G:O2'	35:YA:1884:A:N6	2.48	0.46
35:YA:195:A:H61	35:YA:198:C:H3'	1.81	0.46
35:YA:2150:U:H2'	35:YA:2151:G:H8	1.81	0.46
35:YA:784:A:O4'	37:YD:227:ASN:ND2	2.48	0.46
1:QA:62:U:O2'	1:QA:379:C:O2	2.33	0.46
18:QR:58:LEU:HD23	18:QR:62:GLU:HG3	1.97	0.46
35:RA:323:G:HO2'	35:RA:1205:U:H3	1.64	0.46
30:R5:19:ARG:NH1	35:RA:1264:G:OP1	2.33	0.46
35:RA:746:A:HO2'	35:RA:2611:U:HO2'	1.63	0.46
44:RO:71:ARG:NH1	49:RT:74:ARG:HH12	2.14	0.46
1:XA:323:U:OP1	20:XT:26:ASN:ND2	2.46	0.46
2:XB:69:LEU:HB3	2:XB:162:ILE:HG22	1.97	0.46
2:XB:178:ARG:NH1	2:XB:196:LEU:O	2.49	0.46
35:YA:676:A:H8	35:YA:2069:G:H21	1.64	0.46
35:YA:2404:C:O3'	45:YP:77:ARG:NH2	2.48	0.46
2:QB:16:HIS:HD2	2:QB:210:SER:HA	1.81	0.46
16:QP:53:VAL:HG13	16:QP:79:VAL:HG22	1.97	0.46
35:RA:1048:A:H2	35:RA:1112:G:H21	1.63	0.46
32:R7:49:ARG:NH2	35:RA:128:C:O3'	2.48	0.46
48:RS:36:TYR:HD2	48:RS:52:SER:OG	1.99	0.46
1:XA:486:U:H2'	1:XA:487:A:C8	2.49	0.46
26:Y1:87:PRO:HA	26:Y1:90:ILE:HB	1.98	0.46
35:YA:1153:C:H5'	50:YU:76:TYR:HE2	1.81	0.46
1:QA:150:C:H42	1:QA:171:A:H62	1.64	0.46
10:QJ:7:LYS:HB2	10:QJ:97:GLU:HB2	1.98	0.46
11:XK:19:ALA:HA	11:XK:32:ILE:HA	1.98	0.46
35:YA:2816:C:O2	35:YA:2883:A:O2'	2.30	0.46
35:YA:630:G:N2	35:YA:633:A:OP2	2.38	0.46
35:YA:994:C:OP1	50:YU:53:ARG:NH2	2.48	0.46
37:YD:12:SER:HB2	37:YD:208:LYS:HB3	1.98	0.46
45:YP:106:LEU:HD13	45:YP:112:LEU:HD13	1.98	0.46
4:QD:8:VAL:HG11	4:QD:22:LYS:HD3	1.98	0.46
29:R4:43:TYR:O	29:R4:46:GLN:N	2.47	0.46
30:R5:4:HIS:HB3	30:R5:5:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:RI:79:ILE:HB	42:RI:142:VAL:HG12	1.97	0.46
43:RN:96:GLU:HB2	43:RN:122:VAL:HG12	1.97	0.46
55:YZ:149:SER:OG	55:YZ:150:LEU:N	2.48	0.46
2:QB:60:ASP:O	2:QB:64:ARG:NH1	2.49	0.46
16:QP:14:ASN:HA	16:QP:42:ARG:HH11	1.80	0.46
37:RD:130:ALA:HB2	37:RD:192:THR:HG22	1.97	0.46
38:RE:47:VAL:HG11	38:RE:86:PRO:HD2	1.98	0.46
41:RH:125:VAL:HG22	41:RH:131:VAL:HG23	1.97	0.46
1:XA:1291:G:H4'	9:XI:39:GLY:HA3	1.96	0.46
3:XC:131:ARG:NH1	3:XC:166:GLU:OE1	2.48	0.46
49:YT:27:THR:HB	49:YT:48:ILE:HG13	1.96	0.46
1:QA:1412:C:H2'	1:QA:1413:A:C8	2.51	0.46
2:QB:5:ILE:HG12	2:QB:221:LEU:HB2	1.98	0.46
17:QQ:28:PRO:HA	17:QQ:35:VAL:HA	1.98	0.46
35:RA:1077:A:H5'	35:RA:1078:U:H5''	1.97	0.46
35:RA:2156:G:O6	35:RA:2157:G:N2	2.48	0.46
35:RA:2313:C:O4'	40:RG:40:ASN:ND2	2.49	0.46
35:RA:2795:G:H21	35:RA:2801:A:H62	1.64	0.46
35:RA:630:G:N2	35:RA:633:A:OP2	2.37	0.46
1:XA:909:A:N3	1:XA:1413:A:O2'	2.42	0.46
4:XD:173:TRP:CD1	4:XD:174:LEU:HG	2.50	0.46
35:YA:1204:A:H1'	35:YA:1206:G:C5	2.51	0.46
35:YA:685:A:OP1	35:YA:686:G:N2	2.49	0.46
35:YA:783:A:H8	35:YA:784:A:H4'	1.80	0.46
36:YB:37:C:O2	48:YS:95:HIS:NE2	2.43	0.46
37:YD:123:ALA:HB3	37:YD:131:LEU:HG	1.98	0.46
37:YD:35:LYS:HG2	37:YD:104:TYR:CD2	2.51	0.46
1:QA:859:A:OP2	1:QA:869:G:N2	2.41	0.46
4:QD:105:VAL:HG13	4:QD:110:PHE:HB2	1.98	0.46
11:QK:16:SER:OG	11:QK:106:LYS:NZ	2.46	0.46
1:QA:522:C:H41	12:QL:53:ARG:HH22	1.64	0.46
13:QM:82:MET:CE	13:QM:92:HIS:CB	2.93	0.46
35:RA:2146:C:H4'	35:RA:2147:G:C8	2.51	0.46
35:RA:2851:A:O2'	47:RR:64:ARG:NH2	2.49	0.46
35:RA:587:C:OP2	45:RP:21:ARG:NH2	2.31	0.46
37:RD:35:LYS:HD3	37:RD:104:TYR:CE1	2.50	0.46
35:RA:2851:A:O3'	47:RR:64:ARG:NH2	2.49	0.46
1:XA:952:U:H2'	1:XA:953:G:H8	1.80	0.46
35:YA:2118:U:N3	35:YA:2147:G:O2'	2.45	0.46
35:YA:2659:G:N2	35:YA:2662:A:OP2	2.49	0.46
41:YH:103:LEU:HD22	41:YH:123:PHE:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:YU:92:ARG:HD3	50:YU:94:ASN:HB3	1.97	0.46
30:R5:56:LYS:HE2	30:R5:58:LEU:HD23	1.98	0.45
34:R9:30:PRO:HB3	35:RA:2527:C:H5''	1.97	0.45
35:RA:2572:A:OP1	35:RA:2574:G:O2'	2.31	0.45
43:RN:10:GLU:HA	43:RN:11:PRO:HD3	1.78	0.45
50:RU:66:ASN:HD21	50:RU:70:ARG:HH21	1.63	0.45
35:RA:483:A:O2'	54:RY:49:VAL:O	2.27	0.45
32:Y7:47:ARG:HH22	53:YX:60:ARG:CZ	2.28	0.45
36:YB:80:U:H2'	36:YB:81:G:H21	1.80	0.45
38:YE:16:ARG:HG2	38:YE:21:VAL:HG11	1.98	0.45
38:YE:52:LEU:O	38:YE:74:PRO:HA	2.16	0.45
39:YF:167:ALA:HB1	39:YF:173:VAL:HG11	1.98	0.45
1:QA:1127:G:H21	1:QA:1147:C:H41	1.63	0.45
35:RA:1859:A:N6	35:RA:1883:G:O2'	2.50	0.45
35:RA:270:A:OP2	35:RA:270(Y):G:N1	2.39	0.45
38:RE:8:LYS:O	38:RE:193:GLY:N	2.47	0.45
42:RI:3:VAL:HG12	42:RI:38:LEU:HD23	1.98	0.45
45:RP:7:ARG:HA	45:RP:8:PRO:HD2	1.87	0.45
35:RA:1652:A:N6	47:RR:11:ASN:OD1	2.42	0.45
53:RX:27:THR:HB	53:RX:80:ILE:HG12	1.97	0.45
1:XA:1095:U:P	1:XA:1108:G:H1	2.39	0.45
1:XA:296:U:O2'	1:XA:556:C:O2	2.30	0.45
8:XH:49:GLU:OE2	8:XH:62:TYR:OH	2.23	0.45
11:XK:34:ASP:OD1	11:XK:38:ASN:N	2.50	0.45
19:XS:27:GLU:HG3	19:XS:29:ARG:HG2	1.98	0.45
35:YA:1105:U:H2'	35:YA:1106:G:H8	1.79	0.45
35:YA:141:A:H8	35:YA:1408:C:H1'	1.81	0.45
35:YA:2308:G:H22	35:YA:2311:A:H2	1.64	0.45
35:YA:626:U:O4	45:YP:107:LYS:HE2	2.17	0.45
35:YA:870:A:OP1	46:YQ:6:ARG:NH2	2.49	0.45
2:QB:4:GLU:HG2	2:QB:5:ILE:H	1.81	0.45
5:QE:122:GLU:O	5:QE:126:ARG:NH1	2.49	0.45
1:XA:105:G:OP1	20:XT:22:ARG:NH2	2.50	0.45
35:YA:2580:U:H4'	38:YE:130:GLY:HA3	1.98	0.45
35:YA:2781:A:H5''	35:YA:2782:G:H5'	1.99	0.45
35:YA:742:G:H2'	35:YA:743:G:H8	1.81	0.45
39:YF:113:ALA:HB2	39:YF:183:VAL:HG23	1.98	0.45
41:YH:4:ILE:HG22	41:YH:6:ARG:HG2	1.97	0.45
35:RA:1155:A:H5''	50:RU:55:ARG:HH11	1.81	0.45
35:RA:993:G:OP1	50:RU:50:ARG:NH2	2.47	0.45
38:RE:117:MET:HA	38:RE:122:PHE:N	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y2:17:SER:HB3	27:Y2:20:GLU:OE1	2.17	0.45
38:YE:9:VAL:HB	38:YE:25:VAL:HG23	1.98	0.45
1:QA:950:U:H2'	1:QA:951:G:H8	1.82	0.45
34:R9:25:VAL:HB	34:R9:34:GLN:HB2	1.99	0.45
51:RV:49:THR:HG23	51:RV:50:PRO:CD	2.46	0.45
55:RZ:76:LEU:HA	55:RZ:83:PRO:HA	1.97	0.45
35:YA:1210:A:H8	35:YA:1210:A:H5'	1.80	0.45
40:YG:73:ALA:HB2	40:YG:82:LEU:HD11	1.98	0.45
1:QA:545:C:O2'	1:QA:549:C:OP1	2.35	0.45
2:QB:219:VAL:HA	2:QB:222:ILE:HD12	1.99	0.45
35:RA:1071:G:H22	35:RA:1091:G:H8	1.65	0.45
35:RA:2392:A:H2	35:RA:2424:C:H42	1.63	0.45
36:RB:45:A:O4'	40:RG:95:ARG:NH1	2.50	0.45
46:RQ:12:GLN:HG2	46:RQ:73:PRO:HD2	1.99	0.45
28:Y3:10:LYS:NZ	28:Y3:15:TYR:OH	2.37	0.45
35:YA:2006:C:O2'	35:YA:2823:A:N3	2.49	0.45
37:YD:44:ASN:OD1	37:YD:44:ASN:N	2.46	0.45
42:YI:30:LEU:HB3	42:YI:36:ALA:HB3	1.97	0.45
46:YQ:39:PRO:HB3	46:YQ:99:PRO:HD3	1.99	0.45
55:YZ:47:VAL:O	55:YZ:51:ALA:N	2.42	0.45
12:QL:56:ALA:O	12:QL:68:ALA:N	2.44	0.45
35:RA:2850:A:OP2	35:RA:2866:U:N3	2.44	0.45
35:RA:39:C:O2	39:RF:46:ARG:NH2	2.50	0.45
50:RU:36:ARG:HG2	50:RU:40:PHE:HE1	1.82	0.45
1:XA:1188:A:OP1	9:XI:114:TYR:OH	2.30	0.45
1:XA:1224:G:O2'	1:XA:1322:C:OP2	2.35	0.45
1:XA:1414:U:H3	1:XA:1486:G:H1	1.63	0.45
29:Y4:6:HIS:CE1	40:YG:66:GLN:HA	2.51	0.45
52:YW:73:ALA:HB3	52:YW:106:ILE:HB	1.98	0.45
1:QA:1141:C:H2'	1:QA:1142:G:H8	1.82	0.45
1:QA:1250:A:N3	1:QA:1370:G:O2'	2.44	0.45
2:QB:146:GLN:HG3	2:QB:153:ARG:HH12	1.82	0.45
35:RA:1190:G:H2'	35:RA:1191:G:C8	2.52	0.45
33:R8:5:LYS:HG2	35:RA:242:G:C8	2.52	0.45
37:RD:148:GLU:HB2	37:RD:151:LYS:HD2	1.99	0.45
38:RE:59:VAL:HG11	38:RE:73:GLU:HB2	1.99	0.45
1:XA:23:C:OP2	1:XA:561:U:N3	2.44	0.45
2:XB:178:ARG:HH22	8:XH:74:PRO:HB3	1.80	0.45
5:XE:110:LEU:HD13	5:XE:118:ILE:HG21	1.97	0.45
6:XF:97:PHE:HB2	18:XR:32:ARG:HE	1.82	0.45
27:Y2:18:PRO:HA	27:Y2:21:LEU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Y8:4:MET:HE1	33:Y8:61:LEU:CD1	2.44	0.45
35:YA:1187:G:N2	35:YA:1188:U:O4	2.49	0.45
35:YA:1434:A:H61	35:YA:1558:A:N6	2.15	0.45
46:YQ:77:LYS:NZ	46:YQ:80:GLU:OE2	2.38	0.45
47:YR:13:HIS:NE2	47:YR:15:SER:OG	2.46	0.45
49:YT:24:PRO:HD3	49:YT:52:ILE:HD12	1.98	0.45
17:QQ:45:HIS:CD2	17:QQ:47:PRO:HG3	2.52	0.45
26:R1:7:ILE:HD13	26:R1:91:LYS:HZ3	1.81	0.45
31:R6:6:ARG:HD2	31:R6:7:ILE:HG22	1.99	0.45
32:R7:8:ASN:HB3	32:R7:11:LYS:HB3	1.98	0.45
27:R2:65:ASN:ND2	35:RA:111:A:O3'	2.49	0.45
35:RA:1454:U:O2'	35:RA:1455:G:N7	2.41	0.45
35:RA:627:A:H4'	35:RA:628:G:H5'	1.98	0.45
35:RA:2831:G:OP1	38:RE:58:ARG:NH1	2.50	0.45
49:RT:24:PRO:HA	49:RT:49:VAL:HG23	1.98	0.45
1:XA:157:G:H1	1:XA:164:U:H3	1.64	0.45
1:XA:890:G:O2'	1:XA:906:G:O6	2.28	0.45
1:XA:553:A:O2'	12:XL:29:GLY:O	2.32	0.45
13:XM:17:VAL:O	13:XM:20:THR:OG1	2.26	0.45
35:YA:2315:G:OP1	40:YG:36:LYS:NZ	2.43	0.45
42:YI:130:TYR:HB3	42:YI:136:VAL:HG13	1.99	0.45
35:YA:1652:A:N6	47:YR:11:ASN:OD1	2.46	0.45
1:QA:1077:G:N2	1:QA:1080:A:OP2	2.46	0.45
1:QA:954:G:H21	1:QA:1227:A:H62	1.65	0.45
1:QA:738:C:OP1	6:QF:4:TYR:OH	2.31	0.45
4:QD:68:TYR:HE1	4:QD:103:ASN:HD21	1.57	0.45
8:QH:120:THR:OG1	8:QH:121:ASP:N	2.50	0.45
13:QM:40:ASN:HB3	13:QM:43:THR:HG23	1.99	0.45
13:QM:84:ILE:HD11	13:QM:86:CYS:CB	2.45	0.45
35:RA:2319:G:N1	35:RA:2334:G:OP2	2.45	0.45
49:RT:54:ARG:HG3	49:RT:59:THR:HG21	1.99	0.45
51:RV:49:THR:HG23	51:RV:50:PRO:HD3	1.99	0.45
1:XA:522:C:OP2	12:XL:69:TYR:OH	2.30	0.45
35:YA:2150:U:H2'	35:YA:2151:G:C8	2.52	0.45
50:YU:83:LEU:HD12	50:YU:113:ALA:HB2	1.99	0.45
1:QA:947:G:O3'	13:QM:109:THR:OG1	2.34	0.44
25:R0:55:ARG:NH1	35:RA:2364:C:OP1	2.46	0.44
38:RE:32:PRO:HB3	38:RE:90:THR:HG22	1.98	0.44
39:RF:110:LEU:HD11	39:RF:181:LEU:HB3	1.98	0.44
51:RV:28:GLU:HB2	51:RV:31:ALA:HB2	1.99	0.44
24:XY:53:G:N1	55:YZ:183:LEU:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Y5:2:ALA:HA	35:YA:2015:A:H1'	1.99	0.44
35:YA:2880:C:O3'	47:YR:90:ARG:NH1	2.49	0.44
35:YA:299:A:N3	35:YA:319:C:O2'	2.43	0.44
39:YF:158:THR:O	39:YF:164:ARG:NH2	2.38	0.44
2:QB:53:ARG:HH22	2:QB:199:TYR:HA	1.83	0.44
12:QL:113:ARG:HH21	12:QL:116:SER:HB2	1.82	0.44
19:QS:10:PHE:CD1	19:QS:10:PHE:O	2.70	0.44
35:RA:2723:C:OP2	38:RE:109:LYS:NZ	2.50	0.44
20:XT:74:LYS:HB3	20:XT:75:ASN:H	1.68	0.44
29:Y4:37:SER:HB3	40:YG:112:PRO:HB3	2.00	0.44
1:QA:816:A:OP1	1:QA:1526:G:O2'	2.28	0.44
9:QI:19:LEU:HD22	9:QI:59:PHE:HD2	1.82	0.44
1:QA:552:U:O2'	12:QL:86:ARG:O	2.35	0.44
35:RA:2416:C:H5''	45:RP:64:LYS:HE2	1.99	0.44
43:RN:97:ARG:HA	43:RN:100:GLU:HB2	1.98	0.44
1:XA:247:G:OP2	17:XQ:99:SER:OG	2.36	0.44
1:XA:376:G:H5''	16:XP:5:ARG:HD2	1.99	0.44
18:XR:43:PHE:HE2	18:XR:58:LEU:HD11	1.83	0.44
31:Y6:14:THR:HG1	31:Y6:19:ARG:HE	1.63	0.44
31:Y6:7:ILE:HG13	31:Y6:8:LYS:H	1.81	0.44
35:YA:224:G:O6	35:YA:419:C:O2'	2.30	0.44
1:QA:362:G:N2	1:QA:365:U:OP2	2.49	0.44
35:RA:1863:G:O2'	35:RA:2411:A:O2'	2.27	0.44
44:RO:102:VAL:HG23	44:RO:121:VAL:HG23	1.98	0.44
45:RP:126:VAL:HG13	45:RP:145:PRO:HB2	1.98	0.44
51:RV:72:VAL:HG13	51:RV:85:LYS:HB2	2.00	0.44
9:XI:5:TYR:HE1	9:XI:16:ARG:HB3	1.83	0.44
35:YA:617:G:OP1	39:YF:40:GLN:NE2	2.50	0.44
44:YO:122:LEU:HD13	49:YT:72:VAL:HG11	1.99	0.44
55:YZ:76:LEU:HA	55:YZ:83:PRO:HA	2.00	0.44
1:QA:950:U:H2'	1:QA:951:G:C8	2.53	0.44
3:QC:24:ALA:HB2	3:QC:32:LEU:HD12	1.99	0.44
6:QF:15:ASP:N	6:QF:15:ASP:OD1	2.48	0.44
1:QA:1298:C:C4	7:QG:114:ARG:HD2	2.52	0.44
1:QA:691:G:N7	11:QK:26:ASN:ND2	2.65	0.44
24:QY:19:G:H3'	24:QY:20:G:H8	1.82	0.44
33:R8:26:LYS:NZ	35:RA:2361:A:OP2	2.46	0.44
35:RA:2502:G:H5''	35:RA:2503:A:H5''	1.99	0.44
35:RA:33:U:O4	35:RA:446:G:O2'	2.28	0.44
55:RZ:117:LEU:HD11	55:RZ:172:ALA:HB1	1.99	0.44
1:XA:911:U:OP2	12:XL:97:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:XM:49:THR:HB	13:XM:52:GLU:HG3	1.99	0.44
29:Y4:48:ARG:HH21	29:Y4:51:ASP:HA	1.83	0.44
35:YA:2249:U:N3	35:YA:2253:G:OP2	2.45	0.44
35:YA:860:U:OP2	35:YA:916:G:N1	2.41	0.44
37:YD:231:HIS:CD2	37:YD:249:PRO:HG3	2.53	0.44
49:YT:74:ARG:HG2	49:YT:76:PHE:CE1	2.53	0.44
1:QA:253:U:OP1	17:QQ:67:LYS:NZ	2.37	0.44
1:QA:6:G:H4'	1:QA:298:A:H4'	1.99	0.44
19:QS:9:VAL:CG1	19:QS:39:THR:CB	2.94	0.44
35:RA:1062:G:H2'	35:RA:1063:G:C8	2.52	0.44
35:RA:407:G:H2'	35:RA:408:G:H8	1.81	0.44
36:RB:111:U:H2'	36:RB:112:G:H8	1.82	0.44
37:RD:123:ALA:HB3	37:RD:131:LEU:HG	1.99	0.44
40:RG:71:THR:N	40:RG:89:GLY:O	2.48	0.44
35:RA:2880:C:O3'	47:RR:90:ARG:NH1	2.51	0.44
3:XC:134:ILE:HG23	3:XC:151:VAL:HB	1.99	0.44
5:XE:11:ILE:HD12	5:XE:105:VAL:HG13	1.99	0.44
35:YA:2707:G:H5'	47:YR:68:ARG:HH21	1.83	0.44
55:YZ:94:GLU:CG	55:YZ:95:PRO:CD	2.66	0.44
1:QA:165:C:H2'	1:QA:166:G:C8	2.53	0.44
1:QA:673:G:H2'	1:QA:674:G:C8	2.52	0.44
12:QL:60:LEU:HD21	12:QL:64:TYR:HB2	2.00	0.44
13:QM:91:ARG:HB2	13:QM:98:VAL:HG12	1.99	0.44
35:RA:1568:G:P	37:RD:63:ARG:HH12	2.39	0.44
39:RF:102:PRO:HB2	39:RF:105:VAL:HG23	2.00	0.44
55:RZ:19:ARG:NH1	55:RZ:84:GLU:O	2.51	0.44
8:XH:106:GLY:O	8:XH:122:ARG:NH2	2.35	0.44
20:XT:11:SER:HA	20:XT:13:LEU:HD23	1.99	0.44
35:YA:793:A:OP2	35:YA:2071:A:O2'	2.35	0.44
37:YD:143:HIS:ND1	37:YD:194:GLY:O	2.49	0.44
37:YD:254:THR:OG1	37:YD:254:THR:O	2.35	0.44
1:QA:18:C:H5''	5:QE:127:ASN:HD21	1.83	0.44
9:QI:55:ALA:HA	9:QI:58:HIS:HD2	1.83	0.44
1:QA:35:G:O2'	12:QL:118:SER:O	2.23	0.44
14:QN:24:CYS:HB3	14:QN:28:GLY:H	1.83	0.44
24:QY:25:C:H2'	24:QY:26:G:H8	1.82	0.44
35:RA:1444(A):A:O2'	35:RA:1460:A:N3	2.45	0.44
39:RF:167:ALA:HA	39:RF:170:LEU:HD13	2.00	0.44
52:RW:69:LEU:HD13	52:RW:107:LEU:HD13	1.99	0.44
1:XA:1264:C:H2'	1:XA:1265:G:H8	1.82	0.44
1:XA:632:A:OP1	8:XH:98:LYS:NZ	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:XP:59:TRP:HA	16:XP:62:VAL:HG22	2.00	0.44
42:YI:77:LEU:HD13	42:YI:101:LEU:HD13	2.00	0.44
44:YO:104:ARG:HG3	44:YO:121:VAL:HG12	2.00	0.44
1:QA:1203:C:H5''	14:QN:3:ARG:HH21	1.83	0.44
1:QA:1309:G:N7	13:QM:99:ARG:NH2	2.66	0.44
16:QP:22:THR:HA	16:QP:33:ILE:HG12	2.00	0.44
35:RA:1992:G:OP1	35:RA:1992:G:C8	2.71	0.44
40:RG:38:VAL:HG22	40:RG:93:THR:HG22	2.00	0.44
41:RH:8:PRO:HG2	41:RH:69:ARG:CZ	2.48	0.44
44:RO:71:ARG:NH2	44:RO:122:LEU:OXT	2.39	0.44
44:RO:77:ILE:HD12	49:RT:74:ARG:HD2	2.00	0.44
45:RP:64:LYS:O	45:RP:66:GLY:N	2.51	0.44
1:XA:1318:A:H4'	19:XS:11:VAL:HG21	1.99	0.44
10:XJ:26:ALA:O	10:XJ:30:SER:OG	2.27	0.44
18:XR:74:ARG:HB3	18:XR:81:PHE:CE1	2.52	0.44
25:Y0:33:ALA:N	25:Y0:64:ASP:OD1	2.50	0.44
35:YA:219:G:N3	35:YA:234:C:O2'	2.50	0.44
44:YO:23:ARG:NH2	44:YO:28:SER:O	2.51	0.44
45:YP:126:VAL:HG23	45:YP:145:PRO:HB2	1.99	0.44
46:YQ:8:LYS:HE3	46:YQ:9:TYR:HE1	1.83	0.44
2:QB:200:ILE:HG22	2:QB:202:PRO:HD3	2.00	0.43
9:QI:33:PHE:HE2	9:QI:47:LEU:HD11	1.83	0.43
33:R8:54:GLU:O	33:R8:58:ILE:HG12	2.18	0.43
35:RA:2151:G:H2'	35:RA:2152:G:H8	1.83	0.43
37:RD:67:PHE:HB3	37:RD:153:ALA:HB3	2.00	0.43
1:XA:1286:A:H2'	1:XA:1287:A:H4'	2.00	0.43
1:XA:1404:C:H2'	1:XA:1405:G:C8	2.53	0.43
4:XD:163:GLU:HA	4:XD:166:LYS:HE3	2.00	0.43
13:XM:86:CYS:SG	13:XM:87:TYR:N	2.91	0.43
14:XN:24:CYS:HB3	14:XN:29:ARG:H	1.83	0.43
20:XT:73:HIS:HB3	20:XT:74:LYS:H	1.45	0.43
29:Y4:67:TYR:HB2	29:Y4:68:ARG:H	1.66	0.43
33:Y8:61:LEU:HD23	33:Y8:61:LEU:HA	1.87	0.43
35:YA:1063:G:H22	35:YA:1076:C:H1'	1.83	0.43
35:YA:2119:A:N1	35:YA:2170:A:N6	2.65	0.43
35:YA:2343:C:O2'	35:YA:2373:G:O2'	2.25	0.43
35:YA:2845:G:H2'	35:YA:2846:G:C8	2.53	0.43
35:YA:392:C:H5''	35:YA:409:C:H5''	1.99	0.43
35:YA:956:G:N2	35:YA:960:A:OP2	2.51	0.43
45:YP:90:ARG:HH22	45:YP:105:LEU:HD11	1.83	0.43
48:YS:29:PHE:HB3	48:YS:36:TYR:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:QJ:76:ASN:OD1	10:QJ:76:ASN:N	2.51	0.43
15:QO:87:ILE:HG22	15:QO:88:ARG:H	1.83	0.43
22:QV:63:G:H4'	25:R0:11:ARG:HH12	1.83	0.43
35:RA:1394:U:O2	53:RX:16:LYS:NZ	2.44	0.43
38:RE:54:GLN:HG3	38:RE:55:ASN:H	1.83	0.43
2:XB:95:GLN:HB3	2:XB:96:ARG:H	1.69	0.43
8:XH:19:VAL:HG13	8:XH:21:LYS:HG3	2.00	0.43
9:XI:3:GLN:OE1	9:XI:20:ARG:NE	2.39	0.43
33:Y8:61:LEU:HD13	35:YA:593:G:H4'	1.99	0.43
35:YA:1407:C:H42	35:YA:1595:G:H1	1.66	0.43
35:YA:2298:A:H62	35:YA:2318:G:H8	1.65	0.43
1:QA:258:G:OP1	20:QT:86:ARG:NH1	2.37	0.43
13:QM:49:THR:OG1	13:QM:50:GLU:N	2.51	0.43
35:RA:229:A:H4'	35:RA:230:U:H5'	2.00	0.43
35:RA:861:A:N3	36:RB:79:C:O2'	2.50	0.43
42:RI:69:LYS:HG3	42:RI:136:VAL:HB	1.99	0.43
44:RO:69:ILE:HD12	44:RO:69:ILE:N	2.32	0.43
19:XS:40:ILE:HD11	19:XS:62:ILE:HG12	2.00	0.43
20:XT:75:ASN:N	20:XT:75:ASN:OD1	2.49	0.43
55:YZ:137:ILE:HG23	55:YZ:156:LYS:HB3	1.99	0.43
1:QA:1223:C:P	19:QS:78:ARG:HH12	2.41	0.43
1:QA:790:A:OP1	22:QV:38:A:O2'	2.30	0.43
13:QM:84:ILE:O	19:QS:74:PHE:CE1	2.72	0.43
35:RA:1041:C:H2'	35:RA:1042:G:H8	1.84	0.43
35:RA:2006:C:O2'	35:RA:2823:A:N3	2.50	0.43
33:R8:59:LYS:HG2	45:RP:49:ARG:HE	1.84	0.43
27:Y2:70:GLN:HG3	27:Y2:71:ASN:H	1.83	0.43
33:Y8:29:LYS:HG2	33:Y8:30:ARG:H	1.83	0.43
35:YA:1005:C:O2	35:YA:1138:G:N2	2.41	0.43
35:YA:2630:G:H2'	35:YA:2631:G:C8	2.53	0.43
48:YS:27:SER:HA	48:YS:88:ASP:HB3	2.00	0.43
1:QA:1002:G:H2'	1:QA:1003:G:C8	2.53	0.43
1:QA:1229:A:OP2	13:QM:114:ARG:NH1	2.50	0.43
1:QA:1125:U:O4	10:QJ:5:ARG:NE	2.51	0.43
19:QS:18:LYS:HD2	19:QS:29:ARG:HH22	1.84	0.43
35:RA:500:G:N1	35:RA:503:A:OP2	2.50	0.43
54:RY:99:CYS:SG	54:RY:101:LYS:N	2.91	0.43
29:Y4:67:TYR:HB2	29:Y4:68:ARG:HD3	2.00	0.43
35:YA:83:G:N2	35:YA:103:A:OP2	2.32	0.43
35:YA:1290:C:O2'	35:YA:1536:A:OP2	2.28	0.43
35:YA:764:A:N3	37:YD:213:ARG:NH1	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:YG:43:LEU:HD12	40:YG:90:LEU:HD13	1.99	0.43
41:YH:149:ARG:CZ	41:YH:154:PRO:HG2	2.48	0.43
1:QA:1502:A:H2	1:QA:1505:G:H1	1.66	0.43
10:QJ:27:ALA:HA	10:QJ:30:SER:HB3	1.99	0.43
35:RA:1278:A:H4'	47:RR:34:ILE:HD11	2.00	0.43
1:XA:261:U:OP2	20:XT:79:ARG:NH2	2.52	0.43
35:YA:1667:G:O2'	35:YA:1991:U:O4	2.33	0.43
37:YD:33:LEU:HD21	37:YD:102:LYS:HD2	2.00	0.43
41:YH:103:LEU:HD23	41:YH:115:VAL:HB	2.01	0.43
44:YO:8:LEU:HD13	44:YO:82:ASN:HB3	2.00	0.43
47:YR:3:HIS:O	47:YR:5:LYS:N	2.52	0.43
52:YW:6:ILE:HG12	52:YW:104:THR:HG23	1.99	0.43
32:Y7:47:ARG:HH12	53:YX:60:ARG:HH22	1.67	0.43
2:QB:187:LEU:HA	2:QB:201:ILE:HB	2.01	0.43
4:QD:88:VAL:HG13	5:QE:97:GLY:HA3	1.99	0.43
5:QE:28:PHE:CD2	5:QE:51:VAL:HG13	2.54	0.43
1:QA:599:C:O2'	8:QH:129:VAL:O	2.27	0.43
10:QJ:51:ARG:NE	10:QJ:60:ARG:O	2.49	0.43
13:QM:37:THR:HG23	13:QM:39:ILE:HG12	2.00	0.43
35:RA:2122:U:H2'	35:RA:2123:G:H8	1.83	0.43
35:RA:2503:A:O2'	35:RA:2505:G:OP2	2.25	0.43
35:RA:792:G:N3	35:RA:2072:G:O2'	2.42	0.43
44:RO:71:ARG:HH22	44:RO:122:LEU:C	2.17	0.43
51:RV:40:LEU:HD23	51:RV:47:VAL:HA	2.00	0.43
1:XA:1437:C:H2'	1:XA:1438:G:H8	1.84	0.43
1:XA:522:C:H41	12:XL:53:ARG:HH22	1.66	0.43
2:XB:51:LEU:HD23	2:XB:201:ILE:HD12	2.01	0.43
4:XD:111:ALA:HB1	4:XD:116:GLN:HB3	2.01	0.43
35:YA:2445:G:OP1	39:YF:74:ARG:NH1	2.45	0.43
35:YA:960:A:H61	46:YQ:82:ARG:NH2	2.15	0.43
35:YA:2729:G:H1'	38:YE:187:ALA:HB2	2.00	0.43
44:YO:19:ILE:HG22	44:YO:43:VAL:HA	2.00	0.43
47:YR:59:ASP:N	47:YR:59:ASP:OD1	2.51	0.43
1:QA:1151:A:H2'	1:QA:1152:A:C8	2.54	0.43
37:RD:35:LYS:HB2	37:RD:63:ARG:HA	2.00	0.43
16:XP:18:ARG:NH1	16:XP:32:TYR:OH	2.52	0.43
31:Y6:6:ARG:HG3	31:Y6:7:ILE:H	1.84	0.43
35:YA:2572:A:OP1	35:YA:2574:G:O2'	2.36	0.43
35:YA:2619:C:H5"	38:YE:152:LYS:HD3	2.01	0.43
41:YH:6:ARG:HB2	41:YH:65:HIS:CG	2.54	0.43
1:QA:628:G:H2'	1:QA:629:G:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:QO:76:GLU:HA	15:QO:79:ARG:HH21	1.84	0.43
24:QY:6:U:H2'	24:QY:7:A:H8	1.83	0.43
35:RA:117:G:OP2	35:RA:119:A:O2'	2.28	0.43
24:QY:58:A:C6	55:RZ:183:LEU:HD13	2.54	0.43
1:XA:1376:U:H2'	1:XA:1377:A:C8	2.53	0.43
8:XH:12:ARG:HD3	8:XH:26:VAL:HG22	1.99	0.43
1:XA:35:G:N2	12:XL:118:SER:OG	2.37	0.43
22:XV:15:G:H21	22:XV:21:A:H1'	1.84	0.43
37:YD:245:PRO:HA	37:YD:246:PRO:HD3	1.93	0.43
37:YD:67:PHE:HB3	37:YD:153:ALA:HB3	2.00	0.43
35:YA:1656:C:P	38:YE:136:ARG:HE	2.41	0.43
39:YF:156:LEU:HD21	39:YF:163:VAL:HG12	2.01	0.43
40:YG:135:LEU:HD13	40:YG:140:ILE:HD11	2.01	0.43
35:YA:1138:G:O2'	43:YN:102:ALA:O	2.34	0.43
43:YN:47:ALA:HB2	43:YN:112:LEU:HD11	1.99	0.43
48:YS:110:LEU:HB2	48:YS:112:PHE:CE2	2.54	0.43
55:YZ:54:HIS:HB3	55:YZ:101:PRO:HD3	2.00	0.43
1:QA:1286:A:N3	21:QU:18:TYR:OH	2.52	0.43
3:QC:184:TYR:CD1	3:QC:201:TYR:CE1	3.06	0.43
12:QL:70:ILE:HG12	12:QL:77:LEU:HD12	2.01	0.43
19:QS:31:ILE:HB	19:QS:49:ILE:HD13	2.00	0.43
24:QY:6:U:H2'	24:QY:7:A:C8	2.53	0.43
33:R8:61:LEU:HD13	35:RA:593:G:H4'	2.01	0.43
35:RA:2564:A:OP1	35:RA:2648:C:O2'	2.32	0.43
24:QY:76:A:OP2	35:RA:2602:A:C6	2.72	0.43
37:RD:71:ASP:HB2	37:RD:103:ARG:HH12	1.84	0.43
33:R8:13:ARG:NH1	45:RP:61:ARG:O	2.51	0.43
46:RQ:21:THR:HB	46:RQ:22:LYS:H	1.58	0.43
51:RV:62:LEU:HD21	51:RV:95:LEU:HB2	2.00	0.43
35:YA:1638:C:OP1	35:YA:2710:C:O2'	2.30	0.43
35:YA:579:G:O2'	35:YA:2019:A:OP1	2.33	0.43
39:YF:39:TRP:NE1	39:YF:99:TYR:O	2.45	0.43
1:QA:1314:C:N4	19:QS:2:PRO:O	2.50	0.42
27:R2:9:GLN:HE22	27:R2:56:GLN:HG2	1.83	0.42
31:R6:24:GLU:OE2	35:RA:2286:A:N6	2.51	0.42
35:RA:511:U:O4	35:RA:512:G:N1	2.51	0.42
37:RD:145:VAL:HB	37:RD:155:LEU:HB2	2.00	0.42
40:RG:101:ILE:HG22	40:RG:105:LYS:HE2	2.00	0.42
42:RI:131:LYS:HA	42:RI:132:PRO:HD3	1.91	0.42
45:RP:122:PRO:HB3	45:RP:141:ALA:HB1	2.01	0.42
44:RO:104:ARG:NH2	49:RT:43:GLN:OE1	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:RZ:4:ARG:HD3	55:RZ:60:GLU:OE1	2.19	0.42
55:RZ:74:VAL:HG12	55:RZ:86:VAL:HG23	2.00	0.42
1:XA:1130:A:O5'	9:XI:20:ARG:NH2	2.52	0.42
12:XL:77:LEU:HD21	12:XL:107:ALA:HB2	2.01	0.42
26:Y1:19:GLN:HG3	35:YA:2080:G:H5'	1.99	0.42
35:YA:1508:A:O2'	35:YA:1509:C:O4'	2.32	0.42
35:YA:554:U:H2'	35:YA:556:G:C8	2.54	0.42
50:YU:91:ASP:C	50:YU:93:LYS:H	2.22	0.42
1:QA:1095:U:P	1:QA:1108:G:H1	2.42	0.42
1:QA:1129:C:N4	1:QA:1133:G:O6	2.48	0.42
1:QA:184:G:H2'	1:QA:185:A:C8	2.55	0.42
1:QA:674:G:H2'	1:QA:675:A:C8	2.53	0.42
1:QA:985:C:H2'	1:QA:986:A:H8	1.84	0.42
9:QI:92:TYR:HB3	9:QI:96:LEU:HD23	2.00	0.42
10:QJ:55:LYS:HE3	10:QJ:55:LYS:HB3	1.69	0.42
18:QR:34:TYR:HD1	18:QR:35:ARG:HG3	1.83	0.42
35:RA:224:G:OP2	35:RA:408:G:N2	2.48	0.42
35:RA:581:C:H2'	35:RA:582:G:C8	2.53	0.42
1:XA:1405:G:OP2	57:XA:1670:PAR:O34	2.29	0.42
2:XB:220:ASP:HA	2:XB:223:ILE:HG22	2.01	0.42
33:Y8:4:MET:CE	33:Y8:61:LEU:HD13	2.37	0.42
35:YA:1779:U:OP2	35:YA:1784:A:N6	2.38	0.42
35:YA:639:U:H3	35:YA:649:G:H1	1.67	0.42
37:YD:36:PRO:HA	37:YD:62:TYR:O	2.19	0.42
43:YN:116:LEU:HD23	43:YN:116:LEU:HA	1.88	0.42
47:YR:79:LEU:HA	47:YR:83:ILE:HD12	2.00	0.42
49:YT:60:THR:HG22	49:YT:77:PRO:HA	2.00	0.42
55:YZ:48:PHE:O	55:YZ:52:SER:N	2.50	0.42
1:QA:1151:A:H2'	1:QA:1152:A:H8	1.84	0.42
1:QA:738:C:OP1	6:QF:2:ARG:NH1	2.53	0.42
2:QB:95:GLN:HG3	2:QB:96:ARG:H	1.84	0.42
25:R0:69:PHE:HE2	25:R0:79:VAL:CG2	2.26	0.42
13:QM:57:ARG:NH2	29:R4:32:TYR:OH	2.47	0.42
35:RA:1651:G:OP1	47:RR:40:LYS:NZ	2.37	0.42
35:RA:2210:G:OP1	37:RD:68:LYS:NZ	2.50	0.42
35:RA:2745:C:O2	41:RH:139:GLN:NE2	2.48	0.42
37:RD:69:ARG:HH11	37:RD:105:ILE:HG12	1.84	0.42
37:RD:35:LYS:HD3	37:RD:104:TYR:CZ	2.53	0.42
47:RR:83:ILE:HG23	47:RR:86:ARG:HH21	1.85	0.42
1:XA:619:U:N3	4:XD:134:ASP:OD1	2.40	0.42
7:XG:16:LEU:HD11	9:XI:45:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:XL:124:LYS:HD2	12:XL:125:PRO:HD2	2.00	0.42
12:XL:38:THR:HG23	12:XL:39:VAL:HG23	2.00	0.42
35:YA:2293:C:OP1	48:YS:89:ARG:NH2	2.53	0.42
35:YA:2308:G:H1	35:YA:2311:A:H2	1.67	0.42
35:YA:582:G:OP1	50:YU:14:HIS:ND1	2.50	0.42
35:YA:747:U:H5''	35:YA:748:G:H5'	2.00	0.42
1:QA:1010:G:H2'	1:QA:1011:G:H8	1.85	0.42
1:QA:902:G:H2'	1:QA:903:G:H8	1.85	0.42
35:RA:1067:A:H5''	35:RA:1068:G:C8	2.54	0.42
35:RA:2788:C:O2'	35:RA:2809:A:N3	2.49	0.42
36:RB:80:U:H2'	36:RB:81:G:H21	1.84	0.42
1:XA:542:G:OP1	4:XD:10:ARG:NH2	2.46	0.42
1:XA:812:C:H4'	1:XA:813:U:H5'	2.01	0.42
30:Y5:55:ARG:HA	30:Y5:55:ARG:HD2	1.76	0.42
35:YA:1394:U:O2	53:YX:16:LYS:NZ	2.47	0.42
35:YA:742:G:H2'	35:YA:743:G:C8	2.54	0.42
38:YE:134:ILE:HA	38:YE:137:HIS:CD2	2.54	0.42
40:YG:107:LEU:HD23	40:YG:111:LEU:HD12	2.01	0.42
1:QA:272:C:H2'	1:QA:273:A:H8	1.84	0.42
1:QA:444:C:H2'	1:QA:445:G:C8	2.52	0.42
1:QA:67:C:H2'	1:QA:68:G:C8	2.55	0.42
1:QA:765:G:N2	1:QA:813:U:OP2	2.40	0.42
3:QC:70:VAL:HG12	3:QC:72:LYS:H	1.83	0.42
4:QD:31:CYS:SG	4:QD:32:ALA:N	2.92	0.42
1:QA:429:U:H5'	4:QD:9:CYS:HB2	2.01	0.42
26:R1:47:GLN:NE2	35:RA:2229:C:O2	2.53	0.42
35:RA:1262:A:OP1	52:RW:99:ARG:NH1	2.48	0.42
44:RO:76:ALA:HB3	49:RT:75:ILE:HD12	2.01	0.42
1:XA:940:C:H1'	1:XA:1374:A:H62	1.85	0.42
1:XA:395:C:N4	1:XA:396:G:O6	2.52	0.42
10:XJ:34:VAL:HG23	10:XJ:74:ILE:HG22	2.02	0.42
35:YA:639:U:H2'	35:YA:640:C:C6	2.55	0.42
39:YF:127:GLU:OE1	39:YF:196:LEU:HB2	2.20	0.42
43:YN:130:HIS:HB3	43:YN:134:ARG:NH2	2.34	0.42
35:YA:2405:G:H5'	45:YP:75:ILE:HD13	2.01	0.42
45:YP:98:GLU:HA	45:YP:101:VAL:HG22	2.02	0.42
46:YQ:111:GLU:OE2	46:YQ:133:ARG:NH2	2.52	0.42
48:YS:83:LYS:HG3	48:YS:109:GLY:HA3	2.02	0.42
53:YX:53:LYS:H	53:YX:82:GLN:HB3	1.83	0.42
1:QA:254:G:H2'	1:QA:255:G:H8	1.84	0.42
4:QD:31:CYS:SG	4:QD:33:MET:N	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:QU:10:ARG:HA	21:QU:13:ILE:HD12	2.01	0.42
35:RA:2102:U:H3	35:RA:2187:G:H1	1.68	0.42
35:RA:807:U:O2	39:RF:74:ARG:NH2	2.51	0.42
37:RD:3:VAL:HG23	37:RD:19:ALA:HA	2.00	0.42
53:RX:21:PHE:CE2	53:RX:92:LEU:HB3	2.55	0.42
1:XA:1408:A:N1	57:XA:1670:PAR:O61	2.50	0.42
3:XC:189:ALA:HB3	3:XC:196:LEU:HB2	2.01	0.42
8:XH:86:ILE:HG22	8:XH:93:VAL:HG21	2.01	0.42
35:YA:1105:U:H2'	35:YA:1106:G:C8	2.53	0.42
38:YE:144:ARG:HB3	38:YE:145:LYS:H	1.65	0.42
39:YF:24:LEU:HD23	39:YF:115:ALA:HA	2.00	0.42
44:YO:8:LEU:HB2	44:YO:19:ILE:HG13	2.01	0.42
1:QA:701:C:O2	1:QA:703:G:N1	2.53	0.42
5:QE:12:LEU:HB3	5:QE:31:LEU:HB3	2.01	0.42
12:QL:27:LEU:O	12:QL:33:ARG:NH2	2.52	0.42
17:QQ:4:LYS:HE3	17:QQ:6:LEU:HD21	2.02	0.42
35:RA:2133:G:H2'	35:RA:2157:G:N2	2.34	0.42
26:R1:50:ARG:NH2	35:RA:2199:A:OP1	2.53	0.42
35:RA:2306:C:H3'	35:RA:2307:G:H5''	2.02	0.42
35:RA:574:C:N3	38:RE:145:LYS:NZ	2.68	0.42
40:RG:122:PRO:HB3	40:RG:180:PHE:HD2	1.84	0.42
35:RA:1666:G:OP1	44:RO:66:LYS:HD3	2.19	0.42
50:RU:66:ASN:OD1	50:RU:70:ARG:NE	2.50	0.42
52:RW:88:ARG:NH1	52:RW:94:ASP:OD2	2.52	0.42
13:XM:16:ASP:HB3	13:XM:41:PRO:HB3	2.01	0.42
17:XQ:45:HIS:CD2	17:XQ:47:PRO:HG3	2.55	0.42
55:YZ:80:ARG:HH11	55:YZ:82:ARG:HH12	1.68	0.42
1:QA:464:G:N2	1:QA:467:G:N7	2.68	0.42
2:QB:93:VAL:HG11	2:QB:97:TRP:HD1	1.84	0.42
6:QF:45:LEU:HD12	6:QF:59:TYR:HD1	1.85	0.42
35:RA:1005:C:O2'	43:RN:28:THR:HG21	2.20	0.42
35:RA:307:G:N1	35:RA:310:A:OP2	2.49	0.42
35:RA:363:G:H2'	35:RA:363(A):A:C8	2.54	0.42
35:RA:1567:A:H3'	37:RD:86:PRO:HG3	2.01	0.42
39:RF:167:ALA:HB1	39:RF:173:VAL:HG11	2.02	0.42
51:RV:2:PHE:HB2	51:RV:3:ALA:H	1.72	0.42
55:RZ:89:PHE:HE2	55:RZ:96:VAL:HG11	1.85	0.42
1:XA:781:A:O2'	1:XA:1522:U:O2	2.32	0.42
1:XA:79:G:H2'	1:XA:80:G:C8	2.54	0.42
6:XF:5:GLU:HB3	6:XF:62:TRP:HE1	1.85	0.42
37:YD:25:THR:HG22	37:YD:82:ILE:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:YE:134:ILE:HA	38:YE:137:HIS:HD2	1.85	0.42
40:YG:126:ASP:OD2	40:YG:130:ASN:ND2	2.50	0.42
49:YT:3:ARG:HG3	49:YT:7:ILE:HG12	2.02	0.42
1:QA:1299:A:C8	1:QA:1301:U:H1'	2.54	0.42
13:QM:82:MET:HE3	13:QM:92:HIS:HB3	2.02	0.42
25:R0:26:TYR:HA	25:R0:69:PHE:HE1	1.85	0.42
53:RX:53:LYS:HB2	53:RX:82:GLN:HB3	2.02	0.42
13:XM:47:ASP:N	13:XM:47:ASP:OD1	2.53	0.42
20:XT:29:LYS:O	20:XT:33:ILE:HG12	2.20	0.42
31:Y6:44:ARG:HB2	31:Y6:45:LYS:H	1.67	0.42
40:YG:101:ILE:HG22	40:YG:105:LYS:HE2	2.01	0.42
40:YG:86:MET:HA	40:YG:87:PRO:HD2	1.97	0.42
1:QA:730:G:C5	1:QA:731:G:H1'	2.55	0.42
13:QM:14:ARG:H	13:QM:44:ARG:HA	1.84	0.42
18:QR:35:ARG:HH11	18:QR:35:ARG:HD2	1.70	0.42
35:RA:1902:C:H5'	37:RD:246:PRO:HD3	2.02	0.42
35:YA:2233:U:H2'	35:YA:2234:G:C8	2.55	0.42
35:YA:363:G:H2'	35:YA:363(A):A:H8	1.85	0.42
35:YA:500:G:N1	35:YA:503:A:OP2	2.50	0.42
36:YB:8:U:H3	36:YB:112:G:H1	1.68	0.42
37:YD:145:VAL:HB	37:YD:155:LEU:HB2	2.01	0.42
35:YA:1817:G:OP1	37:YD:88:ARG:NH2	2.53	0.42
45:YP:91:PHE:CE2	45:YP:95:VAL:HG22	2.55	0.42
35:YA:297:C:H5"	54:YY:87:LYS:HG3	2.02	0.42
1:QA:1004:A:P	1:QA:1025:U:H3	2.43	0.41
5:QE:33:VAL:HG13	5:QE:112:LEU:HD12	2.01	0.41
3:QC:37:GLN:NE2	14:QN:52:GLN:OE1	2.38	0.41
10:QJ:61:GLU:OE2	14:QN:58:LYS:HE2	2.20	0.41
27:R2:50:ILE:H	27:R2:50:ILE:HG12	1.70	0.41
35:RA:2618:G:H21	38:RE:150:VAL:HG21	1.85	0.41
38:RE:37:ARG:HB2	38:RE:46:ALA:H	1.85	0.41
50:RU:17:ILE:HG23	50:RU:39:LEU:HD12	2.02	0.41
1:XA:1238:A:H62	1:XA:1301:U:H3	1.68	0.41
2:XB:166:ASP:HB3	2:XB:169:LYS:HB3	2.02	0.41
12:XL:105:TYR:O	12:XL:107:ALA:N	2.53	0.41
18:XR:45:SER:OG	18:XR:47:THR:OG1	2.29	0.41
35:YA:1827:C:O2'	35:YA:1970:A:N3	2.46	0.41
35:YA:2503:A:O2'	35:YA:2505:G:OP2	2.29	0.41
37:YD:31:LYS:HD3	37:YD:94:LEU:HD11	2.02	0.41
41:YH:103:LEU:CD2	41:YH:123:PHE:HE2	2.26	0.41
2:QB:102:LEU:HB3	2:QB:180:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:QM:32:GLU:O	13:QM:36:LYS:HG2	2.20	0.41
31:R6:30:THR:HG23	31:R6:31:PRO:HD3	2.02	0.41
35:RA:1043:C:N3	35:RA:1112:G:N2	2.47	0.41
35:RA:1062:G:H2'	35:RA:1063:G:H8	1.85	0.41
35:RA:2777:G:H5''	35:RA:2778:A:H3'	2.01	0.41
35:RA:2847:U:OP1	49:RT:98:LYS:NZ	2.34	0.41
41:RH:126:PRO:HG2	41:RH:130:ARG:HE	1.85	0.41
46:RQ:56:ARG:HA	46:RQ:56:ARG:HD2	1.89	0.41
50:RU:92:ARG:HD2	51:RV:11:GLN:HB2	2.02	0.41
52:RW:45:TYR:CZ	52:RW:49:LYS:HD2	2.54	0.41
1:XA:824:C:H2'	1:XA:825:G:H8	1.82	0.41
1:XA:7:G:O2'	5:XE:120:THR:O	2.38	0.41
29:Y4:18:CYS:SG	29:Y4:19:GLY:N	2.93	0.41
33:Y8:54:GLU:O	33:Y8:58:ILE:HG12	2.19	0.41
35:YA:2468:G:O2'	35:YA:2481:G:N2	2.54	0.41
35:YA:363(A):A:H2'	35:YA:363(B):G:C8	2.53	0.41
1:QA:1355:G:H2'	1:QA:1356:G:H8	1.85	0.41
24:QY:20:G:OP2	24:QY:60:C:N4	2.54	0.41
25:R0:26:TYR:HA	25:R0:69:PHE:CE1	2.56	0.41
27:R2:4:SER:OG	27:R2:5:GLU:OE1	2.33	0.41
32:R7:49:ARG:HH12	35:RA:1600:C:H4'	1.85	0.41
44:RO:78:ARG:HH12	49:RT:75:ILE:HD11	1.85	0.41
54:RY:46:LYS:HG2	54:RY:60:PHE:CD2	2.56	0.41
55:RZ:91:LEU:HD23	55:RZ:130:PRO:HG3	2.02	0.41
55:RZ:75:ASN:HB2	55:RZ:85:HIS:HB3	2.02	0.41
1:XA:445:G:H2'	1:XA:446:G:C8	2.55	0.41
3:XC:23:TYR:HE1	10:XJ:67:THR:HG23	1.84	0.41
35:YA:1266:G:O2'	35:YA:2012:G:O6	2.32	0.41
52:YW:45:TYR:CZ	52:YW:49:LYS:HD2	2.55	0.41
53:YX:26:TYR:HD2	53:YX:92:LEU:HD22	1.85	0.41
1:QA:1172:C:H2'	1:QA:1173:G:H8	1.85	0.41
1:QA:581:G:OP1	15:QO:65:ARG:NH1	2.53	0.41
1:QA:855:G:OP2	1:QA:871:U:N3	2.44	0.41
4:QD:116:GLN:HE21	4:QD:157:LEU:HD11	1.85	0.41
4:QD:57:ARG:HB3	4:QD:206:PHE:HB2	2.02	0.41
10:QJ:79:ARG:HD3	10:QJ:79:ARG:HA	1.91	0.41
19:QS:63:THR:OG1	19:QS:64:GLU:OE1	2.38	0.41
35:RA:1254:A:H5''	35:RA:1255:U:H5''	2.02	0.41
38:RE:30:PRO:HA	38:RE:92:THR:HA	2.02	0.41
39:RF:11:VAL:HG22	39:RF:125:LEU:HB2	2.02	0.41
41:RH:85:LYS:HB3	41:RH:86:GLU:H	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:RR:57:ARG:HE	47:RR:62:ALA:HB2	1.85	0.41
54:RY:10:GLY:H	54:RY:27:VAL:HG23	1.85	0.41
1:XA:1130:A:N6	1:XA:1131:G:O6	2.53	0.41
1:XA:152:A:H62	1:XA:169:C:N4	2.16	0.41
1:XA:243:A:H4'	1:XA:244:U:H3'	2.01	0.41
1:XA:411:A:C4	1:XA:413:G:H1'	2.55	0.41
1:XA:711:G:H2'	1:XA:712:A:C8	2.55	0.41
1:XA:562:C:H1'	12:XL:15:ARG:HD2	2.02	0.41
26:Y1:97:LEU:HD13	35:YA:270(T):G:H5''	2.02	0.41
35:YA:1056:G:H4'	35:YA:1086:A:H8	1.85	0.41
35:YA:729:G:H5'	35:YA:730:C:H5''	2.01	0.41
2:QB:115:LEU:HD22	2:QB:153:ARG:HD3	2.02	0.41
9:QL:33:PHE:CD1	9:QL:37:PHE:HD2	2.37	0.41
12:QL:85:ILE:HG23	12:QL:98:TYR:HB3	2.02	0.41
13:QM:84:ILE:CG1	13:QM:86:CYS:HB2	2.50	0.41
19:QS:63:THR:OG1	19:QS:64:GLU:N	2.52	0.41
21:QU:6:ARG:HE	21:QU:15:ARG:NH1	2.18	0.41
25:R0:38:VAL:HG21	25:R0:45:PHE:CD2	2.55	0.41
35:RA:195:A:H61	35:RA:198:C:H3'	1.85	0.41
35:RA:2630:G:H2'	35:RA:2631:G:H8	1.86	0.41
35:RA:2849:U:O4	49:RT:23:ARG:NH2	2.38	0.41
35:RA:332:A:O2'	35:RA:334:C:OP2	2.32	0.41
35:RA:2579:C:O2'	38:RE:131:ALA:O	2.34	0.41
40:RG:12:TYR:HA	40:RG:16:ARG:HD3	2.03	0.41
45:RP:121:LYS:O	45:RP:123:LEU:N	2.54	0.41
53:RX:12:VAL:HG12	53:RX:29:TRP:CD2	2.56	0.41
1:XA:861:G:O2'	1:XA:874:G:O2'	2.38	0.41
33:Y8:16:ILE:HD12	33:Y8:63:PRO:HB2	2.02	0.41
35:YA:566:U:P	51:YV:80:GLN:HE21	2.43	0.41
35:YA:1657:C:H4'	38:YE:133:LYS:HB3	2.03	0.41
39:YF:185:ASP:HA	39:YF:188:ARG:HD3	2.03	0.41
1:QA:419:C:OP1	1:QA:513:C:O2'	2.34	0.41
4:QD:140:VAL:HG11	4:QD:146:ILE:HD11	2.03	0.41
4:QD:57:ARG:HH12	5:QE:107:ARG:NH1	2.19	0.41
13:QM:106:ASN:N	13:QM:106:ASN:OD1	2.52	0.41
3:QC:29:TYR:OH	14:QN:54:PRO:O	2.37	0.41
27:R2:41:ILE:HD11	27:R2:44:LEU:HD22	2.03	0.41
35:RA:629:G:N3	35:RA:639:U:O2'	2.52	0.41
41:RH:103:LEU:HD22	41:RH:123:PHE:HD2	1.85	0.41
45:RP:99:LEU:HA	45:RP:102:ARG:NE	2.35	0.41
46:RQ:24:GLY:HA2	46:RQ:67:ARG:HH22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:1345:U:OP1	9:XI:120:ARG:NH1	2.53	0.41
1:XA:437:U:H2'	1:XA:438:G:O4'	2.21	0.41
35:YA:1992:G:N2	35:YA:1996:C:O2'	2.53	0.41
37:YD:241:PRO:O	37:YD:242:ARG:HG2	2.20	0.41
54:YY:90:LEU:HB3	54:YY:91:GLU:H	1.71	0.41
1:QA:1512:U:H3	1:QA:1523:G:H1	1.69	0.41
1:QA:243:A:H4'	1:QA:244:U:H3'	2.03	0.41
1:QA:769:G:OP2	1:QA:803:G:O2'	2.36	0.41
10:QJ:13:HIS:HB3	10:QJ:68:HIS:CD2	2.55	0.41
11:QK:80:VAL:HG13	11:QK:103:LEU:HD12	2.02	0.41
35:RA:1441:G:H2'	35:RA:1442:G:H8	1.84	0.41
35:RA:1588:C:H2'	35:RA:1589:C:H6	1.85	0.41
35:RA:919:G:N2	35:RA:2269:A:OP2	2.54	0.41
35:RA:2345:G:O2'	35:RA:2381:C:O2	2.33	0.41
38:RE:21:VAL:HA	38:RE:22:PRO:HD3	1.93	0.41
40:RG:52:ILE:HG23	40:RG:55:LYS:HB3	2.03	0.41
45:RP:99:LEU:HA	45:RP:102:ARG:HE	1.85	0.41
35:RA:494:G:H4'	52:RW:6:ILE:HB	2.03	0.41
1:XA:1022:G:H2'	1:XA:1023:G:C8	2.56	0.41
9:XI:46:ALA:HA	9:XI:78:LYS:HB2	2.02	0.41
24:XY:19:G:H4'	24:XY:57:G:H22	1.85	0.41
25:Y0:68:GLU:HG3	25:Y0:80:HIS:HB2	2.01	0.41
33:Y8:62:LEU:N	33:Y8:63:PRO:CD	2.83	0.41
55:YZ:59:LEU:HD11	55:YZ:88:PHE:HD2	1.86	0.41
1:QA:1355:G:H2'	1:QA:1356:G:C8	2.56	0.41
9:QI:77:ILE:O	9:QI:81:ILE:HG12	2.20	0.41
16:QP:5:ARG:NH2	16:QP:27:LYS:O	2.53	0.41
30:R5:25:LEU:HD11	52:RW:41:LYS:HE3	2.03	0.41
31:R6:46:HIS:ND1	35:RA:2371:G:O2'	2.35	0.41
35:RA:1467:C:C5	35:RA:1546:C:H2'	2.56	0.41
35:RA:1991:U:C5'	35:RA:1991:U:H6	2.32	0.41
35:RA:259:G:H2'	35:RA:260:G:H8	1.86	0.41
35:RA:2630:G:H2'	35:RA:2631:G:C8	2.55	0.41
35:RA:593:G:H2'	35:RA:594:U:C6	2.55	0.41
35:RA:672:C:H5	45:RP:42:SER:HB2	1.86	0.41
29:R4:7:PRO:HG2	40:RG:65:GLY:HA2	2.03	0.41
51:RV:2:PHE:CD1	51:RV:13:ARG:NH2	2.89	0.41
1:XA:973:G:H3'	1:XA:974:A:H5''	2.03	0.41
26:Y1:7:ILE:HD12	26:Y1:62:VAL:HG21	2.02	0.41
35:YA:2076:U:OP2	35:YA:2238:G:N2	2.37	0.41
35:YA:2661:G:H2'	35:YA:2662:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:2702:U:H5	47:YR:73:VAL:HG21	1.86	0.41
35:YA:458:G:O2'	35:YA:469:G:O6	2.28	0.41
37:YD:232:PRO:HB3	37:YD:244:ARG:NH1	2.36	0.41
40:YG:10:LYS:NZ	40:YG:175:LEU:O	2.54	0.41
5:QE:144:THR:N	5:QE:147:ASP:OD1	2.48	0.41
10:QJ:47:PHE:CE1	10:QJ:63:PHE:HB2	2.56	0.41
3:QC:6:HIS:HB3	14:QN:49:HIS:CD2	2.55	0.41
32:R7:5:TRP:NE1	32:R7:7:PRO:HG3	2.36	0.41
33:R8:34:TRP:CD1	33:R8:35:GLN:HG2	2.56	0.41
35:RA:1817:G:OP1	37:RD:62:TYR:OH	2.27	0.41
35:RA:2055:C:H1'	38:RE:145:LYS:HE3	2.03	0.41
35:RA:2375:G:N2	35:RA:2378:A:OP2	2.49	0.41
35:RA:2656:U:H3	35:RA:2665:A:H2	1.69	0.41
35:RA:907:U:O2'	46:RQ:101:ARG:NH2	2.40	0.41
1:XA:1022:G:H2'	1:XA:1023:G:H8	1.86	0.41
1:XA:1192:C:O2	5:XE:25:ARG:NH2	2.34	0.41
1:XA:884:U:H4'	1:XA:885:G:H5''	2.02	0.41
11:XK:127:LYS:HE3	23:XX:10:G:H5'	2.03	0.41
11:XK:25:TYR:HD1	11:XK:88:GLY:HA2	1.85	0.41
13:XM:108:ARG:HD2	13:XM:114:ARG:HG3	2.03	0.41
28:Y3:26:LEU:O	28:Y3:35:ARG:NE	2.53	0.41
31:Y6:39:TYR:HB3	31:Y6:40:CYS:H	1.76	0.41
35:YA:2100:G:H1	35:YA:2189:U:H3	1.68	0.41
36:YB:111:U:H2'	36:YB:112:G:H8	1.85	0.41
38:YE:12:THR:OG1	38:YE:13:ARG:N	2.53	0.41
41:YH:126:PRO:HB3	41:YH:131:VAL:HA	2.02	0.41
44:YO:64:ARG:HB2	44:YO:83:ALA:HB3	2.03	0.41
1:QA:34:C:H2'	1:QA:35:G:H8	1.85	0.41
9:QI:24:GLY:N	9:QI:60:ASP:OD1	2.44	0.41
16:QP:20:VAL:HG23	16:QP:35:LYS:HA	2.03	0.41
17:QQ:83:ASP:OD1	17:QQ:83:ASP:N	2.53	0.41
21:QU:6:ARG:HE	21:QU:15:ARG:HH11	1.69	0.41
23:QX:15:A:HO2'	23:QX:16:A:H8	1.66	0.41
27:R2:52:ASP:O	27:R2:56:GLN:HG3	2.20	0.41
29:R4:68:ARG:HB3	29:R4:69:LYS:H	1.56	0.41
35:RA:2032:G:H21	38:RE:146:THR:HG1	1.61	0.41
35:RA:2036:C:H2'	35:RA:2037:G:H8	1.86	0.41
35:RA:971:C:O2'	35:RA:983:A:N3	2.38	0.41
35:RA:1142(A):A:H4'	43:RN:25:ARG:HH22	1.86	0.41
1:XA:1237:C:HO2'	1:XA:1300:G:H1	1.69	0.41
10:XJ:57:LYS:CD	10:XJ:60:ARG:HH21	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:1568:G:P	37:YD:63:ARG:HH22	2.42	0.41
39:YF:198:ALA:HA	39:YF:201:VAL:HG12	2.02	0.41
1:QA:67:C:O2'	1:QA:171:A:N3	2.46	0.41
1:QA:346:G:H1'	1:QA:347:G:H5'	2.03	0.41
1:QA:553:A:O2'	12:QL:29:GLY:O	2.34	0.41
26:R1:91:LYS:HB3	26:R1:92:LYS:H	1.58	0.41
33:R8:29:LYS:O	33:R8:33:ASN:ND2	2.38	0.41
35:RA:1012:U:OP1	50:RU:75:ASN:ND2	2.51	0.41
39:RF:24:LEU:HB3	39:RF:115:ALA:HB2	2.02	0.41
39:RF:157:VAL:HB	39:RF:194:MET:HG2	2.03	0.41
42:RI:14:ASP:N	42:RI:14:ASP:OD1	2.54	0.41
44:RO:85:VAL:HG11	44:RO:114:ILE:HD12	2.02	0.41
35:RA:2470:G:H5'	46:RQ:56:ARG:HH21	1.86	0.41
55:RZ:10:ARG:HE	55:RZ:36:LYS:HB3	1.85	0.41
1:XA:25:C:H2'	1:XA:26:A:C8	2.56	0.41
27:Y2:50:ILE:HD12	35:YA:61:G:H5'	2.01	0.41
29:Y4:37:SER:HB2	29:Y4:42:PHE:HB3	2.02	0.41
30:Y5:38:ALA:HB3	30:Y5:40:LYS:NZ	2.31	0.41
33:Y8:29:LYS:HE3	33:Y8:44:LYS:HB2	2.02	0.41
34:Y9:14:CYS:HA	34:Y9:27:CYS:HB2	2.02	0.41
34:Y9:2:LYS:HB2	34:Y9:34:GLN:HG2	2.02	0.41
47:YR:56:LYS:NZ	47:YR:90:ARG:O	2.54	0.41
1:QA:501:C:H2'	1:QA:502:G:H8	1.86	0.40
3:QC:159:GLY:HA2	3:QC:193:TYR:HD2	1.74	0.40
4:QD:165:MET:SD	4:QD:168:ARG:NH1	2.94	0.40
8:QH:49:GLU:HG3	8:QH:51:VAL:HG13	2.03	0.40
18:QR:74:ARG:HB3	18:QR:81:PHE:CE1	2.55	0.40
35:RA:2212:A:H1'	35:RA:2215:G:C4	2.56	0.40
35:RA:571:A:N6	35:RA:2499:C:O3'	2.54	0.40
38:RE:101:ARG:NH1	38:RE:171:GLU:HB2	2.36	0.40
39:RF:29:ASN:ND2	39:RF:32:LEU:HD23	2.33	0.40
39:RF:65:TRP:HZ3	39:RF:75:HIS:HD1	1.69	0.40
40:RG:97:ASP:HA	40:RG:100:TRP:HD1	1.86	0.40
33:R8:59:LYS:HZ1	45:RP:50:ARG:NE	2.19	0.40
50:RU:40:PHE:HB3	51:RV:75:PHE:CD2	2.55	0.40
1:XA:277:C:OP1	17:XQ:68:ARG:NH1	2.54	0.40
1:XA:662:G:H2'	1:XA:663:A:C8	2.56	0.40
33:Y8:26:LYS:HD3	33:Y8:47:LYS:HB3	2.03	0.40
35:YA:1266:G:O6	52:YW:13:SER:OG	2.30	0.40
35:YA:1662:C:O2'	35:YA:2687:U:OP1	2.34	0.40
36:YB:44:G:H1'	36:YB:47:C:N4	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:1565:C:H5''	37:YD:18:VAL:HG21	2.03	0.40
35:YA:1190:G:H5'	45:YP:32:THR:HA	2.03	0.40
47:YR:86:ARG:HH21	47:YR:118:GLU:HB2	1.85	0.40
1:QA:1256:A:OP1	3:QC:26:LYS:NZ	2.39	0.40
5:QE:110:LEU:HD13	5:QE:118:ILE:HG21	2.03	0.40
24:QY:3:G:H22	24:QY:70:U:H3	1.68	0.40
41:RH:41:MET:HG2	41:RH:55:PRO:HD2	2.03	0.40
49:RT:19:LEU:HA	49:RT:20:PRO:HD3	1.97	0.40
50:RU:90:VAL:HG12	50:RU:91:ASP:H	1.86	0.40
1:XA:1302:U:H1'	13:XM:17:VAL:HG11	2.02	0.40
19:XS:64:GLU:O	29:Y4:60:GLN:NE2	2.54	0.40
42:YI:4:ILE:HG12	42:YI:18:VAL:HG22	2.02	0.40
46:YQ:75:THR:HG21	46:YQ:85:LYS:HE3	2.03	0.40
46:YQ:81:VAL:O	46:YQ:82:ARG:NH1	2.45	0.40
47:YR:58:GLY:HA2	47:YR:80:PHE:HE2	1.86	0.40
1:QA:1342:C:H2'	1:QA:1343:G:C8	2.56	0.40
3:QC:153:VAL:HG22	3:QC:198:VAL:HG22	2.02	0.40
1:QA:1111:A:H61	3:QC:177:THR:HG22	1.85	0.40
12:QL:11:VAL:HG11	17:QQ:36:ILE:HG21	2.03	0.40
18:QR:86:VAL:HG12	18:QR:87:ARG:HG2	2.03	0.40
20:QT:37:SER:O	20:QT:41:ILE:HG12	2.22	0.40
30:R5:51:TYR:HB3	30:R5:52:TYR:H	1.48	0.40
35:RA:1193:G:OP1	45:RP:14:LYS:NZ	2.51	0.40
35:RA:1657:C:OP1	38:RE:136:ARG:N	2.54	0.40
35:RA:2577:A:H5''	35:RA:2578:G:H5'	2.03	0.40
35:RA:620:G:H4'	35:RA:621:A:H5''	2.04	0.40
49:RT:73:GLU:OE1	49:RT:103:ARG:NH2	2.52	0.40
1:XA:170:U:H2'	1:XA:171:A:H8	1.86	0.40
1:XA:979:C:O2	14:YN:19:ARG:NE	2.55	0.40
2:XB:31:TYR:HD2	2:XB:202:PRO:HB3	1.86	0.40
3:XC:71:ALA:HA	3:XC:106:VAL:HG22	2.03	0.40
8:XH:39:LEU:HB3	8:XH:45:ILE:HG12	2.03	0.40
25:Y0:46:LYS:HB2	25:Y0:78:TYR:CD1	2.56	0.40
35:YA:1045:A:O2'	35:YA:1046:A:OP2	2.34	0.40
35:YA:30:G:O2'	35:YA:1214:A:N3	2.42	0.40
35:YA:2576:G:O2'	35:YA:2579:C:OP2	2.39	0.40
35:YA:33:U:O4	35:YA:446:G:O2'	2.31	0.40
35:YA:530:G:C5	35:YA:2022:U:H5''	2.55	0.40
24:XY:19:G:C6	35:YA:881:G:H4'	2.57	0.40
43:YN:16:ILE:HG21	43:YN:26:LEU:HD11	2.02	0.40
46:YQ:21:THR:HB	46:YQ:22:LYS:H	1.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:YZ:155:LEU:HD21	55:YZ:163:LEU:HD22	2.03	0.40
1:QA:1292:U:H5'	9:QL:38:GLN:HE22	1.86	0.40
1:QA:427:U:OP2	1:QA:428:G:O2'	2.36	0.40
1:QA:877:C:O2'	8:QH:3:THR:OG1	2.33	0.40
1:QA:985:C:H2'	1:QA:986:A:C8	2.56	0.40
1:QA:392:G:H5'	16:QP:12:LYS:HG3	2.04	0.40
1:QA:1318:A:OP1	19:QS:3:ARG:NH2	2.54	0.40
24:QY:55:U:H5	24:QY:57:G:H8	1.69	0.40
30:R5:51:TYR:HB2	30:R5:56:LYS:HG2	2.03	0.40
33:R8:46:ARG:NH1	35:RA:630:G:OP1	2.55	0.40
35:RA:1024:G:H5''	35:RA:1025:G:H5''	2.03	0.40
35:RA:818:G:N1	35:RA:1188:U:OP2	2.42	0.40
35:RA:514:A:N3	35:RA:581:C:O2'	2.42	0.40
35:RA:845:G:O2'	35:RA:847:U:O4	2.40	0.40
45:RP:115:LEU:HA	45:RP:134:ALA:HB2	2.02	0.40
1:XA:1292:U:H2'	1:XA:1293:G:C8	2.57	0.40
1:XA:19:C:H5''	5:XE:86:ALA:HB3	2.02	0.40
1:XA:130:A:H5'	17:XQ:63:ARG:NH2	2.37	0.40
17:XQ:66:SER:OG	17:XQ:67:LYS:N	2.55	0.40
32:Y7:19:ARG:HD3	35:YA:125:G:H5''	2.03	0.40
35:YA:49:A:N7	35:YA:120:U:H5	2.20	0.40
35:YA:729:G:P	37:YD:13:ARG:HD3	2.61	0.40
37:YD:159:ALA:HB1	37:YD:198:ASN:HB3	2.03	0.40
42:YI:6:LEU:HD13	42:YI:36:ALA:HA	2.02	0.40
35:YA:483:A:O2'	54:YY:49:VAL:O	2.27	0.40
1:QA:627:G:H2'	1:QA:628:G:C8	2.57	0.40
3:QC:134:ILE:HG23	3:QC:151:VAL:HB	2.04	0.40
4:QD:53:ASP:HB3	4:QD:57:ARG:HH12	1.86	0.40
11:QK:43:SER:HB3	11:QK:68:ALA:HB2	2.03	0.40
23:QX:20:C:H2'	23:QX:21:A:C8	2.57	0.40
35:RA:1636:C:H2'	35:RA:1637:A:C8	2.56	0.40
35:RA:446:G:OP1	50:RU:3:ARG:NH1	2.54	0.40
38:RE:201:THR:HG22	38:RE:203:LYS:H	1.87	0.40
39:RF:150:GLY:HA2	39:RF:172:TRP:CD2	2.57	0.40
35:RA:227:A:H5''	45:RP:76:LYS:HD3	2.04	0.40
45:RP:88:LEU:HD12	45:RP:95:VAL:HG11	2.04	0.40
1:XA:170:U:H2'	1:XA:171:A:C8	2.56	0.40
3:XC:8:ILE:HD12	3:XC:16:ARG:NE	2.36	0.40
4:XD:191:ARG:NH2	4:XD:200:GLU:OE1	2.53	0.40
13:XM:16:ASP:N	13:XM:16:ASP:OD1	2.54	0.40
1:XA:626:U:H4'	16:XP:38:TYR:CE2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:468:A:H5''	16:XP:80:PHE:HB3	2.03	0.40
32:Y7:12:ARG:NH2	32:Y7:44:PRO:HB3	2.37	0.40
33:Y8:63:PRO:O	33:Y8:63:PRO:CD	2.70	0.40
39:YF:178:PRO:HB3	39:YF:198:ALA:HB2	2.04	0.40
39:YF:82:ILE:HG13	39:YF:83:PHE:HD1	1.86	0.40
41:YH:54:ARG:NH2	41:YH:57:ASP:OD1	2.55	0.40
45:YP:46:LYS:HB3	45:YP:46:LYS:HE3	1.93	0.40
44:YO:120:GLU:HB2	49:YT:68:TYR:HE2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	235/256 (92%)	206 (88%)	27 (12%)	2 (1%)	17	52
2	XB	235/256 (92%)	207 (88%)	28 (12%)	0	100	100
3	QC	203/239 (85%)	188 (93%)	15 (7%)	0	100	100
3	XC	203/239 (85%)	186 (92%)	17 (8%)	0	100	100
4	QD	206/209 (99%)	199 (97%)	6 (3%)	1 (0%)	29	64
4	XD	206/209 (99%)	199 (97%)	6 (3%)	1 (0%)	29	64
5	QE	149/162 (92%)	138 (93%)	11 (7%)	0	100	100
5	XE	149/162 (92%)	140 (94%)	8 (5%)	1 (1%)	22	57
6	QF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
6	XF	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
7	QG	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
7	XG	153/156 (98%)	145 (95%)	7 (5%)	1 (1%)	22	57
8	QH	136/138 (99%)	121 (89%)	15 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	XH	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
9	QI	125/128 (98%)	111 (89%)	14 (11%)	0	100	100
9	XI	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	19	54
10	QJ	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
10	XJ	97/105 (92%)	84 (87%)	13 (13%)	0	100	100
11	QK	117/129 (91%)	109 (93%)	8 (7%)	0	100	100
11	XK	117/129 (91%)	108 (92%)	9 (8%)	0	100	100
12	QL	123/131 (94%)	107 (87%)	15 (12%)	1 (1%)	19	54
12	XL	123/131 (94%)	108 (88%)	10 (8%)	5 (4%)	3	16
13	QM	119/126 (94%)	99 (83%)	19 (16%)	1 (1%)	19	54
13	XM	119/126 (94%)	102 (86%)	17 (14%)	0	100	100
14	QN	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	9	36
14	XN	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	9	36
15	QO	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
15	XO	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
16	QP	82/88 (93%)	77 (94%)	5 (6%)	0	100	100
16	XP	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
17	QQ	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
17	XQ	98/105 (93%)	95 (97%)	3 (3%)	0	100	100
18	QR	68/88 (77%)	67 (98%)	1 (2%)	0	100	100
18	XR	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
19	QS	82/93 (88%)	69 (84%)	13 (16%)	0	100	100
19	XS	82/93 (88%)	71 (87%)	8 (10%)	3 (4%)	3	19
20	QT	97/106 (92%)	83 (86%)	14 (14%)	0	100	100
20	XT	97/106 (92%)	86 (89%)	8 (8%)	3 (3%)	4	23
21	QU	23/27 (85%)	20 (87%)	3 (13%)	0	100	100
21	XU	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
25	R0	80/85 (94%)	75 (94%)	5 (6%)	0	100	100
25	Y0	80/85 (94%)	76 (95%)	4 (5%)	0	100	100
26	R1	95/98 (97%)	80 (84%)	12 (13%)	3 (3%)	4	22
26	Y1	95/98 (97%)	85 (90%)	8 (8%)	2 (2%)	7	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	R2	67/72 (93%)	59 (88%)	7 (10%)	1 (2%)	10	39
27	Y2	67/72 (93%)	60 (90%)	7 (10%)	0	100	100
28	R3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
29	R4	69/71 (97%)	44 (64%)	18 (26%)	7 (10%)	0	3
29	Y4	69/71 (97%)	41 (59%)	26 (38%)	2 (3%)	4	24
30	R5	57/60 (95%)	48 (84%)	9 (16%)	0	100	100
30	Y5	57/60 (95%)	48 (84%)	9 (16%)	0	100	100
31	R6	47/54 (87%)	31 (66%)	13 (28%)	3 (6%)	1	8
31	Y6	47/54 (87%)	32 (68%)	12 (26%)	3 (6%)	1	8
32	R7	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
32	Y7	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
33	R8	62/65 (95%)	50 (81%)	10 (16%)	2 (3%)	4	22
33	Y8	62/65 (95%)	51 (82%)	10 (16%)	1 (2%)	9	37
34	R9	35/37 (95%)	35 (100%)	0	0	100	100
34	Y9	35/37 (95%)	35 (100%)	0	0	100	100
37	RD	270/276 (98%)	244 (90%)	21 (8%)	5 (2%)	8	33
37	YD	270/276 (98%)	243 (90%)	26 (10%)	1 (0%)	34	69
38	RE	203/206 (98%)	165 (81%)	35 (17%)	3 (2%)	10	39
38	YE	203/206 (98%)	168 (83%)	30 (15%)	5 (2%)	5	27
39	RF	200/210 (95%)	184 (92%)	13 (6%)	3 (2%)	10	39
39	YF	200/210 (95%)	185 (92%)	13 (6%)	2 (1%)	15	49
40	RG	179/182 (98%)	158 (88%)	21 (12%)	0	100	100
40	YG	179/182 (98%)	156 (87%)	22 (12%)	1 (1%)	25	59
41	RH	168/180 (93%)	134 (80%)	30 (18%)	4 (2%)	6	27
41	YH	168/180 (93%)	140 (83%)	26 (16%)	2 (1%)	13	44
42	RI	144/148 (97%)	115 (80%)	21 (15%)	8 (6%)	2	11
42	YI	144/148 (97%)	116 (81%)	22 (15%)	6 (4%)	3	16
43	RN	136/140 (97%)	122 (90%)	13 (10%)	1 (1%)	22	57
43	YN	136/140 (97%)	117 (86%)	18 (13%)	1 (1%)	22	57
44	RO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	YO	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	19	54
45	RP	148/150 (99%)	117 (79%)	27 (18%)	4 (3%)	5	25
45	YP	148/150 (99%)	118 (80%)	28 (19%)	2 (1%)	11	40
46	RQ	139/141 (99%)	111 (80%)	27 (19%)	1 (1%)	22	57
46	YQ	139/141 (99%)	116 (84%)	19 (14%)	4 (3%)	4	24
47	RR	116/118 (98%)	109 (94%)	5 (4%)	2 (2%)	9	36
47	YR	116/118 (98%)	108 (93%)	6 (5%)	2 (2%)	9	36
48	RS	109/112 (97%)	91 (84%)	15 (14%)	3 (3%)	5	25
48	YS	109/112 (97%)	92 (84%)	16 (15%)	1 (1%)	17	52
49	RT	135/146 (92%)	121 (90%)	14 (10%)	0	100	100
49	YT	135/146 (92%)	117 (87%)	17 (13%)	1 (1%)	22	57
50	RU	115/118 (98%)	110 (96%)	4 (4%)	1 (1%)	17	52
50	YU	115/118 (98%)	107 (93%)	5 (4%)	3 (3%)	5	26
51	RV	99/101 (98%)	85 (86%)	12 (12%)	2 (2%)	7	31
51	YV	99/101 (98%)	82 (83%)	16 (16%)	1 (1%)	15	49
52	RW	111/113 (98%)	103 (93%)	8 (7%)	0	100	100
52	YW	111/113 (98%)	106 (96%)	5 (4%)	0	100	100
53	RX	90/96 (94%)	81 (90%)	9 (10%)	0	100	100
53	YX	90/96 (94%)	82 (91%)	7 (8%)	1 (1%)	14	46
54	RY	100/110 (91%)	91 (91%)	9 (9%)	0	100	100
54	YY	100/110 (91%)	94 (94%)	6 (6%)	0	100	100
55	RZ	181/206 (88%)	152 (84%)	24 (13%)	5 (3%)	5	25
55	YZ	181/206 (88%)	158 (87%)	19 (10%)	4 (2%)	6	29
All	All	11470/12126 (95%)	10176 (89%)	1168 (10%)	126 (1%)	14	46

All (126) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	QD	5	ILE
26	R1	92	LYS
29	R4	24	THR
29	R4	43	TYR
31	R6	8	LYS
33	R8	62	LEU

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Mol	Chain	Res	Type
37	RD	33	LEU
41	RH	168	PRO
42	RI	15	VAL
45	RP	108	LYS
47	RR	4	LEU
48	RS	88	ASP
48	RS	89	ARG
50	RU	92	ARG
55	RZ	53	ILE
4	XD	5	ILE
12	XL	105	TYR
12	XL	106	ASP
20	XT	74	LYS
26	Y1	92	LYS
29	Y4	24	THR
38	YE	72	VAL
41	YH	157	TYR
41	YH	168	PRO
42	YI	12	LEU
45	YP	108	LYS
47	YR	4	LEU
50	YU	91	ASP
50	YU	92	ARG
55	YZ	53	ILE
55	YZ	94	GLU
2	QB	208	ILE
14	QN	17	LYS
37	RD	243	GLY
38	RE	83	ASP
42	RI	12	LEU
42	RI	13	GLY
45	RP	15	ARG
47	RR	3	HIS
51	RV	45	THR
51	RV	100	ARG
12	XL	104	VAL
12	XL	116	SER
14	XN	17	LYS
19	XS	27	GLU
20	XT	73	HIS
20	XT	75	ASN
31	Y6	8	LYS

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Mol	Chain	Res	Type
38	YE	132	HIS
39	YF	129	PHE
39	YF	134	GLY
42	YI	15	VAL
43	YN	22	THR
47	YR	3	HIS
48	YS	110	LEU
53	YX	68	ARG
2	QB	238	LEU
13	QM	12	ASN
27	R2	70	GLN
29	R4	23	GLU
31	R6	45	LYS
33	R8	63	PRO
37	RD	32	SER
39	RF	129	PHE
41	RH	40	GLU
42	RI	86	THR
45	RP	6	LEU
19	XS	3	ARG
26	Y1	91	LYS
33	Y8	30	ARG
38	YE	83	ASP
38	YE	129	HIS
42	YI	14	ASP
45	YP	65	ARG
46	YQ	22	LYS
46	YQ	25	ASP
26	R1	91	LYS
29	R4	41	PRO
39	RF	67	GLN
39	RF	130	ALA
41	RH	155	SER
42	RI	134	PRO
48	RS	87	PHE
55	RZ	52	SER
55	RZ	61	LEU
12	XL	115	LYS
31	Y6	7	ILE
40	YG	81	LYS
46	YQ	78	PRO
49	YT	108	ARG

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Mol	Chain	Res	Type
50	YU	90	VAL
29	R4	40	HIS
29	R4	42	PHE
29	R4	44	THR
43	RN	96	GLU
46	RQ	22	LYS
7	XG	8	GLU
19	XS	10	PHE
31	Y6	45	LYS
42	YI	10	GLU
42	YI	16	GLY
51	YV	50	PRO
12	QL	27	LEU
26	R1	54	ALA
38	RE	92	THR
38	RE	93	VAL
45	RP	7	ARG
5	XE	74	GLY
38	YE	131	ALA
44	YO	49	ARG
46	YQ	105	GLU
55	YZ	52	SER
37	RD	123	ALA
55	RZ	180	VAL
37	YD	123	ALA
41	RH	169	VAL
42	RI	16	GLY
42	RI	132	PRO
42	YI	13	GLY
31	R6	7	ILE
42	RI	118	LYS
9	XI	90	PRO
29	Y4	40	HIS
37	RD	36	PRO
55	RZ	111	VAL
55	YZ	61	LEU

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%)	203 (99%)	2 (1%)	76	90
2	XB	205/220 (93%)	204 (100%)	1 (0%)	88	94
3	QC	159/188 (85%)	157 (99%)	2 (1%)	69	87
3	XC	159/188 (85%)	159 (100%)	0	100	100
4	QD	173/181 (96%)	171 (99%)	2 (1%)	71	88
4	XD	173/181 (96%)	172 (99%)	1 (1%)	86	94
5	QE	116/123 (94%)	115 (99%)	1 (1%)	78	91
5	XE	116/123 (94%)	115 (99%)	1 (1%)	78	91
6	QF	90/90 (100%)	90 (100%)	0	100	100
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%)	126 (100%)	0	100	100
8	QH	119/119 (100%)	119 (100%)	0	100	100
8	XH	119/119 (100%)	118 (99%)	1 (1%)	81	92
9	QI	98/99 (99%)	95 (97%)	3 (3%)	40	70
9	XI	98/99 (99%)	97 (99%)	1 (1%)	76	90
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	89/92 (97%)	88 (99%)	1 (1%)	73	89
11	QK	90/99 (91%)	89 (99%)	1 (1%)	73	89
11	XK	90/99 (91%)	89 (99%)	1 (1%)	73	89
12	QL	104/108 (96%)	103 (99%)	1 (1%)	76	90
12	XL	104/108 (96%)	104 (100%)	0	100	100
13	QM	97/101 (96%)	96 (99%)	1 (1%)	76	90
13	XM	97/101 (96%)	97 (100%)	0	100	100
14	QN	49/50 (98%)	49 (100%)	0	100	100
14	XN	49/50 (98%)	49 (100%)	0	100	100
15	QO	79/80 (99%)	77 (98%)	2 (2%)	47	75
15	XO	79/80 (99%)	79 (100%)	0	100	100
16	QP	72/74 (97%)	72 (100%)	0	100	100
16	XP	72/74 (97%)	71 (99%)	1 (1%)	67	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	QQ	95/97 (98%)	94 (99%)	1 (1%)	73	89
17	XQ	95/97 (98%)	95 (100%)	0	100	100
18	QR	61/77 (79%)	59 (97%)	2 (3%)	38	69
18	XR	61/77 (79%)	61 (100%)	0	100	100
19	QS	73/80 (91%)	70 (96%)	3 (4%)	30	64
19	XS	73/80 (91%)	71 (97%)	2 (3%)	44	74
20	QT	76/82 (93%)	76 (100%)	0	100	100
20	XT	76/82 (93%)	76 (100%)	0	100	100
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	19 (95%)	1 (5%)	24	57
25	R0	65/67 (97%)	64 (98%)	1 (2%)	65	85
25	Y0	65/67 (97%)	62 (95%)	3 (5%)	27	59
26	R1	82/83 (99%)	82 (100%)	0	100	100
26	Y1	82/83 (99%)	82 (100%)	0	100	100
27	R2	64/67 (96%)	64 (100%)	0	100	100
27	Y2	64/67 (96%)	62 (97%)	2 (3%)	40	70
28	R3	51/52 (98%)	51 (100%)	0	100	100
28	Y3	51/52 (98%)	51 (100%)	0	100	100
29	R4	63/63 (100%)	59 (94%)	4 (6%)	18	48
29	Y4	63/63 (100%)	62 (98%)	1 (2%)	62	84
30	R5	51/52 (98%)	51 (100%)	0	100	100
30	Y5	51/52 (98%)	50 (98%)	1 (2%)	55	80
31	R6	48/52 (92%)	47 (98%)	1 (2%)	53	79
31	Y6	48/52 (92%)	48 (100%)	0	100	100
32	R7	42/42 (100%)	42 (100%)	0	100	100
32	Y7	42/42 (100%)	41 (98%)	1 (2%)	49	76
33	R8	54/55 (98%)	53 (98%)	1 (2%)	57	81
33	Y8	54/55 (98%)	52 (96%)	2 (4%)	34	66
34	R9	34/34 (100%)	34 (100%)	0	100	100
34	Y9	34/34 (100%)	34 (100%)	0	100	100
37	RD	214/218 (98%)	212 (99%)	2 (1%)	78	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	YD	214/218 (98%)	211 (99%)	3 (1%)	67	86
38	RE	165/166 (99%)	163 (99%)	2 (1%)	71	88
38	YE	165/166 (99%)	163 (99%)	2 (1%)	71	88
39	RF	161/166 (97%)	160 (99%)	1 (1%)	86	94
39	YF	161/166 (97%)	160 (99%)	1 (1%)	86	94
40	RG	155/156 (99%)	154 (99%)	1 (1%)	86	94
40	YG	155/156 (99%)	154 (99%)	1 (1%)	86	94
41	RH	142/148 (96%)	141 (99%)	1 (1%)	84	93
41	YH	142/148 (96%)	141 (99%)	1 (1%)	84	93
42	RI	122/124 (98%)	121 (99%)	1 (1%)	81	92
42	YI	122/124 (98%)	122 (100%)	0	100	100
43	RN	117/119 (98%)	116 (99%)	1 (1%)	78	91
43	YN	117/119 (98%)	117 (100%)	0	100	100
44	RO	100/100 (100%)	98 (98%)	2 (2%)	55	80
44	YO	100/100 (100%)	98 (98%)	2 (2%)	55	80
45	RP	116/116 (100%)	113 (97%)	3 (3%)	46	74
45	YP	116/116 (100%)	115 (99%)	1 (1%)	78	91
46	RQ	111/111 (100%)	109 (98%)	2 (2%)	59	82
46	YQ	111/111 (100%)	108 (97%)	3 (3%)	44	74
47	RR	101/101 (100%)	101 (100%)	0	100	100
47	YR	101/101 (100%)	100 (99%)	1 (1%)	76	90
48	RS	87/88 (99%)	85 (98%)	2 (2%)	50	77
48	YS	87/88 (99%)	84 (97%)	3 (3%)	37	69
49	RT	120/127 (94%)	118 (98%)	2 (2%)	60	83
49	YT	120/127 (94%)	117 (98%)	3 (2%)	47	75
50	RU	93/94 (99%)	92 (99%)	1 (1%)	73	89
50	YU	93/94 (99%)	92 (99%)	1 (1%)	73	89
51	RV	82/82 (100%)	81 (99%)	1 (1%)	71	88
51	YV	82/82 (100%)	80 (98%)	2 (2%)	49	76
52	RW	92/92 (100%)	91 (99%)	1 (1%)	73	89
52	YW	92/92 (100%)	92 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	RX	74/78 (95%)	74 (100%)	0	100	100
53	YX	74/78 (95%)	73 (99%)	1 (1%)	67	86
54	RY	85/91 (93%)	84 (99%)	1 (1%)	71	88
54	YY	85/91 (93%)	85 (100%)	0	100	100
55	RZ	162/179 (90%)	161 (99%)	1 (1%)	86	94
55	YZ	162/179 (90%)	160 (99%)	2 (1%)	71	88
All	All	9688/10064 (96%)	9587 (99%)	101 (1%)	76	90

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	QB	94	ASN
2	QB	226	ARG
3	QC	11	ARG
3	QC	23	TYR
4	QD	59	ARG
4	QD	209	ARG
5	QE	40	ARG
9	QI	33	PHE
9	QI	104	ARG
9	QI	121	ARG
11	QK	12	ARG
12	QL	105	TYR
13	QM	83	ASP
15	QO	18	PHE
15	QO	79	ARG
17	QQ	68	ARG
18	QR	29	PHE
18	QR	34	TYR
19	QS	9	VAL
19	QS	11	VAL
19	QS	44	MET
25	R0	14	ARG
29	R4	16	CYS
29	R4	43	TYR
29	R4	55	ARG
29	R4	67	TYR
31	R6	6	ARG
33	R8	48	PHE
37	RD	6	PHE

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Mol	Chain	Res	Type
37	RD	43	ARG
38	RE	51	PHE
38	RE	84	PHE
39	RF	44	ARG
40	RG	115	ARG
41	RH	152	ARG
42	RI	33	ARG
43	RN	106	MET
44	RO	32	TYR
44	RO	49	ARG
45	RP	7	ARG
45	RP	61	ARG
45	RP	102	ARG
46	RQ	60	ARG
46	RQ	82	ARG
48	RS	17	ARG
48	RS	29	PHE
49	RT	85	LYS
49	RT	115	ARG
50	RU	92	ARG
51	RV	81	TYR
52	RW	92	ARG
54	RY	101	LYS
55	RZ	34	ASN
2	XB	94	ASN
4	XD	47	ARG
5	XE	10	MET
8	XH	104	ARG
9	XI	18	PHE
10	XJ	28	ARG
11	XK	54	ARG
16	XP	38	TYR
19	XS	10	PHE
19	XS	78	ARG
21	XU	24	ARG
25	Y0	14	ARG
25	Y0	45	PHE
25	Y0	74	ARG
27	Y2	59	ARG
27	Y2	65	ASN
29	Y4	68	ARG
30	Y5	37	LYS

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Mol	Chain	Res	Type
32	Y7	49	ARG
33	Y8	62	LEU
33	Y8	65	GLU
37	YD	15	PHE
37	YD	43	ARG
37	YD	62	TYR
38	YE	51	PHE
38	YE	84	PHE
39	YF	38	ARG
40	YG	118	ARG
41	YH	101	ARG
44	YO	64	ARG
44	YO	104	ARG
45	YP	61	ARG
46	YQ	5	ARG
46	YQ	60	ARG
46	YQ	82	ARG
47	YR	94	TYR
48	YS	20	ARG
48	YS	29	PHE
48	YS	106	ARG
49	YT	38	ASN
49	YT	65	LYS
49	YT	100	TYR
50	YU	52	ARG
51	YV	81	TYR
51	YV	91	TYR
53	YX	26	TYR
55	YZ	93	ASP
55	YZ	154	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
2	QB	40	HIS
4	QD	77	ASN
6	QF	84	ASN
7	QG	84	ASN
7	QG	109	ASN
9	QI	58	HIS
10	QJ	33	GLN
13	QM	77	ASN

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Mol	Chain	Res	Type
19	QS	69	HIS
27	R2	9	GLN
29	R4	6	HIS
33	R8	35	GLN
37	RD	116	GLN
39	RF	40	GLN
41	RH	147	ASN
44	RO	5	GLN
46	RQ	12	GLN
47	RR	24	GLN
48	RS	38	GLN
49	RT	58	ASN
50	RU	44	ASN
52	RW	60	ASN
55	RZ	121	HIS
2	XB	16	HIS
2	XB	94	ASN
2	XB	212	GLN
4	XD	161	ASN
7	XG	109	ASN
8	XH	78	GLN
9	XI	31	GLN
9	XI	73	GLN
9	XI	124	GLN
10	XJ	84	GLN
13	XM	101	GLN
15	XO	62	GLN
19	XS	23	ASN
38	YE	143	ASN
39	YF	40	GLN
47	YR	71	GLN
49	YT	38	ASN
52	YW	60	ASN
55	YZ	34	ASN
55	YZ	55	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1522 (98%)	270 (18%)	29 (1%)
1	XA	1498/1522 (98%)	279 (18%)	27 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	QV	76/77 (98%)	15 (19%)	0
22	XV	76/77 (98%)	14 (18%)	0
23	QX	17/19 (89%)	8 (47%)	1 (5%)
23	XX	17/19 (89%)	7 (41%)	1 (5%)
24	QY	74/76 (97%)	28 (37%)	0
24	XY	74/76 (97%)	25 (33%)	0
35	RA	2879/2915 (98%)	587 (20%)	47 (1%)
35	YA	2880/2915 (98%)	587 (20%)	44 (1%)
36	RB	119/122 (97%)	21 (17%)	1 (0%)
36	YB	119/122 (97%)	18 (15%)	0
All	All	9327/9462 (98%)	1859 (19%)	150 (1%)

All (1859) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	31	G
1	QA	32	A
1	QA	39	G
1	QA	48	C
1	QA	50	A
1	QA	51	A
1	QA	54	C
1	QA	64	G
1	QA	65	U
1	QA	66	G
1	QA	78	G
1	QA	79	G
1	QA	90	C
1	QA	91	C
1	QA	95	G
1	QA	101	A
1	QA	108	G
1	QA	116	A
1	QA	121	C
1	QA	129(A)	G
1	QA	144	G
1	QA	146	G
1	QA	163	C
1	QA	169	C
1	QA	173	U
1	QA	174	C

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Mol	Chain	Res	Type
1	QA	182	U
1	QA	187	C
1	QA	191(A)	G
1	QA	195	A
1	QA	197	A
1	QA	209	U
1	QA	210	U
1	QA	216	G
1	QA	244	U
1	QA	245	C
1	QA	247	G
1	QA	251	G
1	QA	267	C
1	QA	270	A
1	QA	281	G
1	QA	289	G
1	QA	306	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	348	G
1	QA	352	C
1	QA	353	A
1	QA	354	G
1	QA	356	A
1	QA	367	U
1	QA	372	C
1	QA	384	G
1	QA	388	G
1	QA	389	A
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

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Mol	Chain	Res	Type
1	QA	422	C
1	QA	423	G
1	QA	429	U
1	QA	440	A
1	QA	452	A
1	QA	466	C
1	QA	467	G
1	QA	484	G
1	QA	485	G
1	QA	486	U
1	QA	496	A
1	QA	497	U
1	QA	505	G
1	QA	508	C
1	QA	509	A
1	QA	510	A
1	QA	511	C
1	QA	518	C
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	572	A
1	QA	573	A
1	QA	576	G
1	QA	577	G
1	QA	579	G
1	QA	607	A
1	QA	618	C
1	QA	620	C
1	QA	630	G
1	QA	631	G
1	QA	652	U
1	QA	653	A
1	QA	665	A
1	QA	671	G
1	QA	688	G
1	QA	693	G

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Mol	Chain	Res	Type
1	QA	701	C
1	QA	702	A
1	QA	703	G
1	QA	704	A
1	QA	723	U
1	QA	724	G
1	QA	731	G
1	QA	748	C
1	QA	753	A
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	815	A
1	QA	817	C
1	QA	819	A
1	QA	820	U
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	872	A
1	QA	889	A
1	QA	902	G
1	QA	914	A
1	QA	927	G
1	QA	934	C
1	QA	935	A
1	QA	948	C
1	QA	960	U
1	QA	966	G
1	QA	968	A
1	QA	969	A
1	QA	971	G
1	QA	972	C
1	QA	974	A

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Mol	Chain	Res	Type
1	QA	976	G
1	QA	977	A
1	QA	981	U
1	QA	982	U
1	QA	991	U
1	QA	992	U
1	QA	993	G
1	QA	994	A
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	1028	C
1	QA	1029	G
1	QA	1030	C
1	QA	1032(A)	G
1	QA	1040	U
1	QA	1054	C
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	1132	C
1	QA	1136	U
1	QA	1137	C
1	QA	1138	G
1	QA	1139	G
1	QA	1146	A
1	QA	1157	A
1	QA	1158	C
1	QA	1159	U
1	QA	1163	C
1	QA	1171	G

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Mol	Chain	Res	Type
1	QA	1178	G
1	QA	1181	G
1	QA	1183	A
1	QA	1187	G
1	QA	1190	G
1	QA	1196	U
1	QA	1197	G
1	QA	1201	A
1	QA	1202	G
1	QA	1211	U
1	QA	1212	U
1	QA	1213	A
1	QA	1225	A
1	QA	1227	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	1282	C
1	QA	1285	A
1	QA	1286	A
1	QA	1287	A
1	QA	1290	G
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	1305	G
1	QA	1321	C
1	QA	1322	C
1	QA	1323	G
1	QA	1326	C
1	QA	1331	G
1	QA	1335	C

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Mol	Chain	Res	Type
1	QA	1336	C
1	QA	1337	G
1	QA	1345	U
1	QA	1346	A
1	QA	1347	G
1	QA	1348	U
1	QA	1353	G
1	QA	1358	U
1	QA	1362(A)	C
1	QA	1370	G
1	QA	1379	G
1	QA	1400	C
1	QA	1419	G
1	QA	1442	G
1	QA	1443	G
1	QA	1446	A
1	QA	1447	G
1	QA	1452	C
1	QA	1453	G
1	QA	1469	G
1	QA	1492	A
1	QA	1497	G
1	QA	1499	A
1	QA	1502	A
1	QA	1503	A
1	QA	1504	G
1	QA	1506	U
1	QA	1517	G
1	QA	1519	A
1	QA	1520	G
1	QA	1525	G
1	QA	1529	G
1	QA	1530	G
22	QV	7	G
22	QV	8	U
22	QV	9	G
22	QV	16	C
22	QV	17	C
22	QV	17(A)	U
22	QV	18	G
22	QV	19	G
22	QV	20	U

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Mol	Chain	Res	Type
22	QV	21	A
22	QV	47	U
22	QV	48	C
22	QV	49	G
22	QV	65	C
22	QV	76	A
23	QX	7	G
23	QX	10	G
23	QX	11	U
23	QX	12	A
23	QX	13	A
23	QX	14	A
23	QX	19	G
23	QX	23	A
24	QY	8	U
24	QY	12	U
24	QY	13	C
24	QY	15	G
24	QY	16	C
24	QY	17	U
24	QY	18	G
24	QY	19	G
24	QY	20	G
24	QY	21	A
24	QY	23	A
24	QY	30	G
24	QY	34	G
24	QY	43	G
24	QY	46	G
24	QY	47	U
24	QY	48	C
24	QY	50	G
24	QY	55	U
24	QY	57	G
24	QY	58	A
24	QY	59	U
24	QY	61	C
24	QY	68	G
24	QY	71	C
24	QY	74	C
24	QY	75	C
24	QY	76	A

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Mol	Chain	Res	Type
35	RA	14	A
35	RA	15	G
35	RA	34	C
35	RA	35	G
35	RA	46	C
35	RA	51	G
35	RA	55	G
35	RA	61	G
35	RA	64	A
35	RA	71	A
35	RA	74	A
35	RA	75	G
35	RA	83	G
35	RA	90	U
35	RA	101	G
35	RA	102	G
35	RA	103	A
35	RA	118	A
35	RA	119	A
35	RA	120	U
35	RA	131	G
35	RA	138	G
35	RA	161	U
35	RA	177	G
35	RA	181	A
35	RA	196	A
35	RA	199	A
35	RA	201	C
35	RA	215	G
35	RA	216	A
35	RA	221	A
35	RA	222	A
35	RA	223	A
35	RA	228	A
35	RA	229	A
35	RA	230	U
35	RA	232	G
35	RA	233	A
35	RA	243	U
35	RA	248	G
35	RA	249	C
35	RA	252	G

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Mol	Chain	Res	Type
35	RA	265	A
35	RA	266	G
35	RA	269	U
35	RA	270(L)	U
35	RA	270(M)	U
35	RA	270(P)	C
35	RA	271(C)	U
35	RA	271	G
35	RA	273(F)	C
35	RA	275	G
35	RA	276	A
35	RA	277	C
35	RA	285	C
35	RA	299	A
35	RA	309	G
35	RA	311	A
35	RA	323	G
35	RA	324	A
35	RA	327	G
35	RA	329	G
35	RA	330	A
35	RA	346	A
35	RA	352	G
35	RA	364	C
35	RA	371	A
35	RA	372	G
35	RA	373	U
35	RA	386	G
35	RA	395	U
35	RA	405	U
35	RA	411	G
35	RA	412	A
35	RA	428	A
35	RA	444	C
35	RA	448	U
35	RA	451	C
35	RA	454	A
35	RA	455	C
35	RA	457	A
35	RA	470	A
35	RA	481	G
35	RA	504	U

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Mol	Chain	Res	Type
35	RA	505	A
35	RA	508	G
35	RA	509	C
35	RA	513	A
35	RA	529	A
35	RA	531	C
35	RA	532	A
35	RA	533	G
35	RA	537	C
35	RA	539	G
35	RA	540	G
35	RA	546	C
35	RA	547	A
35	RA	554	U
35	RA	556	G
35	RA	563	G
35	RA	573	G
35	RA	574	C
35	RA	575	A
35	RA	583	G
35	RA	588	U
35	RA	603	A
35	RA	607	U
35	RA	614	U
35	RA	615	G
35	RA	616	A
35	RA	617	G
35	RA	621	A
35	RA	622	G
35	RA	627	A
35	RA	634	C
35	RA	637	A
35	RA	638	G
35	RA	645	C
35	RA	646	A
35	RA	651	G
35	RA	654	A
35	RA	654(A)	G
35	RA	654(T)	C
35	RA	669	G
35	RA	670	A
35	RA	686	G

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Mol	Chain	Res	Type
35	RA	702	G
35	RA	717	G
35	RA	722	A
35	RA	730	C
35	RA	747	U
35	RA	753	C
35	RA	765	G
35	RA	771	G
35	RA	776	G
35	RA	782	A
35	RA	783	A
35	RA	784	A
35	RA	785	G
35	RA	788	A
35	RA	790	C
35	RA	793	A
35	RA	800	A
35	RA	805	G
35	RA	812	C
35	RA	819	A
35	RA	827	U
35	RA	828	U
35	RA	847	U
35	RA	856	C
35	RA	857	C
35	RA	859	G
35	RA	869	G
35	RA	880	G
35	RA	881	G
35	RA	884	C
35	RA	885	C
35	RA	886	C
35	RA	888	C
35	RA	889	C
35	RA	893	C
35	RA	896	A
35	RA	897	C
35	RA	898	C
35	RA	900	A
35	RA	901	A
35	RA	904	C
35	RA	907	U

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Mol	Chain	Res	Type
35	RA	910	A
35	RA	917	A
35	RA	932	G
35	RA	938	G
35	RA	941	A
35	RA	945	A
35	RA	946	G
35	RA	953	A
35	RA	959	A
35	RA	961	C
35	RA	973	A
35	RA	974	G
35	RA	974(A)	C
35	RA	980	A
35	RA	983	A
35	RA	989	G
35	RA	996	A
35	RA	1003	G
35	RA	1005	C
35	RA	1012	U
35	RA	1013	C
35	RA	1015	G
35	RA	1022	G
35	RA	1023	U
35	RA	1024	G
35	RA	1025	G
35	RA	1026	U
35	RA	1027	A
35	RA	1033	U
35	RA	1044	G
35	RA	1045	A
35	RA	1046	A
35	RA	1049	C
35	RA	1050	A
35	RA	1053	C
35	RA	1055	G
35	RA	1057	A
35	RA	1059	G
35	RA	1060	U
35	RA	1061	U
35	RA	1062	G
35	RA	1065	U

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Mol	Chain	Res	Type
35	RA	1066	U
35	RA	1067	A
35	RA	1068	G
35	RA	1071	G
35	RA	1073	A
35	RA	1076	C
35	RA	1077	A
35	RA	1078	U
35	RA	1079	C
35	RA	1080	C
35	RA	1082	U
35	RA	1083	U
35	RA	1084	A
35	RA	1085	A
35	RA	1086	A
35	RA	1087	G
35	RA	1088	A
35	RA	1090	U
35	RA	1091	G
35	RA	1093	G
35	RA	1095	A
35	RA	1096	A
35	RA	1104	C
35	RA	1105	U
35	RA	1110	G
35	RA	1111	A
35	RA	1112	G
35	RA	1113	U
35	RA	1122	G
35	RA	1131	G
35	RA	1135	C
35	RA	1136	G
35	RA	1139	G
35	RA	1140	C
35	RA	1142(A)	A
35	RA	1168	G
35	RA	1170	G
35	RA	1173	G
35	RA	1174	A
35	RA	1175	U
35	RA	1176	G
35	RA	1179	C

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Mol	Chain	Res	Type
35	RA	1195	G
35	RA	1204	A
35	RA	1205	U
35	RA	1206	G
35	RA	1210	A
35	RA	1211	U
35	RA	1220	A
35	RA	1236	G
35	RA	1238	G
35	RA	1240	U
35	RA	1244	G
35	RA	1252	G
35	RA	1253	A
35	RA	1256	G
35	RA	1271	G
35	RA	1272	A
35	RA	1273	U
35	RA	1284	A
35	RA	1300	U
35	RA	1301	A
35	RA	1312	U
35	RA	1313	U
35	RA	1314	C
35	RA	1319	G
35	RA	1329	U
35	RA	1341	U
35	RA	1349	A
35	RA	1352	U
35	RA	1365	A
35	RA	1368	G
35	RA	1370	C
35	RA	1378	A
35	RA	1379	A
35	RA	1380	G
35	RA	1384	A
35	RA	1385	G
35	RA	1395	A
35	RA	1403	C
35	RA	1404	C
35	RA	1407	C
35	RA	1411	C
35	RA	1416	G

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Mol	Chain	Res	Type
35	RA	1419	A
35	RA	1420	U
35	RA	1421	G
35	RA	1428	C
35	RA	1444(A)	A
35	RA	1445	C
35	RA	1449	A
35	RA	1449(A)	G
35	RA	1455	G
35	RA	1458	C
35	RA	1460	A
35	RA	1461	G
35	RA	1467	C
35	RA	1471	A
35	RA	1482	U
35	RA	1483	G
35	RA	1485	G
35	RA	1490	A
35	RA	1493	C
35	RA	1495	A
35	RA	1497	U
35	RA	1507	A
35	RA	1508	A
35	RA	1510	A
35	RA	1511	A
35	RA	1513	C
35	RA	1514	U
35	RA	1525	G
35	RA	1533	C
35	RA	1535	U
35	RA	1536	A
35	RA	1537	C
35	RA	1538	G
35	RA	1543	A
35	RA	1544	C
35	RA	1545	A
35	RA	1554	A
35	RA	1558	A
35	RA	1559	G
35	RA	1566	A
35	RA	1569	A
35	RA	1578	U

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Mol	Chain	Res	Type
35	RA	1586	A
35	RA	1598	C
35	RA	1608	A
35	RA	1609	A
35	RA	1616	A
35	RA	1617	C
35	RA	1618	A
35	RA	1630(A)	C
35	RA	1640	C
35	RA	1648	C
35	RA	1654	A
35	RA	1667	G
35	RA	1668	A
35	RA	1674	G
35	RA	1675	C
35	RA	1688	U
35	RA	1695	G
35	RA	1703	G
35	RA	1725	G
35	RA	1728	G
35	RA	1729	A
35	RA	1730	U
35	RA	1731	G
35	RA	1734	C
35	RA	1742	C
35	RA	1743	G
35	RA	1756	G
35	RA	1763	G
35	RA	1764	G
35	RA	1773	A
35	RA	1780	A
35	RA	1782	C
35	RA	1787	A
35	RA	1791	A
35	RA	1799	G
35	RA	1800	C
35	RA	1811	G
35	RA	1816	G
35	RA	1820	U
35	RA	1828	G
35	RA	1829	A
35	RA	1835	G

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Mol	Chain	Res	Type
35	RA	1847	A
35	RA	1848	A
35	RA	1858	G
35	RA	1860	G
35	RA	1869	G
35	RA	1872	A
35	RA	1878	G
35	RA	1882	C
35	RA	1885	A
35	RA	1888	G
35	RA	1889	A
35	RA	1900	A
35	RA	1906	G
35	RA	1913	A
35	RA	1929	G
35	RA	1931	U
35	RA	1936	A
35	RA	1938	A
35	RA	1939	U
35	RA	1955	U
35	RA	1963	U
35	RA	1964	G
35	RA	1967	C
35	RA	1969	A
35	RA	1970	A
35	RA	1971	A
35	RA	1972	A
35	RA	1982	C
35	RA	1991	U
35	RA	1992	G
35	RA	1993	U
35	RA	2020	A
35	RA	2023	G
35	RA	2031	A
35	RA	2032	G
35	RA	2033	A
35	RA	2039	C
35	RA	2043	C
35	RA	2052	G
35	RA	2055	C
35	RA	2056	G
35	RA	2059	A

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Mol	Chain	Res	Type
35	RA	2060	A
35	RA	2061	G
35	RA	2062	A
35	RA	2069	G
35	RA	2107	C
35	RA	2111	C
35	RA	2113	U
35	RA	2114	A
35	RA	2115	G
35	RA	2116	G
35	RA	2117	A
35	RA	2119	A
35	RA	2126	A
35	RA	2127	G
35	RA	2128	C
35	RA	2131	G
35	RA	2132	U
35	RA	2133	G
35	RA	2135	A
35	RA	2136	C
35	RA	2145	C
35	RA	2146	C
35	RA	2147	G
35	RA	2148	G
35	RA	2158	A
35	RA	2166	G
35	RA	2168	G
35	RA	2169	A
35	RA	2171	A
35	RA	2173	A
35	RA	2176	A
35	RA	2190	G
35	RA	2198	A
35	RA	2199	A
35	RA	2210	G
35	RA	2211	G
35	RA	2212	A
35	RA	2213	U
35	RA	2215	G
35	RA	2225	A
35	RA	2238	G
35	RA	2239	G

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Mol	Chain	Res	Type
35	RA	2243	U
35	RA	2249	U
35	RA	2266	A
35	RA	2275	C
35	RA	2283	C
35	RA	2284	C
35	RA	2287	A
35	RA	2288	A
35	RA	2307	G
35	RA	2308	G
35	RA	2311	A
35	RA	2319	G
35	RA	2320	A
35	RA	2321	G
35	RA	2325	G
35	RA	2334	G
35	RA	2335	A
35	RA	2345	G
35	RA	2346	A
35	RA	2347	C
35	RA	2350	C
35	RA	2354	G
35	RA	2358	G
35	RA	2372	G
35	RA	2383	G
35	RA	2385	C
35	RA	2392	A
35	RA	2402	C
35	RA	2406	U
35	RA	2410	G
35	RA	2420	C
35	RA	2421	G
35	RA	2423	U
35	RA	2424	C
35	RA	2425	A
35	RA	2429	G
35	RA	2430	A
35	RA	2435	A
35	RA	2439	A
35	RA	2440	C
35	RA	2441	C
35	RA	2445	G

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Mol	Chain	Res	Type
35	RA	2448	A
35	RA	2469	A
35	RA	2470	G
35	RA	2475	C
35	RA	2482	G
35	RA	2484	G
35	RA	2494	G
35	RA	2498	C
35	RA	2502	G
35	RA	2505	G
35	RA	2518	A
35	RA	2519	U
35	RA	2529	G
35	RA	2542	A
35	RA	2543	G
35	RA	2554	U
35	RA	2562	U
35	RA	2564	A
35	RA	2567	G
35	RA	2569	G
35	RA	2573	C
35	RA	2576	G
35	RA	2578	G
35	RA	2582	G
35	RA	2586	C
35	RA	2602	A
35	RA	2609	U
35	RA	2611	U
35	RA	2612	C
35	RA	2615	U
35	RA	2621	A
35	RA	2623	G
35	RA	2629	A
35	RA	2642	G
35	RA	2646	C
35	RA	2654	A
35	RA	2655	G
35	RA	2665	A
35	RA	2673	G
35	RA	2689	U
35	RA	2690	C
35	RA	2700	C

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Mol	Chain	Res	Type
35	RA	2702	U
35	RA	2707	G
35	RA	2712	U
35	RA	2712(A)	A
35	RA	2713	A
35	RA	2714	G
35	RA	2718	G
35	RA	2726	U
35	RA	2732	G
35	RA	2733	A
35	RA	2734	A
35	RA	2739	U
35	RA	2744	G
35	RA	2748	A
35	RA	2757	A
35	RA	2761	G
35	RA	2765	A
35	RA	2766	G
35	RA	2777	G
35	RA	2778	A
35	RA	2779	U
35	RA	2780	G
35	RA	2790	A
35	RA	2791	C
35	RA	2797	U
35	RA	2807	G
35	RA	2818	G
35	RA	2820	A
35	RA	2821	A
35	RA	2823	A
35	RA	2825	C
35	RA	2833	G
35	RA	2834	G
35	RA	2835	A
35	RA	2866	U
35	RA	2872	G
35	RA	2879	C
35	RA	2880	C
35	RA	2882	A
35	RA	2892	A
35	RA	2894	G
36	RB	7	G

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Mol	Chain	Res	Type
36	RB	8	U
36	RB	9	G
36	RB	12	C
36	RB	13	A
36	RB	15	A
36	RB	16	G
36	RB	22	U
36	RB	25	A
36	RB	26	A
36	RB	30	C
36	RB	41	U
36	RB	42	C
36	RB	44	G
36	RB	45	A
36	RB	56	G
36	RB	67	G
36	RB	73	A
36	RB	81	G
36	RB	105	G
36	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	51	A
1	XA	61	G
1	XA	65	U
1	XA	66	G
1	XA	78	G
1	XA	79	G
1	XA	81	G
1	XA	89	U
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

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Mol	Chain	Res	Type
1	XA	144	G
1	XA	147	G
1	XA	163	C
1	XA	169	C
1	XA	172	A
1	XA	173	U
1	XA	174	C
1	XA	187	C
1	XA	188	U
1	XA	190	G
1	XA	191(A)	G
1	XA	195	A
1	XA	197	A
1	XA	201	C
1	XA	209	U
1	XA	216	G
1	XA	220	G
1	XA	244	U
1	XA	245	C
1	XA	247	G
1	XA	251	G
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
1	XA	354	G
1	XA	356	A
1	XA	367	U
1	XA	372	C
1	XA	382	A
1	XA	384	G

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Mol	Chain	Res	Type
1	XA	388	G
1	XA	390	C
1	XA	397	A
1	XA	398	C
1	XA	406	G
1	XA	411	A
1	XA	412	A
1	XA	413	G
1	XA	414	A
1	XA	422	C
1	XA	423	G
1	XA	424	G
1	XA	429	U
1	XA	435	C
1	XA	440	A
1	XA	452	A
1	XA	465	A
1	XA	466	C
1	XA	467	G
1	XA	483	C
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	546	G
1	XA	547	A
1	XA	548	G
1	XA	559	A
1	XA	561	U
1	XA	564	C
1	XA	565	U
1	XA	568	G
1	XA	572	A

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Mol	Chain	Res	Type
1	XA	573	A
1	XA	576	G
1	XA	577	G
1	XA	596	C
1	XA	614	A
1	XA	618	C
1	XA	630	G
1	XA	631	G
1	XA	652	U
1	XA	653	A
1	XA	661	G
1	XA	665	A
1	XA	688	G
1	XA	702	A
1	XA	703	G
1	XA	704	A
1	XA	721	G
1	XA	724	G
1	XA	731	G
1	XA	748	C
1	XA	749	C
1	XA	754	C
1	XA	755	G
1	XA	774	G
1	XA	777	A
1	XA	792	A
1	XA	793	U
1	XA	794	A
1	XA	799	G
1	XA	813	U
1	XA	816	A
1	XA	817	C
1	XA	821	G
1	XA	828	A
1	XA	841	U
1	XA	842	C
1	XA	843	U
1	XA	848	C
1	XA	859	A
1	XA	872	A
1	XA	888	G
1	XA	902	G

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Mol	Chain	Res	Type
1	XA	914	A
1	XA	926	G
1	XA	927	G
1	XA	934	C
1	XA	948	C
1	XA	958	A
1	XA	960	U
1	XA	967	C
1	XA	968	A
1	XA	969	A
1	XA	972	C
1	XA	974	A
1	XA	975	A
1	XA	976	G
1	XA	977	A
1	XA	981	U
1	XA	991	U
1	XA	992	U
1	XA	993	G
1	XA	1004	A
1	XA	1005	A
1	XA	1006	C
1	XA	1009	G
1	XA	1017	G
1	XA	1021	G
1	XA	1024	G
1	XA	1025	U
1	XA	1028	C
1	XA	1029	G
1	XA	1032(A)	G
1	XA	1036	G
1	XA	1042	G
1	XA	1054	C
1	XA	1055	A
1	XA	1066	C
1	XA	1081	G
1	XA	1094	G
1	XA	1095	U
1	XA	1101	A
1	XA	1124	G
1	XA	1125	U
1	XA	1126	U

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Mol	Chain	Res	Type
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	1146	A
1	XA	1152	A
1	XA	1154	G
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	1181	G
1	XA	1182	G
1	XA	1183	A
1	XA	1184	G
1	XA	1187	G
1	XA	1190	G
1	XA	1196	U
1	XA	1197	G
1	XA	1211	U
1	XA	1212	U
1	XA	1238	A
1	XA	1240	U
1	XA	1241	G
1	XA	1256	A
1	XA	1257	U
1	XA	1258	G
1	XA	1260	C
1	XA	1270	C
1	XA	1273	G
1	XA	1280	A
1	XA	1281	U
1	XA	1282	C
1	XA	1286	A
1	XA	1287	A
1	XA	1298	C

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Mol	Chain	Res	Type
1	XA	1300	G
1	XA	1301	U
1	XA	1302	U
1	XA	1303	C
1	XA	1305	G
1	XA	1318	A
1	XA	1320	C
1	XA	1321	C
1	XA	1322	C
1	XA	1323	G
1	XA	1331	G
1	XA	1335	C
1	XA	1336	C
1	XA	1346	A
1	XA	1347	G
1	XA	1353	G
1	XA	1362(A)	C
1	XA	1363	A
1	XA	1364	U
1	XA	1367	C
1	XA	1368	G
1	XA	1370	G
1	XA	1379	G
1	XA	1397	C
1	XA	1398	A
1	XA	1419	G
1	XA	1442	G
1	XA	1443	G
1	XA	1446	A
1	XA	1452	C
1	XA	1453	G
1	XA	1454	G
1	XA	1469	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

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Mol	Chain	Res	Type
1	XA	1519	A
1	XA	1520	G
1	XA	1529	G
1	XA	1530	G
1	XA	1531	A
22	XV	3	C
22	XV	16	C
22	XV	17	C
22	XV	17(A)	U
22	XV	18	G
22	XV	19	G
22	XV	20	U
22	XV	21	A
22	XV	22	G
22	XV	34	C
22	XV	47	U
22	XV	48	C
22	XV	59	A
22	XV	76	A
23	XX	7	G
23	XX	10	G
23	XX	11	U
23	XX	13	A
23	XX	14	A
23	XX	19	G
23	XX	23	A
24	XY	4	G
24	XY	8	U
24	XY	9	A
24	XY	12	U
24	XY	16	C
24	XY	17	U
24	XY	18	G
24	XY	19	G
24	XY	20	G
24	XY	21	A
24	XY	22	G
24	XY	23	A
24	XY	43	G
24	XY	46	G
24	XY	47	U
24	XY	50	G

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Mol	Chain	Res	Type
24	XY	55	U
24	XY	56	C
24	XY	57	G
24	XY	58	A
24	XY	59	U
24	XY	61	C
24	XY	71	C
24	XY	73	A
24	XY	74	C
35	YA	9	U
35	YA	15	G
35	YA	34	C
35	YA	35	G
35	YA	46	C
35	YA	50	U
35	YA	51	G
35	YA	55	G
35	YA	61	G
35	YA	63	U
35	YA	74	A
35	YA	75	G
35	YA	91	A
35	YA	96	G
35	YA	101	G
35	YA	102	G
35	YA	103	A
35	YA	118	A
35	YA	119	A
35	YA	120	U
35	YA	125	G
35	YA	131	G
35	YA	149	A
35	YA	161	U
35	YA	162	U
35	YA	181	A
35	YA	188	G
35	YA	196	A
35	YA	199	A
35	YA	204	A
35	YA	215	G
35	YA	216	A
35	YA	221	A

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Mol	Chain	Res	Type
35	YA	222	A
35	YA	223	A
35	YA	229	A
35	YA	230	U
35	YA	232	G
35	YA	242	G
35	YA	243	U
35	YA	248	G
35	YA	249	C
35	YA	252	G
35	YA	264	C
35	YA	265	A
35	YA	266	G
35	YA	269	U
35	YA	270(L)	U
35	YA	270(M)	U
35	YA	270(N)	G
35	YA	270(P)	C
35	YA	271(A)	C
35	YA	271(B)	G
35	YA	271(C)	U
35	YA	271	G
35	YA	274	G
35	YA	275	G
35	YA	276	A
35	YA	278	A
35	YA	279	C
35	YA	299	A
35	YA	311	A
35	YA	323	G
35	YA	324	A
35	YA	329	G
35	YA	330	A
35	YA	332	A
35	YA	342	G
35	YA	352	G
35	YA	363	G
35	YA	363(F)	A
35	YA	364	C
35	YA	371	A
35	YA	372	G
35	YA	386	G

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Mol	Chain	Res	Type
35	YA	387	U
35	YA	396	G
35	YA	405	U
35	YA	406	G
35	YA	411	G
35	YA	412	A
35	YA	421	U
35	YA	428	A
35	YA	443	A
35	YA	444	C
35	YA	448	U
35	YA	455	C
35	YA	457	A
35	YA	467	G
35	YA	470	A
35	YA	480	A
35	YA	481	G
35	YA	504	U
35	YA	505	A
35	YA	509	C
35	YA	518	G
35	YA	528	A
35	YA	530	G
35	YA	531	C
35	YA	532	A
35	YA	533	G
35	YA	537	C
35	YA	539	G
35	YA	540	G
35	YA	546	C
35	YA	547	A
35	YA	554	U
35	YA	563	G
35	YA	573	G
35	YA	575	A
35	YA	588	U
35	YA	603	A
35	YA	607	U
35	YA	614	U
35	YA	615	G
35	YA	616	A
35	YA	617	G

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Mol	Chain	Res	Type
35	YA	618	G
35	YA	622	G
35	YA	627	A
35	YA	634	C
35	YA	637	A
35	YA	638	G
35	YA	645	C
35	YA	646	A
35	YA	651	G
35	YA	654	A
35	YA	654(A)	G
35	YA	686	G
35	YA	695	G
35	YA	702	G
35	YA	717	G
35	YA	722	A
35	YA	730	C
35	YA	734	A
35	YA	747	U
35	YA	752	A
35	YA	753	C
35	YA	764	A
35	YA	765	G
35	YA	775	G
35	YA	776	G
35	YA	782	A
35	YA	784	A
35	YA	785	G
35	YA	788	A
35	YA	789	A
35	YA	790	C
35	YA	792	G
35	YA	800	A
35	YA	805	G
35	YA	812	C
35	YA	819	A
35	YA	827	U
35	YA	828	U
35	YA	829	A
35	YA	846	C
35	YA	847	U
35	YA	856	C

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Mol	Chain	Res	Type
35	YA	857	C
35	YA	859	G
35	YA	860	U
35	YA	866	A
35	YA	880	G
35	YA	881	G
35	YA	882	G
35	YA	884	C
35	YA	885	C
35	YA	886	C
35	YA	888	C
35	YA	889	C
35	YA	890	A
35	YA	896	A
35	YA	897	C
35	YA	900	A
35	YA	901	A
35	YA	907	U
35	YA	910	A
35	YA	917	A
35	YA	918	A
35	YA	932	G
35	YA	941	A
35	YA	945	A
35	YA	946	G
35	YA	953	A
35	YA	959	A
35	YA	961	C
35	YA	973	A
35	YA	974	G
35	YA	974(A)	C
35	YA	983	A
35	YA	989	G
35	YA	996	A
35	YA	1003	G
35	YA	1005	C
35	YA	1011	G
35	YA	1012	U
35	YA	1013	C
35	YA	1015	G
35	YA	1022	G
35	YA	1023	U

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Mol	Chain	Res	Type
35	YA	1024	G
35	YA	1025	G
35	YA	1026	U
35	YA	1027	A
35	YA	1033	U
35	YA	1045	A
35	YA	1046	A
35	YA	1047	G
35	YA	1050	A
35	YA	1054	A
35	YA	1057	A
35	YA	1059	G
35	YA	1060	U
35	YA	1061	U
35	YA	1062	G
35	YA	1065	U
35	YA	1066	U
35	YA	1067	A
35	YA	1068	G
35	YA	1069	A
35	YA	1071	G
35	YA	1076	C
35	YA	1077	A
35	YA	1078	U
35	YA	1079	C
35	YA	1082	U
35	YA	1083	U
35	YA	1084	A
35	YA	1085	A
35	YA	1086	A
35	YA	1088	A
35	YA	1089	G
35	YA	1093	G
35	YA	1095	A
35	YA	1096	A
35	YA	1097	U
35	YA	1103	A
35	YA	1104	C
35	YA	1110	G
35	YA	1111	A
35	YA	1112	G
35	YA	1122	G

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Mol	Chain	Res	Type
35	YA	1126	A
35	YA	1129	A
35	YA	1130	U
35	YA	1131	G
35	YA	1135	C
35	YA	1136	G
35	YA	1139	G
35	YA	1142	U
35	YA	1142(A)	A
35	YA	1173	G
35	YA	1174	A
35	YA	1175	U
35	YA	1176	G
35	YA	1179	C
35	YA	1195	G
35	YA	1204	A
35	YA	1205	U
35	YA	1210	A
35	YA	1211	U
35	YA	1218	C
35	YA	1220	A
35	YA	1238	G
35	YA	1240	U
35	YA	1250	G
35	YA	1252	G
35	YA	1253	A
35	YA	1256	G
35	YA	1265	A
35	YA	1271	G
35	YA	1272	A
35	YA	1300	U
35	YA	1301	A
35	YA	1306	C
35	YA	1309	G
35	YA	1329	U
35	YA	1341	U
35	YA	1349	A
35	YA	1352	U
35	YA	1365	A
35	YA	1368	G
35	YA	1370	C
35	YA	1379	A

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Mol	Chain	Res	Type
35	YA	1384	A
35	YA	1385	G
35	YA	1386	C
35	YA	1391	U
35	YA	1395	A
35	YA	1407	C
35	YA	1411	C
35	YA	1416	G
35	YA	1419	A
35	YA	1420	U
35	YA	1421	G
35	YA	1427	A
35	YA	1428	C
35	YA	1444(A)	A
35	YA	1449	A
35	YA	1449(A)	G
35	YA	1455	G
35	YA	1458	C
35	YA	1460	A
35	YA	1461	G
35	YA	1467	C
35	YA	1471	A
35	YA	1483	G
35	YA	1485	G
35	YA	1493	C
35	YA	1497	U
35	YA	1507	A
35	YA	1508	A
35	YA	1510	A
35	YA	1511	A
35	YA	1514	U
35	YA	1523	U
35	YA	1534	G
35	YA	1535	U
35	YA	1536	A
35	YA	1537	C
35	YA	1538	G
35	YA	1540	G
35	YA	1543	A
35	YA	1544	C
35	YA	1545	A
35	YA	1558	A

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Mol	Chain	Res	Type
35	YA	1559	G
35	YA	1566	A
35	YA	1569	A
35	YA	1578	U
35	YA	1579	A
35	YA	1581	G
35	YA	1585	C
35	YA	1586	A
35	YA	1598	C
35	YA	1607	C
35	YA	1608	A
35	YA	1609	A
35	YA	1617	C
35	YA	1618	A
35	YA	1640	C
35	YA	1648	C
35	YA	1654	A
35	YA	1668	A
35	YA	1674	G
35	YA	1675	C
35	YA	1693	U
35	YA	1695	G
35	YA	1699	G
35	YA	1700	A
35	YA	1725	G
35	YA	1728	G
35	YA	1729	A
35	YA	1730	U
35	YA	1731	G
35	YA	1733	G
35	YA	1742	C
35	YA	1743	G
35	YA	1754	C
35	YA	1756	G
35	YA	1762	A
35	YA	1763	G
35	YA	1764	G
35	YA	1773	A
35	YA	1780	A
35	YA	1791	A
35	YA	1799	G
35	YA	1800	C

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Mol	Chain	Res	Type
35	YA	1801	G
35	YA	1808	U
35	YA	1811	G
35	YA	1816	G
35	YA	1820	U
35	YA	1828	G
35	YA	1829	A
35	YA	1835	G
35	YA	1847	A
35	YA	1858	G
35	YA	1869	G
35	YA	1872	A
35	YA	1878	G
35	YA	1881	C
35	YA	1882	C
35	YA	1888	G
35	YA	1889	A
35	YA	1896	G
35	YA	1900	A
35	YA	1906	G
35	YA	1919	A
35	YA	1929	G
35	YA	1937	A
35	YA	1938	A
35	YA	1939	U
35	YA	1940	U
35	YA	1955	U
35	YA	1956	U
35	YA	1963	U
35	YA	1964	G
35	YA	1965	C
35	YA	1966	A
35	YA	1967	C
35	YA	1969	A
35	YA	1970	A
35	YA	1971	A
35	YA	1972	A
35	YA	1982	C
35	YA	1991	U
35	YA	1992	G
35	YA	1993	U
35	YA	2020	A

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Mol	Chain	Res	Type
35	YA	2021	C
35	YA	2023	G
35	YA	2031	A
35	YA	2032	G
35	YA	2033	A
35	YA	2039	C
35	YA	2043	C
35	YA	2054	A
35	YA	2055	C
35	YA	2056	G
35	YA	2059	A
35	YA	2060	A
35	YA	2061	G
35	YA	2062	A
35	YA	2069	G
35	YA	2090	G
35	YA	2093	G
35	YA	2099	U
35	YA	2111	C
35	YA	2113	U
35	YA	2114	A
35	YA	2115	G
35	YA	2116	G
35	YA	2119	A
35	YA	2120	G
35	YA	2126	A
35	YA	2127	G
35	YA	2128	C
35	YA	2131	G
35	YA	2132	U
35	YA	2133	G
35	YA	2146	C
35	YA	2147	G
35	YA	2148	G
35	YA	2158	A
35	YA	2165	G
35	YA	2166	G
35	YA	2167	U
35	YA	2168	G
35	YA	2169	A
35	YA	2171	A
35	YA	2173	A

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Mol	Chain	Res	Type
35	YA	2176	A
35	YA	2178	C
35	YA	2190	G
35	YA	2192	G
35	YA	2198	A
35	YA	2210	G
35	YA	2211	G
35	YA	2212	A
35	YA	2213	U
35	YA	2215	G
35	YA	2225	A
35	YA	2234	G
35	YA	2238	G
35	YA	2239	G
35	YA	2243	U
35	YA	2246	G
35	YA	2249	U
35	YA	2269	A
35	YA	2275	C
35	YA	2283	C
35	YA	2287	A
35	YA	2288	A
35	YA	2289	G
35	YA	2307	G
35	YA	2308	G
35	YA	2310	A
35	YA	2311	A
35	YA	2318	G
35	YA	2319	G
35	YA	2320	A
35	YA	2325	G
35	YA	2334	G
35	YA	2336	A
35	YA	2342	C
35	YA	2346	A
35	YA	2347	C
35	YA	2350	C
35	YA	2354	G
35	YA	2377	A
35	YA	2383	G
35	YA	2385	C
35	YA	2403	C

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Mol	Chain	Res	Type
35	YA	2406	U
35	YA	2410	G
35	YA	2423	U
35	YA	2425	A
35	YA	2429	G
35	YA	2430	A
35	YA	2435	A
35	YA	2439	A
35	YA	2440	C
35	YA	2441	C
35	YA	2445	G
35	YA	2448	A
35	YA	2465	C
35	YA	2469	A
35	YA	2470	G
35	YA	2474	C
35	YA	2475	C
35	YA	2478	A
35	YA	2480	C
35	YA	2491	U
35	YA	2494	G
35	YA	2498	C
35	YA	2502	G
35	YA	2505	G
35	YA	2518	A
35	YA	2525	G
35	YA	2529	G
35	YA	2542	A
35	YA	2543	G
35	YA	2554	U
35	YA	2562	U
35	YA	2564	A
35	YA	2567	G
35	YA	2573	C
35	YA	2578	G
35	YA	2586	C
35	YA	2602	A
35	YA	2609	U
35	YA	2611	U
35	YA	2612	C
35	YA	2615	U
35	YA	2629	A

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Mol	Chain	Res	Type
35	YA	2646	C
35	YA	2653	U
35	YA	2654	A
35	YA	2665	A
35	YA	2673	G
35	YA	2679	A
35	YA	2682	U
35	YA	2689	U
35	YA	2690	C
35	YA	2691	C
35	YA	2702	U
35	YA	2707	G
35	YA	2712	U
35	YA	2712(A)	A
35	YA	2713	A
35	YA	2714	G
35	YA	2718	G
35	YA	2726	U
35	YA	2732	G
35	YA	2733	A
35	YA	2744	G
35	YA	2761	G
35	YA	2765	A
35	YA	2766	G
35	YA	2776	A
35	YA	2777	G
35	YA	2778	A
35	YA	2779	U
35	YA	2780	G
35	YA	2790	A
35	YA	2791	C
35	YA	2797	U
35	YA	2798	C
35	YA	2807	G
35	YA	2808	U
35	YA	2818	G
35	YA	2820	A
35	YA	2821	A
35	YA	2823	A
35	YA	2833	G
35	YA	2834	G
35	YA	2835	A

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Mol	Chain	Res	Type
35	YA	2849	U
35	YA	2866	U
35	YA	2872	G
35	YA	2879	C
35	YA	2880	C
35	YA	2891	G
35	YA	2892	A
35	YA	2894	G
36	YB	7	G
36	YB	8	U
36	YB	9	G
36	YB	12	C
36	YB	13	A
36	YB	15	A
36	YB	19	G
36	YB	22	U
36	YB	40	U
36	YB	42	C
36	YB	45	A
36	YB	52	A
36	YB	53	A
36	YB	56	G
36	YB	73	A
36	YB	81	G
36	YB	82	G
36	YB	109	G

All (150) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	QA	115	G
1	QA	181	G
1	QA	243	A
1	QA	244	U
1	QA	250	A
1	QA	266	G
1	QA	328	C
1	QA	410	G
1	QA	412	A
1	QA	484	G
1	QA	485	G
1	QA	509	A

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Mol	Chain	Res	Type
1	QA	687	A
1	QA	703	G
1	QA	753	A
1	QA	792	A
1	QA	812	C
1	QA	913	A
1	QA	992	U
1	QA	1027	C
1	QA	1065	U
1	QA	1285	A
1	QA	1297	C
1	QA	1336	C
1	QA	1346	A
1	QA	1347	G
1	QA	1446	A
1	QA	1498	U
1	QA	1528	U
23	QX	18	G
35	RA	74	A
35	RA	99	U
35	RA	102	G
35	RA	221	A
35	RA	222	A
35	RA	227	A
35	RA	229	A
35	RA	242	G
35	RA	271(B)	G
35	RA	271(C)	U
35	RA	345	A
35	RA	372	G
35	RA	404	C
35	RA	503	A
35	RA	508	G
35	RA	512	G
35	RA	587	C
35	RA	637	A
35	RA	752	A
35	RA	846	C
35	RA	856	C
35	RA	1022	G
35	RA	1026	U
35	RA	1045	A

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Mol	Chain	Res	Type
35	RA	1078	U
35	RA	1085	A
35	RA	1178	C
35	RA	1210	A
35	RA	1312	U
35	RA	1427	A
35	RA	1558	A
35	RA	1653	G
35	RA	1694	C
35	RA	1799	G
35	RA	1819	A
35	RA	1930	G
35	RA	1992	G
35	RA	2060	A
35	RA	2126	A
35	RA	2405	G
35	RA	2439	A
35	RA	2566	A
35	RA	2610	C
35	RA	2689	U
35	RA	2712	U
35	RA	2776	A
35	RA	2832	U
36	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
1	XA	266	G
1	XA	328	C
1	XA	345	C
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

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Mol	Chain	Res	Type
1	XA	753	A
1	XA	793	U
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	1498	U
23	XX	18	G
35	YA	99	U
35	YA	102	G
35	YA	221	A
35	YA	222	A
35	YA	229	A
35	YA	242	G
35	YA	271(B)	G
35	YA	278	A
35	YA	404	C
35	YA	503	A
35	YA	587	C
35	YA	637	A
35	YA	653	A
35	YA	752	A
35	YA	827	U
35	YA	846	C
35	YA	856	C
35	YA	859	G
35	YA	1022	G
35	YA	1026	U
35	YA	1045	A
35	YA	1085	A
35	YA	1178	C
35	YA	1204	A
35	YA	1210	A
35	YA	1427	A
35	YA	1558	A
35	YA	1653	G
35	YA	1694	C
35	YA	1698	A
35	YA	1799	G
35	YA	1819	A

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Mol	Chain	Res	Type
35	YA	1955	U
35	YA	1992	G
35	YA	2126	A
35	YA	2406	U
35	YA	2439	A
35	YA	2566	A
35	YA	2610	C
35	YA	2681	C
35	YA	2689	U
35	YA	2712	U
35	YA	2776	A
35	YA	2832	U

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 855 ligands modelled in this entry, 851 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	$\# Z > 2$
58	SF4	QD	501	-	0,12,12	0.00	-	-		
58	SF4	XD	501	4	0,12,12	0.00	-	-		
57	PAR	QA	1663	-	45,45,45	0.80	0	64,67,67	1.30	8 (12%)
57	PAR	XA	1670	-	45,45,45	0.86	1 (2%)	64,67,67	1.28	7 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SF4	QD	501	-	-	-	0/6/5/5
58	SF4	XD	501	4	-	-	0/6/5/5
57	PAR	QA	1663	-	-	3/18/94/94	0/4/4/4
57	PAR	XA	1670	-	-	3/18/94/94	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	XA	1670	PAR	C24-N24	-2.01	1.44	1.47

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	QA	1663	PAR	C13-O52-C52	-3.20	110.03	117.96
57	XA	1670	PAR	O11-C42-C32	-2.97	102.08	109.18
57	XA	1670	PAR	C13-O52-C52	-2.87	110.85	117.96
57	QA	1663	PAR	C64-C54-C44	-2.68	107.82	113.10
57	QA	1663	PAR	O62-C62-C12	-2.58	105.08	109.81
57	QA	1663	PAR	O33-C33-C23	-2.57	103.05	111.32
57	QA	1663	PAR	O52-C13-C23	2.55	113.24	107.96
57	XA	1670	PAR	O62-C62-C12	-2.42	105.38	109.81
57	XA	1670	PAR	O33-C33-C23	-2.39	103.62	111.32
57	XA	1670	PAR	O52-C13-C23	2.24	112.60	107.96
57	QA	1663	PAR	O11-C42-C32	-2.18	103.98	109.18
57	QA	1663	PAR	C11-C21-N21	-2.18	106.28	110.20
57	XA	1670	PAR	C31-C41-C51	-2.16	106.39	110.24
57	XA	1670	PAR	O11-C11-C21	-2.10	104.59	108.22
57	QA	1663	PAR	C11-O51-C51	2.04	117.69	113.69

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	QA	1663	PAR	O54-C54-C64-N64
57	XA	1670	PAR	O54-C14-O33-C33
57	QA	1663	PAR	O51-C51-C61-O61
57	QA	1663	PAR	C23-C33-O33-C14
57	XA	1670	PAR	C43-C33-O33-C14

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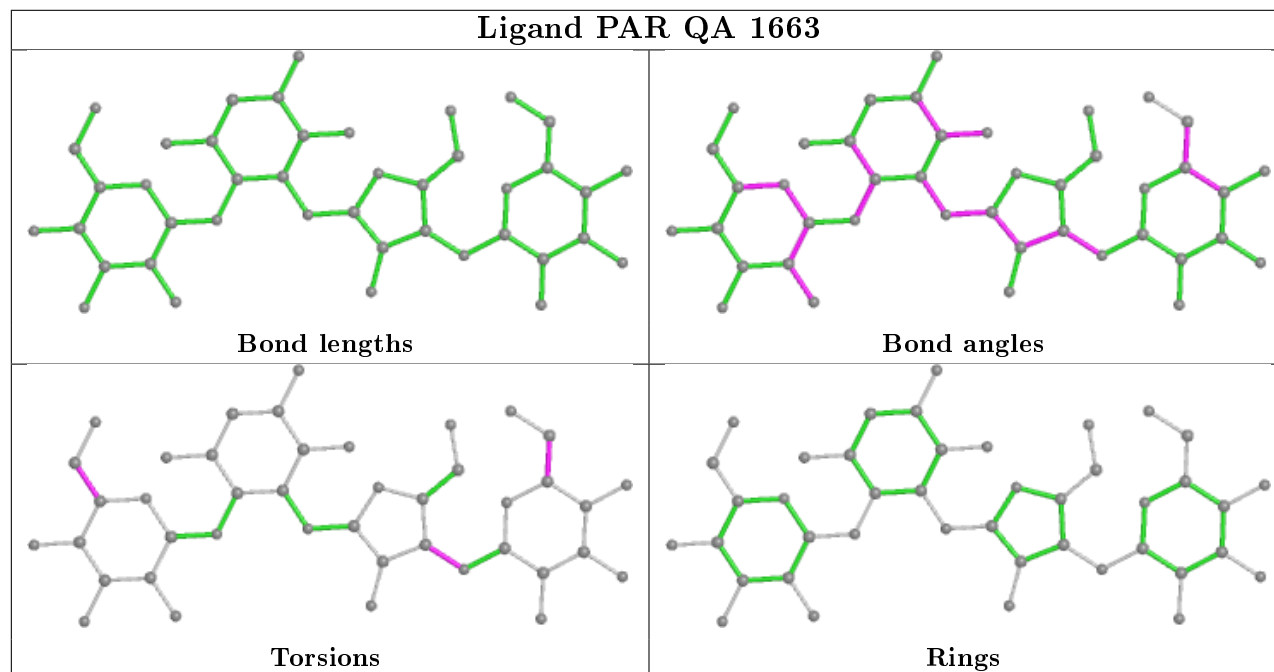
Mol	Chain	Res	Type	Atoms
57	XA	1670	PAR	C23-C33-O33-C14

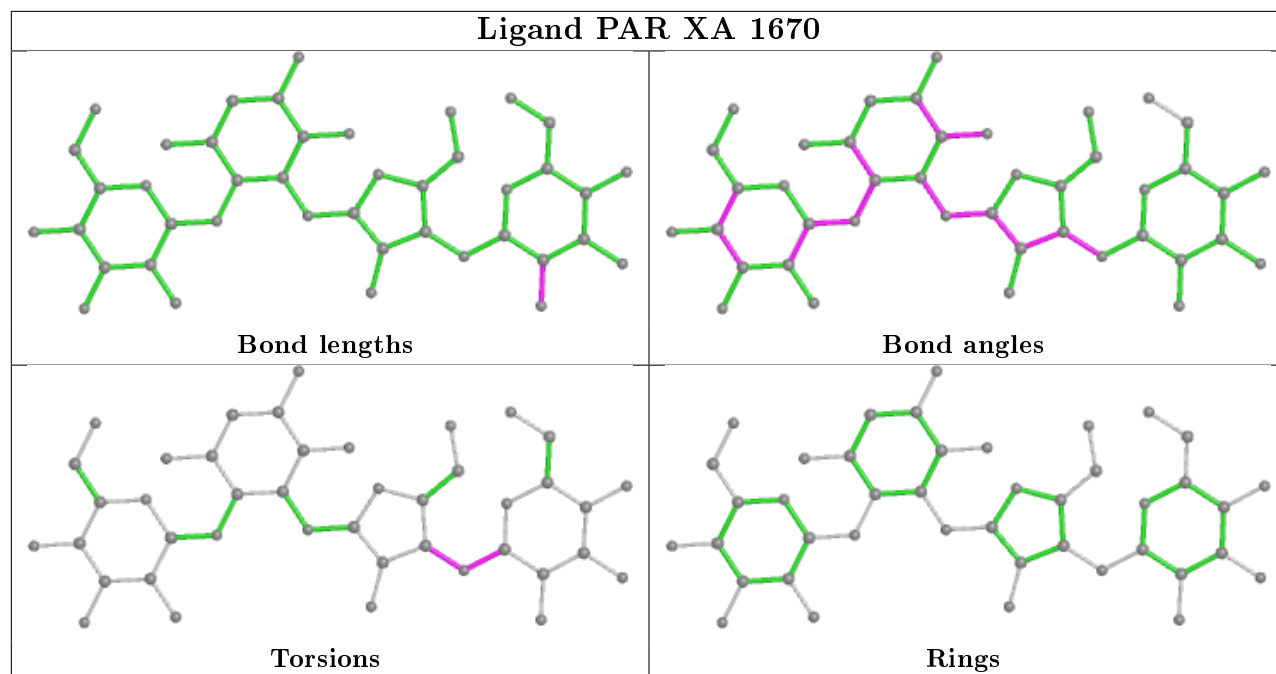
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	XA	1670	PAR	4	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.