



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2020 – 08:18 pm BST

PDB ID : 6BZ6
Title : Thermus thermophilus 70S complex containing 16S G347U ram mutation and empty A site
Authors : Hoffer, E.D.; Maehigashi, T.; Fagan, C.E.; Dunham, C.M.
Deposited on : 2017-12-22
Resolution : 3.18 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

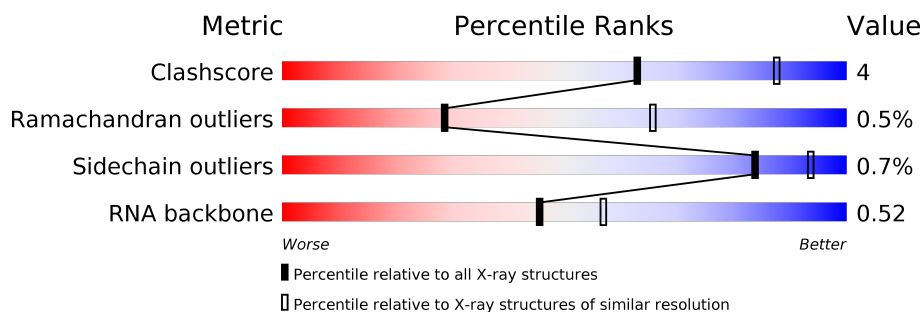
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.18 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	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RNA backbone	3102	1054 (3.50-2.86)


























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	1508	64% 29% 6% ..
1	XA	1508	66% 27% 6% ..
2	QB	256	77% 14% 8%
2	XB	256	79% 13% 8%
3	QC	239	72% 13% 14%
3	XC	239	72% 13% 14%
4	QD	209	87% 12%

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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	132	
12	XL	132	
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	25	
23	XX	25	
24	RA	2915	
24	YA	2915	
25	RB	122	
25	YB	122	
26	RD	276	
26	YD	276	
27	RE	206	
27	YE	206	
28	RF	210	
28	YF	210	
29	RG	182	


























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Mol	Chain	Length	Quality of chain
29	YG	182	 81% 17% ..
30	RH	180	 79% 15% ...
30	YH	180	 78% 16% ...
31	RI	148	 79% 20% .
31	YI	148	 78% 21% .
32	RN	140	 88% 10% ..
32	YN	140	 91% 7% ..
33	RO	122	 89% 11% .
33	YO	122	 91% 8% .
34	RP	150	 79% 21%
34	YP	150	 78% 19% ..
35	RQ	141	 76% 24%
35	YQ	141	 79% 21%
36	RR	118	 86% 13% ..
36	YR	118	 81% 18% .
37	RS	112	 83% 15% ..
37	YS	112	 81% 17% ..
38	RT	146	 71% 22% . 6%
38	YT	146	 68% 25% . 6%
39	RU	118	 84% 14% ..
39	YU	118	 86% 11% ..
40	RV	101	 84% 15% .
40	YV	101	 84% 14% ..
41	RW	113	 88% 12% .
41	YW	113	 89% 11%


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Mol	Chain	Length	Quality of chain
42	RX	96	
42	YX	96	
43	RY	110	
43	YY	110	
44	RZ	206	
44	YZ	206	
45	R0	85	
45	Y0	85	
46	R1	98	
46	Y1	98	
47	R2	72	
47	Y2	72	
48	R3	60	
48	Y3	60	
49	R4	71	
49	Y4	71	
50	R5	60	
50	Y5	60	
51	R6	54	
51	Y6	54	
52	R7	49	
52	Y7	49	
53	R8	65	
53	Y8	65	
54	R9	37	

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Mol	Chain	Length	Quality of chain
54	Y9	37	 81% 19%

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 291753 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	1498	Total	C	N	O	P	0	0	0
			32202	14333	5970	10402	1497			
1	XA	1500	Total	C	N	O	P	0	0	0
			32246	14353	5981	10413	1499			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
QA	347	U	G	engineered mutation	GB 55771382
XA	347	U	G	engineered mutation	GB 55771382

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	QJ	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			
10	XJ	96	Total	C	N	O	S	0	0	0
			777	487	153	136	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QS	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
19	XS	84	Total	C	N	O	S	0	0	0
			674	430	126	116	2			

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 tRNA fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			
22	XV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	12	Total	C	N	O	P	0	0	0
			259	116	48	83	12			
23	XX	11	Total	C	N	O	P	0	0	0
			239	107	46	75	11			

- Molecule 24 is a RNA chain called 23S rRNA.

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

- Molecule 25 is a RNA chain called 5S rRNA.

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

- Molecule 26 is a protein called 50S ribosomal protein L2.

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

- Molecule 27 is a protein called 50S ribosomal protein L3.

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

- Molecule 28 is a protein called 50S ribosomal protein L4.

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

- Molecule 29 is a protein called 50S ribosomal protein L5.

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

- Molecule 30 is a protein called 50S ribosomal protein L6.

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

- Molecule 31 is a protein called 50S ribosomal protein L9.

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

- Molecule 32 is a protein called 50S ribosomal protein L13.

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

- Molecule 33 is a protein called 50S ribosomal protein L14.

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

- Molecule 34 is a protein called 50S ribosomal protein L15.

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

- Molecule 35 is a protein called 50S ribosomal protein L16.

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

- Molecule 36 is a protein called 50S ribosomal protein L17.

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

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

- Molecule 37 is a protein called 50S ribosomal protein L18.

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

- Molecule 38 is a protein called 50S ribosomal protein L19.

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

- Molecule 39 is a protein called 50S ribosomal protein L20.

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

- Molecule 40 is a protein called 50S ribosomal protein L21.

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

- Molecule 41 is a protein called 50S ribosomal protein L22.

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

- Molecule 42 is a protein called 50S ribosomal protein L23.

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

- Molecule 43 is a protein called 50S ribosomal protein L24.

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

- Molecule 44 is a protein called 50S ribosomal protein L25.

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

- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	R0	81	Total	C	N	O	S	0	0	0
			643	398	137	107	1			
45	Y0	75	Total	C	N	O	S	0	0	0
			599	370	127	101	1			

- Molecule 46 is a protein called 50S ribosomal protein L28.

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

- Molecule 47 is a protein called 50S ribosomal protein L29.

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

- Molecule 48 is a protein called 50S ribosomal protein L30.

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

- Molecule 49 is a protein called 50S ribosomal protein L31.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L33.

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

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	R7	47	Total	C	N	O	S	0	0	0
			409	251	102	54	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	Y7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 53 is a protein called 50S ribosomal protein L35.

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

- Molecule 54 is a protein called 50S ribosomal protein L36.

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

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	QA	80	Total	Mg	0	0
			80	80		
55	RP	3	Total	Mg	0	0
			3	3		
55	YA	551	Total	Mg	0	0
			551	551		
55	Y5	1	Total	Mg	0	0
			1	1		
55	RT	1	Total	Mg	0	0
			1	1		
55	RN	1	Total	Mg	0	0
			1	1		
55	XE	1	Total	Mg	0	0
			1	1		
55	XS	1	Total	Mg	0	0
			1	1		
55	Y1	1	Total	Mg	0	0
			1	1		
55	YD	3	Total	Mg	0	0
			3	3		

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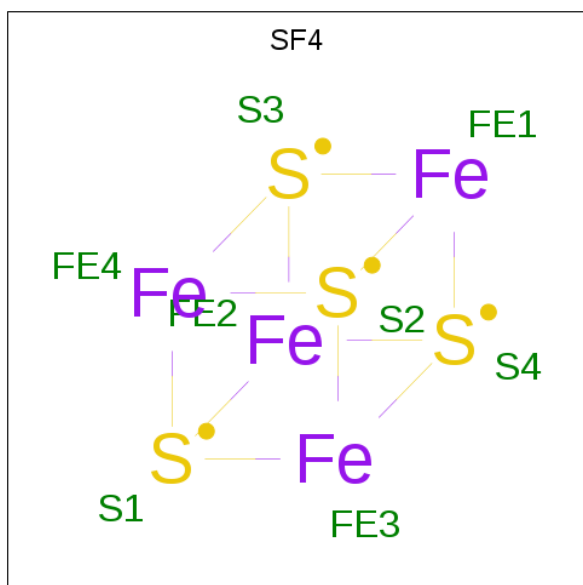
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	XX	1	Total 1	Mg 1	0	0
55	QV	6	Total 6	Mg 6	0	0
55	Y8	2	Total 2	Mg 2	0	0
55	YO	1	Total 1	Mg 1	0	0
55	XA	98	Total 98	Mg 98	0	0
55	YY	1	Total 1	Mg 1	0	0
55	RQ	3	Total 3	Mg 3	0	0
55	R0	2	Total 2	Mg 2	0	0
55	YU	1	Total 1	Mg 1	0	0
55	RO	1	Total 1	Mg 1	0	0
55	QH	1	Total 1	Mg 1	0	0
55	YQ	4	Total 4	Mg 4	0	0
55	QC	1	Total 1	Mg 1	0	0
55	R8	1	Total 1	Mg 1	0	0
55	YX	2	Total 2	Mg 2	0	0
55	RR	2	Total 2	Mg 2	0	0
55	RD	1	Total 1	Mg 1	0	0
55	Y7	1	Total 1	Mg 1	0	0
55	QF	1	Total 1	Mg 1	0	0
55	Y0	2	Total 2	Mg 2	0	0
55	XQ	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	RA	521	Total 521	Mg 521	0	0
55	YF	1	Total 1	Mg 1	0	0
55	YP	2	Total 2	Mg 2	0	0
55	RE	4	Total 4	Mg 4	0	0
55	XL	2	Total 2	Mg 2	0	0
55	YB	12	Total 12	Mg 12	0	0
55	QT	1	Total 1	Mg 1	0	0
55	XV	8	Total 8	Mg 8	0	0
55	RB	11	Total 11	Mg 11	0	0
55	XM	2	Total 2	Mg 2	0	0
55	YE	4	Total 4	Mg 4	0	0

- Molecule 56 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

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

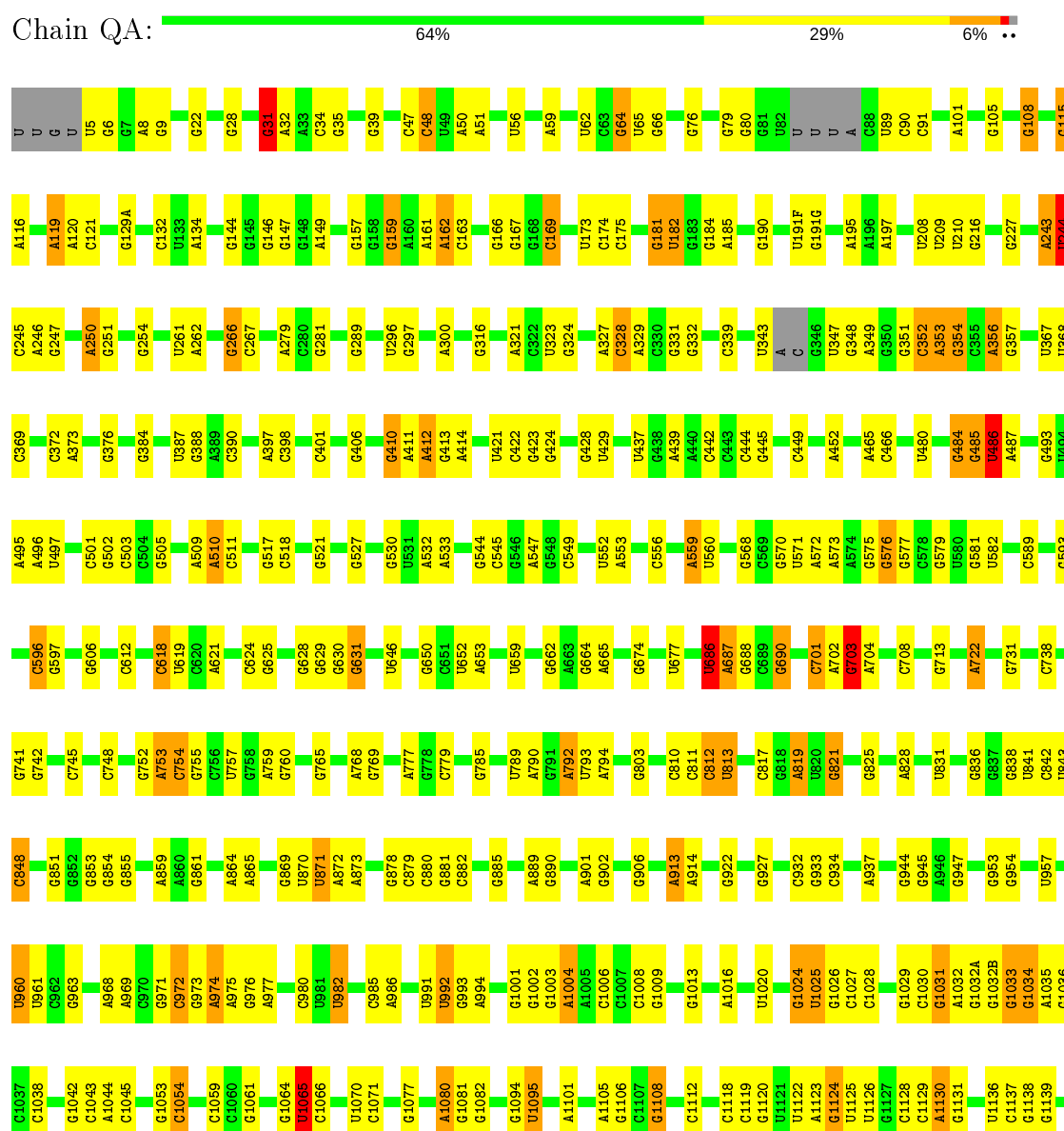
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	Y9	1	Total	Zn	0	0
			1	1		
57	YY	1	Total	Zn	0	0
			1	1		
57	Y6	1	Total	Zn	0	0
			1	1		
57	QN	1	Total	Zn	0	0
			1	1		
57	XN	1	Total	Zn	0	0
			1	1		
57	RY	1	Total	Zn	0	0
			1	1		
57	Y4	1	Total	Zn	0	0
			1	1		
57	R6	1	Total	Zn	0	0
			1	1		
57	Y5	1	Total	Zn	0	0
			1	1		
57	R5	1	Total	Zn	0	0
			1	1		
57	R4	1	Total	Zn	0	0
			1	1		
57	R9	1	Total	Zn	0	0
			1	1		

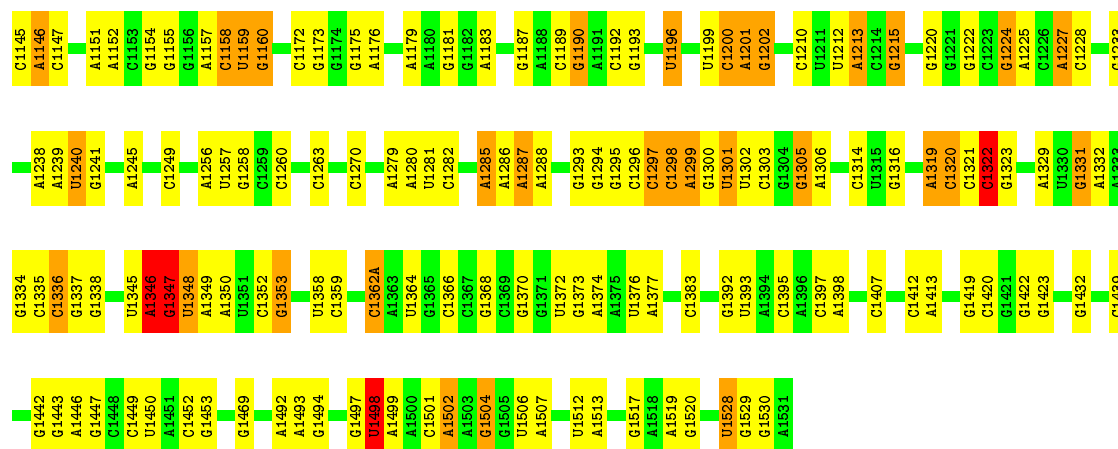
3 Residue-property plots

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

Note EDS failed to run properly.

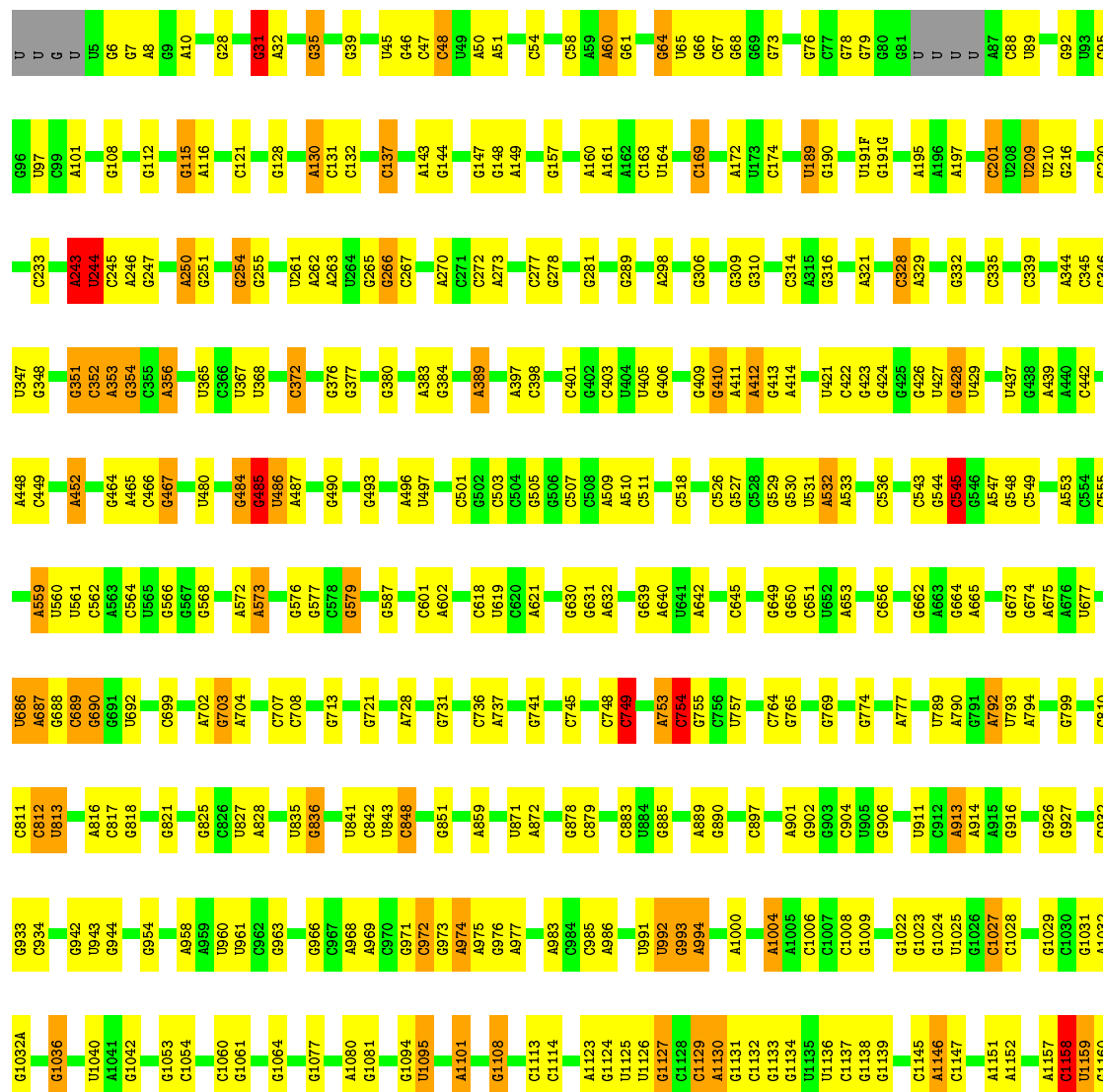
• Molecule 1: 16S rRNA

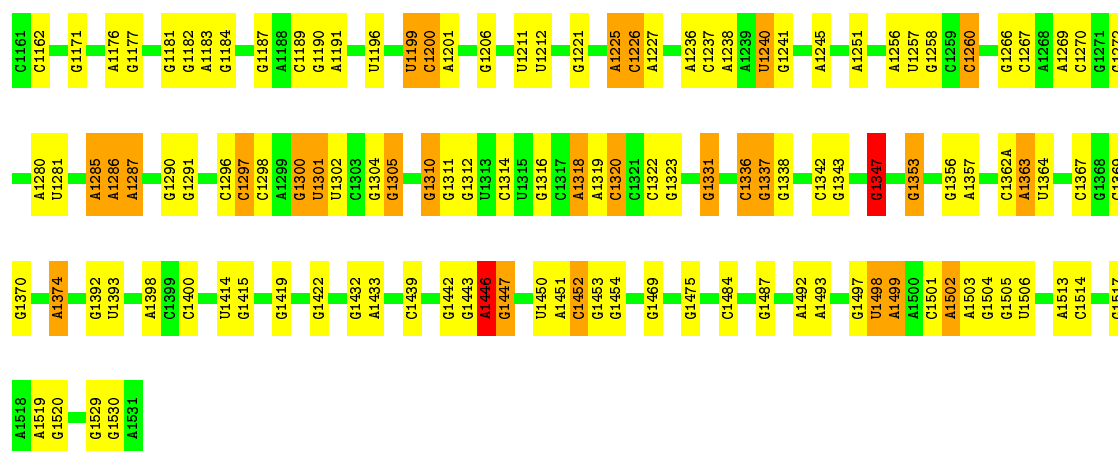




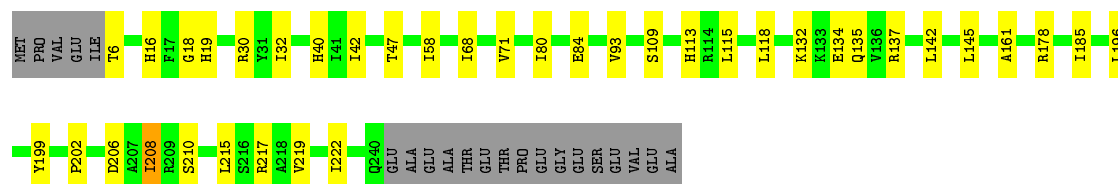
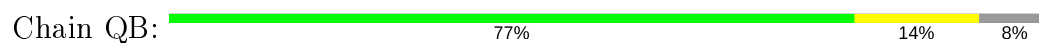
• Molecule 1: 16S rRNA

Chain XA: 66% 27% 6% ..

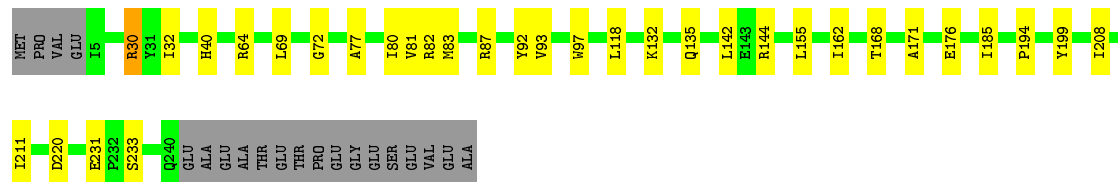
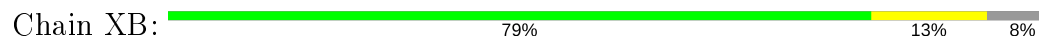




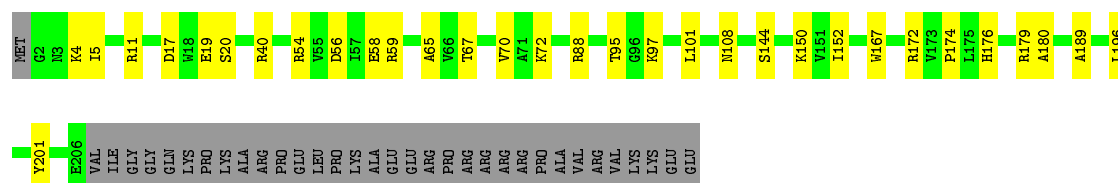
- Molecule 2: 30S ribosomal protein S2



- Molecule 2: 30S ribosomal protein S2

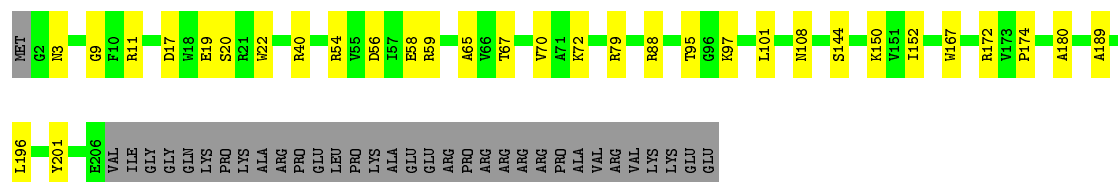


- Molecule 3: 30S ribosomal protein S3



- Molecule 3: 30S ribosomal protein S3





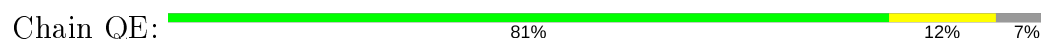
- Molecule 4: 30S ribosomal protein S4



- Molecule 4: 30S ribosomal protein S4



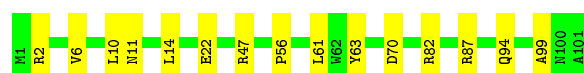
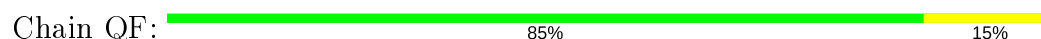
- Molecule 5: 30S ribosomal protein S5



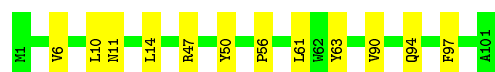
- Molecule 5: 30S ribosomal protein S5




- Molecule 6: 30S ribosomal protein S6



- Molecule 6: 30S ribosomal protein S6



- Molecule 7: 30S ribosomal protein S7

Chain QG:  88% 10% ..




- Molecule 7: 30S ribosomal protein S7

Chain XG:  89% 10% ..




- Molecule 8: 30S ribosomal protein S8

Chain QH:  82% 17% ..




- Molecule 8: 30S ribosomal protein S8

Chain XH:  83% 16% ..



- Molecule 9: 30S ribosomal protein S9

Chain QI:  75% 23% ..



- Molecule 9: 30S ribosomal protein S9

Chain XI:  80% 17% ..



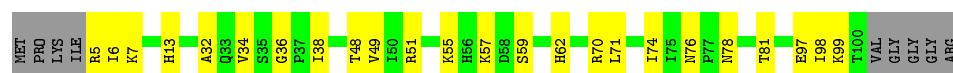
- Molecule 10: 30S ribosomal protein S10

Chain QJ:  70% 25% 6%



- Molecule 10: 30S ribosomal protein S10

Chain XJ: 




- Molecule 11: 30S ribosomal protein S11

Chain QK: 




- Molecule 11: 30S ribosomal protein S11

Chain XK: 




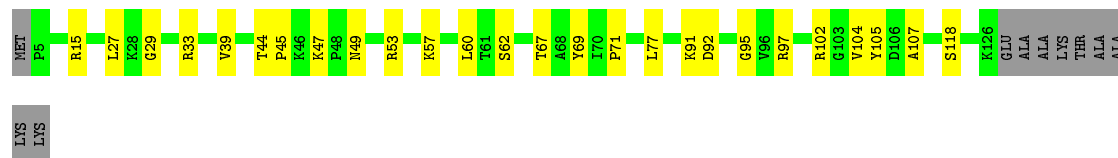
- Molecule 12: 30S ribosomal protein S12

Chain QL: 




- Molecule 12: 30S ribosomal protein S12

Chain XL: 




- Molecule 13: 30S ribosomal protein S13

Chain QM: 




- Molecule 13: 30S ribosomal protein S13

Chain XM: 




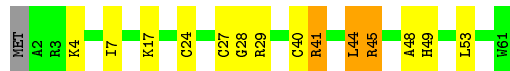
- Molecule 14: 30S ribosomal protein S14 type Z

Chain QN:  75% 20% ..



- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN:  75% 18% 5% .



- Molecule 15: 30S ribosomal protein S15

Chain QO:  92% 7% .




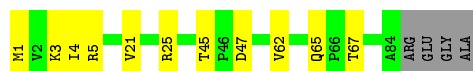
- Molecule 15: 30S ribosomal protein S15

Chain XO:  90% 8% .




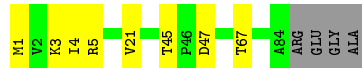
- Molecule 16: 30S ribosomal protein S16

Chain QP:  83% 13% 5%




- Molecule 16: 30S ribosomal protein S16

Chain XP:  86% 9% 5%




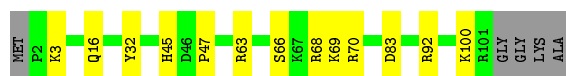
- Molecule 17: 30S ribosomal protein S17

Chain QQ:  89% 7% 5%



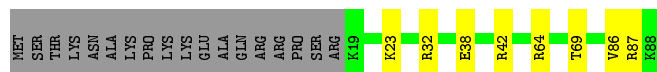
- Molecule 17: 30S ribosomal protein S17

Chain XQ:  83% 12% 5%



- Molecule 18: 30S ribosomal protein S18

Chain QR:  70% 9% 20%



- Molecule 18: 30S ribosomal protein S18

Chain XR:  69% 10% 20%




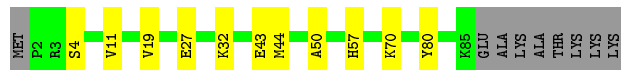
- Molecule 19: 30S ribosomal protein S19

Chain QS:  67% 23% 11%



- Molecule 19: 30S ribosomal protein S19

Chain XS:  78% 12% 10%



- Molecule 20: 30S ribosomal protein S20

Chain QT:  89% 5% 7%




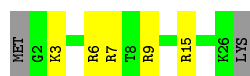
- Molecule 20: 30S ribosomal protein S20

Chain XT:  89% 5% 7%




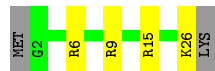
- Molecule 21: 30S ribosomal protein Thx

Chain QU:  74% 19% 7%




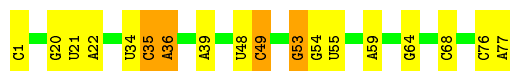
- Molecule 21: 30S ribosomal protein Thx

Chain XU:  78% 15% 7%




- Molecule 22: tRNA fMet

Chain QV:  77% 18% 5%



- Molecule 22: tRNA fMet

Chain XV:  74% 19% 5%




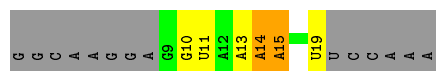
- Molecule 23: messenger RNA

Chain QX:  16% 28% 52%



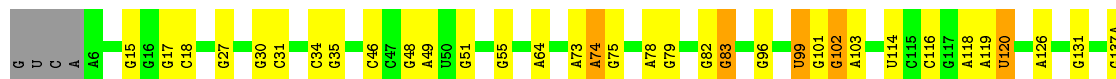
- Molecule 23: messenger RNA

Chain XX:  20% 16% 8% 56%

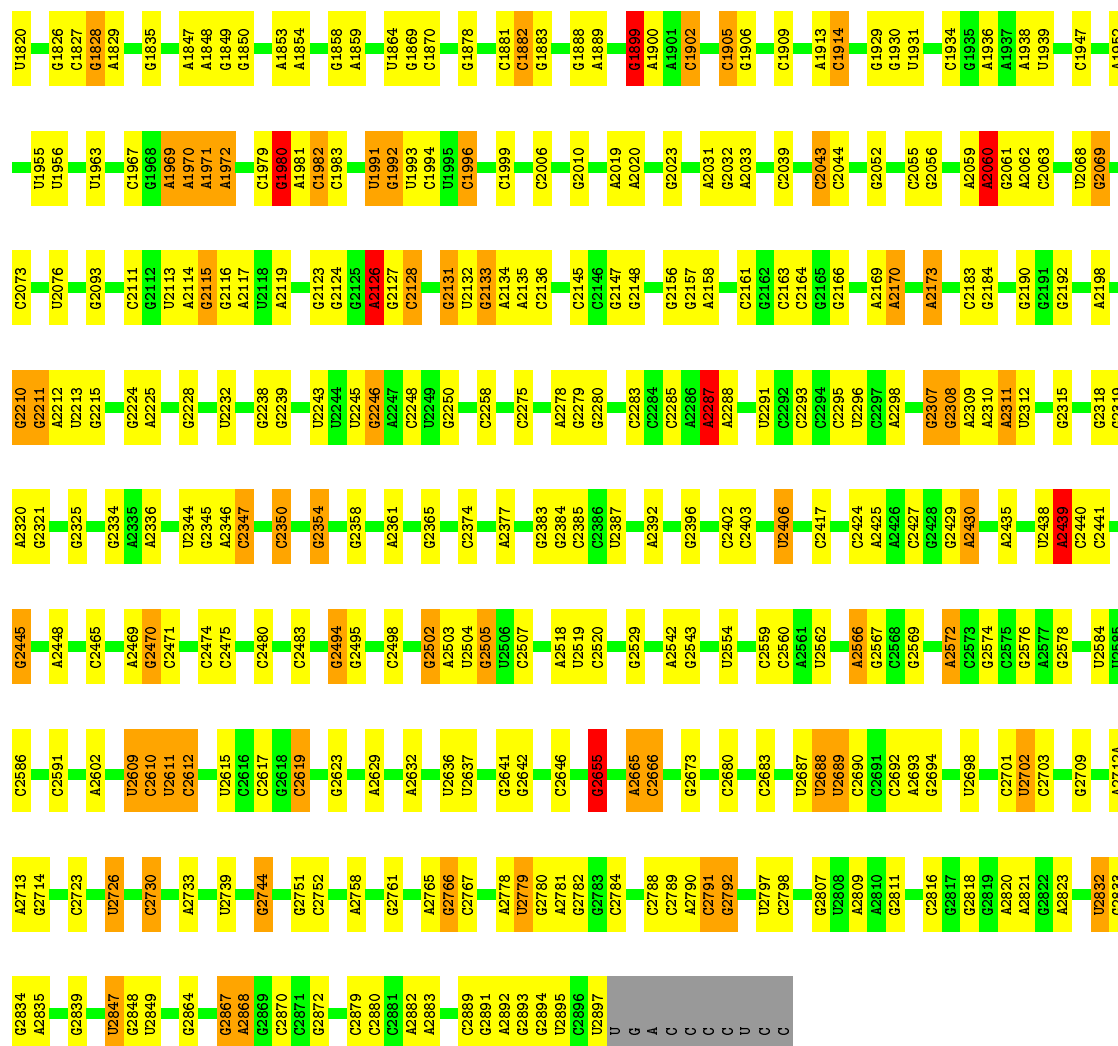


- Molecule 24: 23S rRNA

Chain RA:  67% 26% 6%

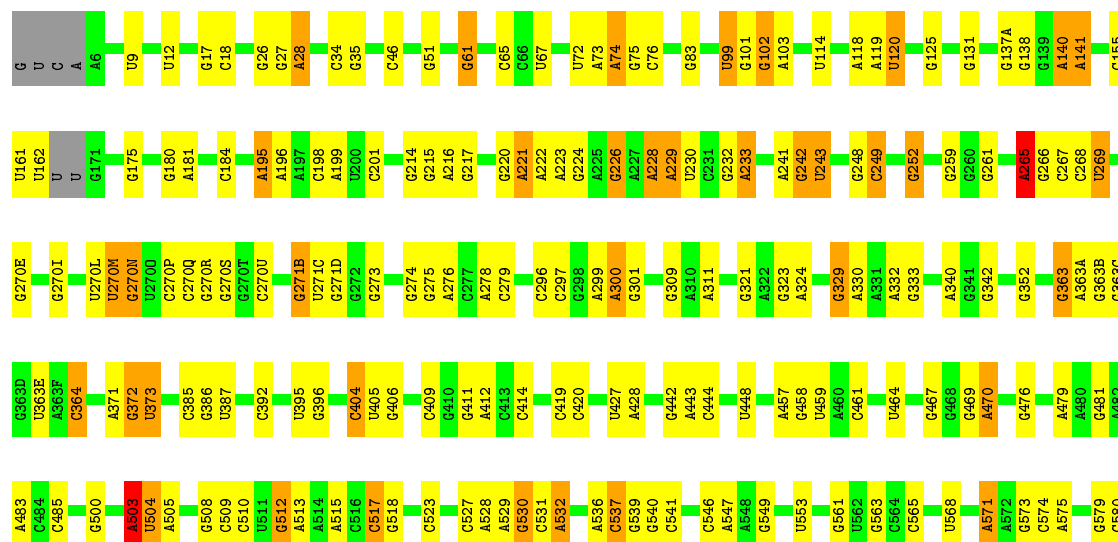


C1886	G138	U269	U328	U448	U554	A654	C790	C907	G1003	A1085	G1203	A1349	A1460	U1578	C1686
A1689	G139	A270	G329	A454	G556	G654A	C791	U907	C1004	A1086	A1204	A1349	G1461	A1578	A1689
C1694	A140	C270H	A330	C455	G563	G654B	G792	A910	G1005	A1087	U1205	U1352	A1471	A1580	C1694
A1698	A141	G270I	G333	C456	C565	C	A793	C914	C1006	A1088	G1206	U1359	C1474	A1583	A1698
G1703	U161	G270J	C336	A457	C565	C	A800	C915	C1007	G1091	U1211	A1359	C1474	C1585	A1698
G1725	U	G270K	C337	C458	C565	C	A800	C916	C1008	G1092	U1211	A1359	C1474	C1586	A1698
G1728	U	U270L	C337	C459	C565	C	A800	C917	C1009	G1093	A1214	C1363	G1479	A1586	G1703
A1729	G171	U270M	C337	C460	C565	C	A800	A917	A1010	G1094	A1214	G1363	G1480	U1590	G1703
U1730	G171	G270N	U339	C461	C565	C	A800	A918	A1011	G1095	A1214	A1365	U1482	G1591	G1725
G1732	G171	U270O	U339	C462	C565	C	A800	A919	U1012	A1096	A1220	A1365	G1483	C1592	G1728
G1733	G171	G270P	C341	C463	C565	C	A800	U922	C1013	U1105	U1234	C1370	G1484	C1593	G1728
C1742	G171	C270Q	G342	C464	C565	C	A800	U922	U1014	U1105	U1234	C1371	G1485	G1593	A1729
G1743	G171	G270R	G343	C465	C565	C	A800	U922	U1015	G1110	G1235	U1372	A1486	G1594	U1730
G1750	G171	G270S	G344	C466	C565	C	A800	U922	U1016	A1111	A1236	C1375	A1487	G1595	G1732
C1754	G171	G270T	G345	C467	C565	C	A800	U922	U1017	A1112	G1237	C1376	A1490	C1598	G1733
A1755	G171	G270U	A346	C468	C565	C	A800	U922	U1018	G1122	G1238	C1377	A1491	C1599	C1742
G1756	G171	G270V	A346	C469	C565	C	A800	U922	U1019	G1123	A1252	C1378	A1492	C1600	A1608
A1762	G171	C270W	G352	A470	C565	C	A800	U922	A1020	G1124	A1253	A1379	A1493	A1610	G1743
G1763	G171	G270X	C364	A480	C565	C	A800	U922	A1021	C1125	G1254	G1380	U1497	C1617	G1750
G1764	G171	U271A	A371	C481	C565	C	A800	U922	U1022	G1126	A1255	A1381	C1504	C1622	C1754
G1769	G171	G271B	G372	C482	C565	C	A800	U922	U1023	A1129	G1256	A1382	C1505	G1622	A1755
A1773	G171	U271C	U373	C483	C565	C	A800	U922	U1024	U1130	C1257	A1383	C1506	G1622	G1756
C1774	G171	G271D	C385	C484	C565	C	A800	U922	G1025	G1131	C1258	U1394	C1507	C1636	A1762
H1775	G171	G272	C385	C485	C565	C	A800	U922	G1026	G1132	A1259	A1395	A1507	A1637	G1763
G1776	G171	C273F	C385	C486	C565	C	A800	U922	A1027	C1133	U1130	U1396	A1508	U1638	G1764
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A1780	G171	G274	C385	C488	C565	C	A800	U922	A1029	G1135	U1132	U1398	A1510	C1640	A1773
C1781	G171	G275	C385	C489	C565	C	A800	U922	A1030	G1136	U1133	U1399	A1511	C1641	C1774
C1782	G171	G276	C385	C490	C565	C	A800	U922	G1042	U1137	U1134	U1400	A1512	C1642	C1782
A1783	G171	C277	C385	C491	C565	C	A800	U922	G1043	G1138	U1135	U1401	A1513	C1643	A1783
A1785	G171	C278	C385	C492	C565	C	A800	U922	G1044	G1139	U1136	U1402	A1514	C1644	A1785
A1786	G171	C288	C385	C493	C565	C	A800	U922	G1045	G1140	U1137	U1403	A1515	C1645	A1786
A1791	G171	A289	C385	C494	C565	C	A800	U922	A1046	G1141	U1138	U1404	A1516	C1646	A1791
G1799	G171	C289	C385	C495	C565	C	A800	U922	A1047	G1142	U1139	U1405	A1517	C1647	G1799
C1800	G171	C296	C385	C496	C565	C	A800	U922	A1048	G1143	U1140	U1406	A1518	C1648	C1800
G1801	G171	C297	C385	C497	C565	C	A800	U922	A1049	G1144	U1141	A1046	A1519	C1649	G1801
C1804	G171	C298	C385	C498	C565	C	A800	U922	A1050	G1145	U1142	A1047	A1520	C1650	C1804
G1816	G171	C299	C385	C499	C565	C	A800	U922	A1051	G1146	U1143	A1048	A1521	C1651	G1816
G1817	G171	A300	C385	C500	C565	C	A800	U922	A1052	G1147	U1144	A1049	A1522	C1652	G1817
U1818	G171	A301	C385	C501	C565	C	A800	U922	A1053	G1148	U1145	A1050	A1523	C1653	U1818
A1819	G171	A302	C385	C502	C565	C	A800	U922	A1054	G1149	U1146	A1051	A1524	C1654	A1819
	G171	A303	C385	C503	C565	C	A800	U922	A1055	G1150	U1147	A1052	A1525	C1655	
	G171	A304	C385	C504	C565	C	A800	U922	A1056	G1151	U1148	A1053	A1526	C1656	
	G171	A305	C385	C505	C565	C	A800	U922	A1057	G1152	U1149	A1054	A1527	C1657	
	G171	A306	C385	C506	C565	C	A800	U922	A1058	G1153	U1150	A1055	A1528	C1658	
	G171	A307	C385	C507	C565	C	A800	U922	A1059	G1154	U1151	A1056	A1529	C1659	
	G171	A308	C385	C508	C565	C	A800	U922	A1060	G1155	U1152	A1057	A1530	C1660	
	G171	A309	C385	C509	C565	C	A800	U922	A1061	G1156	U1153	A1058	A1531	C1661	
	G171	A310	C385	C510	C565	C	A800	U922	A1062	G1157	U1154	A1059	A1532	C1662	
	G171	A311	C385	C511	C565	C	A800	U922	A1063	G1158	U1155	A1060	A1533	C1663	
	G171	A312	C385	C512	C565	C	A800	U922	A1064	G1159	U1156	A1061	A1534	C1664	
	G171	A313	C385	C513	C565	C	A800	U922	A1065	G1160	U1157	A1062	A1535	C1665	
	G171	A314	C385	C514	C565	C	A800	U922	A1066	G1161	U1158	A1063	A1536	C1666	
	G171	A315	C385	C515	C565	C	A800	U922	A1067	G1162	U1159	A1064	A1537	C1667	
	G171	A316	C385	C516	C565	C	A800	U922	A1068	G1163	U1160	A1065	A1538	C1668	
	G171	A317	C385	C517	C565	C	A800	U922	A1069	G1164	U1161	A1066	A1539	C1669	
	G171	A318	C385	C518	C565	C	A800	U922	A1070	G1165	U1162	A1067	A1540	C1670	
	G171	A319	C385	C519	C565	C	A800	U922	A1071	G1166	U1163	A1068	A1541	C1671	
	G171	A320	C385	C520	C565	C	A800	U922	A1072	G1167	U1164	A1069	A1542	C1672	
	G171	A321	C385	C521	C565	C	A800	U922	A1073	G1168	U1165	A1070	A1543	C1673	
	G171	A322	C385	C522	C565	C	A800	U922	A1074	G1169	U1166	A1071	A1544	C1674	
	G171	A323	C385	C523	C565	C	A800	U922	A1075	G1170	U1167	A1072	A1545	C1675	
	G171	A324	C385	C524	C565	C	A800	U922	A1076	G1171	U1168	A1073	A1546	C1676	
	G171	A325	C385	C525	C565	C	A800	U922	A1077	G1172	U1169	A1074	A1547	C1677	
	G171	A326	C385	C526	C565	C	A800	U922	A1078	G1173	U1170	A1075	A1548	C1678	
	G171	A327	C385	C527	C565	C	A800	U922	A1079	G1174	U1171	A1076	A1549	C1679	
	G171	A328	C385	C528	C565	C	A800	U922	A1080	G1175	U1172	A1077	A1550	C1680	
	G171	A329	C385	C529	C565	C	A800	U922	A1081	G1176	U1173	A1078	A1551	C1681	
	G171	A330	C385	C530	C565	C	A800	U922	A1082	G1177	U1174	A1079	A1552	C1682	
	G171	A331	C385	C531	C565	C	A800	U922	A1083	G1178	U1175	A1080	A1553	C1683	
	G171	A332	C385	C532	C565	C	A800	U922	A1084	G1179	U1176	A1081	A1554	C1684	
	G171	A333	C385	C533	C565	C	A800	U922	A1085	G1180	U1177	A1082	A1555	C1685	
	G171	A334	C385	C534	C565	C	A800	U922	A1086	G1181	U1178	A1083	A1556	C1686	
	G171	A335	C385	C535	C565	C	A800	U922	A1087	G1182	U1179	A1084	A1557	C1687	
	G171	A336	C385	C536	C565	C	A800	U922	A1088	G1183	U1180	A1085	A1558	C1688	
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	G171	A339	C385	C539	C565	C	A800	U922	A1091	G1186	U1183	A1088	A1561	C1691	
	G171	A340	C385	C540	C565	C	A800	U922	A1092	G1187	U1184	A1089	A1562	C1692	
	G171	A341	C385	C541	C565	C	A800	U922	A1093	G1188	U1185	A1090	A1563	C1693	
	G171	A342	C385	C542	C565	C	A800	U922	A1094	G1189	U1186	A1091	A1564	C1694	
	G171	A343	C385	C543	C565	C	A800	U922	A1095	G1190	U1187	A1092	A1565	C1695	
	G171	A344	C385	C544	C565	C	A800	U922	A1096	G1191	U1188	A1093	A1566	C1696	
	G171	A345	C385	C545	C565	C	A800	U922	A1097	G1192	U1189	A1094	A1567	C1697	
	G171	A346	C385	C546	C565	C	A800	U922	A1098	G1193	U1190	A1095	A1568	C1698	
	G171	A347	C385	C547	C565	C	A800	U922	A1099	G1194	U1191	A1096	A1569	C1699	
	G171	A348	C385	C548	C565	C	A800	U922	A1100	G1195	U1192	A1097	A1570	C1700	
	G171	A349	C385	C549	C565	C	A800	U922	A1101	G1196	U1193	A1098	A1571	C1701	
	G171	A350	C385	C550	C565	C	A800	U922	A1102	G1197	U1194	A1099	A1572	C1702	
	G171	A351	C385	C551	C565	C	A800	U922	A1103	G1198	U1195	A1100	A1573	C1703	
	G171	A352	C385	C552	C565	C	A800	U922	A1104	G1199					

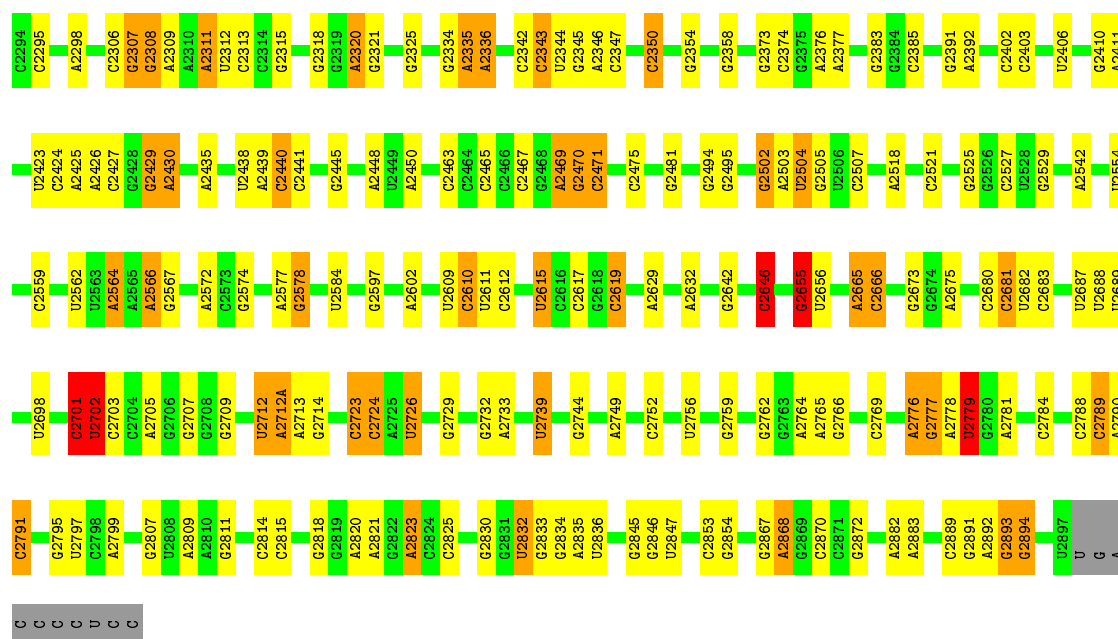


- Molecule 24: 23S rRNA

Chain YA:  66% 25% 6% ..

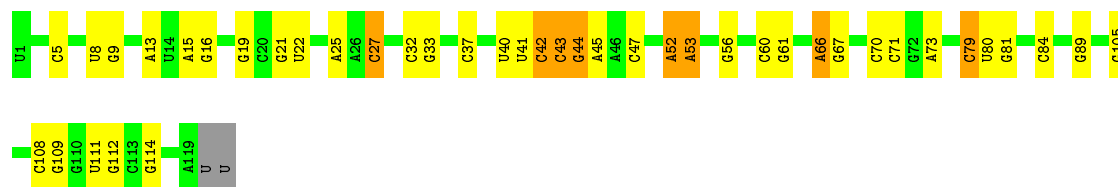


U2180	G2093	A1969	G1858	G1728	G1591	G1487	U1372	G1222	C1104	U1019	U907	A782	g	C584
G2181	G2100	A1970	A1859	A1729	G1595	G1491	C1375	C1223	U1105	A1020	U907	A783	g	C587
G2182	G2100	A1971	A1860	U1730	G1598	G1491	C1375	G1228	G1106	A1021	A910	A784	C	C
G2183	G2105	A1972	G1863	G1731	C1598	G1492	A1378	G1231	C1109	G1023	C915	G785	C	C
G2184	G2106	C1979	U1864	A1732	A1603	C1493	A1379	G1232	G1110	U1024	G916	G786	C	C
G2185	C2107	G1980	G1869	G1743	A1607	C1496	A1384	G1236	G1111	G1025	G917	A788	A	A
G2186	C2108	C1982	C1870	G1750	A1608	U1497	G1386	G1237	G1112	U1026	A918	G789	C	C
U2189	C2111	U1991	A1872	C1754	G1612	G1500	U1391	G1238	G1114	A1027	U930	C791	C	C
G2190	G2112	G1992	G1878	A1755	G1613	C1504	U1394	G1243	G1120	U1033	G931	G792	C	C
G2191	U2113	U1993	C1879	G1756	G1617	C1505	U1396	G1252	G1121	U1035	G932	G794	C	C
G2192	A2114	C1996	C1880	G1762	C1618	C1506	U1398	G1253	G1122	A1046	A941	C795	C	C
A2198	G2115	G1997	C1881	U1763	C1617	A1507	A1395	G1256	C1123	U1047	G942	A800	C	C
A2199	G2116	G1997	C1882	G1764	C1618	A1508	U1396	C1257	C1124	G1055	G943	A801	C	C
C2205	A2117	C1998	G1883	G1776	G1622	A1509	C1399	U1263	G1125	G1056	G944	G805	C	C
U2218	U2118	C1999	G1888	G1769	G1625	A1510	G1402	G1266	A1126	A1050	G945	U677	C	C
A2219	A2119	C2006	A1889	A1773	C1628	A1511	C1402	U1263	U1130	A1054	G946	C812	C	C
G2212	G2121	C2007	G1899	U1773	C1638	G1512	C1407	G1264	G1131	G1055	A953	A819	C	C
U2213	U2122	C2008	G1900	U1774	C1639	A1528	C1407	G1270	C1135	G1056	G956	A820	C	C
G2215	G2123	G2009	G1902	U1775	C1640	A1529	C1411	G1271	G1136	A1057	G957	A821	C	C
G2216	G2124	G2010	G1903	G1776	G1644	A1530	G1416	G1272	G1139	G1058	U958	C825	C	C
A2225	A2126	G2012	G1904	U1779	G1645	G1534	G1417	G1273	U1142	G1059	U959	U826	C	C
G2238	G2127	A2019	C1905	A1780	G1646	U1535	G1418	G1274	U1143	U1060	A960	U827	C	C
G2239	U2132	C2020	G1906	C1781	G1647	A1536	A1419	G1275	A1142	U1061	A961	U828	C	C
G2240	G2133	A2021	G1907	U1785	G1648	C1537	U1420	G1276	A1143	G1062	C961	A829	C	C
A2241	A2134	G2022	C1908	A1784	G1649	G1538	G1421	G1277	G1175	G1071	G981	U847	C	C
G2242	G2135	G2023	A1913	A1786	G1651	G1539	G1422	G1278	G1176	G1072	C982	C846	C	C
U2243	C2136	A2030	C1914	A1787	A1652	G1540	G1423	U1312	C1178	C1076	A983	C856	C	C
U2244	C2140	A2031	A1919	U1788	G1653	U1541	G1424	U1313	C1179	A1077	G987	U858	C	C
U2245	G2141	G2032	C1920	A1791	A1654	A1543	A1427	G1314	C1180	U1078	G988	G859	C	C
G2246	G2141	A2033	G1929	C1795	C1656	A1544	G1428	G1315	G1184	U1082	G989	U860	C	C
A2247	C2145	C2039	U1930	G1799	A1664	C1549	A1444A	U1316	G1190	U1083	C992	A866	C	C
G2258	G2146	U1931	U1931	C1800	G1667	C1567	G1445	G1317	G1195	A1084	C993	A752	C	C
A2266	G2147	C2043	A1936	G1801	A1668	A1568	A1449	G1318	C1196	C994	C994	C753	C	C
A2267	G2148	A2051	A1937	C1804	A1669	G1559	G1449A	G1319	C1197	A1085	C995	C754	C	C
C2275	G2151	G2052	U1938	G1811	G1674	A1566	U1454	G1320	G1198	A1086	C996	C755	C	C
A2278	G2152	C2053	U1939	A1815	C1686	A1567	G1455	G1321	G1199	C997	C997	C756	C	C
G2279	G2153	A2054	U1940	G1816	C1687	A1568	A1460	G1322	C1204	U1089	A1000	U757	C	C
G2280	G2154	C2055	U1955	G1817	C1688	A1569	G1461	G1323	G1205	G1090	C1005	C758	C	C
A2283	G2155	G2056	U1956	U1818	A1689	C1575	C1467	G1324	G1206	U1091	C1006	C759	C	C
C2284	G2156	A2059	C1957	U1819	U1693	U1578	G1467	U1325	G1207	U1092	C1007	C760	C	C
G2284	A2158	A2060	C1958	A1819	C1694	A1579	A1471	G1326	G1208	G1093	U1011	A764	C	C
C2285	G2165	G2061	G1959	G1826	G1695	A1580	G1474	U1327	G1209	U1094	U1012	G765	C	C
A2286	U2167	A2062	U1960	C1827	A1698	G1581	C1474	U1328	G1210	A1095	C1013	C766	C	C
A2287	U2168	U2068	U1963	G1828	A1699	G1582	G1475	U1329	G1211	A1096	G1017	A896	C	C
A2288	A2169	G2069	G1964	A1829	G1703	C1585	G1479	U1330	G1212	U1097	G1018	C897	C	C
G2289	G2170	G2070	C1965	G1835	G1725	A1586	G1480	A1365	A1220	A1103	C1018	A900	C	C
G2290	A2171	A2071	A1966	A1835	G1725	A1587	G1483	G1368	C1221					
U2291	U2172	C2092	C1967	A1847										
C2293	A2173	U2089	G1968											



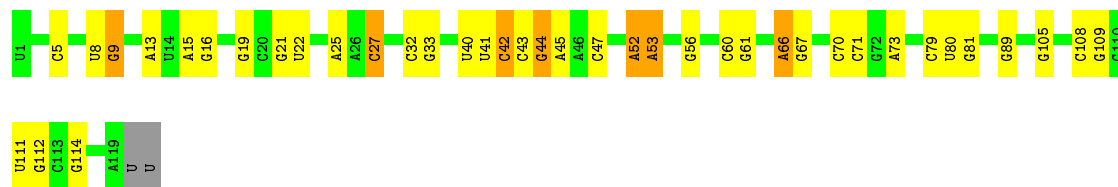
• Molecule 25: 5S rRNA

Chain RB: 64% 28% 7% •



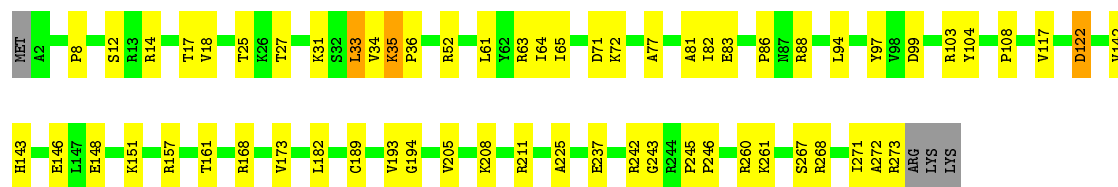
• Molecule 25: 5S rRNA

Chain YB: 66% 27% 6% •

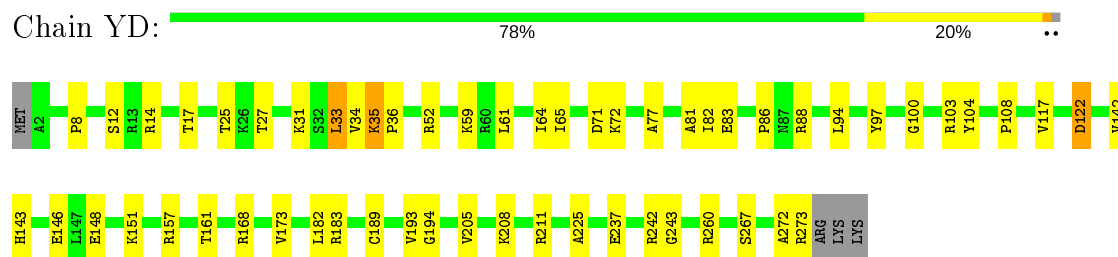


• Molecule 26: 50S ribosomal protein L2

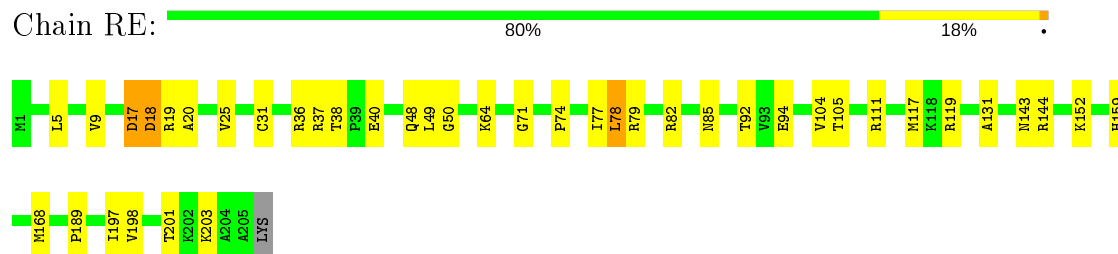
Chain RD: 76% 21% ••



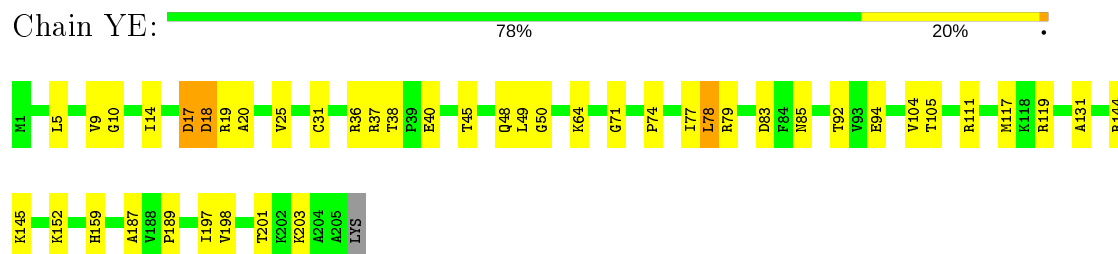
• Molecule 26: 50S ribosomal protein L2



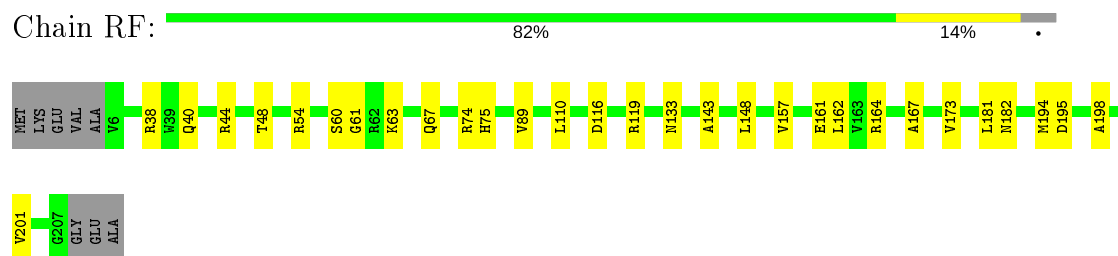
- Molecule 27: 50S ribosomal protein L3



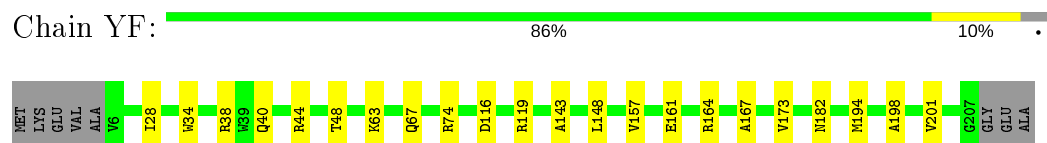
- Molecule 27: 50S ribosomal protein L3



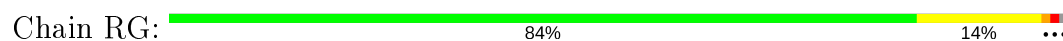
- Molecule 28: 50S ribosomal protein L4

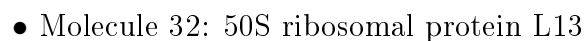


- Molecule 28: 50S ribosomal protein L4



- Molecule 29: 50S ribosomal protein L5





Chain YN:  91% 7% ..



- Molecule 33: 50S ribosomal protein L14

Chain RO:  89% 11% .




- Molecule 33: 50S ribosomal protein L14

Chain YO:  91% 8% .




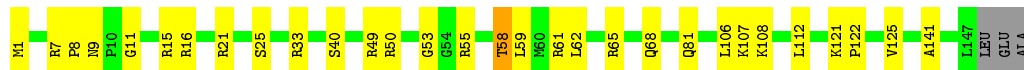
- Molecule 34: 50S ribosomal protein L15

Chain RP:  79% 21%




- Molecule 34: 50S ribosomal protein L15

Chain YP:  78% 19% ..




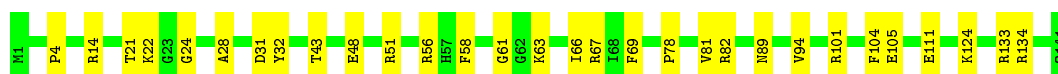
- Molecule 35: 50S ribosomal protein L16

Chain RQ:  76% 24%




- Molecule 35: 50S ribosomal protein L16

Chain YQ:  79% 21%




- Molecule 36: 50S ribosomal protein L17

Chain RR:  86% 13% ..




- Molecule 36: 50S ribosomal protein L17

Chain YR:  81% 18% .




- Molecule 37: 50S ribosomal protein L18

Chain RS:  83% 15% ..



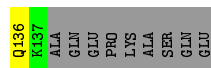
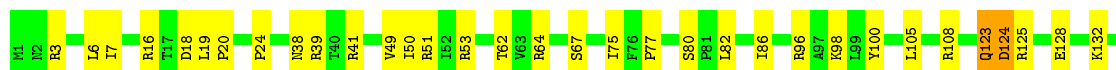
- Molecule 37: 50S ribosomal protein L18

Chain YS:  81% 17% ..



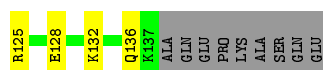
- Molecule 38: 50S ribosomal protein L19

Chain RT:  71% 22% • 6%




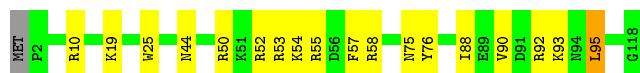
- Molecule 38: 50S ribosomal protein L19

Chain YT:  68% 25% • 6%



- Molecule 39: 50S ribosomal protein L20

Chain RU:  84% 14% ..




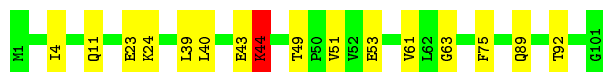
- Molecule 39: 50S ribosomal protein L20

Chain YU:  86% 11% ..




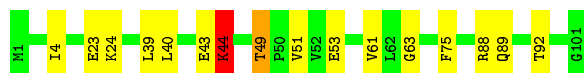
- Molecule 40: 50S ribosomal protein L21

Chain RV:  84% 15% .



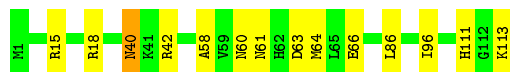
- Molecule 40: 50S ribosomal protein L21

Chain YV:  84% 14% ..



- Molecule 41: 50S ribosomal protein L22

Chain RW:  88% 12% .



- Molecule 41: 50S ribosomal protein L22

Chain YW:  89% 11%




- Molecule 42: 50S ribosomal protein L23

Chain RX:  80% 16% .




- Molecule 42: 50S ribosomal protein L23

Chain YX:  77% 19%




- Molecule 43: 50S ribosomal protein L24

Chain RY:  77% 20%



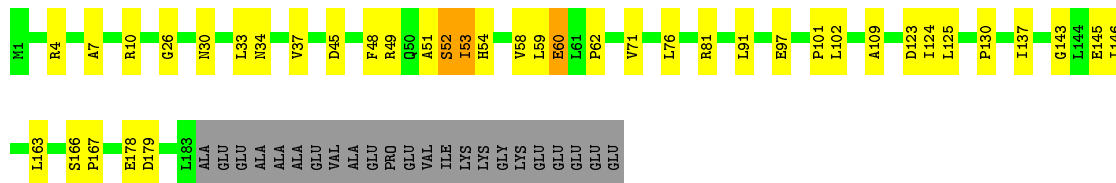
- Molecule 43: 50S ribosomal protein L24

Chain YY:  79% 18%



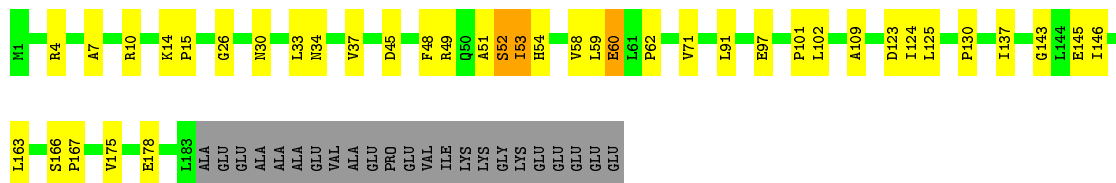
- Molecule 44: 50S ribosomal protein L25

Chain RZ:  69% 18% 11%




- Molecule 44: 50S ribosomal protein L25

Chain YZ:  69% 18% 11%



- Molecule 45: 50S ribosomal protein L27

Chain R0:  75% 20% 5%



- Molecule 45: 50S ribosomal protein L27

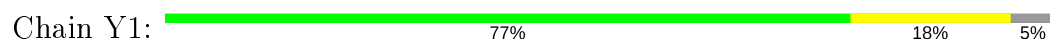
Chain Y0:  68% 20% 12%



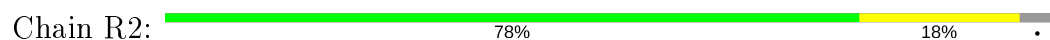
- Molecule 46: 50S ribosomal protein L28



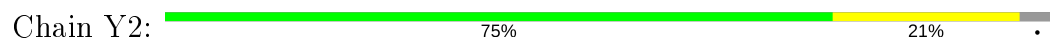
- Molecule 46: 50S ribosomal protein L28



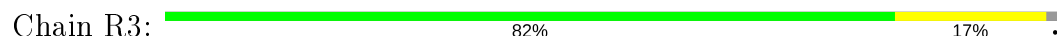
- Molecule 47: 50S ribosomal protein L29



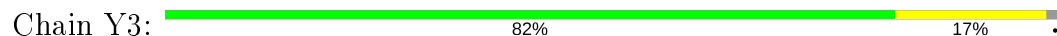
- Molecule 47: 50S ribosomal protein L29



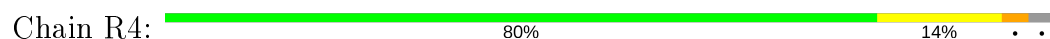
- Molecule 48: 50S ribosomal protein L30

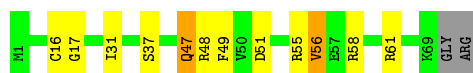


- Molecule 48: 50S ribosomal protein L30



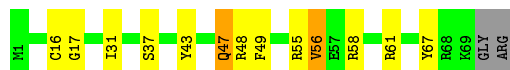
- Molecule 49: 50S ribosomal protein L31





- Molecule 49: 50S ribosomal protein L31

Chain Y4: 79% 15% . .



- Molecule 50: 50S ribosomal protein L32

Chain R5: 83% 15% .



- Molecule 50: 50S ribosomal protein L32

Chain Y5: 80% 18% .



- Molecule 51: 50S ribosomal protein L33

Chain R6: 87% 11% .



- Molecule 51: 50S ribosomal protein L33

Chain Y6: 91% 7% .



- Molecule 52: 50S ribosomal protein L34

Chain R7: 88% 8% .



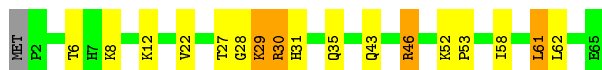
- Molecule 52: 50S ribosomal protein L34

Chain Y7: 86% 12% .



- Molecule 53: 50S ribosomal protein L35

Chain R8: 72% 20% 6%



- Molecule 53: 50S ribosomal protein L35

Chain Y8: 75% 17% 6%



- Molecule 54: 50S ribosomal protein L36

Chain R9: 81% 19%



- Molecule 54: 50S ribosomal protein L36

Chain Y9: 81% 19%



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	209.65Å 447.95Å 618.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	124.48 – 3.18	Depositor
% Data completeness (in resolution range)	99.3 (124.48-3.18)	Depositor
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.12	Depositor
R, R_{free}	0.232 , 0.251	Depositor
Wilson B-factor (Å ²)	76.7	Xtriage
Anisotropy	0.198	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	291753	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	QA	0.76	0/36046	1.03	110/56257 (0.2%)
1	XA	0.88	0/36097	1.04	113/56339 (0.2%)
2	QB	0.32	0/1942	0.58	0/2619
2	XB	0.37	0/1950	0.60	0/2630
3	QC	0.36	0/1629	0.53	0/2195
3	XC	0.36	0/1629	0.53	0/2195
4	QD	0.41	0/1733	0.55	0/2318
4	XD	0.41	0/1733	0.55	0/2318
5	QE	0.36	0/1171	0.55	0/1576
5	XE	0.36	0/1171	0.55	0/1576
6	QF	0.37	0/856	0.52	0/1154
6	XF	0.37	0/856	0.52	0/1154
7	QG	0.34	0/1276	0.47	0/1709
7	XG	0.33	0/1276	0.47	0/1709
8	QH	0.39	0/1128	0.54	0/1517
8	XH	0.39	0/1128	0.54	0/1517
9	QI	0.36	0/1029	0.60	0/1379
9	XI	0.43	1/1017 (0.1%)	0.62	0/1365
10	QJ	0.34	0/814	0.59	0/1095
10	XJ	0.39	0/790	0.60	0/1063
11	QK	0.38	0/900	0.55	0/1213
11	XK	0.43	0/879	0.56	0/1187
12	QL	0.45	0/991	0.64	0/1327
12	XL	0.54	0/972	0.66	0/1301
13	QM	0.36	0/965	0.61	0/1292
13	XM	0.37	0/956	0.63	0/1281
14	QN	0.43	0/501	0.64	1/664 (0.2%)
14	XN	0.43	0/501	0.64	1/664 (0.2%)
15	QO	0.32	0/745	0.51	0/992
15	XO	0.36	0/740	0.51	0/987
16	QP	0.43	0/721	0.56	0/970
16	XP	0.43	0/721	0.56	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.42	0/847	0.54	0/1131
17	XQ	0.42	0/847	0.54	0/1131
18	QR	0.36	0/579	0.56	0/768
18	XR	0.36	0/579	0.56	0/768
19	QS	0.33	0/680	0.67	0/915
19	XS	0.40	0/689	0.66	0/926
20	QT	0.32	0/765	0.57	0/1007
20	XT	0.32	0/765	0.56	0/1007
21	QU	0.40	0/221	0.69	0/288
21	XU	0.40	0/221	0.69	0/288
22	QV	0.85	1/1836 (0.1%)	1.01	6/2859 (0.2%)
22	XV	0.86	1/1836 (0.1%)	1.02	7/2859 (0.2%)
23	QX	0.59	0/290	1.08	2/450 (0.4%)
23	XX	0.65	0/268	0.84	0/416
24	RA	1.03	4/69521 (0.0%)	1.07	285/108529 (0.3%)
24	YA	1.16	8/69543 (0.0%)	1.11	344/108563 (0.3%)
25	RB	0.82	0/2878	1.01	6/4490 (0.1%)
25	YB	0.82	0/2878	1.01	5/4490 (0.1%)
26	RD	0.61	0/2165	0.71	1/2919 (0.0%)
26	YD	0.61	0/2165	0.71	1/2919 (0.0%)
27	RE	0.53	0/1601	0.71	2/2160 (0.1%)
27	YE	0.53	0/1601	0.71	2/2160 (0.1%)
28	RF	0.55	0/1620	0.59	0/2194
28	YF	0.55	0/1620	0.59	0/2194
29	RG	0.40	0/1499	0.65	2/2016 (0.1%)
29	YG	0.40	0/1499	0.65	2/2016 (0.1%)
30	RH	0.41	0/1362	0.65	0/1841
30	YH	0.41	0/1362	0.65	0/1841
31	RI	0.35	0/1151	0.66	0/1558
31	YI	0.35	0/1151	0.66	0/1558
32	RN	0.49	0/1131	0.65	1/1525 (0.1%)
32	YN	0.49	0/1131	0.65	1/1525 (0.1%)
33	RO	0.55	0/943	0.61	0/1269
33	YO	0.55	0/943	0.61	0/1269
34	RP	0.45	0/1162	0.76	1/1544 (0.1%)
34	YP	0.50	0/1139	0.79	1/1514 (0.1%)
35	RQ	0.50	0/1143	0.66	0/1527
35	YQ	0.50	0/1143	0.66	0/1527
36	RR	0.49	0/974	0.69	1/1302 (0.1%)
36	YR	0.51	0/974	0.67	1/1302 (0.1%)
37	RS	0.39	0/892	0.71	0/1187
37	YS	0.39	0/892	0.71	0/1187
38	RT	0.48	0/1155	0.66	1/1542 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YT	0.47	0/1155	0.66	1/1542 (0.1%)
39	RU	0.52	0/982	0.61	0/1306
39	YU	0.52	0/982	0.61	0/1306
40	RV	0.46	0/790	0.67	0/1057
40	YV	0.46	0/790	0.67	0/1057
41	RW	0.54	0/911	0.61	0/1220
41	YW	0.54	0/911	0.61	0/1220
42	RX	0.53	0/739	0.58	0/993
42	YX	0.53	0/739	0.58	0/993
43	RY	0.50	0/831	0.55	0/1108
43	YY	0.50	0/831	0.55	0/1108
44	RZ	0.39	0/1493	0.71	0/2026
44	YZ	0.39	0/1493	0.70	0/2026
45	R0	0.47	0/652	0.56	0/867
45	Y0	0.56	0/607	0.60	0/809
46	R1	0.54	0/770	0.65	0/1022
46	Y1	0.54	0/736	0.65	0/978
47	R2	0.36	0/583	0.53	0/771
47	Y2	0.36	0/583	0.53	0/771
48	R3	0.44	0/474	0.61	0/635
48	Y3	0.43	0/474	0.61	0/635
49	R4	0.36	0/578	0.62	0/776
49	Y4	0.36	0/578	0.62	0/776
50	R5	0.49	0/473	0.56	0/639
50	Y5	0.49	0/473	0.56	0/639
51	R6	0.32	0/460	0.50	0/613
51	Y6	0.32	0/460	0.50	0/613
52	R7	0.52	0/417	0.56	0/550
52	Y7	0.62	0/426	0.59	0/561
53	R8	0.54	0/525	0.83	2/691 (0.3%)
53	Y8	0.54	0/525	0.82	2/691 (0.3%)
54	R9	0.41	0/310	0.49	0/407
54	Y9	0.41	0/310	0.49	0/407
All	All	0.88	15/315585 (0.0%)	0.97	902/471827 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	QD	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	XD	0	2
12	QL	0	2
12	XL	0	2
19	QS	0	1
26	RD	0	4
26	YD	0	4
27	RE	0	4
27	YE	0	4
29	RG	0	1
29	YG	0	1
30	RH	0	2
30	YH	0	2
31	RI	0	2
31	YI	0	2
32	RN	0	1
32	YN	0	1
34	RP	0	1
34	YP	0	3
35	RQ	0	1
35	YQ	0	1
39	RU	0	1
39	YU	0	1
40	RV	0	2
40	YV	0	2
44	RZ	0	4
44	YZ	0	4
47	R2	0	1
47	Y2	0	1
49	R4	0	2
49	Y4	0	2
53	R8	0	4
53	Y8	0	4
All	All	0	71

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	QV	1	C	OP3-P	-10.78	1.48	1.61
22	XV	1	C	OP3-P	-10.77	1.48	1.61
24	YA	1142(A)	A	N9-C4	-5.74	1.34	1.37
24	YA	528	A	N9-C4	-5.62	1.34	1.37
9	XI	121	ARG	C-N	-5.60	1.21	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	YA	782	A	N9-C4	-5.43	1.34	1.37
24	YA	654	A	N9-C4	5.37	1.41	1.37
24	RA	74	A	N9-C4	-5.33	1.34	1.37
24	RA	1899	G	N9-C4	-5.32	1.33	1.38
24	YA	676	A	N9-C4	-5.29	1.34	1.37
24	YA	74	A	N9-C4	-5.25	1.34	1.37
24	YA	2060	A	N9-C4	-5.18	1.34	1.37
24	YA	686	G	C6-N1	-5.18	1.35	1.39
24	RA	2287	A	N9-C4	-5.16	1.34	1.37
24	RA	586	A	N9-C4	-5.13	1.34	1.37

All (902) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	1301	U	N1-C2-O2	13.33	132.13	122.80
1	XA	1158	C	N1-C2-O2	12.35	126.31	118.90
1	QA	1301	U	N3-C2-O2	-11.96	113.83	122.20
1	QA	1158	C	C2-N1-C1'	11.77	131.75	118.80
1	QA	1301	U	C2-N1-C1'	11.74	131.79	117.70
24	RA	856	C	C6-N1-C2	-11.62	115.65	120.30
1	XA	1158	C	C2-N1-C1'	11.59	131.55	118.80
24	RA	1931	U	N3-C2-O2	-10.97	114.52	122.20
1	QA	1158	C	N1-C2-O2	10.62	125.27	118.90
24	YA	860	U	N3-C2-O2	-10.51	114.84	122.20
24	YA	1313	U	C2-N1-C1'	10.50	130.30	117.70
24	RA	1931	U	N1-C2-O2	10.34	130.04	122.80
24	YA	1535	U	N1-C2-O2	10.00	129.80	122.80
1	XA	1301	U	C2-N1-C1'	9.81	129.47	117.70
1	XA	1158	C	N3-C2-O2	-9.70	115.11	121.90
24	RA	828	U	N3-C2-O2	-9.69	115.42	122.20
24	YA	1313	U	N1-C2-O2	9.67	129.57	122.80
1	XA	1301	U	N1-C2-O2	9.67	129.57	122.80
1	QA	1158	C	N3-C2-O2	-9.67	115.13	121.90
24	YA	856	C	C6-N1-C2	-9.63	116.45	120.30
24	RA	1313	U	N3-C2-O2	-9.62	115.47	122.20
1	QA	328	C	N1-C2-O2	9.56	124.64	118.90
24	RA	1313	U	C2-N1-C1'	9.55	129.16	117.70
24	RA	1654	A	O5'-P-OP1	-9.47	97.18	105.70
24	YA	1313	U	N3-C2-O2	-9.42	115.61	122.20
24	YA	120	U	N3-C2-O2	-9.38	115.63	122.20
24	RA	828	U	C2-N1-C1'	9.38	128.95	117.70
24	RA	828	U	N1-C2-O2	9.35	129.34	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	328	C	N1-C2-O2	9.27	124.46	118.90
1	XA	1301	U	N3-C2-O2	-9.26	115.72	122.20
24	RA	456	C	N1-C2-O2	9.25	124.45	118.90
24	YA	1535	U	C2-N1-C1'	9.00	128.50	117.70
24	RA	373	U	C2-N1-C1'	8.93	128.41	117.70
24	RA	1313	U	N1-C2-O2	8.86	129.00	122.80
24	YA	265	A	O4'-C1'-N9	8.85	115.28	108.20
24	RA	1535	U	C2-N1-C1'	8.84	128.31	117.70
24	YA	120	U	N1-C2-O2	8.84	128.98	122.80
24	YA	1535	U	N3-C2-O2	-8.79	116.05	122.20
1	XA	812	C	P-O3'-C3'	8.55	129.96	119.70
1	QA	1158	C	C6-N1-C2	-8.49	116.91	120.30
1	QA	328	C	C2-N1-C1'	8.48	128.13	118.80
24	YA	2868	A	N7-C8-N9	8.41	118.01	113.80
1	XA	449	C	C2-N1-C1'	8.34	127.98	118.80
24	YA	828	U	C2-N1-C1'	8.27	127.62	117.70
1	XA	543	C	C6-N1-C2	-8.23	117.01	120.30
24	RA	856	C	C5-C6-N1	8.22	125.11	121.00
24	YA	1882	C	N1-C2-O2	8.21	123.83	118.90
24	RA	120	U	N1-C2-O2	8.19	128.53	122.80
24	YA	2726	U	N3-C2-O2	-8.17	116.48	122.20
24	RA	456	C	C2-N1-C1'	8.14	127.76	118.80
1	XA	449	C	N1-C2-O2	8.14	123.78	118.90
1	QA	1301	U	C6-N1-C1'	-8.13	109.82	121.20
24	RA	2321	G	C4-N9-C1'	8.06	136.97	126.50
1	QA	1263	C	N1-C2-O2	8.04	123.72	118.90
24	YA	2712	U	N3-C2-O2	-8.03	116.58	122.20
24	YA	2723	C	C6-N1-C2	-8.03	117.09	120.30
24	YA	2868	A	C8-N9-C4	-8.01	102.60	105.80
24	YA	1130	U	P-O3'-C3'	8.00	129.30	119.70
1	QA	1158	C	C6-N1-C1'	-7.97	111.23	120.80
1	XA	1158	C	C6-N1-C1'	-7.93	111.29	120.80
24	RA	1304	C	N1-C2-O2	7.92	123.65	118.90
1	XA	1158	C	C6-N1-C2	-7.92	117.13	120.30
1	XA	328	C	C2-N1-C1'	7.91	127.50	118.80
24	RA	373	U	N1-C2-O2	7.90	128.33	122.80
24	YA	120	U	C2-N1-C1'	7.89	127.17	117.70
24	RA	1535	U	N1-C2-O2	7.88	128.32	122.80
24	YA	2584	U	C2-N1-C1'	7.88	127.15	117.70
1	QA	1322	C	C2-N1-C1'	7.86	127.44	118.80
24	YA	2815	C	C6-N1-C2	-7.85	117.16	120.30
24	RA	2688	U	N3-C2-O2	-7.84	116.71	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	YA	2726	U	N1-C2-O2	7.83	128.28	122.80
1	QA	328	C	N3-C2-O2	-7.83	116.42	121.90
24	RA	373	U	N3-C2-O2	-7.80	116.74	122.20
24	YA	828	U	N3-C2-O2	-7.72	116.80	122.20
24	RA	1899	G	N3-C4-N9	-7.68	121.39	126.00
1	QA	1322	C	N1-C2-O2	7.67	123.50	118.90
24	YA	2210	G	C4-N9-C1'	7.65	136.45	126.50
24	YA	2832	U	P-O3'-C3'	7.62	128.85	119.70
24	YA	1407	C	N1-C2-O2	7.61	123.47	118.90
24	YA	2584	U	N1-C2-O2	7.61	128.12	122.80
24	RA	120	U	N3-C2-O2	-7.57	116.90	122.20
24	RA	530	G	O4'-C1'-N9	7.52	114.22	108.20
1	XA	449	C	N3-C2-O2	-7.48	116.67	121.90
24	RA	613	U	N3-C2-O2	-7.46	116.98	122.20
1	XA	827	U	N3-C2-O2	-7.46	116.98	122.20
24	RA	588	U	C5-C6-N1	7.45	126.43	122.70
24	YA	2726	U	C2-N1-C1'	7.45	126.63	117.70
24	RA	2832	U	P-O3'-C3'	7.44	128.63	119.70
24	YA	503	A	P-O3'-C3'	7.41	128.59	119.70
1	QA	1065	U	P-O3'-C3'	7.41	128.59	119.70
24	YA	860	U	N1-C2-O2	7.40	127.98	122.80
24	YA	2712(A)	A	N7-C8-N9	7.40	117.50	113.80
24	YA	12	U	C2-N1-C1'	7.38	126.55	117.70
24	YA	669	G	C4-N9-C1'	7.34	136.05	126.50
24	RA	120	U	C2-N1-C1'	7.33	126.50	117.70
24	RA	930	U	C2-N1-C1'	7.32	126.48	117.70
24	YA	530	G	O4'-C1'-N9	7.26	114.01	108.20
24	RA	669	G	C4-N9-C1'	7.25	135.93	126.50
24	YA	2779	U	N3-C2-O2	-7.23	117.14	122.20
24	YA	2584	U	N3-C2-O2	-7.23	117.14	122.20
24	RA	1947	C	C6-N1-C2	-7.22	117.41	120.30
24	RA	373	U	C5-C6-N1	7.21	126.31	122.70
24	RA	1535	U	N3-C2-O2	-7.21	117.15	122.20
1	XA	1452	C	N1-C2-O2	7.21	123.22	118.90
24	YA	2705	A	N1-C2-N3	7.20	132.90	129.30
24	RA	2507	C	N1-C2-O2	7.17	123.20	118.90
1	QA	1297	C	P-O3'-C3'	7.16	128.29	119.70
24	YA	1314	C	C6-N1-C2	-7.16	117.44	120.30
24	RA	930	U	N1-C2-O2	7.15	127.80	122.80
24	YA	828	U	N1-C2-O2	7.14	127.80	122.80
1	QA	328	C	P-O3'-C3'	7.14	128.27	119.70
24	RA	613	U	N1-C2-O2	7.14	127.80	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	RA	1558	A	P-O3'-C3'	7.14	128.27	119.70
24	YA	2779	U	C2-N1-C1'	7.14	126.27	117.70
24	RA	2321	G	N3-C4-C5	-7.12	125.04	128.60
24	YA	1882	C	N3-C2-O2	-7.10	116.93	121.90
1	XA	1297	C	P-O3'-C3'	7.09	128.21	119.70
1	QA	792	A	P-O3'-C3'	7.08	128.20	119.70
24	RA	1947	C	N1-C2-O2	7.08	123.15	118.90
24	YA	1534	G	N3-C4-N9	7.08	130.25	126.00
24	YA	2688	U	N3-C2-O2	-7.08	117.25	122.20
24	RA	2870	C	C6-N1-C2	-7.08	117.47	120.30
24	RA	613	U	C2-N1-C1'	7.07	126.18	117.70
24	RA	1543	A	O4'-C1'-N9	7.06	113.85	108.20
24	RA	2584	U	C2-N1-C1'	7.03	126.13	117.70
24	YA	2779	U	N1-C2-O2	7.02	127.72	122.80
24	YA	846	C	P-O3'-C3'	7.02	128.13	119.70
24	YA	856	C	C5-C6-N1	7.02	124.51	121.00
24	YA	1882	C	C6-N1-C2	-7.02	117.49	120.30
24	YA	974(A)	C	N1-C2-O2	6.99	123.10	118.90
24	YA	12	U	N3-C2-O2	-6.99	117.31	122.20
24	YA	1332	G	C4-N9-C1'	6.97	135.57	126.50
24	RA	456	C	C6-N1-C2	-6.97	117.51	120.30
24	RA	1332	G	C4-N9-C1'	6.96	135.55	126.50
24	YA	974(A)	C	N3-C2-O2	-6.96	117.03	121.90
36	RR	75	LEU	CA-CB-CG	6.96	131.30	115.30
24	YA	2681	C	P-O3'-C3'	6.96	128.05	119.70
24	YA	1558	A	P-O3'-C3'	6.96	128.05	119.70
24	YA	12	U	N1-C2-O2	6.94	127.66	122.80
24	YA	621	A	O4'-C1'-N9	6.94	113.75	108.20
24	YA	860	U	C2-N1-C1'	6.94	126.02	117.70
24	YA	2321	G	C4-N9-C1'	6.93	135.51	126.50
24	RA	2559	C	N1-C2-O2	6.91	123.05	118.90
24	YA	783	A	N7-C8-N9	6.91	117.25	113.80
1	QA	1263	C	N3-C2-O2	-6.90	117.07	121.90
1	QA	1322	C	C6-N1-C2	-6.89	117.54	120.30
1	QA	1322	C	N3-C2-O2	-6.89	117.07	121.90
24	YA	2295	C	C6-N1-C2	-6.88	117.55	120.30
24	RA	456	C	N3-C2-O2	-6.87	117.09	121.90
24	RA	846	C	P-O3'-C3'	6.85	127.92	119.70
24	YA	404	C	P-O3'-C3'	6.85	127.92	119.70
24	YA	1882	C	C2-N1-C1'	6.84	126.32	118.80
1	XA	328	C	N3-C2-O2	-6.83	117.12	121.90
1	XA	687	A	P-O3'-C3'	6.83	127.89	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	RA	1899	G	N3-C4-C5	6.82	132.01	128.60
24	YA	783	A	C8-N9-C4	-6.82	103.07	105.80
24	RA	860	U	N3-C2-O2	-6.81	117.43	122.20
24	YA	838	C	N1-C2-O2	6.81	122.98	118.90
1	XA	1158	C	C5-C6-N1	6.80	124.40	121.00
24	RA	1686	C	N1-C2-O2	6.80	122.98	118.90
1	QA	687	A	P-O3'-C3'	6.79	127.85	119.70
24	RA	456	C	C5-C6-N1	6.79	124.39	121.00
24	YA	372	G	P-O3'-C3'	6.79	127.85	119.70
24	YA	2335	A	O4'-C1'-N9	6.79	113.63	108.20
1	XA	789	U	N3-C2-O2	-6.79	117.45	122.20
24	YA	372	G	OP2-P-O3'	6.78	120.11	105.20
1	XA	328	C	P-O3'-C3'	6.77	127.83	119.70
24	YA	2210	G	N3-C4-N9	6.77	130.06	126.00
24	YA	2712	U	P-O3'-C3'	6.75	127.81	119.70
24	YA	271(B)	G	P-O3'-C3'	6.75	127.80	119.70
1	QA	1498	U	P-O3'-C3'	6.74	127.79	119.70
24	YA	537	C	N1-C2-O2	6.74	122.94	118.90
24	RA	1022	G	P-O3'-C3'	6.74	127.78	119.70
24	RA	265	A	O4'-C1'-N9	6.73	113.58	108.20
1	QA	328	C	C6-N1-C2	-6.71	117.61	120.30
24	YA	1026	U	P-O3'-C3'	6.71	127.76	119.70
29	RG	82	LEU	CB-CG-CD1	-6.70	99.60	111.00
34	YP	59	LEU	CA-CB-CG	6.70	130.72	115.30
1	QA	1285	A	P-O3'-C3'	6.70	127.73	119.70
24	YA	2210	G	C8-N9-C1'	-6.70	118.30	127.00
24	YA	1956	U	N3-C2-O2	-6.68	117.52	122.20
1	QA	1528	U	P-O3'-C3'	6.68	127.72	119.70
24	YA	1313	U	C6-N1-C1'	-6.68	111.85	121.20
1	QA	1346	A	P-O3'-C3'	6.68	127.71	119.70
24	YA	459	U	N1-C2-O2	6.68	127.47	122.80
1	XA	992	U	P-O3'-C3'	6.67	127.71	119.70
24	YA	537	C	C6-N1-C2	-6.67	117.63	120.30
29	YG	82	LEU	CB-CG-CD1	-6.67	99.66	111.00
1	XA	1498	U	P-O3'-C3'	6.66	127.69	119.70
1	XA	1499	A	O5'-P-OP1	-6.66	99.71	105.70
1	QA	250	A	P-O3'-C3'	6.66	127.69	119.70
24	RA	2350	C	N1-C2-O2	6.66	122.89	118.90
24	RA	1931	U	C2-N1-C1'	6.65	125.68	117.70
24	RA	2210	G	C4-N9-C1'	6.64	135.14	126.50
1	XA	410	G	OP1-P-O3'	6.64	119.80	105.20
24	YA	1411	C	C6-N1-C2	-6.63	117.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	RA	537	C	C6-N1-C2	-6.63	117.65	120.30
24	YA	1022	G	P-O3'-C3'	6.63	127.65	119.70
24	RA	537	C	C5-C6-N1	6.62	124.31	121.00
24	RA	1980	G	P-O3'-C3'	6.62	127.64	119.70
24	YA	99	U	OP2-P-O3'	6.61	119.73	105.20
24	RA	1881	C	C6-N1-C2	-6.61	117.66	120.30
24	RA	404	C	P-O3'-C3'	6.60	127.62	119.70
1	QA	812	C	P-O3'-C3'	6.57	127.58	119.70
24	RA	930	U	N3-C2-O2	-6.57	117.61	122.20
1	QA	992	U	P-O3'-C3'	6.56	127.57	119.70
1	XA	1285	A	P-O3'-C3'	6.55	127.57	119.70
1	XA	1301	U	C6-N1-C1'	-6.54	112.05	121.20
36	YR	75	LEU	CA-CB-CG	6.53	130.32	115.30
24	RA	1882	C	N1-C2-O2	6.53	122.82	118.90
1	QA	449	C	C2-N1-C1'	6.52	125.97	118.80
24	YA	637	A	P-O3'-C3'	6.52	127.53	119.70
24	YA	758	C	C6-N1-C2	-6.52	117.69	120.30
24	YA	1534	G	N3-C4-C5	-6.52	125.34	128.60
24	RA	637	A	P-O3'-C3'	6.51	127.51	119.70
24	YA	1314	C	C5-C6-N1	6.50	124.25	121.00
24	YA	1653	G	P-O3'-C3'	6.50	127.50	119.70
24	YA	1332	G	C6-C5-N7	-6.49	126.50	130.40
24	YA	2559	C	C6-N1-C2	-6.49	117.70	120.30
24	RA	2321	G	C8-N9-C1'	-6.49	118.56	127.00
1	XA	812	C	OP2-P-O3'	6.49	119.47	105.20
24	RA	2559	C	C6-N1-C2	-6.48	117.71	120.30
1	XA	792	A	O4'-C1'-N9	6.48	113.38	108.20
24	RA	1332	G	C6-C5-N7	-6.47	126.52	130.40
24	YA	99	U	P-O3'-C3'	6.47	127.47	119.70
24	YA	385	C	C6-N1-C2	-6.46	117.71	120.30
24	RA	503	A	P-O3'-C3'	6.45	127.44	119.70
1	XA	1027	C	P-O3'-C3'	6.45	127.44	119.70
1	QA	789	U	N3-C2-O2	-6.44	117.69	122.20
24	YA	1402	C	C6-N1-C2	-6.44	117.72	120.30
24	YA	1786	A	N7-C8-N9	6.44	117.02	113.80
1	QA	1026	G	N3-C4-N9	6.44	129.86	126.00
24	RA	1686	C	N3-C2-O2	-6.44	117.39	121.90
24	YA	1598	C	C6-N1-C2	-6.43	117.73	120.30
24	RA	2688	U	C2-N1-C1'	6.42	125.41	117.70
24	YA	385	C	C2-N1-C1'	6.42	125.86	118.80
24	RA	817	C	C6-N1-C2	-6.42	117.73	120.30
1	XA	189	U	N1-C2-O2	-6.41	118.31	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	RA	1947	C	C5-C6-N1	6.41	124.20	121.00
1	QA	369	C	N1-C2-O2	6.41	122.75	118.90
24	YA	242	G	P-O3'-C3'	6.40	127.38	119.70
24	RA	601	C	C6-N1-C2	-6.40	117.74	120.30
24	RA	1407	C	N1-C2-O2	6.40	122.74	118.90
24	RA	2126	A	P-O3'-C3'	6.39	127.37	119.70
24	YA	669	G	C8-N9-C1'	-6.39	118.69	127.00
1	QA	1347	G	P-O3'-C3'	6.39	127.37	119.70
24	YA	752	A	P-O3'-C3'	6.39	127.37	119.70
1	XA	60	A	P-O3'-C3'	6.38	127.36	119.70
1	XA	449	C	C6-N1-C2	-6.38	117.75	120.30
24	RA	1670	C	N1-C2-O2	6.38	122.73	118.90
24	YA	1967	C	N1-C2-O2	6.34	122.71	118.90
24	YA	1095	A	C2-N3-C4	6.34	113.77	110.60
1	QA	913	A	P-O3'-C3'	6.34	127.30	119.70
24	RA	2655	G	OP2-P-O3'	6.33	119.14	105.20
24	RA	1312	U	P-O3'-C3'	6.33	127.30	119.70
24	RA	752	A	P-O3'-C3'	6.33	127.29	119.70
24	RA	669	G	C8-N9-C1'	-6.32	118.78	127.00
24	RA	1905	C	N1-C2-O2	6.32	122.69	118.90
24	YA	420	C	N1-C2-O2	6.31	122.69	118.90
24	YA	1694	C	P-O3'-C3'	6.31	127.27	119.70
24	YA	1774	C	C5-C6-N1	6.31	124.16	121.00
24	RA	838	C	N1-C2-O2	6.31	122.69	118.90
1	QA	484	G	P-O3'-C3'	6.30	127.27	119.70
1	XA	1452	C	N3-C2-O2	-6.30	117.49	121.90
24	YA	503	A	OP2-P-O3'	6.30	119.06	105.20
24	RA	1375	C	C6-N1-C2	-6.29	117.78	120.30
24	YA	930	U	N3-C2-O2	-6.29	117.80	122.20
24	YA	517	C	C5-C6-N1	6.28	124.14	121.00
24	YA	2210	G	N3-C4-C5	-6.28	125.46	128.60
1	QA	1263	C	C2-N1-C1'	6.28	125.70	118.80
24	YA	930	U	C2-N1-C1'	6.28	125.23	117.70
1	XA	1446	A	P-O3'-C3'	6.27	127.22	119.70
24	RA	2726	U	C2-N1-C1'	6.27	125.22	117.70
23	QX	14	A	C2-N3-C4	6.26	113.73	110.60
24	RA	1026	U	OP1-P-O3'	6.26	118.97	105.20
24	RA	2321	G	N3-C4-N9	6.26	129.75	126.00
24	RA	229	A	P-O3'-C3'	6.26	127.21	119.70
24	RA	2726	U	N3-C2-O2	-6.25	117.82	122.20
24	RA	2498	C	N1-C2-O2	6.25	122.65	118.90
24	YA	2559	C	N1-C2-O2	6.24	122.65	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	1024	G	O5'-P-OP1	6.24	118.19	110.70
24	RA	253	C	C6-N1-C2	-6.24	117.80	120.30
24	YA	385	C	N3-C2-O2	-6.23	117.54	121.90
1	XA	328	C	C6-N1-C2	-6.22	117.81	120.30
1	XA	266	G	P-O3'-C3'	6.22	127.16	119.70
24	RA	1180	C	N1-C2-O2	6.21	122.62	118.90
24	RA	253	C	N1-C2-O2	6.20	122.62	118.90
24	RA	1535	U	C6-N1-C1'	-6.19	112.54	121.20
24	YA	1012	U	OP2-P-O3'	6.19	118.82	105.20
24	RA	2439	A	P-O3'-C3'	6.19	127.13	119.70
1	QA	115	G	P-O3'-C3'	6.16	127.10	119.70
24	YA	267	C	C6-N1-C2	-6.16	117.83	120.30
24	YA	930	U	N1-C2-O2	6.16	127.11	122.80
24	YA	1931	U	N3-C2-O2	-6.16	117.89	122.20
24	YA	635	C	C6-N1-C2	-6.14	117.85	120.30
1	XA	115	G	P-O3'-C3'	6.13	127.05	119.70
24	YA	461	C	C6-N1-C2	-6.12	117.85	120.30
24	YA	1407	C	C5-C6-N1	6.12	124.06	121.00
1	QA	753	A	P-O3'-C3'	6.11	127.04	119.70
24	RA	1786	A	C5-N7-C8	-6.11	100.84	103.90
24	YA	1908	C	C6-N1-C2	-6.11	117.86	120.30
24	RA	1304	C	N3-C2-O2	-6.11	117.62	121.90
24	RA	1934	C	N1-C2-O2	6.11	122.57	118.90
1	XA	530	G	C4-N9-C1'	6.11	134.44	126.50
24	RA	222	A	P-O3'-C3'	6.11	127.03	119.70
24	YA	1314	C	N1-C2-O2	6.11	122.56	118.90
24	RA	2043	C	C6-N1-C2	-6.10	117.86	120.30
1	QA	266	G	P-O3'-C3'	6.09	127.01	119.70
24	RA	1045	A	P-O3'-C3'	6.09	127.00	119.70
24	RA	1786	A	N7-C8-N9	6.09	116.84	113.80
24	YA	2712	U	N1-C2-O2	6.09	127.06	122.80
1	XA	913	A	P-O3'-C3'	6.07	126.98	119.70
24	YA	754	C	C6-N1-C2	-6.06	117.88	120.30
24	YA	140	A	N7-C8-N9	6.06	116.83	113.80
24	RA	1026	U	P-O3'-C3'	6.06	126.97	119.70
24	RA	1005	C	N1-C2-O2	6.05	122.53	118.90
24	RA	2889	C	N1-C2-O2	6.05	122.53	118.90
24	YA	1506	C	C6-N1-C2	-6.04	117.88	120.30
24	YA	1799	G	P-O3'-C3'	6.04	126.95	119.70
1	XA	543	C	N3-C2-O2	-6.04	117.67	121.90
24	RA	1882	C	C6-N1-C2	-6.04	117.89	120.30
24	YA	1332	G	N7-C8-N9	6.03	116.12	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	RA	2559	C	C5-C6-N1	6.03	124.02	121.00
24	YA	537	C	N3-C2-O2	-6.03	117.68	121.90
1	XA	753	A	P-O3'-C3'	6.03	126.93	119.70
1	QA	1200	C	P-O3'-C3'	6.02	126.93	119.70
24	RA	1992	G	P-O3'-C3'	6.02	126.93	119.70
24	YA	1914	C	C2-N1-C1'	6.01	125.41	118.80
24	YA	229	A	P-O3'-C3'	6.01	126.91	119.70
24	RA	285	C	N1-C2-O2	6.01	122.50	118.90
1	QA	410	G	OP1-P-O3'	6.00	118.41	105.20
24	YA	2889	C	N1-C2-O2	6.00	122.50	118.90
1	QA	353	A	OP2-P-O3'	6.00	118.40	105.20
24	RA	1914	C	C2-N1-C1'	6.00	125.40	118.80
24	YA	221	A	P-O3'-C3'	5.99	126.89	119.70
24	YA	2043	C	N1-C2-O2	5.99	122.49	118.90
24	RA	1332	G	N7-C8-N9	5.99	116.09	113.10
24	YA	859	G	P-O3'-C3'	5.98	126.88	119.70
24	YA	974(A)	C	P-O3'-C3'	5.98	126.88	119.70
24	RA	2688	U	N1-C2-O2	5.98	126.99	122.80
24	YA	2769	C	N1-C2-O2	5.98	122.49	118.90
24	YA	2610	C	P-O3'-C3'	5.97	126.87	119.70
1	QA	244	U	P-O3'-C3'	5.97	126.87	119.70
1	XA	1439	C	N1-C2-O2	5.97	122.48	118.90
24	YA	2566	A	P-O3'-C3'	5.97	126.86	119.70
24	RA	1686	C	C6-N1-C2	-5.97	117.91	120.30
24	YA	459	U	N3-C2-O2	-5.97	118.02	122.20
24	YA	992	C	N1-C2-O2	5.97	122.48	118.90
1	XA	410	G	P-O3'-C3'	5.96	126.86	119.70
24	YA	1992	G	P-O3'-C3'	5.96	126.86	119.70
24	RA	1899	G	C4-N9-C1'	-5.96	118.75	126.50
14	QN	44	LEU	CA-CB-CG	5.96	129.01	115.30
14	XN	44	LEU	CA-CB-CG	5.96	129.00	115.30
24	YA	1314	C	C2-N1-C1'	5.95	125.34	118.80
1	QA	254	G	O5'-P-OP1	-5.95	100.35	105.70
24	YA	795	C	C6-N1-C2	-5.95	117.92	120.30
24	YA	1644	C	N1-C2-O2	5.95	122.47	118.90
24	RA	2566	A	P-O3'-C3'	5.94	126.83	119.70
24	RA	1653	G	P-O3'-C3'	5.94	126.83	119.70
1	XA	1310	G	P-O3'-C3'	5.94	126.82	119.70
1	XA	484	G	P-O3'-C3'	5.93	126.82	119.70
22	QV	35	C	P-O3'-C3'	5.92	126.81	119.70
1	XA	233	C	N3-C2-O2	-5.92	117.75	121.90
24	YA	76	C	N1-C2-O2	5.92	122.45	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	YA	1012	U	P-O3'-C3'	5.92	126.81	119.70
1	QA	119	A	P-O3'-C3'	5.92	126.80	119.70
1	XA	244	U	P-O3'-C3'	5.92	126.80	119.70
24	YA	2321	G	C8-N9-C1'	-5.92	119.31	127.00
1	QA	789	U	C2-N1-C1'	5.92	124.80	117.70
24	RA	18	C	C6-N1-C2	-5.92	117.93	120.30
24	YA	838	C	C6-N1-C2	-5.91	117.94	120.30
22	XV	35	C	P-O3'-C3'	5.91	126.79	119.70
24	RA	595	C	C6-N1-C2	-5.91	117.94	120.30
1	XA	412	A	P-O3'-C3'	5.91	126.79	119.70
24	RA	1427	A	P-O3'-C3'	5.90	126.78	119.70
24	RA	1899	G	C8-N9-C1'	5.90	134.67	127.00
24	YA	385	C	N1-C2-O2	5.90	122.44	118.90
24	YA	1085	A	P-O3'-C3'	5.89	126.77	119.70
24	YA	1993	U	O5'-P-OP1	-5.89	100.39	105.70
24	RA	372	G	P-O3'-C3'	5.89	126.77	119.70
1	XA	243	A	P-O3'-C3'	5.89	126.77	119.70
24	RA	1902	C	N1-C2-O2	5.89	122.43	118.90
1	XA	1260	C	C6-N1-C2	-5.89	117.94	120.30
24	RA	1509	C	OP1-P-O3'	5.88	118.14	105.20
24	RA	1257	C	C6-N1-C2	-5.88	117.95	120.30
24	YA	333	G	C4-N9-C1'	5.88	134.14	126.50
24	RA	2726	U	N1-C2-O2	5.87	126.91	122.80
1	XA	377	G	O5'-P-OP1	-5.87	100.42	105.70
24	RA	1267	U	N1-C2-O2	5.87	126.91	122.80
1	XA	328	C	C5-C6-N1	5.87	123.93	121.00
24	RA	2584	U	N1-C2-O2	5.87	126.91	122.80
1	QA	1026	G	C4-N9-C1'	5.87	134.12	126.50
24	RA	676	A	C5-N7-C8	-5.87	100.97	103.90
24	RA	1544	C	N1-C2-O2	5.86	122.42	118.90
1	QA	485	G	P-O3'-C3'	5.85	126.72	119.70
1	XA	810	C	N3-C2-O2	-5.85	117.81	121.90
24	YA	2336	A	C5-C6-N6	-5.84	119.03	123.70
24	RA	512	G	P-O3'-C3'	5.84	126.71	119.70
24	RA	1786	A	C4-C5-N7	5.84	113.62	110.70
24	YA	1958	C	C5-C6-N1	5.84	123.92	121.00
24	YA	783	A	C5-N7-C8	-5.83	100.98	103.90
24	RA	828	U	C6-N1-C1'	-5.83	113.04	121.20
24	YA	541	C	C6-N1-C2	-5.83	117.97	120.30
24	YA	2584	U	C6-N1-C1'	-5.83	113.04	121.20
24	YA	1427	A	P-O3'-C3'	5.82	126.68	119.70
24	RA	731	C	C6-N1-C2	-5.82	117.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	RA	1956	U	N3-C2-O2	-5.82	118.13	122.20
1	XA	233	C	C6-N1-C2	-5.82	117.97	120.30
24	YA	1535	U	C6-N1-C1'	-5.82	113.06	121.20
24	RA	1313	U	C6-N1-C2	-5.81	117.52	121.00
24	RA	221	A	P-O3'-C3'	5.81	126.67	119.70
24	RA	2210	G	C8-N9-C1'	-5.81	119.45	127.00
1	QA	932	C	N1-C2-O2	5.80	122.38	118.90
24	RA	420	C	N1-C2-O2	5.80	122.38	118.90
24	RA	944	G	C4-N9-C1'	5.79	134.03	126.50
24	RA	385	C	N3-C2-O2	-5.79	117.85	121.90
1	QA	754	C	C2-N1-C1'	5.79	125.17	118.80
1	QA	1321	C	C6-N1-C2	-5.78	117.99	120.30
24	YA	2688	U	C2-N1-C1'	5.78	124.64	117.70
24	YA	1407	C	C6-N1-C2	-5.78	117.99	120.30
24	YA	611	C	N1-C2-O2	5.78	122.36	118.90
24	YA	654	A	C2-N3-C4	5.78	113.49	110.60
24	YA	2321	G	N3-C4-N9	5.77	129.46	126.00
24	RA	1376	C	N1-C2-O2	5.77	122.36	118.90
24	RA	1644	C	N1-C2-O2	5.77	122.36	118.90
25	RB	66	A	P-O3'-C3'	5.77	126.62	119.70
24	YA	2465	C	N3-C2-O2	-5.77	117.86	121.90
24	YA	1407	C	N3-C2-O2	-5.76	117.87	121.90
25	YB	66	A	P-O3'-C3'	5.76	126.61	119.70
24	RA	2060	A	P-O3'-C3'	5.75	126.60	119.70
24	RA	1396	U	C2-N1-C1'	5.75	124.60	117.70
24	RA	1983	C	N1-C2-O2	5.75	122.35	118.90
1	QA	1158	C	C5-C6-N1	5.75	123.87	121.00
24	RA	2584	U	N3-C2-O2	-5.74	118.18	122.20
24	YA	1956	U	N1-C2-O2	5.74	126.82	122.80
24	RA	2767	C	C6-N1-C2	-5.74	118.00	120.30
24	YA	1644	C	C6-N1-C2	-5.74	118.00	120.30
1	QA	182	U	C5-C6-N1	5.74	125.57	122.70
1	XA	503	C	C6-N1-C2	-5.74	118.01	120.30
24	YA	1881	C	C6-N1-C2	-5.73	118.01	120.30
24	YA	1992	G	OP2-P-O3'	5.73	117.81	105.20
24	YA	752	A	OP2-P-O3'	5.73	117.81	105.20
24	RA	1992	G	OP2-P-O3'	5.73	117.80	105.20
24	YA	2471	C	N1-C2-O2	5.73	122.34	118.90
24	RA	2610	C	P-O3'-C3'	5.73	126.57	119.70
24	YA	201	C	N1-C2-O2	5.72	122.33	118.90
24	YA	1598	C	C5-C6-N1	5.72	123.86	121.00
24	RA	1947	C	N3-C2-O2	-5.72	117.90	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	RA	2689	U	P-O3'-C3'	5.72	126.56	119.70
24	YA	613	U	C2-N1-C1'	5.71	124.56	117.70
24	YA	613	U	N3-C2-O2	-5.71	118.20	122.20
1	XA	1439	C	C6-N1-C2	-5.71	118.02	120.30
24	RA	817	C	C5-C6-N1	5.70	123.85	121.00
1	QA	243	A	P-O3'-C3'	5.70	126.54	119.70
24	RA	2211	G	C4-N9-C1'	5.70	133.91	126.50
1	QA	686	U	N3-C2-O2	-5.70	118.21	122.20
24	RA	1078	U	P-O3'-C3'	5.70	126.54	119.70
24	YA	459	U	C2-N1-C1'	5.70	124.54	117.70
24	RA	2559	C	N3-C2-O2	-5.70	117.91	121.90
24	RA	1658	C	C5-C6-N1	5.69	123.84	121.00
24	YA	2320	A	C2-N3-C4	5.69	113.44	110.60
24	YA	1386	C	C6-N1-C2	-5.68	118.03	120.30
24	RA	2868	A	N7-C8-N9	5.68	116.64	113.80
34	RP	59	LEU	CA-CB-CG	5.68	128.37	115.30
24	YA	1313	U	C5-C6-N1	5.68	125.54	122.70
24	YA	1474	C	C6-N1-C2	-5.67	118.03	120.30
24	RA	1644	C	C6-N1-C2	-5.67	118.03	120.30
24	RA	1931	U	C5-C4-O4	5.67	129.30	125.90
24	YA	565	C	N1-C2-O2	5.66	122.30	118.90
24	YA	1882	C	C5-C6-N1	5.66	123.83	121.00
24	RA	1656	C	C6-N1-C2	-5.66	118.04	120.30
24	YA	1407	C	C2-N1-C1'	5.66	125.03	118.80
1	QA	1301	U	C5-C6-N1	5.66	125.53	122.70
24	YA	2321	G	N3-C4-C5	-5.65	125.77	128.60
22	XV	53	G	P-O3'-C3'	5.65	126.48	119.70
1	QA	412	A	P-O3'-C3'	5.65	126.48	119.70
24	RA	1313	U	C6-N1-C1'	-5.65	113.29	121.20
24	YA	1905	C	N1-C2-O2	5.64	122.29	118.90
24	RA	99	U	P-O3'-C3'	5.64	126.47	119.70
32	RN	120	LEU	CA-CB-CG	5.64	128.27	115.30
24	YA	1509	C	OP1-P-O3'	5.64	117.60	105.20
24	YA	1460	A	OP2-P-O3'	5.64	117.60	105.20
32	YN	120	LEU	CA-CB-CG	5.63	128.25	115.30
53	Y8	61	LEU	CA-CB-CG	-5.63	102.35	115.30
24	RA	1899	G	C2-N3-C4	-5.63	109.09	111.90
1	XA	254	G	O5'-P-OP1	-5.62	100.64	105.70
24	RA	345	A	P-O3'-C3'	5.62	126.44	119.70
1	QA	1322	C	C5-C6-N1	5.62	123.81	121.00
24	RA	2832	U	OP2-P-O3'	5.62	117.56	105.20
24	YA	268	C	N1-C2-O2	5.61	122.27	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	R8	61	LEU	CA-CB-CG	-5.61	102.39	115.30
24	RA	271(B)	G	P-O3'-C3'	5.61	126.43	119.70
24	YA	2646	C	C6-N1-C2	-5.61	118.06	120.30
24	RA	1474	C	C6-N1-C2	-5.61	118.06	120.30
22	QV	53	G	P-O3'-C3'	5.60	126.42	119.70
1	XA	1452	C	C2-N1-C1'	5.60	124.96	118.80
24	YA	860	U	C6-N1-C2	-5.60	117.64	121.00
24	YA	1402	C	N1-C2-O2	5.59	122.26	118.90
1	QA	810	C	N1-C2-O2	5.59	122.25	118.90
24	YA	1786	A	C4-N9-C1'	5.59	136.37	126.30
1	XA	827	U	C6-N1-C2	-5.58	117.65	121.00
24	RA	2417	C	C6-N1-C2	-5.58	118.07	120.30
24	YA	1411	C	C5-C6-N1	5.57	123.79	121.00
24	YA	1776	G	C4-N9-C1'	5.57	133.75	126.50
24	YA	2868	A	C5-N7-C8	-5.57	101.11	103.90
24	RA	271(B)	G	OP2-P-O3'	5.57	117.45	105.20
24	YA	1781	C	C2-N1-C1'	5.57	124.93	118.80
27	RE	117	MET	CA-CB-CG	5.57	122.77	113.30
24	YA	650	C	C6-N1-C2	-5.57	118.07	120.30
1	XA	810	C	N1-C2-O2	5.57	122.24	118.90
24	YA	201	C	N3-C2-O2	-5.57	118.00	121.90
24	YA	1544	C	N1-C2-O2	5.56	122.24	118.90
24	YA	2559	C	C5-C6-N1	5.56	123.78	121.00
1	XA	543	C	N1-C2-O2	5.56	122.23	118.90
24	YA	18	C	N3-C2-O2	-5.55	118.01	121.90
24	YA	1332	G	C8-N9-C1'	-5.55	119.78	127.00
24	YA	2507	C	N1-C2-O2	5.55	122.23	118.90
24	YA	2723	C	C5-C6-N1	5.55	123.78	121.00
1	QA	1321	C	C5-C6-N1	5.55	123.78	121.00
1	XA	485	G	P-O3'-C3'	5.55	126.36	119.70
1	QA	690	G	O4'-C1'-N9	5.55	112.64	108.20
27	YE	117	MET	CA-CB-CG	5.55	122.73	113.30
24	RA	1332	G	C8-N9-C1'	-5.54	119.79	127.00
24	RA	373	U	C6-N1-C2	-5.54	117.67	121.00
24	YA	1955	U	P-O3'-C3'	5.54	126.35	119.70
24	RA	2586	C	C5-C6-N1	5.54	123.77	121.00
24	YA	753	C	C6-N1-C2	-5.54	118.08	120.30
24	YA	2776	A	P-O3'-C3'	5.54	126.34	119.70
22	QV	49	C	N1-C2-O2	5.53	122.22	118.90
24	RA	2350	C	N3-C2-O2	-5.53	118.03	121.90
24	RA	140	A	N7-C8-N9	5.53	116.56	113.80
24	RA	1914	C	N1-C2-O2	5.53	122.22	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	689	C	N1-C2-O2	5.53	122.22	118.90
24	YA	2559	C	N3-C2-O2	-5.53	118.03	121.90
24	RA	1510	A	C2-N3-C4	5.52	113.36	110.60
1	XA	827	U	C2-N1-C1'	5.52	124.33	117.70
24	YA	1257	C	C6-N1-C2	-5.52	118.09	120.30
1	QA	410	G	P-O3'-C3'	5.52	126.33	119.70
24	RA	114	U	C2-N1-C1'	5.52	124.33	117.70
24	RA	1970	A	O4'-C1'-N9	-5.52	103.79	108.20
24	YA	753	C	C5-C6-N1	5.51	123.76	121.00
22	XV	49	C	N3-C2-O2	-5.51	118.04	121.90
24	YA	654	A	N3-C4-N9	5.51	131.81	127.40
24	YA	2655	G	OP2-P-O3'	5.51	117.33	105.20
24	RA	2586	C	C6-N1-C2	-5.51	118.10	120.30
1	XA	250	A	P-O3'-C3'	5.51	126.31	119.70
1	QA	328	C	C6-N1-C1'	-5.51	114.19	120.80
1	QA	1038	C	N1-C2-O2	5.51	122.20	118.90
24	RA	1363	C	N3-C2-O2	-5.51	118.05	121.90
22	QV	49	C	N3-C2-O2	-5.50	118.05	121.90
24	RA	860	U	C2-N1-C1'	5.50	124.30	117.70
24	RA	2559	C	C2-N1-C1'	5.50	124.85	118.80
1	XA	789	U	C2-N1-C1'	5.50	124.31	117.70
1	XA	1267	C	C6-N1-C2	-5.50	118.10	120.30
24	RA	267	C	N1-C2-O2	5.50	122.20	118.90
24	YA	1264	G	C8-N9-C4	-5.50	104.20	106.40
24	YA	1644	C	N3-C2-O2	-5.50	118.05	121.90
24	RA	1786	A	C4-N9-C1'	5.50	136.19	126.30
22	XV	49	C	N1-C2-O2	5.50	122.20	118.90
24	RA	1827	C	N1-C2-O2	5.49	122.19	118.90
1	XA	754	C	C2-N1-C1'	5.49	124.84	118.80
24	RA	2507	C	N3-C2-O2	-5.49	118.06	121.90
24	YA	67	U	C5-C6-N1	5.49	125.44	122.70
1	QA	1070	U	N3-C2-O2	-5.48	118.36	122.20
25	YB	71	C	N1-C2-O2	5.48	122.19	118.90
24	YA	1827	C	N1-C2-O2	5.48	122.19	118.90
24	RA	1781	C	N1-C2-O2	5.47	122.19	118.90
24	YA	268	C	N3-C2-O2	-5.47	118.07	121.90
24	RA	587	C	P-O3'-C3'	5.47	126.27	119.70
1	QA	1366	C	N1-C2-O2	5.47	122.18	118.90
24	YA	1411	C	N1-C2-O2	5.47	122.18	118.90
24	YA	1109	C	C6-N1-C2	-5.47	118.11	120.30
24	YA	1424	G	O5'-P-OP2	-5.47	100.78	105.70
25	RB	71	C	N1-C2-O2	5.46	122.18	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	932	C	N1-C2-O2	5.46	122.18	118.90
24	YA	654	A	C4-N9-C1'	5.46	136.13	126.30
24	YA	766	C	C6-N1-C2	-5.46	118.12	120.30
24	RA	1005	C	N3-C2-O2	-5.46	118.08	121.90
24	YA	838	C	N3-C2-O2	-5.46	118.08	121.90
24	RA	2498	C	N3-C2-O2	-5.46	118.08	121.90
53	R8	46	ARG	NE-CZ-NH1	-5.46	117.57	120.30
24	YA	1786	A	C8-N9-C4	-5.46	103.62	105.80
24	YA	2712	U	C6-N1-C2	-5.45	117.73	121.00
24	YA	2008	C	C6-N1-C2	-5.45	118.12	120.30
1	QA	1439	C	N1-C2-O2	5.45	122.17	118.90
24	RA	1135	C	N1-C2-O2	5.44	122.17	118.90
24	YA	1640	C	N1-C2-O2	5.44	122.17	118.90
1	XA	449	C	C6-N1-C1'	-5.44	114.27	120.80
24	YA	601	C	C6-N1-C2	-5.44	118.12	120.30
24	YA	1640	C	C6-N1-C2	-5.44	118.12	120.30
24	YA	838	C	C5-C6-N1	5.44	123.72	121.00
1	QA	703	G	P-O3'-C3'	5.43	126.22	119.70
24	YA	1625	C	N1-C2-O2	5.43	122.16	118.90
24	YA	2527	C	N1-C2-O2	5.43	122.16	118.90
24	RA	1234	U	N1-C2-O2	5.43	126.60	122.80
1	XA	897	C	C6-N1-C2	-5.43	118.13	120.30
1	XA	1200	C	P-O3'-C3'	5.43	126.22	119.70
53	Y8	46	ARG	NE-CZ-NH1	-5.43	117.58	120.30
24	RA	1902	C	N3-C2-O2	-5.42	118.10	121.90
24	RA	459	U	N1-C2-O2	5.42	126.60	122.80
24	RA	529	A	C4-N9-C1'	5.42	136.06	126.30
24	YA	1930	G	P-O3'-C3'	5.42	126.20	119.70
24	RA	565	C	N1-C2-O2	5.42	122.15	118.90
24	RA	676	A	O4'-C1'-N9	5.42	112.53	108.20
24	YA	1967	C	N3-C2-O2	-5.41	118.11	121.90
24	RA	503	A	OP2-P-O3'	5.41	117.09	105.20
24	RA	834	C	C6-N1-C2	-5.41	118.14	120.30
24	RA	1909	C	C6-N1-C2	-5.40	118.14	120.30
1	QA	369	C	N3-C2-O2	-5.40	118.12	121.90
24	RA	253	C	N3-C2-O2	-5.40	118.12	121.90
24	RA	1407	C	C5-C6-N1	5.40	123.70	121.00
24	RA	1313	U	C5-C6-N1	5.39	125.40	122.70
24	YA	1914	C	N1-C2-O2	5.39	122.14	118.90
24	YA	1920	C	C5-C6-N1	5.39	123.70	121.00
24	YA	1535	U	C5-C6-N1	5.39	125.40	122.70
24	RA	229	A	OP2-P-O3'	5.39	117.06	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	RA	1065	U	N3-C2-O2	-5.39	118.43	122.20
1	XA	1301	U	C5-C6-N1	5.39	125.39	122.70
24	YA	1021	A	C5-N7-C8	-5.39	101.21	103.90
24	RA	420	C	N3-C2-O2	-5.39	118.13	121.90
24	RA	1234	U	N3-C2-O2	-5.38	118.43	122.20
24	RA	2474	C	N1-C2-O2	5.38	122.13	118.90
1	XA	1114	C	N1-C2-O2	5.38	122.13	118.90
1	XA	353	A	OP2-P-O3'	5.38	117.04	105.20
24	YA	2465	C	N1-C2-O2	5.38	122.13	118.90
1	QA	722	A	C2-N3-C4	5.38	113.29	110.60
24	RA	1180	C	N3-C2-O2	-5.38	118.14	121.90
24	YA	18	C	N1-C2-O2	5.38	122.13	118.90
24	YA	2646	C	N1-C2-O2	5.38	122.12	118.90
24	YA	529	A	C4-N9-C1'	5.37	135.97	126.30
24	YA	837	C	C6-N1-C2	-5.37	118.15	120.30
24	YA	2205	C	N1-C2-O2	5.37	122.12	118.90
24	RA	1644	C	N3-C2-O2	-5.37	118.14	121.90
24	RA	944	G	C8-N9-C1'	-5.37	120.03	127.00
24	YA	2463	C	C6-N1-C2	-5.37	118.15	120.30
24	YA	537	C	C5-C6-N1	5.36	123.68	121.00
1	QA	449	C	N1-C2-O2	5.36	122.12	118.90
24	YA	1779	U	C2-N1-C1'	5.36	124.14	117.70
1	QA	1059	C	C6-N1-C2	-5.36	118.16	120.30
24	YA	2504	U	N1-C2-O2	5.36	126.55	122.80
1	QA	31	G	P-O3'-C3'	5.36	126.13	119.70
24	RA	1956	U	N1-C2-O2	5.36	126.55	122.80
1	QA	1070	U	N1-C2-O2	5.36	126.55	122.80
24	RA	1819	A	P-O3'-C3'	5.35	126.12	119.70
1	QA	1071	C	N1-C2-O2	5.35	122.11	118.90
24	YA	373	U	N3-C2-O2	-5.35	118.46	122.20
24	RA	546	C	N1-C2-O2	5.34	122.11	118.90
24	RA	1396	U	N1-C2-O2	5.34	126.54	122.80
24	YA	333	G	C8-N9-C1'	-5.34	120.06	127.00
1	QA	328	C	C5-C6-N1	5.34	123.67	121.00
1	QA	89	U	N1-C2-O2	5.33	126.53	122.80
1	QA	1026	G	C8-N9-C1'	-5.33	120.06	127.00
1	QA	486	U	C2-N1-C1'	5.33	124.10	117.70
24	RA	1905	C	N3-C2-O2	-5.33	118.17	121.90
24	YA	485	C	C6-N1-C2	-5.33	118.17	120.30
24	RA	2043	C	C5-C6-N1	5.33	123.67	121.00
24	YA	1506	C	N1-C2-O2	5.33	122.10	118.90
24	YA	2825	C	C6-N1-C2	-5.33	118.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	64	G	P-O3'-C3'	5.33	126.09	119.70
24	YA	2350	C	N1-C2-O2	5.32	122.09	118.90
1	XA	904	C	N1-C2-O2	5.32	122.09	118.90
1	XA	1452	C	C6-N1-C2	-5.32	118.17	120.30
24	YA	982	C	C6-N1-C2	-5.32	118.17	120.30
24	RA	2730	C	C6-N1-C2	-5.31	118.17	120.30
24	YA	859	G	OP2-P-O3'	5.31	116.89	105.20
24	YA	1549	C	C6-N1-C2	-5.31	118.17	120.30
24	YA	114	U	C5-C6-N1	5.31	125.36	122.70
24	YA	756	C	N1-C2-O2	5.31	122.09	118.90
24	RA	1882	C	C5-C6-N1	5.31	123.65	121.00
24	RA	74	A	P-O3'-C3'	5.30	126.07	119.70
1	XA	1514	C	C6-N1-C2	-5.30	118.18	120.30
24	YA	1313	U	C6-N1-C2	-5.30	117.82	121.00
24	YA	1881	C	N1-C2-O2	5.30	122.08	118.90
24	RA	1882	C	N3-C2-O2	-5.30	118.19	121.90
24	YA	140	A	C8-N9-C4	-5.30	103.68	105.80
24	YA	1534	G	C4-N9-C1'	5.30	133.39	126.50
24	YA	195	A	P-O3'-C3'	5.29	126.05	119.70
26	RD	34	VAL	C-N-CA	5.29	134.93	121.70
24	YA	1474	C	C5-C6-N1	5.29	123.65	121.00
24	RA	267	C	N3-C2-O2	-5.29	118.20	121.90
24	YA	1930	G	OP2-P-O3'	5.29	116.84	105.20
24	YA	2814	C	N1-C2-O2	5.29	122.07	118.90
26	YD	34	VAL	C-N-CA	5.29	134.92	121.70
1	XA	1290	G	C4-N9-C1'	5.29	133.37	126.50
24	YA	2043	C	C5-C6-N1	5.29	123.64	121.00
1	QA	181	G	P-O3'-C3'	5.29	126.04	119.70
24	YA	1971	A	C2-N3-C4	5.28	113.24	110.60
24	RA	285	C	N3-C2-O2	-5.28	118.20	121.90
24	YA	1804	C	C6-N1-C2	-5.28	118.19	120.30
24	YA	2507	C	C6-N1-C2	-5.28	118.19	120.30
24	YA	591	C	C6-N1-C2	-5.28	118.19	120.30
1	QA	1395	C	N1-C2-O2	5.28	122.07	118.90
1	XA	1225	A	C4-N9-C1'	5.28	135.79	126.30
24	YA	1640	C	C5-C6-N1	5.27	123.64	121.00
22	XV	49	C	C2-N1-C1'	5.27	124.59	118.80
24	YA	1669	A	C2-N3-C4	5.27	113.23	110.60
24	YA	2307	G	C4-N9-C1'	5.27	133.35	126.50
1	QA	1420	C	C6-N1-C2	-5.26	118.19	120.30
24	RA	373	U	C6-N1-C1'	-5.26	113.83	121.20
24	RA	2868	A	C8-N9-C4	-5.26	103.69	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	YA	1204	A	O4'-C1'-N9	5.26	112.41	108.20
24	RA	752	A	OP2-P-O3'	5.26	116.78	105.20
1	QA	1366	C	N3-C2-O2	-5.26	118.22	121.90
24	RA	838	C	N3-C2-O2	-5.26	118.22	121.90
1	XA	365	U	C2-N1-C1'	5.26	124.01	117.70
24	YA	584	C	C6-N1-C2	-5.26	118.20	120.30
24	YA	2702	U	O5'-P-OP2	-5.26	100.97	105.70
24	YA	1931	U	N1-C2-O2	5.26	126.48	122.80
1	XA	31	G	P-O3'-C3'	5.26	126.01	119.70
1	QA	810	C	N3-C2-O2	-5.25	118.22	121.90
23	QX	14	A	N3-C4-N9	5.25	131.60	127.40
24	RA	1658	C	C6-N1-C2	-5.25	118.20	120.30
24	RA	1983	C	N3-C2-O2	-5.25	118.22	121.90
24	YA	2712(A)	A	C5-N7-C8	-5.25	101.27	103.90
1	XA	543	C	C5-C6-N1	5.25	123.62	121.00
25	YB	27	C	C6-N1-C2	-5.25	118.20	120.30
1	QA	1279	A	N7-C8-N9	5.25	116.42	113.80
22	QV	49	C	C2-N1-C1'	5.25	124.57	118.80
22	QV	68	C	N1-C2-O2	5.25	122.05	118.90
24	YA	749	C	N1-C2-O2	5.25	122.05	118.90
24	RA	914	C	C6-N1-C2	-5.24	118.20	120.30
1	XA	1374	A	O4'-C1'-N9	5.24	112.39	108.20
1	QA	1008	C	N1-C2-O2	5.24	122.04	118.90
24	RA	201	C	N1-C2-O2	5.24	122.04	118.90
24	RA	1174	A	C4-N9-C1'	5.24	135.72	126.30
24	RA	595	C	C5-C6-N1	5.23	123.62	121.00
1	XA	690	G	O4'-C1'-N9	5.23	112.39	108.20
24	YA	1695	G	C4-N9-C1'	5.23	133.30	126.50
24	YA	2769	C	N3-C2-O2	-5.23	118.24	121.90
24	YA	2043	C	C6-N1-C2	-5.23	118.21	120.30
24	RA	1979	C	N1-C2-O2	5.23	122.04	118.90
24	RA	2248	C	C6-N1-C2	-5.23	118.21	120.30
24	YA	2089	U	C5-C6-N1	5.23	125.31	122.70
1	XA	530	G	C8-N9-C1'	-5.22	120.21	127.00
24	YA	580	C	C6-N1-C2	-5.22	118.21	120.30
24	YA	1958	C	C6-N1-C2	-5.22	118.21	120.30
24	RA	537	C	N1-C2-O2	5.22	122.03	118.90
24	YA	1121	C	C6-N1-C2	-5.22	118.21	120.30
1	XA	1439	C	N3-C2-O2	-5.22	118.25	121.90
24	RA	273(F)	C	C6-N1-C2	-5.22	118.21	120.30
1	XA	530	G	N3-C4-N9	5.22	129.13	126.00
1	QA	1395	C	C6-N1-C2	-5.21	118.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	RA	2655	G	P-O3'-C3'	5.21	125.96	119.70
1	QA	1336	C	P-O3'-C3'	5.21	125.95	119.70
24	RA	2465	C	N3-C2-O2	-5.21	118.25	121.90
24	YA	1795	C	N1-C2-O2	5.21	122.03	118.90
24	YA	1656	C	C6-N1-C2	-5.21	118.22	120.30
24	RA	721	C	N1-C2-O2	5.21	122.03	118.90
24	RA	1234	U	C2-N1-C1'	5.21	123.95	117.70
25	RB	27	C	C6-N1-C2	-5.21	118.22	120.30
1	QA	960	U	P-O3'-C3'	5.20	125.94	119.70
24	RA	1407	C	C6-N1-C2	-5.20	118.22	120.30
1	XA	764	C	N1-C2-O2	5.20	122.02	118.90
24	YA	141	A	C5-N7-C8	-5.20	101.30	103.90
24	YA	2739	U	N3-C2-O2	-5.20	118.56	122.20
1	QA	1439	C	N3-C2-O2	-5.20	118.26	121.90
24	YA	1402	C	N3-C2-O2	-5.19	118.26	121.90
24	YA	2870	C	N3-C2-O2	-5.19	118.26	121.90
24	RA	456	C	C6-N1-C1'	-5.19	114.57	120.80
24	YA	595	C	C6-N1-C2	-5.19	118.22	120.30
1	QA	913	A	OP2-P-O3'	5.19	116.62	105.20
25	YB	70	C	C6-N1-C2	-5.19	118.22	120.30
24	RA	2073	C	C6-N1-C2	-5.19	118.22	120.30
25	RB	70	C	C6-N1-C2	-5.19	118.22	120.30
24	YA	1314	C	N3-C2-O2	-5.19	118.27	121.90
1	XA	58	C	N1-C2-O2	5.19	122.01	118.90
24	YA	2889	C	N3-C2-O2	-5.18	118.27	121.90
1	XA	530	G	N3-C4-C5	-5.18	126.01	128.60
25	RB	79	C	C6-N1-C2	-5.18	118.23	120.30
24	RA	1312	U	OP2-P-O3'	5.18	116.59	105.20
24	RA	860	U	N1-C2-O2	5.18	126.42	122.80
24	RA	1363	C	N1-C2-O2	5.18	122.01	118.90
24	RA	2210	G	N3-C4-N9	5.17	129.10	126.00
24	RA	2576	G	C4-N9-C1'	5.17	133.22	126.50
1	XA	699	C	C6-N1-C2	-5.17	118.23	120.30
24	YA	1694	C	OP2-P-O3'	5.17	116.58	105.20
24	RA	1085	A	P-O3'-C3'	5.17	125.90	119.70
27	RE	78	LEU	CA-CB-CG	5.17	127.18	115.30
24	RA	897	C	N1-C2-O2	5.16	122.00	118.90
24	RA	1786	A	C6-C5-N7	-5.16	128.69	132.30
24	RA	2723	C	C6-N1-C2	-5.16	118.24	120.30
1	QA	1336	C	OP2-P-O3'	5.15	116.54	105.20
24	RA	930	U	C6-N1-C1'	-5.15	113.98	121.20
24	RA	333	G	C4-N9-C1'	5.15	133.20	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	1158	C	C2-N3-C4	5.15	122.48	119.90
24	YA	269	U	N3-C2-O2	-5.15	118.59	122.20
24	YA	2815	C	N3-C2-O2	-5.15	118.30	121.90
1	XA	897	C	N1-C2-O2	5.15	121.99	118.90
27	YE	78	LEU	CA-CB-CG	5.15	127.14	115.30
1	QA	1322	C	C6-N1-C1'	-5.14	114.63	120.80
24	YA	529	A	N7-C8-N9	5.14	116.37	113.80
1	QA	882	C	N3-C2-O2	-5.14	118.30	121.90
24	YA	1534	G	C2-N3-C4	5.14	114.47	111.90
1	XA	1113	C	C6-N1-C2	-5.14	118.25	120.30
24	YA	1686	C	N1-C2-O2	5.14	121.98	118.90
1	XA	328	C	C6-N1-C1'	-5.13	114.64	120.80
22	XV	68	C	N1-C2-O2	5.13	121.98	118.90
24	RA	2465	C	N1-C2-O2	5.13	121.98	118.90
24	YA	1021	A	C8-N9-C4	-5.13	103.75	105.80
24	RA	1779	U	C2-N1-C1'	5.13	123.85	117.70
24	RA	2617	C	N1-C2-O2	5.13	121.98	118.90
24	YA	1496	A	N7-C8-N9	5.13	116.36	113.80
1	QA	812	C	OP2-P-O3'	5.13	116.48	105.20
1	XA	536	C	C6-N1-C2	-5.12	118.25	120.30
24	YA	1504	C	N1-C2-O2	5.12	121.97	118.90
24	YA	2756	U	OP1-P-O3'	5.12	116.47	105.20
24	RA	1376	C	N3-C2-O2	-5.12	118.32	121.90
24	YA	140	A	C5-N7-C8	-5.12	101.34	103.90
24	RA	343	C	N1-C2-O2	5.12	121.97	118.90
1	QA	169	C	C6-N1-C2	-5.12	118.25	120.30
24	YA	2031	A	O4'-C1'-N9	5.12	112.29	108.20
24	YA	1005	C	N1-C2-O2	5.12	121.97	118.90
24	YA	654	A	N3-C4-C5	-5.11	123.22	126.80
24	YA	1460	A	P-O3'-C3'	5.11	125.83	119.70
1	QA	1383	C	N1-C2-O2	5.11	121.97	118.90
24	YA	753	C	N1-C2-O2	5.11	121.97	118.90
1	QA	1407	C	C6-N1-C2	-5.11	118.26	120.30
24	YA	1026	U	O4'-C1'-N1	5.11	112.28	108.20
1	XA	651	C	N1-C2-O2	5.10	121.96	118.90
24	YA	2688	U	N1-C2-O2	5.10	126.37	122.80
24	YA	2701	C	P-O3'-C3'	5.10	125.82	119.70
24	RA	1804	C	C6-N1-C2	-5.10	118.26	120.30
24	YA	2681	C	OP2-P-O3'	5.09	116.41	105.20
24	YA	613	U	N1-C2-O2	5.09	126.36	122.80
24	RA	273(F)	C	N1-C2-O2	5.09	121.95	118.90
24	RA	1980	G	OP1-P-O3'	5.09	116.39	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	YA	141	A	N7-C8-N9	5.08	116.34	113.80
1	QA	1201	A	P-O3'-C3'	5.08	125.80	119.70
24	YA	2293	C	C6-N1-C2	-5.08	118.27	120.30
1	XA	233	C	N1-C2-O2	5.08	121.95	118.90
1	XA	169	C	C6-N1-C2	-5.07	118.27	120.30
1	XA	703	G	P-O3'-C3'	5.07	125.79	119.70
24	RA	1662	C	C6-N1-C2	-5.07	118.27	120.30
24	YA	243	U	C5-C6-N1	5.07	125.23	122.70
24	YA	114	U	C2-N1-C1'	5.07	123.78	117.70
1	QA	64	G	P-O3'-C3'	5.07	125.78	119.70
1	XA	749	C	C6-N1-C2	-5.07	118.27	120.30
1	XA	1347	G	O4'-C1'-N9	5.07	112.25	108.20
22	XV	66	C	N1-C2-O2	5.07	121.94	118.90
24	YA	269	U	N1-C2-O2	5.07	126.35	122.80
24	YA	1774	C	N1-C2-O2	5.06	121.94	118.90
24	YA	1575	C	N1-C2-O2	5.06	121.94	118.90
24	YA	420	C	N3-C2-O2	-5.06	118.36	121.90
1	XA	645	C	N1-C2-O2	5.06	121.94	118.90
24	RA	461	C	C6-N1-C2	-5.06	118.28	120.30
24	RA	992	C	C6-N1-C2	-5.05	118.28	120.30
24	RA	992	C	N3-C2-O2	-5.05	118.36	121.90
24	RA	2591	C	C6-N1-C2	-5.05	118.28	120.30
24	YA	1528	A	O4'-C1'-N9	5.05	112.24	108.20
24	RA	459	U	N3-C2-O2	-5.05	118.66	122.20
1	XA	1285	A	OP2-P-O3'	5.05	116.31	105.20
24	YA	661	C	C6-N1-C2	-5.05	118.28	120.30
24	YA	2712(A)	A	C8-N9-C4	-5.05	103.78	105.80
24	RA	1314	C	C6-N1-C2	-5.05	118.28	120.30
24	RA	198	C	N1-C2-O2	5.05	121.93	118.90
24	RA	385	C	C2-N1-C1'	5.05	124.35	118.80
24	RA	2044	C	C6-N1-C2	-5.05	118.28	120.30
1	QA	1026	G	N3-C4-C5	-5.04	126.08	128.60
24	YA	2504	U	N3-C2-O2	-5.04	118.67	122.20
1	XA	651	C	N3-C2-O2	-5.04	118.37	121.90
24	YA	2127	G	C8-N9-C4	-5.04	104.38	106.40
1	QA	1045	C	N1-C2-O2	5.04	121.92	118.90
24	YA	537	C	C2-N1-C1'	5.04	124.34	118.80
24	YA	2779	U	C6-N1-C1'	-5.04	114.14	121.20
29	YG	177	GLY	C-N-CA	-5.04	109.09	121.70
38	RT	105	LEU	CA-CB-CG	5.04	126.89	115.30
1	XA	137	C	C6-N1-C2	-5.04	118.28	120.30
24	RA	1402	C	C6-N1-C2	-5.04	118.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	YA	1979	C	C6-N1-C2	-5.04	118.28	120.30
38	YT	105	LEU	CA-CB-CG	5.04	126.88	115.30
24	RA	1994	C	N1-C2-O2	5.03	121.92	118.90
1	XA	545	C	C6-N1-C2	-5.03	118.29	120.30
24	YA	510	C	C5-C6-N1	5.03	123.52	121.00
25	RB	43	C	N1-C2-O2	5.03	121.92	118.90
24	RA	2307	G	C4-N9-C1'	5.03	133.04	126.50
29	RG	177	GLY	C-N-CA	-5.03	109.12	121.70
1	QA	1279	A	C4-N9-C1'	5.03	135.35	126.30
1	XA	314	C	C6-N1-C2	-5.03	118.29	120.30
24	YA	1021	A	N7-C8-N9	5.03	116.31	113.80
24	YA	1399	C	C6-N1-C2	-5.02	118.29	120.30
1	QA	1225	A	C4-N9-C1'	5.02	135.34	126.30
24	YA	1210	A	C3'-C2'-C1'	5.02	105.52	101.50
24	YA	2336	A	C4-C5-N7	5.02	113.21	110.70
1	QA	754	C	N1-C2-O2	5.02	121.91	118.90
24	RA	385	C	N1-C2-O2	5.02	121.91	118.90
24	YA	1879	C	N3-C2-O2	-5.02	118.39	121.90
24	YA	2615	U	N1-C2-O2	5.02	126.31	122.80
24	YA	754	C	C5-C6-N1	5.02	123.51	121.00
24	RA	201	C	N3-C2-O2	-5.01	118.39	121.90
24	RA	904	C	N1-C2-O2	5.01	121.91	118.90
24	YA	611	C	N3-C2-O2	-5.01	118.39	121.90
24	YA	1332	G	N1-C2-N2	-5.01	111.69	116.20
24	YA	1375	C	C6-N1-C2	-5.01	118.29	120.30
24	RA	1881	C	N3-C2-O2	-5.01	118.39	121.90
24	YA	65	C	N1-C2-O2	5.01	121.91	118.90
24	YA	1640	C	C2-N1-C1'	5.01	124.31	118.80
24	RA	1267	U	C2-N1-C1'	5.01	123.71	117.70
24	RA	2471	C	N1-C2-O2	5.00	121.90	118.90
24	RA	1258	C	C6-N1-C2	-5.00	118.30	120.30
1	QA	882	C	N1-C2-O2	5.00	121.90	118.90
24	RA	971	C	C6-N1-C2	-5.00	118.30	120.30
25	YB	79	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (71) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	QD	19	LEU	Peptide
4	QD	33	MET	Peptide
12	QL	104	VAL	Peptide

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Mol	Chain	Res	Type	Group
12	QL	47	LYS	Peptide
19	QS	41	VAL	Peptide
47	R2	46	GLN	Peptide
49	R4	48	ARG	Peptide
49	R4	55	ARG	Peptide
53	R8	28	GLY	Peptide
53	R8	35	GLN	Peptide
53	R8	52	LYS	Peptide
53	R8	62	LEU	Peptide
26	RD	122	ASP	Peptide
26	RD	237	GLU	Peptide
26	RD	33	LEU	Peptide
26	RD	35	LYS	Peptide
27	RE	131	ALA	Peptide
27	RE	17	ASP	Peptide
27	RE	20	ALA	Peptide
27	RE	71	GLY	Peptide
29	RG	82	LEU	Peptide
30	RH	151	ILE	Peptide
30	RH	82	GLY	Peptide
31	RI	119	PRO	Peptide
31	RI	131	LYS	Peptide
32	RN	22	THR	Peptide
34	RP	107	LYS	Peptide
35	RQ	89	ASN	Peptide
39	RU	95	LEU	Peptide
40	RV	44	LYS	Peptide
40	RV	49	THR	Peptide
44	RZ	178	GLU	Peptide
44	RZ	52	SER	Peptide
44	RZ	60	GLU	Peptide
44	RZ	62	PRO	Peptide
4	XD	19	LEU	Peptide
4	XD	33	MET	Peptide
12	XL	104	VAL	Peptide
12	XL	47	LYS	Peptide
47	Y2	46	GLN	Peptide
49	Y4	48	ARG	Peptide
49	Y4	55	ARG	Peptide
53	Y8	28	GLY	Peptide
53	Y8	35	GLN	Peptide
53	Y8	52	LYS	Peptide

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Mol	Chain	Res	Type	Group
53	Y8	62	LEU	Peptide
26	YD	122	ASP	Peptide
26	YD	237	GLU	Peptide
26	YD	33	LEU	Peptide
26	YD	35	LYS	Peptide
27	YE	131	ALA	Peptide
27	YE	17	ASP	Peptide
27	YE	20	ALA	Peptide
27	YE	71	GLY	Peptide
29	YG	82	LEU	Peptide
30	YH	151	ILE	Peptide
30	YH	82	GLY	Peptide
31	YI	119	PRO	Peptide
31	YI	131	LYS	Peptide
32	YN	22	THR	Peptide
34	YP	107	LYS	Peptide
34	YP	25	SER	Peptide
34	YP	9	ASN	Peptide
35	YQ	89	ASN	Peptide
39	YU	95	LEU	Peptide
40	YV	44	LYS	Peptide
40	YV	49	THR	Peptide
44	YZ	178	GLU	Peptide
44	YZ	52	SER	Peptide
44	YZ	60	GLU	Peptide
44	YZ	62	PRO	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32202	0	16255	204	0
1	XA	32246	0	16277	177	0
2	QB	1907	0	1958	20	0
2	XB	1915	0	1969	17	0
3	QC	1605	0	1668	21	0
3	XC	1605	0	1668	20	2
4	QD	1703	0	1766	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	XD	1703	0	1767	22	0
5	QE	1155	0	1213	11	0
5	XE	1155	0	1213	7	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	10	0
8	QH	1108	0	1164	16	0
8	XH	1108	0	1165	15	0
9	QI	1010	0	1037	26	0
9	XI	998	0	1023	16	0
10	QJ	801	0	849	18	0
10	XJ	777	0	816	19	0
11	QK	885	0	904	19	2
11	XK	864	0	881	15	0
12	QL	975	0	1062	12	0
12	XL	956	0	1046	16	0
13	QM	955	0	1021	14	0
13	XM	946	0	1008	17	0
14	QN	492	0	529	7	0
14	XN	492	0	529	8	0
15	QO	734	0	771	5	0
15	XO	729	0	768	4	0
16	QP	705	0	725	7	0
16	XP	705	0	725	4	0
17	QQ	834	0	904	6	0
17	XQ	834	0	904	13	0
18	QR	574	0	644	6	0
18	XR	574	0	644	7	0
19	QS	665	0	686	15	0
19	XS	674	0	699	8	0
20	QT	763	0	860	5	0
20	XT	763	0	861	5	0
21	QU	217	0	234	5	0
21	XU	217	0	234	4	0
22	QV	1644	0	836	3	0
22	XV	1644	0	836	4	0
23	QX	259	0	129	2	0
23	XX	239	0	119	1	0
24	RA	62071	0	31285	264	0
24	YA	62091	0	31293	267	0
25	RB	2573	0	1306	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	YB	2573	0	1306	13	0
26	RD	2115	0	2195	42	0
26	YD	2115	0	2195	40	0
27	RE	1568	0	1634	25	0
27	YE	1568	0	1634	26	0
28	RF	1585	0	1632	20	0
28	YF	1585	0	1632	15	0
29	RG	1474	0	1535	17	0
29	YG	1474	0	1535	20	0
30	RH	1336	0	1418	19	0
30	YH	1336	0	1418	20	1
31	RI	1136	0	1223	17	0
31	YI	1136	0	1223	19	0
32	RN	1104	0	1180	9	0
32	YN	1104	0	1180	5	0
33	RO	933	0	996	12	0
33	YO	933	0	996	10	0
34	RP	1145	0	1227	22	0
34	YP	1122	0	1206	22	0
35	RQ	1122	0	1179	25	0
35	YQ	1122	0	1179	21	0
36	RR	960	0	1021	9	0
36	YR	960	0	1021	13	0
37	RS	882	0	943	11	0
37	YS	882	0	943	14	0
38	RT	1141	0	1202	22	0
38	YT	1141	0	1202	23	0
39	RU	964	0	1022	19	0
39	YU	964	0	1021	18	0
40	RV	779	0	852	11	0
40	YV	779	0	852	10	3
41	RW	900	0	964	7	2
41	YW	900	0	964	5	0
42	RX	725	0	778	10	0
42	YX	725	0	778	13	0
43	RY	818	0	909	14	4
43	YY	818	0	909	12	3
44	RZ	1461	0	1493	22	0
44	YZ	1461	0	1493	21	0
45	R0	643	0	667	11	0
45	Y0	599	0	617	12	0
46	R1	763	0	848	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	Y1	729	0	802	9	0
47	R2	581	0	629	6	0
47	Y2	581	0	629	7	4
48	R3	469	0	518	8	0
48	Y3	469	0	518	6	0
49	R4	565	0	557	7	0
49	Y4	565	0	557	8	0
50	R5	459	0	476	8	0
50	Y5	459	0	479	8	3
51	R6	453	0	473	5	0
51	Y6	453	0	473	3	0
52	R7	409	0	454	2	0
52	Y7	418	0	467	5	0
53	R8	517	0	582	14	0
53	Y8	517	0	582	9	0
54	R9	307	0	335	4	0
54	Y9	307	0	335	4	0
55	QA	80	0	0	0	0
55	QC	1	0	0	0	0
55	QF	1	0	0	0	0
55	QH	1	0	0	0	0
55	QT	1	0	0	0	0
55	QV	6	0	0	0	0
55	R0	2	0	0	0	0
55	R8	1	0	0	0	0
55	RA	521	0	0	0	0
55	RB	11	0	0	0	0
55	RD	1	0	0	0	0
55	RE	4	0	0	0	0
55	RN	1	0	0	0	0
55	RO	1	0	0	0	0
55	RP	3	0	0	0	0
55	RQ	3	0	0	0	0
55	RR	2	0	0	0	0
55	RT	1	0	0	0	0
55	XA	98	0	0	0	0
55	XE	1	0	0	0	0
55	XL	2	0	0	0	0
55	XM	2	0	0	0	0
55	XQ	1	0	0	0	0
55	XS	1	0	0	0	0
55	XV	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	XX	1	0	0	0	0
55	Y0	2	0	0	0	0
55	Y1	1	0	0	0	0
55	Y5	1	0	0	0	0
55	Y7	1	0	0	0	0
55	Y8	2	0	0	0	0
55	YA	551	0	0	0	0
55	YB	12	0	0	0	0
55	YD	3	0	0	0	0
55	YE	4	0	0	0	0
55	YF	1	0	0	0	0
55	YO	1	0	0	0	0
55	YP	2	0	0	0	0
55	YQ	4	0	0	0	0
55	YU	1	0	0	0	0
55	YX	2	0	0	0	0
55	YY	1	0	0	0	0
56	QD	8	0	0	0	0
56	XD	8	0	0	0	0
57	QN	1	0	0	0	0
57	R4	1	0	0	0	0
57	R5	1	0	0	0	0
57	R6	1	0	0	0	0
57	R9	1	0	0	0	0
57	RY	1	0	0	0	0
57	XN	1	0	0	0	0
57	Y4	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y6	1	0	0	0	0
57	Y9	1	0	0	0	0
57	YY	1	0	0	0	0
All	All	291753	0	197645	1817	12

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 4.

All (1817) 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)
24:RA:602:G:HO2'	24:RA:604:G:HO2'	1.26	0.80
46:Y1:91:LYS:HE2	46:Y1:92:LYS:HE2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:664:G:H22	1:QA:741:G:H1	1.36	0.74
1:XA:686:U:H1'	11:XK:42:TRP:HE1	1.54	0.73
24:RA:676:A:H8	24:RA:2069:G:H21	1.36	0.72
1:QA:1422:G:H5''	33:RO:48:PRO:HB3	1.72	0.72
24:RA:883:G:H1	24:RA:893:C:H42	1.36	0.72
31:RI:27:ARG:HB2	46:R1:71:TYR:HE2	1.55	0.71
24:RA:994:C:OP1	39:RU:53:ARG:NH2	2.24	0.71
24:YA:249:C:O2	53:Y8:12:LYS:NZ	2.24	0.71
16:XP:1:MET:SD	16:XP:3:LYS:NZ	2.64	0.71
24:YA:958:U:OP2	35:YQ:14:ARG:NH1	2.24	0.70
36:YR:24:GLN:HE21	36:YR:36:THR:HG21	1.56	0.70
1:QA:147:G:H1	1:QA:175:C:H42	1.39	0.70
1:QA:677:U:H3	1:QA:713:G:H22	1.39	0.69
16:QP:1:MET:SD	16:QP:3:LYS:NZ	2.64	0.69
1:XA:189:U:O2	17:XQ:63:ARG:NH2	2.25	0.69
24:RA:1817:G:OP1	26:RD:88:ARG:NH2	2.25	0.69
24:YA:1817:G:OP1	26:YD:88:ARG:NH2	2.26	0.69
24:YA:2666:C:O2	30:YH:152:ARG:NH1	2.26	0.69
30:RH:130:ARG:HH12	30:RH:132:ARG:HH21	1.41	0.68
1:QA:1316:G:H22	1:QA:1319:A:H5''	1.56	0.68
19:XS:50:ALA:HB1	19:XS:57:HIS:HB3	1.75	0.68
16:QP:45:THR:HG22	16:QP:47:ASP:H	1.59	0.68
16:XP:45:THR:HG22	16:XP:47:ASP:H	1.59	0.68
46:Y1:83:GLU:HG2	46:Y1:85:LEU:H	1.57	0.67
24:YA:2245:U:H5'	24:YA:2246:G:H5'	1.77	0.67
30:YH:130:ARG:HH12	30:YH:132:ARG:HH21	1.41	0.67
24:RA:2784:C:O2'	27:RE:37:ARG:NH1	2.28	0.67
10:XJ:7:LYS:HB2	10:XJ:97:GLU:HB2	1.76	0.67
32:YN:133:GLN:HG2	32:YN:135:PRO:HD3	1.77	0.67
24:RA:1043:C:H42	24:RA:1112:G:H1	1.43	0.66
24:RA:1568:G:H5''	26:RD:61:LEU:HD23	1.77	0.66
24:YA:996:A:OP2	39:YU:92:ARG:NH2	2.28	0.66
24:YA:141:A:H8	24:YA:1595:G:H21	1.42	0.66
24:YA:1863:G:HO2'	24:YA:2411:A:HO2'	1.41	0.66
24:YA:1568:G:H5''	26:YD:61:LEU:HD23	1.77	0.66
24:YA:2784:C:O2'	27:YE:37:ARG:NH1	2.28	0.66
26:RD:35:LYS:NZ	26:RD:64:ILE:O	2.28	0.66
24:RA:1980:G:O2'	24:RA:1982:C:OP2	2.14	0.66
12:QL:117:ARG:HB2	12:QL:122:THR:HB	1.76	0.66
32:RN:133:GLN:HG2	32:RN:135:PRO:HD3	1.77	0.65
24:YA:517:C:OP1	50:Y5:16:ARG:NH2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:RA:2296:U:OP2	37:RS:9:ARG:NH1	2.29	0.65
2:QB:185:ILE:HG22	2:QB:199:TYR:HB2	1.78	0.65
17:QQ:66:SER:O	17:QQ:70:ARG:NH1	2.30	0.65
24:RA:27:G:N2	24:RA:513:A:OP2	2.29	0.65
26:RD:8:PRO:HB3	26:RD:14:ARG:HB3	1.79	0.65
17:XQ:66:SER:O	17:XQ:70:ARG:NH1	2.30	0.65
24:YA:676:A:H8	24:YA:2069:G:H21	1.43	0.65
1:QA:963:G:H21	10:QJ:55:LYS:HD3	1.62	0.64
24:RA:301:G:OP2	43:RY:84:ARG:NH2	2.24	0.64
45:R0:27:GLU:HG3	45:R0:68:GLU:HA	1.79	0.64
26:YD:8:PRO:HB3	26:YD:14:ARG:HB3	1.79	0.64
24:RA:309:G:N3	24:RA:329:G:O2'	2.30	0.64
27:YE:5:LEU:HG	27:YE:49:LEU:HD23	1.80	0.64
24:YA:994:C:OP1	39:YU:53:ARG:NH2	2.30	0.64
2:XB:185:ILE:HG22	2:XB:199:TYR:HB2	1.79	0.64
26:YD:35:LYS:NZ	26:YD:64:ILE:O	2.28	0.64
24:YA:571:A:H5'	24:YA:2030:A:H62	1.63	0.64
24:YA:259:G:H21	24:YA:621:A:H8	1.46	0.64
1:QA:825:G:O2'	8:QH:12:ARG:NH2	2.31	0.64
24:RA:630:G:OP1	53:R8:46:ARG:NH1	2.23	0.64
1:QA:439:A:OP2	1:QA:493:G:N1	2.31	0.63
9:QI:112:LYS:HA	9:QI:119:ALA:HB2	1.80	0.63
1:XA:403:C:OP2	4:XD:74:GLN:NE2	2.31	0.63
5:QE:102:ALA:HB1	5:QE:106:PRO:HG2	1.79	0.63
5:XE:102:ALA:HB1	5:XE:106:PRO:HG2	1.80	0.63
4:QD:100:ARG:NH2	4:QD:136:PRO:O	2.32	0.63
35:RQ:60:ARG:H	44:RZ:179:ASP:HB2	1.63	0.63
46:R1:87:PRO:HA	46:R1:90:ILE:HG22	1.80	0.63
29:RG:29:TRP:O	29:RG:33:ARG:NH1	2.31	0.63
29:YG:29:TRP:O	29:YG:33:ARG:NH1	2.31	0.63
24:RA:1607:C:N4	24:RA:1622:G:OP2	2.32	0.63
49:Y4:16:CYS:SG	49:Y4:17:GLY:N	2.72	0.63
3:QC:172:ARG:HG2	3:QC:174:PRO:HD3	1.80	0.63
9:QI:28:VAL:HG22	9:QI:63:ILE:HB	1.80	0.63
24:YA:2680:C:H5'	27:YE:189:PRO:HA	1.79	0.63
24:RA:2470:G:H5'	35:RQ:56:ARG:HH21	1.62	0.62
24:YA:630:G:OP1	53:Y8:46:ARG:NH1	2.24	0.62
24:YA:1124:C:O2	54:Y9:36:GLN:NE2	2.32	0.62
24:YA:1826:G:O2'	26:YD:242:ARG:NH2	2.32	0.62
1:QA:1031:G:H2'	1:QA:1032:A:H8	1.65	0.62
3:QC:150:LYS:HE2	3:QC:152:ILE:HD11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:RA:1826:G:O2'	26:RD:242:ARG:NH2	2.31	0.62
25:RB:33:G:OP2	29:RG:96:ARG:NH2	2.31	0.62
24:YA:1055:G:H22	24:YA:1104:C:H42	1.47	0.62
24:RA:2006:C:O2'	24:RA:2823:A:N3	2.32	0.62
24:RA:2788:C:O2'	24:RA:2809:A:N3	2.33	0.62
4:XD:100:ARG:NH2	4:XD:136:PRO:O	2.32	0.62
24:YA:1859:A:N6	24:YA:1883:G:O2'	2.33	0.62
12:QL:60:LEU:HD12	12:QL:62:SER:H	1.65	0.62
1:QA:1329:A:N7	21:QU:7:ARG:NH2	2.46	0.62
24:RA:2119:A:N6	24:RA:2170:A:N7	2.48	0.62
50:Y5:20:ARG:HA	50:Y5:23:HIS:HD2	1.65	0.62
24:RA:442:G:H1'	28:RF:48:THR:HG21	1.82	0.62
1:XA:246:A:OP2	17:XQ:100:LYS:NZ	2.33	0.62
45:Y0:27:GLU:HG3	45:Y0:68:GLU:HA	1.81	0.62
49:R4:47:GLN:HG2	49:R4:49:PHE:HB3	1.81	0.61
50:R5:20:ARG:HA	50:R5:23:HIS:HD2	1.65	0.61
24:RA:2135:A:H62	24:RA:2156:G:H21	1.45	0.61
1:XA:1422:G:H5''	33:YO:48:PRO:HB3	1.82	0.61
3:XC:172:ARG:HG2	3:XC:174:PRO:HD3	1.80	0.61
43:YY:47:LYS:NZ	43:YY:48:ALA:O	2.33	0.61
2:XB:118:LEU:HB3	2:XB:142:LEU:HD12	1.82	0.61
3:XC:150:LYS:HE2	3:XC:152:ILE:HD11	1.80	0.61
46:Y1:18:ILE:HG12	46:Y1:37:ILE:HG12	1.82	0.61
19:QS:19:VAL:HG11	19:QS:44:MET:HG2	1.82	0.61
49:R4:16:CYS:SG	49:R4:17:GLY:N	2.72	0.61
27:RE:5:LEU:HG	27:RE:49:LEU:HD23	1.80	0.61
24:RA:907:U:O2'	35:RQ:101:ARG:NH2	2.33	0.61
10:XJ:38:ILE:HD11	10:XJ:71:LEU:HD23	1.83	0.61
24:RA:819:A:OP2	24:RA:1187:G:N2	2.32	0.61
19:XS:32:LYS:HA	19:XS:50:ALA:HB3	1.82	0.61
1:QA:1119:C:OP2	9:QI:9:ARG:NH2	2.32	0.61
1:XA:842:C:O2'	1:XA:848:C:N4	2.34	0.61
34:RP:68:GLN:HG2	53:R8:12:LYS:HG2	1.81	0.61
24:YA:2795:G:N2	24:YA:2799:A:OP2	2.33	0.61
24:RA:955:C:OP1	35:RQ:85:LYS:NZ	2.30	0.61
1:XA:971:G:N2	1:XA:1363:A:OP2	2.33	0.61
11:XK:86:GLY:O	11:XK:91:ARG:NH1	2.33	0.61
24:RA:1411:C:H42	24:RA:1591:G:H1	1.47	0.61
1:XA:1127:G:H1'	1:XA:1147:C:H42	1.66	0.61
1:XA:414:A:OP2	1:XA:428:G:N2	2.31	0.61
49:Y4:47:GLN:HG2	49:Y4:49:PHE:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:YA:273:G:H1	24:YA:364:C:H42	1.49	0.61
26:YD:260:ARG:NH1	26:YD:267:SER:OG	2.32	0.61
37:YS:20:ARG:NH1	45:Y0:48:GLY:O	2.32	0.61
34:RP:58:THR:O	34:RP:61:ARG:NH2	2.33	0.61
34:RP:62:LEU:HD12	53:R8:30:ARG:HH21	1.65	0.61
25:YB:9:G:OP1	37:YS:15:ARG:NH1	2.31	0.61
46:R1:51:VAL:HG11	46:R1:74:VAL:HG21	1.82	0.61
39:RU:50:ARG:O	39:RU:54:LYS:NZ	2.34	0.60
3:QC:108:ASN:HD21	3:QC:144:SER:HB2	1.66	0.60
46:R1:65:SER:HG	46:R1:66:HIS:HD1	1.49	0.60
24:RA:2156:G:O6	24:RA:2157:G:N2	2.34	0.60
39:YU:50:ARG:O	39:YU:54:LYS:NZ	2.34	0.60
1:QA:452:A:H62	1:QA:480:U:H3	1.47	0.60
24:RA:1019:U:H3	24:RA:1142(A):A:H62	1.48	0.60
24:YA:593:G:H4'	53:Y8:61:LEU:HD13	1.83	0.60
24:RA:1171:G:N7	24:RA:1174:A:N6	2.49	0.60
24:RA:2612:C:OP2	50:R5:2:ALA:N	2.34	0.60
24:YA:309:G:N3	24:YA:329:G:O2'	2.34	0.60
24:RA:1667:G:O2'	24:RA:1991:U:O4	2.19	0.60
24:YA:1980:G:O2'	24:YA:1982:C:OP2	2.17	0.60
24:YA:888:C:H3'	24:YA:889:C:H4'	1.83	0.60
10:QJ:3:LYS:N	10:QJ:74:ILE:O	2.34	0.60
24:RA:1652:A:OP1	36:RR:8:ARG:NH1	2.34	0.60
35:YQ:81:VAL:O	35:YQ:82:ARG:NE	2.33	0.60
1:QA:593:G:H1	1:QA:646:U:H3	1.50	0.60
26:RD:260:ARG:NH1	26:RD:267:SER:OG	2.32	0.60
3:QC:150:LYS:HE3	3:QC:167:TRP:HE1	1.67	0.60
24:RA:1365:A:O2'	46:R1:11:ARG:NH2	2.34	0.60
24:RA:956:G:OP2	35:RQ:14:ARG:NH2	2.34	0.60
1:XA:244:U:OP2	17:XQ:100:LYS:NZ	2.34	0.60
24:RA:918:A:N3	25:RB:80:U:O2'	2.31	0.60
24:RA:993:G:OP1	39:RU:50:ARG:NH2	2.35	0.60
1:XA:1227:A:OP1	19:XS:80:TYR:OH	2.18	0.60
24:YA:1056:G:H4'	24:YA:1086:A:H8	1.66	0.60
24:YA:1971:A:OP2	26:YD:242:ARG:NH2	2.34	0.60
24:RA:1791:A:N6	24:RA:1828:G:O2'	2.32	0.60
37:YS:20:ARG:NH2	45:Y0:51:VAL:O	2.31	0.60
3:XC:108:ASN:HD21	3:XC:144:SER:HB2	1.66	0.59
1:QA:31:G:O2'	1:QA:48:C:N4	2.34	0.59
1:XA:1393:U:HO2'	1:XA:1501:C:HO2'	1.50	0.59
12:XL:60:LEU:HD12	12:XL:62:SER:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:RA:458:G:N2	24:RA:470:A:OP2	2.32	0.59
24:RA:83:G:H1	24:RA:102:G:HO2'	1.49	0.59
24:YA:270(I):G:H1	24:YA:270(Q):C:H42	1.48	0.59
43:YY:102:CYS:SG	43:YY:103:GLY:N	2.75	0.59
24:RA:259:G:H21	24:RA:621:A:H8	1.49	0.59
1:XA:261:U:OP2	20:XT:79:ARG:NH2	2.35	0.59
8:XH:91:ARG:NE	17:XQ:32:TYR:O	2.33	0.59
24:YA:2495:G:H5''	35:YQ:81:VAL:HG12	1.84	0.59
24:RA:530:G:O2'	24:RA:532:A:N7	2.36	0.59
26:YD:27:THR:HG21	26:YD:81:ALA:HB1	1.84	0.59
32:YN:96:GLU:HB2	32:YN:122:VAL:HG12	1.85	0.59
19:QS:18:LYS:HG2	19:QS:31:ILE:HD12	1.84	0.59
3:XC:150:LYS:HE3	3:XC:167:TRP:HE1	1.67	0.59
24:YA:2183:C:H2'	24:YA:2184:G:H8	1.68	0.59
1:QA:261:U:OP2	20:QT:79:ARG:NH2	2.35	0.59
10:QJ:38:ILE:HD11	10:QJ:71:LEU:HD23	1.83	0.59
35:RQ:81:VAL:O	35:RQ:82:ARG:NE	2.33	0.59
24:YA:442:G:H1'	28:YF:48:THR:HG21	1.85	0.59
9:QI:121:ARG:NH1	9:QI:122:ALA:O	2.36	0.59
24:RA:1264:G:OP1	50:R5:19:ARG:NH2	2.28	0.59
24:YA:1607:C:N4	24:YA:1622:G:OP2	2.33	0.59
2:QB:118:LEU:HB3	2:QB:142:LEU:HD12	1.84	0.59
26:RD:27:THR:HG21	26:RD:81:ALA:HB1	1.84	0.59
1:XA:765:G:N2	1:XA:813:U:OP2	2.34	0.59
27:RE:50:GLY:HA2	27:RE:77:ILE:HA	1.85	0.59
24:RA:662:G:OP1	34:RP:15:ARG:NH1	2.35	0.59
43:RY:102:CYS:SG	43:RY:103:GLY:N	2.75	0.59
6:QF:94:GLN:OE1	18:QR:32:ARG:NH1	2.36	0.58
19:QS:12:ASP:OD2	19:QS:35:SER:OG	2.20	0.58
2:XB:82:ARG:NH1	2:XB:92:TYR:OH	2.36	0.58
9:QI:21:PRO:HA	9:QI:59:PHE:HA	1.85	0.58
19:QS:50:ALA:HB1	19:QS:57:HIS:HB3	1.86	0.58
26:RD:143:HIS:ND1	26:RD:194:GLY:O	2.32	0.58
24:YA:776:G:N7	24:YA:793:A:O2'	2.37	0.58
4:QD:15:GLU:OE2	4:QD:59:ARG:NH1	2.37	0.58
24:YA:265:A:N6	24:YA:427:U:O2'	2.36	0.58
26:YD:168:ARG:HG2	26:YD:173:VAL:HG12	1.85	0.58
27:YE:18:ASP:HB3	38:YT:82:LEU:HD11	1.85	0.58
36:YR:88:ARG:NH2	36:YR:89:ASP:OD1	2.36	0.58
24:RA:141:A:H8	24:RA:1595:G:H21	1.52	0.58
1:XA:437:U:O2	4:XD:119:GLN:NE2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:YE:50:GLY:HA2	27:YE:77:ILE:HA	1.85	0.58
49:R4:56:VAL:HG23	49:R4:58:ARG:HG3	1.86	0.58
46:R1:83:GLU:HG2	46:R1:85:LEU:H	1.68	0.58
24:RA:1012:U:OP1	39:RU:75:ASN:ND2	2.35	0.58
24:RA:1899:G:H22	24:RA:1902:C:H41	1.50	0.58
32:RN:96:GLU:HB2	32:RN:122:VAL:HG12	1.85	0.58
1:XA:544:G:OP1	4:XD:59:ARG:NH2	2.37	0.58
24:YA:2789:C:O2	24:YA:2894:G:N2	2.36	0.58
24:YA:458:G:N2	24:YA:470:A:OP2	2.33	0.58
10:QJ:45:ARG:HB3	10:QJ:65:LEU:HB3	1.84	0.58
24:RA:1530:G:H1	24:RA:1541:U:H3	1.52	0.58
26:RD:168:ARG:HG2	26:RD:173:VAL:HG12	1.86	0.58
1:XA:439:A:OP2	1:XA:493:G:N1	2.30	0.58
46:Y1:87:PRO:HA	46:Y1:90:ILE:HG22	1.85	0.58
24:RA:2115:G:N1	24:RA:2164:C:OP2	2.37	0.58
24:YA:1689:A:H62	24:YA:1698:A:H2	1.50	0.58
24:YA:321:G:O2'	24:YA:340:A:N3	2.36	0.58
36:RR:88:ARG:NH2	36:RR:89:ASP:OD1	2.37	0.57
4:XD:15:GLU:OE2	4:XD:59:ARG:NH1	2.37	0.57
46:R1:52:ARG:HH11	46:R1:57:GLU:HB2	1.69	0.57
11:XK:83:ILE:HG12	11:XK:109:VAL:HB	1.85	0.57
18:XR:32:ARG:HA	18:XR:69:THR:HG21	1.87	0.57
24:YA:458:G:O2'	24:YA:469:G:O6	2.23	0.57
27:RE:105:THR:HB	27:RE:197:ILE:HG23	1.86	0.57
34:RP:18:ARG:HE	34:RP:27:HIS:HE1	1.52	0.57
1:XA:427:U:OP1	4:XD:13:ARG:NH2	2.36	0.57
2:XB:80:ILE:HD11	2:XB:208:ILE:HG23	1.85	0.57
45:Y0:70:GLN:OE1	45:Y0:80:HIS:NE2	2.37	0.57
1:QA:316:G:OP2	1:QA:351:G:O2'	2.22	0.57
24:RA:1111:A:H5'	30:RH:3:ARG:HH21	1.67	0.57
31:RI:99:GLU:OE2	31:RI:103:ARG:NH2	2.38	0.57
1:XA:405:U:O4	4:XD:2:GLY:N	2.37	0.57
13:XM:83:ASP:OD1	13:XM:93:ARG:NH2	2.34	0.57
49:Y4:56:VAL:HG23	49:Y4:58:ARG:HG3	1.86	0.57
25:RB:37:C:O2	37:RS:95:HIS:NE2	2.36	0.57
44:RZ:145:GLU:HG3	44:RZ:146:ILE:HG12	1.86	0.57
1:XA:1392:G:H21	1:XA:1502:A:H8	1.52	0.57
3:XC:95:THR:HG22	3:XC:97:LYS:H	1.70	0.57
24:YA:1089:G:N2	24:YA:1090:U:O4	2.38	0.57
24:YA:1019:U:H3	24:YA:1142(A):A:H62	1.50	0.57
24:YA:297:C:OP1	43:YY:87:LYS:NZ	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1159:U:O2'	1:QA:1160:G:N7	2.37	0.57
1:QA:1240:U:OP1	7:QG:119:ARG:NH2	2.37	0.57
1:QA:559:A:H4'	1:QA:560:U:H3'	1.87	0.57
2:QB:68:ILE:HG12	2:QB:161:ALA:HB3	1.87	0.57
36:RR:104:ARG:HG3	36:RR:107:ASP:HB3	1.86	0.57
1:QA:581:G:O3'	15:QO:64:ARG:NH2	2.37	0.57
3:XC:20:SER:HB2	3:XC:40:ARG:HH22	1.70	0.57
12:XL:71:PRO:O	12:XL:102:ARG:NH1	2.38	0.57
24:YA:620:G:H4'	24:YA:621:A:H5''	1.87	0.57
24:RA:2848:G:O2'	24:RA:2867:G:N2	2.36	0.57
33:YO:80:ASP:OD2	38:YT:64:ARG:NH2	2.38	0.57
40:YV:24:LYS:HA	40:YV:92:THR:HG23	1.87	0.57
9:QI:104:ARG:NH1	9:QI:105:ASP:O	2.38	0.57
24:RA:2068:U:H3	24:RA:2430:A:H2	1.51	0.57
40:RV:24:LYS:HA	40:RV:92:THR:HG23	1.87	0.57
11:XK:34:ASP:OD1	11:XK:38:ASN:N	2.38	0.57
51:Y6:10:LEU:HD13	51:Y6:19:ARG:HG2	1.87	0.57
30:YH:153:LYS:HB3	30:YH:161:GLY:HA2	1.86	0.57
24:RA:630:G:N2	24:RA:633:A:OP2	2.32	0.56
30:RH:46:GLU:OE1	30:RH:51:ARG:NH1	2.38	0.56
19:XS:19:VAL:HG11	19:XS:44:MET:HG2	1.85	0.56
24:YA:1270:C:H5''	24:YA:1271:G:H5'	1.87	0.56
24:YA:2068:U:H3	24:YA:2430:A:H2	1.53	0.56
27:YE:105:THR:HB	27:YE:197:ILE:HG23	1.86	0.56
3:QC:95:THR:HG22	3:QC:97:LYS:H	1.70	0.56
24:RA:1220:A:OP2	39:RU:19:LYS:NZ	2.32	0.56
24:RA:1479:G:OP2	24:RA:1510:A:N6	2.38	0.56
24:RA:2680:C:OP2	27:RE:111:ARG:NH2	2.35	0.56
1:XA:954:G:H21	1:XA:1227:A:H62	1.51	0.56
24:YA:2392:A:H2	24:YA:2424:C:H42	1.53	0.56
1:QA:738:C:OP1	6:QF:2:ARG:NH1	2.37	0.56
24:RA:860:U:H2'	24:RA:861:A:H8	1.70	0.56
44:YZ:145:GLU:HG3	44:YZ:146:ILE:HG12	1.87	0.56
1:QA:339:C:OP2	33:RO:97:ARG:NH1	2.39	0.56
9:XI:21:PRO:HA	9:XI:59:PHE:HA	1.87	0.56
24:YA:184:C:O2'	24:YA:217:G:N3	2.38	0.56
24:YA:2882:A:OP1	36:YR:96:ARG:NH1	2.38	0.56
44:YZ:10:ARG:NH2	44:YZ:37:VAL:O	2.39	0.56
24:RA:1490:A:O2'	26:RD:99:ASP:OD1	2.23	0.56
30:RH:153:LYS:HB3	30:RH:161:GLY:HA2	1.86	0.56
13:XM:3:ARG:HA	13:XM:9:ILE:HG21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:XR:86:VAL:HG12	18:XR:87:ARG:HG2	1.88	0.56
24:YA:2469:A:H2	24:YA:2481:G:H21	1.52	0.56
30:YH:46:GLU:OE1	30:YH:51:ARG:NH1	2.38	0.56
2:QB:6:THR:O	2:QB:217:ARG:NH1	2.38	0.56
3:QC:88:ARG:HE	3:QC:101:LEU:HB3	1.71	0.56
11:QK:18:ARG:HG2	11:QK:81:ASP:HB2	1.88	0.56
24:RA:1542:G:O6	24:RA:1543:A:N6	2.39	0.56
13:XM:19:LEU:HD21	13:XM:56:LEU:HD11	1.88	0.56
29:YG:47:LYS:HD3	29:YG:81:LYS:HB2	1.87	0.56
3:QC:20:SER:HB2	3:QC:40:ARG:HH22	1.70	0.56
24:RA:2308:G:H22	24:RA:2311:A:H2	1.52	0.56
26:RD:146:GLU:HB2	26:RD:189:CYS:HB3	1.88	0.56
1:QA:297:G:N2	1:QA:300:A:OP2	2.36	0.56
1:QA:624:C:H2'	1:QA:625:G:H8	1.71	0.56
1:XA:8:A:N6	4:XD:205:GLU:O	2.39	0.56
14:XM:27:CYS:SG	14:XM:28:GLY:N	2.78	0.56
24:YA:2470:G:H5'	35:YQ:56:ARG:HH21	1.71	0.56
7:QG:116:ALA:HA	7:QG:119:ARG:HE	1.71	0.56
24:RA:2285:C:OP2	51:R6:6:ARG:NH1	2.39	0.56
53:Y8:29:LYS:O	53:Y8:31:HIS:N	2.38	0.56
1:QA:227:G:N2	16:QP:62:VAL:O	2.31	0.56
24:RA:1341:U:OP2	24:RA:1394:U:O2'	2.24	0.56
24:YA:2701:C:H3'	24:YA:2702:U:H5''	1.87	0.56
24:YA:675:A:OP1	28:YF:63:LYS:NZ	2.31	0.56
24:YA:2115:G:N2	24:YA:2165:G:N7	2.53	0.55
24:YA:2154:G:H2'	24:YA:2155:G:H8	1.71	0.55
24:YA:2313:C:H5''	29:YG:91:ARG:HD3	1.87	0.55
1:QA:986:A:N3	19:QS:52:TYR:OH	2.34	0.55
1:QA:8:A:N6	4:QD:205:GLU:O	2.38	0.55
29:RG:47:LYS:HD3	29:RG:81:LYS:HB2	1.88	0.55
1:XA:587:G:N2	1:XA:754:C:OP2	2.39	0.55
2:XB:168:THR:HA	2:XB:171:ALA:HB2	1.89	0.55
3:XC:70:VAL:HG12	3:XC:72:LYS:H	1.72	0.55
24:YA:1195:G:O6	34:YP:16:ARG:NH2	2.38	0.55
24:YA:2502:G:H5''	24:YA:2503:A:H5''	1.87	0.55
1:QA:933:G:O6	7:QG:3:ARG:NH2	2.39	0.55
1:XA:690:G:H22	11:XK:55:LYS:HZ1	1.53	0.55
13:XM:14:ARG:NH2	13:XM:16:ASP:OD2	2.39	0.55
24:YA:226:G:O2'	24:YA:228:A:N6	2.40	0.55
26:YD:146:GLU:HB2	26:YD:189:CYS:HB3	1.88	0.55
24:YA:907:U:O2'	35:YQ:101:ARG:NH2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:811:C:O2'	1:QA:901:A:N1	2.39	0.55
1:QA:1128:C:OP1	9:QL:66:ARG:NH2	2.40	0.55
14:QN:27:CYS:SG	14:QN:28:GLY:N	2.79	0.55
1:QA:244:U:OP2	17:QQ:100:LYS:NZ	2.40	0.55
24:RA:587:C:OP2	34:RP:21:ARG:NH1	2.39	0.55
33:RO:80:ASP:OD2	38:RT:64:ARG:NH2	2.39	0.55
1:XA:128:G:O2'	17:XQ:3:LYS:NZ	2.35	0.55
1:XA:825:G:O2'	8:XH:12:ARG:NH2	2.36	0.55
1:XA:662:G:O2'	1:XA:836:G:OP1	2.25	0.55
3:XC:88:ARG:HE	3:XC:101:LEU:HB3	1.71	0.55
1:XA:254:G:O2'	17:XQ:16:GLN:O	2.23	0.55
54:Y9:2:LYS:NZ	54:Y9:31:LYS:O	2.39	0.55
2:QB:47:THR:HA	2:QB:202:PRO:HG2	1.88	0.55
18:QR:32:ARG:HA	18:QR:69:THR:HG21	1.87	0.55
1:QA:1314:C:N4	19:QS:2:PRO:O	2.38	0.55
1:XA:1151:A:O2'	10:XJ:70:ARG:NH2	2.39	0.55
3:XC:19:GLU:O	3:XC:40:ARG:NH2	2.39	0.55
1:QA:1249:C:O2'	9:QL:73:GLN:NE2	2.38	0.55
1:QA:945:G:N2	1:QA:1334:G:O2'	2.39	0.55
11:QK:86:GLY:O	11:QK:91:ARG:NH1	2.40	0.55
13:QM:93:ARG:NH1	24:RA:888:C:OP1	2.40	0.55
24:RA:1969:A:O2'	24:RA:1972:A:N3	2.34	0.55
24:RA:338:G:OP1	43:RY:4:LYS:NZ	2.39	0.55
24:RA:503:A:H4'	24:RA:504:U:H5'	1.87	0.55
24:RA:859:G:N2	24:RA:917:A:OP2	2.38	0.55
30:RH:12:PRO:HG2	30:RH:13:LYS:HG2	1.88	0.55
1:QA:618:C:H5'	1:QA:619:U:H5''	1.88	0.55
18:QR:86:VAL:HG12	18:QR:87:ARG:HG2	1.88	0.55
54:R9:2:LYS:NZ	54:R9:31:LYS:O	2.39	0.55
33:RO:104:ARG:HH11	33:RO:121:VAL:HG12	1.72	0.55
44:RZ:10:ARG:NH2	44:RZ:37:VAL:O	2.39	0.55
1:XA:972:C:OP2	10:XJ:57:LYS:NZ	2.39	0.55
6:XF:94:GLN:OE1	18:XR:32:ARG:NH1	2.40	0.55
1:QA:690:G:H22	11:QK:55:LYS:HZ1	1.55	0.55
24:RA:1124:C:O2	54:R9:36:GLN:NE2	2.39	0.55
30:YH:12:PRO:HG2	30:YH:13:LYS:HG2	1.88	0.55
33:YO:104:ARG:HH11	33:YO:121:VAL:HG12	1.72	0.55
54:R9:25:VAL:HB	54:R9:34:GLN:HB2	1.89	0.55
24:RA:1059:G:O6	24:RA:1079:C:N4	2.40	0.55
1:XA:707:C:OP1	11:XK:85:ARG:NH1	2.39	0.55
7:XG:111:ARG:NH2	7:XG:126:ASP:OD2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:YA:857:C:OP2	45:Y0:77:ARG:NH2	2.39	0.55
24:YA:1103:A:H5'	24:YA:1104:C:H5	1.72	0.55
28:YF:116:ASP:OD1	28:YF:119:ARG:NH2	2.39	0.55
43:RY:47:LYS:NZ	43:RY:48:ALA:O	2.33	0.55
1:XA:1123:A:H4'	10:XJ:36:GLY:HA3	1.87	0.55
1:XA:316:G:OP2	1:XA:351:G:O2'	2.22	0.55
12:XL:45:PRO:HB3	12:XL:92:ASP:HB3	1.89	0.55
1:QA:1210:C:O2'	1:QA:1213:A:O2'	2.25	0.54
1:QA:765:G:N2	1:QA:813:U:OP2	2.33	0.54
1:QA:973:G:O6	1:QA:974:A:N6	2.41	0.54
8:QH:106:GLY:O	8:QH:122:ARG:NH2	2.38	0.54
51:R6:10:LEU:HD13	51:R6:19:ARG:HG2	1.87	0.54
24:RA:2680:C:H5'	27:RE:189:PRO:HA	1.88	0.54
24:YA:1530:G:O6	24:YA:1542:G:N2	2.40	0.54
1:QA:437:U:H3	1:QA:495:A:H62	1.54	0.54
1:QA:757:U:O2'	1:QA:879:C:O2	2.25	0.54
24:RA:958:U:OP2	35:RQ:14:ARG:NH1	2.39	0.54
2:XB:69:LEU:HB3	2:XB:162:ILE:HG22	1.89	0.54
7:XG:116:ALA:HA	7:XG:119:ARG:HE	1.71	0.54
1:QA:674:G:OP1	6:QF:87:ARG:NH2	2.40	0.54
37:RS:15:ARG:NE	37:RS:88:ASP:OD1	2.40	0.54
1:XA:642:A:N3	8:XH:113:SER:OG	2.34	0.54
1:XA:677:U:H3	1:XA:713:G:H22	1.54	0.54
24:YA:1310:G:OP2	52:Y7:9:ARG:NE	2.34	0.54
1:QA:838:G:H1	1:QA:848:C:H42	1.54	0.54
7:QG:150:ALA:HB1	11:QK:57:THR:HG21	1.90	0.54
8:QH:12:ARG:HD2	8:QH:26:VAL:HG12	1.88	0.54
24:RA:414:C:O2	24:RA:1864:U:O2'	2.24	0.54
36:RR:12:ARG:O	36:RR:17:ARG:NH2	2.40	0.54
47:Y2:17:SER:HB2	47:Y2:20:GLU:HG2	1.89	0.54
3:QC:19:GLU:O	3:QC:40:ARG:NH2	2.39	0.54
24:RA:2791:C:H4'	24:RA:2792:G:H5'	1.88	0.54
1:XA:993:G:O2'	1:XA:994:A:N7	2.40	0.54
8:XH:12:ARG:HD2	8:XH:26:VAL:HG12	1.88	0.54
24:YA:1359:A:H62	24:YA:1372:U:H3	1.54	0.54
27:YE:201:THR:HG22	27:YE:203:LYS:H	1.72	0.54
28:YF:116:ASP:OD2	34:YP:1:MET:N	2.35	0.54
40:YV:23:GLU:OE2	40:YV:89:GLN:NE2	2.35	0.54
3:QC:70:VAL:HG12	3:QC:72:LYS:H	1.72	0.54
1:QA:619:U:N3	4:QD:134:ASP:OD1	2.35	0.54
24:RA:782:A:O2'	26:RD:225:ALA:O	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:XB:72:GLY:HA3	2:XB:81:VAL:HG21	1.89	0.54
1:XA:191(G):G:O2'	20:XT:101:GLY:O	2.25	0.54
24:YA:1791:A:N6	24:YA:1828:G:O2'	2.38	0.54
26:YD:143:HIS:ND1	26:YD:194:GLY:O	2.32	0.54
30:YH:149:ARG:NH2	30:YH:167:GLU:OE2	2.41	0.54
38:RT:77:PRO:HB2	38:RT:80:SER:HB2	1.89	0.54
54:Y9:25:VAL:HB	54:Y9:34:GLN:HB2	1.89	0.54
1:QA:35:G:N3	12:QL:118:SER:OG	2.41	0.54
1:QA:745:C:OP1	1:QA:851:G:O2'	2.26	0.54
6:QF:99:ALA:HB1	18:QR:23:LYS:HE3	1.89	0.54
24:RA:2298:A:H62	24:RA:2318:G:H8	1.56	0.54
24:YA:2655:G:N2	24:YA:2665:A:OP2	2.41	0.54
37:YS:15:ARG:NE	37:YS:88:ASP:OD1	2.40	0.54
1:QA:323:U:OP1	20:QT:26:ASN:ND2	2.39	0.54
1:QA:662:G:O2'	1:QA:836:G:OP1	2.24	0.54
24:RA:2387:U:O2'	45:R0:19:LYS:NZ	2.40	0.54
24:RA:768:G:O2'	24:RA:1379:A:N6	2.41	0.54
24:RA:2882:A:OP1	36:RR:96:ARG:NH1	2.40	0.54
1:XA:811:C:O2'	1:XA:901:A:N1	2.41	0.54
8:XH:106:GLY:O	8:XH:122:ARG:NH2	2.38	0.54
24:YA:2680:C:OP2	27:YE:111:ARG:NH2	2.31	0.54
1:QA:686:U:H1'	11:QK:42:TRP:HE1	1.72	0.54
26:RD:81:ALA:HB3	26:RD:94:LEU:HB3	1.90	0.54
27:RE:201:THR:HG22	27:RE:203:LYS:H	1.72	0.54
27:RE:9:VAL:HB	27:RE:25:VAL:HG23	1.90	0.54
40:RV:23:GLU:OE2	40:RV:89:GLN:NE2	2.35	0.54
2:XB:30:ARG:HH21	2:XB:194:PRO:HG2	1.73	0.54
25:RB:80:U:H2'	25:RB:81:G:H21	1.74	0.53
39:RU:44:ASN:HD21	40:RV:75:PHE:HB3	1.73	0.53
24:YA:138:G:N2	42:YX:44:GLU:OE1	2.29	0.53
44:YZ:48:PHE:HA	44:YZ:51:ALA:HB3	1.90	0.53
24:RA:297:C:OP1	43:RY:87:LYS:NZ	2.41	0.53
39:RU:90:VAL:HG22	40:RV:39:LEU:HD23	1.89	0.53
1:QA:1123:A:H4'	10:QJ:36:GLY:HA3	1.88	0.53
27:RE:78:LEU:HG	27:RE:79:ARG:HG2	1.90	0.53
47:Y2:22:GLU:OE2	47:Y2:68:ARG:NH2	2.42	0.53
27:YE:9:VAL:HB	27:YE:25:VAL:HG23	1.90	0.53
36:YR:24:GLN:HE22	36:YR:40:LYS:HB3	1.73	0.53
1:QA:1077:G:N2	1:QA:1080:A:OP2	2.41	0.53
1:QA:376:G:H1	1:QA:387:U:H3	1.55	0.53
28:RF:116:ASP:OD1	28:RF:119:ARG:NH2	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:RV:61:VAL:HG12	40:RV:63:GLY:H	1.74	0.53
1:XA:143:A:H2	1:XA:220:G:H1	1.55	0.53
1:XA:490:G:OP2	4:XD:132:ARG:NH2	2.42	0.53
24:YA:1454:U:O2'	24:YA:1455:G:N7	2.35	0.53
33:YO:7:TYR:HE1	33:YO:44:LYS:HG3	1.74	0.53
34:YP:49:ARG:HH11	53:Y8:58:ILE:HG22	1.72	0.53
36:YR:86:ARG:NH2	36:YR:118:GLU:OXT	2.41	0.53
1:QA:1002:G:H2'	1:QA:1003:G:H8	1.74	0.53
10:QJ:28:ARG:NH2	10:QJ:34:VAL:O	2.41	0.53
24:RA:270(T):G:H5''	46:R1:97:LEU:HD22	1.90	0.53
47:R2:17:SER:HB2	47:R2:20:GLU:HG2	1.89	0.53
24:RA:1638:C:O2	24:RA:2698:U:O2'	2.27	0.53
32:RN:58:ASP:OD1	32:RN:58:ASP:N	2.41	0.53
33:RO:7:TYR:HE1	33:RO:44:LYS:HG3	1.74	0.53
1:XA:278:G:OP2	17:XQ:92:ARG:NH2	2.41	0.53
34:YP:62:LEU:HD12	53:Y8:30:ARG:HH21	1.73	0.53
30:YH:164:TYR:HB2	30:YH:167:GLU:HB2	1.90	0.53
1:QA:581:G:OP1	15:QO:65:ARG:NH1	2.41	0.53
47:R2:22:GLU:OE2	47:R2:68:ARG:NH2	2.42	0.53
29:RG:37:VAL:HG22	29:RG:159:VAL:HG12	1.89	0.53
1:XA:356:A:N3	1:XA:368:U:O2'	2.39	0.53
24:YA:587:C:OP2	34:YP:21:ARG:NH1	2.39	0.53
25:YB:80:U:H2'	25:YB:81:G:H21	1.73	0.53
44:YZ:52:SER:O	44:YZ:54:HIS:N	2.39	0.53
1:QA:768:A:N3	1:QA:1512:U:O2'	2.41	0.53
1:QA:701:C:O2	1:QA:703:G:N1	2.41	0.53
10:XJ:51:ARG:O	14:XN:45:ARG:NH1	2.42	0.53
13:XM:47:ASP:N	13:XM:47:ASP:OD1	2.40	0.53
24:YA:630:G:N2	24:YA:633:A:OP2	2.39	0.53
36:YR:104:ARG:HG3	36:YR:107:ASP:HB3	1.90	0.53
24:RA:1153:C:H5'	39:RU:76:TYR:HE2	1.72	0.53
24:RA:995:C:O2	32:RN:3:THR:OG1	2.26	0.53
30:RH:164:TYR:HB2	30:RH:167:GLU:HB2	1.90	0.53
1:XA:157:G:H1	1:XA:164:U:H3	1.55	0.53
46:Y1:51:VAL:HG11	46:Y1:74:VAL:HG21	1.90	0.53
46:Y1:52:ARG:HH11	46:Y1:57:GLU:HB2	1.73	0.53
24:YA:1084:A:N1	24:YA:1085:A:N6	2.56	0.53
38:YT:77:PRO:HB2	38:YT:80:SER:HB2	1.89	0.53
5:QE:98:THR:HB	5:QE:117:ASP:HB3	1.91	0.53
1:QA:1346:A:H5''	9:QI:120:ARG:HH12	1.74	0.53
1:XA:526:C:OP2	12:XL:91:LYS:NZ	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:YW:86:LEU:HD22	41:YW:96:ILE:HD11	1.90	0.53
9:QI:93:ARG:HH12	9:QI:102:LEU:HD22	1.74	0.53
24:RA:296:C:O3'	43:RY:95:LYS:NZ	2.41	0.53
26:RD:31:LYS:HB3	26:RD:35:LYS:HG3	1.91	0.53
24:YA:1728:G:N1	24:YA:1730:U:OP2	2.41	0.53
24:YA:180:G:N2	24:YA:215:G:O6	2.41	0.53
27:YE:78:LEU:HG	27:YE:79:ARG:HG2	1.90	0.53
31:YI:99:GLU:OE2	31:YI:103:ARG:NH2	2.38	0.53
1:QA:1175:G:H2'	1:QA:1176:A:H8	1.74	0.52
2:QB:178:ARG:NH2	2:QB:196:LEU:O	2.42	0.52
24:RA:1971:A:OP2	26:RD:242:ARG:NH2	2.39	0.52
28:RF:161:GLU:OE1	28:RF:164:ARG:NH2	2.42	0.52
30:RH:149:ARG:NH2	30:RH:167:GLU:OE2	2.41	0.52
24:YA:1652:A:OP1	36:YR:8:ARG:NH1	2.42	0.52
26:YD:31:LYS:HB3	26:YD:35:LYS:HG3	1.91	0.52
31:YI:5:LEU:HD21	31:YI:12:LEU:HB3	1.91	0.52
24:RA:1061:U:OP2	24:RA:1070:A:O2'	2.26	0.52
24:RA:1485:G:H1	24:RA:1504:C:H42	1.56	0.52
24:RA:2052:G:H4'	27:RE:143:ASN:H	1.75	0.52
24:YA:2788:C:O2'	24:YA:2809:A:N3	2.40	0.52
29:YG:161:THR:HG22	29:YG:163:ALA:H	1.73	0.52
32:YN:58:ASP:OD1	32:YN:58:ASP:N	2.41	0.52
24:RA:517:C:OP1	50:R5:16:ARG:NH2	2.42	0.52
44:RZ:48:PHE:HA	44:RZ:51:ALA:HB3	1.90	0.52
24:YA:2140:C:H2'	24:YA:2141:G:H8	1.75	0.52
29:YG:37:VAL:HG22	29:YG:159:VAL:HG12	1.90	0.52
1:QA:1061:G:OP1	10:QJ:59:SER:OG	2.24	0.52
1:QA:576:G:N2	1:QA:759:A:OP1	2.40	0.52
53:R8:29:LYS:O	53:R8:31:HIS:N	2.38	0.52
24:RA:2494:G:OP1	45:R0:3:HIS:N	2.42	0.52
26:RD:71:ASP:HB2	26:RD:103:ARG:HH12	1.74	0.52
24:YA:1394:U:O2	42:YX:16:LYS:NZ	2.39	0.52
26:YD:71:ASP:HB2	26:YD:103:ARG:HH12	1.74	0.52
35:YQ:31:ASP:OD1	35:YQ:134:ARG:NH1	2.42	0.52
44:YZ:102:LEU:HD11	44:YZ:124:ILE:HG13	1.92	0.52
1:QA:1128:C:H1'	1:QA:1146:A:H61	1.75	0.52
42:RX:26:TYR:HE2	42:RX:89:ILE:H	1.57	0.52
8:XH:9:MET:HG3	8:XH:26:VAL:HG11	1.92	0.52
24:YA:2438:U:O2'	24:YA:2440:C:OP1	2.28	0.52
39:YU:90:VAL:HG11	40:YV:40:LEU:HG	1.92	0.52
1:QA:742:G:OP2	15:QO:35:ARG:NH2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:RA:2392:A:H2	24:RA:2424:C:H42	1.57	0.52
24:RA:392:C:H5''	24:RA:409:C:H5''	1.92	0.52
24:RA:2666:C:O2	30:RH:152:ARG:NH1	2.42	0.52
40:YV:61:VAL:HG12	40:YV:63:GLY:H	1.74	0.52
44:YZ:45:ASP:OD1	44:YZ:49:ARG:NE	2.43	0.52
1:QA:957:U:OP1	19:QS:81:ARG:NH2	2.42	0.52
24:RA:1009:A:OP2	32:RN:37:LYS:NZ	2.43	0.52
29:RG:161:THR:HG22	29:RG:163:ALA:H	1.73	0.52
34:RP:52:GLU:OE2	34:RP:58:THR:OG1	2.27	0.52
44:RZ:45:ASP:OD1	44:RZ:49:ARG:NE	2.43	0.52
1:XA:545:C:OP1	4:XD:61:LYS:NZ	2.41	0.52
24:YA:1341:U:OP2	24:YA:1394:U:O2'	2.21	0.52
26:YD:81:ALA:HB3	26:YD:94:LEU:HB3	1.90	0.52
42:YX:26:TYR:HE2	42:YX:89:ILE:H	1.58	0.52
5:QE:78:HIS:HE1	5:QE:80:ILE:HD13	1.75	0.52
7:QG:111:ARG:NH2	7:QG:126:ASP:OD2	2.37	0.52
30:RH:8:PRO:HG2	30:RH:69:ARG:HE	1.75	0.52
41:RW:86:LEU:HD22	41:RW:96:ILE:HD11	1.90	0.52
25:YB:5:C:O2'	25:YB:27:C:O2	2.28	0.52
24:YA:782:A:O2'	26:YD:225:ALA:O	2.28	0.52
24:RA:2701:C:H3'	24:RA:2702:U:H5''	1.91	0.52
31:RI:5:LEU:HD21	31:RI:12:LEU:HB3	1.91	0.52
1:XA:790:A:OP1	22:XV:39:A:O2'	2.25	0.52
24:YA:820:A:N3	24:YA:943:U:O2'	2.41	0.52
24:YA:993:G:OP1	39:YU:50:ARG:NH2	2.42	0.52
28:YF:40:GLN:HE22	28:YF:182:ASN:HB2	1.75	0.52
1:QA:357:G:O2'	31:YI:89:TYR:O	2.25	0.52
8:QH:9:MET:HG3	8:QH:26:VAL:HG11	1.92	0.52
24:RA:2502:G:H5''	24:RA:2503:A:H5''	1.91	0.52
25:RB:5:C:O2'	25:RB:27:C:O2	2.28	0.52
44:RZ:52:SER:O	44:RZ:54:HIS:N	2.39	0.52
29:YG:142:PRO:HB2	49:Y4:31:ILE:HG21	1.91	0.52
5:QE:137:GLU:OE1	5:QE:140:ARG:NH1	2.43	0.51
1:QA:947:G:O3'	13:QM:109:THR:OG1	2.28	0.51
24:RA:2495:G:H5''	35:RQ:81:VAL:HG12	1.93	0.51
1:XA:1245:A:OP2	21:XU:9:ARG:NH2	2.43	0.51
1:XA:1251:A:N3	1:XA:1369:C:O2'	2.38	0.51
50:Y5:41:PRO:O	50:Y5:44:THR:OG1	2.28	0.51
24:RA:184:C:O2'	24:RA:217:G:N3	2.37	0.51
28:RF:198:ALA:HA	28:RF:201:VAL:HG12	1.92	0.51
35:RQ:31:ASP:OD1	35:RQ:134:ARG:NH1	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:1286:A:H2'	1:XA:1287:A:H4'	1.92	0.51
1:XA:745:C:OP1	1:XA:851:G:O2'	2.27	0.51
5:XE:98:THR:HB	5:XE:117:ASP:HB3	1.91	0.51
21:XU:6:ARG:HH21	21:XU:15:ARG:HH21	1.58	0.51
24:YA:1999:C:O2	24:YA:2687:U:O2'	2.26	0.51
24:YA:629:G:N3	24:YA:639:U:O2'	2.43	0.51
42:YX:53:LYS:NZ	42:YX:55:ASN:OD1	2.44	0.51
1:QA:1222:G:OP1	19:QS:78:ARG:NH1	2.32	0.51
1:QA:954:G:H21	1:QA:1227:A:H62	1.57	0.51
3:QC:17:ASP:O	3:QC:54:ARG:NH2	2.43	0.51
45:R0:39:ARG:NH1	45:R0:58:THR:OG1	2.43	0.51
1:XA:689:C:H3'	1:XA:690:G:H21	1.75	0.51
24:YA:224:G:O6	24:YA:419:C:O2'	2.27	0.51
1:QA:444:C:H2'	1:QA:445:G:H8	1.74	0.51
24:RA:480:A:O2'	43:RY:46:LYS:O	2.28	0.51
1:XA:963:G:H21	10:XJ:55:LYS:HD3	1.76	0.51
24:YA:626:U:O4	34:YP:81:GLN:NE2	2.44	0.51
31:YI:78:THR:HG22	31:YI:141:LYS:HE3	1.92	0.51
2:QB:115:LEU:HD13	2:QB:145:LEU:HB3	1.91	0.51
24:RA:1270:C:H5''	24:RA:1271:G:H5'	1.92	0.51
24:RA:527:C:N4	24:RA:2779:U:OP2	2.41	0.51
29:RG:55:LYS:NZ	29:RG:59:GLU:OE2	2.44	0.51
1:XA:748:C:H1'	1:XA:749:C:H5	1.75	0.51
1:XA:8:A:N6	4:XD:208:SER:O	2.43	0.51
24:YA:2467:C:O2	35:YQ:124:LYS:NZ	2.36	0.51
24:YA:26:G:H1'	24:YA:515:A:H61	1.76	0.51
28:YF:161:GLU:OE1	28:YF:164:ARG:NH2	2.42	0.51
4:QD:62:GLN:HE22	4:QD:65:ARG:HH21	1.59	0.51
26:RD:122:ASP:OD1	26:RD:122:ASP:N	2.40	0.51
31:RI:78:THR:HG22	31:RI:141:LYS:HE3	1.92	0.51
1:XA:1101:A:N6	2:XB:176:GLU:OE2	2.44	0.51
2:XB:231:GLU:HG3	2:XB:233:SER:H	1.75	0.51
6:XF:50:TYR:OH	18:XR:75:ILE:O	2.28	0.51
35:YQ:28:ALA:HB3	35:YQ:67:ARG:HH12	1.76	0.51
1:QA:1372:U:H5''	9:QI:71:SER:HB3	1.93	0.51
26:RD:148:GLU:HB2	26:RD:151:LYS:HD2	1.93	0.51
27:RE:104:VAL:HG22	27:RE:198:VAL:HG22	1.93	0.51
24:YA:2153:G:H2'	24:YA:2154:G:H8	1.74	0.51
24:YA:605:C:O2	24:YA:657:U:O2'	2.27	0.51
26:YD:148:GLU:HB2	26:YD:151:LYS:HD2	1.93	0.51
3:XC:17:ASP:O	3:XC:54:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:YG:55:LYS:NZ	29:YG:59:GLU:OE2	2.44	0.51
24:RA:605:C:O2	24:RA:657:U:O2'	2.29	0.51
28:RF:40:GLN:HE22	28:RF:182:ASN:HB2	1.75	0.51
1:XA:31:G:O2'	1:XA:48:C:N4	2.43	0.51
1:QA:1013:G:N2	1:QA:1016:A:OP2	2.40	0.51
1:QA:1032(B):G:N2	1:QA:1033:G:O6	2.44	0.51
1:QA:1306:A:N6	1:QA:1331:G:O2'	2.44	0.51
1:QA:570:G:O6	1:QA:865:A:N6	2.43	0.51
2:QB:71:VAL:HA	2:QB:93:VAL:HB	1.93	0.51
46:R1:18:ILE:HG12	46:R1:37:ILE:HG12	1.93	0.51
24:RA:2245:U:H5'	24:RA:2246:G:H5'	1.93	0.51
5:XE:137:GLU:OE1	5:XE:140:ARG:NH1	2.43	0.51
1:XA:376:G:H5''	16:XP:5:ARG:HB2	1.93	0.51
54:Y9:27:CYS:SG	54:Y9:28:GLU:N	2.84	0.51
24:YA:1818:U:H2'	26:YD:157:ARG:HG2	1.92	0.51
28:YF:198:ALA:HA	28:YF:201:VAL:HG12	1.92	0.51
32:YN:6:PRO:HG3	32:YN:41:ASP:HB2	1.93	0.51
1:QA:878:G:H5'	8:QH:89:PRO:HG2	1.92	0.50
3:QC:189:ALA:HB3	3:QC:196:LEU:HB2	1.93	0.50
24:RA:998:C:OP2	39:RU:58:ARG:NH1	2.44	0.50
25:RB:111:U:H2'	25:RB:112:G:H8	1.75	0.50
5:XE:78:HIS:HE1	5:XE:80:ILE:HD13	1.75	0.50
48:Y3:15:TYR:O	48:Y3:20:LYS:NZ	2.44	0.50
24:YA:1059:G:H22	24:YA:1062:G:H4'	1.76	0.50
37:YS:25:ARG:NH1	37:YS:42:ASP:OD2	2.44	0.50
13:QM:47:ASP:N	13:QM:47:ASP:OD1	2.38	0.50
24:RA:2637:U:H5''	27:RE:82:ARG:NH1	2.27	0.50
29:RG:173:LEU:O	29:RG:178:PHE:N	2.41	0.50
30:RH:86:GLU:HB2	30:RH:165:ALA:H	1.76	0.50
18:XR:38:GLU:O	18:XR:42:ARG:NH1	2.45	0.50
24:YA:1063:G:H22	24:YA:1076:C:H1'	1.76	0.50
31:YI:79:ILE:HB	31:YI:142:VAL:HA	1.93	0.50
1:QA:937:A:N6	1:QA:1345:U:O4	2.41	0.50
1:QA:1432:G:OP1	38:RT:108:ARG:N	2.40	0.50
1:QA:34:C:H2'	1:QA:35:G:H8	1.77	0.50
9:QI:113:LYS:HB2	9:QI:119:ALA:HA	1.94	0.50
18:QR:38:GLU:O	18:QR:42:ARG:NH1	2.45	0.50
24:RA:2126:A:N6	24:RA:2163:C:O2'	2.44	0.50
42:RX:53:LYS:NZ	42:RX:55:ASN:OD1	2.44	0.50
28:YF:167:ALA:HB1	28:YF:173:VAL:HG11	1.93	0.50
24:YA:2683:C:OP1	38:YT:53:ARG:NH2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:356:A:N3	1:QA:368:U:O2'	2.37	0.50
4:QD:116:GLN:HE21	4:QD:157:LEU:HD21	1.76	0.50
21:QU:6:ARG:HH21	21:QU:15:ARG:HH21	1.58	0.50
54:R9:27:CYS:SG	54:R9:28:GLU:N	2.84	0.50
34:RP:135:LEU:HG	34:RP:139:LYS:HE2	1.93	0.50
37:RS:25:ARG:NH1	37:RS:42:ASP:OD2	2.44	0.50
4:XD:62:GLN:HE22	4:XD:65:ARG:HH21	1.59	0.50
45:Y0:10:THR:HG22	45:Y0:12:ASN:H	1.77	0.50
24:YA:523:C:O2	24:YA:553:U:O2'	2.28	0.50
26:YD:122:ASP:OD1	26:YD:122:ASP:N	2.40	0.50
1:QA:1320:C:O2	19:QS:36:ARG:NH2	2.43	0.50
1:QA:296:U:O2'	1:QA:556:C:O2	2.28	0.50
24:RA:83:G:O2'	24:RA:102:G:N2	2.44	0.50
24:RA:603:A:N1	24:RA:625:G:O2'	2.38	0.50
1:XA:1004:A:H1'	1:XA:1036:G:H22	1.75	0.50
1:XA:656:C:O2	15:XO:28:GLN:NE2	2.43	0.50
1:XA:911:U:OP2	12:XL:97:ARG:NH2	2.41	0.50
3:XC:19:GLU:HG2	3:XC:54:ARG:HE	1.77	0.50
10:XJ:78:ASN:O	10:XJ:81:THR:OG1	2.28	0.50
24:YA:1664:A:H61	24:YA:1996:C:H42	1.60	0.50
1:QA:953:G:N7	13:QM:104:ARG:NH2	2.58	0.50
1:QA:1443:G:N2	24:RA:2864:G:OP1	2.40	0.50
24:RA:517:C:O2'	41:RW:18:ARG:NH2	2.37	0.50
24:RA:2619:C:H5"	27:RE:152:LYS:HA	1.92	0.50
1:XA:1191:A:OP2	3:XC:3:ASN:ND2	2.44	0.50
1:XA:559:A:OP1	5:XE:126:ARG:NH2	2.45	0.50
24:YA:574:C:N3	27:YE:145:LYS:NZ	2.58	0.50
25:YB:111:U:H2'	25:YB:112:G:H8	1.75	0.50
24:RA:2632:A:O2'	24:RA:2811:G:O2'	2.23	0.50
31:RI:129:THR:HA	31:RI:137:PRO:HA	1.93	0.50
44:RZ:4:ARG:HG2	44:RZ:58:VAL:HB	1.93	0.50
31:YI:129:THR:HA	31:YI:137:PRO:HA	1.93	0.50
1:QA:1305:G:N2	1:QA:1332:A:OP2	2.44	0.50
1:QA:1393:U:HO2'	1:QA:1501:C:HO2'	1.56	0.50
1:QA:708:C:OP1	11:QK:85:ARG:NH2	2.34	0.50
24:RA:249:C:O2	53:R8:12:LYS:NZ	2.41	0.50
30:RH:88:LEU:HA	30:RH:130:ARG:HA	1.94	0.50
35:RQ:28:ALA:HB3	35:RQ:67:ARG:HH12	1.76	0.50
44:RZ:102:LEU:HD11	44:RZ:124:ILE:HG13	1.92	0.50
30:YH:86:GLU:HB2	30:YH:165:ALA:H	1.76	0.50
37:YS:26:LEU:HB3	37:YS:87:PHE:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:571:U:O4	1:QA:864:A:N6	2.44	0.50
5:QE:33:VAL:HG11	5:QE:109:ILE:HA	1.94	0.50
9:QI:42:ARG:NH1	9:QI:71:SER:OG	2.45	0.50
50:R5:41:PRO:O	50:R5:44:THR:OG1	2.28	0.50
25:RB:114:G:O2'	37:RS:50:SER:OG	2.29	0.50
27:RE:36:ARG:NH1	27:RE:85:ASN:OD1	2.45	0.50
28:RF:63:LYS:HE2	28:RF:67:GLN:HB2	1.94	0.50
24:RA:138:G:N2	42:RX:44:GLU:OE1	2.30	0.50
1:XA:352:C:O2'	1:XA:354:G:OP1	2.23	0.50
1:XA:639:G:H2'	1:XA:640:A:H8	1.77	0.50
5:XE:33:VAL:HG11	5:XE:109:ILE:HA	1.94	0.50
13:XM:58:GLU:O	13:XM:62:ASN:ND2	2.45	0.50
24:YA:1266:G:O2'	24:YA:2012:G:O6	2.25	0.50
24:YA:2470:G:OP1	35:YQ:56:ARG:NH2	2.45	0.50
24:YA:2572:A:H2'	27:YE:144:ARG:HD3	1.94	0.50
24:YA:83:G:H1	24:YA:102:G:HO2'	1.57	0.50
30:YH:88:LEU:HA	30:YH:130:ARG:HA	1.94	0.50
24:RA:270(R):G:H21	46:R1:78:LYS:HD2	1.77	0.49
34:RP:49:ARG:HH11	53:R8:58:ILE:HG22	1.77	0.49
24:RA:987:G:O2'	24:RA:1000:A:N3	2.43	0.49
28:RF:167:ALA:HB1	28:RF:173:VAL:HG11	1.93	0.49
1:XA:1158:C:O2	1:XA:1159:U:O2'	2.31	0.49
16:XP:4:ILE:HG12	16:XP:21:VAL:HG12	1.94	0.49
1:QA:831:U:H3	1:QA:855:G:H1	1.59	0.49
11:QK:52:GLY:H	11:QK:55:LYS:HE2	1.77	0.49
12:QL:113:ARG:HH21	12:QL:116:SER:HB2	1.76	0.49
26:RD:182:LEU:H	26:RD:272:ALA:HB3	1.77	0.49
31:RI:79:ILE:HB	31:RI:142:VAL:HA	1.93	0.49
3:XC:189:ALA:HB3	3:XC:196:LEU:HB2	1.93	0.49
4:XD:116:GLN:HE21	4:XD:157:LEU:HD21	1.76	0.49
30:YH:8:PRO:HG2	30:YH:69:ARG:HE	1.75	0.49
44:YZ:163:LEU:HD13	44:YZ:167:PRO:HD3	1.94	0.49
13:QM:99:ARG:HB2	13:QM:101:GLN:HE22	1.77	0.49
24:RA:2285:C:OP1	51:R6:29:ASN:ND2	2.46	0.49
24:RA:2655:G:N2	24:RA:2665:A:OP2	2.45	0.49
24:YA:2108:C:O2	24:YA:2181:G:N2	2.31	0.49
24:YA:2777:G:OP2	24:YA:2781:A:O2'	2.29	0.49
33:YO:19:ILE:HG22	33:YO:43:VAL:HA	1.94	0.49
1:QA:544:G:OP1	4:QD:59:ARG:NH2	2.45	0.49
48:R3:15:TYR:O	48:R3:20:LYS:NZ	2.44	0.49
24:RA:2010:G:H5''	41:RW:42:ARG:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:YA:2151:G:H2'	24:YA:2152:G:C8	2.47	0.49
24:YA:598:G:H5'	34:YP:11:GLY:HA3	1.95	0.49
31:YI:88:ILE:HB	31:YI:121:LYS:HG3	1.95	0.49
3:QC:19:GLU:HG2	3:QC:54:ARG:HE	1.77	0.49
16:QP:4:ILE:HG12	16:QP:21:VAL:HG12	1.94	0.49
24:RA:458:G:O2'	24:RA:469:G:O6	2.23	0.49
27:RE:18:ASP:HB3	38:RT:82:LEU:HD11	1.94	0.49
34:RP:115:LEU:HA	34:RP:134:ALA:HB2	1.95	0.49
1:XA:335:C:O2'	1:XA:1433:A:N3	2.41	0.49
24:YA:1510:A:O2'	24:YA:1511:A:N7	2.44	0.49
1:QA:552:U:O2'	12:QL:86:ARG:O	2.30	0.49
11:QK:34:ASP:OD1	11:QK:38:ASN:N	2.46	0.49
24:RA:1818:U:H2'	26:RD:157:ARG:HG2	1.95	0.49
26:RD:36:PRO:HB2	26:RD:61:LEU:HD12	1.95	0.49
33:RO:19:ILE:HG22	33:RO:43:VAL:HA	1.94	0.49
1:XA:243:A:H4'	1:XA:244:U:H3'	1.95	0.49
24:YA:987:G:O2'	24:YA:1000:A:N3	2.37	0.49
28:YF:63:LYS:HE2	28:YF:67:GLN:HB2	1.94	0.49
39:YU:95:LEU:HD13	40:YV:4:ILE:HD12	1.93	0.49
44:YZ:4:ARG:HG2	44:YZ:58:VAL:HB	1.93	0.49
1:QA:166:G:H2'	1:QA:167:G:H8	1.78	0.49
38:RT:24:PRO:HA	38:RT:49:VAL:HG13	1.94	0.49
1:XA:464:G:N2	1:XA:467:G:N7	2.61	0.49
24:YA:2185:C:H2'	24:YA:2186:G:H8	1.77	0.49
31:YI:79:ILE:N	31:YI:141:LYS:O	2.42	0.49
1:XA:339:C:H5	33:YO:97:ARG:HH12	1.61	0.49
44:YZ:102:LEU:HD23	44:YZ:137:ILE:HB	1.95	0.49
1:QA:1392:G:H21	1:QA:1502:A:H8	1.61	0.49
1:QA:348:G:H2'	1:QA:349:A:H8	1.77	0.49
13:QM:3:ARG:HA	13:QM:9:ILE:HG21	1.94	0.49
38:RT:124:ASP:O	38:RT:128:GLU:N	2.46	0.49
1:XA:1240:U:OP1	7:XG:119:ARG:NH2	2.46	0.49
9:XI:46:ALA:HB2	9:XI:74:ILE:HG23	1.94	0.49
27:YE:104:VAL:HG22	27:YE:198:VAL:HG22	1.93	0.49
33:YO:2:ILE:HB	33:YO:33:ALA:HB3	1.95	0.49
1:QA:1350:A:N7	9:QI:118:LYS:NZ	2.60	0.49
13:QM:40:ASN:HB3	13:QM:43:THR:HG23	1.95	0.49
24:RA:1045:A:H5''	24:RA:1111:A:H61	1.78	0.49
24:RA:1689:A:OP2	24:RA:1698:A:N6	2.41	0.49
24:RA:2816:C:O2	24:RA:2883:A:O2'	2.28	0.49
43:RY:15:VAL:HG21	43:RY:42:VAL:HG11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:YA:805:G:N2	24:YA:829:A:OP1	2.45	0.49
26:YD:182:LEU:H	26:YD:272:ALA:HB3	1.77	0.49
38:YT:62:THR:HG22	38:YT:75:ILE:HG12	1.95	0.49
3:QC:58:GLU:HB2	3:QC:65:ALA:HB3	1.95	0.49
11:QK:21:ILE:HB	11:QK:84:VAL:HG12	1.95	0.49
24:RA:2692:C:O2	24:RA:2847:U:O2'	2.28	0.49
35:RQ:43:THR:HG22	35:RQ:94:VAL:HG12	1.95	0.49
24:RA:495:G:H21	41:RW:61:ASN:HD21	1.59	0.49
7:XG:94:ARG:NH1	7:XG:98:SER:OG	2.46	0.49
10:XJ:6:ILE:HG22	10:XJ:98:ILE:HG13	1.94	0.49
24:YA:1998:G:O2'	24:YA:2724:C:O2'	2.29	0.49
24:YA:2125:G:O2'	24:YA:2173:A:N6	2.45	0.49
1:QA:1498:U:OP2	23:QX:16:A:O2'	2.31	0.48
9:QI:5:TYR:HE1	9:QI:16:ARG:HB2	1.78	0.48
1:QA:35:G:O2'	12:QL:118:SER:O	2.27	0.48
24:RA:2730:C:O2'	27:RE:168:MET:O	2.29	0.48
28:RF:195:ASP:OD1	28:RF:195:ASP:N	2.38	0.48
1:XA:1367:C:OP1	9:XI:115:GLY:N	2.39	0.48
1:XA:943:U:H1'	9:XI:124:GLN:HE22	1.77	0.48
24:YA:513:A:O2'	24:YA:1217:C:OP1	2.29	0.48
24:YA:1693:U:O2	26:YD:14:ARG:NH1	2.46	0.48
25:YB:114:G:O2'	37:YS:50:SER:OG	2.22	0.48
9:QI:128:ARG:NH2	22:QV:34:U:OP2	2.37	0.48
32:RN:6:PRO:HG3	32:RN:41:ASP:HB2	1.93	0.48
37:RS:26:LEU:HB3	37:RS:87:PHE:HA	1.94	0.48
10:XJ:48:THR:HG23	10:XJ:62:HIS:HB3	1.94	0.48
27:YE:36:ARG:NH1	27:YE:85:ASN:OD1	2.45	0.48
1:QA:1314:C:OP2	19:QS:4:SER:OG	2.26	0.48
1:QA:954:G:O6	13:QM:104:ARG:NH1	2.46	0.48
33:RO:2:ILE:HB	33:RO:33:ALA:HB3	1.95	0.48
1:XA:426:G:OP1	4:XD:38:TYR:OH	2.23	0.48
24:YA:1510:A:O2'	24:YA:1512:G:N7	2.37	0.48
24:YA:2306:C:N4	29:YG:42:GLY:O	2.43	0.48
38:YT:24:PRO:HA	38:YT:49:VAL:HG13	1.94	0.48
12:QL:124:LYS:HD2	12:QL:125:PRO:HD2	1.96	0.48
28:RF:116:ASP:OD2	34:RP:1:MET:N	2.38	0.48
31:RI:79:ILE:N	31:RI:141:LYS:O	2.42	0.48
3:XC:58:GLU:HB2	3:XC:65:ALA:HB3	1.94	0.48
1:XA:933:G:O6	7:XG:3:ARG:NH2	2.46	0.48
24:YA:2424:C:O2	24:YA:2429:G:O2'	2.27	0.48
35:YQ:48:GLU:OE2	35:YQ:51:ARG:NH2	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:368:U:OP1	31:YI:91:SER:OG	2.26	0.48
2:QB:16:HIS:HA	2:QB:210:SER:HB2	1.94	0.48
7:QG:94:ARG:NH1	7:QG:98:SER:OG	2.46	0.48
45:R0:32:ARG:N	45:R0:35:ASN:OD1	2.46	0.48
24:RA:2224:G:OP1	26:RD:268:ARG:NH1	2.46	0.48
24:RA:2683:C:OP1	38:RT:53:ARG:NH2	2.42	0.48
24:RA:746:A:O2'	24:RA:2611:U:O2'	2.30	0.48
1:XA:201:C:H42	1:XA:216:G:H1	1.61	0.48
36:YR:3:HIS:O	36:YR:5:LYS:N	2.47	0.48
1:QA:501:C:H2'	1:QA:502:G:H8	1.79	0.48
24:RA:270(U):C:H2'	24:RA:270(V):G:H8	1.77	0.48
44:RZ:163:LEU:HD13	44:RZ:167:PRO:HD3	1.94	0.48
44:RZ:7:ALA:HB2	44:RZ:59:LEU:HB3	1.95	0.48
1:XA:835:U:H3	1:XA:851:G:H1	1.62	0.48
1:QA:1504:G:OP1	1:QA:1507:A:O2'	2.28	0.48
13:QM:49:THR:HG22	13:QM:51:ALA:H	1.78	0.48
24:RA:1899:G:N2	24:RA:1902:C:H41	2.12	0.48
24:RA:2739:U:O2	24:RA:2766:G:N2	2.47	0.48
24:RA:861:A:N3	25:RB:79:C:O2'	2.43	0.48
31:RI:88:ILE:HB	31:RI:121:LYS:HG3	1.95	0.48
9:XI:112:LYS:HA	9:XI:119:ALA:HB2	1.96	0.48
46:Y1:17:SER:HB2	46:Y1:40:ARG:HD2	1.94	0.48
27:YE:119:ARG:NH1	27:YE:159:HIS:O	2.47	0.48
33:RO:104:ARG:NH1	33:RO:121:VAL:O	2.47	0.48
34:RP:65:ARG:O	34:RP:68:GLN:NE2	2.47	0.48
35:RQ:48:GLU:OE2	35:RQ:51:ARG:NH2	2.35	0.48
1:XA:1450:U:O2'	1:XA:1451:A:N7	2.37	0.48
11:XK:17:GLY:HA2	11:XK:35:PRO:HD3	1.95	0.48
24:YA:2791:C:OP1	24:YA:2893:G:N2	2.47	0.48
24:YA:603:A:N1	24:YA:625:G:O2'	2.39	0.48
24:YA:662:G:OP1	34:YP:15:ARG:NH1	2.46	0.48
38:YT:124:ASP:O	38:YT:128:GLU:N	2.46	0.48
24:RA:116:C:O2'	24:RA:126:A:N3	2.38	0.48
24:RA:2503:A:O2'	24:RA:2505:G:OP2	2.22	0.48
29:YG:179:PRO:HB3	49:Y4:43:TYR:HE1	1.78	0.48
24:YA:1196:C:O2'	24:YA:1228:G:O2'	2.27	0.48
26:YD:77:ALA:HB3	26:YD:117:VAL:HG13	1.96	0.48
34:YP:68:GLN:HG2	53:Y8:12:LYS:HG2	1.95	0.48
9:QI:29:ASN:HD21	9:QI:65:VAL:HB	1.79	0.48
17:QQ:83:ASP:OD1	17:QQ:83:ASP:N	2.47	0.48
24:RA:137(A):G:H21	42:RX:41:ASN:HD21	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:RA:224:G:O6	24:RA:419:C:O2'	2.29	0.48
27:RE:119:ARG:NH1	27:RE:159:HIS:O	2.47	0.48
24:RA:252:G:OP2	34:RP:50:ARG:NH1	2.47	0.48
1:XA:1022:G:H2'	1:XA:1023:G:H8	1.79	0.48
2:XB:77:ALA:HB2	2:XB:211:ILE:HD13	1.96	0.48
1:XA:675:A:H1'	11:XK:116:HIS:CD2	2.49	0.48
11:XK:21:ILE:HG13	11:XK:30:VAL:HG12	1.96	0.48
24:RA:593:G:H4'	53:R8:61:LEU:HD13	1.96	0.47
24:RA:1061:U:H5''	24:RA:1070:A:H1'	1.95	0.47
24:RA:1689:A:H62	24:RA:1698:A:H2	1.61	0.47
12:XL:53:ARG:HH12	12:XL:92:ASP:HB2	1.78	0.47
45:Y0:46:LYS:HD2	45:Y0:78:TYR:HE1	1.79	0.47
24:YA:2289:G:N2	24:YA:2344:U:O2	2.46	0.47
24:YA:918:A:N3	25:YB:80:U:O2'	2.45	0.47
1:QA:159:G:H21	1:QA:162:A:H8	1.62	0.47
2:QB:219:VAL:HA	2:QB:222:ILE:HD12	1.96	0.47
1:QA:545:C:H5'	4:QD:72:GLU:HG3	1.96	0.47
24:RA:2354:G:H4'	45:R0:35:ASN:HD22	1.79	0.47
9:XI:13:ALA:HB2	9:XI:68:GLY:HA3	1.95	0.47
24:YA:1779:U:OP2	24:YA:1784:A:N6	2.42	0.47
24:YA:587:C:O2	34:YP:33:ARG:NH2	2.47	0.47
1:QA:1122:U:O4	1:QA:1123:A:N6	2.47	0.47
8:QH:10:LEU:HD22	8:QH:83:ILE:HD11	1.96	0.47
11:QK:22:HIS:HB3	11:QK:29:ILE:HG23	1.97	0.47
48:R3:39:ASP:OD1	48:R3:44:ARG:NH2	2.46	0.47
1:XA:757:U:O2'	1:XA:879:C:O2	2.30	0.47
8:XH:10:LEU:HD22	8:XH:83:ILE:HD11	1.96	0.47
47:Y2:4:SER:OG	47:Y2:5:GLU:N	2.48	0.47
24:YA:1184:G:P	48:Y3:29:ARG:HH12	2.38	0.47
24:YA:1417:C:O2'	24:YA:1587:A:N3	2.41	0.47
24:YA:829:A:N7	24:YA:2247:A:O2'	2.46	0.47
1:QA:1034:G:H2'	1:QA:1035:A:C8	2.49	0.47
1:QA:589:C:H42	1:QA:650:G:H1	1.63	0.47
2:QB:80:ILE:HD11	2:QB:208:ILE:HG23	1.96	0.47
4:QD:14:ARG:HD2	4:QD:40:PRO:HD2	1.97	0.47
24:RA:2611:U:C4	50:R5:3:LYS:HG2	2.48	0.47
26:RD:77:ALA:HB3	26:RD:117:VAL:HG13	1.96	0.47
24:YA:2151:G:H2'	24:YA:2152:G:H8	1.78	0.47
24:YA:2308:G:H22	24:YA:2311:A:H2	1.62	0.47
33:YO:104:ARG:NH1	33:YO:121:VAL:O	2.47	0.47
6:QF:6:VAL:HB	6:QF:63:TYR:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:RA:2128:C:H1'	24:RA:2173:A:H2	1.79	0.47
24:RA:265:A:N6	24:RA:427:U:O2'	2.47	0.47
24:RA:626:U:H5''	24:RA:627:A:H5'	1.97	0.47
36:RR:33:ARG:HD3	36:RR:113:LEU:HD11	1.96	0.47
17:XQ:83:ASP:OD1	17:XQ:83:ASP:N	2.47	0.47
1:XA:263:A:OP2	20:XT:79:ARG:NH1	2.48	0.47
35:YQ:43:THR:HG22	35:YQ:94:VAL:HG12	1.95	0.47
38:YT:3:ARG:HB2	38:YT:6:LEU:HB3	1.96	0.47
43:YY:15:VAL:HG21	43:YY:42:VAL:HG11	1.95	0.47
10:QJ:7:LYS:HB2	10:QJ:97:GLU:HB2	1.97	0.47
24:RA:1491:G:H2'	24:RA:1492:G:H8	1.79	0.47
4:XD:14:ARG:HD2	4:XD:40:PRO:HD2	1.97	0.47
46:Y1:80:LEU:HD12	46:Y1:81:LYS:HG2	1.97	0.47
24:YA:1139:G:O2'	24:YA:1143:A:N1	2.40	0.47
24:YA:220:G:O2'	24:YA:233:A:N3	2.44	0.47
1:QA:108:G:N2	1:QA:108:G:OP2	2.48	0.47
1:QA:414:A:OP2	1:QA:428:G:N2	2.34	0.47
2:QB:32:ILE:HD11	2:QB:40:HIS:HB3	1.96	0.47
9:QI:42:ARG:NH1	9:QI:71:SER:O	2.44	0.47
38:RT:3:ARG:HB2	38:RT:6:LEU:HB3	1.96	0.47
24:RA:1155:A:O3'	39:RU:55:ARG:NH1	2.48	0.47
1:XA:1432:G:OP1	38:YT:108:ARG:N	2.46	0.47
1:XA:452:A:H62	1:XA:480:U:H3	1.63	0.47
1:XA:1286:A:H5''	21:XU:26:LYS:HD2	1.97	0.47
29:YG:173:LEU:O	29:YG:178:PHE:N	2.41	0.47
27:YE:14:ILE:HG13	38:YT:14:TYR:HE2	1.80	0.47
1:QA:134:A:H61	16:QP:25:ARG:HH12	1.61	0.47
53:R8:6:THR:OG1	53:R8:8:LYS:NZ	2.48	0.47
24:RA:1045:A:O4'	24:RA:1111:A:N6	2.48	0.47
24:RA:2123:G:H2'	24:RA:2124:G:H8	1.79	0.47
34:RP:101:VAL:HB	34:RP:106:LEU:HB2	1.97	0.47
38:RT:50:ILE:HD11	38:RT:100:TYR:HA	1.97	0.47
38:RT:62:THR:HG22	38:RT:75:ILE:HG12	1.95	0.47
1:XA:309:G:H2'	1:XA:310:G:H8	1.79	0.47
1:XA:618:C:H5'	1:XA:619:U:H5''	1.97	0.47
1:XA:878:G:H5'	8:XH:89:PRO:HG2	1.97	0.47
14:YN:48:ALA:HB2	14:YN:53:LEU:HD12	1.97	0.47
26:YD:36:PRO:HB2	26:YD:61:LEU:HD12	1.95	0.47
1:QA:1172:C:H2'	1:QA:1173:G:C8	2.50	0.47
1:QA:1245:A:OP2	21:QU:9:ARG:NH2	2.47	0.47
24:RA:1203:G:O6	24:RA:1204:A:N6	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:RA:489:G:N2	24:RA:1321:A:OP1	2.48	0.47
24:RA:242:G:O2'	24:RA:254:G:O6	2.27	0.47
31:RI:123:LEU:HD23	31:RI:142:VAL:HG22	1.96	0.47
1:XA:1129:C:OP1	9:XI:62:TYR:OH	2.28	0.47
9:XI:5:TYR:HE1	9:XI:16:ARG:HB2	1.80	0.47
6:XF:97:PHE:HB2	18:XR:32:ARG:HE	1.80	0.47
24:YA:1110:G:O3'	30:YH:3:ARG:NH2	2.47	0.47
24:YA:994:C:OP2	39:YU:54:LYS:NZ	2.42	0.47
28:YF:143:ALA:HB1	28:YF:148:LEU:HB2	1.96	0.47
1:QA:1287:A:H2	1:QA:1353:G:H1'	1.79	0.47
1:QA:596:C:H2'	1:QA:597:G:H8	1.80	0.47
36:RR:3:HIS:O	36:RR:5:LYS:N	2.48	0.47
1:XA:1305:G:N2	1:XA:1331:G:H2'	2.30	0.47
31:YI:123:LEU:HD23	31:YI:142:VAL:HG22	1.96	0.47
24:YA:831:G:N2	34:YP:53:GLY:O	2.38	0.47
34:YP:58:THR:O	34:YP:61:ARG:NH2	2.40	0.47
36:YR:51:LEU:HD22	36:YR:66:VAL:HG13	1.97	0.47
7:QG:15:ASP:OD1	7:QG:44:TYR:OH	2.33	0.47
27:RE:17:ASP:O	27:RE:19:ARG:N	2.48	0.47
29:RG:67:LYS:HD2	29:RG:68:PRO:HD2	1.97	0.47
14:YN:24:CYS:HB3	14:YN:29:ARG:H	1.80	0.47
14:YN:4:LYS:HA	14:YN:7:ILE:HG12	1.97	0.47
24:YA:1598:C:O3'	42:YX:35:THR:OG1	2.32	0.47
26:YD:25:THR:HG22	26:YD:82:ILE:H	1.80	0.47
38:YT:20:PRO:HD2	38:YT:86:ILE:HG23	1.97	0.47
1:QA:1002:G:H2'	1:QA:1003:G:C8	2.49	0.46
26:RD:25:THR:HG22	26:RD:82:ILE:H	1.80	0.46
44:RZ:102:LEU:HD23	44:RZ:137:ILE:HB	1.95	0.46
24:YA:1062:G:N2	24:YA:1077:A:N1	2.63	0.46
24:YA:1728:G:H8	24:YA:1732:A:H62	1.61	0.46
24:YA:612:G:N2	24:YA:616:A:O2'	2.48	0.46
26:YD:83:GLU:OE1	26:YD:104:TYR:OH	2.33	0.46
30:YH:106:THR:HG22	30:YH:112:PRO:HB3	1.97	0.46
38:YT:50:ILE:HD11	38:YT:100:TYR:HA	1.97	0.46
1:QA:530:G:N2	1:QA:530:G:OP2	2.46	0.46
4:QD:10:ARG:HG3	4:QD:40:PRO:HG3	1.98	0.46
1:QA:1347:G:O6	9:QI:10:ARG:NH2	2.49	0.46
24:RA:1131:G:HO2'	24:RA:1132:A:H8	1.63	0.46
24:RA:2310:A:N6	29:RG:79:ASN:OD1	2.48	0.46
33:RO:120:GLU:OE1	38:RT:67:SER:OG	2.33	0.46
24:YA:1264:G:OP1	50:Y5:19:ARG:NH2	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:YA:2315:G:OP1	29:YG:36:LYS:NZ	2.48	0.46
27:YE:74:PRO:HG2	27:YE:77:ILE:HG22	1.97	0.46
44:YZ:7:ALA:HB2	44:YZ:59:LEU:HB3	1.95	0.46
10:QJ:51:ARG:O	14:QN:45:ARG:NH1	2.43	0.46
28:RF:143:ALA:HB1	28:RF:148:LEU:HB2	1.96	0.46
30:RH:106:THR:HG22	30:RH:112:PRO:HB3	1.97	0.46
1:XA:736:C:O2'	6:XF:90:VAL:O	2.31	0.46
8:XH:12:ARG:HH12	8:XH:27:PRO:HD3	1.81	0.46
13:XM:99:ARG:HB2	13:XM:101:GLN:HE22	1.81	0.46
24:YA:1612:C:O2'	52:Y7:5:TRP:O	2.29	0.46
53:Y8:6:THR:OG1	53:Y8:8:LYS:NZ	2.48	0.46
24:YA:1754:C:P	38:YT:96:ARG:HH12	2.38	0.46
35:YQ:21:THR:HB	35:YQ:22:LYS:H	1.56	0.46
1:QA:1199:U:O2'	1:QA:1202:G:OP1	2.34	0.46
1:QA:606:G:H22	1:QA:631:G:H5'	1.80	0.46
8:QH:12:ARG:HH12	8:QH:27:PRO:HD3	1.81	0.46
8:QH:49:GLU:OE2	8:QH:62:TYR:OH	2.28	0.46
14:QN:48:ALA:HB2	14:QN:53:LEU:HD12	1.97	0.46
24:RA:2293:C:O2'	37:RS:93:LYS:NZ	2.48	0.46
1:XA:1221:G:OP1	1:XA:1320:C:N4	2.42	0.46
1:XA:131:C:O2'	1:XA:262:A:N3	2.40	0.46
24:YA:1860:G:H1	24:YA:1882:C:H42	1.63	0.46
1:QA:855:G:OP2	1:QA:871:U:N3	2.43	0.46
24:RA:583:G:H5''	39:RU:10:ARG:HH12	1.80	0.46
24:RA:389:G:H22	34:RP:72:PRO:HD3	1.81	0.46
1:XA:1131:G:OP1	9:XI:20:ARG:NH2	2.44	0.46
24:YA:17:G:H4'	39:YU:25:TRP:HE1	1.80	0.46
24:YA:61:G:H1'	47:Y2:47:ASN:HD22	1.80	0.46
24:YA:793:A:OP2	24:YA:2071:A:O2'	2.31	0.46
24:YA:2619:C:H5''	27:YE:152:LYS:HA	1.97	0.46
42:YX:54:VAL:HG22	42:YX:81:VAL:HG23	1.98	0.46
24:RA:1568:G:OP1	26:RD:63:ARG:NH1	2.35	0.46
27:RE:74:PRO:HG2	27:RE:77:ILE:HG22	1.97	0.46
32:RN:60:ILE:H	32:RN:60:ILE:HG13	1.57	0.46
4:XD:10:ARG:HG3	4:XD:40:PRO:HG3	1.97	0.46
13:XM:66:LEU:HB3	13:XM:67:GLU:H	1.57	0.46
48:Y3:39:ASP:OD1	48:Y3:44:ARG:NH2	2.46	0.46
24:YA:363:G:H2'	24:YA:363(A):A:H8	1.81	0.46
1:QA:352:C:O2'	1:QA:354:G:OP1	2.24	0.46
11:QK:24:SER:OG	11:QK:25:TYR:N	2.48	0.46
14:QN:4:LYS:HA	14:QN:7:ILE:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:RA:523:C:O2	24:RA:553:U:O2'	2.34	0.46
4:XD:57:ARG:NH2	4:XD:205:GLU:OE2	2.43	0.46
24:YA:2006:C:O2'	24:YA:2823:A:N3	2.48	0.46
13:XM:93:ARG:NH1	24:YA:888:C:OP1	2.49	0.46
24:YA:674:G:H1'	28:YF:74:ARG:HD3	1.97	0.46
29:YG:67:LYS:HD2	29:YG:68:PRO:HD2	1.97	0.46
1:QA:1224:G:H1	1:QA:1362(A):C:H42	1.62	0.46
1:QA:246:A:OP2	17:QQ:100:LYS:NZ	2.49	0.46
4:QD:57:ARG:NH2	5:QE:107:ARG:HD3	2.31	0.46
47:R2:4:SER:OG	47:R2:5:GLU:N	2.48	0.46
24:RA:2365:G:O6	53:R8:43:GLN:NE2	2.46	0.46
27:RE:31:CYS:HB3	27:RE:49:LEU:HG	1.98	0.46
24:YA:2343:C:O2'	24:YA:2373:G:O2'	2.25	0.46
24:YA:27:G:N2	24:YA:512:G:H2'	2.31	0.46
24:YA:601:C:O2'	24:YA:605:C:OP1	2.33	0.46
35:YQ:111:GLU:OE1	35:YQ:133:ARG:NH2	2.49	0.46
42:YX:26:TYR:HD2	42:YX:89:ILE:HD12	1.81	0.46
1:QA:1119:C:H2'	1:QA:1120:G:H8	1.80	0.46
1:QA:1288:A:N3	1:QA:1352:C:O2'	2.39	0.46
11:QK:57:THR:HG22	11:QK:59:TYR:H	1.81	0.46
1:QA:1493:A:H2	23:QX:20:U:H1'	1.81	0.46
49:R4:51:ASP:OD1	49:R4:51:ASP:N	2.47	0.46
25:RB:52:A:HO2'	25:RB:53:A:H8	1.60	0.46
29:RG:114:ILE:HB	29:RG:117:PHE:HB2	1.98	0.46
1:XA:1061:G:OP1	10:XJ:59:SER:OG	2.33	0.46
7:XG:15:ASP:OD1	7:XG:44:TYR:OH	2.33	0.46
1:XA:553:A:O2'	12:XL:29:GLY:O	2.30	0.46
12:XL:67:THR:OG1	12:XL:95:GLY:O	2.32	0.46
24:YA:2354:G:H4'	45:Y0:35:ASN:HD22	1.81	0.46
24:YA:1899:G:H21	24:YA:1902:C:H41	1.64	0.46
24:YA:2122:U:H2'	24:YA:2123:G:C8	2.51	0.46
24:YA:2154:G:H2'	24:YA:2155:G:C8	2.51	0.46
44:YZ:53:ILE:HG22	44:YZ:71:VAL:HG13	1.98	0.46
1:QA:279:A:OP2	17:QQ:95:TYR:OH	2.27	0.46
9:QI:63:ILE:HG21	9:QI:77:ILE:HG12	1.97	0.46
1:QA:1296:C:OP1	13:QM:44:ARG:NH2	2.49	0.46
24:RA:300:A:OP1	43:RY:86:ARG:NH2	2.49	0.46
1:XA:501:C:O2	1:XA:549:C:O2'	2.29	0.46
1:XA:35:G:N2	12:XL:118:SER:OG	2.39	0.46
24:YA:536:A:P	39:YU:53:ARG:HH11	2.39	0.46
24:YA:787:U:H5''	24:YA:788:A:H5'	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:YH:89:ILE:HG22	30:YH:162:ILE:HG23	1.98	0.46
1:QA:972:C:OP2	10:QJ:57:LYS:NZ	2.42	0.45
24:RA:2287:A:N6	24:RA:2344:U:H3	2.14	0.45
24:RA:2572:A:OP1	24:RA:2574:G:O2'	2.29	0.45
3:XC:56:ASP:HB2	3:XC:67:THR:HB	1.98	0.45
6:XF:6:VAL:HB	6:XF:63:TYR:HB2	1.97	0.45
1:XA:1226:C:O2'	13:XM:111:LYS:NZ	2.49	0.45
24:YA:2134:A:N6	24:YA:2156:G:O2'	2.49	0.45
1:QA:890:G:O2'	1:QA:906:G:O6	2.31	0.45
30:RH:152:ARG:HE	30:RH:153:LYS:HD2	1.82	0.45
42:RX:26:TYR:HD2	42:RX:89:ILE:HD12	1.81	0.45
13:XM:8:GLU:OE2	29:YG:115:ARG:NH2	2.49	0.45
24:YA:2285:C:OP2	51:Y6:6:ARG:NH1	2.49	0.45
24:YA:2133:G:O2'	24:YA:2158:A:N1	2.49	0.45
24:RA:1566:A:P	26:RD:211:ARG:HH21	2.39	0.45
27:RE:38:THR:OG1	27:RE:40:GLU:OE1	2.34	0.45
1:XA:1443:G:H5''	1:XA:1446:A:H2	1.82	0.45
24:YA:1598:C:H5'	42:YX:36:LYS:HB2	1.98	0.45
27:YE:17:ASP:O	27:YE:19:ARG:N	2.48	0.45
35:YQ:4:PRO:HG3	35:YQ:69:PHE:HE2	1.82	0.45
1:QA:1349:A:H62	1:QA:1373:G:H21	1.63	0.45
26:RD:142:VAL:HG23	26:RD:193:VAL:HA	1.99	0.45
38:RT:123:GLN:O	38:RT:125:ARG:N	2.50	0.45
1:XA:1151:A:H2'	1:XA:1152:A:H8	1.81	0.45
1:XA:380:G:N2	1:XA:383:A:OP2	2.46	0.45
10:XJ:49:VAL:HG23	14:YN:41:ARG:HB2	1.98	0.45
38:YT:123:GLN:O	38:YT:125:ARG:N	2.50	0.45
1:QA:944:G:N1	1:QA:1338:G:OP2	2.46	0.45
35:RQ:4:PRO:HG3	35:RQ:69:PHE:HE2	1.82	0.45
1:XA:10:A:HO2'	1:XA:507:C:HO2'	1.62	0.45
1:XA:769:G:H4'	1:XA:1513:A:H4'	1.99	0.45
10:XJ:34:VAL:HG22	10:XJ:74:ILE:HG22	1.99	0.45
14:YN:29:ARG:HD3	14:YN:40:CYS:HB2	1.99	0.45
24:YA:2030:A:H4'	24:YA:2031:A:H8	1.81	0.45
1:QA:503:C:OP2	12:QL:116:SER:OG	2.25	0.45
3:QC:56:ASP:HB2	3:QC:67:THR:HB	1.98	0.45
13:QM:108:ARG:HE	13:QM:114:ARG:HD2	1.81	0.45
14:QN:24:CYS:HB3	14:QN:29:ARG:H	1.80	0.45
35:RQ:66:ILE:HA	35:RQ:104:PHE:HA	1.99	0.45
39:RU:90:VAL:HG11	40:RV:40:LEU:HG	1.98	0.45
4:XD:155:LEU:HD23	4:XD:155:LEU:HA	1.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:XH:34:GLU:OE1	8:XH:37:ARG:NH2	2.50	0.45
29:YG:108:ASN:HA	49:Y4:37:SER:HB3	1.99	0.45
27:YE:38:THR:OG1	27:YE:40:GLU:OE1	2.34	0.45
34:YP:122:PRO:HB3	34:YP:141:ALA:HB1	1.98	0.45
44:YZ:109:ALA:HB3	44:YZ:143:GLY:HA2	1.98	0.45
6:QF:10:LEU:HD13	6:QF:61:LEU:HD13	1.99	0.45
24:RA:2258:C:O2'	24:RA:2427:C:OP2	2.27	0.45
24:RA:674:G:H1'	28:RF:74:ARG:HD3	1.98	0.45
29:RG:71:THR:N	29:RG:89:GLY:O	2.49	0.45
35:RQ:111:GLU:OE1	35:RQ:133:ARG:NH2	2.49	0.45
36:RR:38:VAL:HG22	36:RR:112:ALA:HB2	1.99	0.45
43:RY:14:LEU:HB2	43:RY:75:ILE:HD11	1.98	0.45
44:RZ:53:ILE:HG22	44:RZ:71:VAL:HG13	1.98	0.45
1:XA:1314:C:OP2	19:XS:4:SER:OG	2.30	0.45
1:XA:67:C:H2'	1:XA:68:G:C8	2.52	0.45
11:XK:21:ILE:HB	11:XK:84:VAL:HG12	1.97	0.45
35:YQ:28:ALA:N	35:YQ:105:GLU:OE2	2.50	0.45
1:QA:1224:G:O2'	1:QA:1322:C:OP2	2.34	0.45
10:QJ:39:PRO:HB3	10:QJ:70:ARG:NH1	2.32	0.45
24:RA:500:G:N1	24:RA:503:A:OP2	2.47	0.45
24:RA:859:G:O2'	24:RA:916:G:O6	2.30	0.45
38:RT:20:PRO:HD2	38:RT:86:ILE:HG23	1.97	0.45
44:RZ:109:ALA:HB3	44:RZ:143:GLY:HA2	1.98	0.45
1:XA:1130:A:O2'	9:XI:3:GLN:NE2	2.49	0.45
1:XA:1133:G:H2'	1:XA:1134:G:H8	1.82	0.45
24:YA:2010:G:H5''	41:YW:42:ARG:HB2	1.99	0.45
36:YR:30:THR:O	36:YR:78:LYS:NZ	2.50	0.45
3:QC:59:ARG:HH12	3:QC:97:LYS:HE3	1.82	0.45
5:QE:110:LEU:HD13	5:QE:118:ILE:HD13	1.99	0.45
24:RA:243:U:P	53:R8:8:LYS:HZ1	2.39	0.45
24:RA:270(I):G:H2'	24:RA:270(J):G:C8	2.52	0.45
30:RH:89:ILE:HG22	30:RH:162:ILE:HG23	1.98	0.45
2:XB:132:LYS:HA	2:XB:135:GLN:HB2	1.99	0.45
25:YB:44:G:O2'	25:YB:47:C:N4	2.49	0.45
29:YG:71:THR:N	29:YG:89:GLY:O	2.49	0.45
8:QH:34:GLU:OE1	8:QH:37:ARG:NH2	2.50	0.45
9:QI:42:ARG:NH2	9:QI:75:ASP:OD2	2.43	0.45
24:RA:1083:U:O2'	24:RA:1086:A:N1	2.50	0.45
24:RA:1173:G:N2	24:RA:1175:U:O4	2.45	0.45
24:RA:1779:U:OP2	24:RA:1784:A:N6	2.37	0.45
24:RA:2291:U:O2'	24:RA:2374:C:O2	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:RO:7:TYR:CE1	33:RO:44:LYS:HG3	2.51	0.45
1:XA:464:G:N1	1:XA:467:G:OP2	2.48	0.45
12:XL:53:ARG:HB3	12:XL:69:TYR:HE1	1.82	0.45
52:Y7:10:ARG:HE	52:Y7:14:LYS:HD2	1.82	0.45
24:YA:579:G:O2'	24:YA:2019:A:OP1	2.35	0.45
24:YA:2572:A:OP1	24:YA:2574:G:O2'	2.33	0.45
24:YA:300:A:OP1	43:YY:86:ARG:NH2	2.50	0.45
24:YA:530:G:O2'	24:YA:532:A:N7	2.49	0.45
43:YY:14:LEU:HB2	43:YY:75:ILE:HD11	1.98	0.45
41:RW:58:ALA:HB1	41:RW:64:MET:HB2	1.99	0.44
15:XO:17:ARG:HH12	15:XO:77:ARG:NH1	2.15	0.44
24:YA:1651:G:OP1	36:YR:40:LYS:NZ	2.46	0.44
26:YD:142:VAL:HG23	26:YD:193:VAL:HA	1.99	0.44
1:QA:1213:A:N6	1:QA:1215:G:N3	2.65	0.44
14:QN:29:ARG:HD3	14:QN:40:CYS:HB2	1.99	0.44
19:QS:45:VAL:HG13	19:QS:63:THR:HA	1.98	0.44
45:R0:70:GLN:OE1	45:R0:80:HIS:NE2	2.48	0.44
46:R1:80:LEU:HD12	46:R1:81:LYS:HG2	1.99	0.44
24:RA:2781:A:H5''	24:RA:2782:G:H5'	1.99	0.44
42:RX:54:VAL:HG22	42:RX:81:VAL:HG23	1.98	0.44
1:XA:1318:A:H4'	19:XS:11:VAL:HG21	1.99	0.44
12:XL:39:VAL:HB	12:XL:57:LYS:HB2	1.99	0.44
46:Y1:60:PHE:HB3	46:Y1:62:VAL:HG13	1.98	0.44
24:YA:28:A:N6	24:YA:512:G:O2'	2.51	0.44
24:YA:531:C:OP1	24:YA:561:G:N1	2.50	0.44
38:YT:16:ARG:NH2	38:YT:18:ASP:OD2	2.50	0.44
24:YA:296:C:O3'	43:YY:95:LYS:NZ	2.49	0.44
46:R1:91:LYS:HE2	46:R1:92:LYS:HE2	1.98	0.44
13:XM:80:ARG:HD2	49:Y4:58:ARG:HD3	1.98	0.44
24:YA:1667:G:O2'	24:YA:1991:U:O4	2.26	0.44
24:YA:2376:A:N6	37:YS:89:ARG:HD3	2.32	0.44
28:YF:34:TRP:CE3	34:YP:8:PRO:HB3	2.52	0.44
1:QA:1376:U:H2'	1:QA:1377:A:C8	2.52	0.44
24:RA:1296:G:OP1	24:RA:2709:G:O2'	2.22	0.44
24:RA:1592:C:H2'	24:RA:1593:G:H8	1.82	0.44
24:RA:1754:C:OP1	38:RT:96:ARG:NH1	2.50	0.44
39:RU:88:ILE:HG23	39:RU:90:VAL:HG23	2.00	0.44
42:RX:5:TYR:O	47:R2:36:ARG:NH2	2.50	0.44
1:XA:579:G:H5'	1:XA:728:A:H1'	2.00	0.44
48:Y3:12:PRO:HB2	48:Y3:20:LYS:HG2	1.99	0.44
24:YA:1479:G:N7	24:YA:1510:A:N6	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:YA:2105:C:H2'	24:YA:2106:G:H8	1.82	0.44
24:YA:27:G:H22	24:YA:512:G:H2'	1.83	0.44
27:YE:48:GLN:OE1	27:YE:64:LYS:NZ	2.50	0.44
35:YQ:66:ILE:HA	35:YQ:104:PHE:HA	1.99	0.44
39:YU:88:ILE:HG23	39:YU:90:VAL:HG23	2.00	0.44
40:YV:4:ILE:O	40:YV:39:LEU:N	2.50	0.44
1:QA:501:C:H1'	1:QA:549:C:H1'	1.98	0.44
35:RQ:28:ALA:N	35:RQ:105:GLU:OE2	2.50	0.44
38:RT:16:ARG:NH2	38:RT:18:ASP:OD2	2.50	0.44
52:Y7:5:TRP:NE1	52:Y7:7:PRO:HG3	2.33	0.44
24:YA:1537:C:H2'	24:YA:1538:G:C8	2.52	0.44
24:YA:1613:G:O2'	52:Y7:3:ARG:NE	2.40	0.44
24:YA:2258:C:O2'	24:YA:2427:C:OP2	2.35	0.44
24:YA:252:G:OP2	34:YP:50:ARG:NH1	2.50	0.44
24:YA:270(M):U:OP1	24:YA:270(N):G:N2	2.51	0.44
24:YA:500:G:N1	24:YA:503:A:OP2	2.50	0.44
24:YA:825:C:O2	34:YP:55:ARG:NH2	2.51	0.44
25:YB:40:U:H3	25:YB:43:C:H5"	1.82	0.44
26:YD:72:LYS:HG3	26:YD:97:TYR:CE2	2.53	0.44
38:YT:3:ARG:HG3	38:YT:7:ILE:HG12	1.99	0.44
24:RA:1849:G:H2'	24:RA:1850:G:H8	1.82	0.44
24:RA:2287:A:H62	24:RA:2344:U:H3	1.64	0.44
24:RA:1567:A:H3'	26:RD:86:PRO:HG3	1.98	0.44
1:XA:1502:A:H2	1:XA:1505:G:H1	1.64	0.44
24:YA:2123:G:H2'	24:YA:2124:G:C8	2.53	0.44
24:YA:363(A):A:H2'	24:YA:363(B):G:H8	1.83	0.44
1:QA:690:G:H22	11:QK:55:LYS:NZ	2.16	0.44
13:QM:80:ARG:HD2	49:R4:58:ARG:HD3	1.98	0.44
24:RA:1799:G:N2	24:RA:1818:U:O2'	2.50	0.44
24:RA:2445:G:P	28:RF:74:ARG:HH22	2.40	0.44
36:RR:103:ARG:NH1	41:RW:40:ASN:OD1	2.45	0.44
44:RZ:30:ASN:OD1	44:RZ:33:LEU:N	2.46	0.44
1:XA:1446:A:O2'	1:XA:1447:G:O4'	2.36	0.44
1:XA:209:U:H1'	1:XA:216:G:C2	2.53	0.44
24:YA:2123:G:H2'	24:YA:2124:G:H8	1.83	0.44
24:YA:2646:C:OP2	24:YA:2732:G:O2'	2.22	0.44
24:YA:414:C:O2	24:YA:1864:U:O2'	2.25	0.44
30:YH:152:ARG:HE	30:YH:153:LYS:HD2	1.82	0.44
24:YA:1243:G:H4'	34:YP:7:ARG:HH21	1.82	0.44
1:QA:1054:C:O2	1:QA:1196:U:N3	2.50	0.44
13:QM:14:ARG:NH2	13:QM:16:ASP:OD2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:RA:818:G:N1	24:RA:1188:U:OP2	2.33	0.44
24:RA:2744:G:N2	30:RH:143:GLN:OE1	2.37	0.44
34:RP:114:ILE:HD13	34:RP:125:VAL:HG21	1.98	0.44
1:XA:1356:G:H2'	1:XA:1357:A:C8	2.53	0.44
4:XD:119:GLN:HE21	4:XD:123:HIS:CE1	2.35	0.44
13:XM:15:VAL:HG22	13:XM:45:VAL:HB	2.00	0.44
24:YA:1338:G:N7	42:YX:62:LYS:NZ	2.55	0.44
25:YB:33:G:H5'	29:YG:2:PRO:HG3	1.99	0.44
24:YA:1500:G:H21	26:YD:100:GLY:HA3	1.83	0.44
31:YI:56:LYS:O	31:YI:60:GLU:N	2.50	0.44
1:QA:132:C:O3'	20:QT:74:LYS:NZ	2.51	0.44
1:QA:664:G:OP1	18:QR:64:ARG:NE	2.44	0.44
1:QA:986:A:O2'	19:QS:55:LYS:O	2.35	0.44
12:QL:103:GLY:N	12:QL:107:ALA:O	2.50	0.44
24:RA:1598:C:O3'	42:RX:35:THR:OG1	2.36	0.44
24:RA:579:G:O2'	24:RA:2019:A:OP1	2.33	0.44
24:RA:223:A:O2'	24:RA:420:C:O2	2.29	0.44
24:RA:463:G:N2	24:RA:466:A:OP2	2.46	0.44
25:RB:40:U:H3	25:RB:43:C:H5''	1.82	0.44
27:RE:92:THR:HG23	27:RE:94:GLU:H	1.82	0.44
34:RP:121:LYS:HD3	34:RP:122:PRO:HD2	2.00	0.44
35:RQ:80:GLU:HB2	45:R0:7:LEU:HG	2.00	0.44
1:XA:1296:C:OP1	13:XM:44:ARG:NH2	2.51	0.44
15:XO:7:GLU:OE2	15:XO:38:ARG:NH2	2.47	0.44
22:XV:20:G:O6	29:YG:83:ARG:NH2	2.39	0.44
24:YA:2215:G:H2'	24:YA:2216:G:H8	1.83	0.44
27:YE:31:CYS:HB3	27:YE:49:LEU:HG	1.98	0.44
27:YE:92:THR:HG23	27:YE:94:GLU:H	1.82	0.44
29:YG:114:ILE:HB	29:YG:117:PHE:HB2	1.98	0.44
4:QD:119:GLN:HE21	4:QD:123:HIS:CE1	2.35	0.43
11:QK:83:ILE:HG12	11:QK:109:VAL:HG22	2.00	0.43
12:QL:117:ARG:NH2	12:QL:124:LYS:HD3	2.33	0.43
45:R0:46:LYS:HD2	45:R0:78:TYR:HE1	1.83	0.43
24:RA:2791:C:OP1	24:RA:2893:G:N2	2.51	0.43
24:RA:336:C:O2'	43:RY:35:TYR:OH	2.36	0.43
25:RB:22:U:H3	25:RB:61:G:H1	1.65	0.43
43:RY:29:GLU:HB3	43:RY:38:ILE:HD12	2.00	0.43
7:XG:15:ASP:HB3	7:XG:19:GLY:H	1.83	0.43
50:Y5:20:ARG:HA	50:Y5:23:HIS:CD2	2.48	0.43
24:YA:2146:C:H4'	24:YA:2147:G:C8	2.53	0.43
24:YA:363(B):G:H2'	24:YA:363(C):G:H8	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:YD:108:PRO:HB3	26:YD:143:HIS:CE1	2.53	0.43
35:YQ:63:LYS:HD2	44:YZ:175:VAL:HG21	1.99	0.43
38:YT:51:ARG:HG2	38:YT:98:LYS:HE3	1.99	0.43
1:QA:1065:U:H6	1:QA:1190:G:H21	1.64	0.43
1:QA:552:U:H2'	1:QA:553:A:H8	1.82	0.43
24:RA:1819:A:H5''	26:RD:161:THR:HG21	1.99	0.43
24:RA:2572:A:H2'	27:RE:144:ARG:HD3	2.00	0.43
26:RD:108:PRO:HB3	26:RD:143:HIS:CE1	2.53	0.43
26:RD:17:THR:HB	26:RD:205:VAL:H	1.83	0.43
29:RG:16:ARG:NH2	29:RG:28:VAL:O	2.51	0.43
24:RA:1006:C:H5'	32:RN:28:THR:HG23	2.00	0.43
35:RQ:135:ASP:OD2	44:RZ:81:ARG:NH2	2.45	0.43
1:XA:1060:C:H2'	1:XA:1061:G:H8	1.83	0.43
1:XA:1095:U:P	1:XA:1108:G:H1	2.41	0.43
1:XA:112:G:H4'	1:XA:389:A:H4'	2.00	0.43
1:XA:573:A:N3	1:XA:883:C:O2'	2.44	0.43
11:XK:34:ASP:OD1	11:XK:37:GLY:N	2.51	0.43
12:XL:27:LEU:O	12:XL:33:ARG:NH2	2.50	0.43
24:YA:1223:C:OP2	40:YV:88:ARG:NH1	2.45	0.43
24:YA:2853:C:H2'	24:YA:2854:G:H8	1.83	0.43
24:YA:301:G:OP2	43:YY:84:ARG:NH2	2.50	0.43
41:YW:58:ALA:HB1	41:YW:64:MET:HB2	1.99	0.43
1:QA:1124:G:H3'	1:QA:1145:C:N4	2.33	0.43
25:RB:44:G:O2'	25:RB:47:C:N4	2.49	0.43
1:XA:890:G:O2'	1:XA:906:G:O6	2.27	0.43
6:XF:10:LEU:HD13	6:XF:61:LEU:HD13	1.99	0.43
8:XH:121:ASP:OD1	8:XH:121:ASP:N	2.51	0.43
38:YT:132:LYS:O	38:YT:136:GLN:NE2	2.51	0.43
8:QH:100:ILE:HA	8:QH:101:PRO:HD3	1.87	0.43
24:RA:984:A:H5''	24:RA:985:C:H5	1.84	0.43
39:RU:44:ASN:ND2	40:RV:75:PHE:HB3	2.32	0.43
1:XA:1053:G:N7	1:XA:1199:U:H2'	2.33	0.43
1:XA:265:G:H4'	17:XQ:66:SER:HA	1.99	0.43
53:Y8:22:VAL:HB	53:Y8:53:PRO:HB3	2.00	0.43
24:YA:1057:A:N6	24:YA:1087:G:OP2	2.51	0.43
24:YA:1113:U:H2'	24:YA:1114:G:C8	2.53	0.43
25:YB:22:U:H3	25:YB:61:G:H1	1.65	0.43
35:YQ:58:PHE:HD2	35:YQ:61:GLY:HA3	1.84	0.43
38:YT:19:LEU:HD22	38:YT:86:ILE:HG22	2.00	0.43
42:YX:57:LEU:HG	42:YX:78:LYS:HB2	2.01	0.43
44:YZ:97:GLU:HG2	44:YZ:125:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:985:C:H2'	1:QA:986:A:C8	2.53	0.43
2:QB:132:LYS:HA	2:QB:135:GLN:HB2	2.00	0.43
10:QJ:4:ILE:HG12	10:QJ:100:THR:HG22	2.01	0.43
9:QI:128:ARG:NH1	22:QV:36:A:OP2	2.52	0.43
24:RA:2232:U:OP2	46:R1:40:ARG:NH2	2.52	0.43
24:RA:1782:C:H1'	24:RA:2609:U:H5''	2.01	0.43
24:RA:270(S):G:H2'	24:RA:270(T):G:H8	1.84	0.43
38:RT:51:ARG:HG2	38:RT:98:LYS:HE3	1.99	0.43
39:RU:92:ARG:HD2	40:RV:11:GLN:HB2	2.00	0.43
42:RX:57:LEU:HG	42:RX:78:LYS:HB2	2.00	0.43
1:XA:1237:C:O3'	1:XA:1300:G:N2	2.50	0.43
13:XM:3:ARG:HH21	13:XM:7:VAL:HA	1.83	0.43
45:Y0:23:VAL:HG13	45:Y0:38:VAL:HG22	1.99	0.43
24:YA:1930:G:N2	24:YA:1969:A:OP2	2.31	0.43
24:YA:2134:A:OP2	24:YA:2157:G:N2	2.46	0.43
28:YF:28:ILE:H	28:YF:28:ILE:HG13	1.67	0.43
39:YU:57:PHE:HA	39:YU:57:PHE:HD1	1.76	0.43
40:YV:43:GLU:HG3	40:YV:44:LYS:H	1.83	0.43
1:QA:1095:U:P	1:QA:1108:G:H1	2.41	0.43
1:QA:191(F):U:H2'	1:QA:191(G):G:H8	1.84	0.43
1:QA:575:G:HO2'	1:QA:821:G:H5'	1.84	0.43
7:QG:15:ASP:HB3	7:QG:19:GLY:H	1.83	0.43
45:R0:23:VAL:HG13	45:R0:38:VAL:HG22	2.00	0.43
48:R3:12:PRO:HB2	48:R3:20:LYS:HG2	1.99	0.43
24:RA:2693:A:H2'	24:RA:2694:G:H8	1.83	0.43
24:RA:776:G:N7	24:RA:793:A:O2'	2.52	0.43
30:RH:146:ALA:O	30:RH:150:ALA:N	2.52	0.43
38:RT:132:LYS:O	38:RT:136:GLN:NE2	2.51	0.43
44:RZ:97:GLU:HG2	44:RZ:125:LEU:HD11	2.00	0.43
1:XA:486:U:H2'	1:XA:487:A:H8	1.83	0.43
3:XC:59:ARG:HH12	3:XC:97:LYS:HE3	1.82	0.43
15:XO:24:SER:OG	15:XO:25:THR:N	2.52	0.43
44:YZ:30:ASN:OD1	44:YZ:33:LEU:N	2.46	0.43
1:QA:1035:A:N6	1:QA:1036:G:N3	2.66	0.43
1:QA:1105:A:H2'	1:QA:1106:G:H8	1.83	0.43
1:QA:1118:C:H1'	1:QA:1179:A:C4	2.54	0.43
1:QA:501:C:O2	1:QA:549:C:O2'	2.29	0.43
1:QA:853:G:H2'	1:QA:854:G:H8	1.83	0.43
1:QA:922:G:H4'	5:QE:20:GLN:HA	2.01	0.43
24:RA:1590:U:H2'	24:RA:1591:G:H8	1.84	0.43
24:RA:527:C:N3	24:RA:2779:U:H5''	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:RA:78:A:H2'	24:RA:79:G:H8	1.84	0.43
30:RH:107:VAL:HG11	30:RH:162:ILE:HD11	2.01	0.43
1:XA:1145:C:H4'	1:XA:1146:A:H8	1.83	0.43
1:XA:1342:C:H4'	9:XI:125:TYR:HB3	2.00	0.43
24:YA:1535:U:N3	24:YA:1537:C:H1'	2.33	0.43
24:YA:1638:C:O2	24:YA:2698:U:O2'	2.36	0.43
24:YA:476:G:N1	24:YA:479:A:OP2	2.42	0.43
24:YA:536:A:OP1	39:YU:53:ARG:NH1	2.51	0.43
7:QG:115:ARG:HB2	7:QG:118:VAL:HG22	2.01	0.43
20:QT:26:ASN:HB2	20:QT:71:THR:HG23	2.00	0.43
24:RA:1195:G:O6	34:RP:16:ARG:NH2	2.51	0.43
24:RA:1565:C:H5''	26:RD:18:VAL:HG11	2.01	0.43
24:RA:1999:C:O2	24:RA:2687:U:O2'	2.33	0.43
31:RI:88:ILE:HG22	31:RI:90:GLY:H	1.84	0.43
35:RQ:58:PHE:HD2	35:RQ:61:GLY:HA3	1.84	0.43
38:RT:19:LEU:HD22	38:RT:86:ILE:HG22	2.00	0.43
38:RT:3:ARG:HG3	38:RT:7:ILE:HG12	1.99	0.43
39:RU:95:LEU:HD13	40:RV:4:ILE:HD12	2.00	0.43
40:RV:43:GLU:HG3	40:RV:44:LYS:H	1.83	0.43
1:XA:692:U:OP1	11:XK:124:LYS:NZ	2.36	0.43
9:XI:114:TYR:HE2	10:XJ:59:SER:HA	1.83	0.43
24:YA:2285:C:OP1	51:Y6:29:ASN:ND2	2.51	0.43
24:YA:1231:G:H2'	24:YA:1232:G:H8	1.84	0.43
24:YA:1567:A:H3'	26:YD:86:PRO:HG3	2.01	0.43
24:YA:1800:C:OP2	26:YD:183:ARG:NH1	2.42	0.43
24:YA:363(A):A:H2'	24:YA:363(B):G:C8	2.54	0.43
24:YA:881:G:H3'	24:YA:882:G:C8	2.53	0.43
26:YD:65:ILE:HD12	26:YD:88:ARG:CZ	2.49	0.43
10:QJ:48:THR:HA	10:QJ:62:HIS:HB3	2.01	0.43
50:R5:20:ARG:HA	50:R5:23:HIS:CD2	2.48	0.43
24:RA:30:G:O2'	24:RA:1214:A:N3	2.46	0.43
26:RD:65:ILE:HD12	26:RD:88:ARG:CZ	2.49	0.43
34:RP:106:LEU:HD21	34:RP:112:LEU:HD13	2.00	0.43
1:XA:944:G:N1	1:XA:1338:G:OP2	2.40	0.43
1:XA:664:G:H22	1:XA:741:G:H1	1.65	0.43
5:XE:110:LEU:HD13	5:XE:118:ILE:HD13	1.99	0.43
8:XH:17:THR:O	8:XH:78:GLN:NE2	2.50	0.43
24:YA:776:G:N2	24:YA:2241:A:OP1	2.48	0.43
24:YA:2291:U:O2'	24:YA:2374:C:O2	2.34	0.43
24:YA:2632:A:O2'	24:YA:2811:G:O2'	2.28	0.43
29:YG:16:ARG:NH2	29:YG:28:VAL:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1154:G:H2'	1:QA:1155:G:H8	1.83	0.43
1:QA:149:A:H4'	1:QA:1450:U:C4	2.54	0.43
8:QH:121:ASP:N	8:QH:121:ASP:OD1	2.51	0.43
24:RA:411:G:OP2	24:RA:2406:U:O2'	2.33	0.43
1:XA:1236:A:H4'	1:XA:1304:G:H4'	2.00	0.43
1:XA:1287:A:H2	1:XA:1353:G:H1'	1.84	0.43
1:XA:191(F):U:H2'	1:XA:191(G):G:H8	1.84	0.43
1:XA:401:C:O2'	1:XA:621:A:N3	2.43	0.43
2:XB:32:ILE:HD11	2:XB:40:HIS:HB3	2.00	0.43
24:YA:270(E):G:H1	24:YA:270(U):C:H42	1.67	0.43
24:YA:607:U:H3	24:YA:621:A:H2	1.66	0.43
24:YA:994:C:H3'	39:YU:54:LYS:HE3	2.01	0.43
26:YD:17:THR:O	26:YD:211:ARG:NH1	2.50	0.43
27:YE:10:GLY:HA3	38:YT:8:LYS:HD3	2.01	0.43
3:QC:11:ARG:HH21	3:QC:180:ALA:HB3	1.84	0.42
9:QI:111:ARG:HG3	14:QN:61:TRP:NE1	2.34	0.42
11:QK:93:GLN:OE1	11:QK:96:ARG:NH2	2.50	0.42
24:RA:956:G:H2'	24:RA:957:A:H2'	2.00	0.42
31:RI:56:LYS:O	31:RI:60:GLU:N	2.50	0.42
35:RQ:24:GLY:H	35:RQ:101:ARG:NE	2.17	0.42
1:XA:372:C:H42	1:XA:389:A:H62	1.65	0.42
9:XI:9:ARG:HG2	9:XI:14:VAL:HG22	2.01	0.42
24:YA:527:C:N4	24:YA:2779:U:OP2	2.44	0.42
34:YP:106:LEU:HD21	34:YP:112:LEU:HD13	2.01	0.42
1:QA:401:C:O2'	1:QA:621:A:N3	2.48	0.42
1:QA:628:G:H2'	1:QA:629:G:C8	2.54	0.42
47:R2:14:ARG:NH1	47:R2:66:GLU:OE1	2.52	0.42
24:RA:220:G:O2'	24:RA:233:A:N3	2.43	0.42
24:RA:321:G:O2'	24:RA:340:A:N3	2.48	0.42
31:RI:40:THR:O	31:RI:44:LEU:N	2.41	0.42
1:XA:1347:G:N2	1:XA:1374:A:OP2	2.45	0.42
7:XG:115:ARG:HB2	7:XG:118:VAL:HG22	2.01	0.42
12:XL:77:LEU:HD21	12:XL:107:ALA:HB2	2.01	0.42
20:XT:26:ASN:HB2	20:XT:71:THR:HG23	2.00	0.42
24:YA:1022:G:N2	24:YA:1023:U:O4	2.51	0.42
24:YA:2293:C:O2'	37:YS:93:LYS:NZ	2.52	0.42
34:YP:65:ARG:O	34:YP:68:GLN:NE2	2.52	0.42
4:QD:57:ARG:NH2	4:QD:205:GLU:OE2	2.43	0.42
7:QG:73:MET:HG2	7:QG:90:GLU:HA	2.02	0.42
9:QI:20:ARG:O	9:QI:60:ASP:N	2.48	0.42
45:R0:38:VAL:HG21	45:R0:45:PHE:HD2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:RA:31:C:O2'	24:RA:1238:G:OP1	2.37	0.42
24:RA:1359:A:H62	24:RA:1372:U:H3	1.67	0.42
24:RA:2311:A:H1'	29:RG:82:LEU:HD11	2.01	0.42
31:RI:2:LYS:HA	31:RI:20:ASP:HA	2.01	0.42
35:RQ:137:TYR:HB3	44:RZ:76:LEU:HD11	2.01	0.42
1:XA:148:G:H2'	1:XA:149:A:H8	1.84	0.42
1:XA:409:G:OP1	4:XD:24:GLU:N	2.53	0.42
10:XJ:5:ARG:N	10:XJ:99:LYS:O	2.52	0.42
24:YA:2445:G:P	28:YF:74:ARG:HH22	2.43	0.42
30:YH:146:ALA:O	30:YH:150:ALA:N	2.52	0.42
41:YW:35:ILE:O	41:YW:39:THR:OG1	2.29	0.42
1:QA:1239:A:O2'	1:QA:1298:C:N4	2.52	0.42
1:QA:819:A:H8	1:QA:819:A:H5'	1.85	0.42
2:QB:19:HIS:CD2	2:QB:206:ASP:HB2	2.54	0.42
4:QD:98:GLU:HA	4:QD:103:ASN:HD22	1.84	0.42
12:QL:33:ARG:NH2	12:QL:61:THR:OG1	2.52	0.42
50:R5:16:ARG:NH1	50:R5:17:ASP:OD1	2.52	0.42
24:RA:577:G:O2'	24:RA:1254:A:OP1	2.34	0.42
24:RA:2637:U:H5''	27:RE:82:ARG:HH12	1.84	0.42
1:XA:649:G:H2'	1:XA:650:G:H8	1.84	0.42
9:XI:65:VAL:HG21	9:XI:73:GLN:HG3	2.01	0.42
12:XL:44:THR:HA	12:XL:45:PRO:HD3	1.83	0.42
13:XM:16:ASP:HB3	13:XM:41:PRO:HB3	2.02	0.42
24:YA:1819:A:H5''	26:YD:161:THR:HG21	2.00	0.42
24:YA:2577:A:H5''	24:YA:2578:G:H5'	2.01	0.42
26:YD:148:GLU:OE1	26:YD:151:LYS:NZ	2.45	0.42
33:YO:7:TYR:CE1	33:YO:44:LYS:HG3	2.51	0.42
35:YQ:24:GLY:H	35:YQ:101:ARG:NE	2.17	0.42
44:YZ:163:LEU:HD22	44:YZ:167:PRO:HG3	2.01	0.42
2:QB:134:GLU:HA	2:QB:137:ARG:HB3	2.01	0.42
10:QJ:45:ARG:O	10:QJ:65:LEU:N	2.44	0.42
1:QA:659:U:OP1	15:QO:9:GLN:NE2	2.52	0.42
53:R8:22:VAL:HB	53:R8:53:PRO:HB3	2.00	0.42
24:RA:1141:U:H1'	24:RA:1142(A):A:C6	2.54	0.42
24:RA:49:A:H61	24:RA:177:G:H2'	1.85	0.42
24:RA:48:G:N2	24:RA:49:A:N1	2.67	0.42
31:RI:2:LYS:HG2	31:RI:20:ASP:HB3	2.01	0.42
35:RQ:32:TYR:CE1	35:RQ:133:ARG:HG3	2.54	0.42
1:XA:985:C:H2'	1:XA:986:A:H8	1.84	0.42
3:XC:11:ARG:HH21	3:XC:180:ALA:HB3	1.85	0.42
45:Y0:46:LYS:HB2	45:Y0:78:TYR:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Y2:14:ARG:NH1	47:Y2:66:GLU:OE1	2.52	0.42
24:YA:1105:U:H2'	24:YA:1106:G:H8	1.84	0.42
24:YA:1018:C:O3'	24:YA:1120:G:N2	2.52	0.42
1:QA:376:G:H5''	16:QP:5:ARG:HB2	2.01	0.42
26:RD:245:PRO:HA	26:RD:246:PRO:HD3	1.85	0.42
1:XA:1266:G:N2	1:XA:1269:A:OP2	2.45	0.42
1:XA:1336:C:O2	1:XA:1337:G:N1	2.53	0.42
1:XA:255:G:OP1	17:XQ:69:LYS:NZ	2.46	0.42
4:XD:23:GLY:N	4:XD:26:CYS:SG	2.73	0.42
1:XA:562:C:H1'	12:XL:15:ARG:HD2	2.00	0.42
45:Y0:23:VAL:HB	45:Y0:26:TYR:HE1	1.83	0.42
24:YA:1035:U:H2'	24:YA:1036:G:C8	2.54	0.42
24:YA:2729:G:H1'	27:YE:187:ALA:HB2	2.01	0.42
31:YI:2:LYS:HA	31:YI:20:ASP:HA	2.02	0.42
35:YQ:32:TYR:CE1	35:YQ:133:ARG:HG3	2.54	0.42
43:YY:29:GLU:HB3	43:YY:38:ILE:HD12	2.00	0.42
1:QA:1347:G:N2	1:QA:1374:A:OP2	2.33	0.42
6:QF:70:ASP:OD1	6:QF:70:ASP:N	2.53	0.42
17:QQ:45:HIS:CD2	17:QQ:47:PRO:HG3	2.54	0.42
48:R3:18:ASP:N	48:R3:18:ASP:OD1	2.53	0.42
24:RA:387:U:P	46:R1:20:ARG:HH12	2.42	0.42
31:RI:129:THR:HG22	31:RI:137:PRO:HB3	2.02	0.42
32:RN:54:VAL:HB	32:RN:122:VAL:HG22	2.02	0.42
1:XA:1343:G:H1'	9:XI:121:ARG:NH1	2.34	0.42
1:XA:148:G:H2'	1:XA:149:A:C8	2.54	0.42
1:XA:690:G:H22	11:XK:55:LYS:NZ	2.17	0.42
26:YD:17:THR:HB	26:YD:205:VAL:H	1.83	0.42
26:YD:31:LYS:HD2	26:YD:31:LYS:HA	1.89	0.42
37:YS:3:ARG:HE	37:YS:4:LEU:HD13	1.85	0.42
39:YU:49:HIS:O	39:YU:53:ARG:N	2.46	0.42
12:QL:53:ARG:HH12	12:QL:92:ASP:HB2	1.85	0.42
24:RA:1636:C:H2'	24:RA:1637:A:C8	2.55	0.42
24:RA:2228:G:OP1	26:RD:261:LYS:NZ	2.36	0.42
26:RD:72:LYS:HG3	26:RD:97:TYR:CE2	2.53	0.42
37:RS:34:HIS:CD2	37:RS:54:LEU:HD12	2.54	0.42
38:RT:39:ARG:HH22	38:RT:41:ARG:HD3	1.85	0.42
2:XB:93:VAL:HG21	2:XB:97:TRP:HD1	1.84	0.42
8:XH:49:GLU:OE2	8:XH:62:TYR:OH	2.28	0.42
47:Y2:51:ARG:HH11	47:Y2:55:ARG:NH2	2.18	0.42
24:YA:2168:G:N1	24:YA:2171:A:N7	2.55	0.42
25:YB:42:C:O2	29:YG:93:THR:N	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:YS:85:VAL:HG22	37:YS:110:LEU:HD22	2.02	0.42
1:QA:486:U:H2'	1:QA:487:A:H8	1.85	0.42
6:QF:22:GLU:OE2	6:QF:82:ARG:NH2	2.47	0.42
15:QO:24:SER:OG	15:QO:25:THR:N	2.52	0.42
24:RA:1015:G:H2'	24:RA:1016:G:H8	1.84	0.42
24:RA:1510:A:O2'	24:RA:1511:A:N7	2.53	0.42
24:RA:270(H):C:H2'	24:RA:270(I):G:C8	2.55	0.42
1:XA:132:C:O3'	20:XT:74:LYS:NZ	2.50	0.42
1:XA:1291:G:O2'	9:XI:38:GLN:OE1	2.34	0.42
45:Y0:38:VAL:HG21	45:Y0:45:PHE:HD2	1.85	0.42
50:Y5:16:ARG:NH1	50:Y5:17:ASP:OD1	2.52	0.42
24:YA:2845:G:H2'	24:YA:2846:G:H8	1.84	0.42
37:YS:34:HIS:CD2	37:YS:54:LEU:HD12	2.54	0.42
1:QA:769:G:H4'	1:QA:1513:A:H4'	2.02	0.42
24:RA:1184:G:P	48:R3:29:ARG:HH12	2.43	0.42
24:RA:288:C:H2'	24:RA:289:A:H8	1.83	0.42
1:XA:1022:G:H2'	1:XA:1023:G:C8	2.55	0.42
24:YA:698:C:O2'	24:YA:734:A:N6	2.53	0.42
31:YI:2:LYS:HG2	31:YI:20:ASP:HB3	2.01	0.42
44:YZ:14:LYS:HA	44:YZ:15:PRO:HD3	1.90	0.42
10:QJ:51:ARG:NH2	10:QJ:61:GLU:HB3	2.35	0.41
11:QK:18:ARG:HA	11:QK:81:ASP:H	1.85	0.41
24:RA:1645:G:H5''	24:RA:1646:C:H5'	2.02	0.41
39:RU:52:ARG:NH1	39:RU:55:ARG:HH21	2.18	0.41
1:XA:971:G:H5''	1:XA:972:C:H5''	2.02	0.41
31:YI:88:ILE:HG22	31:YI:90:GLY:H	1.84	0.41
34:YP:33:ARG:HD3	34:YP:40:SER:HA	2.01	0.41
39:YU:58:ARG:HH11	39:YU:93:LYS:HE2	1.85	0.41
1:QA:161:A:O2'	1:QA:162:A:O4'	2.38	0.41
1:QA:510:A:OP2	4:QD:49:ARG:NH2	2.53	0.41
1:QA:612:C:O2	1:QA:629:G:N2	2.53	0.41
1:QA:790:A:OP1	22:QV:39:A:O2'	2.31	0.41
8:QH:17:THR:O	8:QH:78:GLN:NE2	2.50	0.41
1:QA:779:C:H5''	11:QK:122:LYS:HG2	2.01	0.41
11:QK:58:PRO:HB2	11:QK:93:GLN:HG3	2.02	0.41
24:RA:1412:A:H2'	24:RA:1413:G:C8	2.55	0.41
24:RA:586:A:N1	24:RA:809:G:O2'	2.40	0.41
31:RI:13:GLY:HA3	31:RI:17:GLN:HG2	2.02	0.41
35:RQ:21:THR:HB	35:RQ:22:LYS:H	1.55	0.41
33:RO:76:ALA:HB3	38:RT:75:ILE:HD12	2.02	0.41
42:RX:25:LYS:HB3	42:RX:80:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:28:G:H1	1:XA:555:C:H42	1.68	0.41
1:XA:448:A:OP2	1:XA:485:G:N2	2.38	0.41
4:XD:98:GLU:HA	4:XD:103:ASN:HD22	1.84	0.41
7:XG:73:MET:HG2	7:XG:90:GLU:HA	2.02	0.41
24:YA:195:A:N6	24:YA:198:C:OP2	2.53	0.41
24:YA:2023:G:H5'	24:YA:2617:C:H4'	2.02	0.41
30:YH:107:VAL:HG11	30:YH:162:ILE:HD11	2.01	0.41
44:YZ:123:ASP:N	44:YZ:123:ASP:OD1	2.52	0.41
1:QA:1294:G:H2'	1:QA:1295:G:C8	2.56	0.41
2:QB:109:SER:O	2:QB:113:HIS:ND1	2.37	0.41
2:QB:18:GLY:H	2:QB:42:ILE:HD12	1.85	0.41
24:RA:2347:C:HO2'	51:R6:21:TYR:HH	1.67	0.41
24:RA:729:G:H5'	24:RA:730:C:H5''	2.02	0.41
28:RF:157:VAL:HB	28:RF:194:MET:HB3	2.03	0.41
44:RZ:123:ASP:N	44:RZ:123:ASP:OD1	2.52	0.41
1:XA:674:G:H2'	1:XA:675:A:C8	2.56	0.41
3:XC:150:LYS:HB3	3:XC:201:TYR:HB2	2.03	0.41
24:YA:503:A:H4'	24:YA:504:U:H5'	2.01	0.41
31:YI:13:GLY:HA3	31:YI:17:GLN:HG2	2.02	0.41
1:QA:1004:A:P	1:QA:1025:U:H3	2.44	0.41
1:QA:1422:G:H2'	1:QA:1423:G:H8	1.85	0.41
3:QC:5:ILE:HD12	10:QJ:51:ARG:HH12	1.84	0.41
5:QE:75:THR:OG1	5:QE:76:ILE:N	2.54	0.41
1:QA:1147:C:O2	9:QI:16:ARG:NH2	2.53	0.41
10:QJ:13:HIS:HA	10:QJ:16:LEU:HB3	2.02	0.41
48:R3:48:GLU:HA	48:R3:51:ALA:HB2	2.03	0.41
51:R6:10:LEU:HG	51:R6:54:ILE:HG13	2.03	0.41
24:RA:2131:G:N2	24:RA:2158:A:N7	2.68	0.41
24:RA:2183:C:H2'	24:RA:2184:G:C8	2.55	0.41
26:RD:182:LEU:HB2	26:RD:271:ILE:HB	2.02	0.41
26:RD:83:GLU:OE1	26:RD:104:TYR:OH	2.33	0.41
38:RT:128:GLU:O	38:RT:132:LYS:N	2.49	0.41
44:RZ:91:LEU:HD12	44:RZ:130:PRO:HB3	2.02	0.41
1:XA:1151:A:H2'	1:XA:1152:A:C8	2.55	0.41
1:XA:1414:U:H2'	1:XA:1415:G:H8	1.86	0.41
6:XF:47:ARG:NH2	6:XF:56:PRO:HB2	2.35	0.41
17:XQ:45:HIS:CD2	17:XQ:47:PRO:HG3	2.54	0.41
21:XU:6:ARG:HE	21:XU:15:ARG:NH2	2.18	0.41
24:YA:1263:U:H1'	50:Y5:10:LYS:HG3	2.03	0.41
24:YA:1385:G:O2'	24:YA:1396:U:O2	2.31	0.41
24:YA:270(R):G:H2'	24:YA:270(S):G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:YI:129:THR:HG22	31:YI:137:PRO:HB3	2.02	0.41
33:YO:7:TYR:HD1	33:YO:7:TYR:HA	1.76	0.41
44:YZ:91:LEU:HD12	44:YZ:130:PRO:HB3	2.03	0.41
1:QA:1294:G:H2'	1:QA:1295:G:H8	1.85	0.41
4:QD:23:GLY:N	4:QD:26:CYS:SG	2.73	0.41
6:QF:47:ARG:NH2	6:QF:56:PRO:HB2	2.35	0.41
24:RA:2361:A:O5'	53:R8:27:THR:OG1	2.38	0.41
24:RA:1423:G:OP1	24:RA:1492:G:O2'	2.36	0.41
25:RB:84:C:OP1	48:R3:15:TYR:OH	2.34	0.41
24:RA:586:A:H5'	28:RF:89:VAL:HG21	2.01	0.41
37:RS:85:VAL:HG22	37:RS:110:LEU:HD22	2.02	0.41
1:XA:708:C:OP1	11:XK:85:ARG:NH2	2.43	0.41
2:XB:155:LEU:HD13	2:XB:155:LEU:HA	1.88	0.41
7:XG:66:VAL:HG12	7:XG:70:LYS:HE3	2.02	0.41
19:XS:43:GLU:OE2	49:Y4:67:TYR:OH	2.38	0.41
26:YD:35:LYS:HD2	26:YD:104:TYR:CZ	2.56	0.41
31:YI:76:THR:OG1	31:YI:139:GLN:NE2	2.53	0.41
39:YU:44:ASN:HD21	40:YV:75:PHE:HB3	1.84	0.41
1:QA:1129:C:H4'	1:QA:1130:A:H8	1.86	0.41
1:QA:1192:C:OP2	3:QC:4:LYS:NZ	2.40	0.41
1:QA:501:C:H2'	1:QA:502:G:C8	2.56	0.41
1:QA:62:U:H3	1:QA:105:G:H1	1.67	0.41
7:QG:66:VAL:HG12	7:QG:70:LYS:HE3	2.02	0.41
21:QU:6:ARG:HE	21:QU:15:ARG:NH2	2.18	0.41
46:R1:52:ARG:NH2	46:R1:55:GLY:O	2.53	0.41
24:RA:1899:G:O2'	24:RA:1900:A:H5''	2.21	0.41
26:RD:35:LYS:HD2	26:RD:104:TYR:CZ	2.56	0.41
31:RI:76:THR:OG1	31:RI:139:GLN:NE2	2.53	0.41
1:XA:1077:G:N2	1:XA:1080:A:OP2	2.48	0.41
1:XA:529:G:O6	12:XL:49:ASN:ND2	2.48	0.41
10:XJ:32:ALA:HB3	10:XJ:76:ASN:HB2	2.02	0.41
22:XV:15:G:H1	22:XV:49:C:H5	1.68	0.41
24:YA:1491:G:H2'	24:YA:1492:G:H8	1.86	0.41
24:YA:1311:G:H21	24:YA:1603:A:H62	1.68	0.41
30:YH:12:PRO:HB3	30:YH:48:GLY:HA2	2.03	0.41
24:YA:137(A):G:H21	42:YX:41:ASN:HD21	1.68	0.41
44:YZ:10:ARG:HH22	44:YZ:26:GLY:H	1.69	0.41
1:QA:28:G:O2'	1:QA:296:U:OP1	2.31	0.41
5:QE:78:HIS:HB3	8:QH:107:LEU:HD12	2.03	0.41
11:QK:38:ASN:HA	11:QK:39:PRO:HD3	1.94	0.41
24:RA:1328:G:N2	24:RA:1330:C:O2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:RA:2133:G:N7	24:RA:2157:G:N1	2.68	0.41
37:RS:3:ARG:HE	37:RS:4:LEU:HD13	1.85	0.41
1:XA:674:G:H2'	1:XA:675:A:H8	1.84	0.41
6:XF:11:ASN:HB3	6:XF:14:LEU:HG	2.03	0.41
1:XA:277:C:H5''	17:XQ:68:ARG:HH21	1.85	0.41
24:YA:1888:G:N2	24:YA:1888:G:OP2	2.51	0.41
24:YA:2723:C:OP1	36:YR:3:HIS:ND1	2.48	0.41
24:YA:694:U:OP1	26:YD:59:LYS:NZ	2.38	0.41
1:QA:56:U:H4'	31:YI:82:ARG:HH12	1.85	0.41
37:YS:18:ILE:HA	37:YS:18:ILE:HD13	1.92	0.41
1:QA:769:G:OP2	1:QA:803:G:O2'	2.35	0.41
6:QF:11:ASN:HB3	6:QF:14:LEU:HG	2.03	0.41
46:R1:17:SER:HB2	46:R1:40:ARG:HD2	2.01	0.41
24:RA:1952:A:N3	24:RA:2560:C:O2'	2.46	0.41
27:RE:48:GLN:OE1	27:RE:64:LYS:NZ	2.50	0.41
30:RH:154:PRO:HA	30:RH:161:GLY:HA3	2.02	0.41
24:RA:1666:G:HO2'	33:RO:6:THR:HG1	1.59	0.41
1:XA:673:G:H2'	1:XA:674:G:C8	2.55	0.41
2:XB:30:ARG:HD3	2:XB:30:ARG:H	1.85	0.41
10:XJ:5:ARG:HH21	10:XJ:99:LYS:HD2	1.86	0.41
48:Y3:18:ASP:OD1	48:Y3:18:ASP:N	2.53	0.41
24:YA:941:A:O2'	24:YA:1190:G:O3'	2.37	0.41
24:YA:2116:G:N1	24:YA:2165:G:O6	2.54	0.41
24:YA:363(B):G:H2'	24:YA:363(C):G:C8	2.56	0.41
25:YB:52:A:HO2'	25:YB:53:A:H8	1.65	0.41
37:YS:61:ASN:O	37:YS:64:GLU:N	2.54	0.41
38:YT:42:ILE:H	38:YT:42:ILE:HG13	1.78	0.41
1:QA:1293:G:H2'	1:QA:1294:G:C8	2.56	0.41
1:QA:1319:A:OP1	19:QS:3:ARG:NH1	2.54	0.41
1:QA:1412:C:H2'	1:QA:1413:A:C8	2.56	0.41
1:QA:880:C:H2'	1:QA:881:G:H8	1.86	0.41
1:QA:1112:C:H1'	3:QC:179:ARG:HH11	1.86	0.41
1:QA:1348:U:H4'	9:QI:120:ARG:HD2	2.03	0.41
13:QM:3:ARG:HH12	29:RG:113:ARG:HH21	1.69	0.41
47:R2:51:ARG:HH11	47:R2:55:ARG:NH2	2.18	0.41
29:RG:142:PRO:HB2	49:R4:31:ILE:HG21	2.03	0.41
53:R8:61:LEU:HA	53:R8:61:LEU:HD23	1.82	0.41
28:RF:63:LYS:NZ	28:RF:75:HIS:O	2.39	0.41
24:RA:2483:C:N3	35:RQ:124:LYS:HE3	2.36	0.41
1:XA:272:C:H2'	1:XA:273:A:H8	1.84	0.41
2:XB:87:ARG:NH1	2:XB:220:ASP:OD1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:XH:20:TYR:HE2	8:XH:75:ARG:HD2	1.86	0.41
1:XA:1320:C:H5'	19:XS:70:LYS:HG3	2.02	0.41
24:YA:392:C:H5''	24:YA:409:C:H5''	2.03	0.41
30:YH:107:VAL:HB	30:YH:153:LYS:HZ2	1.86	0.41
32:YN:54:VAL:HB	32:YN:122:VAL:HG22	2.02	0.41
1:QA:1119:C:H2'	1:QA:1120:G:C8	2.56	0.41
2:QB:84:GLU:HB3	2:QB:219:VAL:HG21	2.01	0.41
5:QE:143:ARG:NE	8:QH:77:GLU:OE2	2.52	0.41
10:QJ:30:SER:HB2	10:QJ:80:LYS:HG3	2.03	0.41
52:R7:13:ALA:HB2	52:R7:46:VAL:HG11	2.02	0.41
24:RA:1288:U:O3'	24:RA:1647:G:N2	2.53	0.41
24:RA:1853:A:H2'	24:RA:1854:A:C8	2.56	0.41
24:RA:2438:U:O3'	24:RA:2439:A:H3'	2.21	0.41
28:RF:110:LEU:HD11	28:RF:181:LEU:HG	2.03	0.41
28:RF:133:ASN:H	28:RF:162:LEU:HD13	1.86	0.41
34:RP:62:LEU:HD12	53:R8:30:ARG:NH2	2.34	0.41
43:RY:13:VAL:HG12	43:RY:74:PRO:HA	2.03	0.41
44:RZ:163:LEU:HD22	44:RZ:167:PRO:HG3	2.02	0.41
1:XA:1004:A:H1'	1:XA:1036:G:H1	1.86	0.41
1:XA:736:C:H2'	1:XA:737:A:H8	1.86	0.41
8:XH:97:VAL:HG21	8:XH:128:GLY:HA2	2.03	0.41
1:XA:1484:C:O2'	24:YA:1960:A:O2'	2.28	0.41
30:YH:91:GLY:HA3	30:YH:94:TYR:CD2	2.56	0.41
1:QA:1320:C:C2	19:QS:72:GLY:HA3	2.55	0.41
1:QA:1352:C:OP1	21:QU:3:LYS:NZ	2.39	0.41
1:QA:184:G:H2'	1:QA:185:A:H8	1.86	0.41
52:R7:5:TRP:NE1	52:R7:7:PRO:HG3	2.36	0.41
24:RA:1412:A:H2'	24:RA:1413:G:H8	1.86	0.41
24:RA:1859:A:N6	24:RA:1883:G:O2'	2.53	0.41
40:RV:51:VAL:HG12	40:RV:53:GLU:H	1.86	0.41
1:XA:1133:G:H2'	1:XA:1134:G:C8	2.56	0.41
1:XA:1189:C:OP1	10:XJ:51:ARG:NH2	2.43	0.41
1:XA:1316:G:N2	1:XA:1319:A:OP2	2.52	0.41
18:XR:74:ARG:HD3	18:XR:81:PHE:HA	2.03	0.41
24:YA:261:G:HO2'	24:YA:609(A):G:HO2'	1.64	0.41
24:YA:956:G:OP2	35:YQ:14:ARG:NH2	2.53	0.41
26:YD:12:SER:HB2	26:YD:208:LYS:HB3	2.03	0.41
44:YZ:54:HIS:ND1	44:YZ:101:PRO:HG3	2.36	0.41
1:QA:1151:A:H2'	1:QA:1152:A:H8	1.86	0.40
1:QA:1220:G:OP1	19:QS:37:ARG:NH2	2.53	0.40
1:QA:1298:C:H4'	1:QA:1299:A:C4	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:581:G:N2	1:QA:582:U:O4	2.54	0.40
1:QA:982:U:O2	1:QA:1222:G:N1	2.44	0.40
3:QC:150:LYS:HB3	3:QC:201:TYR:HB2	2.03	0.40
24:RA:1664:A:H61	24:RA:1996:C:H42	1.69	0.40
24:RA:673:C:OP1	28:RF:54:ARG:NH1	2.50	0.40
25:RB:60:C:H2'	25:RB:61:G:H8	1.87	0.40
26:RD:12:SER:HB2	26:RD:208:LYS:HB3	2.03	0.40
25:RB:42:C:O2'	29:RG:67:LYS:O	2.25	0.40
34:RP:37:GLY:O	34:RP:40:SER:OG	2.31	0.40
24:RA:2295:C:H5	37:RS:13:ARG:HH12	1.69	0.40
43:RY:11:ASP:OD1	43:RY:11:ASP:N	2.54	0.40
1:XA:130:A:N3	1:XA:263:A:O2'	2.46	0.40
1:XA:532:A:H2	1:XA:1206:G:H21	1.68	0.40
1:XA:601:C:H2'	1:XA:602:A:H8	1.85	0.40
1:XA:7:G:H5'	1:XA:298:A:O4'	2.21	0.40
11:XK:43:SER:HB3	11:XK:68:ALA:HB2	2.03	0.40
3:XC:9:GLY:HA3	14:XN:49:HIS:HA	2.03	0.40
24:YA:2298:A:H62	24:YA:2318:G:H8	1.69	0.40
36:YR:79:LEU:HD12	36:YR:83:ILE:HB	2.03	0.40
39:YU:92:ARG:HD3	39:YU:92:ARG:HH11	1.76	0.40
1:QA:1151:A:H2'	1:QA:1152:A:C8	2.57	0.40
1:QA:1175:G:H2'	1:QA:1176:A:C8	2.53	0.40
2:QB:58:ILE:HD11	2:QB:185:ILE:HD13	2.03	0.40
4:QD:173:TRP:CD1	4:QD:174:LEU:HG	2.57	0.40
1:QA:191(G):G:O2'	20:QT:101:GLY:O	2.39	0.40
24:RA:1535:U:H5'	24:RA:1537:C:N3	2.36	0.40
24:RA:17:G:H4'	39:RU:25:TRP:HE1	1.86	0.40
24:RA:807:U:O2'	24:RA:2060:A:N1	2.43	0.40
24:RA:271(D):G:H2'	24:RA:272:G:H8	1.87	0.40
39:RU:58:ARG:HH11	39:RU:93:LYS:HE2	1.85	0.40
13:XM:87:TYR:O	13:XM:91:ARG:HG2	2.22	0.40
24:YA:1087:G:C4	24:YA:1089:G:H1'	2.56	0.40
24:YA:2521:C:O2'	24:YA:2564:A:N3	2.47	0.40
24:YA:2883:A:OP1	50:Y5:52:TYR:OH	2.27	0.40
27:YE:45:THR:O	27:YE:83:ASP:N	2.50	0.40
31:YI:40:THR:O	31:YI:44:LEU:N	2.41	0.40
34:YP:121:LYS:HD3	34:YP:122:PRO:HD2	2.03	0.40
38:YT:91:ARG:HB2	38:YT:121:ILE:HG13	2.04	0.40
39:YU:52:ARG:NH1	39:YU:55:ARG:HH21	2.18	0.40
1:QA:1189:C:O2'	3:QC:176:HIS:ND1	2.50	0.40
1:QA:324:G:N1	1:QA:327:A:OP2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:QB:84:GLU:HG3	2:QB:215:LEU:HB3	2.04	0.40
48:R3:29:ARG:HH11	48:R3:29:ARG:HD2	1.75	0.40
24:RA:1423:G:H2'	24:RA:1424:G:H8	1.86	0.40
24:RA:2123:G:H2'	24:RA:2124:G:C8	2.55	0.40
24:RA:270:A:OP2	24:RA:270(Y):G:N1	2.55	0.40
26:RD:17:THR:O	26:RD:211:ARG:NH1	2.50	0.40
29:RG:108:ASN:HA	49:R4:37:SER:HB3	2.02	0.40
30:RH:12:PRO:HB3	30:RH:48:GLY:HA2	2.03	0.40
34:RP:9:ASN:N	34:RP:9:ASN:OD1	2.53	0.40
41:RW:111:HIS:HD2	41:RW:113:LYS:H	1.70	0.40
44:RZ:10:ARG:HH22	44:RZ:26:GLY:H	1.69	0.40
1:XA:73:G:H1	1:XA:97:U:H3	1.69	0.40
23:XX:14:A:H3'	23:XX:15:A:C8	2.55	0.40
24:YA:1931:U:H6	24:YA:1931:U:H2'	1.73	0.40
24:YA:483:A:O4'	43:YY:48:ALA:HB1	2.21	0.40
25:YB:60:C:H2'	25:YB:61:G:H8	1.87	0.40
41:YW:111:HIS:HD2	41:YW:113:LYS:H	1.69	0.40
42:YX:25:LYS:HB3	42:YX:80:ILE:HD11	2.02	0.40
1:QA:1043:C:H2'	1:QA:1044:A:C8	2.56	0.40
8:QH:97:VAL:HG21	8:QH:128:GLY:HA2	2.03	0.40
8:QH:20:TYR:HE2	8:QH:75:ARG:HD2	1.85	0.40
16:QP:3:LYS:HG3	16:QP:65:GLN:O	2.22	0.40
24:RA:1068:G:N2	24:RA:1095:A:O2'	2.54	0.40
24:RA:372:G:N2	24:RA:401:A:OP2	2.54	0.40
24:RA:855:G:H1	24:RA:922:U:H3	1.70	0.40
26:RD:72:LYS:HG3	26:RD:97:TYR:HE2	1.87	0.40
44:RZ:54:HIS:ND1	44:RZ:101:PRO:HG3	2.36	0.40
1:XA:45:U:H2'	1:XA:46:G:C8	2.57	0.40
42:YX:11:PRO:HD3	47:Y2:37:PHE:CD1	2.55	0.40
24:YA:1296:G:OP1	24:YA:2709:G:O2'	2.24	0.40
24:YA:2702:U:H1'	24:YA:2703:C:H5	1.86	0.40
24:YA:1566:A:P	26:YD:211:ARG:HH21	2.44	0.40
30:YH:154:PRO:HA	30:YH:161:GLY:HA3	2.02	0.40
34:YP:7:ARG:HA	34:YP:8:PRO:HD2	1.95	0.40
43:YY:13:VAL:HG12	43:YY:74:PRO:HA	2.03	0.40
1:QA:59:A:H3'	1:QA:331:G:H22	1.87	0.40
1:QA:861:G:O6	1:QA:869:G:N2	2.54	0.40
24:RA:2250:G:C4	35:RQ:82:ARG:HG3	2.56	0.40
28:RF:182:ASN:N	28:RF:182:ASN:OD1	2.54	0.40
28:RF:60:SER:OG	28:RF:61:GLY:N	2.55	0.40
1:XA:1152:A:H5''	10:XJ:13:HIS:ND1	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:973:G:H3'	1:XA:974:A:H5''	2.03	0.40
3:XC:20:SER:OG	3:XC:22:TRP:NE1	2.50	0.40
22:XV:59:A:O2'	22:XV:61:U:OP2	2.26	0.40
48:Y3:48:GLU:HA	48:Y3:51:ALA:HB2	2.03	0.40
24:YA:1407:C:H42	24:YA:1595:G:H1	1.69	0.40
24:YA:1423:G:OP1	24:YA:1492:G:O2'	2.39	0.40
24:YA:730:C:OP1	24:YA:1775:U:O2'	2.31	0.40
28:YF:157:VAL:HB	28:YF:194:MET:HB3	2.02	0.40
38:YT:39:ARG:HH22	38:YT:41:ARG:HD3	1.85	0.40
40:YV:51:VAL:HG12	40:YV:53:GLU:H	1.86	0.40
43:YY:11:ASP:N	43:YY:11:ASP:OD1	2.54	0.40

All (12) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:RY:21:LYS:NZ	47:Y2:71:ASN:CB[3_555]	1.64	0.56
43:RY:19:LYS:O	47:Y2:71:ASN:ND2[3_555]	1.79	0.41
41:RW:63:ASP:OD1	43:YY:92:ASN:ND2[3_555]	1.88	0.32
40:YV:49:THR:O	50:Y5:59:GLU:OE2[4_445]	1.90	0.30
40:YV:49:THR:OG1	50:Y5:60:VAL:O[4_445]	1.91	0.29
43:RY:21:LYS:NZ	47:Y2:71:ASN:CG[3_555]	2.03	0.17
30:YH:46:GLU:OE2	43:YY:23:ARG:NH1[4_445]	2.05	0.15
40:YV:49:THR:OG1	50:Y5:59:GLU:OE2[4_445]	2.10	0.10
11:QK:99:GLN:OE1	3:XC:79:ARG:NE[4_555]	2.12	0.08
43:RY:19:LYS:C	47:Y2:71:ASN:ND2[3_555]	2.13	0.07
11:QK:99:GLN:NE2	3:XC:79:ARG:NE[4_555]	2.14	0.06
41:RW:60:ASN:OD1	43:YY:91:GLU:O[3_555]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	233/256 (91%)	205 (88%)	27 (12%)	1 (0%)	34	69
2	XB	234/256 (91%)	210 (90%)	24 (10%)	0	100	100
3	QC	203/239 (85%)	188 (93%)	15 (7%)	0	100	100
3	XC	203/239 (85%)	188 (93%)	15 (7%)	0	100	100
4	QD	206/209 (99%)	193 (94%)	13 (6%)	0	100	100
4	XD	206/209 (99%)	193 (94%)	13 (6%)	0	100	100
5	QE	149/162 (92%)	142 (95%)	6 (4%)	1 (1%)	22	60
5	XE	149/162 (92%)	142 (95%)	6 (4%)	1 (1%)	22	60
6	QF	99/101 (98%)	99 (100%)	0	0	100	100
6	XF	99/101 (98%)	99 (100%)	0	0	100	100
7	QG	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
7	XG	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
8	QH	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
8	XH	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
9	QI	125/128 (98%)	114 (91%)	11 (9%)	0	100	100
9	XI	124/128 (97%)	114 (92%)	10 (8%)	0	100	100
10	QJ	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
10	XJ	94/105 (90%)	83 (88%)	11 (12%)	0	100	100
11	QK	117/129 (91%)	109 (93%)	8 (7%)	0	100	100
11	XK	114/129 (88%)	107 (94%)	7 (6%)	0	100	100
12	QL	123/132 (93%)	104 (85%)	19 (15%)	0	100	100
12	XL	120/132 (91%)	105 (88%)	14 (12%)	1 (1%)	19	56
13	QM	118/126 (94%)	101 (86%)	16 (14%)	1 (1%)	19	56
13	XM	117/126 (93%)	100 (86%)	17 (14%)	0	100	100
14	QN	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	9	40
14	XN	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	9	40
15	QO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
15	XO	85/89 (96%)	85 (100%)	0	0	100	100
16	QP	82/88 (93%)	81 (99%)	1 (1%)	0	100	100
16	XP	82/88 (93%)	81 (99%)	1 (1%)	0	100	100
17	QQ	98/105 (93%)	97 (99%)	1 (1%)	0	100	100
17	XQ	98/105 (93%)	97 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	QR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
18	XR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
19	QS	81/93 (87%)	71 (88%)	10 (12%)	0	100	100
19	XS	82/93 (88%)	66 (80%)	15 (18%)	1 (1%)	13	48
20	QT	97/106 (92%)	90 (93%)	7 (7%)	0	100	100
20	XT	97/106 (92%)	90 (93%)	7 (7%)	0	100	100
21	QU	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
21	XU	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
26	RD	270/276 (98%)	246 (91%)	23 (8%)	1 (0%)	34	69
26	YD	270/276 (98%)	246 (91%)	23 (8%)	1 (0%)	34	69
27	RE	203/206 (98%)	165 (81%)	37 (18%)	1 (0%)	29	66
27	YE	203/206 (98%)	165 (81%)	37 (18%)	1 (0%)	29	66
28	RF	200/210 (95%)	186 (93%)	14 (7%)	0	100	100
28	YF	200/210 (95%)	186 (93%)	14 (7%)	0	100	100
29	RG	179/182 (98%)	152 (85%)	26 (14%)	1 (1%)	25	63
29	YG	179/182 (98%)	152 (85%)	26 (14%)	1 (1%)	25	63
30	RH	172/180 (96%)	149 (87%)	19 (11%)	4 (2%)	6	32
30	YH	172/180 (96%)	149 (87%)	19 (11%)	4 (2%)	6	32
31	RI	144/148 (97%)	126 (88%)	16 (11%)	2 (1%)	11	44
31	YI	144/148 (97%)	126 (88%)	16 (11%)	2 (1%)	11	44
32	RN	136/140 (97%)	124 (91%)	11 (8%)	1 (1%)	22	60
32	YN	136/140 (97%)	124 (91%)	11 (8%)	1 (1%)	22	60
33	RO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
33	YO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
34	RP	148/150 (99%)	122 (82%)	25 (17%)	1 (1%)	22	60
34	YP	145/150 (97%)	115 (79%)	29 (20%)	1 (1%)	22	60
35	RQ	139/141 (99%)	117 (84%)	21 (15%)	1 (1%)	22	60
35	YQ	139/141 (99%)	117 (84%)	21 (15%)	1 (1%)	22	60
36	RR	115/118 (98%)	107 (93%)	8 (7%)	0	100	100
36	YR	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	17	54
37	RS	109/112 (97%)	91 (84%)	17 (16%)	1 (1%)	17	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	YS	109/112 (97%)	91 (84%)	17 (16%)	1 (1%)	17	54
38	RT	135/146 (92%)	120 (89%)	13 (10%)	2 (2%)	10	43
38	YT	135/146 (92%)	120 (89%)	13 (10%)	2 (2%)	10	43
39	RU	115/118 (98%)	107 (93%)	8 (7%)	0	100	100
39	YU	115/118 (98%)	107 (93%)	8 (7%)	0	100	100
40	RV	99/101 (98%)	84 (85%)	14 (14%)	1 (1%)	15	52
40	YV	99/101 (98%)	84 (85%)	14 (14%)	1 (1%)	15	52
41	RW	111/113 (98%)	105 (95%)	5 (4%)	1 (1%)	17	54
41	YW	111/113 (98%)	105 (95%)	5 (4%)	1 (1%)	17	54
42	RX	90/96 (94%)	87 (97%)	3 (3%)	0	100	100
42	YX	90/96 (94%)	86 (96%)	4 (4%)	0	100	100
43	RY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
43	YY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
44	RZ	181/206 (88%)	148 (82%)	30 (17%)	3 (2%)	9	40
44	YZ	181/206 (88%)	148 (82%)	30 (17%)	3 (2%)	9	40
45	R0	79/85 (93%)	76 (96%)	3 (4%)	0	100	100
45	Y0	73/85 (86%)	69 (94%)	4 (6%)	0	100	100
46	R1	95/98 (97%)	84 (88%)	11 (12%)	0	100	100
46	Y1	91/98 (93%)	80 (88%)	11 (12%)	0	100	100
47	R2	67/72 (93%)	62 (92%)	4 (6%)	1 (2%)	10	43
47	Y2	67/72 (93%)	62 (92%)	4 (6%)	1 (2%)	10	43
48	R3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
48	Y3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
49	R4	67/71 (94%)	55 (82%)	11 (16%)	1 (2%)	10	43
49	Y4	67/71 (94%)	55 (82%)	11 (16%)	1 (2%)	10	43
50	R5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
50	Y5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
51	R6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
51	Y6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
52	R7	45/49 (92%)	45 (100%)	0	0	100	100
52	Y7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	R8	62/65 (95%)	49 (79%)	11 (18%)	2 (3%)	4	23
53	Y8	62/65 (95%)	49 (79%)	11 (18%)	2 (3%)	4	23
54	R9	35/37 (95%)	35 (100%)	0	0	100	100
54	Y9	35/37 (95%)	35 (100%)	0	0	100	100
All	All	11452/12128 (94%)	10380 (91%)	1015 (9%)	57 (0%)	29	66

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
27	RE	18	ASP
31	RI	15	VAL
38	RT	124	ASP
44	RZ	53	ILE
12	XL	105	TYR
27	YE	18	ASP
31	YI	15	VAL
38	YT	124	ASP
44	YZ	53	ILE
14	QN	17	LYS
53	R8	29	LYS
53	R8	30	ARG
14	XN	17	LYS
34	YP	108	LYS
53	Y8	29	LYS
53	Y8	30	ARG
26	RD	243	GLY
30	RH	86	GLU
32	RN	22	THR
34	RP	108	LYS
38	RT	123	GLN
26	YD	243	GLY
30	YH	86	GLU
32	YN	22	THR
38	YT	123	GLN
29	RG	81	LYS
30	RH	87	LEU
30	RH	152	ARG
35	RQ	78	PRO
47	R2	70	GLN
49	R4	47	GLN
29	YG	81	LYS

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Mol	Chain	Res	Type
30	YH	87	LEU
30	YH	152	ARG
35	YQ	78	PRO
47	Y2	70	GLN
49	Y4	47	GLN
2	QB	208	ILE
13	QM	14	ARG
30	RH	12	PRO
40	RV	44	LYS
44	RZ	60	GLU
19	XS	27	GLU
30	YH	12	PRO
40	YV	44	LYS
44	YZ	60	GLU
37	RS	62	LYS
41	RW	66	GLU
36	YR	4	LEU
37	YS	62	LYS
41	YW	66	GLU
31	RI	16	GLY
31	YI	16	GLY
5	QE	74	GLY
5	XE	74	GLY
44	RZ	166	SER
44	YZ	166	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	203/220 (92%)	202 (100%)	1 (0%)	88	95
2	XB	204/220 (93%)	200 (98%)	4 (2%)	55	79
3	QC	159/188 (85%)	159 (100%)	0	100	100
3	XC	159/188 (85%)	159 (100%)	0	100	100
4	QD	180/181 (99%)	180 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	XD	180/181 (99%)	180 (100%)	0	100	100
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%)	125 (99%)	1 (1%)	81	92
7	XG	126/127 (99%)	125 (99%)	1 (1%)	81	92
8	QH	118/119 (99%)	118 (100%)	0	100	100
8	XH	118/119 (99%)	118 (100%)	0	100	100
9	QI	98/99 (99%)	96 (98%)	2 (2%)	55	79
9	XI	97/99 (98%)	97 (100%)	0	100	100
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	86/92 (94%)	86 (100%)	0	100	100
11	QK	90/99 (91%)	90 (100%)	0	100	100
11	XK	88/99 (89%)	88 (100%)	0	100	100
12	QL	104/109 (95%)	104 (100%)	0	100	100
12	XL	103/109 (94%)	103 (100%)	0	100	100
13	QM	96/101 (95%)	96 (100%)	0	100	100
13	XM	95/101 (94%)	95 (100%)	0	100	100
14	QN	49/50 (98%)	46 (94%)	3 (6%)	18	51
14	XN	49/50 (98%)	46 (94%)	3 (6%)	18	51
15	QO	79/80 (99%)	79 (100%)	0	100	100
15	XO	79/80 (99%)	79 (100%)	0	100	100
16	QP	72/74 (97%)	71 (99%)	1 (1%)	67	85
16	XP	72/74 (97%)	71 (99%)	1 (1%)	67	85
17	QQ	95/97 (98%)	95 (100%)	0	100	100
17	XQ	95/97 (98%)	95 (100%)	0	100	100
18	QR	61/77 (79%)	61 (100%)	0	100	100
18	XR	61/77 (79%)	61 (100%)	0	100	100
19	QS	72/80 (90%)	72 (100%)	0	100	100
19	XS	73/80 (91%)	73 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	QT	76/82 (93%)	76 (100%)	0	100	100
20	XT	76/82 (93%)	76 (100%)	0	100	100
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	20 (100%)	0	100	100
26	RD	214/218 (98%)	211 (99%)	3 (1%)	67	85
26	YD	214/218 (98%)	211 (99%)	3 (1%)	67	85
27	RE	165/166 (99%)	165 (100%)	0	100	100
27	YE	165/166 (99%)	165 (100%)	0	100	100
28	RF	161/166 (97%)	159 (99%)	2 (1%)	71	87
28	YF	161/166 (97%)	159 (99%)	2 (1%)	71	87
29	RG	155/156 (99%)	154 (99%)	1 (1%)	86	94
29	YG	155/156 (99%)	154 (99%)	1 (1%)	86	94
30	RH	145/148 (98%)	141 (97%)	4 (3%)	43	73
30	YH	145/148 (98%)	141 (97%)	4 (3%)	43	73
31	RI	122/124 (98%)	122 (100%)	0	100	100
31	YI	122/124 (98%)	122 (100%)	0	100	100
32	RN	117/119 (98%)	116 (99%)	1 (1%)	78	91
32	YN	117/119 (98%)	116 (99%)	1 (1%)	78	91
33	RO	100/100 (100%)	99 (99%)	1 (1%)	76	89
33	YO	100/100 (100%)	99 (99%)	1 (1%)	76	89
34	RP	116/116 (100%)	116 (100%)	0	100	100
34	YP	114/116 (98%)	112 (98%)	2 (2%)	59	81
35	RQ	111/111 (100%)	111 (100%)	0	100	100
35	YQ	111/111 (100%)	111 (100%)	0	100	100
36	RR	100/101 (99%)	99 (99%)	1 (1%)	76	89
36	YR	100/101 (99%)	100 (100%)	0	100	100
37	RS	87/88 (99%)	86 (99%)	1 (1%)	73	88
37	YS	87/88 (99%)	86 (99%)	1 (1%)	73	88
38	RT	120/127 (94%)	119 (99%)	1 (1%)	81	92
38	YT	120/127 (94%)	119 (99%)	1 (1%)	81	92
39	RU	93/94 (99%)	92 (99%)	1 (1%)	73	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	YU	93/94 (99%)	92 (99%)	1 (1%)	73	88
40	RV	82/82 (100%)	82 (100%)	0	100	100
40	YV	82/82 (100%)	82 (100%)	0	100	100
41	RW	92/92 (100%)	90 (98%)	2 (2%)	52	78
41	YW	92/92 (100%)	90 (98%)	2 (2%)	52	78
42	RX	74/78 (95%)	73 (99%)	1 (1%)	67	85
42	YX	74/78 (95%)	73 (99%)	1 (1%)	67	85
43	RY	88/91 (97%)	88 (100%)	0	100	100
43	YY	88/91 (97%)	88 (100%)	0	100	100
44	RZ	162/179 (90%)	161 (99%)	1 (1%)	86	94
44	YZ	162/179 (90%)	161 (99%)	1 (1%)	86	94
45	R0	65/67 (97%)	64 (98%)	1 (2%)	65	85
45	Y0	61/67 (91%)	60 (98%)	1 (2%)	62	83
46	R1	82/83 (99%)	82 (100%)	0	100	100
46	Y1	78/83 (94%)	78 (100%)	0	100	100
47	R2	64/67 (96%)	64 (100%)	0	100	100
47	Y2	64/67 (96%)	64 (100%)	0	100	100
48	R3	51/52 (98%)	50 (98%)	1 (2%)	55	79
48	Y3	51/52 (98%)	50 (98%)	1 (2%)	55	79
49	R4	62/63 (98%)	60 (97%)	2 (3%)	39	70
49	Y4	62/63 (98%)	60 (97%)	2 (3%)	39	70
50	R5	51/52 (98%)	51 (100%)	0	100	100
50	Y5	51/52 (98%)	51 (100%)	0	100	100
51	R6	51/52 (98%)	51 (100%)	0	100	100
51	Y6	51/52 (98%)	51 (100%)	0	100	100
52	R7	40/42 (95%)	40 (100%)	0	100	100
52	Y7	41/42 (98%)	41 (100%)	0	100	100
53	R8	54/55 (98%)	54 (100%)	0	100	100
53	Y8	54/55 (98%)	54 (100%)	0	100	100
54	R9	34/34 (100%)	34 (100%)	0	100	100
54	Y9	34/34 (100%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	9687/10066 (96%)	9619 (99%)	68 (1%)	84	93

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	QB	30	ARG
5	QE	73	ASN
7	QG	94	ARG
9	QI	10	ARG
9	QI	111	ARG
14	QN	41	ARG
14	QN	44	LEU
14	QN	45	ARG
16	QP	67	THR
26	RD	33	LEU
26	RD	52	ARG
26	RD	273	ARG
28	RF	38	ARG
28	RF	44	ARG
29	RG	40	ASN
30	RH	23	ARG
30	RH	69	ARG
30	RH	149	ARG
30	RH	152	ARG
32	RN	115	ARG
33	RO	97	ARG
36	RR	3	HIS
37	RS	3	ARG
38	RT	38	ASN
39	RU	57	PHE
41	RW	15	ARG
41	RW	40	ASN
42	RX	66	LEU
44	RZ	34	ASN
45	R0	14	ARG
48	R3	30	ARG
49	R4	56	VAL
49	R4	61	ARG
2	XB	30	ARG
2	XB	64	ARG
2	XB	83	MET
2	XB	144	ARG

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Mol	Chain	Res	Type
5	XE	73	ASN
7	XG	94	ARG
14	XN	41	ARG
14	XN	44	LEU
14	XN	45	ARG
16	XP	67	THR
26	YD	33	LEU
26	YD	52	ARG
26	YD	273	ARG
28	YF	38	ARG
28	YF	44	ARG
29	YG	40	ASN
30	YH	23	ARG
30	YH	69	ARG
30	YH	149	ARG
30	YH	152	ARG
32	YN	115	ARG
33	YO	97	ARG
34	YP	58	THR
34	YP	125	VAL
37	YS	3	ARG
38	YT	38	ASN
39	YU	57	PHE
41	YW	15	ARG
41	YW	40	ASN
42	YX	66	LEU
44	YZ	34	ASN
45	Y0	14	ARG
48	Y3	30	ARG
49	Y4	56	VAL
49	Y4	61	ARG

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

Mol	Chain	Res	Type
2	QB	212	GLN
3	QC	37	GLN
4	QD	123	HIS
5	QE	73	ASN
6	QF	7	ASN
7	QG	68	ASN
9	QI	73	GLN

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Mol	Chain	Res	Type
9	QI	124	GLN
26	RD	87	ASN
27	RE	159	HIS
28	RF	40	GLN
30	RH	74	ASN
31	RI	104	GLN
34	RP	27	HIS
38	RT	38	ASN
39	RU	94	ASN
41	RW	61	ASN
42	RX	41	ASN
50	R5	23	HIS
2	XB	40	HIS
4	XD	119	GLN
5	XE	73	ASN
6	XF	7	ASN
7	XG	68	ASN
9	XI	29	ASN
9	XI	124	GLN
26	YD	87	ASN
26	YD	227	ASN
28	YF	40	GLN
30	YH	74	ASN
31	YI	104	GLN
34	YP	27	HIS
35	YQ	123	HIS
36	YR	24	GLN
38	YT	38	ASN
39	YU	94	ASN
42	YX	41	ASN
47	Y2	46	GLN
47	Y2	47	ASN
50	Y5	23	HIS
51	Y6	46	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1496/1508 (99%)	280 (18%)	35 (2%)
1	XA	1498/1508 (99%)	281 (18%)	31 (2%)
22	QV	76/77 (98%)	14 (18%)	2 (2%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	XV	76/77 (98%)	14 (18%)	2 (2%)
23	QX	11/25 (44%)	5 (45%)	1 (9%)
23	XX	10/25 (40%)	6 (60%)	0
24	RA	2879/2915 (98%)	577 (20%)	38 (1%)
24	YA	2880/2915 (98%)	573 (19%)	40 (1%)
25	RB	119/122 (97%)	22 (18%)	2 (1%)
25	YB	119/122 (97%)	22 (18%)	2 (1%)
All	All	9164/9294 (98%)	1794 (19%)	153 (1%)

All (1794) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	9	G
1	QA	22	G
1	QA	32	A
1	QA	39	G
1	QA	47	C
1	QA	48	C
1	QA	50	A
1	QA	51	A
1	QA	64	G
1	QA	65	U
1	QA	66	G
1	QA	76	G
1	QA	79	G
1	QA	80	G
1	QA	90	C
1	QA	91	C
1	QA	101	A
1	QA	108	G
1	QA	116	A
1	QA	120	A
1	QA	121	C
1	QA	129(A)	G
1	QA	144	G
1	QA	146	G
1	QA	157	G
1	QA	159	G
1	QA	162	A
1	QA	163	C
1	QA	169	C

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Mol	Chain	Res	Type
1	QA	173	U
1	QA	174	C
1	QA	182	U
1	QA	190	G
1	QA	195	A
1	QA	197	A
1	QA	208	U
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	262	A
1	QA	267	C
1	QA	281	G
1	QA	289	G
1	QA	321	A
1	QA	328	C
1	QA	329	A
1	QA	332	G
1	QA	343	U
1	QA	347	U
1	QA	352	C
1	QA	353	A
1	QA	354	G
1	QA	356	A
1	QA	367	U
1	QA	372	C
1	QA	373	A
1	QA	384	G
1	QA	388	G
1	QA	390	C
1	QA	397	A
1	QA	398	C
1	QA	406	G
1	QA	411	A
1	QA	412	A
1	QA	413	G
1	QA	421	U
1	QA	422	C

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Mol	Chain	Res	Type
1	QA	423	G
1	QA	424	G
1	QA	429	U
1	QA	442	C
1	QA	465	A
1	QA	466	C
1	QA	485	G
1	QA	486	U
1	QA	496	A
1	QA	497	U
1	QA	505	G
1	QA	509	A
1	QA	510	A
1	QA	511	C
1	QA	517	G
1	QA	518	C
1	QA	521	G
1	QA	527	G
1	QA	532	A
1	QA	533	A
1	QA	547	A
1	QA	559	A
1	QA	568	G
1	QA	572	A
1	QA	573	A
1	QA	576	G
1	QA	577	G
1	QA	579	G
1	QA	596	C
1	QA	618	C
1	QA	630	G
1	QA	631	G
1	QA	652	U
1	QA	653	A
1	QA	665	A
1	QA	686	U
1	QA	688	G
1	QA	701	C
1	QA	702	A
1	QA	703	G
1	QA	704	A
1	QA	722	A

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Mol	Chain	Res	Type
1	QA	731	G
1	QA	748	C
1	QA	752	G
1	QA	754	C
1	QA	755	G
1	QA	760	G
1	QA	777	A
1	QA	785	G
1	QA	792	A
1	QA	793	U
1	QA	794	A
1	QA	813	U
1	QA	817	C
1	QA	819	A
1	QA	821	G
1	QA	828	A
1	QA	841	U
1	QA	842	C
1	QA	843	U
1	QA	848	C
1	QA	859	A
1	QA	870	U
1	QA	871	U
1	QA	872	A
1	QA	873	A
1	QA	885	G
1	QA	889	A
1	QA	902	G
1	QA	914	A
1	QA	927	G
1	QA	934	C
1	QA	960	U
1	QA	961	U
1	QA	968	A
1	QA	969	A
1	QA	971	G
1	QA	972	C
1	QA	974	A
1	QA	975	A
1	QA	976	G
1	QA	977	A
1	QA	980	C

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Mol	Chain	Res	Type
1	QA	982	U
1	QA	991	U
1	QA	992	U
1	QA	993	G
1	QA	994	A
1	QA	1001	G
1	QA	1004	A
1	QA	1006	C
1	QA	1009	G
1	QA	1020	U
1	QA	1024	G
1	QA	1025	U
1	QA	1027	C
1	QA	1028	C
1	QA	1029	G
1	QA	1030	C
1	QA	1031	G
1	QA	1032(A)	G
1	QA	1033	G
1	QA	1034	G
1	QA	1042	G
1	QA	1053	G
1	QA	1054	C
1	QA	1064	G
1	QA	1065	U
1	QA	1066	C
1	QA	1080	A
1	QA	1081	G
1	QA	1082	G
1	QA	1094	G
1	QA	1095	U
1	QA	1101	A
1	QA	1108	G
1	QA	1124	G
1	QA	1125	U
1	QA	1126	U
1	QA	1130	A
1	QA	1131	G
1	QA	1136	U
1	QA	1137	C
1	QA	1138	G
1	QA	1139	G

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Mol	Chain	Res	Type
1	QA	1146	A
1	QA	1157	A
1	QA	1158	C
1	QA	1159	U
1	QA	1160	G
1	QA	1181	G
1	QA	1183	A
1	QA	1187	G
1	QA	1190	G
1	QA	1193	G
1	QA	1196	U
1	QA	1200	C
1	QA	1201	A
1	QA	1202	G
1	QA	1212	U
1	QA	1213	A
1	QA	1215	G
1	QA	1224	G
1	QA	1227	A
1	QA	1228	C
1	QA	1233	G
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	1286	A
1	QA	1287	A
1	QA	1297	C
1	QA	1298	C
1	QA	1299	A
1	QA	1300	G
1	QA	1301	U
1	QA	1302	U
1	QA	1303	C
1	QA	1305	G

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Mol	Chain	Res	Type
1	QA	1319	A
1	QA	1320	C
1	QA	1322	C
1	QA	1323	G
1	QA	1331	G
1	QA	1335	C
1	QA	1336	C
1	QA	1337	G
1	QA	1346	A
1	QA	1347	G
1	QA	1348	U
1	QA	1353	G
1	QA	1358	U
1	QA	1359	C
1	QA	1362(A)	C
1	QA	1364	U
1	QA	1368	G
1	QA	1370	G
1	QA	1397	C
1	QA	1398	A
1	QA	1419	G
1	QA	1442	G
1	QA	1446	A
1	QA	1447	G
1	QA	1449	C
1	QA	1452	C
1	QA	1453	G
1	QA	1469	G
1	QA	1492	A
1	QA	1494	G
1	QA	1497	G
1	QA	1499	A
1	QA	1502	A
1	QA	1504	G
1	QA	1506	U
1	QA	1517	G
1	QA	1519	A
1	QA	1520	G
1	QA	1529	G
1	QA	1530	G
22	QV	20	G
22	QV	21	U

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Mol	Chain	Res	Type
22	QV	22	A
22	QV	35	C
22	QV	36	A
22	QV	48	U
22	QV	49	C
22	QV	53	G
22	QV	54	G
22	QV	55	U
22	QV	59	A
22	QV	64	G
22	QV	76	C
22	QV	77	A
23	QX	10	G
23	QX	12	A
23	QX	13	A
23	QX	15	A
23	QX	19	U
24	RA	15	G
24	RA	34	C
24	RA	35	G
24	RA	46	C
24	RA	51	G
24	RA	55	G
24	RA	64	A
24	RA	73	A
24	RA	74	A
24	RA	75	G
24	RA	82	G
24	RA	83	G
24	RA	96	G
24	RA	101	G
24	RA	102	G
24	RA	103	A
24	RA	118	A
24	RA	119	A
24	RA	120	U
24	RA	131	G
24	RA	140	A
24	RA	177	G
24	RA	181	A
24	RA	196	A
24	RA	199	A

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Mol	Chain	Res	Type
24	RA	214	G
24	RA	215	G
24	RA	216	A
24	RA	221	A
24	RA	222	A
24	RA	223	A
24	RA	226	G
24	RA	228	A
24	RA	229	A
24	RA	230	U
24	RA	232	G
24	RA	233	A
24	RA	248	G
24	RA	249	C
24	RA	252	G
24	RA	265	A
24	RA	266	G
24	RA	269	U
24	RA	270(L)	U
24	RA	270(M)	U
24	RA	270(N)	G
24	RA	270(P)	C
24	RA	271(C)	U
24	RA	275	G
24	RA	276	A
24	RA	277	C
24	RA	283	A
24	RA	299	A
24	RA	304	G
24	RA	311	A
24	RA	317	G
24	RA	323	G
24	RA	324	A
24	RA	327	G
24	RA	329	G
24	RA	330	A
24	RA	342	G
24	RA	346	A
24	RA	352	G
24	RA	364	C
24	RA	371	A
24	RA	372	G

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Mol	Chain	Res	Type
24	RA	373	U
24	RA	386	G
24	RA	395	U
24	RA	405	U
24	RA	406	G
24	RA	407	G
24	RA	411	G
24	RA	412	A
24	RA	428	A
24	RA	444	C
24	RA	448	U
24	RA	454	A
24	RA	455	C
24	RA	456	C
24	RA	457	A
24	RA	464	U
24	RA	467	G
24	RA	470	A
24	RA	481	G
24	RA	504	U
24	RA	505	A
24	RA	509	C
24	RA	513	A
24	RA	527	C
24	RA	529	A
24	RA	531	C
24	RA	532	A
24	RA	533	G
24	RA	537	C
24	RA	539	G
24	RA	540	G
24	RA	546	C
24	RA	547	A
24	RA	549	G
24	RA	556	G
24	RA	563	G
24	RA	573	G
24	RA	574	C
24	RA	575	A
24	RA	588	U
24	RA	603	A
24	RA	607	U

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Mol	Chain	Res	Type
24	RA	614	U
24	RA	615	G
24	RA	617	G
24	RA	621	A
24	RA	622	G
24	RA	627	A
24	RA	634	C
24	RA	637	A
24	RA	638	G
24	RA	645	C
24	RA	646	A
24	RA	651	G
24	RA	652	C
24	RA	654	A
24	RA	654(A)	G
24	RA	669	G
24	RA	686	G
24	RA	702	G
24	RA	717	G
24	RA	722	A
24	RA	730	C
24	RA	753	C
24	RA	765	G
24	RA	776	G
24	RA	782	A
24	RA	783	A
24	RA	784	A
24	RA	785	G
24	RA	790	C
24	RA	791	C
24	RA	800	A
24	RA	805	G
24	RA	812	C
24	RA	819	A
24	RA	827	U
24	RA	828	U
24	RA	831	G
24	RA	847	U
24	RA	856	C
24	RA	857	C
24	RA	859	G
24	RA	869	G

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Mol	Chain	Res	Type
24	RA	882	G
24	RA	884	C
24	RA	885	C
24	RA	886	C
24	RA	888	C
24	RA	889	C
24	RA	896	A
24	RA	897	C
24	RA	900	A
24	RA	901	A
24	RA	907	U
24	RA	910	A
24	RA	914	C
24	RA	915	C
24	RA	917	A
24	RA	918	A
24	RA	932	G
24	RA	938	G
24	RA	941	A
24	RA	945	A
24	RA	946	G
24	RA	953	A
24	RA	957	A
24	RA	959	A
24	RA	961	C
24	RA	973	A
24	RA	974	G
24	RA	974(A)	C
24	RA	980	A
24	RA	983	A
24	RA	989	G
24	RA	996	A
24	RA	1003	G
24	RA	1005	C
24	RA	1008	C
24	RA	1011	G
24	RA	1012	U
24	RA	1013	C
24	RA	1017	G
24	RA	1020	A
24	RA	1022	G
24	RA	1023	U

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Mol	Chain	Res	Type
24	RA	1025	G
24	RA	1026	U
24	RA	1027	A
24	RA	1033	U
24	RA	1042	G
24	RA	1044	G
24	RA	1045	A
24	RA	1046	A
24	RA	1050	A
24	RA	1054	A
24	RA	1055	G
24	RA	1060	U
24	RA	1061	U
24	RA	1062	G
24	RA	1065	U
24	RA	1066	U
24	RA	1070	A
24	RA	1071	G
24	RA	1077	A
24	RA	1078	U
24	RA	1079	C
24	RA	1082	U
24	RA	1083	U
24	RA	1084	A
24	RA	1085	A
24	RA	1086	A
24	RA	1087	G
24	RA	1088	A
24	RA	1091	G
24	RA	1093	G
24	RA	1096	A
24	RA	1105	U
24	RA	1110	G
24	RA	1111	A
24	RA	1112	G
24	RA	1122	G
24	RA	1126	A
24	RA	1129	A
24	RA	1130	U
24	RA	1131	G
24	RA	1135	C
24	RA	1136	G

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Mol	Chain	Res	Type
24	RA	1139	G
24	RA	1140	C
24	RA	1142	U
24	RA	1142(A)	A
24	RA	1155	A
24	RA	1173	G
24	RA	1174	A
24	RA	1175	U
24	RA	1176	G
24	RA	1179	C
24	RA	1181	C
24	RA	1195	G
24	RA	1204	A
24	RA	1205	U
24	RA	1206	G
24	RA	1210	A
24	RA	1211	U
24	RA	1220	A
24	RA	1236	G
24	RA	1238	G
24	RA	1252	G
24	RA	1253	A
24	RA	1256	G
24	RA	1265	A
24	RA	1271	G
24	RA	1272	A
24	RA	1273	U
24	RA	1300	U
24	RA	1301	A
24	RA	1309	G
24	RA	1312	U
24	RA	1313	U
24	RA	1314	C
24	RA	1321	A
24	RA	1329	U
24	RA	1349	A
24	RA	1352	U
24	RA	1365	A
24	RA	1370	C
24	RA	1378	A
24	RA	1379	A
24	RA	1380	G

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Mol	Chain	Res	Type
24	RA	1384	A
24	RA	1385	G
24	RA	1395	A
24	RA	1407	C
24	RA	1408	C
24	RA	1411	C
24	RA	1416	G
24	RA	1419	A
24	RA	1420	U
24	RA	1421	G
24	RA	1428	C
24	RA	1444(A)	A
24	RA	1445	C
24	RA	1449	A
24	RA	1449(A)	G
24	RA	1455	G
24	RA	1458	C
24	RA	1460	A
24	RA	1461	G
24	RA	1471	A
24	RA	1474	C
24	RA	1482	U
24	RA	1483	G
24	RA	1487	G
24	RA	1493	C
24	RA	1497	U
24	RA	1504	C
24	RA	1505	C
24	RA	1506	C
24	RA	1507	A
24	RA	1508	A
24	RA	1510	A
24	RA	1514	U
24	RA	1515	C
24	RA	1533	C
24	RA	1534	G
24	RA	1535	U
24	RA	1536	A
24	RA	1537	C
24	RA	1543	A
24	RA	1544	C
24	RA	1545	A

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Mol	Chain	Res	Type
24	RA	1547	C
24	RA	1558	A
24	RA	1559	G
24	RA	1560	G
24	RA	1566	A
24	RA	1569	A
24	RA	1578	U
24	RA	1580	A
24	RA	1583	A
24	RA	1586	A
24	RA	1598	C
24	RA	1607	C
24	RA	1608	A
24	RA	1609	A
24	RA	1610	A
24	RA	1617	C
24	RA	1640	C
24	RA	1648	C
24	RA	1654	A
24	RA	1667	G
24	RA	1668	A
24	RA	1674	G
24	RA	1675	C
24	RA	1694	C
24	RA	1703	G
24	RA	1725	G
24	RA	1728	G
24	RA	1729	A
24	RA	1731	G
24	RA	1733	G
24	RA	1742	C
24	RA	1743	G
24	RA	1750	G
24	RA	1756	G
24	RA	1762	A
24	RA	1763	G
24	RA	1764	G
24	RA	1769	G
24	RA	1773	A
24	RA	1774	C
24	RA	1776	G
24	RA	1780	A

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Mol	Chain	Res	Type
24	RA	1791	A
24	RA	1799	G
24	RA	1800	C
24	RA	1801	G
24	RA	1816	G
24	RA	1820	U
24	RA	1828	G
24	RA	1829	A
24	RA	1835	G
24	RA	1847	A
24	RA	1848	A
24	RA	1858	G
24	RA	1869	G
24	RA	1870	C
24	RA	1878	G
24	RA	1882	C
24	RA	1888	G
24	RA	1889	A
24	RA	1899	G
24	RA	1905	C
24	RA	1906	G
24	RA	1913	A
24	RA	1914	C
24	RA	1929	G
24	RA	1930	G
24	RA	1936	A
24	RA	1938	A
24	RA	1939	U
24	RA	1955	U
24	RA	1963	U
24	RA	1967	C
24	RA	1969	A
24	RA	1970	A
24	RA	1971	A
24	RA	1972	A
24	RA	1981	A
24	RA	1982	C
24	RA	1991	U
24	RA	1992	G
24	RA	1993	U
24	RA	1996	C
24	RA	2020	A

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Mol	Chain	Res	Type
24	RA	2023	G
24	RA	2031	A
24	RA	2032	G
24	RA	2033	A
24	RA	2039	C
24	RA	2043	C
24	RA	2055	C
24	RA	2056	G
24	RA	2059	A
24	RA	2060	A
24	RA	2061	G
24	RA	2062	A
24	RA	2063	C
24	RA	2069	G
24	RA	2076	U
24	RA	2093	G
24	RA	2111	C
24	RA	2113	U
24	RA	2114	A
24	RA	2115	G
24	RA	2116	G
24	RA	2117	A
24	RA	2126	A
24	RA	2127	G
24	RA	2128	C
24	RA	2131	G
24	RA	2132	U
24	RA	2133	G
24	RA	2134	A
24	RA	2136	C
24	RA	2145	C
24	RA	2147	G
24	RA	2148	G
24	RA	2161	C
24	RA	2166	G
24	RA	2169	A
24	RA	2170	A
24	RA	2173	A
24	RA	2190	G
24	RA	2192	G
24	RA	2198	A
24	RA	2210	G

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Mol	Chain	Res	Type
24	RA	2211	G
24	RA	2212	A
24	RA	2213	U
24	RA	2215	G
24	RA	2225	A
24	RA	2238	G
24	RA	2239	G
24	RA	2243	U
24	RA	2246	G
24	RA	2275	C
24	RA	2278	A
24	RA	2279	G
24	RA	2280	G
24	RA	2283	C
24	RA	2287	A
24	RA	2288	A
24	RA	2307	G
24	RA	2308	G
24	RA	2309	A
24	RA	2311	A
24	RA	2312	U
24	RA	2315	G
24	RA	2319	G
24	RA	2320	A
24	RA	2325	G
24	RA	2334	G
24	RA	2336	A
24	RA	2345	G
24	RA	2346	A
24	RA	2347	C
24	RA	2350	C
24	RA	2354	G
24	RA	2358	G
24	RA	2377	A
24	RA	2383	G
24	RA	2384	G
24	RA	2385	C
24	RA	2396	G
24	RA	2402	C
24	RA	2403	C
24	RA	2406	U
24	RA	2425	A

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Mol	Chain	Res	Type
24	RA	2429	G
24	RA	2430	A
24	RA	2435	A
24	RA	2439	A
24	RA	2440	C
24	RA	2441	C
24	RA	2445	G
24	RA	2448	A
24	RA	2469	A
24	RA	2470	G
24	RA	2475	C
24	RA	2480	C
24	RA	2494	G
24	RA	2502	G
24	RA	2504	U
24	RA	2505	G
24	RA	2518	A
24	RA	2519	U
24	RA	2520	C
24	RA	2529	G
24	RA	2542	A
24	RA	2543	G
24	RA	2554	U
24	RA	2562	U
24	RA	2567	G
24	RA	2569	G
24	RA	2572	A
24	RA	2578	G
24	RA	2602	A
24	RA	2609	U
24	RA	2611	U
24	RA	2612	C
24	RA	2615	U
24	RA	2619	C
24	RA	2623	G
24	RA	2629	A
24	RA	2636	U
24	RA	2641	G
24	RA	2642	G
24	RA	2646	C
24	RA	2655	G
24	RA	2665	A

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Mol	Chain	Res	Type
24	RA	2666	C
24	RA	2673	G
24	RA	2688	U
24	RA	2689	U
24	RA	2690	C
24	RA	2702	U
24	RA	2703	C
24	RA	2712(A)	A
24	RA	2713	A
24	RA	2714	G
24	RA	2726	U
24	RA	2733	A
24	RA	2744	G
24	RA	2751	G
24	RA	2752	C
24	RA	2758	A
24	RA	2761	G
24	RA	2765	A
24	RA	2766	G
24	RA	2778	A
24	RA	2779	U
24	RA	2780	G
24	RA	2789	C
24	RA	2790	A
24	RA	2791	C
24	RA	2792	G
24	RA	2797	U
24	RA	2798	C
24	RA	2807	G
24	RA	2818	G
24	RA	2820	A
24	RA	2821	A
24	RA	2833	G
24	RA	2834	G
24	RA	2835	A
24	RA	2839	G
24	RA	2847	U
24	RA	2849	U
24	RA	2867	G
24	RA	2868	A
24	RA	2872	G
24	RA	2879	C

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Mol	Chain	Res	Type
24	RA	2880	C
24	RA	2891	G
24	RA	2892	A
24	RA	2894	G
24	RA	2895	U
24	RA	2897	U
25	RB	8	U
25	RB	9	G
25	RB	13	A
25	RB	15	A
25	RB	16	G
25	RB	19	G
25	RB	21	G
25	RB	25	A
25	RB	32	C
25	RB	41	U
25	RB	42	C
25	RB	44	G
25	RB	45	A
25	RB	52	A
25	RB	53	A
25	RB	56	G
25	RB	67	G
25	RB	73	A
25	RB	89	G
25	RB	105	G
25	RB	108	C
25	RB	109	G
1	XA	6	G
1	XA	32	A
1	XA	35	G
1	XA	39	G
1	XA	47	C
1	XA	48	C
1	XA	50	A
1	XA	51	A
1	XA	54	C
1	XA	61	G
1	XA	65	U
1	XA	66	G
1	XA	76	G
1	XA	79	G

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Mol	Chain	Res	Type
1	XA	88	C
1	XA	89	U
1	XA	92	G
1	XA	95	G
1	XA	101	A
1	XA	108	G
1	XA	116	A
1	XA	121	C
1	XA	130	A
1	XA	137	C
1	XA	144	G
1	XA	147	G
1	XA	160	A
1	XA	161	A
1	XA	163	C
1	XA	169	C
1	XA	172	A
1	XA	174	C
1	XA	190	G
1	XA	195	A
1	XA	197	A
1	XA	201	C
1	XA	209	U
1	XA	210	U
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	306	G
1	XA	321	A
1	XA	328	C
1	XA	329	A
1	XA	332	G
1	XA	344	A
1	XA	345	C
1	XA	346	G
1	XA	347	U
1	XA	348	G

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Mol	Chain	Res	Type
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	384	G
1	XA	389	A
1	XA	397	A
1	XA	398	C
1	XA	406	G
1	XA	411	A
1	XA	412	A
1	XA	413	G
1	XA	421	U
1	XA	422	C
1	XA	423	G
1	XA	424	G
1	XA	428	G
1	XA	429	U
1	XA	442	C
1	XA	452	A
1	XA	465	A
1	XA	466	C
1	XA	467	G
1	XA	485	G
1	XA	486	U
1	XA	496	A
1	XA	497	U
1	XA	505	G
1	XA	509	A
1	XA	510	A
1	XA	511	C
1	XA	518	C
1	XA	527	G
1	XA	531	U
1	XA	532	A
1	XA	533	A
1	XA	545	C
1	XA	547	A
1	XA	548	G

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Mol	Chain	Res	Type
1	XA	559	A
1	XA	561	U
1	XA	564	C
1	XA	566	G
1	XA	568	G
1	XA	572	A
1	XA	573	A
1	XA	576	G
1	XA	577	G
1	XA	579	G
1	XA	630	G
1	XA	631	G
1	XA	632	A
1	XA	653	A
1	XA	665	A
1	XA	686	U
1	XA	688	G
1	XA	702	A
1	XA	703	G
1	XA	704	A
1	XA	721	G
1	XA	731	G
1	XA	749	C
1	XA	753	A
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	818	G
1	XA	821	G
1	XA	828	A
1	XA	836	G
1	XA	841	U
1	XA	843	U
1	XA	848	C

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Mol	Chain	Res	Type
1	XA	859	A
1	XA	871	U
1	XA	872	A
1	XA	885	G
1	XA	889	A
1	XA	902	G
1	XA	914	A
1	XA	916	G
1	XA	926	G
1	XA	927	G
1	XA	934	C
1	XA	942	G
1	XA	958	A
1	XA	960	U
1	XA	961	U
1	XA	966	G
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	983	A
1	XA	991	U
1	XA	992	U
1	XA	993	G
1	XA	994	A
1	XA	1000	A
1	XA	1004	A
1	XA	1006	C
1	XA	1008	C
1	XA	1009	G
1	XA	1024	G
1	XA	1025	U
1	XA	1028	C
1	XA	1029	G
1	XA	1031	G
1	XA	1032	A
1	XA	1032(A)	G
1	XA	1036	G
1	XA	1040	U

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Mol	Chain	Res	Type
1	XA	1042	G
1	XA	1054	C
1	XA	1064	G
1	XA	1081	G
1	XA	1094	G
1	XA	1095	U
1	XA	1101	A
1	XA	1108	G
1	XA	1124	G
1	XA	1125	U
1	XA	1126	U
1	XA	1127	G
1	XA	1129	C
1	XA	1130	A
1	XA	1132	C
1	XA	1136	U
1	XA	1137	C
1	XA	1138	G
1	XA	1139	G
1	XA	1146	A
1	XA	1157	A
1	XA	1158	C
1	XA	1159	U
1	XA	1160	G
1	XA	1162	C
1	XA	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	1199	U
1	XA	1201	A
1	XA	1211	U
1	XA	1212	U
1	XA	1225	A
1	XA	1226	C
1	XA	1238	A

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Mol	Chain	Res	Type
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	1272	G
1	XA	1280	A
1	XA	1281	U
1	XA	1286	A
1	XA	1287	A
1	XA	1298	C
1	XA	1300	G
1	XA	1301	U
1	XA	1302	U
1	XA	1305	G
1	XA	1310	G
1	XA	1311	G
1	XA	1312	G
1	XA	1318	A
1	XA	1320	C
1	XA	1322	C
1	XA	1323	G
1	XA	1331	G
1	XA	1336	C
1	XA	1337	G
1	XA	1347	G
1	XA	1353	G
1	XA	1362(A)	C
1	XA	1363	A
1	XA	1364	U
1	XA	1370	G
1	XA	1398	A
1	XA	1400	C
1	XA	1419	G
1	XA	1442	G
1	XA	1446	A
1	XA	1447	G
1	XA	1452	C
1	XA	1453	G
1	XA	1454	G

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Mol	Chain	Res	Type
1	XA	1469	G
1	XA	1475	G
1	XA	1487	G
1	XA	1492	A
1	XA	1493	A
1	XA	1497	G
1	XA	1499	A
1	XA	1502	A
1	XA	1504	G
1	XA	1506	U
1	XA	1517	G
1	XA	1519	A
1	XA	1520	G
1	XA	1529	G
1	XA	1530	G
22	XV	20	G
22	XV	21	U
22	XV	22	A
22	XV	35	C
22	XV	36	A
22	XV	48	U
22	XV	49	C
22	XV	53	G
22	XV	54	G
22	XV	55	U
22	XV	59	A
22	XV	64	G
22	XV	76	C
22	XV	77	A
23	XX	10	G
23	XX	11	U
23	XX	13	A
23	XX	14	A
23	XX	15	A
23	XX	19	U
24	YA	9	U
24	YA	28	A
24	YA	34	C
24	YA	35	G
24	YA	46	C
24	YA	51	G
24	YA	61	G

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Mol	Chain	Res	Type
24	YA	72	U
24	YA	73	A
24	YA	74	A
24	YA	75	G
24	YA	99	U
24	YA	101	G
24	YA	102	G
24	YA	103	A
24	YA	118	A
24	YA	119	A
24	YA	120	U
24	YA	125	G
24	YA	131	G
24	YA	140	A
24	YA	155	C
24	YA	161	U
24	YA	162	U
24	YA	175	G
24	YA	181	A
24	YA	196	A
24	YA	199	A
24	YA	214	G
24	YA	216	A
24	YA	221	A
24	YA	222	A
24	YA	223	A
24	YA	226	G
24	YA	228	A
24	YA	229	A
24	YA	230	U
24	YA	232	G
24	YA	233	A
24	YA	241	A
24	YA	242	G
24	YA	243	U
24	YA	248	G
24	YA	249	C
24	YA	252	G
24	YA	265	A
24	YA	266	G
24	YA	269	U
24	YA	270(L)	U

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Mol	Chain	Res	Type
24	YA	270(M)	U
24	YA	270(N)	G
24	YA	270(P)	C
24	YA	271(B)	G
24	YA	271(C)	U
24	YA	271(D)	G
24	YA	274	G
24	YA	275	G
24	YA	276	A
24	YA	278	A
24	YA	279	C
24	YA	299	A
24	YA	300	A
24	YA	311	A
24	YA	323	G
24	YA	324	A
24	YA	329	G
24	YA	330	A
24	YA	332	A
24	YA	342	G
24	YA	352	G
24	YA	363	G
24	YA	363(E)	U
24	YA	364	C
24	YA	371	A
24	YA	372	G
24	YA	373	U
24	YA	386	G
24	YA	387	U
24	YA	395	U
24	YA	396	G
24	YA	405	U
24	YA	406	G
24	YA	411	G
24	YA	412	A
24	YA	428	A
24	YA	443	A
24	YA	444	C
24	YA	448	U
24	YA	457	A
24	YA	464	U
24	YA	467	G

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Mol	Chain	Res	Type
24	YA	470	A
24	YA	481	G
24	YA	504	U
24	YA	505	A
24	YA	508	G
24	YA	509	C
24	YA	512	G
24	YA	518	G
24	YA	532	A
24	YA	537	C
24	YA	539	G
24	YA	540	G
24	YA	546	C
24	YA	547	A
24	YA	549	G
24	YA	563	G
24	YA	568	U
24	YA	571	A
24	YA	573	G
24	YA	575	A
24	YA	603	A
24	YA	607	U
24	YA	614	U
24	YA	615	G
24	YA	617	G
24	YA	621	A
24	YA	622	G
24	YA	627	A
24	YA	634	C
24	YA	637	A
24	YA	638	G
24	YA	645	C
24	YA	646	A
24	YA	651	G
24	YA	654	A
24	YA	654(A)	G
24	YA	654(B)	C
24	YA	670	A
24	YA	686	G
24	YA	717	G
24	YA	722	A
24	YA	730	C

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Mol	Chain	Res	Type
24	YA	753	C
24	YA	764	A
24	YA	765	G
24	YA	775	G
24	YA	776	G
24	YA	782	A
24	YA	784	A
24	YA	785	G
24	YA	790	C
24	YA	791	C
24	YA	800	A
24	YA	805	G
24	YA	812	C
24	YA	819	A
24	YA	827	U
24	YA	828	U
24	YA	831	G
24	YA	847	U
24	YA	856	C
24	YA	857	C
24	YA	860	U
24	YA	866	A
24	YA	881	G
24	YA	882	G
24	YA	884	C
24	YA	885	C
24	YA	886	C
24	YA	888	C
24	YA	889	C
24	YA	896	A
24	YA	897	C
24	YA	900	A
24	YA	907	U
24	YA	910	A
24	YA	915	C
24	YA	917	A
24	YA	918	A
24	YA	932	G
24	YA	941	A
24	YA	945	A
24	YA	946	G
24	YA	953	A

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Mol	Chain	Res	Type
24	YA	957	A
24	YA	959	A
24	YA	961	C
24	YA	973	A
24	YA	974	G
24	YA	974(A)	C
24	YA	975	G
24	YA	980	A
24	YA	983	A
24	YA	989	G
24	YA	996	A
24	YA	1005	C
24	YA	1011	G
24	YA	1012	U
24	YA	1013	C
24	YA	1017	G
24	YA	1021	A
24	YA	1022	G
24	YA	1023	U
24	YA	1025	G
24	YA	1026	U
24	YA	1027	A
24	YA	1033	U
24	YA	1046	A
24	YA	1047	G
24	YA	1050	A
24	YA	1054	A
24	YA	1059	G
24	YA	1060	U
24	YA	1061	U
24	YA	1062	G
24	YA	1067	A
24	YA	1068	G
24	YA	1069	A
24	YA	1070	A
24	YA	1071	G
24	YA	1073	A
24	YA	1076	C
24	YA	1077	A
24	YA	1078	U
24	YA	1082	U
24	YA	1083	U

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Mol	Chain	Res	Type
24	YA	1084	A
24	YA	1085	A
24	YA	1086	A
24	YA	1088	A
24	YA	1089	G
24	YA	1090	U
24	YA	1093	G
24	YA	1096	A
24	YA	1097	U
24	YA	1103	A
24	YA	1104	C
24	YA	1110	G
24	YA	1111	A
24	YA	1122	G
24	YA	1126	A
24	YA	1131	G
24	YA	1135	C
24	YA	1136	G
24	YA	1139	G
24	YA	1142	U
24	YA	1142(A)	A
24	YA	1151	G
24	YA	1173	G
24	YA	1174	A
24	YA	1175	U
24	YA	1176	G
24	YA	1179	C
24	YA	1180	C
24	YA	1204	A
24	YA	1205	U
24	YA	1206	G
24	YA	1211	U
24	YA	1220	A
24	YA	1221	C
24	YA	1236	G
24	YA	1238	G
24	YA	1252	G
24	YA	1253	A
24	YA	1256	G
24	YA	1265	A
24	YA	1271	G
24	YA	1272	A

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Mol	Chain	Res	Type
24	YA	1275	A
24	YA	1300	U
24	YA	1301	A
24	YA	1329	U
24	YA	1341	U
24	YA	1349	A
24	YA	1352	U
24	YA	1365	A
24	YA	1368	G
24	YA	1378	A
24	YA	1379	A
24	YA	1384	A
24	YA	1385	G
24	YA	1391	U
24	YA	1407	C
24	YA	1411	C
24	YA	1416	G
24	YA	1419	A
24	YA	1420	U
24	YA	1421	G
24	YA	1428	C
24	YA	1444(A)	A
24	YA	1445	C
24	YA	1449	A
24	YA	1449(A)	G
24	YA	1455	G
24	YA	1460	A
24	YA	1461	G
24	YA	1467	C
24	YA	1471	A
24	YA	1482	U
24	YA	1483	G
24	YA	1487	G
24	YA	1493	C
24	YA	1496	A
24	YA	1497	U
24	YA	1506	C
24	YA	1507	A
24	YA	1508	A
24	YA	1510	A
24	YA	1511	A
24	YA	1534	G

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Mol	Chain	Res	Type
24	YA	1535	U
24	YA	1536	A
24	YA	1537	C
24	YA	1540	G
24	YA	1543	A
24	YA	1544	C
24	YA	1545	A
24	YA	1558	A
24	YA	1559	G
24	YA	1566	A
24	YA	1569	A
24	YA	1578	U
24	YA	1579	A
24	YA	1581	G
24	YA	1585	C
24	YA	1586	A
24	YA	1587	A
24	YA	1591	G
24	YA	1598	C
24	YA	1608	A
24	YA	1617	C
24	YA	1618	A
24	YA	1640	C
24	YA	1646	C
24	YA	1648	C
24	YA	1654	A
24	YA	1674	G
24	YA	1693	U
24	YA	1695	G
24	YA	1703	G
24	YA	1725	G
24	YA	1728	G
24	YA	1729	A
24	YA	1730	U
24	YA	1731	G
24	YA	1732	A
24	YA	1743	G
24	YA	1750	G
24	YA	1754	C
24	YA	1756	G
24	YA	1762	A
24	YA	1763	G

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Mol	Chain	Res	Type
24	YA	1764	G
24	YA	1769	G
24	YA	1773	A
24	YA	1774	C
24	YA	1780	A
24	YA	1787	A
24	YA	1791	A
24	YA	1799	G
24	YA	1800	C
24	YA	1801	G
24	YA	1811	G
24	YA	1815	A
24	YA	1816	G
24	YA	1828	G
24	YA	1829	A
24	YA	1835	G
24	YA	1847	A
24	YA	1858	G
24	YA	1869	G
24	YA	1870	C
24	YA	1872	A
24	YA	1878	G
24	YA	1882	C
24	YA	1889	A
24	YA	1903	G
24	YA	1906	G
24	YA	1913	A
24	YA	1914	C
24	YA	1919	A
24	YA	1929	G
24	YA	1930	G
24	YA	1931	U
24	YA	1936	A
24	YA	1938	A
24	YA	1939	U
24	YA	1940	U
24	YA	1955	U
24	YA	1956	U
24	YA	1960	A
24	YA	1963	U
24	YA	1965	C
24	YA	1967	C

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Mol	Chain	Res	Type
24	YA	1969	A
24	YA	1970	A
24	YA	1971	A
24	YA	1972	A
24	YA	1982	C
24	YA	1991	U
24	YA	1992	G
24	YA	1993	U
24	YA	2020	A
24	YA	2021	C
24	YA	2023	G
24	YA	2031	A
24	YA	2032	G
24	YA	2033	A
24	YA	2039	C
24	YA	2043	C
24	YA	2051	A
24	YA	2052	G
24	YA	2054	A
24	YA	2055	C
24	YA	2056	G
24	YA	2059	A
24	YA	2060	A
24	YA	2061	G
24	YA	2062	A
24	YA	2069	G
24	YA	2093	G
24	YA	2100	G
24	YA	2111	C
24	YA	2112	G
24	YA	2114	A
24	YA	2115	G
24	YA	2116	G
24	YA	2118	U
24	YA	2119	A
24	YA	2120	G
24	YA	2126	A
24	YA	2127	G
24	YA	2132	U
24	YA	2133	G
24	YA	2136	C
24	YA	2145	C

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Mol	Chain	Res	Type
24	YA	2146	C
24	YA	2147	G
24	YA	2148	G
24	YA	2156	G
24	YA	2158	A
24	YA	2166	G
24	YA	2168	G
24	YA	2169	A
24	YA	2171	A
24	YA	2173	A
24	YA	2180	U
24	YA	2189	U
24	YA	2190	G
24	YA	2192	G
24	YA	2198	A
24	YA	2210	G
24	YA	2211	G
24	YA	2212	A
24	YA	2215	G
24	YA	2225	A
24	YA	2238	G
24	YA	2239	G
24	YA	2243	U
24	YA	2266	A
24	YA	2267	A
24	YA	2275	C
24	YA	2278	A
24	YA	2280	G
24	YA	2283	C
24	YA	2287	A
24	YA	2288	A
24	YA	2307	G
24	YA	2308	G
24	YA	2309	A
24	YA	2311	A
24	YA	2312	U
24	YA	2320	A
24	YA	2325	G
24	YA	2334	G
24	YA	2335	A
24	YA	2336	A
24	YA	2342	C

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Mol	Chain	Res	Type
24	YA	2343	C
24	YA	2345	G
24	YA	2346	A
24	YA	2347	C
24	YA	2350	C
24	YA	2358	G
24	YA	2377	A
24	YA	2383	G
24	YA	2385	C
24	YA	2391	G
24	YA	2402	C
24	YA	2403	C
24	YA	2406	U
24	YA	2410	G
24	YA	2423	U
24	YA	2425	A
24	YA	2426	A
24	YA	2429	G
24	YA	2430	A
24	YA	2435	A
24	YA	2439	A
24	YA	2440	C
24	YA	2441	C
24	YA	2448	A
24	YA	2450	A
24	YA	2469	A
24	YA	2470	G
24	YA	2471	C
24	YA	2475	C
24	YA	2494	G
24	YA	2502	G
24	YA	2504	U
24	YA	2505	G
24	YA	2518	A
24	YA	2525	G
24	YA	2529	G
24	YA	2542	A
24	YA	2554	U
24	YA	2562	U
24	YA	2564	A
24	YA	2567	G
24	YA	2578	G

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Mol	Chain	Res	Type
24	YA	2597	G
24	YA	2602	A
24	YA	2609	U
24	YA	2611	U
24	YA	2612	C
24	YA	2615	U
24	YA	2619	C
24	YA	2629	A
24	YA	2642	G
24	YA	2646	C
24	YA	2655	G
24	YA	2656	U
24	YA	2665	A
24	YA	2666	C
24	YA	2673	G
24	YA	2675	A
24	YA	2682	U
24	YA	2689	U
24	YA	2701	C
24	YA	2702	U
24	YA	2707	G
24	YA	2712	U
24	YA	2712(A)	A
24	YA	2713	A
24	YA	2714	G
24	YA	2724	C
24	YA	2726	U
24	YA	2733	A
24	YA	2739	U
24	YA	2744	G
24	YA	2749	A
24	YA	2752	C
24	YA	2759	G
24	YA	2762	G
24	YA	2764	A
24	YA	2765	A
24	YA	2766	G
24	YA	2777	G
24	YA	2778	A
24	YA	2779	U
24	YA	2789	C
24	YA	2790	A

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Mol	Chain	Res	Type
24	YA	2791	C
24	YA	2797	U
24	YA	2807	G
24	YA	2818	G
24	YA	2820	A
24	YA	2821	A
24	YA	2823	A
24	YA	2830	G
24	YA	2833	G
24	YA	2834	G
24	YA	2835	A
24	YA	2836	U
24	YA	2847	U
24	YA	2867	G
24	YA	2868	A
24	YA	2872	G
24	YA	2891	G
24	YA	2892	A
24	YA	2893	G
24	YA	2894	G
25	YB	8	U
25	YB	9	G
25	YB	13	A
25	YB	15	A
25	YB	16	G
25	YB	19	G
25	YB	21	G
25	YB	25	A
25	YB	32	C
25	YB	41	U
25	YB	42	C
25	YB	44	G
25	YB	45	A
25	YB	52	A
25	YB	53	A
25	YB	56	G
25	YB	67	G
25	YB	73	A
25	YB	89	G
25	YB	105	G
25	YB	108	C
25	YB	109	G

All (153) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	QA	5	U
1	QA	31	G
1	QA	64	G
1	QA	115	G
1	QA	119	A
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
1	QA	687	A
1	QA	703	G
1	QA	753	A
1	QA	792	A
1	QA	812	C
1	QA	913	A
1	QA	960	U
1	QA	992	U
1	QA	1065	U
1	QA	1200	C
1	QA	1201	A
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
22	QV	35	C
22	QV	53	G
23	QX	14	A
24	RA	74	A
24	RA	99	U
24	RA	221	A
24	RA	222	A

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Mol	Chain	Res	Type
24	RA	229	A
24	RA	271(B)	G
24	RA	345	A
24	RA	372	G
24	RA	404	C
24	RA	503	A
24	RA	512	G
24	RA	587	C
24	RA	637	A
24	RA	752	A
24	RA	846	C
24	RA	856	C
24	RA	1022	G
24	RA	1026	U
24	RA	1045	A
24	RA	1078	U
24	RA	1085	A
24	RA	1178	C
24	RA	1210	A
24	RA	1312	U
24	RA	1427	A
24	RA	1558	A
24	RA	1653	G
24	RA	1819	A
24	RA	1980	G
24	RA	1992	G
24	RA	2060	A
24	RA	2126	A
24	RA	2439	A
24	RA	2566	A
24	RA	2610	C
24	RA	2689	U
24	RA	2832	U
24	RA	2867	G
25	RB	66	A
25	RB	108	C
1	XA	31	G
1	XA	60	A
1	XA	64	G
1	XA	78	G
1	XA	115	G
1	XA	243	A

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Mol	Chain	Res	Type
1	XA	244	U
1	XA	250	A
1	XA	266	G
1	XA	328	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
1	XA	753	A
1	XA	812	C
1	XA	913	A
1	XA	992	U
1	XA	1027	C
1	XA	1200	C
1	XA	1285	A
1	XA	1297	C
1	XA	1310	G
1	XA	1336	C
1	XA	1446	A
1	XA	1498	U
1	XA	1503	A
22	XV	35	C
22	XV	53	G
24	YA	99	U
24	YA	221	A
24	YA	229	A
24	YA	242	G
24	YA	271(B)	G
24	YA	278	A
24	YA	372	G
24	YA	404	C
24	YA	503	A
24	YA	637	A
24	YA	752	A
24	YA	846	C
24	YA	856	C
24	YA	859	G
24	YA	974(A)	C

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Mol	Chain	Res	Type
24	YA	1022	G
24	YA	1026	U
24	YA	1085	A
24	YA	1109	C
24	YA	1130	U
24	YA	1178	C
24	YA	1210	A
24	YA	1379	A
24	YA	1427	A
24	YA	1460	A
24	YA	1558	A
24	YA	1653	G
24	YA	1694	C
24	YA	1799	G
24	YA	1913	A
24	YA	1930	G
24	YA	1955	U
24	YA	1992	G
24	YA	2566	A
24	YA	2610	C
24	YA	2681	C
24	YA	2712	U
24	YA	2776	A
24	YA	2832	U
24	YA	2867	G
25	YB	66	A
25	YB	108	C

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1358 ligands modelled in this entry, 1356 are monoatomic - leaving 2 for Mogul analysis.

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

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

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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