Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 11:28 PM EDT

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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

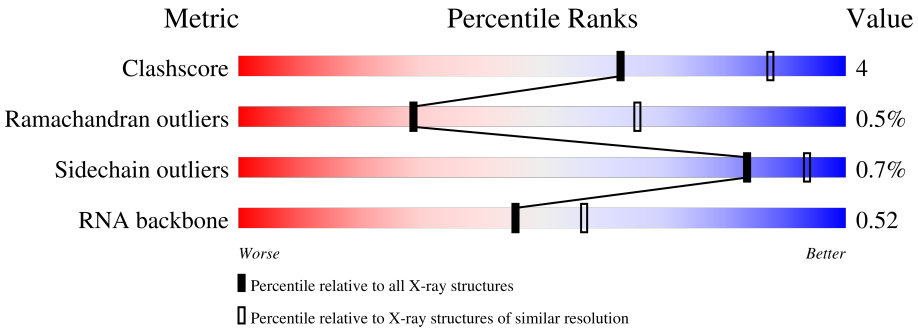
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.18 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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	QA	1508	64% 29% 6% ••
1	XA	1508	66% 27% 6% ••
2	QB	256	77% 14% 8%
2	XB	256	79% 12% 8%
3	QC	239	72% 13% 14%
3	XC	239	72% 13% 14%

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Mol	Chain	Length	Quality of chain
4	QD	209	87% 12%
4	XD	209	85% 14%
5	QE	162	81% 12% 7%
5	XE	162	84% 9% 7%
6	QF	101	85% 15%
6	XF	101	88% 12%
7	QG	156	88% 10% ••
7	XG	156	89% 10% ••
8	QH	138	82% 17% •
8	XH	138	83% 16% •
9	QI	128	75% 23% ••
9	XI	128	80% 17% ••
10	QJ	105	70% 25% 6%
10	XJ	105	69% 23% 9%
11	QK	129	72% 20% 8%
11	XK	129	75% 15% 10%
12	QL	132	81% 14% 5%
12	XL	132	73% 20% 8%
13	QM	126	81% 13% • 5%
13	XM	126	75% 20% 6%
14	QN	61	75% 20% ••
14	XN	61	75% 18% 5% •
15	QO	89	92% 7% •
15	XO	89	90% 8% •
16	QP	88	83% 13% 5%

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Mol	Chain	Length	Quality of chain
16	XP	88	86% 9% 5%
17	QQ	105	89% 7% 5%
17	XQ	105	83% 12% 5%
18	QR	88	70% 9% 20%
18	XR	88	69% 10% 20%
19	QS	93	67% 23% 11%
19	XS	93	78% 12% 10%
20	QT	106	89% 5% 7%
20	XT	106	89% 5% 7%
21	QU	27	74% 19% 7%
21	XU	27	78% 15% 7%
22	QV	77	77% 18% 5%
22	XV	77	74% 19% 5%
23	QX	25	16% 28% 52%
23	XX	25	20% 16% 8% 56%
24	RA	2915	67% 26% 6%
24	YA	2915	66% 25% 6%
25	RB	122	64% 28% 7%
25	YB	122	66% 27% 6%
26	RD	276	76% 21%
26	YD	276	78% 20%
27	RE	206	80% 18%
27	YE	206	78% 20%
28	RF	210	82% 14%
28	YF	210	86% 10%

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Mol	Chain	Length	Quality of chain
29	RG	182	84% 14%
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%

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Mol	Chain	Length	Quality of chain
41	YW	113	89% 11%
42	RX	96	80% 16%
42	YX	96	77% 19%
43	RY	110	77% 20%
43	YY	110	79% 18%
44	RZ	206	69% 18% 11%
44	YZ	206	69% 18% 11%
45	R0	85	75% 20% 5%
45	Y0	85	68% 20% 12%
46	R1	98	74% 24%
46	Y1	98	77% 18% 5%
47	R2	72	78% 18%
47	Y2	72	75% 21%
48	R3	60	82% 17%
48	Y3	60	82% 17%
49	R4	71	80% 14%
49	Y4	71	79% 15%
50	R5	60	83% 15%
50	Y5	60	80% 18%
51	R6	54	87% 11%
51	Y6	54	91% 7%
52	R7	49	88% 8%
52	Y7	49	86% 12%
53	R8	65	72% 20% 6%
53	Y8	65	75% 17% 6%

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Mol	Chain	Length	Quality of chain
54	R9	37	
54	Y9	37	

2 Entry composition (i)

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 960	C 599	N 202	O 159	0	0	0

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

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

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

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

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

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

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

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

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

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

- 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	0	0	0
			469	298	90	81			
48	Y3	59	Total	C	N	O	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 418	C 257	N 104	O 55	S 2	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	QA	80	Total 80	Mg 80	0	0
55	QC	1	Total 1	Mg 1	0	0
55	QF	1	Total 1	Mg 1	0	0
55	QH	1	Total 1	Mg 1	0	0
55	QT	1	Total 1	Mg 1	0	0
55	QV	6	Total 6	Mg 6	0	0
55	RA	521	Total 521	Mg 521	0	0
55	RB	11	Total 11	Mg 11	0	0
55	RD	1	Total 1	Mg 1	0	0
55	RE	4	Total 4	Mg 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	RN	1	Total Mg 1 1	0	0
55	RO	1	Total Mg 1 1	0	0
55	RP	3	Total Mg 3 3	0	0
55	RQ	3	Total Mg 3 3	0	0
55	RR	2	Total Mg 2 2	0	0
55	RT	1	Total Mg 1 1	0	0
55	R0	2	Total Mg 2 2	0	0
55	R8	1	Total Mg 1 1	0	0
55	XA	98	Total Mg 98 98	0	0
55	XE	1	Total Mg 1 1	0	0
55	XL	2	Total Mg 2 2	0	0
55	XM	2	Total Mg 2 2	0	0
55	XQ	1	Total Mg 1 1	0	0
55	XS	1	Total Mg 1 1	0	0
55	XV	8	Total Mg 8 8	0	0
55	XX	1	Total Mg 1 1	0	0
55	YA	551	Total Mg 551 551	0	0
55	YB	12	Total Mg 12 12	0	0
55	YD	3	Total Mg 3 3	0	0
55	YE	4	Total Mg 4 4	0	0
55	YF	1	Total Mg 1 1	0	0

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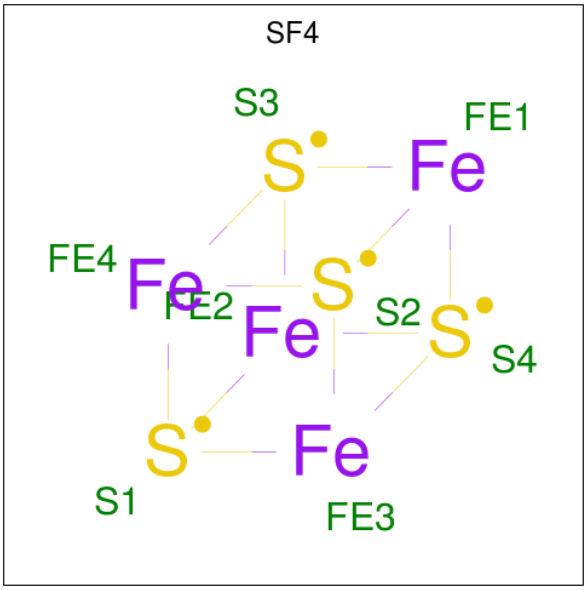
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	YO	1	Total Mg 1 1	0	0
55	YP	2	Total Mg 2 2	0	0
55	YQ	4	Total Mg 4 4	0	0
55	YU	1	Total Mg 1 1	0	0
55	YX	2	Total Mg 2 2	0	0
55	YY	1	Total Mg 1 1	0	0
55	Y0	2	Total Mg 2 2	0	0
55	Y1	1	Total Mg 1 1	0	0
55	Y5	1	Total Mg 1 1	0	0
55	Y7	1	Total Mg 1 1	0	0
55	Y8	2	Total Mg 2 2	0	0

- Molecule 56 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

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

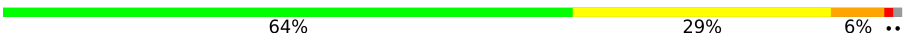
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	QN	1	Total Zn 1 1	0	0
57	RY	1	Total Zn 1 1	0	0
57	R4	1	Total Zn 1 1	0	0
57	R5	1	Total Zn 1 1	0	0
57	R6	1	Total Zn 1 1	0	0
57	R9	1	Total Zn 1 1	0	0
57	XN	1	Total Zn 1 1	0	0
57	YY	1	Total Zn 1 1	0	0
57	Y4	1	Total Zn 1 1	0	0
57	Y5	1	Total Zn 1 1	0	0
57	Y6	1	Total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

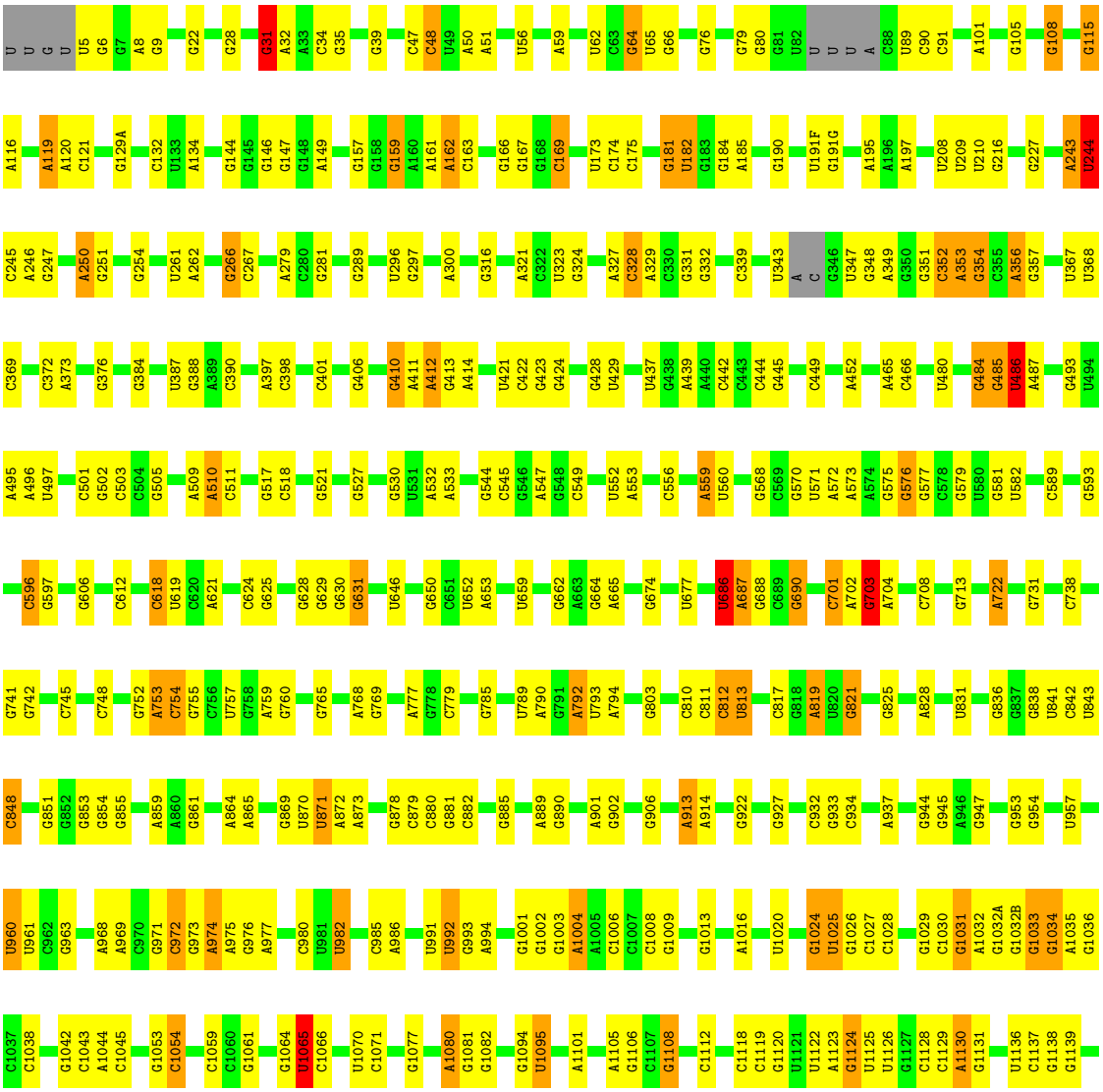
3 Residue-property plots (i)

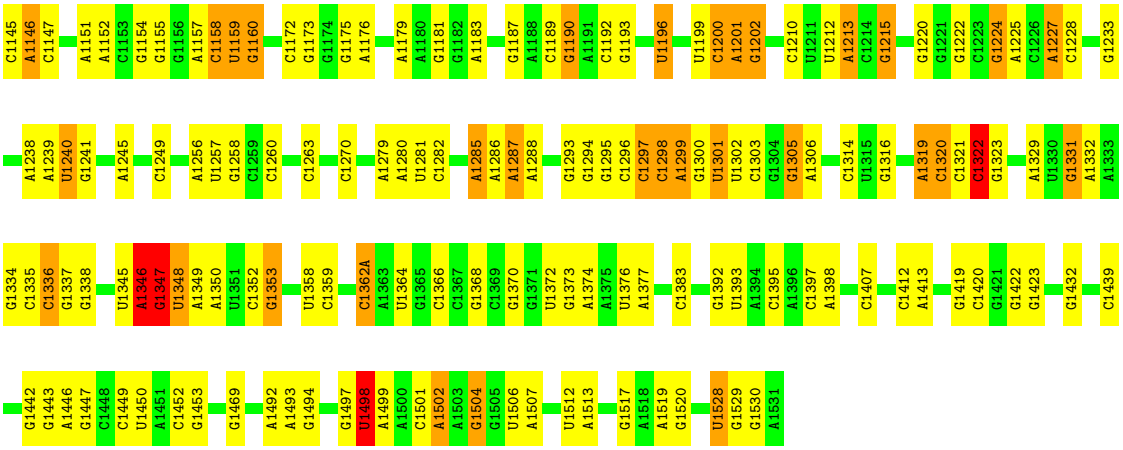
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS failed to run properly.

- Molecule 1: 16S rRNA

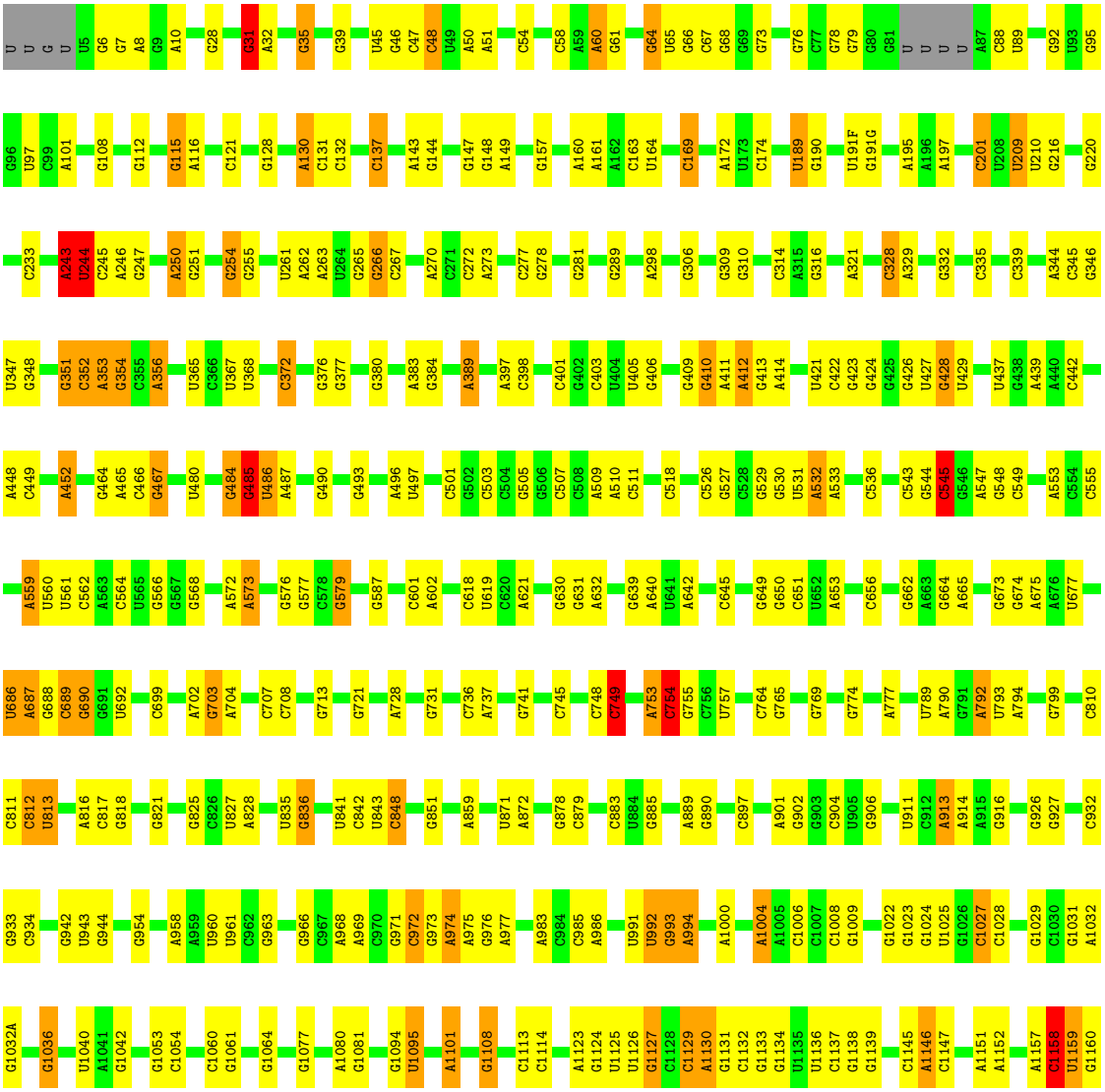
Chain QA: 

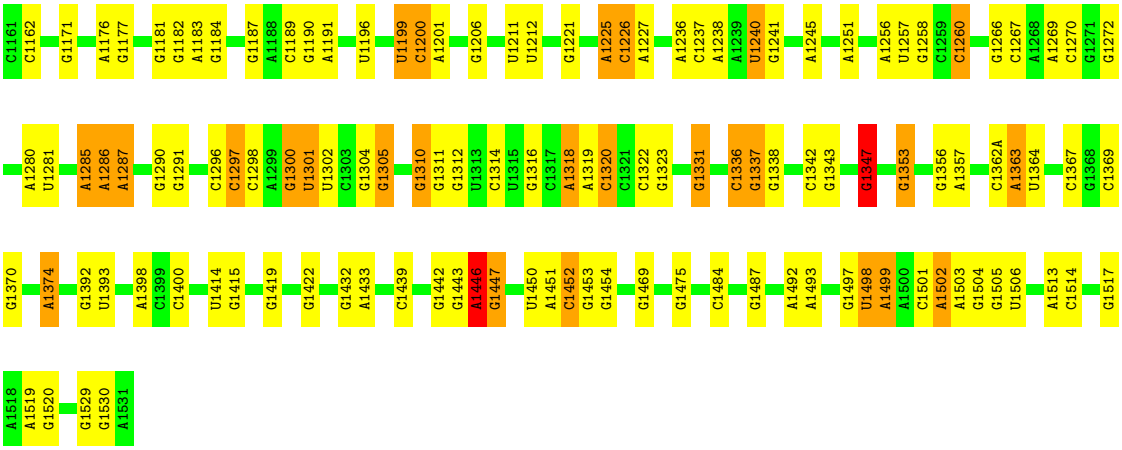




• Molecule 1: 16S rRNA

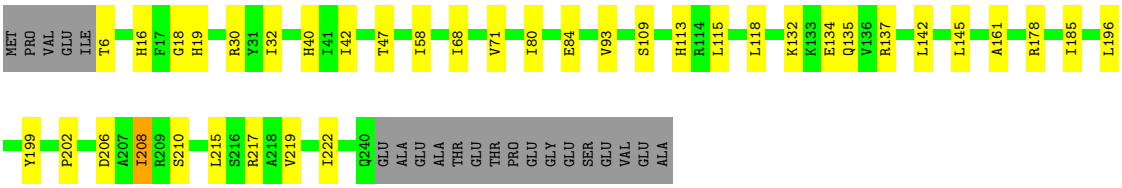
Chain XA:





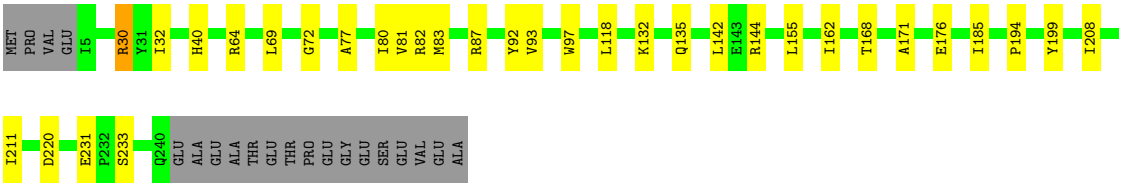
• Molecule 2: 30S ribosomal protein S2

Chain QB:



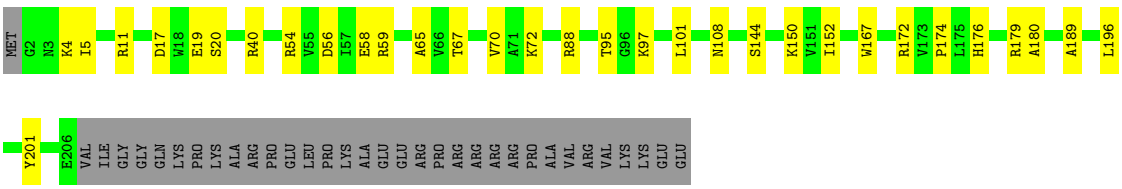
• Molecule 2: 30S ribosomal protein S2

Chain XB:



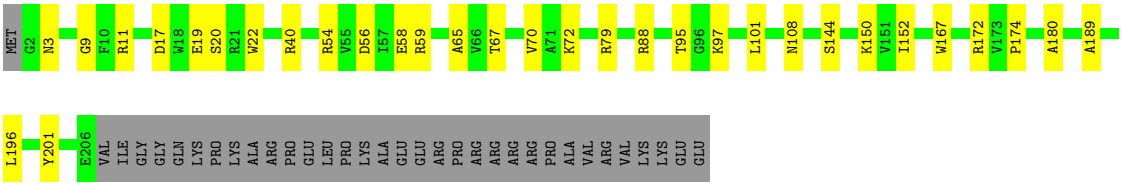
• Molecule 3: 30S ribosomal protein S3

Chain QC:



• Molecule 3: 30S ribosomal protein S3

Chain XC:

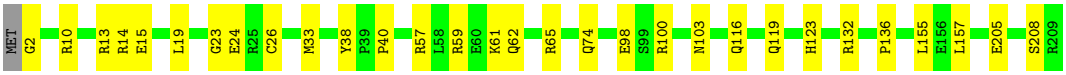


• Molecule 4: 30S ribosomal protein S4

Chain QD:

• Molecule 4: 30S ribosomal protein S4

Chain XD:



• Molecule 5: 30S ribosomal protein S5

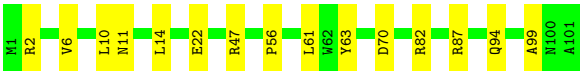
Chain QE:

• Molecule 5: 30S ribosomal protein S5

Chain XE:

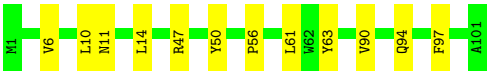
• Molecule 6: 30S ribosomal protein S6

Chain QF:



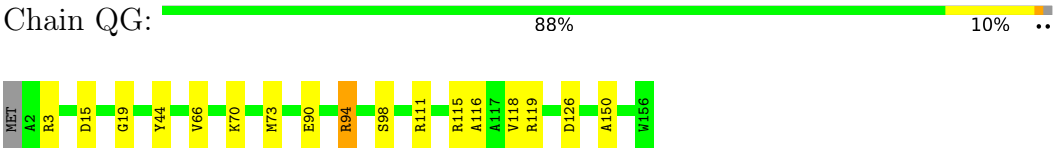
• Molecule 6: 30S ribosomal protein S6

Chain XF:



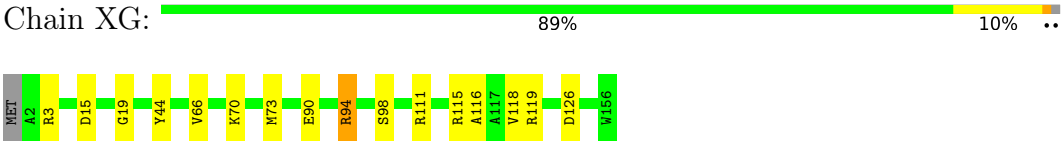
• Molecule 7: 30S ribosomal protein S7

Chain QG:



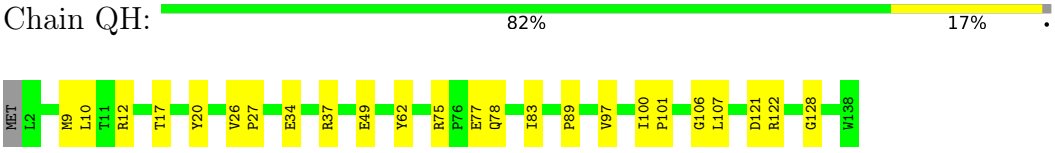
• Molecule 7: 30S ribosomal protein S7

Chain XG:



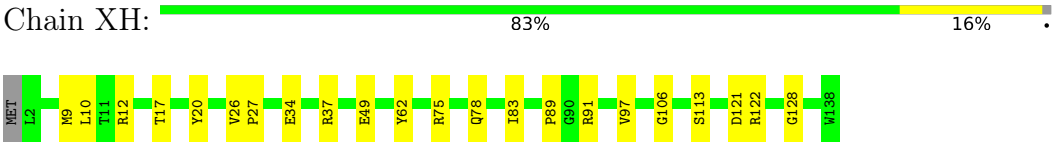
• Molecule 8: 30S ribosomal protein S8

Chain QH:



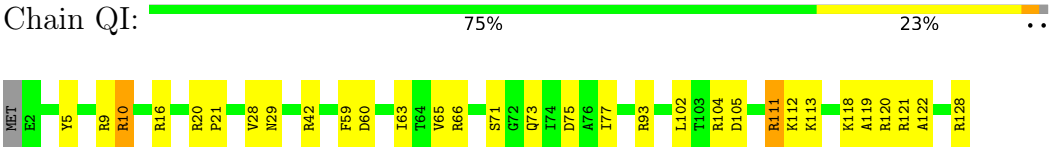
• Molecule 8: 30S ribosomal protein S8

Chain XH:



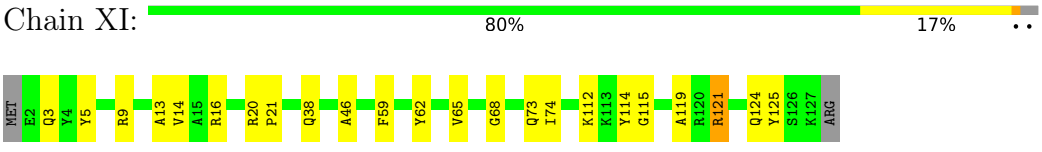
• Molecule 9: 30S ribosomal protein S9

Chain QI:



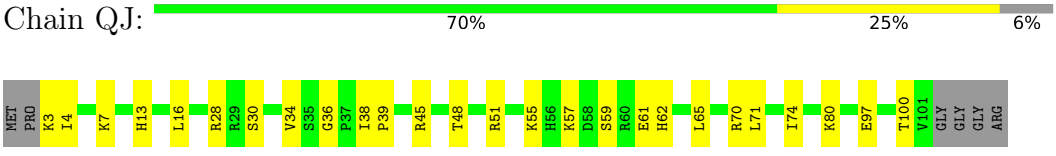
• Molecule 9: 30S ribosomal protein S9

Chain XI:



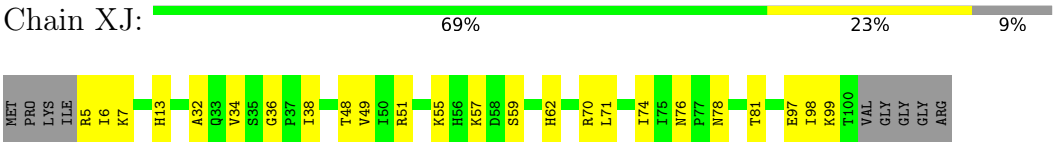
• Molecule 10: 30S ribosomal protein S10

Chain QJ:



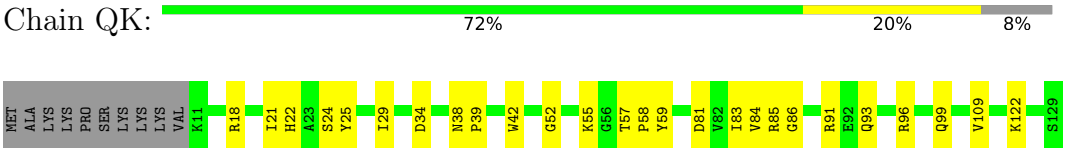
• Molecule 10: 30S ribosomal protein S10

Chain XJ:



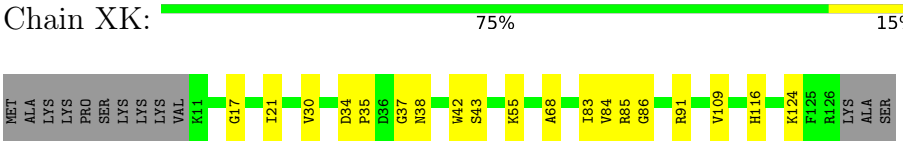
• Molecule 11: 30S ribosomal protein S11

Chain QK:



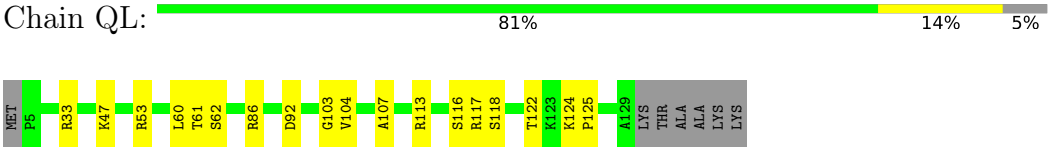
• Molecule 11: 30S ribosomal protein S11

Chain XK:



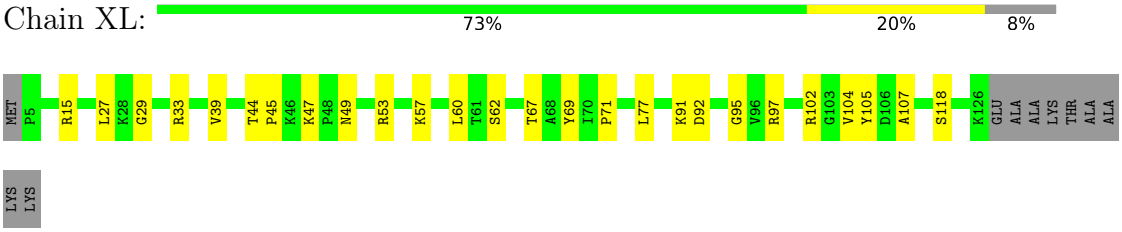
• Molecule 12: 30S ribosomal protein S12

Chain QL:



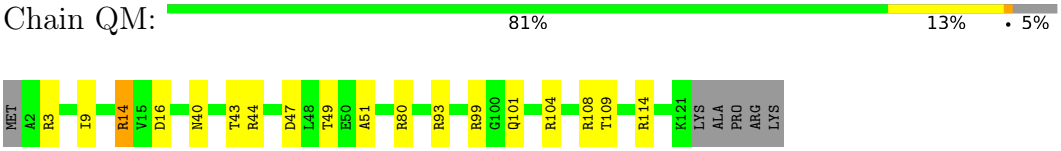
• Molecule 12: 30S ribosomal protein S12

Chain XL:



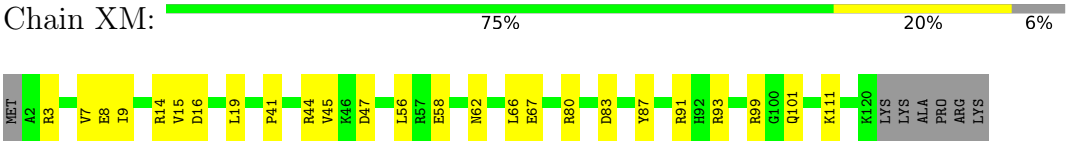
• Molecule 13: 30S ribosomal protein S13

Chain QM:



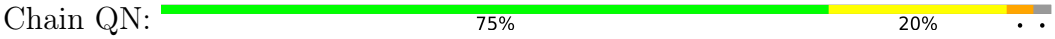
• Molecule 13: 30S ribosomal protein S13

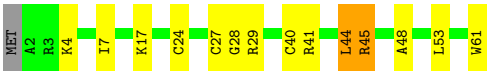
Chain XM:



• Molecule 14: 30S ribosomal protein S14 type Z

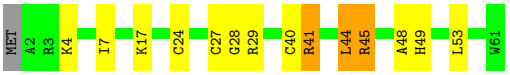
Chain QN:





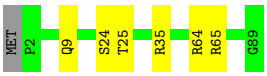
• Molecule 14: 30S ribosomal protein S14 type Z

Chain XN:



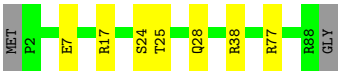
• Molecule 15: 30S ribosomal protein S15

Chain QO:



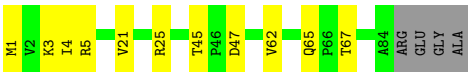
• Molecule 15: 30S ribosomal protein S15

Chain XO:



• Molecule 16: 30S ribosomal protein S16

Chain QP:



• Molecule 16: 30S ribosomal protein S16

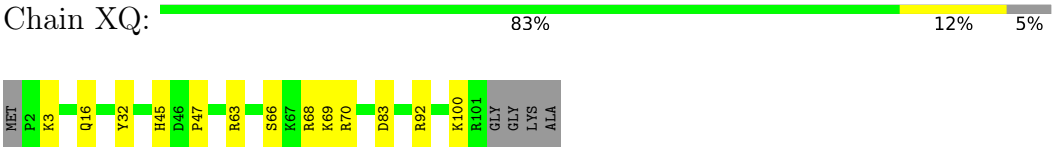
Chain XP:

• Molecule 17: 30S ribosomal protein S17

Chain QQ:

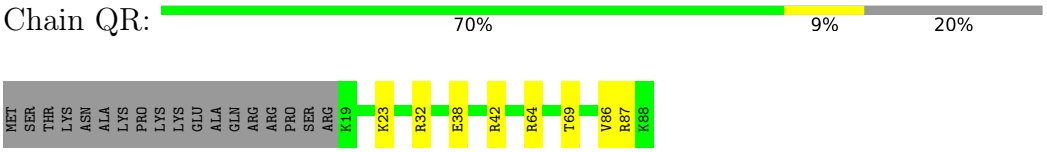
• Molecule 17: 30S ribosomal protein S17

Chain XQ:



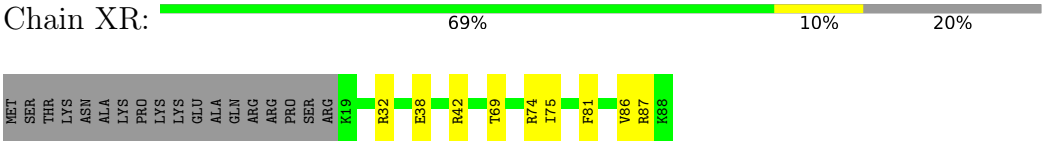
• Molecule 18: 30S ribosomal protein S18

Chain QR:



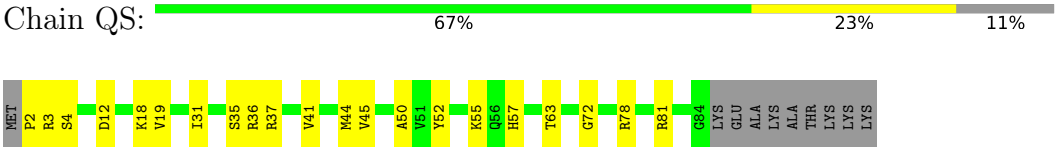
• Molecule 18: 30S ribosomal protein S18

Chain XR:



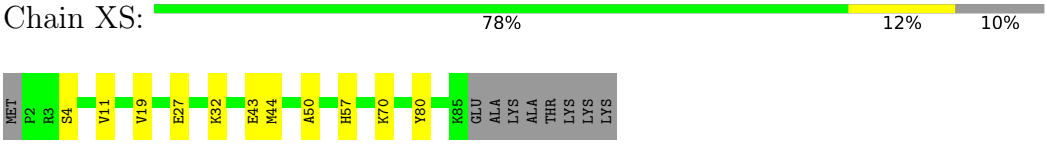
• Molecule 19: 30S ribosomal protein S19

Chain QS:



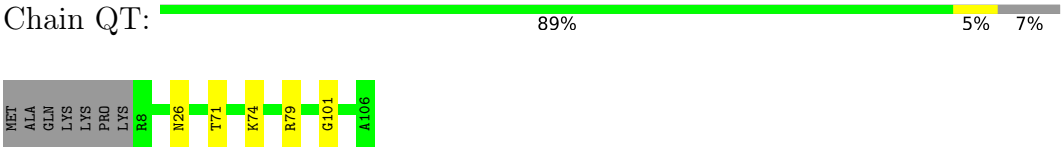
• Molecule 19: 30S ribosomal protein S19

Chain XS:



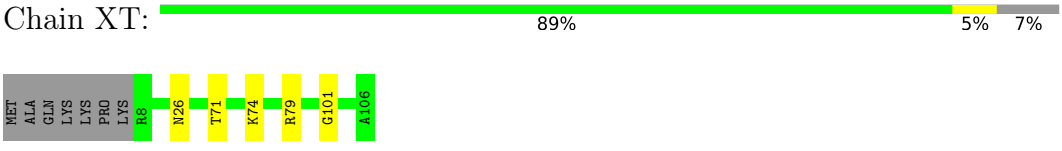
• Molecule 20: 30S ribosomal protein S20

Chain QT:



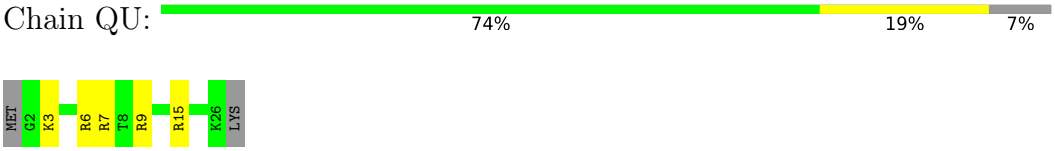
• Molecule 20: 30S ribosomal protein S20

Chain XT:



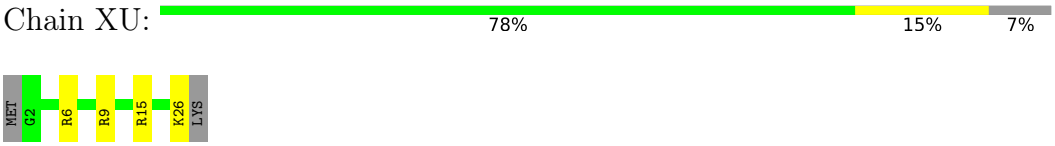
• Molecule 21: 30S ribosomal protein Thx

Chain QU:



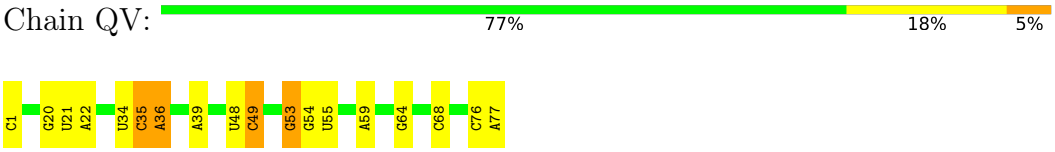
• Molecule 21: 30S ribosomal protein Thx

Chain XU:



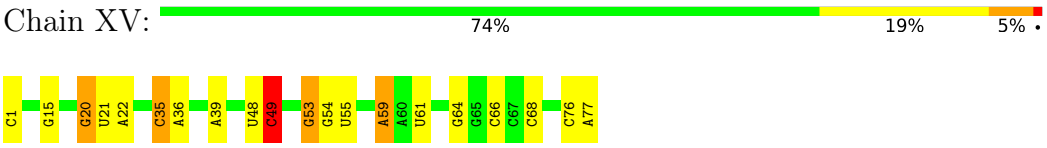
• Molecule 22: tRNA fMet

Chain QV:



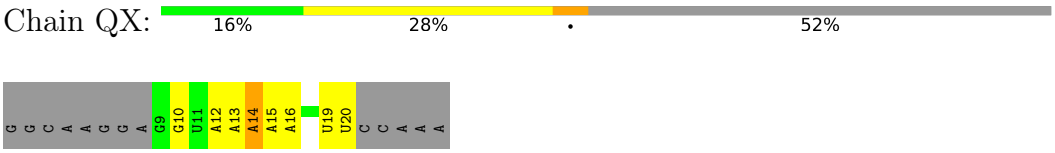
• Molecule 22: tRNA fMet

Chain XV:



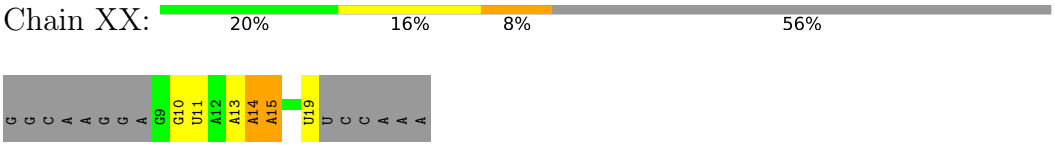
• Molecule 23: messenger RNA

Chain QX:



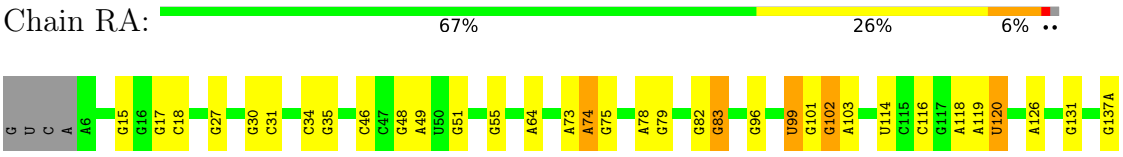
• Molecule 23: messenger RNA

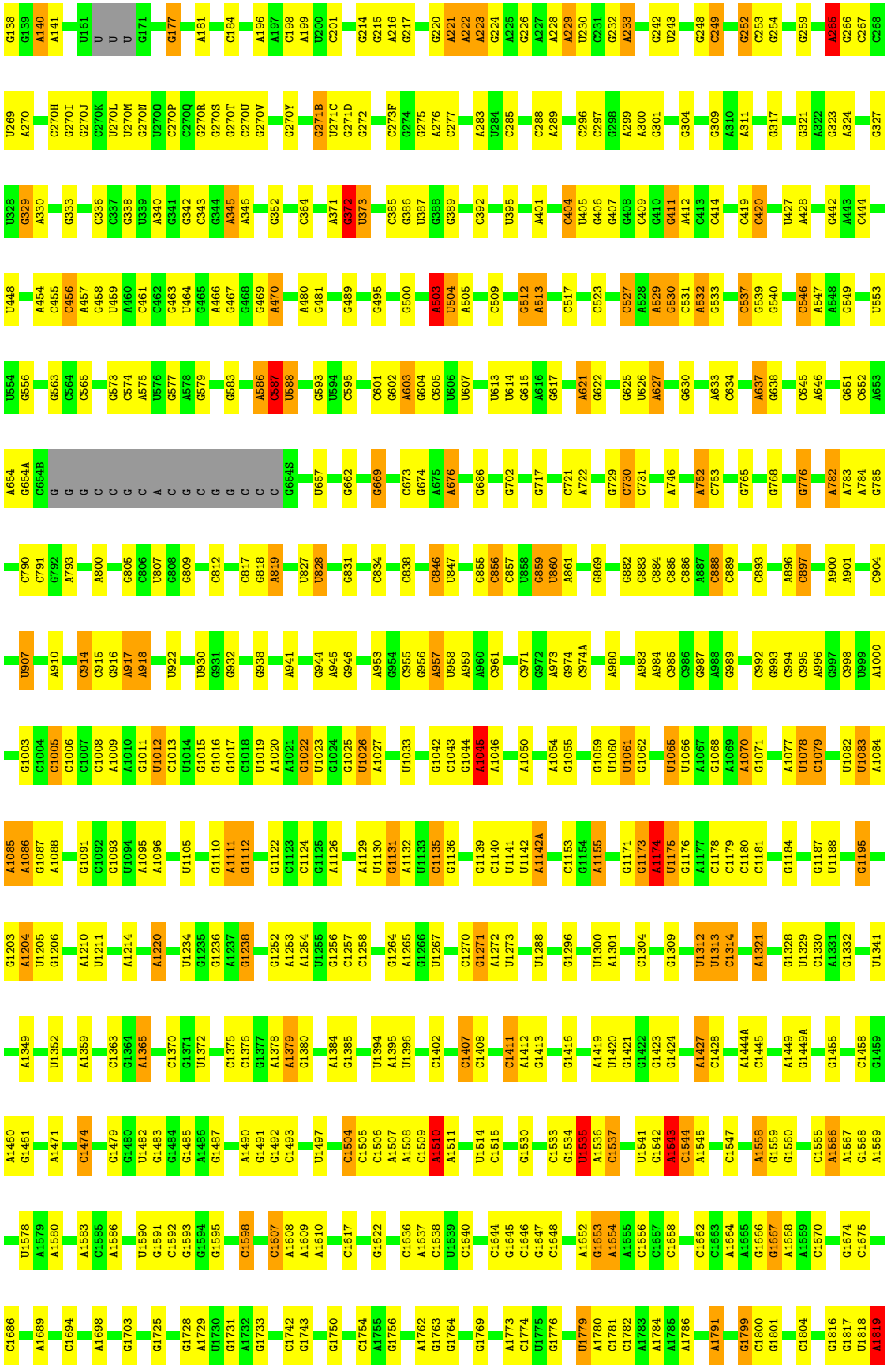
Chain XX:

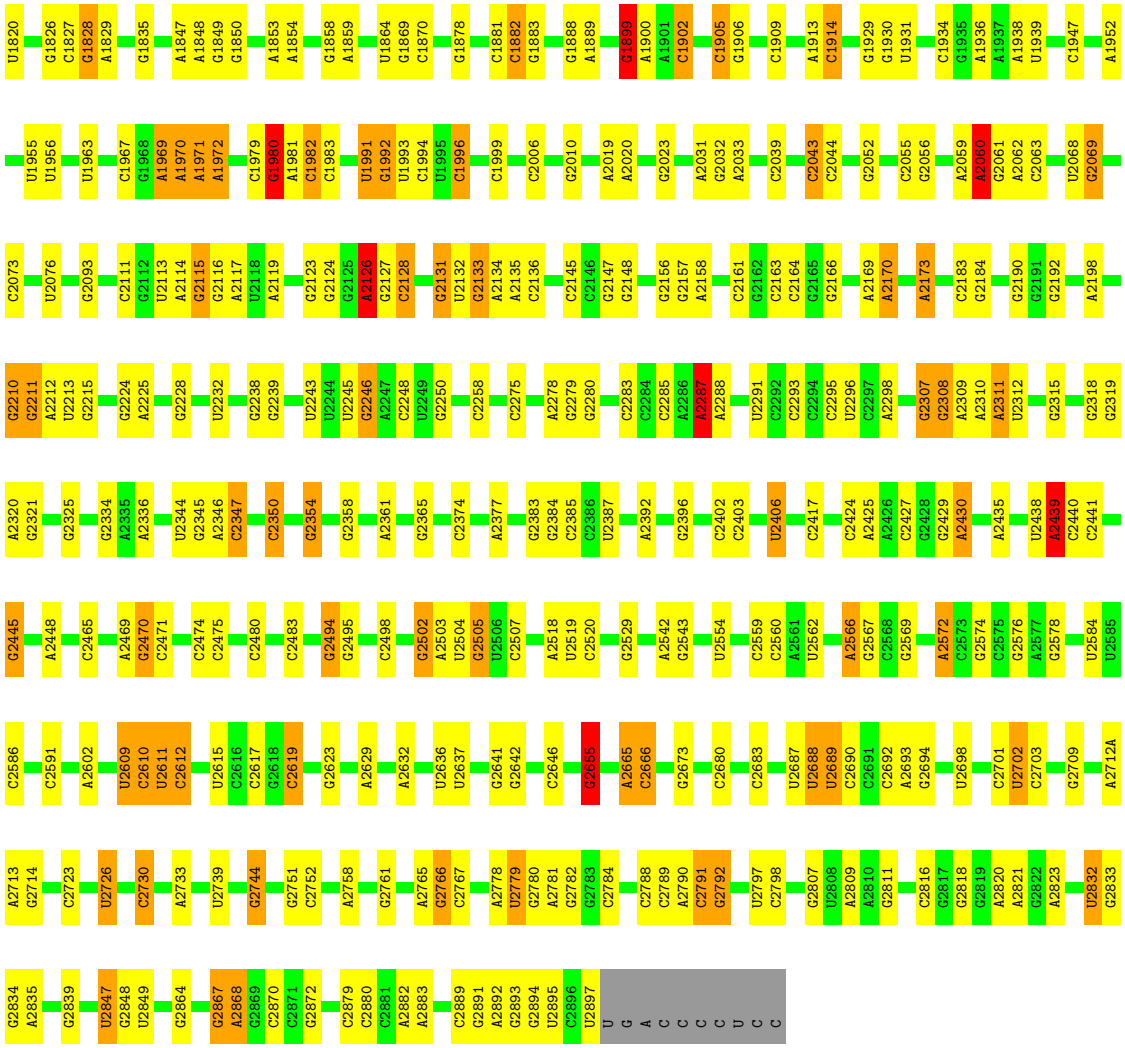


• Molecule 24: 23S rRNA

Chain RA:

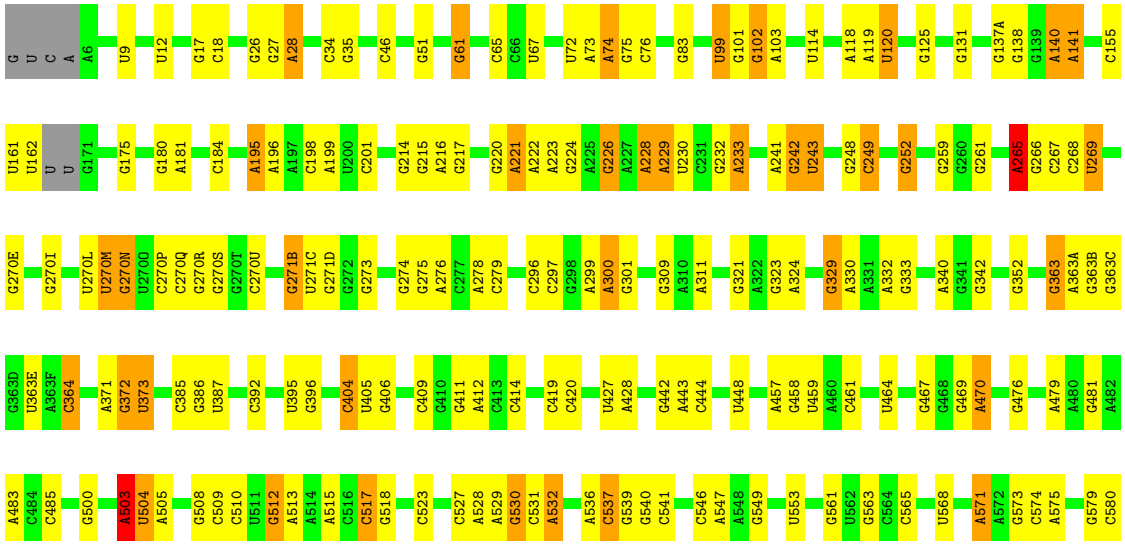


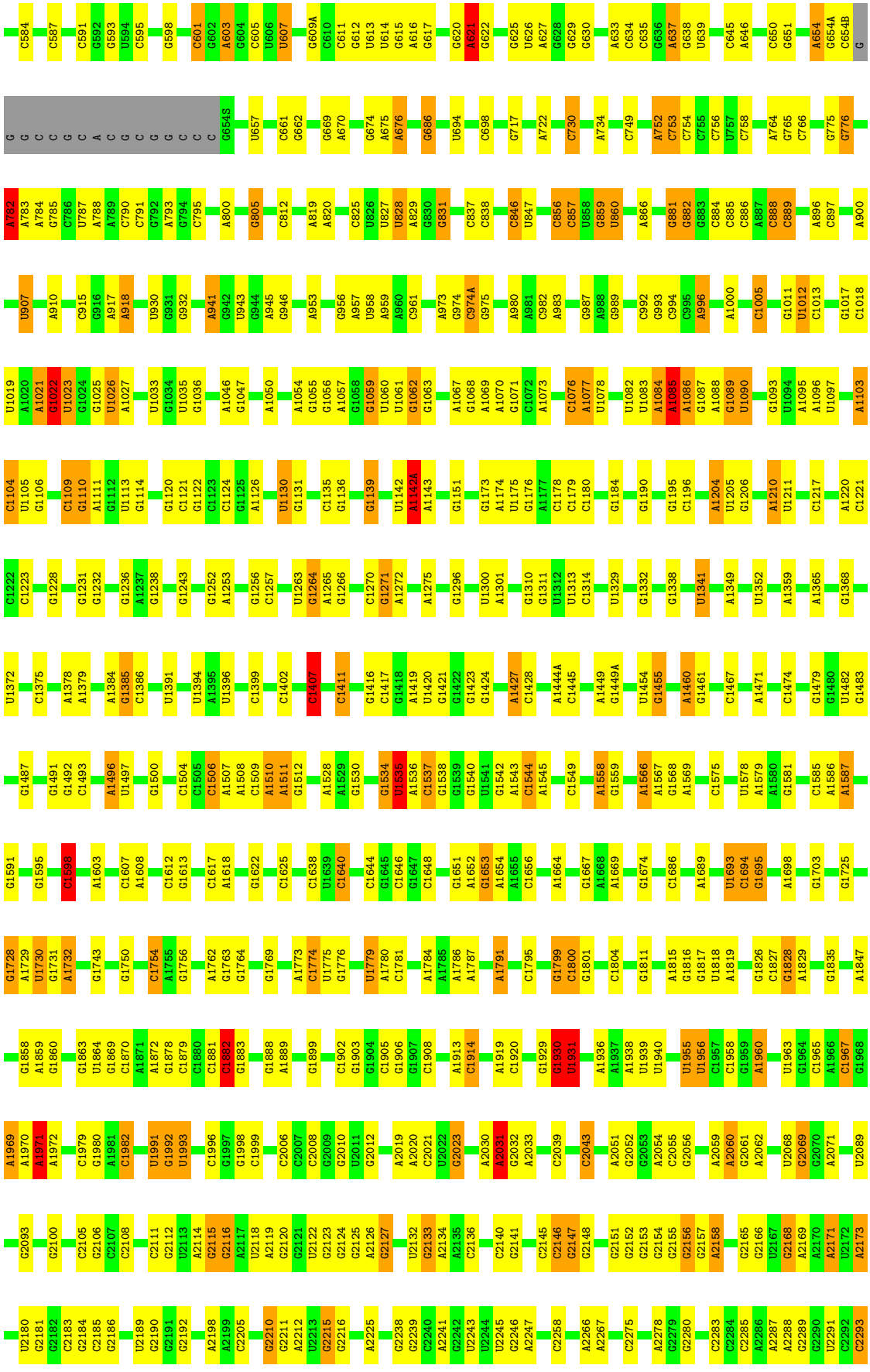




• Molecule 24: 23S rRNA

Chain YA:

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G C C C G C A C G C G C C G654S U657 C661 G662 G669 A670 G674 A675 A676 G686 U694 C698 G717 A722 C730 A734 C749 A752 C753 C754 C755 C756 U757 C758 A764 G765 C766 G775 G776
A782 A783 A784 G785 C786 U787 A788 A789 C790 C791 G792 A793 G794 C795 A800 G805 C812 A819 A820 C825 U826 U827 U828 A829 G830 G831 C837 C838 C846 U847 C856 C857 U858 G859 U860 A866 A881 G882 G883 C884 C885 C886 A887 C888 C889 A896 C897 A900
U907 A910 C915 G916 A917 A918 U930 G931 G932 A941 G942 U943 G944 A945 G946 A953 A956 A957 U958 A959 A960 C961 A973 G974 C974A G975 A980 A981 C982 A983 G987 A988 G989 C992 G993 C994 C995 A996 A1000 C1005 G1011 U1012 C1013 G1017 C1018
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C1104 U1105 G1106 C1109 G1110 A1111 G1112 U1113 G1114 G1120 C1121 G1122 C1123 C1124 G1125 A1126 U1130 G1131 C1135 G1136 G1139 U1142 A1142A A1143 G1151 G1173 A1174 U1175 G1176 A1177 C1178 C1179 C1180 G1184 G1190 G1195 C1196 A1204 U1205 G1206 A1210 U1211 C1217 A1220 C1221
C1222 C1223 G1228 G1231 G1232 G1236 A1237 G1238 G1243 G1252 A1253 G1256 C1257 U1263 G1264 A1265 G1266 C1270 G1271 A1272 A1275 G1296 U1300 A1301 G1310 G1311 U1312 U1313 C1314 U1329 G1332 G1338 U1341 A1349 U1352 A1359 A1365 G1368
U1372 C1375 A1378 A1379 A1384 G1385 C1386 U1391 U1394 A1395 U1396 C1399 C1402 C1407 C1411 G1416 C1417 G1418 A1419 U1420 G1421 G1422 G1423 G1424 A1427 C1428 A1444A C1445 A1449 G1449A U1454 G1455 A1460 G1461 C1467 A1471 C1474 G1479 G1480 U1482 G1483
G1487 G1491 G1492 C1493 A1496 U1497 G1500 C1504 C1505 C1506 A1507 A1508 C1509 A1510 A1511 G1512 A1528 A1529 G1530 G1534 U1535 A1536 C1537 G1538 G1539 G1540 U1541 G1542 A1543 C1544 A1545 C1549 A1558 G1559 A1566 A1567 G1568 A1569 C1575 U1578 A1579 A1580 G1581 C1585 A1586 A1587
G1591 G1595 C1598 A1603 C1607 A1608 C1612 G1613 C1617 A1618 G1622 C1625 C1638 U1639 C1640 C1644 G1645 C1646 G1647 C1648 G1651 A1652 G1653 A1654 A1655 C1656 A1664 G1667 A1668 A1669 G1674 C1686 A1689 U1693 C1694 G1695 A1698 G1703 G1725
G1728 A1729 U1730 G1731 A1732 G1743 G1750 C1754 A1755 G1756 A1762 G1763 G1764 G1769 A1773 C1774 U1775 G1776 U1779 A1780 C1781 A1784 A1785 A1786 A1787 A1791 C1795 G1799 C1800 G1801 C1804 G1811 A1815 G1816 G1817 U1818 A1819 G1826 C1827 G1828 A1829 G1835 A1847
G1858 A1859 G1860 G1863 U1864 G1869 C1870 A1871 A1872 G1878 C1879 C1880 C1881 C1882 G1883 G1888 A1889 G1899 C1902 G1903 G1904 C1905 G1906 G1907 C1908 A1913 C1914 A1919 C1920 G1929 G1930 U1931 A1936 A1937 A1938 U1939 U1940 U1955 U1956 C1957 C1958 G1959 A1960 U1963 G1964 C1965 A1966 C1967 G1968
A1969 A1970 A1971 A1972 C1979 G1980 A1981 C1982 U1991 G1992 U1993 C1996 G1997 G1998 C1999 C2006 C2007 C2008 G2009 G2010 U2011 G2012 A2019 A2020 C2021 U2022 G2023 A2030 A2031 G2032 A2033 C2039 C2043 A2051 G2052 G2053 A2054 C2055 G2056 A2059 A2060 G2061 A2062 U2068 G2069 G2070 A2071 U2089
G2093 G2100 C2105 G2106 C2107 C2108 C2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 U2132 G2133 A2134 A2135 C2136 C2140 G2141 C2145 C2146 G2147 G2148 G2151 G2152 G2153 G2154 G2155 G2156 G2157 A2158 G2165 G2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173
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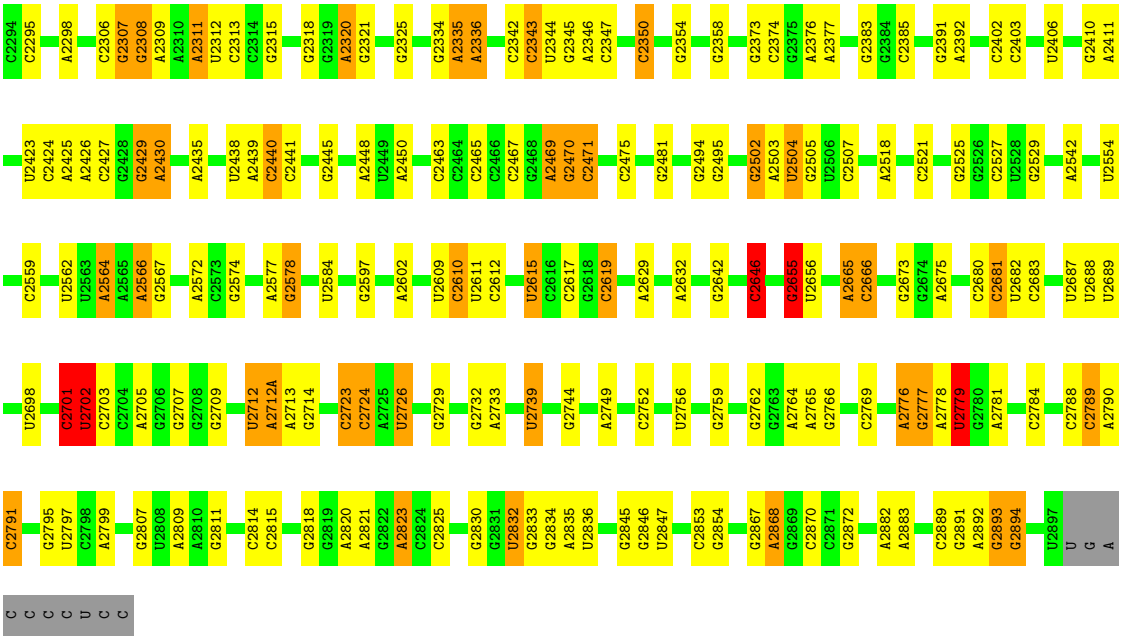
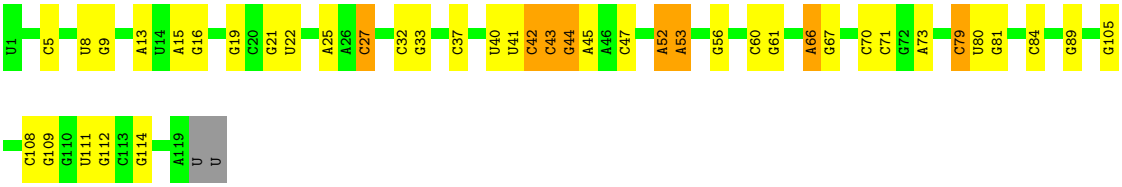


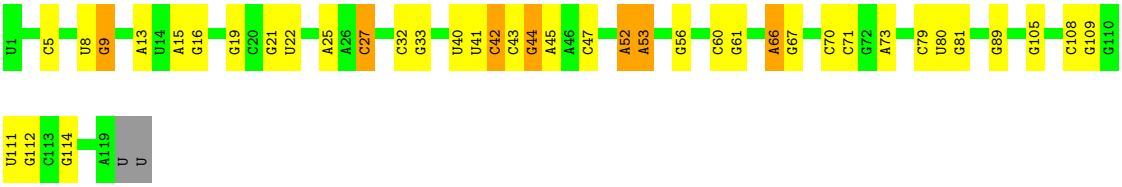
• Molecule 25: 5S rRNA

Chain RB:



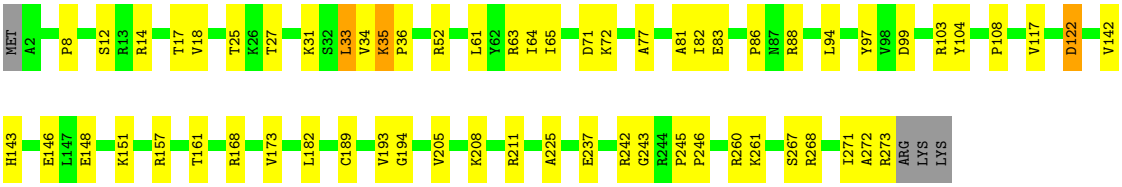
• Molecule 25: 5S rRNA

Chain YB:



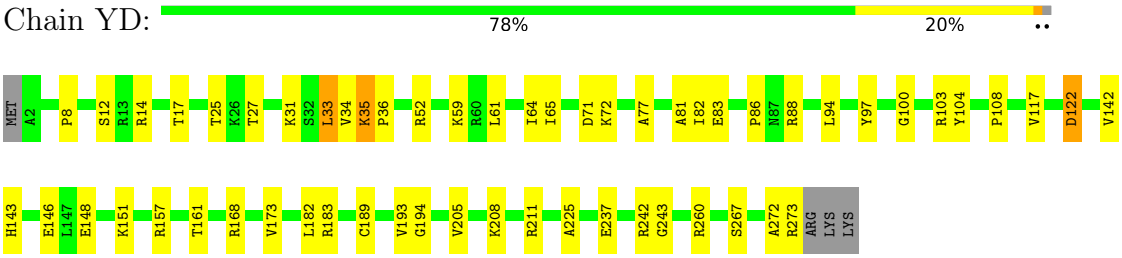
• Molecule 26: 50S ribosomal protein L2

Chain RD:



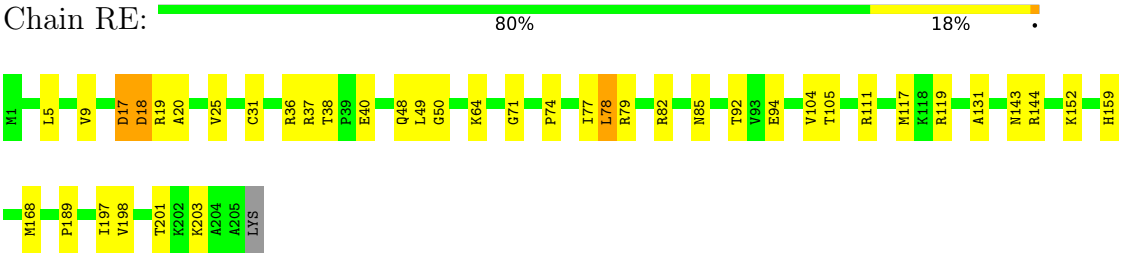
• Molecule 26: 50S ribosomal protein L2

Chain YD:



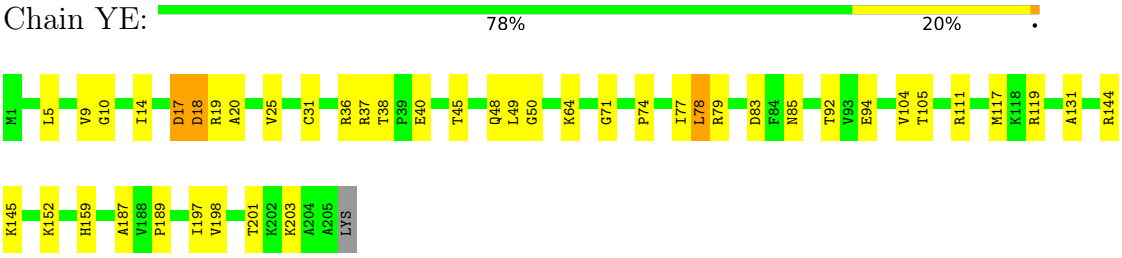
• Molecule 27: 50S ribosomal protein L3

Chain RE:



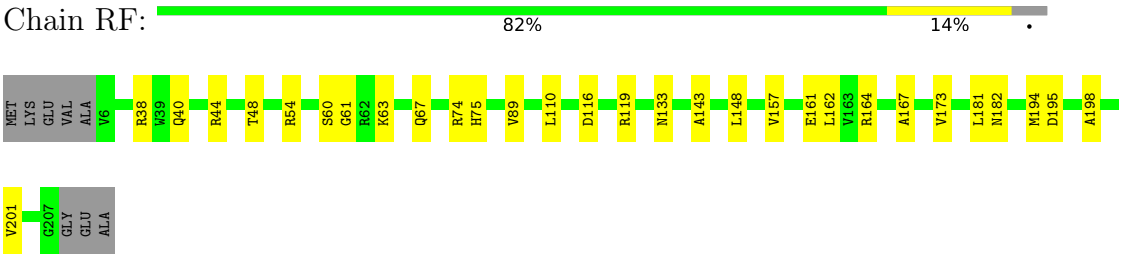
• Molecule 27: 50S ribosomal protein L3

Chain YE:



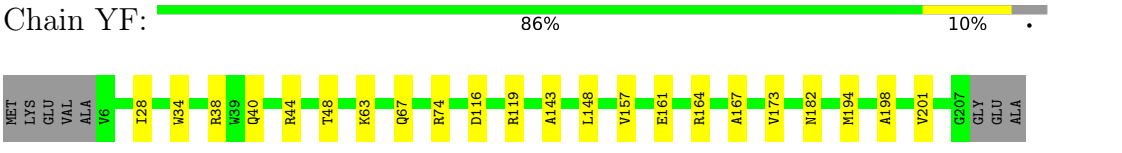
• Molecule 28: 50S ribosomal protein L4

Chain RF:



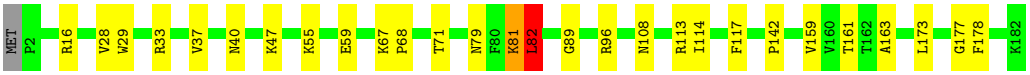
• Molecule 28: 50S ribosomal protein L4

Chain YF:



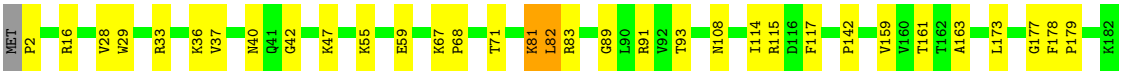
• Molecule 29: 50S ribosomal protein L5

Chain RG:



• Molecule 29: 50S ribosomal protein L5

Chain YG:

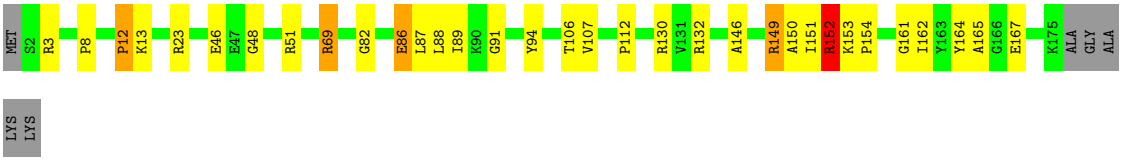


• Molecule 30: 50S ribosomal protein L6

Chain RH:

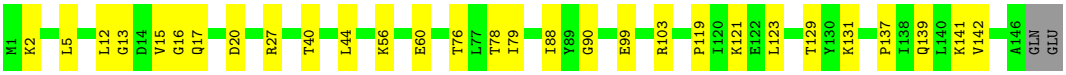
• Molecule 30: 50S ribosomal protein L6

Chain YH:



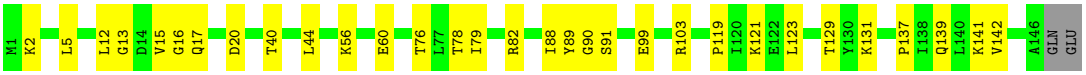
• Molecule 31: 50S ribosomal protein L9

Chain RI:



• Molecule 31: 50S ribosomal protein L9

Chain YI:

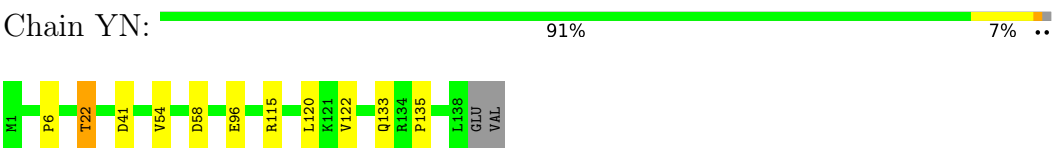


• Molecule 32: 50S ribosomal protein L13

Chain RN:

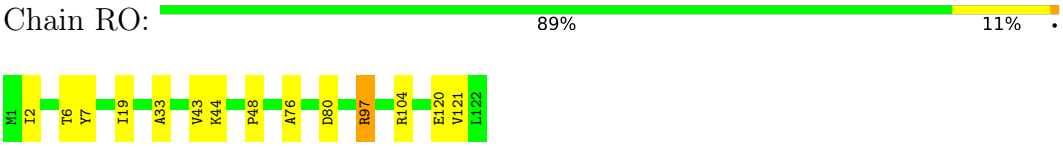
• Molecule 32: 50S ribosomal protein L13

Chain YN:



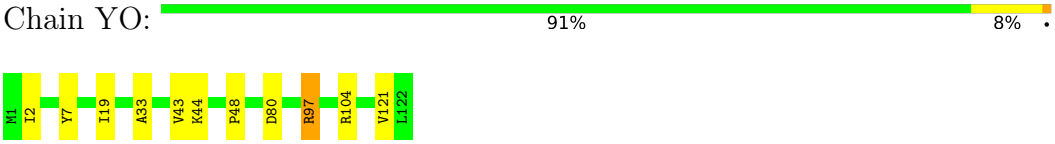
• Molecule 33: 50S ribosomal protein L14

Chain RO:



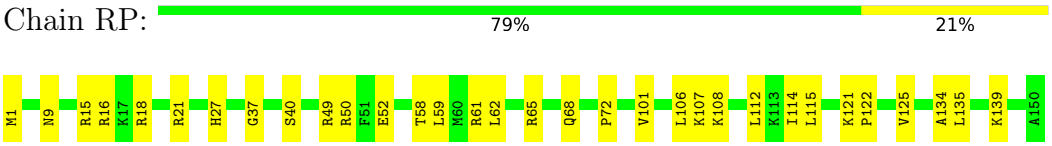
• Molecule 33: 50S ribosomal protein L14

Chain YO:



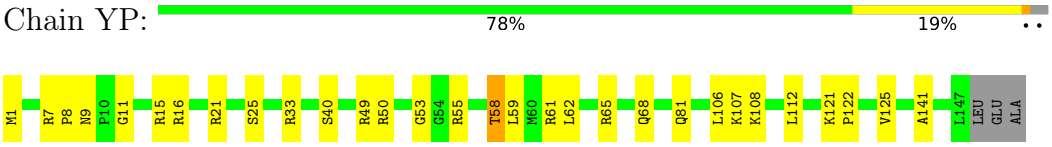
• Molecule 34: 50S ribosomal protein L15

Chain RP:



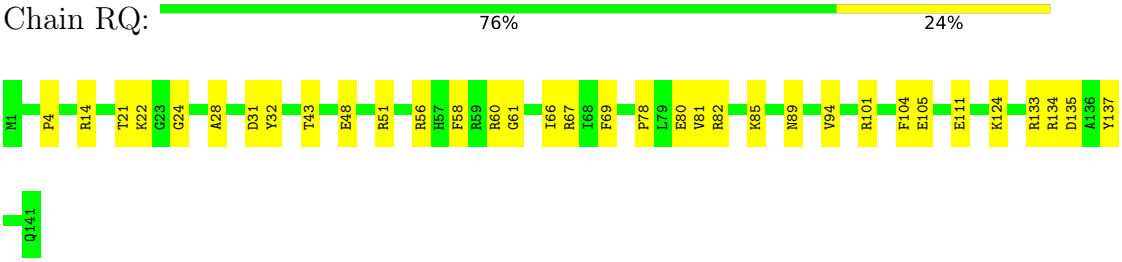
• Molecule 34: 50S ribosomal protein L15

Chain YP:



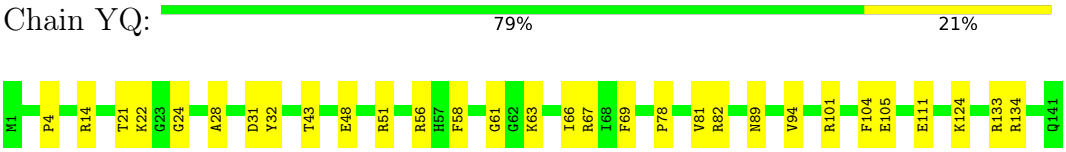
• Molecule 35: 50S ribosomal protein L16

Chain RQ:



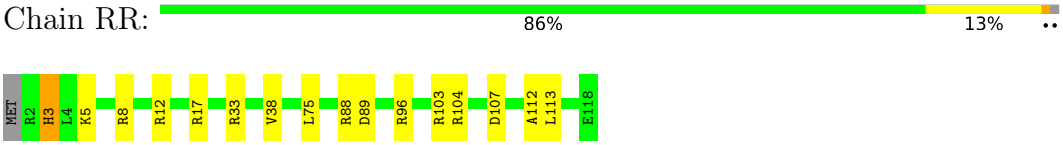
• Molecule 35: 50S ribosomal protein L16

Chain YQ:



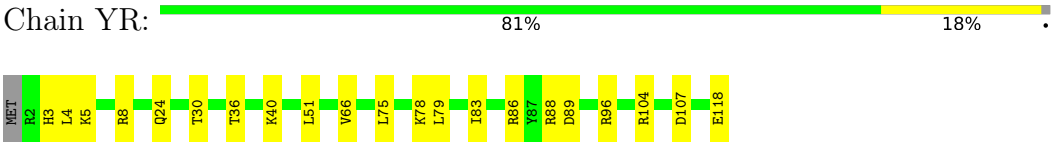
• Molecule 36: 50S ribosomal protein L17

Chain RR:



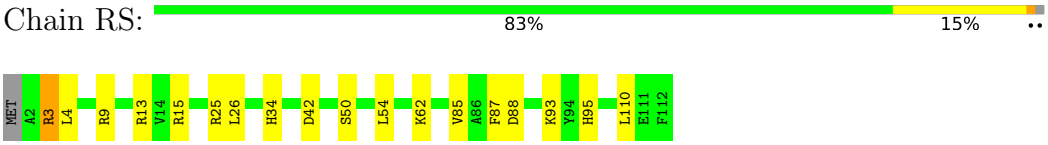
• Molecule 36: 50S ribosomal protein L17

Chain YR:



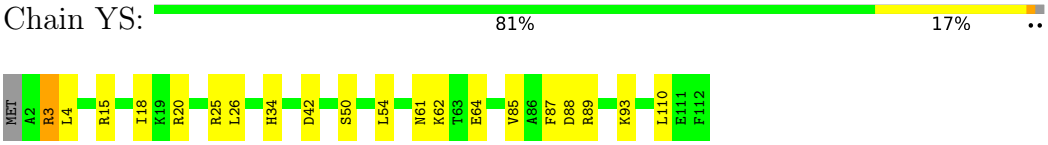
• Molecule 37: 50S ribosomal protein L18

Chain RS:



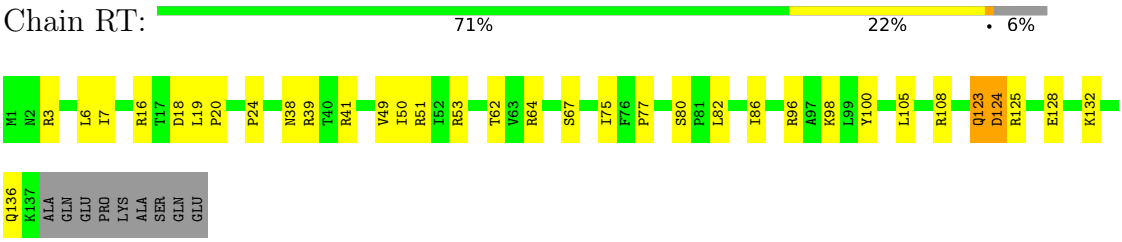
• Molecule 37: 50S ribosomal protein L18

Chain YS:



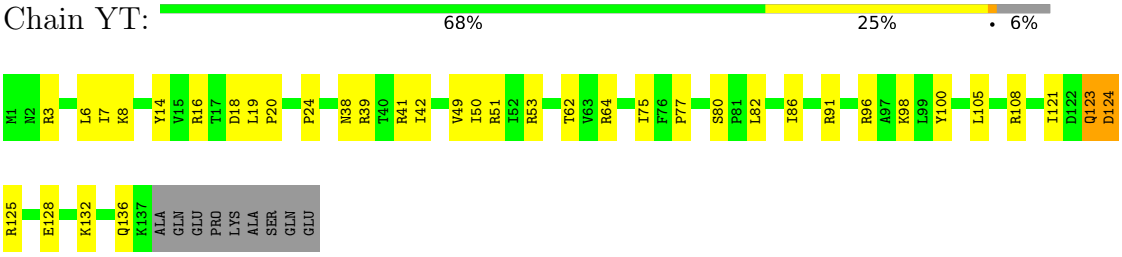
• Molecule 38: 50S ribosomal protein L19

Chain RT:



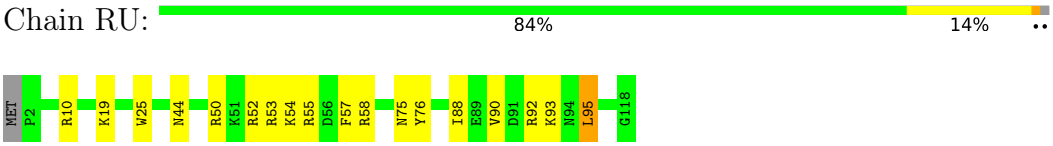
• Molecule 38: 50S ribosomal protein L19

Chain YT:



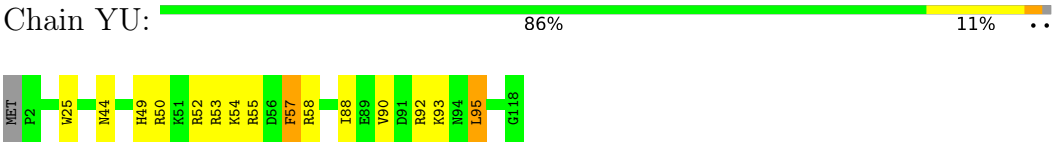
• Molecule 39: 50S ribosomal protein L20

Chain RU:



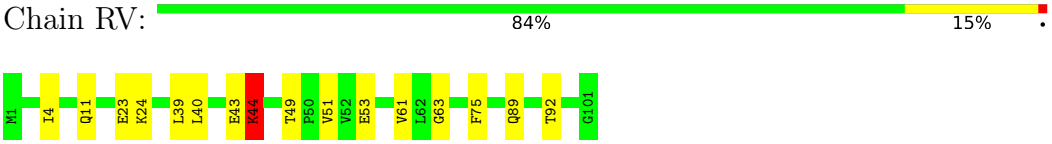
• Molecule 39: 50S ribosomal protein L20

Chain YU:



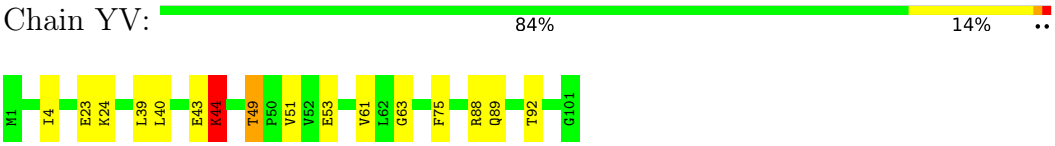
• Molecule 40: 50S ribosomal protein L21

Chain RV:



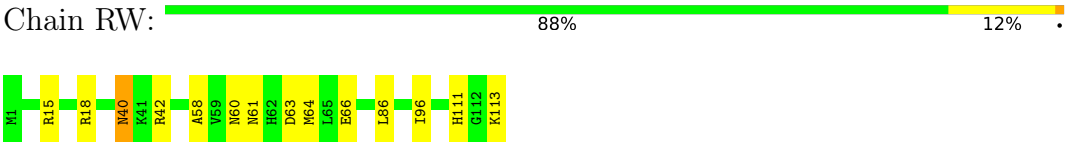
• Molecule 40: 50S ribosomal protein L21

Chain YV:



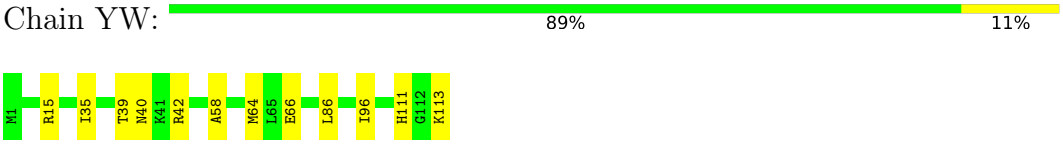
• Molecule 41: 50S ribosomal protein L22

Chain RW:



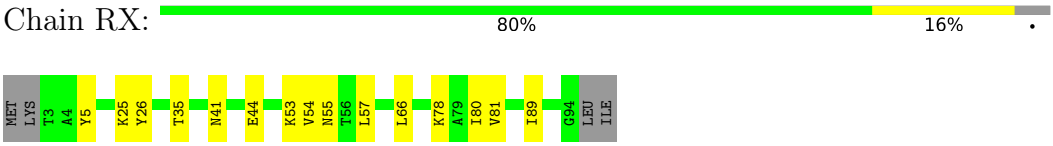
• Molecule 41: 50S ribosomal protein L22

Chain YW:



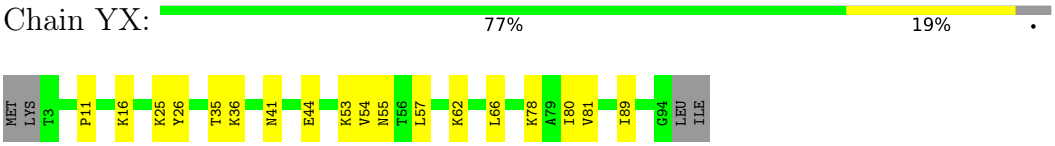
• Molecule 42: 50S ribosomal protein L23

Chain RX:



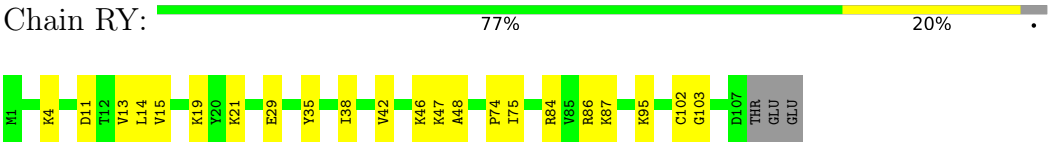
• Molecule 42: 50S ribosomal protein L23

Chain YX:



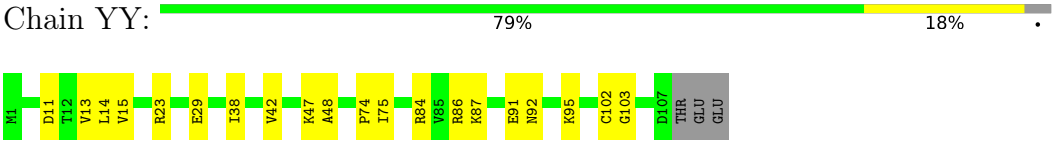
• Molecule 43: 50S ribosomal protein L24

Chain RY:



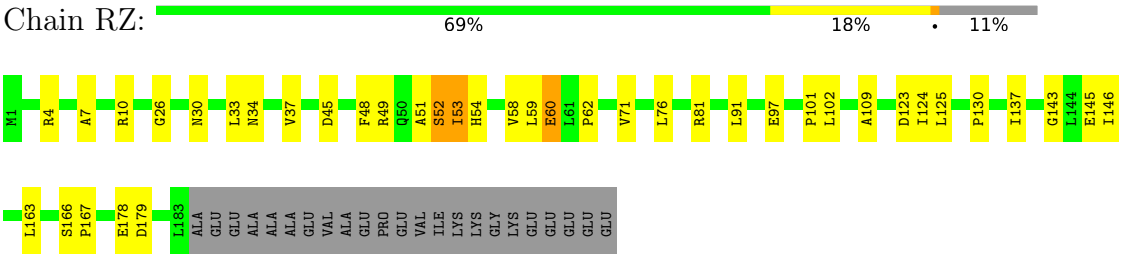
• Molecule 43: 50S ribosomal protein L24

Chain YY:



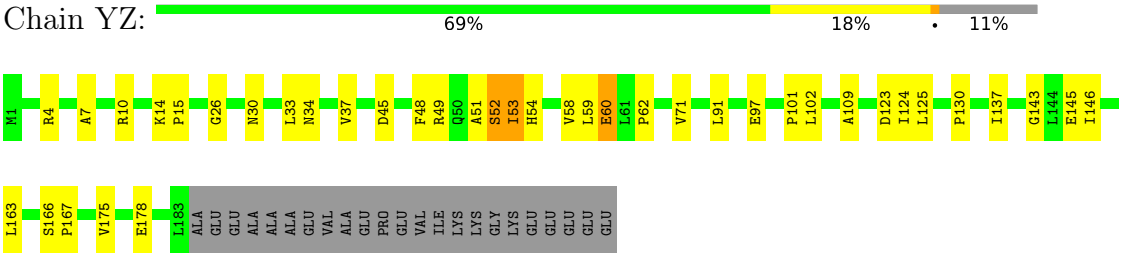
• Molecule 44: 50S ribosomal protein L25

Chain RZ:



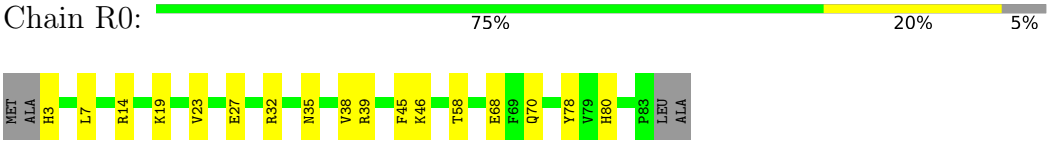
• Molecule 44: 50S ribosomal protein L25

Chain YZ:



• Molecule 45: 50S ribosomal protein L27

Chain R0:

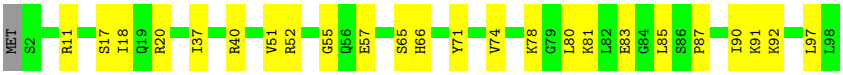


• Molecule 45: 50S ribosomal protein L27

Chain Y0:

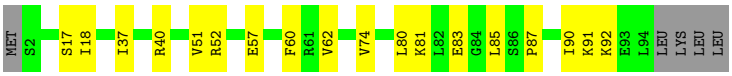
• Molecule 46: 50S ribosomal protein L28

Chain R1:



• Molecule 46: 50S ribosomal protein L28

Chain Y1:



• Molecule 47: 50S ribosomal protein L29

Chain R2:

• Molecule 47: 50S ribosomal protein L29

Chain Y2:

• Molecule 48: 50S ribosomal protein L30

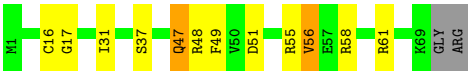
Chain R3:

• Molecule 48: 50S ribosomal protein L30

Chain Y3:

• Molecule 49: 50S ribosomal protein L31

Chain R4:



• Molecule 49: 50S ribosomal protein L31

Chain Y4:

• Molecule 50: 50S ribosomal protein L32

Chain R5:

• Molecule 50: 50S ribosomal protein L32

Chain Y5:

• Molecule 51: 50S ribosomal protein L33

Chain R6:

• Molecule 51: 50S ribosomal protein L33

Chain Y6:

• Molecule 52: 50S ribosomal protein L34

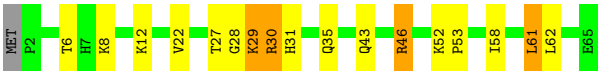
Chain R7:

• Molecule 52: 50S ribosomal protein L34

Chain Y7:

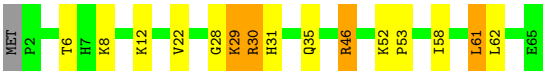
• Molecule 53: 50S ribosomal protein L35

Chain R8:



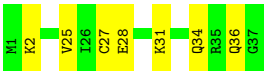
• Molecule 53: 50S ribosomal protein L35

Chain Y8:



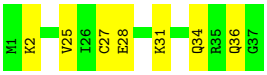
• Molecule 54: 50S ribosomal protein L36

Chain R9:



• Molecule 54: 50S ribosomal protein L36

Chain Y9:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	QA	0.76	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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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:1568:G:H5"	26:YD:61:LEU:HD23	1.77	0.66
24:YA:1863:G:HO2'	24:YA:2411:A:HO2'	1.41	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:259:G:H21	24:YA:621:A:H8	1.46	0.64
24:YA:571:A:H5'	24:YA:2030:A:H62	1.63	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
29:RG:29:TRP:O	29:RG:33:ARG:NH1	2.31	0.63
46:R1:87:PRO:HA	46:R1:90:ILE:HG22	1.80	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
1:QA:1329:A:N7	21:QU:7:ARG:NH2	2.46	0.62
12:QL:60:LEU:HD12	12:QL:62:SER:H	1.65	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
24:RA:2135:A:H62	24:RA:2156:G:H21	1.45	0.61
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
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
24:RA:907:U:O2'	35:RQ:101:ARG:NH2	2.33	0.61
27:RE:5:LEU:HG	27:RE:49:LEU:HD23	1.80	0.61
49:R4:16:CYS:SG	49:R4:17:GLY:N	2.72	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:414:A:OP2	1:XA:428:G:N2	2.31	0.61
1:XA:1127:G:H1'	1:XA:1147:C:H42	1.66	0.61
24:YA:273:G:H1	24:YA:364:C:H42	1.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
49:Y4:47:GLN:HG2	49:Y4:49:PHE:HB3	1.81	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
24:RA:2156:G:O6	24:RA:2157:G:N2	2.34	0.60
46:R1:65:SER:HG	46:R1:66:HIS:HD1	1.49	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:888:C:H3'	24:YA:889:C:H4'	1.83	0.60
24:YA:1980:G:O2'	24:YA:1982:C:OP2	2.17	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:956:G:OP2	35:RQ:14:ARG:NH2	2.34	0.60
24:RA:1365:A:O2'	46:R1:11: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:83:G:H1	24:RA:102:G:HO2'	1.49	0.59
24:RA:458:G:N2	24:RA:470:A:OP2	2.32	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
24:RA:662:G:OP1	34:RP:15:ARG:NH1	2.35	0.59
27:RE:50:GLY:HA2	27:RE:77:ILE:HA	1.85	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
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
46:R1:83:GLU:HG2	46:R1:85:LEU:H	1.68	0.58
1:XA:544:G:OP1	4:XD:59:ARG:NH2	2.37	0.58
24:YA:458:G:N2	24:YA:470:A:OP2	2.33	0.58
24:YA:2789:C:O2	24:YA:2894:G:N2	2.36	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:321:G:O2'	24:YA:340:A:N3	2.36	0.58
24:YA:1689:A:H62	24:YA:1698:A:H2	1.50	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:1019:U:H3	24:YA:1142(A):A:H62	1.50	0.57
24:YA:1089:G:N2	24:YA:1090:U:O4	2.38	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:559:A:H4'	1:QA:560:U:H3'	1.87	0.57
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
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
30:YH:153:LYS:HB3	30:YH:161:GLY:HA2	1.86	0.57
51:Y6:10:LEU:HD13	51:Y6:19:ARG:HG2	1.87	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: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
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
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:XN:27:CYS:SG	14:XN: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:675:A:OP1	28:YF:63:LYS:NZ	2.31	0.56
24:YA:2701:C:H3'	24:YA:2702:U:H5"	1.87	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:8:A:N6	4:QD:205:GLU:O	2.38	0.55
1:QA:986:A:N3	19:QS:52:TYR:OH	2.34	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
24:YA:907:U:O2'	35:YQ:101:ARG:NH2	2.37	0.55
26:YD:146:GLU:HB2	26:YD:189:CYS:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:244:U:OP2	17:QQ:100:LYS:NZ	2.40	0.55
1:QA:811:C:O2'	1:QA:901:A:N1	2.39	0.55
1:QA:1128:C:OP1	9:QI:66:ARG:NH2	2.40	0.55
14:QN:27:CYS:SG	14:QN:28:GLY:N	2.79	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:254:G:O2'	17:XQ:16:GLN:O	2.23	0.55
1:XA:662:G:O2'	1:XA:836:G:OP1	2.25	0.55
1:XA:825:G:O2'	8:XH:12:ARG:NH2	2.36	0.55
3:XC:88:ARG:HE	3:XC:101:LEU:HB3	1.71	0.55
54:Y9:2:LYS:NZ	54:Y9:31:LYS:O	2.39	0.55
1:QA:1314:C:N4	19:QS:2:PRO:O	2.38	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: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:945:G:N2	1:QA:1334:G:O2'	2.39	0.55
1:QA:1249:C:O2'	9:QI:73:GLN:NE2	2.38	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: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
24:RA:1969:A:O2'	24:RA:1972:A:N3	2.34	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
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
54:R9:2:LYS:NZ	54:R9:31:LYS: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
24:RA:1059:G:O6	24:RA:1079:C:N4	2.40	0.55
54:R9:25:VAL:HB	54:R9:34:GLN:HB2	1.89	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:316:G:OP2	1:XA:351:G:O2'	2.22	0.55
1:XA:1123:A:H4'	10:XJ:36:GLY:HA3	1.87	0.55
12:XL:45:PRO:HB3	12:XL:92:ASP:HB3	1.89	0.55
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
1:QA:1210:C:O2'	1:QA:1213:A:O2'	2.25	0.54
8:QH:106:GLY:O	8:QH:122:ARG:NH2	2.38	0.54
24:RA:2680:C:H5'	27:RE:189:PRO:HA	1.88	0.54
51:R6:10:LEU:HD13	51:R6:19:ARG:HG2	1.87	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
1:QA:619:U:N3	4:QD:134:ASP:OD1	2.35	0.54
3:QC:70:VAL:HG12	3:QC:72:LYS:H	1.72	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)
1:XA:191(G):G:O2'	20:XT:101:GLY:O	2.25	0.54
2:XB:72:GLY:HA3	2:XB:81:VAL:HG21	1.89	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:768:G:O2'	24:RA:1379:A:N6	2.41	0.54
24:RA:2387:U:O2'	45:R0:19:LYS:NZ	2.40	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:9:VAL:HB	27:RE:25:VAL:HG23	1.90	0.54
27:RE:201:THR:HG22	27:RE:203:LYS:H	1.72	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
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
47:Y2:22:GLU:OE2	47:Y2:68:ARG:NH2	2.42	0.53
1:QA:376:G:H1	1:QA:387:U:H3	1.55	0.53
1:QA:1077:G:N2	1:QA:1080:A:OP2	2.41	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
24:RA:1638:C:O2	24:RA:2698:U:O2'	2.27	0.53
32:RN:58:ASP:N	32:RN:58:ASP:OD1	2.41	0.53
33:RO:7:TYR:HE1	33:RO:44:LYS:HG3	1.74	0.53
47:R2:17:SER:HB2	47:R2:20:GLU:HG2	1.89	0.53
1:XA:278:G:OP2	17:XQ:92:ARG:NH2	2.41	0.53
30:YH:164:TYR:HB2	30:YH:167:GLU:HB2	1.90	0.53
34:YP:62:LEU:HD12	53:Y8:30:ARG:HH21	1.73	0.53
1:QA:581:G:OP1	15:QO:65:ARG:NH1	2.41	0.53
29:RG:37:VAL:HG22	29:RG:159:VAL:HG12	1.89	0.53
47:R2:22:GLU:OE2	47:R2:68:ARG:NH2	2.42	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:701:C:O2	1:QA:703:G:N1	2.41	0.53
1:QA:768:A:N3	1:QA:1512:U:O2'	2.41	0.53
10:XJ:51:ARG:O	14:XN:45:ARG:NH1	2.42	0.53
13:XM:47:ASP:OD1	13:XM:47:ASP:N	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:995:C:O2	32:RN:3:THR:OG1	2.26	0.53
24:RA:1153:C:H5'	39:RU:76:TYR:HE2	1.72	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
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
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
1:QA:1346:A:H5"	9:QI:120:ARG:HH12	1.74	0.53
5:QE:98:THR:HB	5:QE:117:ASP:HB3	1.91	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:180:G:N2	24:YA:215:G:O6	2.41	0.53
24:YA:1728:G:N1	24:YA:1730:U:OP2	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:576:G:N2	1:QA:759:A:OP1	2.40	0.52
1:QA:1061:G:OP1	10:QJ:59:SER:OG	2.24	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
53:R8:29:LYS:O	53:R8:31:HIS:N	2.38	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:392:C:H5"	24:RA:409:C:H5"	1.92	0.52
24:RA:2392:A:H2	24:RA:2424:C:H42	1.57	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
24:YA:782:A:O2'	26:YD:225:ALA:O	2.28	0.52
25:YB:5:C:O2'	25:YB:27:C:O2	2.28	0.52
1:QA:357:G:O2'	31:YI:89:TYR:O	2.25	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
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
1:QA:947:G:O3'	13:QM:109:THR:OG1	2.28	0.51
5:QE:137:GLU:OE1	5:QE:140:ARG:NH1	2.43	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:745:C:OP1	1:XA:851:G:O2'	2.27	0.51
1:XA:1286:A:H2'	1:XA:1287:A:H4'	1.92	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:629:G:N3	24:YA:639:U:O2'	2.43	0.51
24:YA:1999:C:O2	24:YA:2687:U:O2'	2.26	0.51
42:YX:53:LYS:NZ	42:YX:55:ASN:OD1	2.44	0.51
1:QA:954:G:H21	1:QA:1227:A:H62	1.57	0.51
1:QA:1222:G:OP1	19:QS:78:ARG:NH1	2.32	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:527:C:N4	24:RA:2779:U:OP2	2.41	0.51
24:RA:1270:C:H5"	24:RA:1271:G:H5'	1.92	0.51
29:RG:55:LYS:NZ	29:RG:59:GLU:OE2	2.44	0.51
1:XA:8:A:N6	4:XD:208:SER:O	2.43	0.51
1:XA:748:C:H1'	1:XA:749:C:H5	1.75	0.51
24:YA:26:G:H1'	24:YA:515:A:H61	1.76	0.51
24:YA:2467:C:O2	35:YQ:124:LYS:NZ	2.36	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:N	26:RD:122:ASP:OD1	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:605:C:O2	24:YA:657:U:O2'	2.27	0.51
24:YA:2153:G:H2'	24:YA:2154:G:H8	1.74	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:570:G:O6	1:QA:865:A:N6	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
2:QB:71:VAL:HA	2:QB:93:VAL:HB	1.93	0.51
24:RA:2245:U:H5'	24:RA:2246:G:H5'	1.93	0.51
46:R1:18:ILE:HG12	46:R1:37:ILE:HG12	1.93	0.51
1:XA:376:G:H5"	16:XP:5:ARG:HB2	1.93	0.51
5:XE:137:GLU:OE1	5:XE:140:ARG:NH1	2.43	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
54:Y9:27:CYS:SG	54:Y9:28:GLU:N	2.84	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
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
48:Y3:15:TYR:O	48:Y3:20:LYS:NZ	2.44	0.50
13:QM:47:ASP:OD1	13:QM:47:ASP:N	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:34:C:H2'	1:QA:35:G:H8	1.77	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
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
24:YA:2683:C:OP1	38:YT:53:ARG:NH2	2.42	0.50
28:YF:167:ALA:HB1	28:YF:173:VAL:HG11	1.93	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
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
54:R9:27:CYS:SG	54:R9:28:GLU:N	2.84	0.50
4:XD:62:GLN:HE22	4:XD:65:ARG:HH21	1.59	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
45:Y0:10:THR:HG22	45:Y0:12:ASN:H	1.77	0.50
1:QA:296:U:O2'	1:QA:556:C:O2	2.28	0.50
1:QA:1320:C:O2	19:QS:36:ARG:NH2	2.43	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: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
1:XA:1004:A:H1'	1:XA:1036:G:H22	1.75	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:559:A:OP1	5:XE:126:ARG:NH2	2.45	0.50
1:XA:1191:A:OP2	3:XC:3:ASN:ND2	2.44	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:708:C:OP1	11:QK:85:ARG:NH2	2.34	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
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
24:RA:138:G:N2	42:RX:44:GLU:OE1	2.30	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
50:R5:41:PRO:O	50:R5:44:THR:OG1	2.28	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:83:G:H1	24:YA:102:G:HO2'	1.57	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
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
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
34:RP:49:ARG:HH11	53:R8:58:ILE:HG22	1.77	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
24:RA:2010:G:H5"	41:RW:42:ARG:HB2	1.94	0.49
48:R3:15:TYR:O	48:R3:20:LYS:NZ	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:YA:598:G:H5'	34:YP:11:GLY:HA3	1.95	0.49
24:YA:2151:G:H2'	24:YA:2152:G:C8	2.47	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:339:C:H5	33:YO:97:ARG:HH12	1.61	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
44:YZ:102:LEU:HD23	44:YZ:137:ILE:HB	1.95	0.49
1:QA:348:G:H2'	1:QA:349:A:H8	1.77	0.49
1:QA:1392:G:H21	1:QA:1502:A:H8	1.61	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:495:G:H21	41:RW:61:ASN:HD21	1.59	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
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:35:G:O2'	12:QL:118:SER:O	2.27	0.48
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
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:943:U:H1'	9:XI:124:GLN:HE22	1.77	0.48
1:XA:1367:C:OP1	9:XI:115:GLY:N	2.39	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:954:G:O6	13:QM:104:ARG:NH1	2.46	0.48
1:QA:1314:C:OP2	19:QS:4:SER:OG	2.26	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
1:XA:933:G:O6	7:XG:3:ARG:NH2	2.46	0.48
3:XC:58:GLU:HB2	3:XC:65:ALA:HB3	1.94	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
24:RA:746:A:O2'	24:RA:2611:U:O2'	2.30	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
45:R0:32:ARG:N	45:R0:35:ASN:OD1	2.46	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:7:ALA:HB2	44:RZ:59:LEU:HB3	1.95	0.48
44:RZ:163:LEU:HD13	44:RZ:167:PRO:HD3	1.94	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:861:A:N3	25:RB:79:C:O2'	2.43	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
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
27:YE:119:ARG:NH1	27:YE:159:HIS:O	2.47	0.48
46:Y1:17:SER:HB2	46:Y1:40:ARG:HD2	1.94	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: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
24:YA:2791:C:OP1	24:YA:2893:G:N2	2.47	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
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
29:YG:179:PRO:HB3	49:Y4:43:TYR:HE1	1.78	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:N	17:QQ:83:ASP:OD1	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
24:RA:252:G:OP2	34:RP:50:ARG:NH1	2.47	0.48
27:RE:119:ARG:NH1	27:RE:159:HIS:O	2.47	0.48
1:XA:675:A:H1'	11:XK:116:HIS:CD2	2.49	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
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
24:YA:918:A:N3	25:YB:80:U:O2'	2.45	0.47
24:YA:2289:G:N2	24:YA:2344:U:O2	2.46	0.47
45:Y0:46:LYS:HD2	45:Y0:78:TYR:HE1	1.79	0.47
1:QA:159:G:H21	1:QA:162:A:H8	1.62	0.47
1:QA:545:C:H5'	4:QD:72:GLU:HG3	1.96	0.47
2:QB:219:VAL:HA	2:QB:222:ILE:HD12	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:587:C:O2	34:YP:33:ARG:NH2	2.47	0.47
24:YA:1779:U:OP2	24:YA:1784:A:N6	2.42	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
24:YA:829:A:N7	24:YA:2247:A:O2'	2.46	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
47:Y2:4:SER:OG	47:Y2:5:GLU:N	2.48	0.47
1:QA:589:C:H42	1:QA:650:G:H1	1.63	0.47
1:QA:1034:G:H2'	1:QA:1035:A:C8	2.49	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: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
24:RA:2128:C:H1'	24:RA:2173:A:H2	1.79	0.47
36:RR:33:ARG:HD3	36:RR:113:LEU:HD11	1.96	0.47
1:XA:263:A:OP2	20:XT:79:ARG:NH1	2.48	0.47
17:XQ:83:ASP:N	17:XQ:83:ASP:OD1	2.47	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
24:YA:220:G:O2'	24:YA:233:A:N3	2.44	0.47
24:YA:1139:G:O2'	24:YA:1143:A:N1	2.40	0.47
46:Y1:80:LEU:HD12	46:Y1:81:LYS:HG2	1.97	0.47
1:QA:108:G:OP2	1:QA:108:G:N2	2.48	0.47
1:QA:134:A:H61	16:QP:25:ARG:HH12	1.61	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
24:RA:1045:A:O4'	24:RA:1111:A:N6	2.48	0.47
24:RA:1155:A:O3'	39:RU:55:ARG:NH1	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:3:ARG:HB2	38:RT:6:LEU:HB3	1.96	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
53:R8:6:THR:OG1	53:R8:8:LYS:NZ	2.48	0.47
1:XA:309:G:H2'	1:XA:310:G:H8	1.79	0.47
1:XA:452:A:H62	1:XA:480:U:H3	1.63	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
1:XA:1286:A:H5"	21:XU:26:LYS:HD2	1.97	0.47
1:XA:1432:G:OP1	38:YT:108:ARG:N	2.46	0.47
14:XN:48:ALA:HB2	14:XN:53:LEU:HD12	1.97	0.47
26:YD:36:PRO:HB2	26:YD:61:LEU:HD12	1.95	0.47
27:YE:14:ILE:HG13	38:YT:14:TYR:HE2	1.80	0.47
29:YG:173:LEU:O	29:YG:178:PHE:N	2.41	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:242:G:O2'	24:RA:254:G:O6	2.27	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:1203:G:O6	24:RA:1204:A:N6	2.48	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
6:XF:97:PHE:HB2	18:XR:32:ARG:HE	1.80	0.47
9:XI:5:TYR:HE1	9:XI:16:ARG:HB2	1.80	0.47
24:YA:994:C:OP2	39:YU:54:LYS:NZ	2.42	0.47
24:YA:1110:G:O3'	30:YH:3:ARG:NH2	2.47	0.47
28:YF:143:ALA:HB1	28:YF:148:LEU:HB2	1.96	0.47
1:QA:596:C:H2'	1:QA:597:G:H8	1.80	0.47
1:QA:1287:A:H2	1:QA:1353:G:H1'	1.79	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
24:YA:831:G:N2	34:YP:53:GLY:O	2.38	0.47
31:YI:123:LEU:HD23	31:YI:142:VAL:HG22	1.96	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:XN:4:LYS:HA	14:XN:7:ILE:HG12	1.97	0.47
14:XN:24:CYS:HB3	14:XN:29:ARG:H	1.80	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:612:G:N2	24:YA:616:A:O2'	2.48	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
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:OP2	1:QA:530:G:N2	2.46	0.46
1:QA:1347:G:O6	9:QI:10:ARG:NH2	2.49	0.46
4:QD:10:ARG:HG3	4:QD:40:PRO:HG3	1.98	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
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
53:Y8:6:THR:OG1	53:Y8:8:LYS:NZ	2.48	0.46
1:QA:606:G:H22	1:QA:631:G:H5'	1.80	0.46
1:QA:1199:U:O2'	1:QA:1202:G:OP1	2.34	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:131:C:O2'	1:XA:262:A:N3	2.40	0.46
1:XA:1221:G:OP1	1:XA:1320:C:N4	2.42	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:389:G:H22	34:RP:72:PRO:HD3	1.81	0.46
24:RA:583:G:H5"	39:RU:10:ARG:HH12	1.80	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
24:YA:363:G:H2'	24:YA:363(A):A:H8	1.81	0.46
48:Y3:39:ASP:OD1	48:Y3:44:ARG:NH2	2.46	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
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
24:YA:2006:C:O2'	24:YA:2823:A:N3	2.48	0.46
29:YG:67:LYS:HD2	29:YG:68:PRO:HD2	1.97	0.46
1:QA:246:A:OP2	17:QQ:100:LYS:NZ	2.49	0.46
1:QA:1224:G:H1	1:QA:1362(A):C:H42	1.62	0.46
4:QD:57:ARG:NH2	5:QE:107:ARG:HD3	2.31	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
47:R2:4:SER:OG	47:R2:5:GLU:N	2.48	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
24:YA:2343:C:O2'	24:YA:2373:G:O2'	2.25	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
1:QA:1493:A:H2	23:QX:20:U:H1'	1.81	0.46
11:QK:57:THR:HG22	11:QK:59:TYR:H	1.81	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
49:R4:51:ASP:N	49:R4:51:ASP:OD1	2.47	0.46
1:XA:553:A:O2'	12:XL:29:GLY:O	2.30	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
12:XL:67:THR:OG1	12:XL:95:GLY:O	2.32	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
24:YA:2354:G:H4'	45:Y0:35:ASN:HD22	1.81	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
1:QA:1296:C:OP1	13:QM:44:ARG:NH2	2.49	0.46
9:QI:63:ILE:HG21	9:QI:77:ILE:HG12	1.97	0.46
24:RA:300:A:OP1	43:RY:86:ARG:NH2	2.49	0.46
1:XA:35:G:N2	12:XL:118:SER:OG	2.39	0.46
1:XA:501:C:O2	1:XA:549:C:O2'	2.29	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
1:XA:1226:C:O2'	13:XM:111:LYS:NZ	2.49	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
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:2133:G:O2'	24:YA:2158:A:N1	2.49	0.45
24:YA:2285:C:OP2	51:Y6:6:ARG:NH1	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:380:G:N2	1:XA:383:A:OP2	2.46	0.45
1:XA:1151:A:H2'	1:XA:1152:A:H8	1.81	0.45
10:XJ:49:VAL:HG23	14:XN: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:XN:29:ARG:HD3	14:XN: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:HA	4:XD:155:LEU:HD23	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
27:YE:38:THR:OG1	27:YE:40:GLU:OE1	2.34	0.45
29:YG:108:ASN:HA	49:Y4:37:SER:HB3	1.99	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:674:G:H1'	28:RF:74:ARG:HD3	1.98	0.45
24:RA:2258:C:O2'	24:RA:2427:C:OP2	2.27	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:67:C:H2'	1:XA:68:G:C8	2.52	0.45
1:XA:1314:C:OP2	19:XS:4:SER:OG	2.30	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
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
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
43:YY:14:LEU:HB2	43:YY:75:ILE:HD11	1.98	0.45
52:Y7:10:ARG:HE	52:Y7:14:LYS:HD2	1.82	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
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
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
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
24:YA:28:A:N6	24:YA:512:G:O2'	2.51	0.44
24:YA:296:C:O3'	43:YY:95:LYS:NZ	2.49	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
46:Y1:60:PHE:HB3	46:Y1:62:VAL:HG13	1.98	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
24:YA:27:G:H22	24:YA:512:G:H2'	1.83	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
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
48:Y3:12:PRO:HB2	48:Y3:20:LYS:HG2	1.99	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
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
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
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
52:Y7:5:TRP:NE1	52:Y7:7:PRO:HG3	2.33	0.44
24:RA:1567:A:H3'	26:RD:86:PRO:HG3	1.98	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
1:XA:1502:A:H2	1:XA:1505:G:H1	1.64	0.44
24:YA:363(A):A:H2'	24:YA:363(B):G:H8	1.83	0.44
24:YA:2123:G:H2'	24:YA:2124:G:C8	2.53	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:209:U:H1'	1:XA:216:G:C2	2.53	0.44
1:XA:1446:A:O2'	1:XA:1447:G:O4'	2.36	0.44
24:YA:414:C:O2	24:YA:1864:U:O2'	2.25	0.44
24:YA:1243:G:H4'	34:YP:7:ARG:HH21	1.82	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
30:YH:152:ARG:HE	30:YH:153:LYS:HD2	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
24:YA:1500:G:H21	26:YD:100:GLY:HA3	1.83	0.44
25:YB:33:G:H5'	29:YG:2:PRO:HG3	1.99	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: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
24:RA:579:G:O2'	24:RA:2019:A:OP1	2.33	0.44
24:RA:1598:C:O3'	42:RX:35:THR:OG1	2.36	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
24:RA:336:C:O2'	43:RY:35:TYR:OH	2.36	0.43
24:RA:2791:C:OP1	24:RA:2893:G:N2	2.51	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
45:R0:46:LYS:HD2	45:R0:78:TYR:HE1	1.83	0.43
7:XG:15:ASP:HB3	7:XG:19:GLY:H	1.83	0.43
24:YA:363(B):G:H2'	24:YA:363(C):G:H8	1.83	0.43
24:YA:2146:C:H4'	24:YA:2147:G:C8	2.53	0.43
26:YD:108:PRO:HB3	26:YD:143:HIS:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
50:Y5:20:ARG:HA	50:Y5:23:HIS:CD2	2.48	0.43
1:QA:552:U:H2'	1:QA:553:A:H8	1.82	0.43
1:QA:1065:U:H6	1:QA:1190:G:H21	1.64	0.43
24:RA:1006:C:H5'	32:RN:28:THR:HG23	2.00	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:17:THR:HB	26:RD:205:VAL:H	1.83	0.43
26:RD:108:PRO:HB3	26:RD:143:HIS:CE1	2.53	0.43
29:RG:16:ARG:NH2	29:RG:28:VAL:O	2.51	0.43
35:RQ:135:ASP:OD2	44:RZ:81:ARG:NH2	2.45	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
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
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:301:G:OP2	43:YY:84: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
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:265:G:H4'	17:XQ:66:SER:HA	1.99	0.43
1:XA:1053:G:N7	1:XA:1199:U:H2'	2.33	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
53:Y8:22:VAL:HB	53:Y8:53:PRO:HB3	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
9:QI:128:ARG:NH1	22:QV:36:A:OP2	2.52	0.43
10:QJ:4:ILE:HG12	10:QJ:100:THR:HG22	2.01	0.43
24:RA:270(S):G:H2'	24:RA:270(T):G:H8	1.84	0.43
24:RA:1782:C:H1'	24:RA:2609:U:H5"	2.01	0.43
24:RA:2232:U:OP2	46:R1:40:ARG:NH2	2.52	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
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:HD1	39:YU:57:PHE:HA	1.76	0.43
40:YV:43:GLU:HG3	40:YV:44:LYS:H	1.83	0.43
45:Y0:23:VAL:HG13	45:Y0:38:VAL:HG22	1.99	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
1:QA:1095:U:P	1:QA:1108:G:H1	2.41	0.43
7:QG:15:ASP:HB3	7:QG:19:GLY:H	1.83	0.43
24:RA:776:G:N7	24:RA:793:A:O2'	2.52	0.43
24:RA:2693:A:H2'	24:RA:2694:G:H8	1.83	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
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
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: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
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
24:RA:78:A:H2'	24:RA:79: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:1590:U:H2'	24:RA:1591: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: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
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
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:3:ARG:HG3	38:RT:7:ILE:HG12	1.99	0.43
38:RT:19:LEU:HD22	38:RT:86:ILE:HG22	2.00	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: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
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:2285:C:OP1	51:Y6:29:ASN:ND2	2.51	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
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
50:R5:20:ARG:HA	50:R5:23:HIS:CD2	2.48	0.43
1:XA:664:G:H22	1:XA:741:G:H1	1.65	0.43
1:XA:944:G:N1	1:XA:1338:G:OP2	2.40	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:149:A:H4'	1:QA:1450:U:C4	2.54	0.43
1:QA:1154:G:H2'	1:QA:1155:G:H8	1.83	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: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
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
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
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
47:R2:14:ARG:NH1	47:R2:66:GLU:OE1	2.52	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
24:RA:31:C:O2'	24:RA:1238:G:OP1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
45:R0:38:VAL:HG21	45:R0:45:PHE:HD2	1.85	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:819:A:H5'	1:QA:819:A:H8	1.85	0.42
1:QA:1239:A:O2'	1:QA:1298:C:N4	2.52	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
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
50:R5:16:ARG:NH1	50:R5:17:ASP:OD1	2.52	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
1:QA:659:U:OP1	15:QO:9:GLN:NE2	2.52	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
24:RA:48:G:N2	24:RA:49:A:N1	2.67	0.42
24:RA:49:A:H61	24:RA:177:G:H2'	1.85	0.42
24:RA:1141:U:H1'	24:RA:1142(A):A:C6	2.54	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
53:R8:22:VAL:HB	53:R8:53:PRO:HB3	2.00	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
24:YA:1018:C:O3'	24:YA:1120:G:N2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:YA:1105:U:H2'	24:YA:1106:G:H8	1.84	0.42
45:Y0:46:LYS:HB2	45:Y0:78:TYR:CD1	2.54	0.42
47:Y2:14:ARG:NH1	47:Y2:66:GLU:OE1	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:255:G:OP1	17:XQ:69:LYS:NZ	2.46	0.42
1:XA:562:C:H1'	12:XL:15:ARG:HD2	2.00	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
4:XD:23:GLY:N	4:XD:26:CYS:SG	2.73	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
45:Y0:23:VAL:HB	45:Y0:26:TYR:HE1	1.83	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
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
48:R3:18:ASP:OD1	48:R3:18:ASP:N	2.53	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
1:XA:1343:G:H1'	9:XI:121:ARG:NH1	2.34	0.42
26:YD:17:THR:HB	26:YD:205:VAL:H	1.83	0.42
26:YD:31:LYS:HA	26:YD:31:LYS:HD2	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
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
37:YS:85:VAL:HG22	37:YS:110:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Y2:51:ARG:HH11	47:Y2:55:ARG:NH2	2.18	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:270(H):C:H2'	24:RA:270(I):G:C8	2.55	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
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
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
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
1:QA:769:G:H4'	1:QA:1513:A:H4'	2.02	0.42
24:RA:288:C:H2'	24:RA:289:A:H8	1.83	0.42
24:RA:1184:G:P	48:R3:29:ARG:HH12	2.43	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:779:C:H5"	11:QK:122:LYS:HG2	2.01	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
11:QK:58:PRO:HB2	11:QK:93:GLN:HG3	2.02	0.41
24:RA:586:A:N1	24:RA:809:G:O2'	2.40	0.41
24:RA:1412:A:H2'	24:RA:1413:G:C8	2.55	0.41
31:RI:13:GLY:HA3	31:RI:17:GLN:HG2	2.02	0.41
33:RO:76:ALA:HB3	38:RT:75:ILE:HD12	2.02	0.41
35:RQ:21:THR:HB	35:RQ:22:LYS:H	1.55	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:OD1	44:YZ:123:ASP:N	2.52	0.41
1:QA:1294:G:H2'	1:QA:1295:G:C8	2.56	0.41
2:QB:18:GLY:H	2:QB:42:ILE:HD12	1.85	0.41
2:QB:109:SER:O	2:QB:113:HIS:ND1	2.37	0.41
24:RA:729:G:H5'	24:RA:730:C:H5"	2.02	0.41
24:RA:2347:C:HO2'	51:R6:21:TYR:HH	1.67	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:1147:C:O2	9:QI:16:ARG:NH2	2.53	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
10:QJ:13:HIS:HA	10:QJ:16:LEU:HB3	2.02	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:83:GLU:OE1	26:RD:104:TYR:OH	2.33	0.41
26:RD:182:LEU:HB2	26:RD:271:ILE:HB	2.02	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
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
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:270(R):G:H2'	24:YA:270(S):G:C8	2.55	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

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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:586:A:H5'	28:RF:89:VAL:HG21	2.01	0.41
24:RA:1423:G:OP1	24:RA:1492:G:O2'	2.36	0.41
24:RA:2361:A:O5'	53:R8:27:THR:OG1	2.38	0.41
25:RB:84:C:OP1	48:R3:15:TYR:OH	2.34	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:62:U:H3	1:QA:105:G:H1	1.67	0.41
1:QA:501:C:H2'	1:QA:502:G:C8	2.56	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
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
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
46:R1:52:ARG:NH2	46:R1:55:GLY:O	2.53	0.41
1:XA:529:G:O6	12:XL:49:ASN:ND2	2.48	0.41
1:XA:1077:G:N2	1:XA:1080:A:OP2	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:137(A):G:H21	42:YX:41:ASN:HD21	1.68	0.41
24:YA:1311:G:H21	24:YA:1603:A:H62	1.68	0.41
24:YA:1491:G:H2'	24:YA:1492:G:H8	1.86	0.41
30:YH:12:PRO:HB3	30:YH:48:GLY:HA2	2.03	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
1:QA:56:U:H4'	31:YI:82:ARG:HH12	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:RA:1328:G:N2	24:RA:1330:C:O2	2.54	0.41
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:277:C:H5"	17:XQ:68:ARG:HH21	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
24:YA:694:U:OP1	26:YD:59:LYS:NZ	2.38	0.41
24:YA:1888:G:OP2	24:YA:1888:G:N2	2.51	0.41
24:YA:2723:C:OP1	36:YR:3:HIS:ND1	2.48	0.41
37:YS:18:ILE:HD13	37:YS:18:ILE:HA	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
24:RA:1666:G:HO2'	33:RO:6:THR:HG1	1.59	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
46:R1:17:SER:HB2	46:R1:40:ARG:HD2	2.01	0.41
1:XA:673:G:H2'	1:XA:674:G:C8	2.55	0.41
2:XB:30:ARG:H	2:XB:30:ARG:HD3	1.85	0.41
10:XJ:5:ARG:HH21	10:XJ:99:LYS:HD2	1.86	0.41
24:YA:363(B):G:H2'	24:YA:363(C):G:C8	2.56	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
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
48:Y3:18:ASP:OD1	48:Y3:18:ASP:N	2.53	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:1119:C:H2'	1:QA:1120:G:C8	2.56	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:1348:U:H4'	9:QI:120:ARG:HD2	2.03	0.41
1:QA:1412:C:H2'	1:QA:1413:A: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
13:QM:3:ARG:HH12	29:RG:113:ARG:HH21	1.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:RA:2483:C:N3	35:RQ:124:LYS:HE3	2.36	0.41
28:RF:63:LYS:NZ	28:RF:75:HIS:O	2.39	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
29:RG:142:PRO:HB2	49:R4:31:ILE:HG21	2.03	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
47:R2:51:ARG:HH11	47:R2:55:ARG:NH2	2.18	0.41
52:R7:13:ALA:HB2	52:R7:46:VAL:HG11	2.02	0.41
53:R8:61:LEU:HD23	53:R8:61:LEU:HA	1.82	0.41
1:XA:272:C:H2'	1:XA:273:A:H8	1.84	0.41
1:XA:736:C:H2'	1:XA:737:A:H8	1.86	0.41
1:XA:1004:A:H1'	1:XA:1036:G:H1	1.86	0.41
1:XA:1320:C:H5'	19:XS:70:LYS:HG3	2.02	0.41
1:XA:1484:C:O2'	24:YA:1960:A:O2'	2.28	0.41
2:XB:87:ARG:NH1	2:XB:220:ASP:OD1	2.53	0.41
8:XH:20:TYR:HE2	8:XH:75:ARG:HD2	1.86	0.41
8:XH:97:VAL:HG21	8:XH:128:GLY:HA2	2.03	0.41
24:YA:392:C:H5"	24:YA:409:C:H5"	2.03	0.41
30:YH:91:GLY:HA3	30:YH:94:TYR:CD2	2.56	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:184:G:H2'	1:QA:185:A:H8	1.86	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
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
52:R7:5:TRP:NE1	52:R7:7:PRO:HG3	2.36	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: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
1:QA:1151:A:H2'	1:QA:1152:A:H8	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:QC:150:LYS:HB3	3:QC:201:TYR:HB2	2.03	0.40
24:RA:673:C:OP1	28:RF:54:ARG:NH1	2.50	0.40
24:RA:1664:A:H61	24:RA:1996:C:H42	1.69	0.40
24:RA:2295:C:H5	37:RS:13:ARG:HH12	1.69	0.40
25:RB:42:C:O2'	29:RG:67:LYS:O	2.25	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
34:RP:37:GLY:O	34:RP:40:SER:OG	2.31	0.40
43:RY:11:ASP:OD1	43:RY:11:ASP:N	2.54	0.40
1:XA:7:G:H5'	1:XA:298:A:O4'	2.21	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
3:XC:9:GLY:HA3	14:XN:49:HIS:HA	2.03	0.40
11:XK:43:SER:HB3	11:XK:68:ALA:HB2	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:HH11	39:YU:92:ARG:HD3	1.76	0.40
1:QA:191(G):G:O2'	20:QT:101:GLY:O	2.39	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
24:RA:17:G:H4'	39:RU:25:TRP:HE1	1.86	0.40
24:RA:271(D):G:H2'	24:RA:272:G:H8	1.87	0.40
24:RA:807:U:O2'	24:RA:2060:A:N1	2.43	0.40
24:RA:1535:U:H5'	24:RA:1537:C:N3	2.36	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:324:G:N1	1:QA:327:A:OP2	2.54	0.40
1:QA:1189:C:O2'	3:QC:176:HIS:ND1	2.50	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
24:RA:270:A:OP2	24:RA:270(Y):G:N1	2.55	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
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:OD1	34:RP:9:ASN:N	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
48:R3:29:ARG:HH11	48:R3:29:ARG:HD2	1.75	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:483:A:O4'	43:YY:48:ALA:HB1	2.21	0.40
24:YA:1931:U:H6	24:YA:1931:U:H2'	1.73	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:20:TYR:HE2	8:QH:75:ARG:HD2	1.85	0.40
8:QH:97:VAL:HG21	8:QH:128:GLY:HA2	2.03	0.40
16:QP:3:LYS:HG3	16:QP:65:GLN:O	2.22	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
24:RA:1068:G:N2	24:RA:1095:A:O2'	2.54	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
24:YA:1296:G:OP1	24:YA:2709:G:O2'	2.24	0.40
24:YA:1566:A:P	26:YD:211:ARG:HH21	2.44	0.40
24:YA:2702:U:H1'	24:YA:2703:C:H5	1.86	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
42:YX:11:PRO:HD3	47:Y2:37:PHE:CD1	2.55	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:60:SER:OG	28:RF:61:GLY:N	2.55	0.40
28:RF:182:ASN:OD1	28:RF:182:ASN:N	2.54	0.40
1:XA:973:G:H3'	1:XA:974:A:H5"	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:1152:A:H5"	10:XJ:13:HIS:ND1	2.37	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
24:YA:730:C:OP1	24:YA:1775:U:O2'	2.31	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
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
48:Y3:48:GLU:HA	48:Y3:51:ALA:HB2	2.03	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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	QB	233/256 (91%)	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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	QB	203/220 (92%)	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

Sometimes 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 (i)

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 monosaccharides 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	XD	301	4	0,12,12	-	-	-		
56	SF4	QD	301	4	0,12,12	-	-	-		

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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