



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2024 – 07:38 PM EST

PDB ID : 6BZ8
Title : Thermus thermophilus 70S containing 16S G347U point mutation and near-cognate ASL Leucine in A site
Authors : Hoffer, E.D.; Maehigashi, T.; Fagan, C.E.; Dunham, C.M.
Deposited on : 2017-12-22
Resolution : 3.74 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

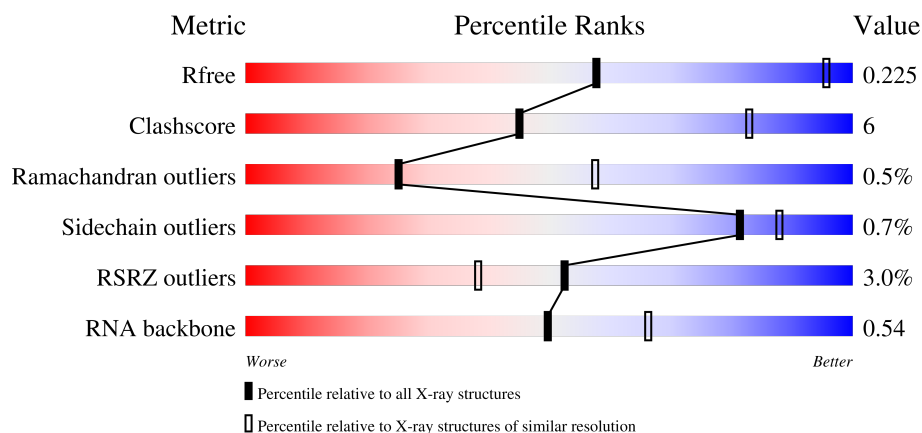
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.74 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.







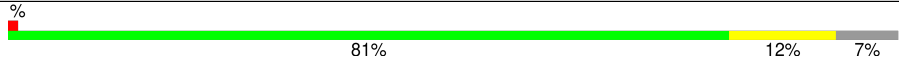
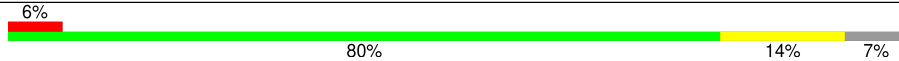
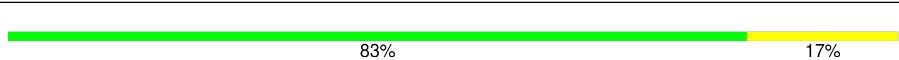
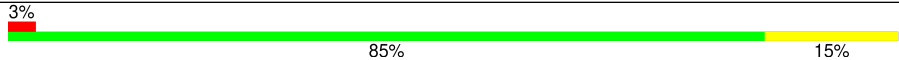
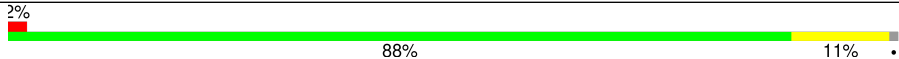
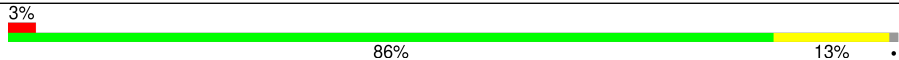
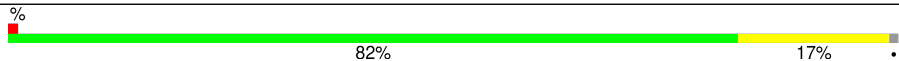
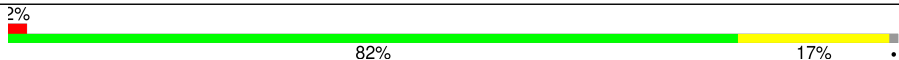


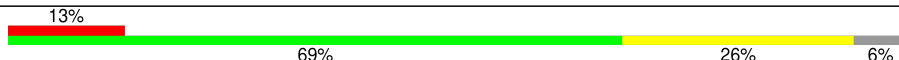
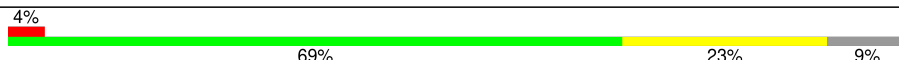
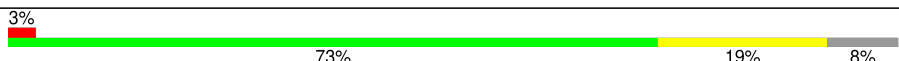
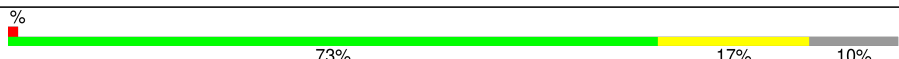
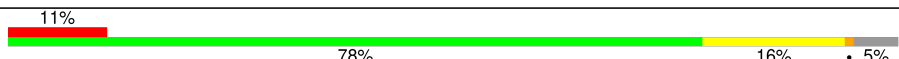

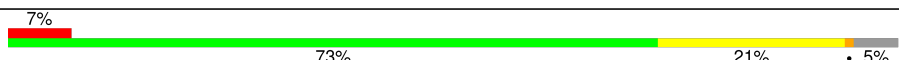
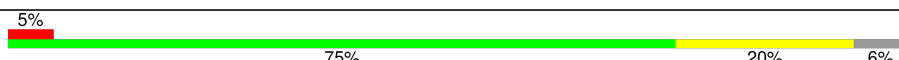
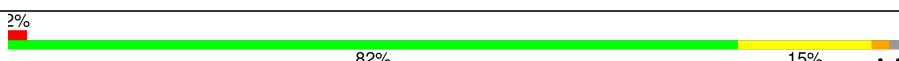
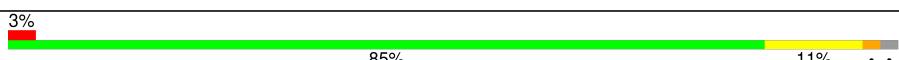
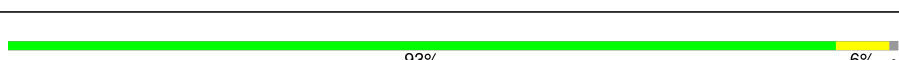
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1104 (3.88-3.60)
Clashscore	180529	1161 (3.88-3.60)
Ramachandran outliers	177936	1139 (3.88-3.60)
Sidechain outliers	177891	1134 (3.88-3.60)
RSRZ outliers	164620	1104 (3.88-3.60)
RNA backbone	3690	1123 (4.46-3.00)

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

Mol	Chain	Length	Quality of chain
1	QA	1508	<div> <div>2%</div> <div>54% 36% 8% ..</div> </div>
1	XA	1508	<div> <div>2%</div> <div>54% 35% 8% ..</div> </div>
2	QB	256	<div> <div>2%</div> <div>70% 21% 8%</div> </div>
2	XB	256	<div> <div>2%</div> <div>74% 18% 8%</div> </div>

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Mol	Chain	Length	Quality of chain
3	QC	239	
3	XC	239	
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126	
13	XM	126	
14	QN	61	
14	XN	61	
15	QO	89	

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Mol	Chain	Length	Quality of chain
15	XO	89	
16	QP	88	
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	QW	77	
22	XV	77	
22	XW	77	
23	QX	25	
23	XX	25	
24	QY	17	
24	XY	17	
25	RA	2915	
25	YA	2915	
26	RB	122	
26	YB	122	

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Mol	Chain	Length	Quality of chain
27	RD	276	
27	YD	276	
28	RE	206	
28	YE	206	
29	RF	210	
29	YF	210	
30	RG	182	
30	YG	182	
31	RH	180	
31	YH	180	
32	RI	148	
32	YI	148	
33	RN	140	
33	YN	140	
34	RO	122	
34	YO	122	
35	RP	150	
35	YP	150	
36	RQ	141	
36	YQ	141	
37	RR	118	
37	YR	118	
38	RS	112	
38	YS	112	
39	RT	146	

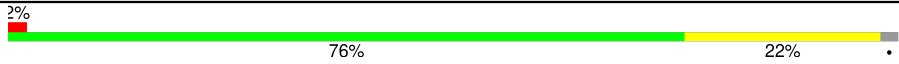
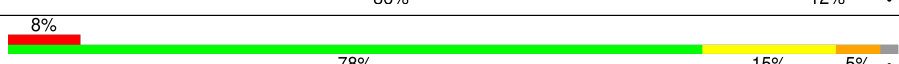

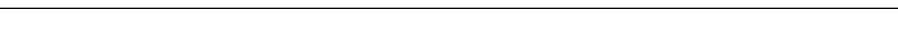
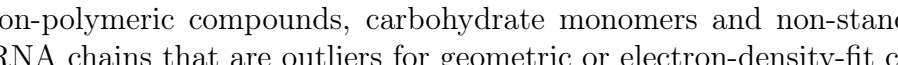
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Mol	Chain	Length	Quality of chain
39	YT	146	
40	RU	118	
40	YU	118	
41	RV	101	
41	YV	101	
42	RW	113	
42	YW	113	
43	RX	96	
43	YX	96	
44	RY	110	
44	YY	110	
45	RZ	206	
45	YZ	206	
46	R0	85	
46	Y0	85	
47	R1	98	
47	Y1	98	
48	R2	72	
48	Y2	72	
49	R3	60	
49	Y3	60	
50	R4	71	
50	Y4	71	
51	R5	60	
51	Y5	60	

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Mol	Chain	Length	Quality of chain
52	R6	54	
52	Y6	54	
53	R7	49	
53	Y7	49	
54	R8	65	
54	Y8	65	
55	R9	37	
55	Y9	37	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	RA	3213	-	-	-	X
56	MG	RA	3409	-	-	-	X
56	MG	YA	3520	-	-	-	X

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 295646 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QA	1500	Total	C	N	O	P	0	0	0
			32244	14352	5978	10415	1499			
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	QW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	XV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			
22	XW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	8	Total	C	N	O	P	0	0	0
			167	75	27	57	8			
23	XX	11	Total	C	N	O	P	0	0	0
			230	105	42	73	10			

- Molecule 24 is a RNA chain called ASL Leu.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	17	Total	C	N	O	P	0	0	0
			362	162	65	118	17			
24	XY	17	Total	C	N	O	P	0	0	0
			362	162	65	118	17			

- Molecule 25 is a RNA chain called 23S rRNA.

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

- Molecule 26 is a RNA chain called 5S rRNA.

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

- Molecule 27 is a protein called 50S ribosomal protein L2.

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

- Molecule 28 is a protein called 50S ribosomal protein L3.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

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

- Molecule 31 is a protein called 50S ribosomal protein L6.

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

- Molecule 32 is a protein called 50S ribosomal protein L9.

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

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

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

- Molecule 35 is a protein called 50S ribosomal protein L15.

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

- Molecule 36 is a protein called 50S ribosomal protein L16.

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

- Molecule 37 is a protein called 50S ribosomal protein L17.

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

- Molecule 38 is a protein called 50S ribosomal protein L18.

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

- Molecule 39 is a protein called 50S ribosomal protein L19.

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

- Molecule 40 is a protein called 50S ribosomal protein L20.

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

- Molecule 41 is a protein called 50S ribosomal protein L21.

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

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

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

- Molecule 44 is a protein called 50S ribosomal protein L24.

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

- Molecule 45 is a protein called 50S ribosomal protein L25.

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

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	R0	81	Total	C	N	O	S	0	0	0
			643	398	137	107	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	Y0	75	Total	C	N	O	S	0	0	0
			599	370	127	101	1			

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

- Molecule 48 is a protein called 50S ribosomal protein L29.

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

- Molecule 49 is a protein called 50S ribosomal protein L30.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L32.

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

- Molecule 52 is a protein called 50S ribosomal protein L33.

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

- Molecule 53 is a protein called 50S ribosomal protein L34.

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

- Molecule 54 is a protein called 50S ribosomal protein L35.

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

- Molecule 55 is a protein called 50S ribosomal protein L36.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QA	72	Total	Mg	0	0
			72	72		
56	QC	1	Total	Mg	0	0
			1	1		
56	QF	1	Total	Mg	0	0
			1	1		
56	QH	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QV	6	Total 6	Mg 6	0	0
56	QX	1	Total 1	Mg 1	0	0
56	QY	1	Total 1	Mg 1	0	0
56	RA	513	Total 513	Mg 513	0	0
56	RB	11	Total 11	Mg 11	0	0
56	RE	3	Total 3	Mg 3	0	0
56	RN	1	Total 1	Mg 1	0	0
56	RO	1	Total 1	Mg 1	0	0
56	RP	2	Total 2	Mg 2	0	0
56	RQ	2	Total 2	Mg 2	0	0
56	RR	2	Total 2	Mg 2	0	0
56	RT	1	Total 1	Mg 1	0	0
56	RY	1	Total 1	Mg 1	0	0
56	R0	3	Total 3	Mg 3	0	0
56	R8	1	Total 1	Mg 1	0	0
56	XA	80	Total 80	Mg 80	0	0
56	XC	1	Total 1	Mg 1	0	0
56	XE	1	Total 1	Mg 1	0	0
56	XL	1	Total 1	Mg 1	0	0
56	XM	1	Total 1	Mg 1	0	0
56	XQ	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	XS	1	Total 1	Mg 1	0	0
56	XV	8	Total 8	Mg 8	0	0
56	XX	1	Total 1	Mg 1	0	0
56	YA	541	Total 541	Mg 541	0	0
56	YB	12	Total 12	Mg 12	0	0
56	YD	1	Total 1	Mg 1	0	0
56	YE	3	Total 3	Mg 3	0	0
56	YO	1	Total 1	Mg 1	0	0
56	YP	4	Total 4	Mg 4	0	0
56	YQ	3	Total 3	Mg 3	0	0
56	YX	2	Total 2	Mg 2	0	0
56	YY	1	Total 1	Mg 1	0	0
56	Y0	2	Total 2	Mg 2	0	0
56	Y5	1	Total 1	Mg 1	0	0
56	Y7	1	Total 1	Mg 1	0	0
56	Y8	1	Total 1	Mg 1	0	0

- Molecule 57 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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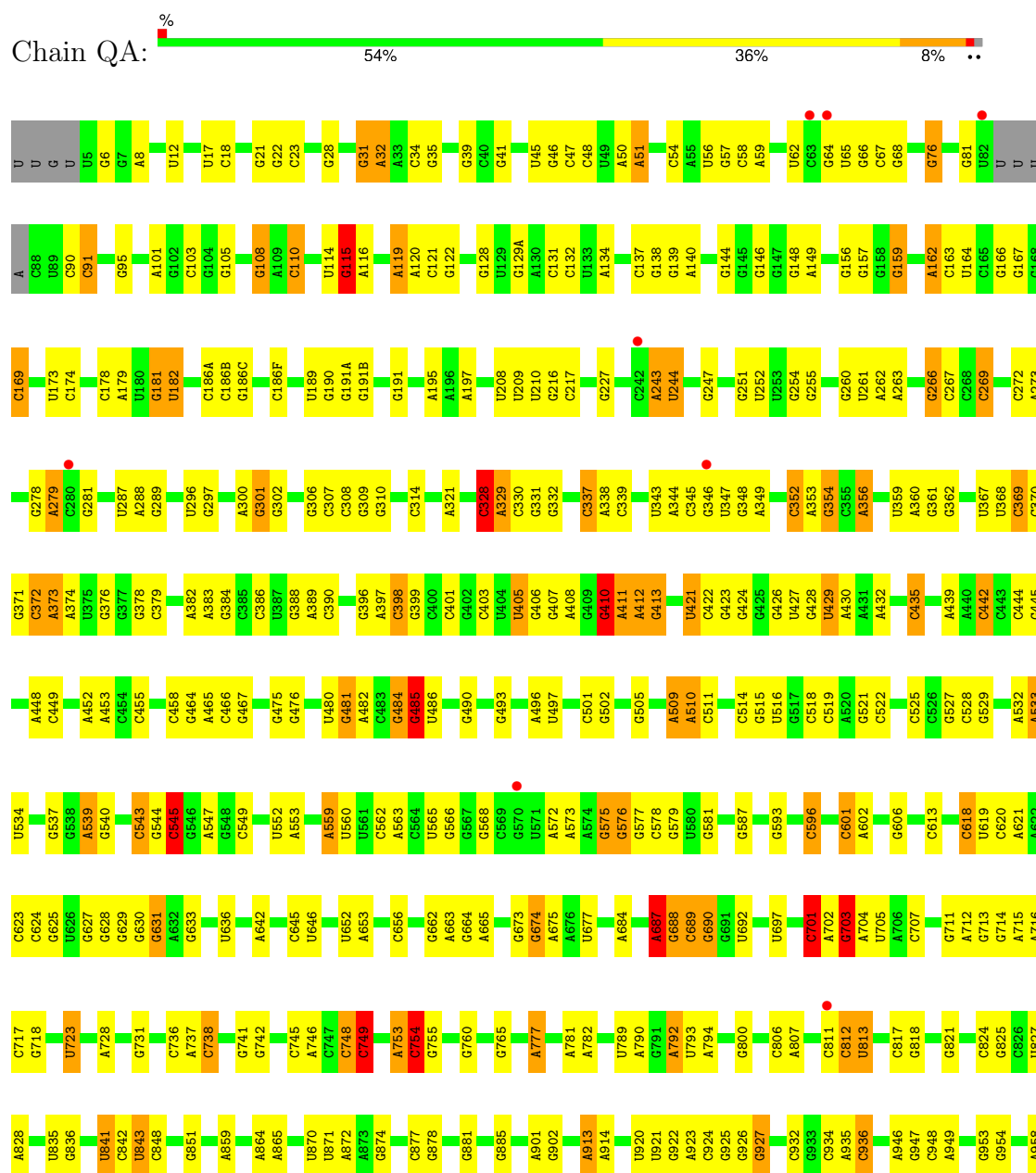
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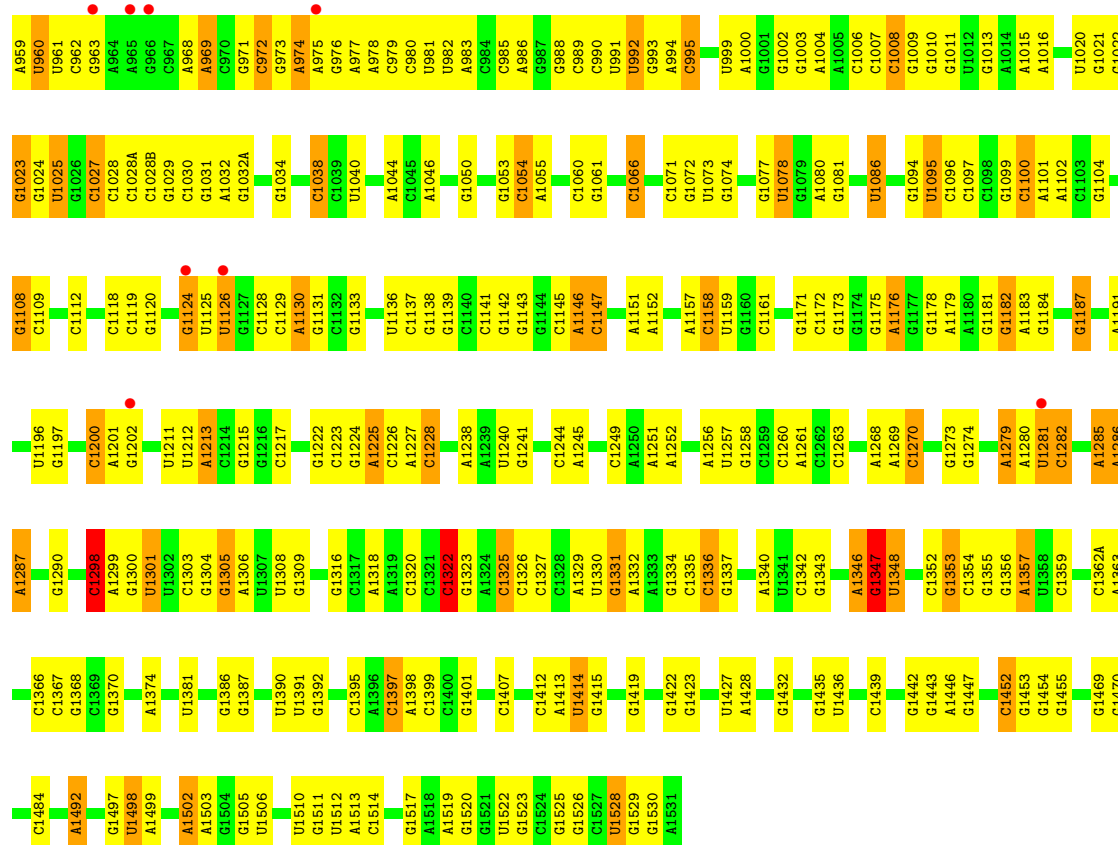
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	Y6	1	Total 1	Zn 1	0	0
58	Y9	1	Total 1	Zn 1	0	0

3 Residue-property plots

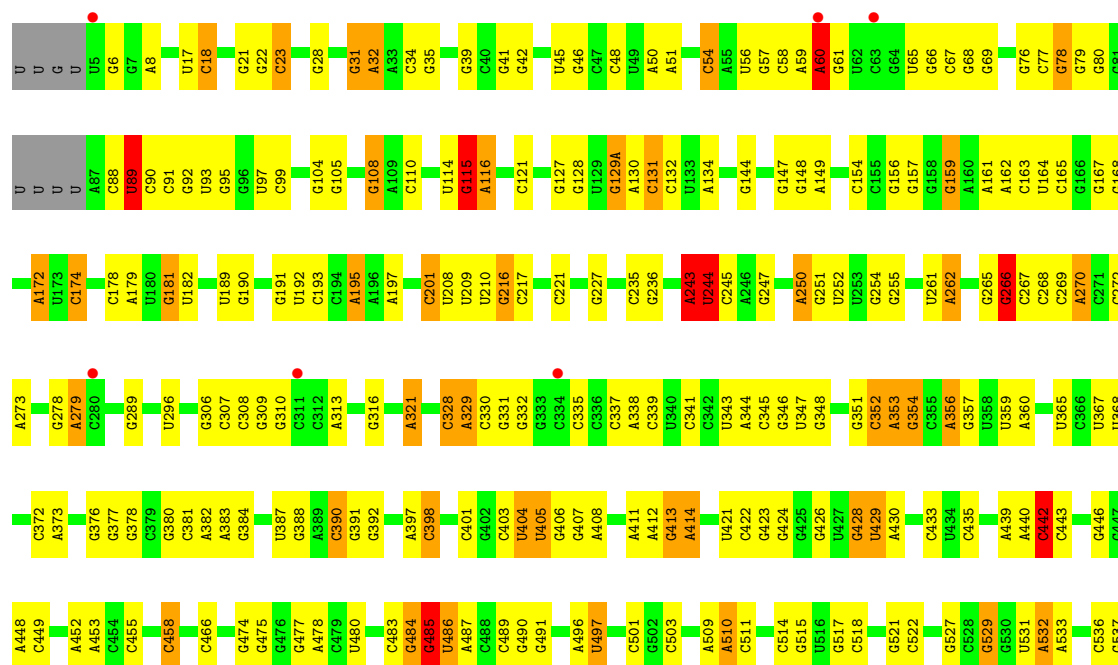
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

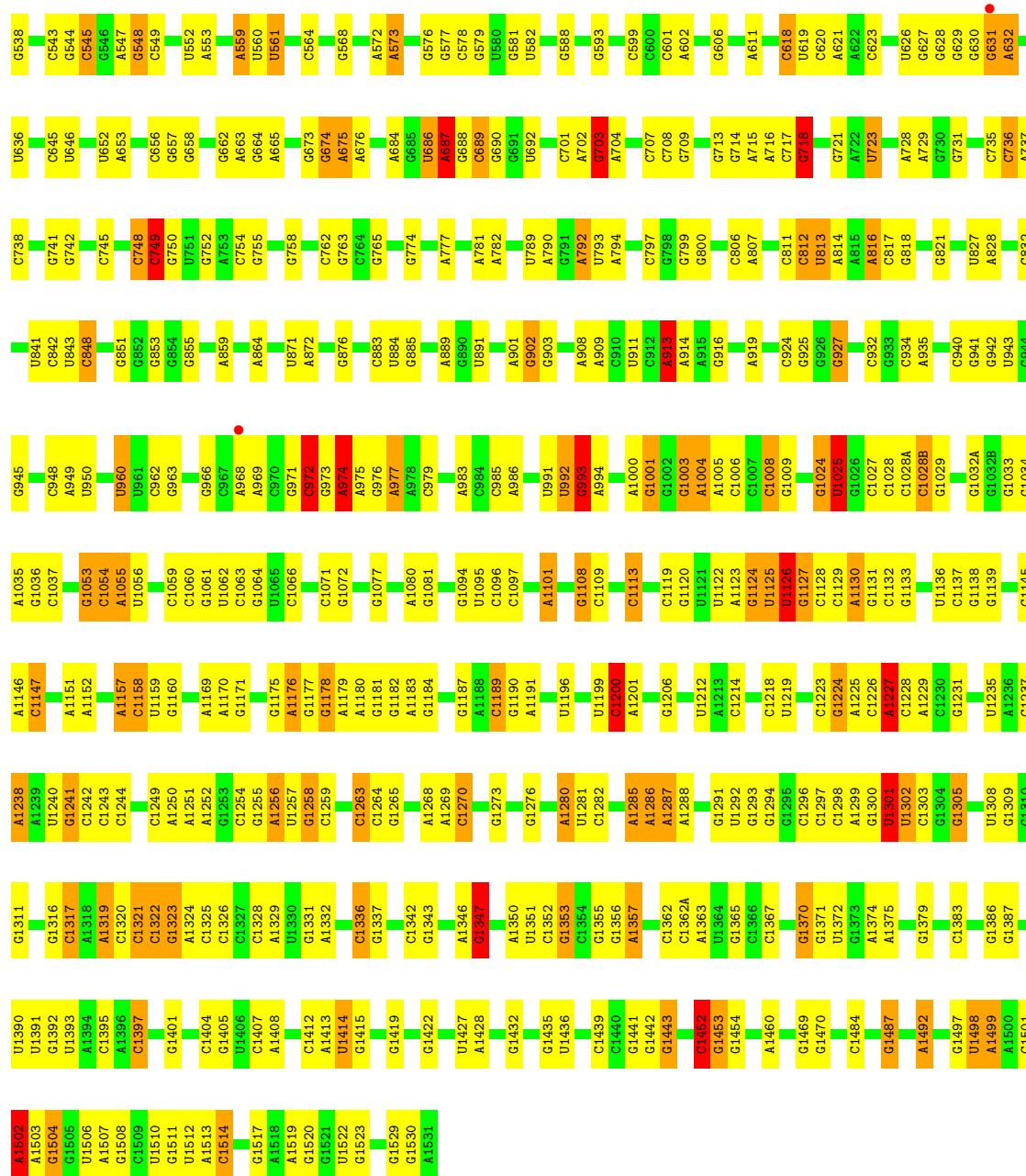
• Molecule 1: 16S rRNA



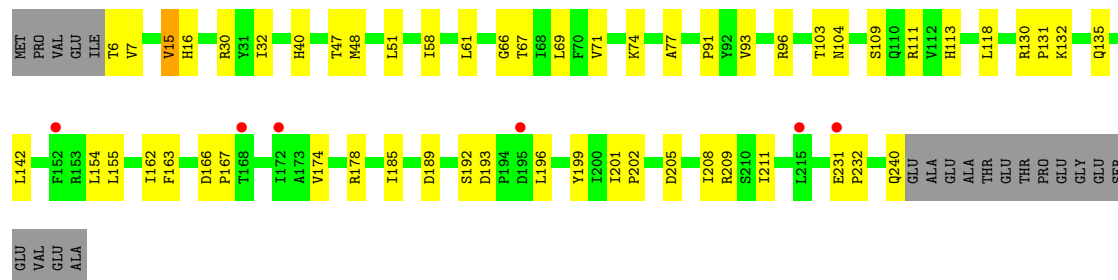
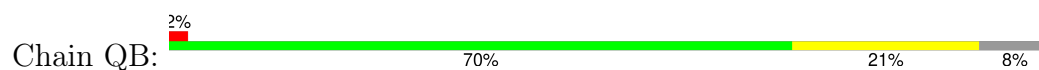


• Molecule 1: 16S rRNA

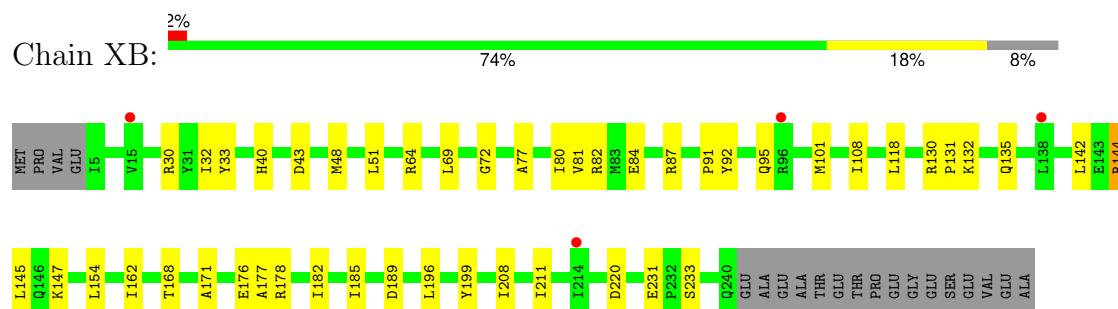




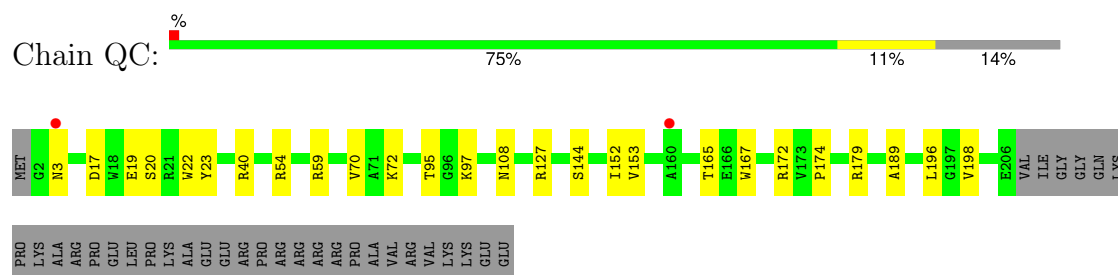
• Molecule 2: 30S ribosomal protein S2



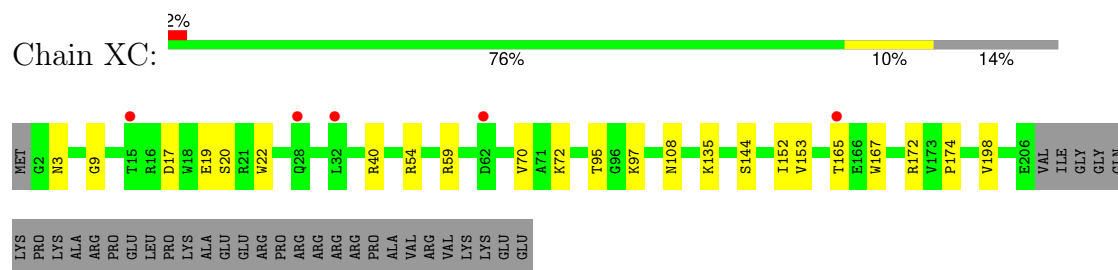
- Molecule 2: 30S ribosomal protein S2



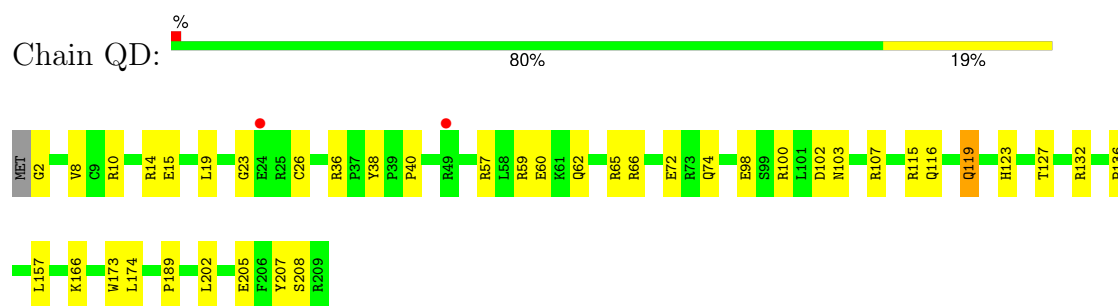
- Molecule 3: 30S ribosomal protein S3



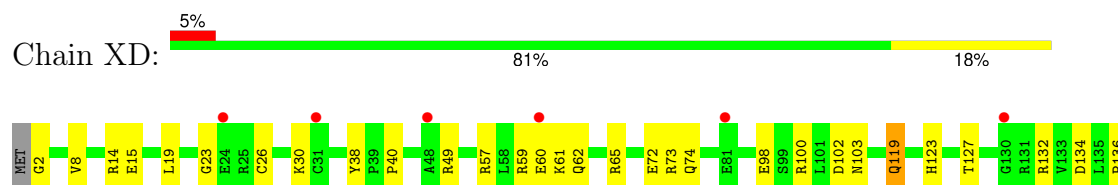
- Molecule 3: 30S ribosomal protein S3



- Molecule 4: 30S ribosomal protein S4

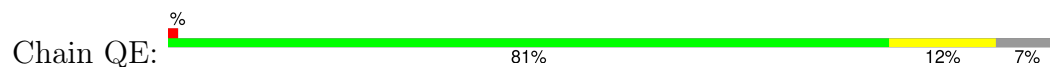


- Molecule 4: 30S ribosomal protein S4

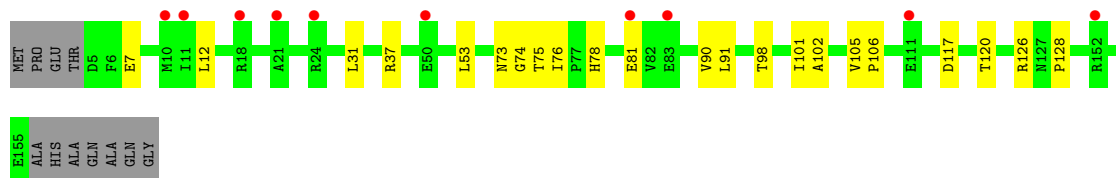
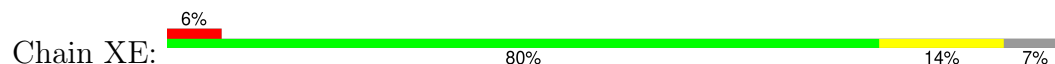




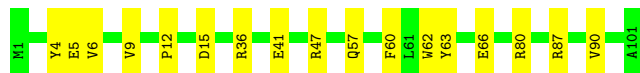
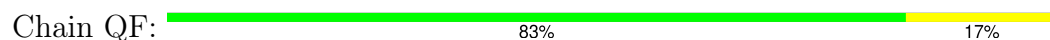
- Molecule 5: 30S ribosomal protein S5



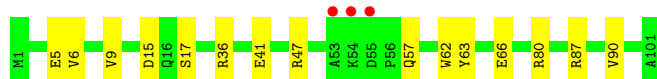
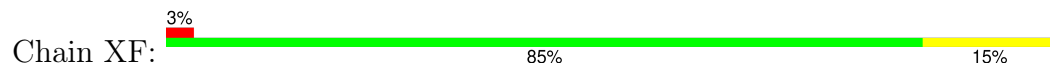
- Molecule 5: 30S ribosomal protein S5



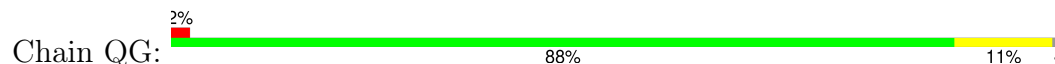
- Molecule 6: 30S ribosomal protein S6



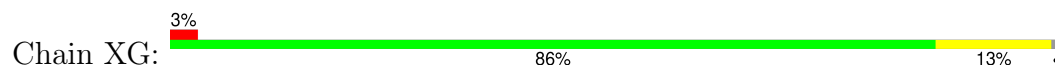
- Molecule 6: 30S ribosomal protein S6



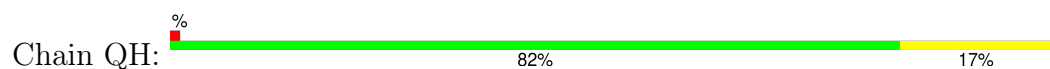
- Molecule 7: 30S ribosomal protein S7



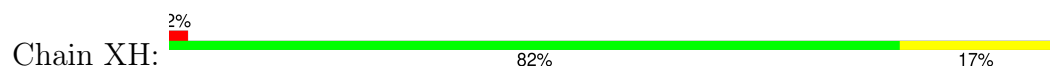
- Molecule 7: 30S ribosomal protein S7



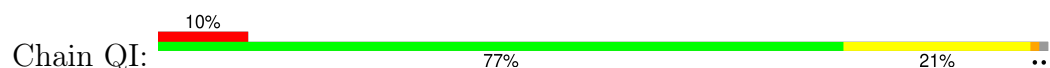
- Molecule 8: 30S ribosomal protein S8



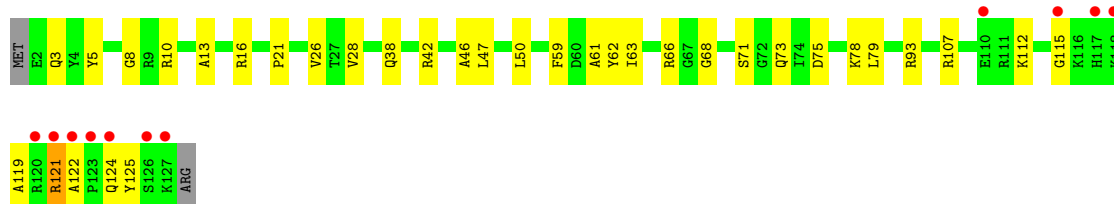
- Molecule 8: 30S ribosomal protein S8



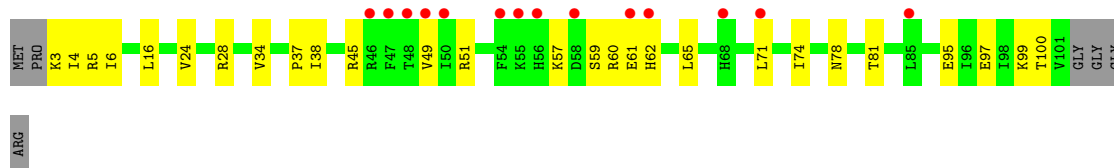
- Molecule 9: 30S ribosomal protein S9



- Molecule 9: 30S ribosomal protein S9



- Molecule 10: 30S ribosomal protein S10




- Molecule 10: 30S ribosomal protein S10




VAL
GLY
GLY
GLY
ARG

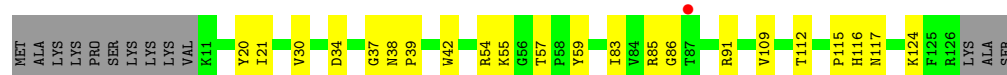
- Molecule 11: 30S ribosomal protein S11

Chain QK: 




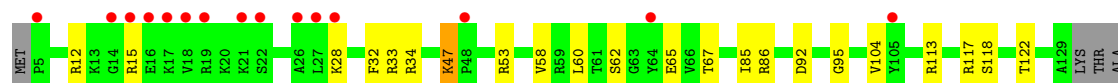
- Molecule 11: 30S ribosomal protein S11

Chain XK: 




- Molecule 12: 30S ribosomal protein S12

Chain QL: 



ALA
LYS
LYS


- Molecule 12: 30S ribosomal protein S12

Chain XL: 



ALA
ALA
LYS
THR
ALA
LYS
LYS

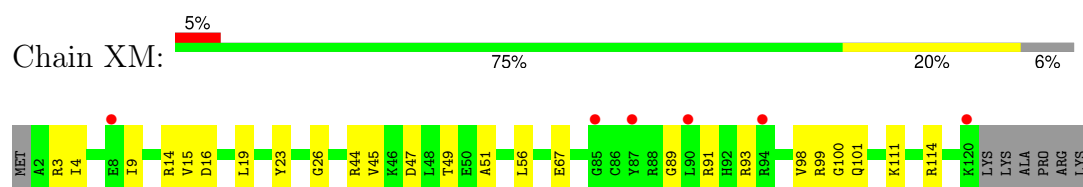
- Molecule 13: 30S ribosomal protein S13

Chain QM: 

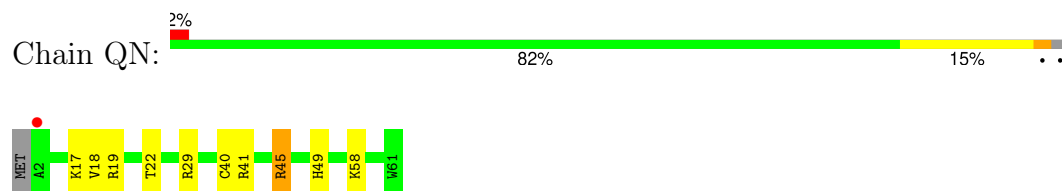


PRO
ARG
LYS

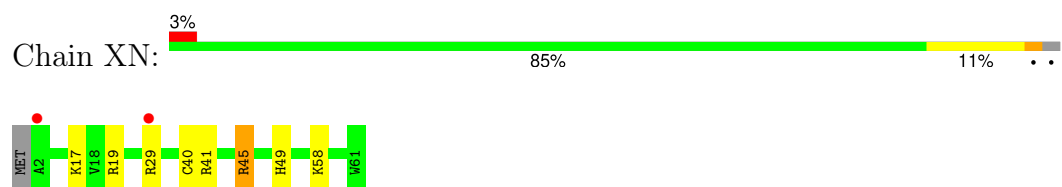
- Molecule 13: 30S ribosomal protein S13



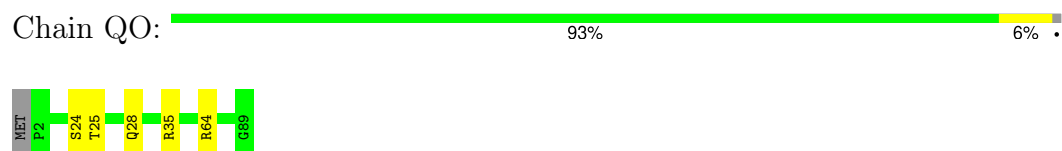
- Molecule 14: 30S ribosomal protein S14 type Z



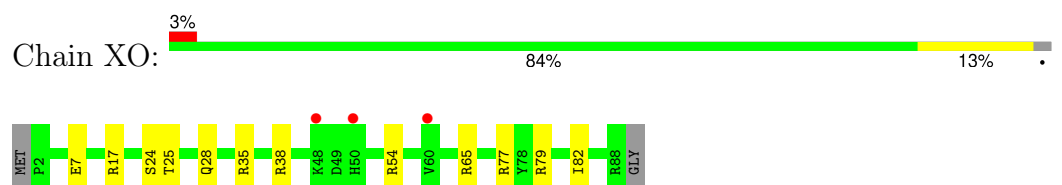
- Molecule 14: 30S ribosomal protein S14 type Z



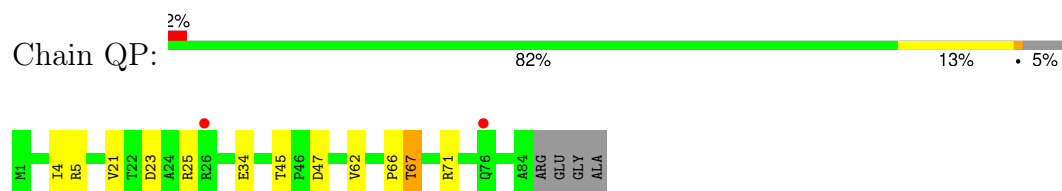
- Molecule 15: 30S ribosomal protein S15



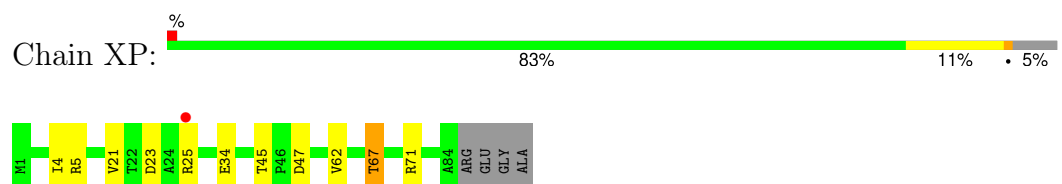
- Molecule 15: 30S ribosomal protein S15



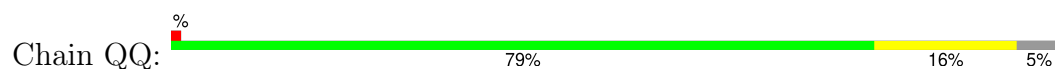
- Molecule 16: 30S ribosomal protein S16



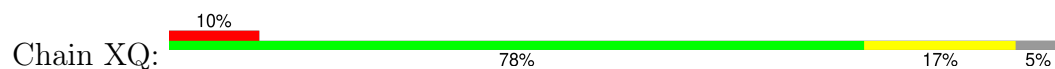
- Molecule 16: 30S ribosomal protein S16



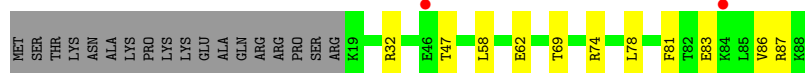
- Molecule 17: 30S ribosomal protein S17



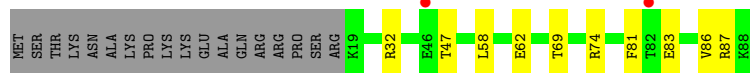
- Molecule 17: 30S ribosomal protein S17



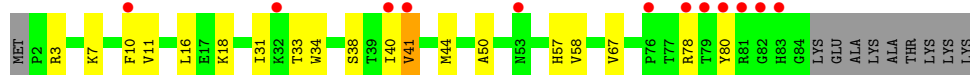
- Molecule 18: 30S ribosomal protein S18



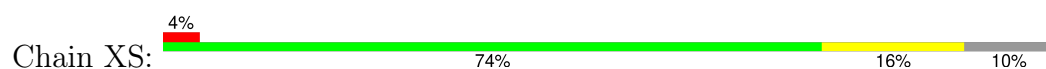
- Molecule 18: 30S ribosomal protein S18



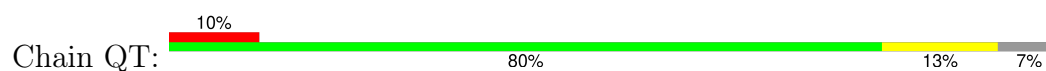
- Molecule 19: 30S ribosomal protein S19

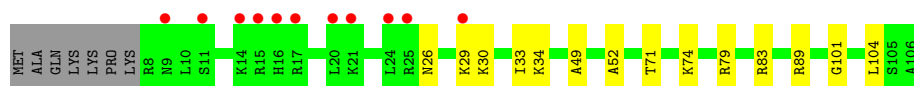


- Molecule 19: 30S ribosomal protein S19

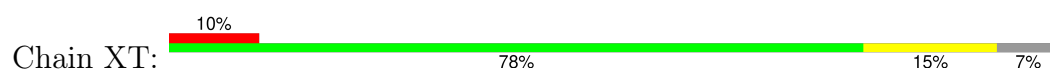


- Molecule 20: 30S ribosomal protein S20





- Molecule 20: 30S ribosomal protein S20



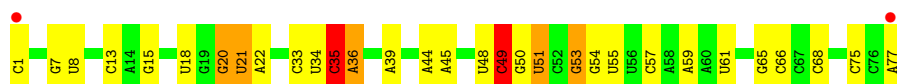
- Molecule 21: 30S ribosomal protein Thx



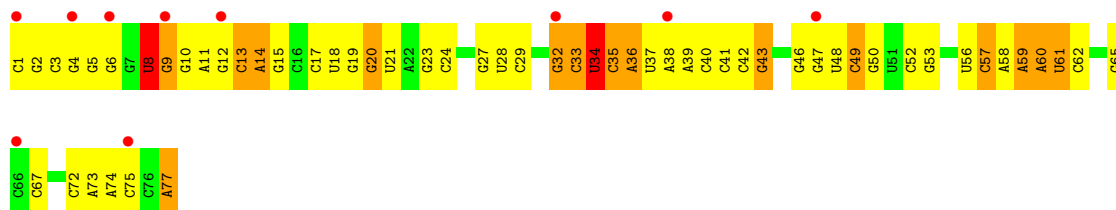
- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: tRNA fMet



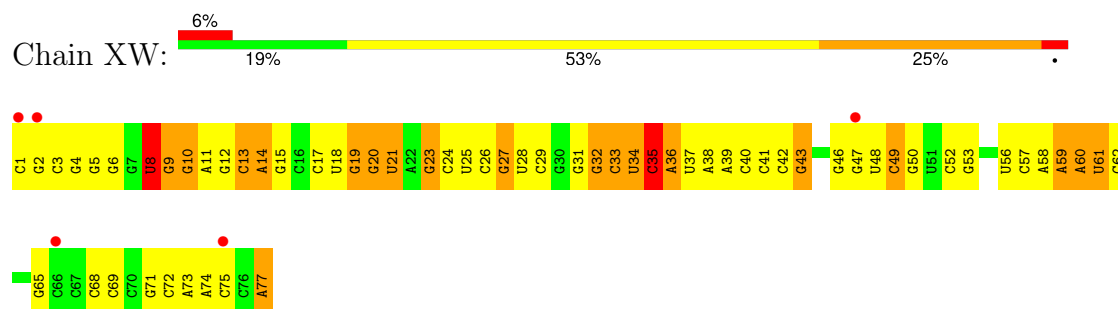
- Molecule 22: tRNA fMet



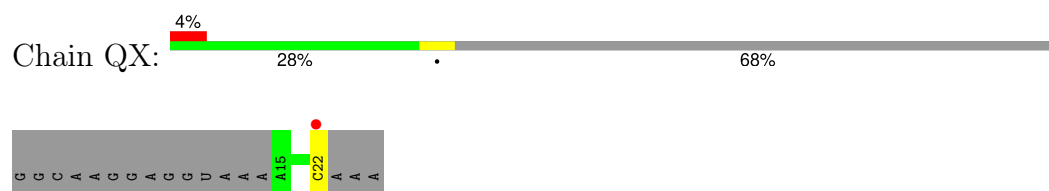
- Molecule 22: tRNA fMet



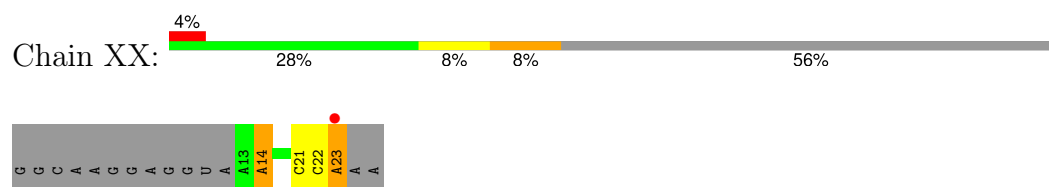
- Molecule 22: tRNA fMet



- Molecule 23: messenger RNA



- Molecule 23: messenger RNA



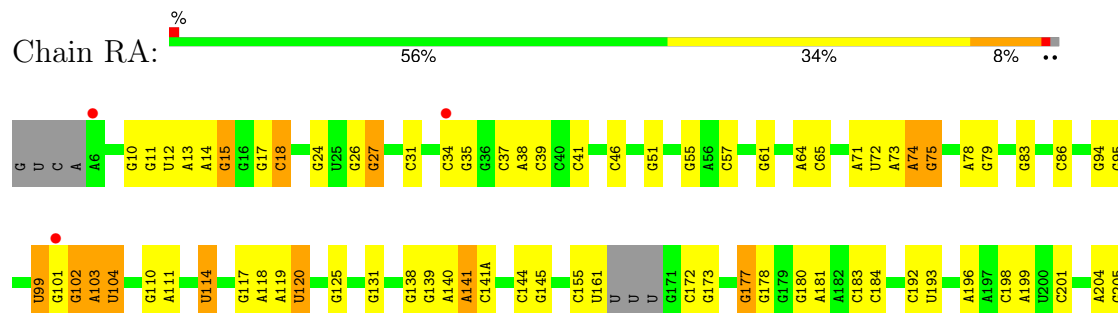
- Molecule 24: ASL Leu



- Molecule 24: ASL Leu

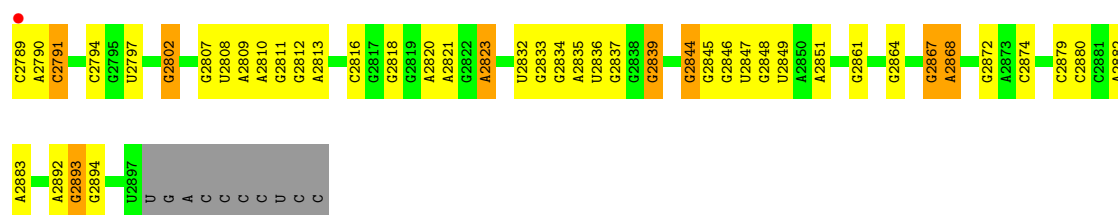


- Molecule 25: 23S rRNA

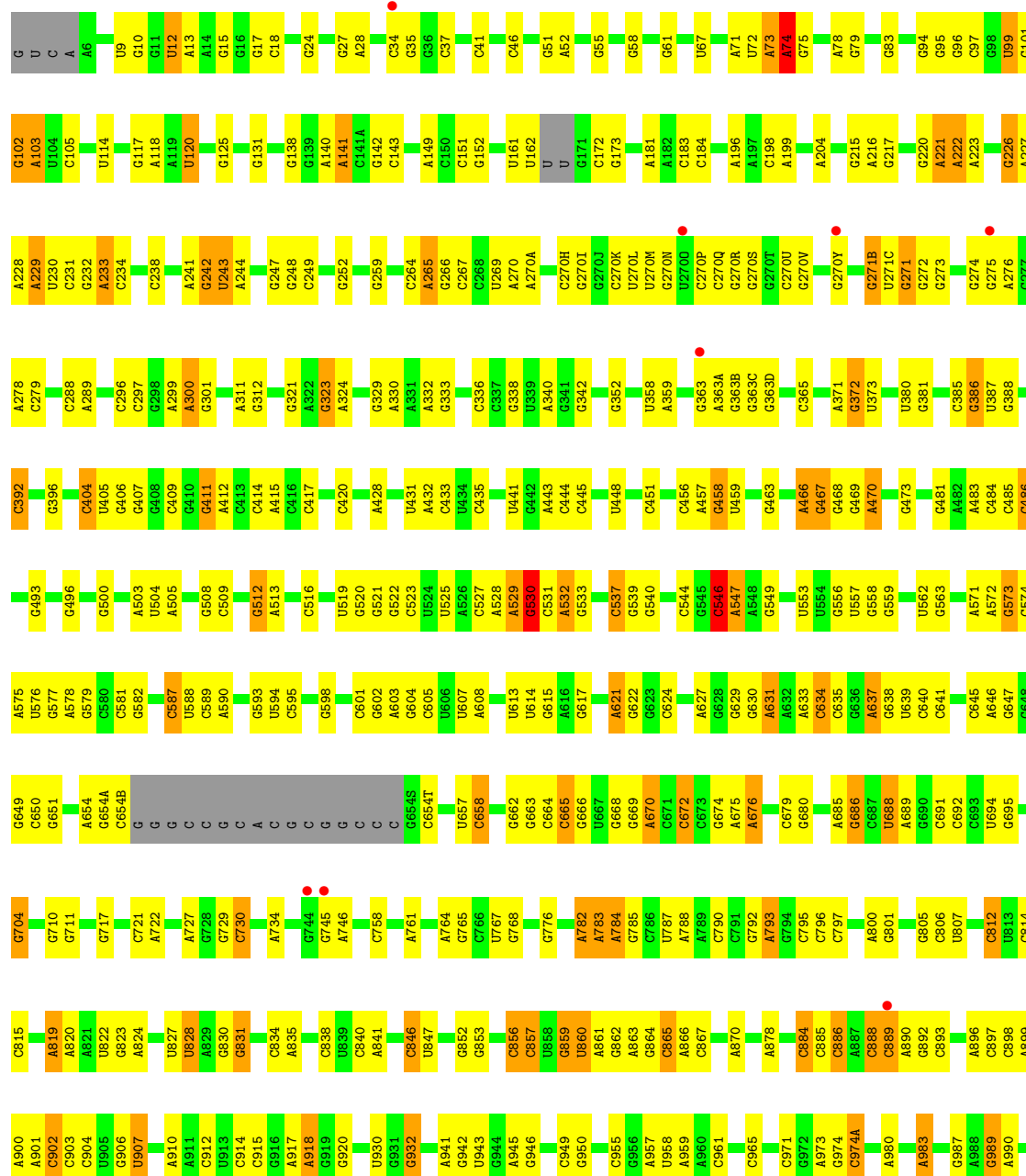




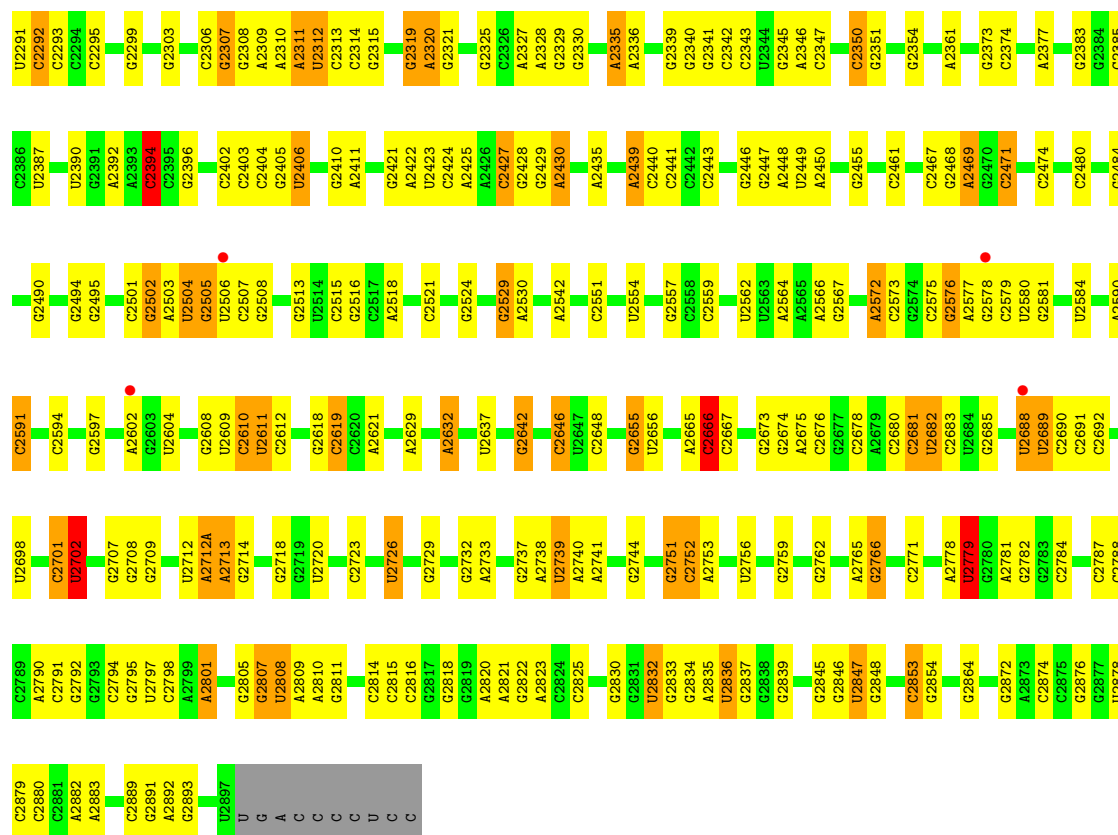
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G2708	G2618	G2519	A2430	G2239	G2141	A2060	U1956	G1846	G1763	C1644	A1545	
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G2713	C2626	C2539	A2335	U2246	C2147	C2065	U1963	A1853	G1773	G1651	C1554	C1462
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G2718	C2628	A2542	G2444	U2249	U2150	U2068	A1966	A1859	G1776	C1657	G1559	G1472
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G2731	U2637	C2556		A2269	C2162	A2082	C1979		A1785	A1664	U1578	G1484
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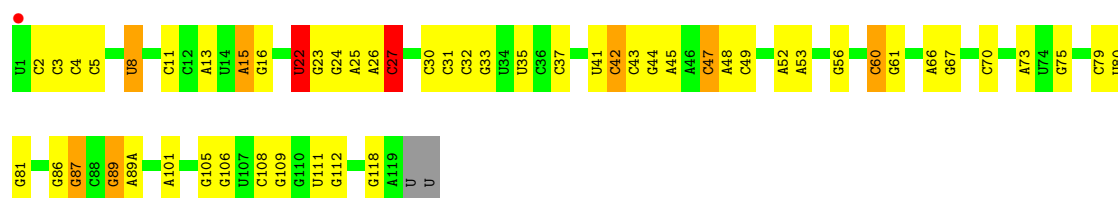
• Molecule 25: 23S rRNA



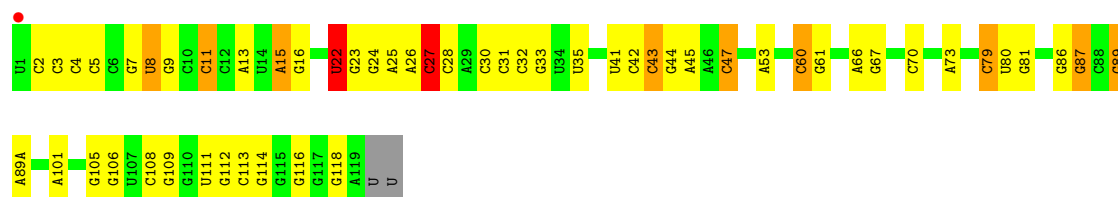




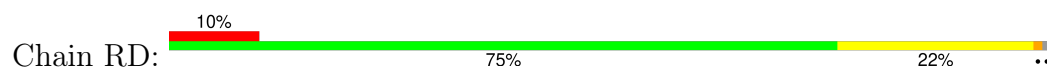
• Molecule 26: 5S rRNA

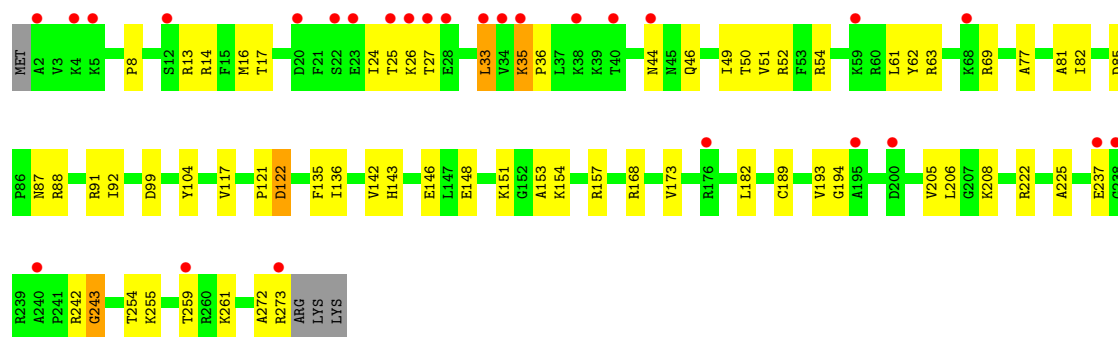


• Molecule 26: 5S rRNA

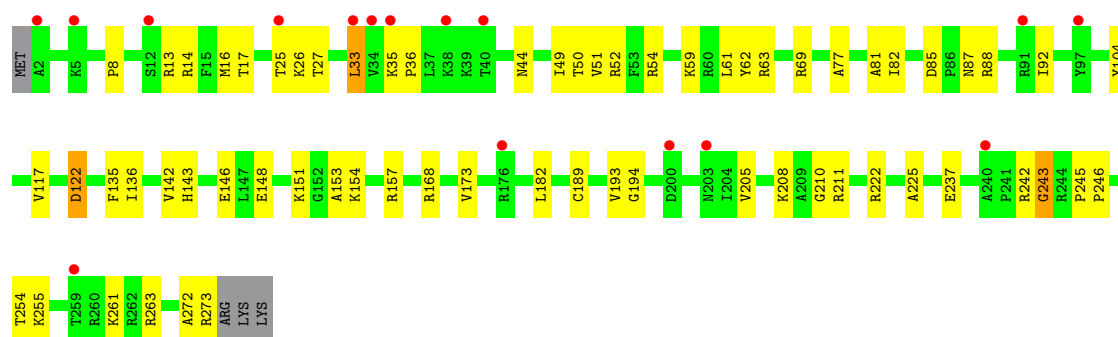
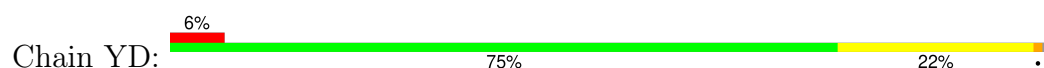


• Molecule 27: 50S ribosomal protein L2

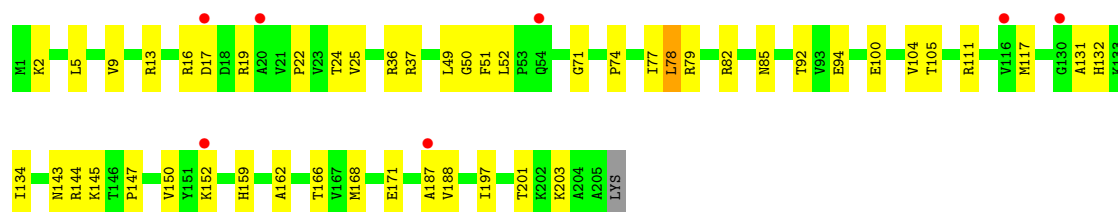
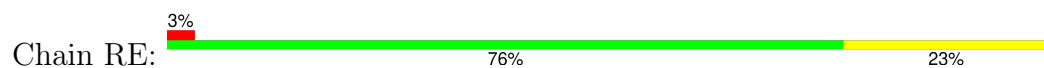




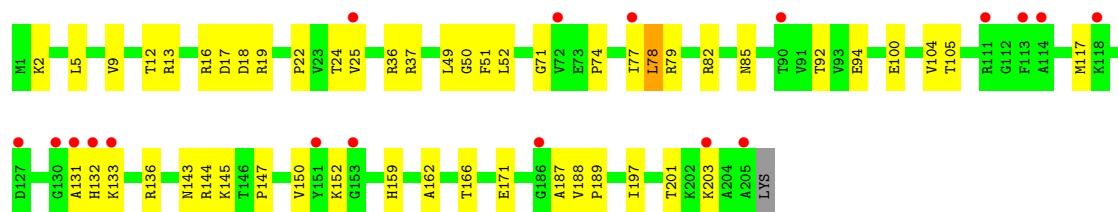
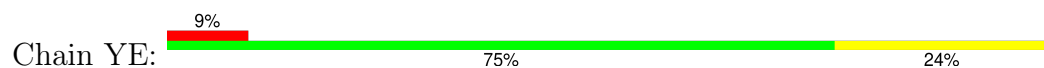
• Molecule 27: 50S ribosomal protein L2



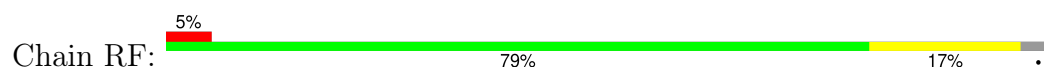
• Molecule 28: 50S ribosomal protein L3

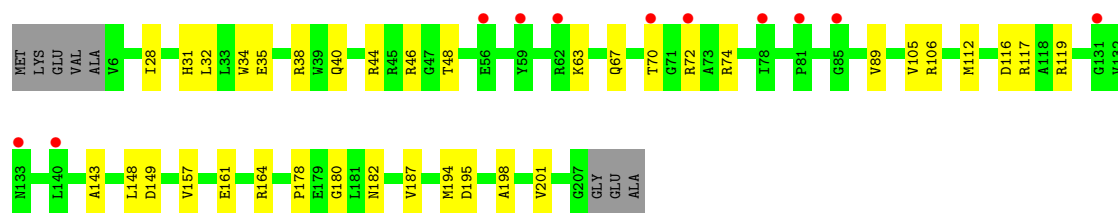


• Molecule 28: 50S ribosomal protein L3

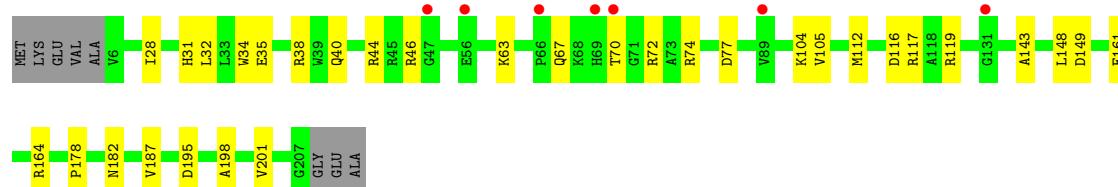
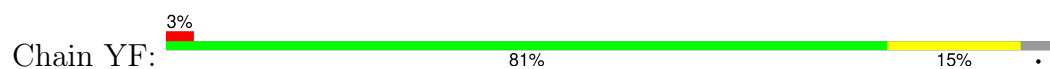


• Molecule 29: 50S ribosomal protein L4

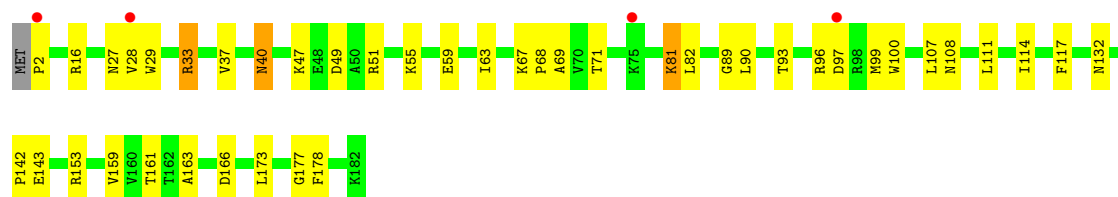
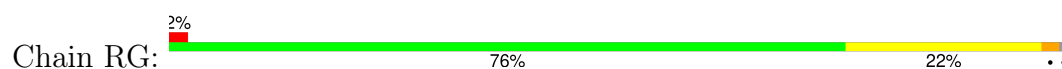




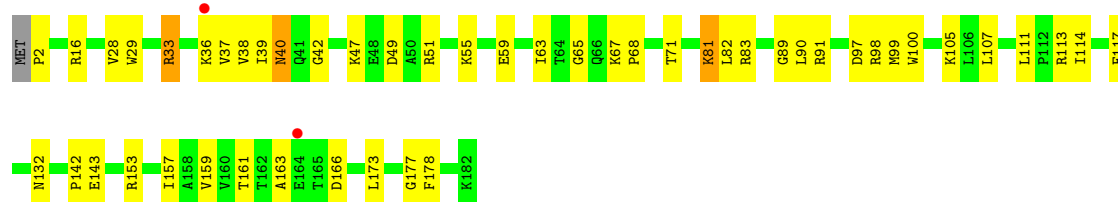
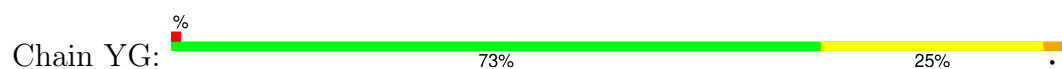
• Molecule 29: 50S ribosomal protein L4



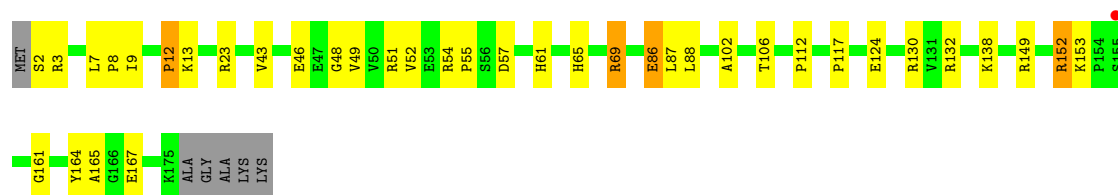
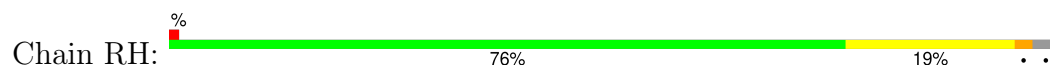
• Molecule 30: 50S ribosomal protein L5



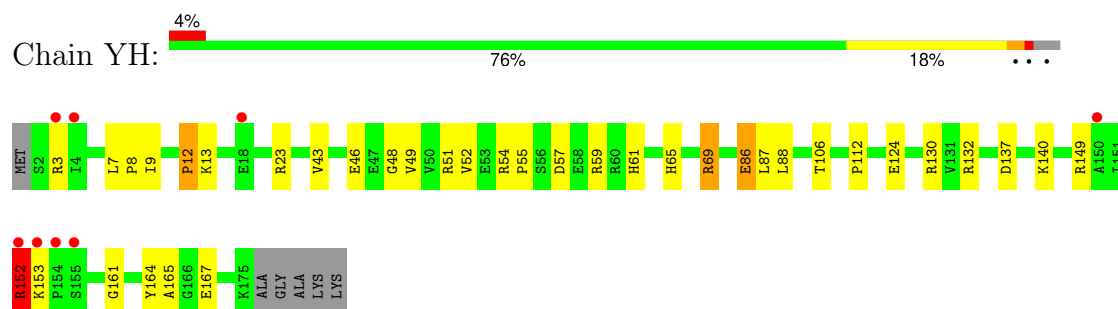
• Molecule 30: 50S ribosomal protein L5



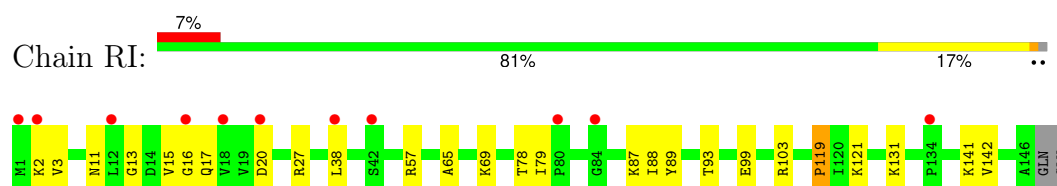
• Molecule 31: 50S ribosomal protein L6



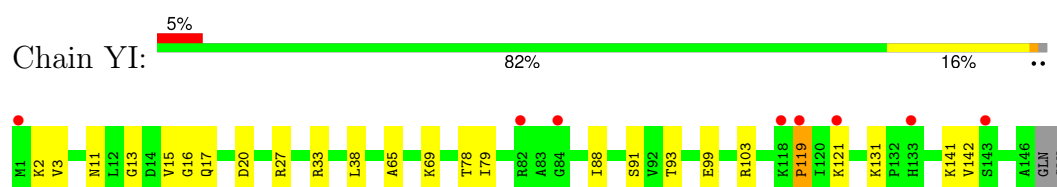
- Molecule 31: 50S ribosomal protein L6



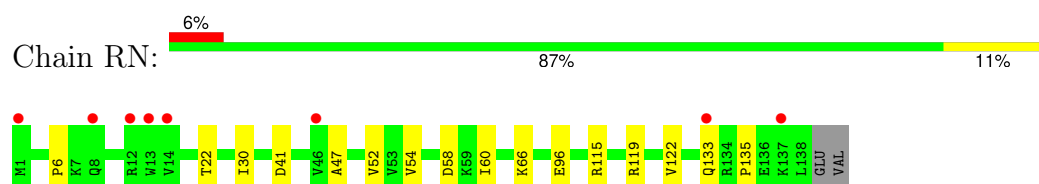
- Molecule 32: 50S ribosomal protein L9



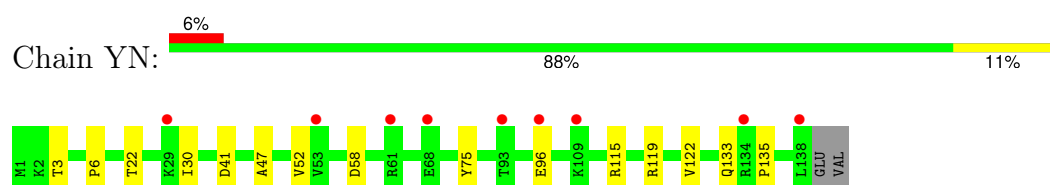
- Molecule 32: 50S ribosomal protein L9



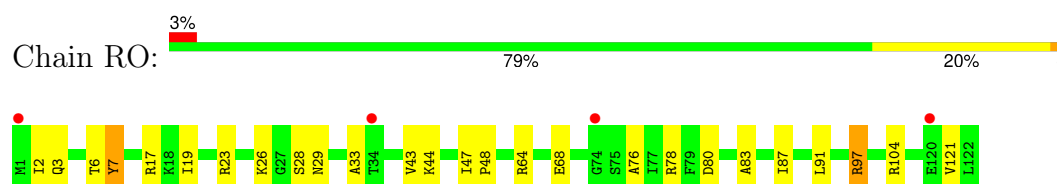
- Molecule 33: 50S ribosomal protein L13



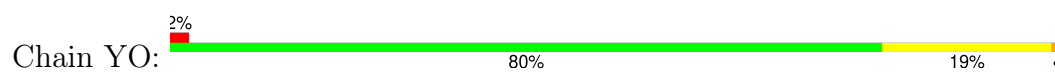
- Molecule 33: 50S ribosomal protein L13



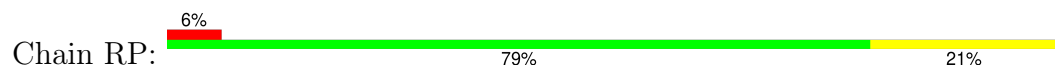
- Molecule 34: 50S ribosomal protein L14



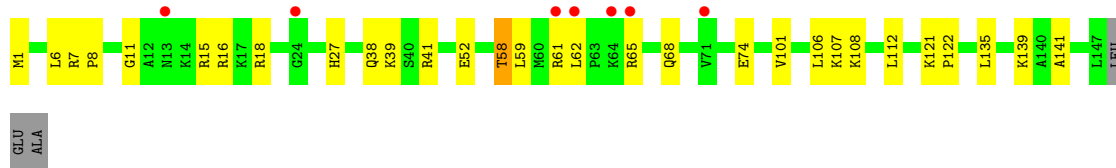
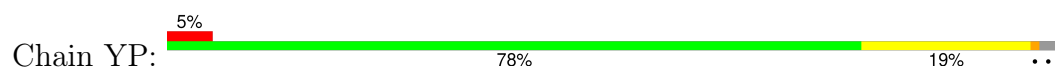
- Molecule 34: 50S ribosomal protein L14



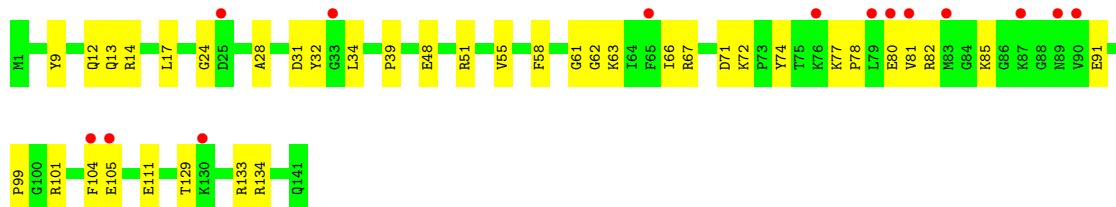
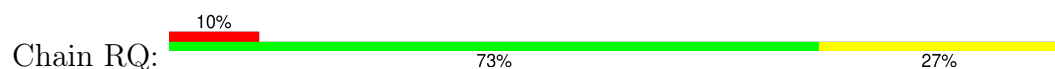
- Molecule 35: 50S ribosomal protein L15



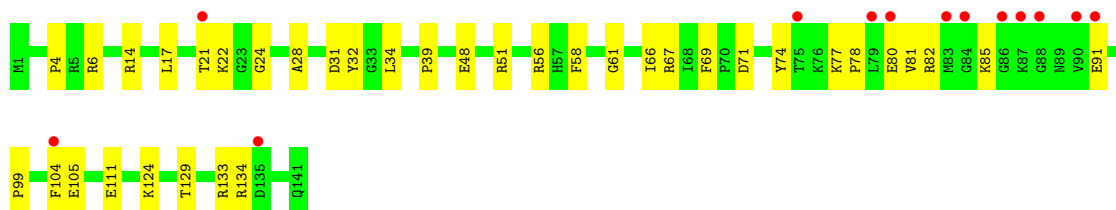
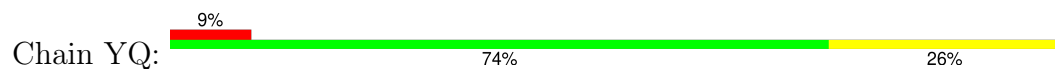
- Molecule 35: 50S ribosomal protein L15



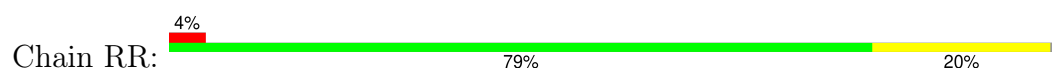
- Molecule 36: 50S ribosomal protein L16



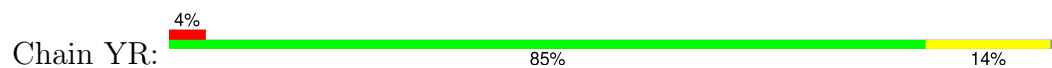
- Molecule 36: 50S ribosomal protein L16



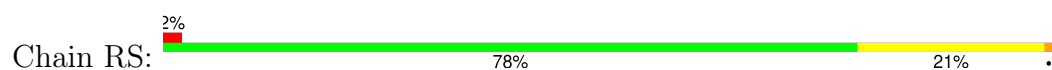
- Molecule 37: 50S ribosomal protein L17



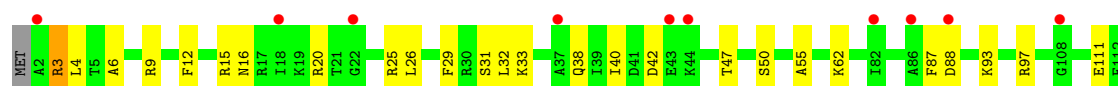
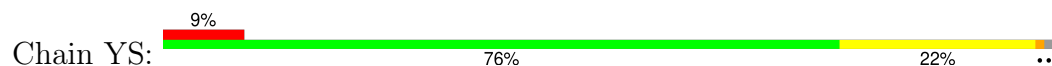
- Molecule 37: 50S ribosomal protein L17



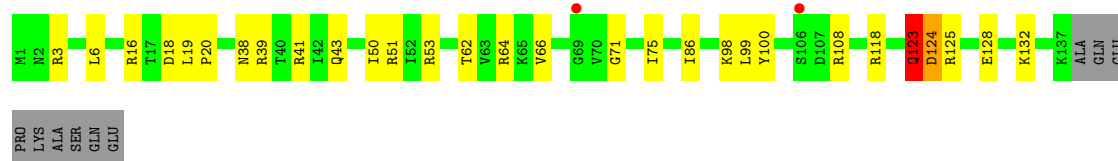
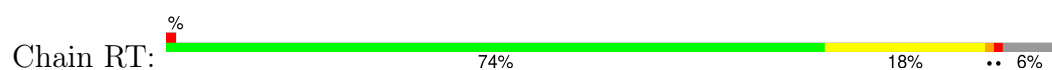
- Molecule 38: 50S ribosomal protein L18



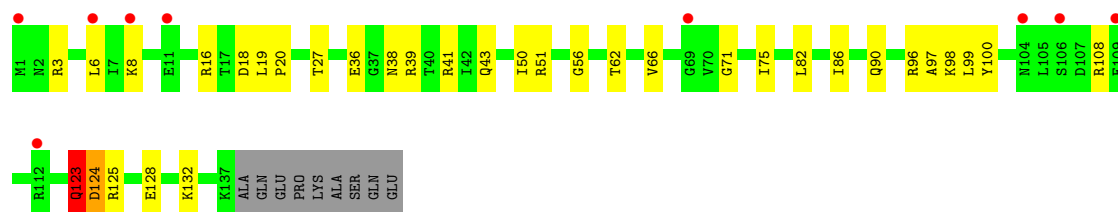
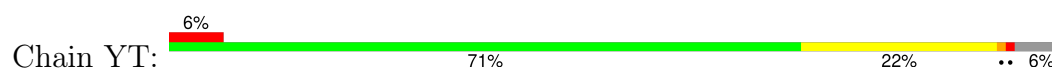
- Molecule 38: 50S ribosomal protein L18



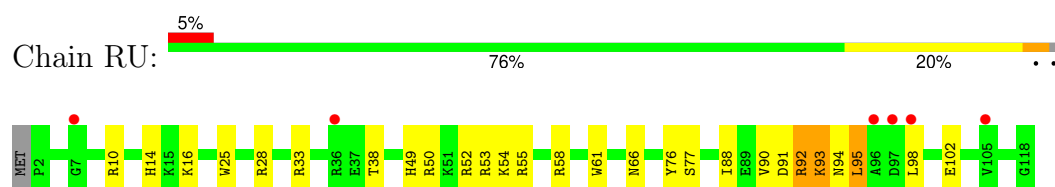
- Molecule 39: 50S ribosomal protein L19



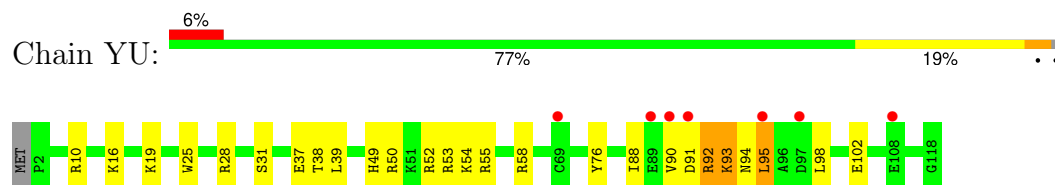
- Molecule 39: 50S ribosomal protein L19



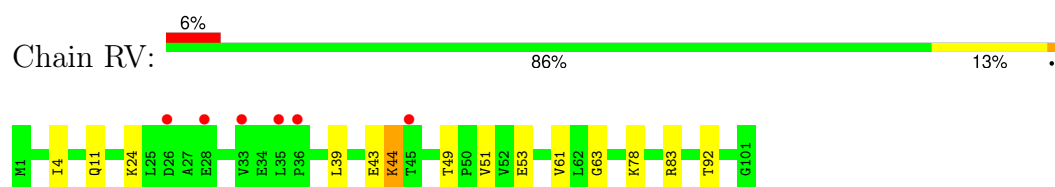
- Molecule 40: 50S ribosomal protein L20



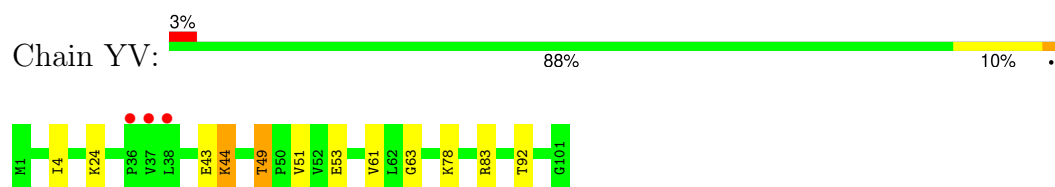
- Molecule 40: 50S ribosomal protein L20



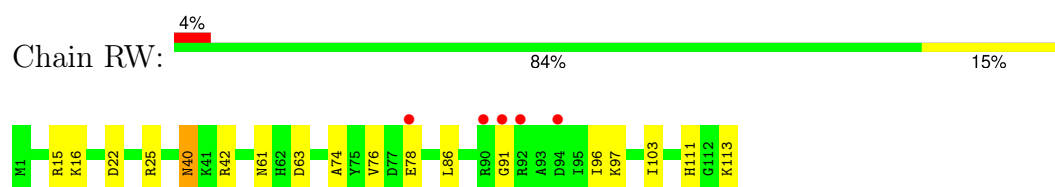
- Molecule 41: 50S ribosomal protein L21



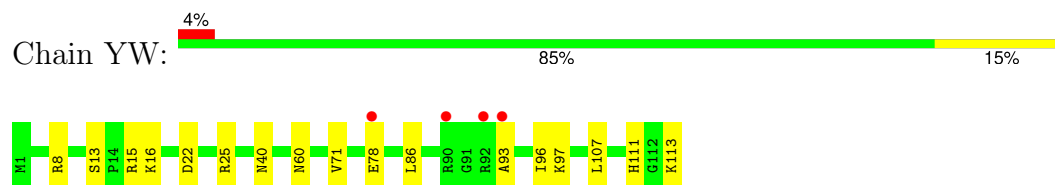
- Molecule 41: 50S ribosomal protein L21



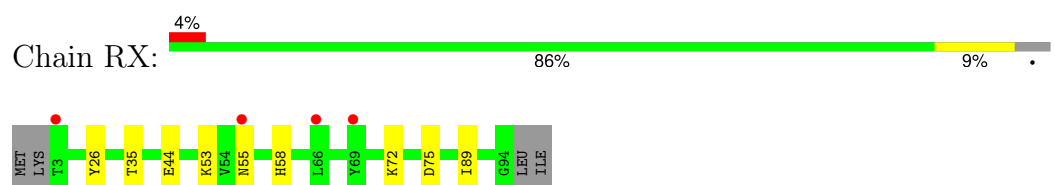
- Molecule 42: 50S ribosomal protein L22




- Molecule 42: 50S ribosomal protein L22



- Molecule 43: 50S ribosomal protein L23




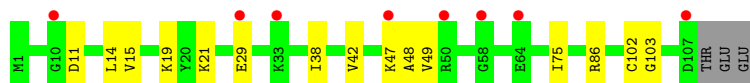
- Molecule 43: 50S ribosomal protein L23

Chain YX:  85% 10%




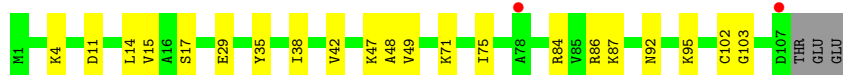
- Molecule 44: 50S ribosomal protein L24

Chain RY:  7% 84% 14%



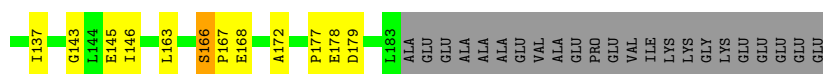
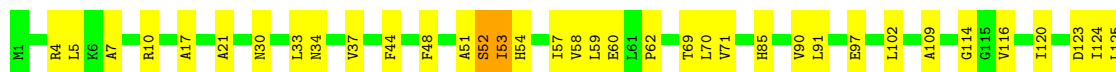
- Molecule 44: 50S ribosomal protein L24

Chain YY:  2% 78% 19%



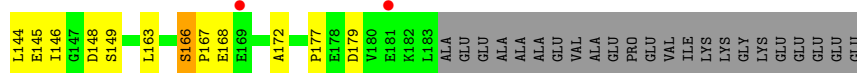
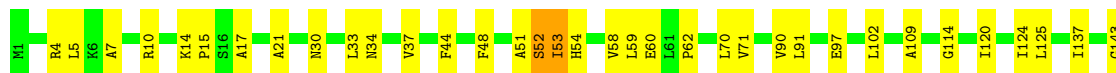
- Molecule 45: 50S ribosomal protein L25

Chain RZ:  66% 22% 11%




- Molecule 45: 50S ribosomal protein L25

Chain YZ:  66% 21% 11%

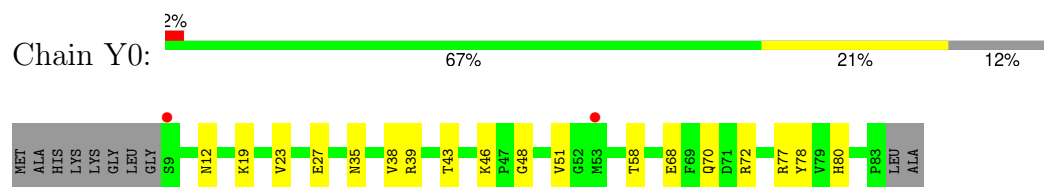


- Molecule 46: 50S ribosomal protein L27

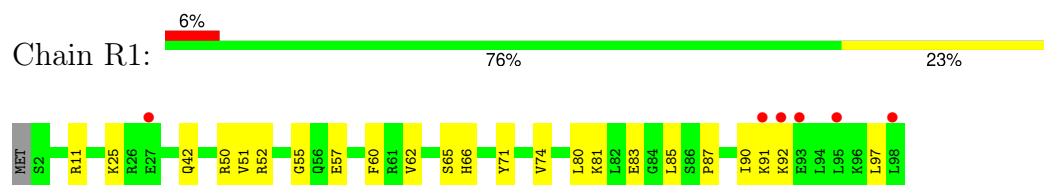
Chain R0:  6% 78% 18% 5%



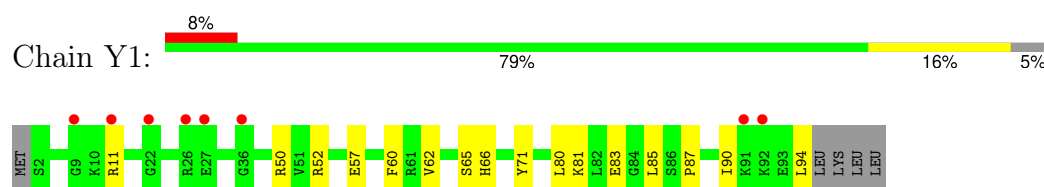
• Molecule 46: 50S ribosomal protein L27



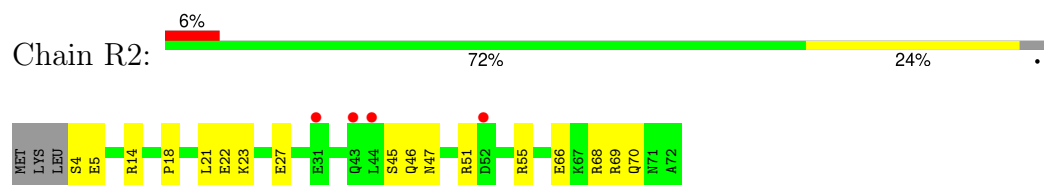
• Molecule 47: 50S ribosomal protein L28



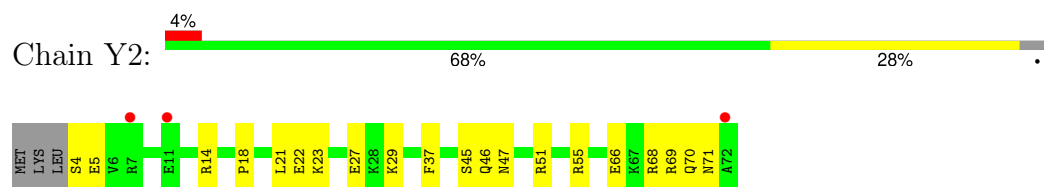
• Molecule 47: 50S ribosomal protein L28



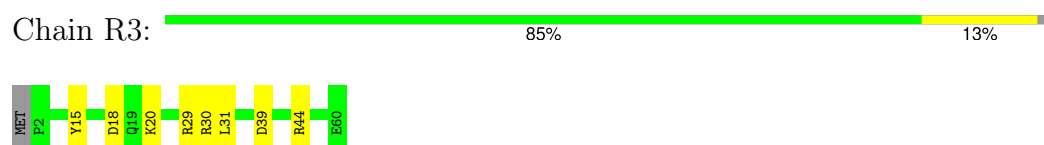
• Molecule 48: 50S ribosomal protein L29



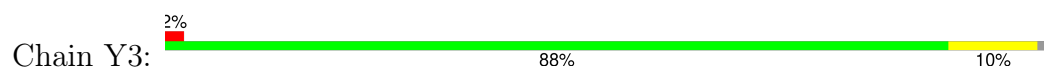
• Molecule 48: 50S ribosomal protein L29



• Molecule 49: 50S ribosomal protein L30

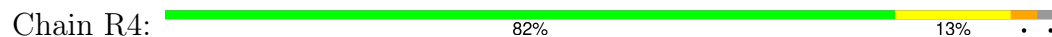


• Molecule 49: 50S ribosomal protein L30

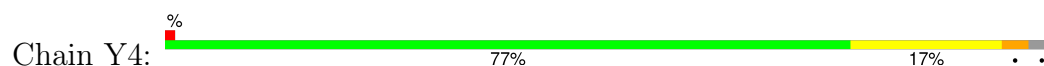




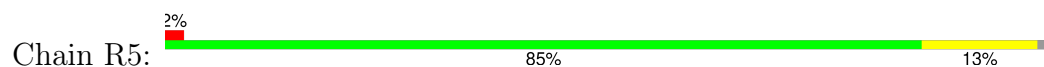
- Molecule 50: 50S ribosomal protein L31



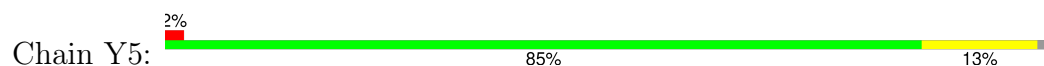
- Molecule 50: 50S ribosomal protein L31



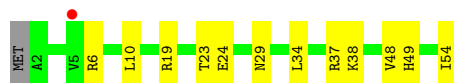
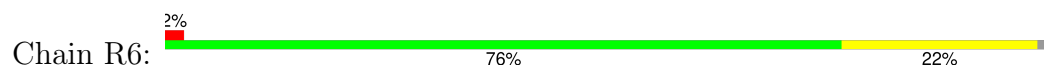
- Molecule 51: 50S ribosomal protein L32



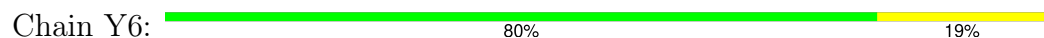
- Molecule 51: 50S ribosomal protein L32



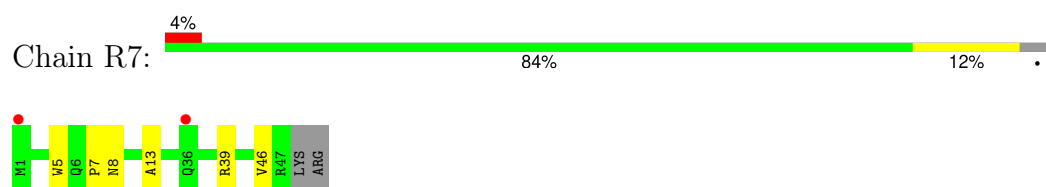
- Molecule 52: 50S ribosomal protein L33



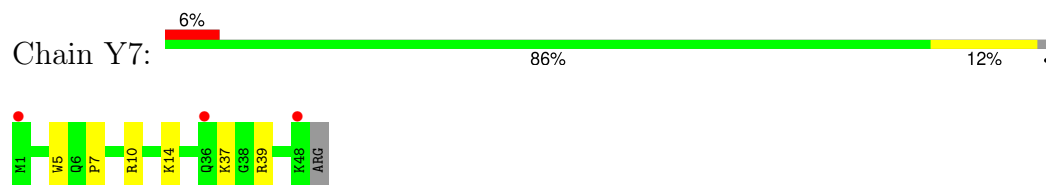
- Molecule 52: 50S ribosomal protein L33



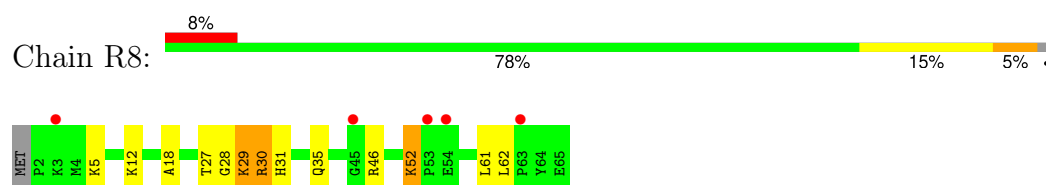
- Molecule 53: 50S ribosomal protein L34



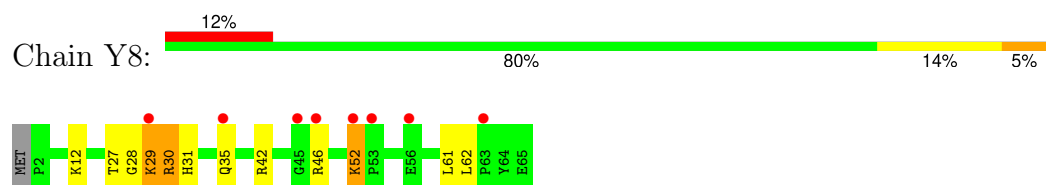
- Molecule 53: 50S ribosomal protein L34



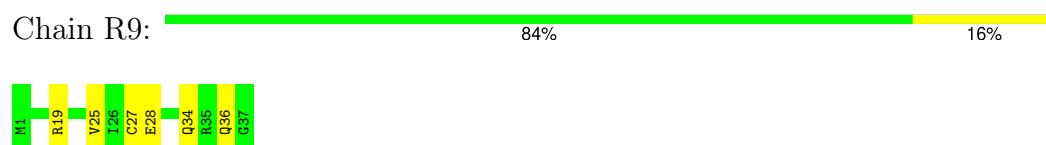
- Molecule 54: 50S ribosomal protein L35



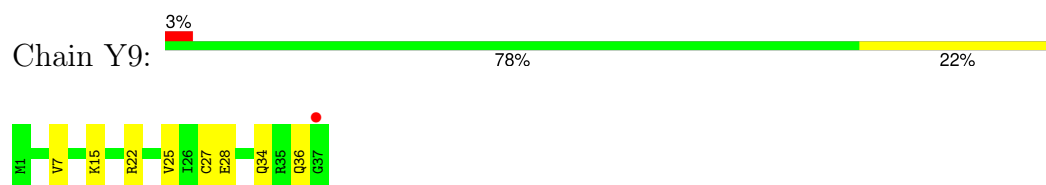
- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



- Molecule 55: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.81Å 448.83Å 618.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	134.68 – 3.74 134.68 – 3.74	Depositor EDS
% Data completeness (in resolution range)	100.0 (134.68-3.74) 100.0 (134.68-3.74)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.58Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.204 , 0.225 0.205 , 0.225	Depositor DCC
R_{free} test set	569907 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	112.7	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 139.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	295646	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	QA	0.96	0/36094	1.18	226/56334 (0.4%)
1	XA	0.96	0/36097	1.18	214/56339 (0.4%)
2	QB	0.40	0/1942	0.62	0/2619
2	XB	0.40	0/1950	0.59	0/2630
3	QC	0.39	0/1629	0.56	0/2195
3	XC	0.39	0/1629	0.56	0/2195
4	QD	0.45	0/1733	0.57	0/2318
4	XD	0.45	0/1733	0.57	0/2318
5	QE	0.42	0/1171	0.58	0/1576
5	XE	0.42	0/1171	0.58	0/1576
6	QF	0.44	0/856	0.58	0/1154
6	XF	0.44	0/856	0.58	0/1154
7	QG	0.36	0/1276	0.51	0/1709
7	XG	0.36	0/1276	0.51	0/1709
8	QH	0.44	0/1128	0.57	0/1517
8	XH	0.44	0/1128	0.56	0/1517
9	QI	0.44	0/1029	0.64	0/1379
9	XI	0.43	1/1017 (0.1%)	0.61	0/1365
10	QJ	0.42	0/814	0.62	1/1095 (0.1%)
10	XJ	0.40	0/790	0.61	1/1063 (0.1%)
11	QK	0.45	0/900	0.55	0/1213
11	XK	0.42	0/879	0.54	0/1187
12	QL	0.50	0/991	0.66	0/1327
12	XL	0.57	1/972 (0.1%)	0.68	0/1301
13	QM	0.41	0/965	0.62	0/1292
13	XM	0.39	0/956	0.61	0/1281
14	QN	0.51	0/501	0.60	0/664
14	XN	0.51	0/501	0.60	0/664
15	QO	0.40	0/745	0.55	0/992
15	XO	0.39	0/740	0.53	0/987
16	QP	0.49	0/721	0.58	0/970
16	XP	0.49	0/721	0.58	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.45	0/847	0.58	0/1131
17	XQ	0.45	0/847	0.58	0/1131
18	QR	0.39	0/579	0.62	0/768
18	XR	0.39	0/579	0.63	0/768
19	QS	0.38	0/680	0.71	1/915 (0.1%)
19	XS	0.40	0/689	0.66	0/926
20	QT	0.35	0/765	0.61	0/1007
20	XT	0.35	0/765	0.61	0/1007
21	QU	0.46	0/221	0.74	0/288
21	XU	0.46	0/221	0.74	0/288
22	QV	0.94	1/1836 (0.1%)	1.22	21/2859 (0.7%)
22	QW	0.31	0/1832	0.96	2/2855 (0.1%)
22	XV	0.94	1/1836 (0.1%)	1.22	21/2859 (0.7%)
22	XW	0.29	0/1832	0.94	2/2855 (0.1%)
23	QX	0.99	0/185	0.85	0/285
23	XX	1.03	1/257 (0.4%)	0.85	0/398
24	QY	0.78	0/404	1.11	0/627
24	XY	0.78	0/404	1.11	0/627
25	RA	1.12	5/69521 (0.0%)	1.24	583/108529 (0.5%)
25	YA	1.16	13/69543 (0.0%)	1.25	546/108563 (0.5%)
26	RB	0.81	0/2878	1.23	25/4490 (0.6%)
26	YB	0.81	0/2878	1.22	25/4490 (0.6%)
27	RD	0.60	0/2165	0.71	1/2919 (0.0%)
27	YD	0.60	0/2165	0.71	1/2919 (0.0%)
28	RE	0.52	0/1601	0.71	2/2160 (0.1%)
28	YE	0.52	0/1601	0.71	2/2160 (0.1%)
29	RF	0.58	0/1620	0.62	0/2194
29	YF	0.58	0/1620	0.62	0/2194
30	RG	0.40	0/1499	0.66	1/2016 (0.0%)
30	YG	0.40	0/1499	0.66	1/2016 (0.0%)
31	RH	0.41	0/1362	0.64	0/1841
31	YH	0.41	0/1362	0.64	0/1841
32	RI	0.37	0/1151	0.65	0/1558
32	YI	0.37	0/1151	0.65	0/1558
33	RN	0.50	0/1131	0.64	0/1525
33	YN	0.50	0/1131	0.64	0/1525
34	RO	0.55	0/943	0.61	0/1269
34	YO	0.55	0/943	0.61	0/1269
35	RP	0.47	0/1162	0.76	1/1544 (0.1%)
35	YP	0.49	0/1139	0.76	1/1514 (0.1%)
36	RQ	0.48	0/1143	0.66	0/1527
36	YQ	0.48	0/1143	0.66	0/1527
37	RR	0.49	0/974	0.69	1/1302 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	YR	0.50	0/974	0.66	1/1302 (0.1%)
38	RS	0.38	0/892	0.70	0/1187
38	YS	0.38	0/892	0.70	0/1187
39	RT	0.46	0/1155	0.66	0/1542
39	YT	0.46	0/1155	0.66	0/1542
40	RU	0.52	0/982	0.61	0/1306
40	YU	0.52	0/982	0.61	0/1306
41	RV	0.47	0/790	0.67	0/1057
41	YV	0.46	0/790	0.67	0/1057
42	RW	0.54	0/911	0.61	0/1220
42	YW	0.55	0/911	0.61	0/1220
43	RX	0.56	0/739	0.58	0/993
43	YX	0.56	0/739	0.58	0/993
44	RY	0.53	0/831	0.56	0/1108
44	YY	0.53	0/831	0.56	0/1108
45	RZ	0.39	0/1493	0.71	0/2026
45	YZ	0.39	0/1493	0.71	0/2026
46	R0	0.51	0/652	0.57	0/867
46	Y0	0.47	0/607	0.56	0/809
47	R1	0.58	1/770 (0.1%)	0.64	0/1022
47	Y1	0.56	0/736	0.65	0/978
48	R2	0.40	0/583	0.52	0/771
48	Y2	0.40	0/583	0.52	0/771
49	R3	0.44	0/474	0.60	0/635
49	Y3	0.44	0/474	0.60	0/635
50	R4	0.37	0/578	0.64	0/776
50	Y4	0.37	0/578	0.64	0/776
51	R5	0.50	0/473	0.58	0/639
51	Y5	0.50	0/473	0.58	0/639
52	R6	0.34	0/460	0.51	0/613
52	Y6	0.34	0/460	0.51	0/613
53	R7	0.52	0/417	0.59	0/550
53	Y7	0.60	0/426	0.62	0/561
54	R8	0.55	0/525	0.76	0/691
54	Y8	0.55	0/525	0.76	0/691
55	R9	0.44	0/310	0.50	0/407
55	Y9	0.43	0/310	0.50	0/407
All	All	0.93	24/319989 (0.0%)	1.10	1680/478685 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	QB	0	1
4	QD	0	1
4	XD	0	1
12	QL	0	2
12	XL	0	2
13	QM	0	1
27	RD	0	4
27	YD	0	4
28	RE	0	3
28	YE	0	3
30	RG	0	1
30	YG	0	1
31	RH	0	1
31	YH	0	1
32	RI	0	3
32	YI	0	3
35	RP	0	1
35	YP	0	1
37	RR	0	1
39	RT	0	1
39	YT	0	1
40	RU	0	2
40	YU	0	2
41	RV	0	2
41	YV	0	2
45	RZ	0	4
45	YZ	0	4
50	R4	0	1
50	Y4	0	1
54	R8	0	4
54	Y8	0	4
All	All	0	63

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	XV	1	C	OP3-P	-10.70	1.48	1.61
22	QV	1	C	OP3-P	-10.69	1.48	1.61
25	YA	74	A	N9-C4	-6.89	1.33	1.37
25	RA	74	A	N9-C4	-6.79	1.33	1.37
23	XX	21	C	O3'-P	-6.62	1.53	1.61
12	XL	104	VAL	CB-CG2	-5.78	1.40	1.52
25	YA	1378	A	N9-C4	-5.62	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	RA	1021	A	N9-C4	-5.49	1.34	1.37
25	RA	2448	A	N9-C4	-5.48	1.34	1.37
47	R1	42	GLN	C-N	-5.47	1.21	1.34
25	RA	2287	A	N9-C4	-5.46	1.34	1.37
25	YA	654	A	N9-C4	5.39	1.41	1.37
25	YA	556	G	N9-C8	-5.39	1.34	1.37
25	RA	783	A	N7-C5	-5.35	1.36	1.39
25	YA	265	A	N9-C4	-5.34	1.34	1.37
25	YA	1510	A	N9-C4	5.32	1.41	1.37
9	XI	121	ARG	C-N	-5.22	1.22	1.34
25	YA	2060	A	N9-C4	-5.17	1.34	1.37
25	YA	783	A	N7-C5	-5.14	1.36	1.39
25	YA	1287	A	N7-C5	-5.12	1.36	1.39
25	YA	1095	A	N9-C4	5.10	1.41	1.37
25	YA	528	A	N9-C4	-5.06	1.34	1.37
25	YA	1142(A)	A	N9-C4	-5.06	1.34	1.37
25	YA	2542	A	N9-C4	-5.05	1.34	1.37

All (1680) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	1158	C	C2-N1-C1'	13.01	133.12	118.80
1	QA	1301	U	N1-C2-O2	12.90	131.83	122.80
1	XA	1158	C	N1-C2-O2	12.82	126.59	118.90
1	QA	328	C	N1-C2-O2	12.57	126.44	118.90
1	QA	1301	U	N3-C2-O2	-12.21	113.65	122.20
1	XA	1158	C	C2-N1-C1'	12.12	132.13	118.80
25	RA	2474	C	N1-C2-O2	12.10	126.16	118.90
1	QA	1158	C	N1-C2-O2	12.03	126.12	118.90
1	QA	1301	U	C2-N1-C1'	11.97	132.06	117.70
1	XA	458	C	N3-C2-O2	-11.90	113.57	121.90
25	RA	2506	U	C2-N1-C1'	11.84	131.91	117.70
1	XA	1301	U	C2-N1-C1'	11.56	131.57	117.70
25	YA	546	C	N1-C2-O2	11.55	125.83	118.90
1	XA	1054	C	N1-C2-O2	11.44	125.76	118.90
25	RA	2506	U	N1-C2-O2	11.29	130.71	122.80
25	RA	828	U	C2-N1-C1'	11.16	131.10	117.70
1	XA	328	C	N1-C2-O2	11.06	125.54	118.90
1	XA	1301	U	N3-C2-O2	-11.04	114.47	122.20
25	RA	856	C	C6-N1-C2	-11.02	115.89	120.30
25	RA	2702	U	C2-N1-C1'	10.95	130.84	117.70
1	XA	1054	C	C2-N1-C1'	10.92	130.81	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	1301	U	N1-C2-O2	10.78	130.35	122.80
25	RA	2474	C	C2-N1-C1'	10.78	130.65	118.80
26	YB	31	C	N1-C2-O2	10.70	125.32	118.90
26	RB	31	C	N1-C2-O2	10.70	125.32	118.90
26	RB	31	C	C2-N1-C1'	10.57	130.43	118.80
26	YB	31	C	C2-N1-C1'	10.54	130.40	118.80
1	QA	1322	C	C2-N1-C1'	10.46	130.31	118.80
1	XA	754	C	C2-N1-C1'	10.45	130.29	118.80
25	RA	2474	C	N3-C2-O2	-10.43	114.60	121.90
25	RA	2666	C	N1-C2-O2	10.36	125.12	118.90
25	YA	546	C	C2-N1-C1'	10.32	130.16	118.80
1	QA	328	C	C2-N1-C1'	10.28	130.11	118.80
25	RA	1931	U	N3-C2-O2	-10.28	115.00	122.20
1	QA	1086	U	N1-C2-O2	10.18	129.93	122.80
1	QA	328	C	N3-C2-O2	-10.13	114.81	121.90
1	XA	328	C	C2-N1-C1'	10.10	129.91	118.80
25	RA	1774	C	N1-C2-O2	10.09	124.95	118.90
25	RA	2506	U	N3-C2-O2	-10.06	115.16	122.20
25	YA	856	C	C6-N1-C2	-9.86	116.36	120.30
25	YA	1535	U	N1-C2-O2	9.80	129.66	122.80
25	RA	2128	C	N1-C2-O2	9.76	124.75	118.90
25	YA	828	U	C2-N1-C1'	9.73	129.37	117.70
25	YA	1535	U	C2-N1-C1'	9.72	129.36	117.70
25	RA	2394	C	N1-C2-O2	9.64	124.69	118.90
1	QA	1322	C	N1-C2-O2	9.62	124.67	118.90
25	RA	1313	U	C2-N1-C1'	9.58	129.20	117.70
25	RA	1313	U	N3-C2-O2	-9.57	115.50	122.20
25	YA	1774	C	N1-C2-O2	9.56	124.63	118.90
25	YA	1931	U	N1-C2-O2	9.56	129.49	122.80
25	RA	1774	C	N3-C2-O2	-9.52	115.23	121.90
1	QA	1158	C	N3-C2-O2	-9.51	115.24	121.90
1	XA	1158	C	N3-C2-O2	-9.48	115.26	121.90
25	RA	2702	U	N1-C2-O2	9.48	129.43	122.80
25	RA	860	U	N3-C2-O2	-9.47	115.57	122.20
1	QA	936	C	N1-C2-O2	9.46	124.58	118.90
25	YA	1914	C	N1-C2-O2	9.41	124.55	118.90
25	RA	1505	C	C2-N1-C1'	9.39	129.13	118.80
25	RA	546	C	N1-C2-O2	9.39	124.53	118.90
25	YA	2666	C	N1-C2-O2	9.38	124.53	118.90
25	YA	1535	U	N3-C2-O2	-9.37	115.64	122.20
25	YA	1774	C	N3-C2-O2	-9.37	115.34	121.90
25	YA	860	U	N3-C2-O2	-9.37	115.64	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	RA	2702	U	N3-C2-O2	-9.32	115.67	122.20
25	RA	1931	U	N1-C2-O2	9.26	129.28	122.80
1	XA	458	C	N1-C2-O2	9.22	124.43	118.90
25	YA	1931	U	N3-C2-O2	-9.16	115.79	122.20
25	YA	1313	U	C2-N1-C1'	9.15	128.68	117.70
1	QA	1158	C	C6-N1-C1'	-9.11	109.86	120.80
25	YA	1914	C	C2-N1-C1'	9.07	128.78	118.80
26	RB	11	C	N1-C2-O2	9.06	124.34	118.90
25	YA	1956	U	N3-C2-O2	-9.05	115.87	122.20
1	QA	186(F)	C	N3-C2-O2	-9.04	115.58	121.90
26	YB	11	C	N1-C2-O2	9.03	124.32	118.90
1	XA	328	C	N3-C2-O2	-8.90	115.67	121.90
25	RA	265	A	O4'-C1'-N9	8.88	115.30	108.20
25	YA	867	C	N1-C2-O2	8.88	124.22	118.90
25	YA	546	C	N3-C2-O2	-8.82	115.72	121.90
25	RA	1686	C	C2-N1-C1'	8.81	128.49	118.80
1	XA	1054	C	N3-C2-O2	-8.79	115.75	121.90
25	RA	546	C	C6-N1-C2	-8.78	116.79	120.30
25	RA	1914	C	C2-N1-C1'	8.67	128.34	118.80
25	YA	2310	A	N1-C6-N6	-8.67	113.40	118.60
25	RA	2688	U	C2-N1-C1'	8.65	128.08	117.70
22	XV	33	C	N1-C2-O2	8.58	124.05	118.90
25	YA	265	A	O4'-C1'-N9	8.57	115.05	108.20
1	QA	1086	U	N3-C2-O2	-8.56	116.20	122.20
25	RA	1313	U	N1-C2-O2	8.55	128.78	122.80
25	YA	1313	U	N3-C2-O2	-8.54	116.22	122.20
1	XA	1158	C	C6-N1-C1'	-8.53	110.56	120.80
22	QV	33	C	N1-C2-O2	8.50	124.00	118.90
1	QA	410	G	OP1-P-O3'	8.50	123.89	105.20
25	RA	893	C	N1-C2-O2	8.48	123.99	118.90
25	RA	2394	C	N3-C2-O2	-8.47	115.97	121.90
25	YA	1314	C	C2-N1-C1'	8.46	128.11	118.80
1	QA	1158	C	C6-N1-C2	-8.46	116.92	120.30
25	RA	2688	U	N3-C2-O2	-8.45	116.28	122.20
25	RA	1314	C	C2-N1-C1'	8.45	128.09	118.80
25	RA	1411	C	C2-N1-C1'	8.40	128.04	118.80
25	RA	669	G	C4-N9-C1'	8.39	137.41	126.50
1	XA	1054	C	C6-N1-C1'	-8.39	110.73	120.80
25	RA	1882	C	C2-N1-C1'	8.38	128.01	118.80
1	QA	961	U	N3-C2-O2	-8.37	116.34	122.20
25	YA	231	C	C2-N1-C1'	8.37	128.01	118.80
25	YA	2814	C	N3-C2-O2	-8.36	116.05	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	YA	12	U	N3-C2-O2	-8.36	116.35	122.20
25	RA	2506	U	C6-N1-C1'	-8.35	109.51	121.20
1	XA	754	C	N1-C2-O2	8.31	123.89	118.90
25	YA	2814	C	N1-C2-O2	8.31	123.89	118.90
1	XA	812	C	P-O3'-C3'	8.31	129.67	119.70
25	YA	2666	C	N3-C2-O2	-8.30	116.09	121.90
25	YA	860	U	N1-C2-O2	8.29	128.61	122.80
1	QA	1322	C	N3-C2-O2	-8.29	116.10	121.90
25	RA	1065	U	N1-C2-O2	8.26	128.58	122.80
25	RA	2712	U	N3-C2-O2	-8.26	116.42	122.20
25	RA	898	C	N1-C2-O2	8.23	123.84	118.90
25	YA	1411	C	C2-N1-C1'	8.22	127.84	118.80
25	YA	2506	U	N1-C2-O2	8.20	128.54	122.80
25	RA	2137	C	C2-N1-C1'	8.20	127.82	118.80
25	YA	1882	C	C2-N1-C1'	8.19	127.80	118.80
25	YA	2506	U	C2-N1-C1'	8.16	127.49	117.70
25	RA	2128	C	C2-N1-C1'	8.12	127.74	118.80
25	YA	867	C	C2-N1-C1'	8.09	127.70	118.80
25	YA	120	U	C2-N1-C1'	8.07	127.38	117.70
25	RA	1914	C	N1-C2-O2	8.07	123.74	118.90
25	YA	1417	C	C2-N1-C1'	8.07	127.67	118.80
1	XA	442	C	C2-N1-C1'	8.05	127.65	118.80
1	XA	792	A	O4'-C1'-N9	8.05	114.64	108.20
1	QA	1054	C	N1-C2-O2	8.04	123.73	118.90
25	YA	1882	C	C5-C6-N1	8.03	125.02	121.00
26	YB	31	C	N3-C2-O2	-8.03	116.28	121.90
1	QA	674	G	C8-N9-C4	-8.02	103.19	106.40
1	XA	154	C	N3-C2-O2	-8.01	116.29	121.90
25	RA	2456	C	C6-N1-C2	-8.00	117.10	120.30
25	YA	2115	G	N3-C4-C5	-7.99	124.60	128.60
25	RA	1065	U	N3-C2-O2	-7.99	116.61	122.20
26	RB	31	C	N3-C2-O2	-7.99	116.31	121.90
25	YA	435	C	N1-C2-O2	7.97	123.68	118.90
25	YA	1407	C	C2-N1-C1'	7.94	127.53	118.80
25	YA	867	C	N3-C2-O2	-7.93	116.35	121.90
25	RA	749	C	N1-C2-O2	7.92	123.65	118.90
25	YA	2128	C	C2-N1-C1'	7.91	127.50	118.80
1	QA	1301	U	C6-N1-C1'	-7.91	110.13	121.20
25	YA	2161	C	N1-C2-O2	7.91	123.64	118.90
25	RA	2666	C	N3-C2-O2	-7.90	116.37	121.90
25	RA	2752	C	N1-C2-O2	7.90	123.64	118.90
25	YA	2115	G	C4-N9-C1'	7.88	136.75	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	YA	120	U	N1-C2-O2	7.87	128.31	122.80
25	YA	1411	C	C6-N1-C2	-7.84	117.17	120.30
25	RA	2712	U	N1-C2-O2	7.83	128.28	122.80
1	QA	1322	C	C6-N1-C2	-7.82	117.17	120.30
25	YA	856	C	C5-C6-N1	7.82	124.91	121.00
25	YA	1658	C	C5-C6-N1	7.80	124.90	121.00
25	RA	856	C	C5-C6-N1	7.80	124.90	121.00
25	YA	1686	C	C2-N1-C1'	7.80	127.38	118.80
25	RA	546	C	C5-C6-N1	7.80	124.90	121.00
25	YA	1882	C	C6-N1-C2	-7.80	117.18	120.30
25	RA	1881	C	C2-N1-C1'	7.79	127.37	118.80
25	YA	1658	C	C6-N1-C2	-7.77	117.19	120.30
25	RA	708	C	C2-N1-C1'	7.77	127.35	118.80
25	YA	12	U	N1-C2-O2	7.77	128.24	122.80
1	QA	1263	C	C2-N1-C1'	7.76	127.34	118.80
25	YA	12	U	C2-N1-C1'	7.75	127.00	117.70
25	RA	546	C	N3-C2-O2	-7.75	116.48	121.90
25	RA	860	U	N1-C2-O2	7.72	128.21	122.80
25	YA	537	C	C2-N1-C1'	7.70	127.27	118.80
1	XA	754	C	C6-N1-C1'	-7.69	111.57	120.80
25	YA	1313	U	N1-C2-O2	7.69	128.18	122.80
22	QV	66	C	C2-N1-C1'	7.68	127.25	118.80
22	XV	66	C	C2-N1-C1'	7.67	127.24	118.80
25	YA	1640	C	N1-C2-O2	7.66	123.50	118.90
25	RA	1407	C	C2-N1-C1'	7.66	127.22	118.80
25	RA	828	U	N1-C2-O2	7.64	128.15	122.80
1	XA	1158	C	C6-N1-C2	-7.63	117.25	120.30
25	RA	537	C	C2-N1-C1'	7.62	127.19	118.80
25	YA	930	U	N3-C2-O2	-7.62	116.87	122.20
25	RA	1742	C	C6-N1-C2	-7.61	117.25	120.30
25	YA	537	C	C5-C6-N1	7.60	124.80	121.00
25	YA	9	U	N1-C2-O2	7.60	128.12	122.80
25	YA	1914	C	N3-C2-O2	-7.60	116.58	121.90
25	RA	2726	U	N1-C2-O2	7.59	128.11	122.80
25	RA	2474	C	C6-N1-C2	-7.57	117.27	120.30
1	XA	1439	C	C2-N1-C1'	7.56	127.12	118.80
1	XA	307	C	N1-C2-O2	7.56	123.44	118.90
1	XA	328	C	C6-N1-C2	-7.56	117.28	120.30
25	RA	2666	C	C2-N1-C1'	7.56	127.11	118.80
1	QA	410	G	P-O3'-C3'	7.55	128.77	119.70
25	YA	676	A	N7-C8-N9	7.54	117.57	113.80
26	YB	11	C	C2-N1-C1'	7.53	127.08	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	792	A	O4'-C1'-N9	7.53	114.22	108.20
1	XA	1301	U	C6-N1-C1'	-7.53	110.66	121.20
25	YA	1404	C	C2-N1-C1'	7.51	127.06	118.80
26	RB	27	C	N1-C2-O2	7.51	123.41	118.90
25	RA	1658	C	C5-C6-N1	7.50	124.75	121.00
26	RB	11	C	C2-N1-C1'	7.50	127.05	118.80
25	YA	2889	C	C2-N1-C1'	7.50	127.05	118.80
25	YA	1510	A	C2-N3-C4	7.49	114.35	110.60
25	YA	2666	C	C6-N1-C2	-7.49	117.30	120.30
25	RA	2474	C	C6-N1-C1'	-7.49	111.82	120.80
25	RA	1474	C	C2-N1-C1'	7.48	127.02	118.80
25	YA	1407	C	C6-N1-C2	-7.47	117.31	120.30
25	YA	2115	G	N3-C4-N9	7.46	130.47	126.00
25	RA	1640	C	N1-C2-O2	7.45	123.37	118.90
25	RA	2128	C	N3-C2-O2	-7.45	116.69	121.90
25	YA	2739	U	N3-C2-O2	-7.44	116.99	122.20
25	YA	1314	C	C6-N1-C2	-7.44	117.33	120.30
25	YA	1474	C	C2-N1-C1'	7.44	126.98	118.80
25	RA	828	U	C6-N1-C1'	-7.43	110.80	121.20
26	YB	27	C	N1-C2-O2	7.42	123.36	118.90
25	RA	1514	U	N1-C2-O2	7.42	127.99	122.80
1	XA	252	U	C2-N1-C1'	7.42	126.60	117.70
25	YA	1406	U	C2-N1-C1'	7.42	126.60	117.70
25	RA	2726	U	C2-N1-C1'	7.41	126.60	117.70
25	YA	930	U	N1-C2-O2	7.41	127.98	122.80
25	RA	2702	U	C5-C6-N1	7.40	126.40	122.70
25	YA	2321	G	N3-C4-C5	-7.40	124.90	128.60
1	QA	749	C	N3-C2-O2	-7.40	116.72	121.90
26	RB	31	C	C6-N1-C1'	-7.39	111.93	120.80
25	RA	1513	C	C2-N1-C1'	7.39	126.93	118.80
1	XA	960	U	N1-C2-O2	7.39	127.97	122.80
25	YA	2506	U	N3-C2-O2	-7.39	117.03	122.20
25	YA	1956	U	N1-C2-O2	7.37	127.96	122.80
25	RA	2163	C	N1-C2-O2	7.37	123.32	118.90
25	RA	828	U	N3-C2-O2	-7.36	117.05	122.20
25	RA	1882	C	C5-C6-N1	7.36	124.68	121.00
25	RA	1504	C	C2-N1-C1'	7.36	126.90	118.80
26	YB	31	C	C6-N1-C1'	-7.36	111.97	120.80
25	YA	120	U	N3-C2-O2	-7.36	117.05	122.20
25	RA	904	C	C2-N1-C1'	7.35	126.89	118.80
25	RA	1658	C	C6-N1-C2	-7.35	117.36	120.30
25	YA	2688	U	N3-C2-O2	-7.34	117.06	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	RA	1065	U	C2-N1-C1'	7.33	126.50	117.70
25	RA	1407	C	C6-N1-C2	-7.32	117.37	120.30
25	YA	2394	C	N1-C2-O2	7.32	123.29	118.90
25	RA	2712	U	C2-N1-C1'	7.31	126.47	117.70
25	YA	1095	A	C2-N3-C4	7.31	114.25	110.60
25	YA	1406	U	C5-C6-N1	7.31	126.36	122.70
26	YB	11	C	N3-C2-O2	-7.31	116.78	121.90
25	YA	546	C	C6-N1-C2	-7.30	117.38	120.30
26	RB	11	C	N3-C2-O2	-7.30	116.79	121.90
25	RA	269	U	N3-C2-O2	-7.29	117.10	122.20
25	YA	893	C	C2-N1-C1'	7.29	126.81	118.80
25	YA	1005	C	N1-C2-O2	7.28	123.27	118.90
25	RA	898	C	N3-C2-O2	-7.28	116.80	121.90
25	RA	2726	U	N3-C2-O2	-7.27	117.11	122.20
1	QA	328	C	P-O3'-C3'	7.27	128.43	119.70
25	RA	1931	U	C2-N1-C1'	7.26	126.42	117.70
25	YA	828	U	N3-C2-O2	-7.26	117.12	122.20
25	YA	2832	U	P-O3'-C3'	7.26	128.41	119.70
25	RA	2210	G	C4-N9-C1'	7.25	135.93	126.50
25	YA	537	C	C6-N1-C2	-7.25	117.40	120.30
1	XA	1158	C	C5-C6-N1	7.25	124.62	121.00
25	RA	192	C	N1-C2-O2	7.23	123.24	118.90
25	YA	1005	C	C2-N1-C1'	7.21	126.74	118.80
26	RB	43	C	N1-C2-O2	7.21	123.22	118.90
25	YA	1931	U	C2-N1-C1'	7.20	126.34	117.70
25	YA	1407	C	N1-C2-O2	7.20	123.22	118.90
1	QA	1322	C	C6-N1-C1'	-7.20	112.17	120.80
25	RA	2196	C	C2-N1-C1'	7.18	126.70	118.80
1	QA	1439	C	C2-N1-C1'	7.18	126.70	118.80
25	YA	1496	A	N7-C8-N9	7.18	117.39	113.80
25	RA	1105	U	N3-C2-O2	-7.17	117.18	122.20
25	RA	2168	G	C4-N9-C1'	7.17	135.81	126.50
1	XA	827	U	N3-C2-O2	-7.16	117.19	122.20
26	YB	43	C	N1-C2-O2	7.16	123.19	118.90
25	RA	1956	U	N3-C2-O2	-7.16	117.19	122.20
1	QA	1027	C	OP1-P-O3'	7.15	120.92	105.20
25	YA	1509	C	OP1-P-O3'	7.14	120.91	105.20
1	QA	1357	A	C8-N9-C4	-7.13	102.95	105.80
25	YA	546	C	C6-N1-C1'	-7.13	112.25	120.80
1	QA	1027	C	P-O3'-C3'	7.12	128.25	119.70
25	YA	2666	C	C2-N1-C1'	7.12	126.63	118.80
22	QV	33	C	C2-N1-C1'	7.11	126.62	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	RA	1509	C	OP1-P-O3'	7.11	120.84	105.20
25	RA	2874	C	N1-C2-O2	7.11	123.17	118.90
25	RA	2868	A	N7-C8-N9	7.11	117.35	113.80
25	YA	1424	G	O5'-P-OP1	-7.11	99.31	105.70
1	XA	330	C	N1-C2-O2	7.10	123.16	118.90
25	RA	120	U	N1-C2-O2	7.10	127.77	122.80
25	YA	9	U	N3-C2-O2	-7.10	117.23	122.20
25	YA	650	C	N3-C2-O2	-7.10	116.93	121.90
25	RA	1514	U	C2-N1-C1'	7.10	126.22	117.70
25	YA	2787	C	C2-N1-C1'	7.10	126.61	118.80
25	RA	227	A	P-O3'-C3'	7.09	128.21	119.70
25	RA	1105	U	N1-C2-O2	7.09	127.76	122.80
25	YA	2507	C	C5-C6-N1	7.08	124.54	121.00
1	XA	754	C	N3-C2-O2	-7.08	116.94	121.90
25	RA	537	C	C5-C6-N1	7.07	124.54	121.00
25	RA	2739	U	N3-C2-O2	-7.07	117.25	122.20
1	QA	328	C	C6-N1-C1'	-7.06	112.32	120.80
1	QA	328	C	C6-N1-C2	-7.06	117.47	120.30
1	QA	1347	G	P-O3'-C3'	7.06	128.18	119.70
22	XV	33	C	C2-N1-C1'	7.05	126.56	118.80
25	RA	456	C	C5-C6-N1	7.05	124.53	121.00
25	RA	1505	C	N1-C2-O2	7.05	123.13	118.90
25	RA	2702	U	C6-N1-C1'	-7.05	111.33	121.20
25	YA	1741	C	C2-N1-C1'	7.05	126.55	118.80
1	QA	596	C	C6-N1-C2	-7.05	117.48	120.30
1	XA	812	C	OP2-P-O3'	7.05	120.70	105.20
25	YA	2321	G	C4-N9-C1'	7.04	135.66	126.50
1	QA	1263	C	N1-C2-O2	7.04	123.13	118.90
25	YA	9	U	C2-N1-C1'	7.04	126.15	117.70
25	YA	1026	U	P-O3'-C3'	7.04	128.15	119.70
25	YA	435	C	N3-C2-O2	-7.03	116.98	121.90
22	QV	33	C	N3-C2-O2	-7.03	116.98	121.90
22	XV	33	C	N3-C2-O2	-7.03	116.98	121.90
25	YA	965	C	C6-N1-C2	-7.02	117.49	120.30
25	YA	404	C	P-O3'-C3'	7.02	128.12	119.70
1	XA	442	C	C6-N1-C2	-7.01	117.50	120.30
25	YA	1640	C	C5-C6-N1	7.00	124.50	121.00
25	YA	1180	C	C2-N1-C1'	7.00	126.50	118.80
25	YA	269	U	N3-C2-O2	-7.00	117.30	122.20
1	QA	843	U	C5-C6-N1	7.00	126.20	122.70
1	XA	458	C	C6-N1-C2	-6.99	117.50	120.30
1	XA	827	U	C2-N1-C1'	6.99	126.09	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	YA	114	U	C2-N1-C1'	6.99	126.08	117.70
1	XA	110	C	N1-C2-O2	6.98	123.09	118.90
25	YA	1534	G	N3-C4-N9	6.98	130.19	126.00
1	QA	936	C	N3-C2-O2	-6.97	117.02	121.90
25	YA	1332	G	C6-C5-N7	-6.97	126.22	130.40
25	RA	1598	C	C2-N1-C1'	6.96	126.46	118.80
25	YA	1332	G	C4-N9-C1'	6.96	135.55	126.50
1	XA	1302	U	C2-N1-C1'	6.95	126.04	117.70
25	RA	1882	C	C6-N1-C2	-6.95	117.52	120.30
25	RA	2666	C	C6-N1-C2	-6.95	117.52	120.30
1	QA	1158	C	C5-C6-N1	6.93	124.46	121.00
25	RA	1514	U	N3-C2-O2	-6.93	117.35	122.20
25	YA	1835	G	N3-C4-N9	6.92	130.15	126.00
1	QA	442	C	C2-N1-C1'	6.92	126.41	118.80
1	QA	789	U	N3-C2-O2	-6.92	117.36	122.20
25	YA	556	G	C4-N9-C1'	6.92	135.49	126.50
25	YA	2559	C	N1-C2-O2	6.92	123.05	118.90
25	RA	669	G	C8-N9-C1'	-6.91	118.02	127.00
25	RA	2688	U	N1-C2-O2	6.91	127.63	122.80
25	RA	1992	G	P-O3'-C3'	6.90	127.98	119.70
25	RA	1026	U	P-O3'-C3'	6.90	127.97	119.70
26	YB	31	C	C6-N1-C2	-6.89	117.54	120.30
25	YA	1742	C	C6-N1-C2	-6.88	117.55	120.30
25	RA	1045	A	P-O3'-C3'	6.88	127.96	119.70
26	RB	31	C	C6-N1-C2	-6.88	117.55	120.30
1	XA	674	G	C8-N9-C4	-6.88	103.65	106.40
25	YA	556	G	N7-C8-N9	6.88	116.54	113.10
25	RA	435	C	N1-C2-O2	6.88	123.03	118.90
25	RA	1774	C	C2-N1-C1'	6.88	126.36	118.80
25	RA	456	C	C6-N1-C2	-6.87	117.55	120.30
25	RA	1411	C	C6-N1-C2	-6.87	117.55	120.30
1	XA	23	C	C5-C6-N1	6.87	124.44	121.00
1	XA	449	C	C2-N1-C1'	6.86	126.34	118.80
1	QA	843	U	C2-N1-C1'	6.85	125.92	117.70
25	RA	1537	C	N1-C2-O2	6.85	123.01	118.90
25	RA	2137	C	N1-C2-O2	6.85	123.01	118.90
25	RA	1406	U	N1-C2-O2	6.84	127.59	122.80
25	RA	269	U	N1-C2-O2	6.84	127.59	122.80
25	YA	1411	C	C5-C6-N1	6.84	124.42	121.00
25	RA	1406	U	N3-C2-O2	-6.84	117.41	122.20
1	XA	687	A	P-O3'-C3'	6.83	127.89	119.70
1	XA	960	U	N3-C2-O2	-6.83	117.42	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	YA	271(B)	G	P-O3'-C3'	6.83	127.89	119.70
25	RA	1022	G	P-O3'-C3'	6.83	127.89	119.70
25	YA	420	C	C2-N1-C1'	6.83	126.31	118.80
25	RA	120	U	C2-N1-C1'	6.82	125.89	117.70
25	YA	1929	G	OP1-P-O3'	6.82	120.21	105.20
25	RA	1505	C	C6-N1-C1'	-6.82	112.61	120.80
1	QA	442	C	C6-N1-C2	-6.81	117.58	120.30
1	XA	328	C	P-O3'-C3'	6.81	127.87	119.70
1	QA	435	C	C2-N1-C1'	6.81	126.29	118.80
25	RA	2064	C	C6-N1-C2	-6.80	117.58	120.30
25	YA	2681	C	P-O3'-C3'	6.79	127.85	119.70
25	RA	2321	G	C4-N9-C1'	6.79	135.33	126.50
25	YA	1835	G	C4-N9-C1'	6.79	135.33	126.50
25	YA	2559	C	C6-N1-C2	-6.79	117.59	120.30
25	RA	1558	A	P-O3'-C3'	6.78	127.84	119.70
28	RE	78	LEU	CA-CB-CG	6.78	130.89	115.30
25	YA	1474	C	C6-N1-C2	-6.78	117.59	120.30
28	YE	78	LEU	CA-CB-CG	6.78	130.89	115.30
25	RA	1332	G	C6-C5-N7	-6.76	126.34	130.40
1	QA	1285	A	P-O3'-C3'	6.76	127.81	119.70
25	RA	2666	C	C5-C6-N1	6.75	124.38	121.00
1	QA	1357	A	N7-C8-N9	6.75	117.17	113.80
1	XA	960	U	C2-N1-C1'	6.75	125.80	117.70
1	QA	169	C	N1-C2-O2	6.75	122.95	118.90
25	RA	2832	U	P-O3'-C3'	6.75	127.80	119.70
1	QA	1528	U	P-O3'-C3'	6.74	127.79	119.70
25	YA	721	C	C2-N1-C1'	6.74	126.22	118.80
25	YA	1180	C	N1-C2-O2	6.74	122.95	118.90
25	YA	676	A	C8-N9-C4	-6.74	103.10	105.80
25	YA	1558	A	P-O3'-C3'	6.74	127.79	119.70
25	YA	1914	C	C6-N1-C1'	-6.73	112.72	120.80
25	YA	1549	C	N1-C2-O2	6.73	122.94	118.90
25	YA	2683	C	C6-N1-C2	-6.73	117.61	120.30
25	RA	1915	U	N1-C2-O2	6.73	127.51	122.80
25	YA	1474	C	C5-C6-N1	6.72	124.36	121.00
25	RA	537	C	C6-N1-C2	-6.72	117.61	120.30
1	XA	328	C	C6-N1-C1'	-6.72	112.73	120.80
25	YA	1774	C	C6-N1-C2	-6.71	117.61	120.30
1	QA	1054	C	N3-C2-O2	-6.71	117.20	121.90
25	RA	546	C	C2-N1-C1'	6.71	126.18	118.80
25	RA	1406	U	C2-N1-C1'	6.71	125.75	117.70
25	YA	2161	C	N3-C2-O2	-6.71	117.21	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	269	C	C2-N1-C1'	6.70	126.17	118.80
1	XA	154	C	N1-C2-O2	6.69	122.91	118.90
25	RA	828	U	C5-C6-N1	6.69	126.04	122.70
25	RA	1411	C	N1-C2-O2	6.69	122.91	118.90
25	YA	828	U	N1-C2-O2	6.68	127.48	122.80
25	YA	846	C	P-O3'-C3'	6.68	127.72	119.70
25	RA	1323	U	C2-N1-C1'	6.68	125.72	117.70
25	YA	867	C	C6-N1-C2	-6.67	117.63	120.30
25	RA	2559	C	N1-C2-O2	6.67	122.90	118.90
1	QA	435	C	C5-C6-N1	6.67	124.33	121.00
25	RA	1686	C	C6-N1-C2	-6.67	117.63	120.30
25	YA	1992	G	P-O3'-C3'	6.66	127.69	119.70
1	QA	1498	U	P-O3'-C3'	6.66	127.69	119.70
25	YA	2248	C	C2-N1-C1'	6.66	126.13	118.80
25	YA	1306	C	C6-N1-C2	-6.66	117.64	120.30
25	RA	1411	C	C5-C6-N1	6.66	124.33	121.00
1	QA	687	A	P-O3'-C3'	6.65	127.68	119.70
25	YA	856	C	N3-C2-O2	-6.65	117.25	121.90
25	RA	1882	C	N1-C2-O2	6.64	122.88	118.90
25	YA	459	U	N1-C2-O2	6.63	127.44	122.80
25	RA	2115	G	N3-C4-C5	-6.63	125.29	128.60
1	QA	789	U	C2-N1-C1'	6.62	125.65	117.70
25	YA	654(T)	C	N1-C2-O2	6.62	122.88	118.90
25	YA	2065	C	C5-C6-N1	6.62	124.31	121.00
25	RA	1754	C	C6-N1-C2	-6.62	117.65	120.30
25	RA	193	U	N3-C2-O2	-6.62	117.57	122.20
25	YA	1549	C	C2-N1-C1'	6.62	126.08	118.80
25	RA	1424	G	O5'-P-OP1	-6.61	99.75	105.70
25	RA	915	C	C2-N1-C1'	6.61	126.07	118.80
1	QA	843	U	N1-C2-O2	6.61	127.42	122.80
1	XA	1285	A	P-O3'-C3'	6.60	127.62	119.70
1	QA	1109	C	N1-C2-O2	6.60	122.86	118.90
1	XA	1109	C	N1-C2-O2	6.59	122.85	118.90
25	RA	2874	C	N3-C2-O2	-6.58	117.29	121.90
1	XA	1024	G	O5'-P-OP1	6.58	118.60	110.70
1	QA	484	G	P-O3'-C3'	6.58	127.60	119.70
25	RA	1462	C	N3-C2-O2	-6.58	117.29	121.90
25	RA	1742	C	C5-C6-N1	6.58	124.29	121.00
25	YA	2504	U	N1-C2-O2	6.58	127.41	122.80
25	RA	2321	G	N3-C4-C5	-6.58	125.31	128.60
1	XA	435	C	C5-C6-N1	6.58	124.29	121.00
25	RA	392	C	C2-N1-C1'	6.58	126.04	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	YA	2584	U	C2-N1-C1'	6.58	125.59	117.70
25	RA	1915	U	N3-C2-O2	-6.58	117.60	122.20
25	RA	867	C	N1-C2-O2	6.58	122.84	118.90
25	RA	749	C	N3-C2-O2	-6.57	117.30	121.90
25	RA	404	C	P-O3'-C3'	6.57	127.59	119.70
25	RA	846	C	P-O3'-C3'	6.57	127.58	119.70
1	XA	690	G	O4'-C1'-N9	6.56	113.45	108.20
25	RA	1914	C	N3-C2-O2	-6.56	117.31	121.90
1	XA	1498	U	P-O3'-C3'	6.55	127.56	119.70
25	YA	537	C	N1-C2-O2	6.55	122.83	118.90
25	RA	898	C	C2-N1-C1'	6.55	126.00	118.80
25	YA	1022	G	P-O3'-C3'	6.54	127.55	119.70
1	QA	58	C	C6-N1-C2	-6.54	117.68	120.30
1	XA	1317	C	N1-C2-O2	6.54	122.83	118.90
25	RA	1774	C	C6-N1-C2	-6.54	117.68	120.30
25	YA	546	C	C5-C6-N1	6.53	124.27	121.00
25	RA	530	G	N1-C6-O6	-6.53	115.98	119.90
25	RA	859	G	OP2-P-O3'	6.53	119.56	105.20
25	RA	1474	C	C6-N1-C2	-6.53	117.69	120.30
25	RA	544	C	C6-N1-C2	-6.52	117.69	120.30
25	RA	2248	C	C2-N1-C1'	6.52	125.97	118.80
25	YA	856	C	N1-C2-O2	6.52	122.81	118.90
1	QA	1054	C	C2-N1-C1'	6.52	125.97	118.80
25	YA	231	C	N1-C2-O2	6.52	122.81	118.90
25	YA	912	C	C2-N1-C1'	6.52	125.97	118.80
25	RA	2307	G	C4-N9-C1'	6.52	134.97	126.50
25	YA	859	G	OP2-P-O3'	6.51	119.53	105.20
1	XA	1147	C	N1-C2-O2	6.51	122.81	118.90
25	YA	2808	U	N3-C2-O2	-6.51	117.64	122.20
25	RA	1437	C	C2-N1-C1'	6.50	125.95	118.80
25	RA	1881	C	C6-N1-C2	-6.50	117.70	120.30
25	YA	2739	U	N1-C2-O2	6.50	127.35	122.80
1	XA	1439	C	N1-C2-O2	6.49	122.80	118.90
22	XV	66	C	N1-C2-O2	6.49	122.79	118.90
25	YA	1774	C	C2-N1-C1'	6.49	125.94	118.80
25	YA	2720	U	N3-C2-O2	-6.49	117.66	122.20
25	YA	2128	C	N1-C2-O2	6.48	122.79	118.90
25	RA	1407	C	N1-C2-O2	6.48	122.79	118.90
25	RA	2096	U	N1-C2-O2	6.47	127.33	122.80
25	YA	2115	G	C8-N9-C1'	-6.47	118.59	127.00
25	RA	1012	U	OP2-P-O3'	6.47	119.43	105.20
25	YA	2461	C	C2-N1-C1'	6.47	125.92	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	QV	66	C	N1-C2-O2	6.47	122.78	118.90
25	RA	1437	C	C6-N1-C2	-6.47	117.71	120.30
25	RA	2730	C	C6-N1-C2	-6.46	117.72	120.30
25	RA	2752	C	C2-N1-C1'	6.46	125.91	118.80
25	RA	2832	U	OP2-P-O3'	6.46	119.42	105.20
1	QA	812	C	P-O3'-C3'	6.45	127.44	119.70
25	YA	1417	C	C5-C6-N1	6.45	124.22	121.00
25	RA	1537	C	N3-C2-O2	-6.45	117.39	121.90
25	RA	637	A	P-O3'-C3'	6.44	127.43	119.70
25	RA	2210	G	C8-N9-C1'	-6.44	118.62	127.00
25	RA	1437	C	C5-C6-N1	6.44	124.22	121.00
25	YA	556	G	C6-C5-N7	-6.44	126.54	130.40
1	QA	1346	A	P-O3'-C3'	6.44	127.42	119.70
1	QA	1330	U	C2-N1-C1'	6.44	125.42	117.70
25	RA	860	U	C2-N1-C1'	6.44	125.42	117.70
1	QA	932	C	C2-N1-C1'	6.43	125.88	118.80
25	RA	859	G	P-O3'-C3'	6.43	127.42	119.70
1	XA	60	A	P-O3'-C3'	6.43	127.42	119.70
25	RA	965	C	C6-N1-C2	-6.43	117.73	120.30
25	RA	1686	C	N1-C2-O2	6.43	122.76	118.90
25	RA	880	G	C4-N9-C1'	6.42	134.85	126.50
25	YA	2701	C	C6-N1-C2	-6.42	117.73	120.30
25	RA	271(B)	G	P-O3'-C3'	6.42	127.41	119.70
25	RA	1992	G	OP2-P-O3'	6.42	119.33	105.20
25	RA	1675	C	N1-C2-O2	6.42	122.75	118.90
1	XA	328	C	C5-C6-N1	6.42	124.21	121.00
1	XA	992	U	P-O3'-C3'	6.42	127.40	119.70
25	YA	1267	U	C2-N1-C1'	6.42	125.40	117.70
25	RA	285	C	N1-C2-O2	6.42	122.75	118.90
25	RA	2752	C	N3-C2-O2	-6.41	117.41	121.90
25	RA	243	U	C5-C6-N1	6.40	125.90	122.70
1	QA	992	U	P-O3'-C3'	6.40	127.38	119.70
25	YA	1535	U	C6-N1-C1'	-6.40	112.25	121.20
25	RA	1078	U	P-O3'-C3'	6.39	127.38	119.70
25	RA	1549	C	C2-N1-C1'	6.39	125.83	118.80
1	XA	1347	G	OP2-P-O3'	6.39	119.27	105.20
25	RA	31	C	C5-C6-N1	6.39	124.20	121.00
25	YA	1407	C	C5-C6-N1	6.39	124.20	121.00
25	RA	1180	C	C2-N1-C1'	6.39	125.83	118.80
25	RA	1462	C	C6-N1-C2	-6.38	117.75	120.30
25	YA	2126	A	P-O3'-C3'	6.38	127.35	119.70
1	QA	995	C	C6-N1-C2	-6.37	117.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	RA	904	C	C5-C6-N1	6.37	124.19	121.00
25	RA	1741	C	C6-N1-C2	-6.37	117.75	120.30
1	QA	110	C	N1-C2-O2	6.37	122.72	118.90
25	RA	544	C	C2-N1-C1'	6.37	125.80	118.80
1	QA	913	A	P-O3'-C3'	6.36	127.33	119.70
25	RA	2720	U	N3-C2-O2	-6.36	117.75	122.20
25	YA	860	U	C2-N1-C1'	6.36	125.33	117.70
25	RA	1314	C	C6-N1-C2	-6.35	117.76	120.30
25	RA	1314	C	N1-C2-O2	6.35	122.71	118.90
25	RA	1644	C	C6-N1-C2	-6.35	117.76	120.30
25	RA	2115	G	C4-N9-C1'	6.35	134.75	126.50
25	YA	654	A	C2-N3-C4	6.35	113.78	110.60
25	RA	2591	C	C6-N1-C2	-6.34	117.76	120.30
25	YA	1534	G	N3-C4-C5	-6.34	125.43	128.60
25	RA	1012	U	P-O3'-C3'	6.34	127.31	119.70
1	XA	307	C	N3-C2-O2	-6.33	117.47	121.90
25	RA	2519	U	O5'-P-OP1	-6.33	100.00	105.70
25	YA	2319	G	N3-C4-N9	6.33	129.80	126.00
25	YA	2513	G	O5'-P-OP2	-6.33	100.00	105.70
1	QA	529	G	C5-C6-O6	-6.33	124.80	128.60
25	YA	269	U	N1-C2-O2	6.33	127.23	122.80
25	YA	373	U	N3-C2-O2	-6.32	117.78	122.20
25	RA	234	C	N1-C2-O2	6.31	122.69	118.90
25	YA	1462	C	N1-C2-O2	6.31	122.69	118.90
22	QV	33	C	C6-N1-C2	-6.31	117.78	120.30
1	QA	458	C	C6-N1-C2	-6.30	117.78	120.30
1	XA	435	C	C2-N1-C1'	6.30	125.73	118.80
1	QA	1109	C	N3-C2-O2	-6.30	117.49	121.90
25	YA	1109	C	P-O3'-C3'	6.30	127.25	119.70
1	XA	266	G	P-O3'-C3'	6.29	127.25	119.70
1	XA	675	A	N7-C8-N9	6.29	116.94	113.80
25	YA	795	C	C6-N1-C2	-6.29	117.79	120.30
1	QA	481	G	P-O3'-C3'	6.28	127.23	119.70
25	RA	2126	A	P-O3'-C3'	6.28	127.23	119.70
25	RA	222	A	P-O3'-C3'	6.27	127.23	119.70
25	RA	795	C	C6-N1-C2	-6.27	117.79	120.30
1	QA	458	C	N3-C2-O2	-6.27	117.51	121.90
25	RA	141	A	N7-C8-N9	6.27	116.94	113.80
25	YA	2688	U	C2-N1-C1'	6.27	125.22	117.70
25	RA	2248	C	N1-C2-O2	6.27	122.66	118.90
1	QA	1439	C	N1-C2-O2	6.27	122.66	118.90
1	QA	674	G	N9-C4-C5	6.26	107.91	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	RB	79	C	C6-N1-C2	-6.26	117.79	120.30
25	RA	1956	U	N1-C2-O2	6.26	127.18	122.80
25	RA	2115	G	N3-C4-N9	6.26	129.76	126.00
25	YA	1404	C	C5-C6-N1	6.26	124.13	121.00
25	RA	1505	C	C5-C6-N1	6.26	124.13	121.00
25	YA	242	G	P-O3'-C3'	6.26	127.21	119.70
1	QA	1147	C	N1-C2-O2	6.25	122.65	118.90
25	RA	1950	G	C4-N9-C1'	6.25	134.63	126.50
25	RA	915	C	C6-N1-C2	-6.25	117.80	120.30
1	XA	993	G	C6-C5-N7	-6.25	126.65	130.40
27	YD	69	ARG	NE-CZ-NH1	-6.25	117.17	120.30
1	QA	1066	C	N1-C2-O2	6.25	122.65	118.90
25	YA	797	C	C5-C6-N1	6.24	124.12	121.00
25	YA	1406	U	N1-C2-O2	6.24	127.17	122.80
1	XA	675	A	C8-N9-C4	-6.24	103.30	105.80
27	RD	69	ARG	NE-CZ-NH1	-6.24	117.18	120.30
25	YA	2682	U	N1-C2-O2	6.24	127.17	122.80
25	RA	1543	A	O4'-C1'-N9	6.24	113.19	108.20
25	RA	2739	U	N1-C2-O2	6.24	127.17	122.80
1	XA	115	G	P-O3'-C3'	6.24	127.18	119.70
25	RA	2096	U	N3-C2-O2	-6.23	117.84	122.20
25	RA	2439	A	P-O3'-C3'	6.23	127.18	119.70
25	RA	104	U	N1-C2-O2	6.23	127.16	122.80
25	YA	828	U	C6-N1-C1'	-6.23	112.48	121.20
25	RA	1510	A	C2-N3-C4	6.23	113.71	110.60
1	XA	455	C	C2-N1-C1'	6.23	125.65	118.80
25	YA	2439	A	P-O3'-C3'	6.23	127.17	119.70
35	YP	59	LEU	CA-CB-CG	6.23	129.62	115.30
25	RA	867	C	N3-C2-O2	-6.22	117.54	121.90
25	RA	2065	C	C5-C6-N1	6.22	124.11	121.00
1	QA	455	C	C2-N1-C1'	6.22	125.64	118.80
26	YB	79	C	C6-N1-C2	-6.22	117.81	120.30
1	XA	690	G	C4-N9-C1'	6.22	134.58	126.50
25	YA	234	C	N1-C2-O2	6.21	122.63	118.90
1	XA	620	C	N1-C2-O2	6.21	122.63	118.90
1	QA	307	C	N1-C2-O2	6.21	122.63	118.90
25	RA	1947	C	C2-N1-C1'	6.21	125.63	118.80
25	YA	1835	G	N3-C4-C5	-6.21	125.50	128.60
25	RA	2394	C	C2-N1-C1'	6.21	125.63	118.80
1	QA	449	C	C2-N1-C1'	6.21	125.62	118.80
25	RA	676	A	N7-C8-N9	6.20	116.90	113.80
25	RA	898	C	C6-N1-C2	-6.20	117.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	RA	2137	C	C6-N1-C2	-6.20	117.82	120.30
25	RA	1046	A	C2-N3-C4	6.20	113.70	110.60
1	XA	435	C	C6-N1-C2	-6.20	117.82	120.30
25	YA	1509	C	P-O3'-C3'	6.20	127.14	119.70
1	XA	353	A	OP2-P-O3'	6.19	118.82	105.20
1	XA	993	G	C4-N9-C1'	6.19	134.55	126.50
25	YA	2099	U	N1-C2-O2	6.19	127.13	122.80
25	RA	1462	C	N1-C2-O2	6.19	122.61	118.90
25	RA	2471	C	N1-C2-O2	6.19	122.61	118.90
25	YA	1686	C	N1-C2-O2	6.19	122.61	118.90
25	YA	222	A	P-O3'-C3'	6.18	127.12	119.70
1	QA	1330	U	N3-C2-O2	-6.18	117.87	122.20
1	XA	932	C	C2-N1-C1'	6.18	125.60	118.80
25	RA	1537	C	C6-N1-C2	-6.18	117.83	120.30
22	XV	33	C	C6-N1-C2	-6.17	117.83	120.30
25	YA	1234	U	N3-C2-O2	-6.17	117.88	122.20
25	YA	2099	U	N3-C2-O2	-6.17	117.88	122.20
25	YA	1406	U	N3-C2-O2	-6.16	117.89	122.20
25	YA	637	A	P-O3'-C3'	6.16	127.09	119.70
25	YA	486	C	C6-N1-C2	-6.16	117.84	120.30
25	RA	544	C	C5-C6-N1	6.15	124.08	121.00
25	RA	1474	C	N1-C2-O2	6.15	122.59	118.90
1	QA	1322	C	C5-C6-N1	6.15	124.08	121.00
25	YA	797	C	C6-N1-C2	-6.15	117.84	120.30
25	YA	2557	G	C4-N9-C1'	6.15	134.49	126.50
1	XA	442	C	C5-C6-N1	6.15	124.07	121.00
10	QJ	16	LEU	CA-CB-CG	6.14	129.43	115.30
25	RA	114	U	C2-N1-C1'	6.14	125.07	117.70
25	RA	1598	C	C6-N1-C2	-6.14	117.84	120.30
1	XA	1514	C	C6-N1-C2	-6.14	117.84	120.30
25	RA	193	U	N1-C2-O2	6.14	127.10	122.80
25	RA	1417	C	C5-C6-N1	6.14	124.07	121.00
25	YA	930	U	C2-N1-C1'	6.14	125.06	117.70
25	YA	2682	U	N3-C2-O2	-6.14	117.90	122.20
25	RA	1914	C	C6-N1-C1'	-6.13	113.44	120.80
1	XA	221	C	C6-N1-C2	-6.13	117.85	120.30
25	YA	2815	C	C6-N1-C2	-6.13	117.85	120.30
1	QA	1439	C	C6-N1-C2	-6.13	117.85	120.30
1	XA	913	A	P-O3'-C3'	6.13	127.05	119.70
1	QA	753	A	P-O3'-C3'	6.13	127.05	119.70
1	QA	936	C	C2-N1-C1'	6.12	125.54	118.80
25	RA	1407	C	C5-C6-N1	6.12	124.06	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	993	G	N3-C4-N9	6.12	129.67	126.00
25	RA	1549	C	N1-C2-O2	6.12	122.57	118.90
25	YA	544	C	C5-C6-N1	6.12	124.06	121.00
1	XA	433	C	C6-N1-C2	-6.12	117.85	120.30
25	YA	859	G	P-O3'-C3'	6.12	127.04	119.70
25	YA	466	A	C8-N9-C4	-6.12	103.35	105.80
25	RA	456	C	N1-C2-O2	6.11	122.57	118.90
1	XA	1158	C	C2-N3-C4	6.11	122.95	119.90
25	YA	2320	A	C2-N3-C4	6.10	113.65	110.60
25	RA	104	U	N3-C2-O2	-6.10	117.93	122.20
25	RA	1312	U	P-O3'-C3'	6.10	127.02	119.70
25	RA	1294	U	N3-C2-O2	-6.10	117.93	122.20
25	YA	2063	C	N1-C2-O2	6.09	122.56	118.90
1	XA	78	G	OP1-P-O3'	6.09	118.61	105.20
25	YA	828	U	C5-C6-N1	6.09	125.75	122.70
25	RA	2712	U	P-O3'-C3'	6.09	127.01	119.70
26	RB	11	C	C6-N1-C2	-6.09	117.86	120.30
26	YB	70	C	C6-N1-C2	-6.09	117.86	120.30
25	RA	2847	U	N1-C2-O2	6.08	127.06	122.80
25	YA	544	C	C6-N1-C2	-6.08	117.87	120.30
25	YA	650	C	N1-C2-O2	6.08	122.55	118.90
25	RA	279	C	C2-N1-C1'	6.08	125.49	118.80
25	RA	333	G	C4-N9-C1'	6.08	134.40	126.50
25	YA	806	C	C6-N1-C2	-6.08	117.87	120.30
25	YA	1264	G	C8-N9-C4	-6.07	103.97	106.40
25	RA	1598	C	N1-C2-O2	6.07	122.54	118.90
25	YA	18	C	C6-N1-C2	-6.07	117.87	120.30
25	YA	796	C	C6-N1-C2	-6.07	117.87	120.30
25	RA	1332	G	C4-N9-C1'	6.07	134.39	126.50
25	YA	2507	C	C6-N1-C2	-6.07	117.87	120.30
1	XA	31	G	P-O3'-C3'	6.06	126.97	119.70
25	YA	2655	G	P-O3'-C3'	6.06	126.97	119.70
25	YA	140	A	N7-C8-N9	6.06	116.83	113.80
25	YA	1081	U	N1-C2-O2	6.06	127.04	122.80
25	YA	373	U	N1-C2-O2	6.06	127.04	122.80
1	QA	1325	C	N1-C2-O2	6.06	122.53	118.90
25	RA	1513	C	N1-C2-O2	6.05	122.53	118.90
26	YB	22	U	C2-N1-C1'	6.05	124.97	117.70
25	RA	192	C	N3-C2-O2	-6.05	117.66	121.90
1	QA	1301	U	C5-C6-N1	6.05	125.73	122.70
26	RB	22	U	C2-N1-C1'	6.05	124.96	117.70
1	XA	789	U	N3-C2-O2	-6.05	117.97	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	YA	2248	C	N1-C2-O2	6.05	122.53	118.90
25	YA	1332	G	N7-C8-N9	6.05	116.12	113.10
25	YA	1404	C	N1-C2-O2	6.04	122.53	118.90
25	YA	2584	U	N1-C2-O2	6.04	127.03	122.80
25	RA	1979	C	C6-N1-C2	-6.04	117.88	120.30
25	RA	2168	G	C8-N9-C1'	-6.04	119.15	127.00
25	RA	2481	G	P-O3'-C3'	6.04	126.95	119.70
26	YB	11	C	C6-N1-C2	-6.04	117.88	120.30
25	RA	2506	U	C5-C6-N1	6.04	125.72	122.70
1	QA	1147	C	N3-C2-O2	-6.04	117.67	121.90
1	XA	718	G	C4-C5-N7	6.04	113.22	110.80
25	YA	231	C	C6-N1-C1'	-6.04	113.56	120.80
25	YA	893	C	N1-C2-O2	6.04	122.52	118.90
25	RA	1833	U	N3-C2-O2	-6.03	117.98	122.20
25	YA	2490	G	C4-N9-C1'	6.03	134.34	126.50
25	RA	141	A	C5-N7-C8	-6.03	100.89	103.90
25	RA	708	C	N1-C2-O2	6.03	122.52	118.90
25	RA	1961	C	N1-C2-O2	6.03	122.52	118.90
25	YA	2853	C	C6-N1-C2	-6.03	117.89	120.30
1	QA	266	G	P-O3'-C3'	6.03	126.93	119.70
1	QA	1225	A	C4-N9-C1'	6.03	137.15	126.30
26	RB	70	C	C6-N1-C2	-6.03	117.89	120.30
25	YA	2254	C	N1-C2-O2	6.03	122.52	118.90
25	RA	285	C	C2-N1-C1'	6.02	125.42	118.80
25	YA	1640	C	C2-N1-C1'	6.02	125.42	118.80
26	RB	31	C	C5-C6-N1	6.02	124.01	121.00
25	YA	1604	C	C6-N1-C2	-6.02	117.89	120.30
25	YA	1915	U	N1-C2-O2	6.02	127.01	122.80
1	QA	533	A	P-O3'-C3'	6.01	126.92	119.70
25	RA	2210	G	N3-C4-N9	6.01	129.61	126.00
26	RB	30	C	C6-N1-C2	-6.01	117.90	120.30
25	RA	537	C	N1-C2-O2	6.01	122.50	118.90
25	YA	1390	U	N3-C2-O2	-6.01	117.99	122.20
1	XA	449	C	N1-C2-O2	6.01	122.50	118.90
25	YA	676	A	C5-N7-C8	-6.01	100.90	103.90
25	RA	456	C	C2-N1-C1'	6.00	125.41	118.80
25	YA	392	C	C2-N1-C1'	6.00	125.41	118.80
1	QA	182	U	C5-C6-N1	6.00	125.70	122.70
25	YA	838	C	C6-N1-C2	-6.00	117.90	120.30
26	YB	31	C	C5-C6-N1	6.00	124.00	121.00
1	QA	115	G	P-O3'-C3'	6.00	126.89	119.70
25	YA	2688	U	N1-C2-O2	6.00	127.00	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	497	U	N3-C2-O2	-6.00	118.00	122.20
26	YB	47	C	N1-C2-O2	5.99	122.50	118.90
1	QA	703	G	P-O3'-C3'	5.99	126.89	119.70
25	YA	1779	U	C2-N1-C1'	5.99	124.89	117.70
25	RA	2490	G	C4-N9-C1'	5.98	134.28	126.50
25	RA	2868	A	C8-N9-C4	-5.98	103.41	105.80
25	YA	1950	G	C4-N9-C1'	5.98	134.28	126.50
25	RA	267	C	C6-N1-C2	-5.98	117.91	120.30
1	XA	252	U	C5-C6-N1	5.98	125.69	122.70
25	YA	1741	C	C6-N1-C2	-5.97	117.91	120.30
25	RA	2667	C	N1-C2-O2	5.97	122.48	118.90
25	YA	2702	U	C5-C6-N1	5.97	125.68	122.70
25	YA	97	C	N1-C2-O2	5.97	122.48	118.90
25	RA	880	G	C8-N9-C1'	-5.96	119.25	127.00
25	YA	1982	C	C2-N1-C1'	5.96	125.36	118.80
25	YA	2196	C	C2-N1-C1'	5.96	125.36	118.80
25	YA	1404	C	C6-N1-C2	-5.96	117.92	120.30
25	YA	1992	G	OP2-P-O3'	5.96	118.32	105.20
26	YB	30	C	C6-N1-C2	-5.96	117.92	120.30
25	YA	1012	U	P-O3'-C3'	5.96	126.85	119.70
25	RA	1313	U	C6-N1-C1'	-5.95	112.86	121.20
25	YA	1333	C	N1-C2-O2	5.95	122.47	118.90
25	YA	650	C	C6-N1-C2	-5.95	117.92	120.30
1	XA	335	C	C6-N1-C2	-5.95	117.92	120.30
25	YA	2210	G	N3-C4-N9	5.95	129.57	126.00
1	QA	749	C	N1-C2-O2	5.95	122.47	118.90
25	RA	1694	C	P-O3'-C3'	5.95	126.84	119.70
25	RA	74	A	O4'-C1'-N9	-5.95	103.44	108.20
1	XA	110	C	N3-C2-O2	-5.95	117.74	121.90
25	YA	669	G	C4-N9-C1'	5.95	134.23	126.50
25	RA	1510	A	N3-C4-N9	5.94	132.15	127.40
25	RA	2712(A)	A	N7-C8-N9	5.94	116.77	113.80
25	YA	1411	C	N1-C2-O2	5.94	122.47	118.90
25	YA	1835	G	C8-N9-C1'	-5.94	119.27	127.00
1	XA	1317	C	N3-C2-O2	-5.94	117.74	121.90
25	YA	1513	C	C6-N1-C2	-5.94	117.92	120.30
25	YA	2814	C	C2-N1-C1'	5.94	125.33	118.80
25	RA	893	C	C2-N1-C1'	5.93	125.32	118.80
26	RB	47	C	N1-C2-O2	5.93	122.46	118.90
25	YA	229	A	P-O3'-C3'	5.93	126.81	119.70
1	XA	1025	U	N1-C2-O2	5.92	126.94	122.80
25	RA	229	A	P-O3'-C3'	5.92	126.80	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	993	G	C8-N9-C1'	-5.91	119.31	127.00
25	YA	1496	A	C8-N9-C4	-5.91	103.44	105.80
1	XA	221	C	C2-N1-C1'	5.91	125.30	118.80
1	QA	1407	C	C6-N1-C2	-5.91	117.94	120.30
25	RA	2730	C	C2-N1-C1'	5.91	125.30	118.80
25	YA	1656	C	C6-N1-C2	-5.91	117.94	120.30
25	YA	1407	C	N3-C2-O2	-5.91	117.77	121.90
25	YA	2591	C	C6-N1-C2	-5.91	117.94	120.30
1	XA	543	C	C6-N1-C2	-5.90	117.94	120.30
25	YA	1390	U	C2-N1-C1'	5.90	124.78	117.70
25	YA	1640	C	C6-N1-C2	-5.90	117.94	120.30
25	RA	1085	A	P-O3'-C3'	5.90	126.78	119.70
25	RA	1445	C	N1-C2-O2	5.90	122.44	118.90
25	RA	2702	U	C6-N1-C2	-5.90	117.46	121.00
25	YA	529	A	C8-N9-C4	-5.90	103.44	105.80
25	RA	817	C	C6-N1-C2	-5.89	117.94	120.30
1	XA	89	U	P-O3'-C3'	5.89	126.77	119.70
1	XA	1439	C	C6-N1-C2	-5.89	117.94	120.30
25	YA	243	U	C5-C6-N1	5.89	125.64	122.70
25	YA	544	C	C2-N1-C1'	5.89	125.28	118.80
25	RA	242	G	P-O3'-C3'	5.89	126.77	119.70
25	RA	312	G	C4-N9-C1'	5.89	134.16	126.50
1	QA	481	G	OP2-P-O3'	5.88	118.15	105.20
25	RA	2342	C	C6-N1-C2	-5.88	117.95	120.30
25	YA	1882	C	N1-C2-O2	5.88	122.43	118.90
1	QA	620	C	N1-C2-O2	5.88	122.43	118.90
25	RA	904	C	N1-C2-O2	5.88	122.43	118.90
25	YA	234	C	C6-N1-C2	-5.88	117.95	120.30
1	QA	674	G	N7-C8-N9	5.87	116.04	113.10
1	XA	738	C	C5-C6-N1	5.87	123.94	121.00
1	XA	1302	U	N1-C2-O2	5.87	126.91	122.80
1	XA	1439	C	C5-C6-N1	5.87	123.94	121.00
25	RA	1474	C	C5-C6-N1	5.87	123.94	121.00
25	YA	2559	C	C5-C6-N1	5.87	123.94	121.00
26	RB	27	C	C2-N1-C1'	5.87	125.25	118.80
1	QA	405	U	N1-C2-O2	5.87	126.91	122.80
26	RB	27	C	C5-C6-N1	5.86	123.93	121.00
26	YB	27	C	C2-N1-C1'	5.86	125.25	118.80
25	RA	1323	U	N3-C4-O4	5.86	123.50	119.40
25	YA	1256	G	C4-N9-C1'	5.86	134.11	126.50
25	YA	267	C	C6-N1-C2	-5.85	117.96	120.30
25	YA	1306	C	C5-C6-N1	5.85	123.92	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	RA	893	C	C5-C6-N1	5.85	123.92	121.00
26	RB	22	U	N3-C2-O2	-5.85	118.11	122.20
25	YA	1905	C	N1-C2-O2	5.84	122.41	118.90
25	RA	1640	C	N3-C2-O2	-5.84	117.81	121.90
25	RA	102	G	P-O3'-C3'	5.84	126.71	119.70
26	YB	22	U	N3-C2-O2	-5.84	118.11	122.20
1	QA	701	C	P-O3'-C3'	5.84	126.70	119.70
25	YA	2394	C	N3-C2-O2	-5.83	117.81	121.90
25	RA	1686	C	C6-N1-C1'	-5.83	113.80	120.80
25	RA	2168	G	N3-C4-C5	-5.83	125.68	128.60
37	RR	75	LEU	CA-CB-CG	5.83	128.72	115.30
1	XA	484	G	P-O3'-C3'	5.83	126.70	119.70
22	QV	35	C	P-O3'-C3'	5.83	126.70	119.70
25	RA	2066	C	N1-C2-O2	5.83	122.40	118.90
25	RA	2163	C	N3-C2-O2	-5.83	117.82	121.90
25	RA	2559	C	N3-C2-O2	-5.83	117.82	121.90
25	YA	97	C	N3-C2-O2	-5.83	117.82	121.90
25	YA	1437	C	C6-N1-C2	-5.82	117.97	120.30
25	YA	2557	G	C6-C5-N7	-5.82	126.91	130.40
25	RA	1679	U	N3-C2-O2	-5.82	118.13	122.20
25	RA	2730	C	C5-C6-N1	5.82	123.91	121.00
1	XA	827	U	N1-C2-O2	5.82	126.87	122.80
1	XA	1336	C	P-O3'-C3'	5.82	126.68	119.70
25	RA	2471	C	C2-N1-C1'	5.82	125.20	118.80
25	YA	1893	C	N1-C2-O2	5.82	122.39	118.90
25	RA	2168	G	N3-C4-N9	5.82	129.49	126.00
22	QV	66	C	C5-C6-N1	5.81	123.91	121.00
25	RA	120	U	N3-C2-O2	-5.81	118.13	122.20
25	YA	243	U	N1-C2-O2	5.81	126.87	122.80
25	RA	1513	C	C6-N1-C2	-5.81	117.98	120.30
25	YA	2766	G	C4-N9-C1'	5.81	134.05	126.50
25	RA	1881	C	C5-C6-N1	5.80	123.90	121.00
22	XV	49	C	N1-C2-O2	5.80	122.38	118.90
25	RA	2254	C	N1-C2-O2	5.79	122.38	118.90
25	RA	2787	C	C2-N1-C1'	5.79	125.17	118.80
1	QA	328	C	C5-C6-N1	5.79	123.90	121.00
25	YA	445	C	N3-C2-O2	-5.79	117.84	121.90
25	YA	1078	U	P-O3'-C3'	5.79	126.65	119.70
22	XV	35	C	P-O3'-C3'	5.79	126.64	119.70
25	RA	974(A)	C	P-O3'-C3'	5.79	126.64	119.70
25	RA	1506	C	N1-C2-O2	5.79	122.37	118.90
25	YA	459	U	N3-C2-O2	-5.79	118.15	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	YA	1417	C	C6-N1-C2	-5.78	117.99	120.30
25	RA	269	U	C2-N1-C1'	5.78	124.64	117.70
25	YA	1313	U	C6-N1-C1'	-5.78	113.11	121.20
22	XV	66	C	C5-C6-N1	5.78	123.89	121.00
25	YA	974(A)	C	N1-C2-O2	5.78	122.37	118.90
25	YA	2610	C	P-O3'-C3'	5.78	126.63	119.70
25	RA	904	C	C6-N1-C2	-5.77	117.99	120.30
1	QA	442	C	N1-C2-O2	5.77	122.36	118.90
22	QV	49	C	N1-C2-O2	5.77	122.36	118.90
25	RA	2056	G	C4-N9-C1'	5.77	134.00	126.50
25	YA	1979	C	C6-N1-C2	-5.77	117.99	120.30
25	RA	1370	C	C2-N1-C1'	5.77	125.14	118.80
25	RA	1830	C	C2-N1-C1'	5.77	125.14	118.80
25	YA	97	C	C6-N1-C2	-5.77	117.99	120.30
1	XA	645	C	N1-C2-O2	5.76	122.36	118.90
25	YA	1506	C	N1-C2-O2	5.76	122.36	118.90
25	YA	1549	C	C5-C6-N1	5.76	123.88	121.00
1	XA	88	C	N3-C2-O2	-5.76	117.87	121.90
1	QA	435	C	N1-C2-O2	5.76	122.36	118.90
25	RA	2065	C	C6-N1-C2	-5.76	118.00	120.30
1	XA	1301	U	C5-C6-N1	5.76	125.58	122.70
25	RA	1656	C	C6-N1-C2	-5.76	118.00	120.30
1	XA	536	C	C2-N1-C1'	5.76	125.13	118.80
25	RA	1504	C	N1-C2-O2	5.75	122.35	118.90
25	RA	1528	A	N7-C8-N9	5.75	116.68	113.80
25	RA	1947	C	C6-N1-C2	-5.75	118.00	120.30
25	YA	1294	U	N3-C2-O2	-5.75	118.17	122.20
1	QA	1347	G	OP2-P-O3'	5.75	117.84	105.20
25	RA	669	G	N3-C4-C5	-5.75	125.73	128.60
25	YA	1920	C	N1-C2-O2	5.75	122.35	118.90
25	YA	2321	G	N3-C4-N9	5.75	129.45	126.00
25	RA	2128	C	C6-N1-C1'	-5.75	113.91	120.80
1	XA	1502	A	C6-C5-N7	-5.75	128.28	132.30
25	YA	2726	U	N1-C2-O2	5.75	126.82	122.80
1	XA	58	C	C6-N1-C2	-5.74	118.00	120.30
1	XA	1514	C	C5-C6-N1	5.74	123.87	121.00
25	YA	2064	C	C6-N1-C2	-5.74	118.00	120.30
25	RA	1407	C	N3-C2-O2	-5.74	117.88	121.90
25	RA	1658	C	C2-N1-C1'	5.74	125.11	118.80
25	RA	1786	A	C4-C5-N7	5.74	113.57	110.70
1	XA	1028(B)	C	C6-N1-C2	-5.74	118.00	120.30
25	RA	1741	C	C2-N1-C1'	5.74	125.11	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	RA	1893	C	C2-N1-C1'	5.74	125.11	118.80
25	YA	2480	C	N3-C2-O2	-5.74	117.89	121.90
26	YB	27	C	C5-C6-N1	5.73	123.87	121.00
25	RA	1779	U	C2-N1-C1'	5.73	124.58	117.70
1	QA	843	U	N3-C2-O2	-5.73	118.19	122.20
1	XA	308	C	N1-C2-O2	5.73	122.34	118.90
25	YA	2504	U	N3-C2-O2	-5.73	118.19	122.20
1	XA	1502	A	C4-N9-C1'	5.73	136.61	126.30
25	RA	797	C	C5-C6-N1	5.72	123.86	121.00
1	QA	369	C	C6-N1-C2	-5.72	118.01	120.30
25	RA	2642	G	C4-N9-C1'	5.72	133.94	126.50
25	RA	2689	U	P-O3'-C3'	5.72	126.57	119.70
1	XA	1407	C	C6-N1-C2	-5.72	118.01	120.30
25	RA	1157	G	C4-N9-C1'	5.72	133.94	126.50
1	XA	404	U	N3-C2-O2	-5.72	118.19	122.20
1	QA	1298	C	P-O3'-C3'	5.71	126.55	119.70
25	RA	2794	C	N1-C2-O2	5.71	122.33	118.90
1	XA	529	G	C5-C6-O6	-5.71	125.18	128.60
25	RA	893	C	N3-C2-O2	-5.71	117.91	121.90
25	RA	2847	U	N3-C2-O2	-5.70	118.21	122.20
25	YA	2295	C	C6-N1-C2	-5.70	118.02	120.30
1	QA	705	U	N3-C2-O2	-5.70	118.21	122.20
1	XA	723	U	N1-C2-O2	5.70	126.79	122.80
25	YA	1742	C	C5-C6-N1	5.70	123.85	121.00
25	RA	2006	C	C2-N1-C1'	5.69	125.06	118.80
25	RA	2776	A	P-O3'-C3'	5.69	126.53	119.70
1	QA	749	C	C6-N1-C2	-5.69	118.03	120.30
25	YA	1804	C	C6-N1-C2	-5.68	118.03	120.30
25	RA	758	C	N3-C2-O2	-5.68	117.92	121.90
25	YA	41	C	C2-N1-C1'	5.68	125.05	118.80
25	RA	595	C	C5-C6-N1	5.68	123.84	121.00
1	QA	186(A)	C	N3-C2-O2	-5.68	117.92	121.90
25	RA	312	G	C8-N9-C1'	-5.68	119.62	127.00
25	RA	2512	C	C5-C6-N1	5.68	123.84	121.00
25	YA	2752	C	N1-C2-O2	5.68	122.31	118.90
37	YR	75	LEU	CA-CB-CG	5.68	128.36	115.30
25	RA	1333	C	C6-N1-C2	-5.68	118.03	120.30
1	QA	789	U	C6-N1-C2	-5.68	117.59	121.00
25	RA	2739	U	C2-N1-C1'	5.68	124.51	117.70
1	XA	449	C	C6-N1-C2	-5.67	118.03	120.30
1	QA	932	C	C6-N1-C2	-5.67	118.03	120.30
25	YA	1402	C	C6-N1-C2	-5.67	118.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	RA	1791	A	O5'-P-OP1	-5.67	100.60	105.70
1	XA	1109	C	N3-C2-O2	-5.67	117.93	121.90
1	QA	186(F)	C	C6-N1-C2	-5.67	118.03	120.30
25	YA	1905	C	N3-C2-O2	-5.67	117.93	121.90
25	RA	1513	C	C5-C6-N1	5.66	123.83	121.00
25	RA	243	U	N1-C2-O2	5.66	126.76	122.80
25	YA	1686	C	C6-N1-C1'	-5.65	114.02	120.80
25	YA	654	A	N3-C4-N9	5.65	131.92	127.40
1	QA	1225	A	N7-C8-N9	5.65	116.62	113.80
25	RA	2712(A)	A	C8-N9-C4	-5.65	103.54	105.80
25	RA	512	G	P-O3'-C3'	5.65	126.48	119.70
1	QA	1325	C	N3-C2-O2	-5.65	117.95	121.90
25	RA	2559	C	C6-N1-C2	-5.65	118.04	120.30
25	YA	556	G	C8-N9-C1'	-5.64	119.66	127.00
25	RA	1046	A	N3-C4-N9	5.64	131.91	127.40
25	RA	2056	G	C4-C5-N7	5.64	113.06	110.80
25	YA	2506	U	C6-N1-C1'	-5.64	113.30	121.20
1	XA	181	G	P-O3'-C3'	5.64	126.47	119.70
25	RA	392	C	C5-C6-N1	5.64	123.82	121.00
25	YA	1510	A	N3-C4-N9	5.64	131.91	127.40
25	YA	1776	G	C4-N9-C1'	5.64	133.83	126.50
25	RA	1427	A	P-O3'-C3'	5.63	126.46	119.70
1	QA	314	C	C2-N1-C1'	5.63	124.99	118.80
25	RA	41	C	C2-N1-C1'	5.63	125.00	118.80
25	RA	243	U	N3-C2-O2	-5.63	118.26	122.20
25	RA	2874	C	C2-N1-C1'	5.63	124.99	118.80
25	YA	234	C	N3-C2-O2	-5.63	117.96	121.90
25	RA	221	A	P-O3'-C3'	5.63	126.45	119.70
25	RA	271(B)	G	OP2-P-O3'	5.63	117.58	105.20
25	YA	1899	G	C6-C5-N7	-5.63	127.02	130.40
1	QA	1038	C	N1-C2-O2	5.62	122.28	118.90
1	XA	449	C	N3-C2-O2	-5.62	117.96	121.90
25	YA	2043	C	C5-C6-N1	5.62	123.81	121.00
25	YA	312	G	C4-N9-C1'	5.62	133.81	126.50
25	YA	1791	A	O5'-P-OP1	-5.62	100.64	105.70
1	QA	1023	G	OP1-P-O3'	5.62	117.56	105.20
25	RA	984	A	C8-N9-C4	-5.62	103.55	105.80
25	RA	1314	C	C6-N1-C1'	-5.62	114.06	120.80
25	RA	1504	C	C5-C6-N1	5.62	123.81	121.00
25	RA	2766	G	C4-N9-C1'	5.62	133.81	126.50
1	XA	307	C	C2-N1-C1'	5.62	124.98	118.80
25	RA	2584	U	C2-N1-C1'	5.62	124.44	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	RA	1605	C	C6-N1-C2	-5.62	118.05	120.30
25	YA	2559	C	N3-C2-O2	-5.61	117.97	121.90
25	RA	2210	G	N3-C4-C5	-5.61	125.80	128.60
1	QA	217	C	C2-N1-C1'	5.61	124.97	118.80
25	YA	2128	C	C6-N1-C1'	-5.61	114.07	120.80
25	RA	183	C	C6-N1-C2	-5.61	118.06	120.30
1	XA	244	U	P-O3'-C3'	5.61	126.43	119.70
25	YA	445	C	C6-N1-C2	-5.61	118.06	120.30
1	XA	442	C	N1-C2-O2	5.61	122.26	118.90
1	QA	596	C	C5-C6-N1	5.60	123.80	121.00
1	QA	962	C	N1-C2-O2	5.60	122.26	118.90
1	XA	623	C	C5-C6-N1	5.60	123.80	121.00
25	RA	99	U	P-O3'-C3'	5.60	126.42	119.70
25	RA	1644	C	C2-N1-C1'	5.60	124.96	118.80
25	YA	2311	A	N7-C8-N9	5.60	116.60	113.80
1	QA	738	C	C6-N1-C2	-5.59	118.06	120.30
25	RA	1376	C	C2-N1-C1'	5.59	124.95	118.80
1	QA	960	U	N1-C2-O2	5.59	126.71	122.80
25	RA	2350	C	C2-N1-C1'	5.59	124.95	118.80
1	XA	749	C	C6-N1-C2	-5.59	118.06	120.30
25	YA	783	A	C5-N7-C8	-5.59	101.11	103.90
1	XA	1225	A	C4-N9-C1'	5.58	136.35	126.30
1	QA	23	C	C5-C6-N1	5.58	123.79	121.00
1	QA	1439	C	C5-C6-N1	5.58	123.79	121.00
1	XA	1301	U	C6-N1-C2	-5.58	117.65	121.00
25	YA	41	C	C6-N1-C2	-5.58	118.07	120.30
1	QA	252	U	C2-N1-C1'	5.58	124.40	117.70
25	RA	1445	C	C2-N1-C1'	5.58	124.94	118.80
25	YA	2814	C	C6-N1-C2	-5.58	118.07	120.30
25	RA	1394	U	C5-C6-N1	5.58	125.49	122.70
25	YA	2073	C	C6-N1-C2	-5.58	118.07	120.30
25	RA	2787	C	N1-C2-O2	5.58	122.25	118.90
25	YA	433	C	C6-N1-C2	-5.58	118.07	120.30
25	YA	812	C	C6-N1-C2	-5.58	118.07	120.30
25	YA	1390	U	N1-C2-O2	5.58	126.70	122.80
25	RA	795	C	C5-C6-N1	5.57	123.79	121.00
25	RA	2688	U	C6-N1-C1'	-5.57	113.40	121.20
25	YA	198	C	C2-N1-C1'	5.57	124.93	118.80
25	RA	1256	G	C4-N9-C1'	5.57	133.74	126.50
25	YA	1915	U	N3-C2-O2	-5.57	118.30	122.20
25	RA	2468	G	C4-N9-C1'	5.57	133.74	126.50
25	YA	2006	C	N1-C2-O2	5.57	122.24	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	YA	2099	U	C2-N1-C1'	5.57	124.38	117.70
1	QA	119	A	P-O3'-C3'	5.56	126.38	119.70
25	RA	2161	C	N1-C2-O2	5.56	122.24	118.90
25	YA	420	C	N1-C2-O2	5.56	122.24	118.90
25	RA	1046	A	C4-N9-C1'	5.56	136.31	126.30
25	RA	1398	C	C2-N1-C1'	5.56	124.92	118.80
25	YA	658	C	C5-C6-N1	5.56	123.78	121.00
25	YA	1549	C	C6-N1-C2	-5.56	118.08	120.30
1	QA	980	C	N3-C2-O2	-5.56	118.01	121.90
25	YA	1314	C	C5-C6-N1	5.56	123.78	121.00
1	XA	645	C	C2-N1-C1'	5.56	124.91	118.80
25	YA	2015	A	C8-N9-C4	-5.56	103.58	105.80
1	QA	1347	G	N3-C4-N9	-5.55	122.67	126.00
25	YA	2468	G	C4-N9-C1'	5.55	133.72	126.50
1	XA	1347	G	O4'-C1'-N9	5.55	112.64	108.20
1	XA	1395	C	N1-C2-O2	5.55	122.23	118.90
25	RA	2720	U	N1-C2-O2	5.55	126.69	122.80
1	XA	485	G	P-O3'-C3'	5.55	126.36	119.70
25	YA	1915	U	C2-N1-C1'	5.55	124.36	117.70
25	RA	2847	U	C2-N1-C1'	5.55	124.36	117.70
25	YA	1005	C	C5-C6-N1	5.55	123.77	121.00
25	RA	1026	U	OP1-P-O3'	5.54	117.40	105.20
25	RA	2137	C	C5-C6-N1	5.54	123.77	121.00
1	QA	1008	C	C2-N1-C1'	5.54	124.90	118.80
25	YA	2066	C	N1-C2-O2	5.54	122.22	118.90
1	QA	31	G	P-O3'-C3'	5.54	126.35	119.70
25	RA	676	A	C8-N9-C4	-5.54	103.58	105.80
1	XA	738	C	C6-N1-C2	-5.54	118.08	120.30
1	XA	1452	C	C2-N1-C1'	5.54	124.89	118.80
25	YA	1188	U	N1-C2-O2	5.54	126.68	122.80
25	YA	1781	C	N1-C2-O2	5.54	122.22	118.90
25	YA	1510	A	N3-C4-C5	-5.54	122.92	126.80
25	RA	2456	C	C5-C6-N1	5.54	123.77	121.00
25	RA	650	C	N1-C2-O2	5.53	122.22	118.90
26	RB	27	C	N3-C2-O2	-5.53	118.03	121.90
25	YA	529	A	N7-C8-N9	5.53	116.57	113.80
25	YA	1095	A	N3-C4-N9	5.53	131.83	127.40
25	YA	1417	C	C6-N1-C1'	-5.53	114.16	120.80
1	QA	1330	U	N1-C2-O2	5.53	126.67	122.80
1	QA	1395	C	C2-N1-C1'	5.53	124.88	118.80
25	RA	1398	C	C6-N1-C2	-5.53	118.09	120.30
25	YA	1332	G	C8-N9-C1'	-5.53	119.81	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	YA	1694	C	P-O3'-C3'	5.53	126.34	119.70
1	QA	269	C	N1-C2-O2	5.53	122.22	118.90
35	RP	59	LEU	CA-CB-CG	5.53	128.02	115.30
25	RA	1670	C	N1-C2-O2	5.53	122.22	118.90
25	YA	183	C	N1-C2-O2	5.53	122.22	118.90
25	YA	1427	A	P-O3'-C3'	5.53	126.33	119.70
25	YA	2507	C	N1-C2-O2	5.53	122.22	118.90
25	RA	1742	C	C2-N1-C1'	5.53	124.88	118.80
25	RA	2196	C	N1-C2-O2	5.53	122.22	118.90
1	XA	1126	U	O5'-P-OP2	-5.53	100.73	105.70
25	RA	1544	C	N1-C2-O2	5.52	122.21	118.90
25	YA	1504	C	N1-C2-O2	5.52	122.21	118.90
22	QV	68	C	C2-N1-C1'	5.52	124.88	118.80
1	XA	1357	A	N7-C8-N9	5.52	116.56	113.80
1	QA	1270	C	C5-C6-N1	5.52	123.76	121.00
25	YA	898	C	C6-N1-C2	-5.52	118.09	120.30
1	XA	501	C	C6-N1-C2	-5.51	118.09	120.30
22	XV	68	C	C2-N1-C1'	5.51	124.87	118.80
25	YA	530	G	N1-C6-O6	-5.51	116.59	119.90
25	RA	650	C	N3-C2-O2	-5.51	118.04	121.90
25	YA	634	C	N1-C2-O2	5.51	122.21	118.90
25	YA	2210	G	C4-N9-C1'	5.51	133.66	126.50
1	QA	1200	C	P-O3'-C3'	5.51	126.31	119.70
22	QV	53	G	P-O3'-C3'	5.51	126.31	119.70
25	RA	1686	C	C5-C6-N1	5.51	123.75	121.00
25	YA	898	C	C2-N1-C1'	5.51	124.86	118.80
25	YA	2557	G	N3-C4-N9	5.51	129.30	126.00
25	RA	2342	C	C2-N1-C1'	5.50	124.86	118.80
25	RA	333	G	C8-N9-C1'	-5.50	119.85	127.00
25	YA	624	C	C6-N1-C2	-5.50	118.10	120.30
25	YA	912	C	N1-C2-O2	5.50	122.20	118.90
25	RA	435	C	N3-C2-O2	-5.50	118.05	121.90
25	RA	2844	G	C4-N9-C1'	5.50	133.65	126.50
1	XA	1499	A	O5'-P-OP1	-5.50	100.75	105.70
25	YA	1406	U	C6-N1-C2	-5.50	117.70	121.00
25	RA	373	U	N3-C2-O2	-5.49	118.36	122.20
1	QA	405	U	C2-N1-C1'	5.49	124.29	117.70
25	RA	589	C	C5-C6-N1	5.49	123.75	121.00
25	YA	688	U	C5-C6-N1	5.49	125.44	122.70
25	RA	41	C	C6-N1-C2	-5.49	118.11	120.30
25	RA	1505	C	C6-N1-C2	-5.48	118.11	120.30
25	RA	2073	C	C6-N1-C2	-5.48	118.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	YA	796	C	C5-C6-N1	5.48	123.74	121.00
25	YA	2642	G	C4-N9-C1'	5.48	133.63	126.50
25	RA	634	C	C6-N1-C2	-5.48	118.11	120.30
1	QA	1263	C	C6-N1-C1'	-5.48	114.22	120.80
25	RA	141(A)	C	C6-N1-C2	-5.48	118.11	120.30
25	RA	923	C	C5-C6-N1	5.48	123.74	121.00
1	XA	1054	C	C5-C6-N1	5.48	123.74	121.00
25	YA	2808	U	C2-N1-C1'	5.48	124.28	117.70
1	QA	1452	C	N1-C2-O2	5.48	122.19	118.90
25	RA	2868	A	C5-N7-C8	-5.48	101.16	103.90
25	YA	1514	U	N1-C2-O2	5.48	126.64	122.80
25	YA	1833	U	N3-C2-O2	-5.48	118.37	122.20
25	YA	1474	C	N1-C2-O2	5.47	122.19	118.90
25	YA	2808	U	N1-C2-O2	5.47	126.63	122.80
25	RA	37	C	C6-N1-C2	-5.47	118.11	120.30
25	RA	1516	U	C2-N1-C1'	5.47	124.27	117.70
1	XA	689	C	C2-N1-C1'	5.47	124.82	118.80
25	YA	1964	G	O4'-C1'-N9	-5.47	103.82	108.20
25	YA	1204	A	O4'-C1'-N9	5.47	112.58	108.20
1	QA	723	U	N3-C2-O2	-5.47	118.37	122.20
25	RA	1202	C	N1-C2-O2	5.47	122.18	118.90
25	YA	221	A	P-O3'-C3'	5.47	126.26	119.70
25	YA	1675	C	N1-C2-O2	5.47	122.18	118.90
25	YA	1741	C	N1-C2-O2	5.47	122.18	118.90
1	XA	1025	U	C2-N1-C1'	5.47	124.26	117.70
25	YA	758	C	N3-C2-O2	-5.47	118.07	121.90
25	YA	1462	C	N3-C2-O2	-5.47	118.07	121.90
1	XA	405	U	C2-N1-C1'	5.47	124.26	117.70
22	XV	53	G	P-O3'-C3'	5.47	126.26	119.70
25	YA	795	C	C5-C6-N1	5.47	123.73	121.00
25	RA	1950	G	O4'-C1'-N9	5.46	112.57	108.20
25	RA	57	C	C5-C6-N1	5.46	123.73	121.00
25	YA	312	G	C8-N9-C1'	-5.46	119.90	127.00
25	RA	503	A	P-O3'-C3'	5.46	126.25	119.70
1	XA	31	G	OP1-P-O3'	5.46	117.21	105.20
25	RA	2107	C	C2-N1-C1'	5.46	124.80	118.80
25	RA	373	U	N1-C2-O2	5.46	126.62	122.80
25	YA	1430	C	C5-C6-N1	5.45	123.73	121.00
25	YA	1635	G	C4-N9-C1'	5.45	133.59	126.50
25	YA	1893	C	C2-N1-C1'	5.45	124.80	118.80
25	RA	1903	G	O5'-P-OP1	-5.45	100.80	105.70
25	YA	2787	C	N1-C2-O2	5.45	122.17	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	RA	12	U	N3-C2-O2	-5.45	118.39	122.20
25	RA	1679	U	C2-N1-C1'	5.45	124.24	117.70
25	RA	2556	C	N1-C2-O2	5.45	122.17	118.90
25	YA	595	C	C6-N1-C2	-5.45	118.12	120.30
25	YA	1081	U	N3-C2-O2	-5.45	118.39	122.20
25	RA	74	A	C2-N3-C4	-5.45	107.88	110.60
22	QV	66	C	C6-N1-C2	-5.45	118.12	120.30
25	RA	1742	C	N1-C2-O2	5.45	122.17	118.90
25	RA	31	C	C6-N1-C2	-5.44	118.12	120.30
25	RA	2056	G	C8-N9-C1'	-5.44	119.92	127.00
1	XA	54	C	N3-C2-O2	-5.44	118.09	121.90
1	XA	243	A	P-O3'-C3'	5.44	126.23	119.70
25	YA	99	U	P-O3'-C3'	5.44	126.23	119.70
25	YA	2559	C	C2-N1-C1'	5.44	124.78	118.80
25	YA	2683	C	N3-C2-O2	-5.43	118.10	121.90
1	QA	1182	G	P-O3'-C3'	5.43	126.22	119.70
25	RA	2655	G	OP2-P-O3'	5.43	117.15	105.20
1	XA	250	A	P-O3'-C3'	5.43	126.22	119.70
1	QA	738	C	C5-C6-N1	5.43	123.71	121.00
25	YA	2307	G	C4-N9-C1'	5.43	133.55	126.50
26	YB	27	C	N3-C2-O2	-5.43	118.10	121.90
25	RA	1881	C	N1-C2-O2	5.42	122.15	118.90
25	YA	2056	G	C4-N9-C1'	5.42	133.55	126.50
25	YA	730	C	C6-N1-C2	-5.42	118.13	120.30
1	QA	1279	A	N7-C8-N9	5.42	116.51	113.80
25	RA	279	C	C6-N1-C2	-5.42	118.13	120.30
22	XV	66	C	C6-N1-C2	-5.42	118.13	120.30
25	YA	2584	U	N3-C2-O2	-5.42	118.41	122.20
25	RA	721	C	C2-N1-C1'	5.42	124.76	118.80
1	QA	936	C	C6-N1-C2	-5.42	118.13	120.30
1	QA	442	C	C5-C6-N1	5.41	123.71	121.00
1	QA	1126	U	O5'-P-OP2	-5.41	100.83	105.70
1	QA	1270	C	C6-N1-C2	-5.41	118.14	120.30
25	YA	654	A	C4-N9-C1'	5.41	136.04	126.30
25	YA	1045	A	P-O3'-C3'	5.41	126.20	119.70
1	XA	32	A	O5'-P-OP1	-5.41	100.83	105.70
1	XA	754	C	C6-N1-C2	-5.41	118.14	120.30
1	QA	1187	G	C4-N9-C1'	5.41	133.53	126.50
25	RA	1256	G	C8-N9-C1'	-5.41	119.97	127.00
1	XA	1362	C	C6-N1-C2	-5.41	118.14	120.30
1	QA	1158	C	C2-N3-C4	5.41	122.60	119.90
22	QV	33	C	C5-C6-N1	5.41	123.70	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	RA	1644	C	N3-C2-O2	-5.41	118.12	121.90
25	YA	672	C	C6-N1-C2	-5.41	118.14	120.30
25	YA	2557	G	C8-N9-C1'	-5.41	119.97	127.00
25	RA	120	U	C6-N1-C1'	-5.40	113.63	121.20
25	YA	102	G	P-O3'-C3'	5.40	126.19	119.70
25	RA	2196	C	C6-N1-C2	-5.40	118.14	120.30
26	RB	27	C	C6-N1-C2	-5.40	118.14	120.30
1	QA	435	C	C6-N1-C2	-5.40	118.14	120.30
25	RA	2164	C	N1-C2-O2	5.40	122.14	118.90
25	YA	904	C	C2-N1-C1'	5.40	124.74	118.80
1	QA	169	C	N3-C2-O2	-5.40	118.12	121.90
1	XA	1054	C	C6-N1-C2	-5.40	118.14	120.30
25	YA	2726	U	N3-C2-O2	-5.39	118.42	122.20
25	RA	1267	U	C2-N1-C1'	5.39	124.17	117.70
25	YA	2321	G	C8-N9-C1'	-5.39	120.00	127.00
1	QA	509	A	OP1-P-O3'	5.38	117.04	105.20
1	QA	563	A	C4-N9-C1'	5.38	135.99	126.30
25	RA	155	C	N1-C2-O2	5.38	122.13	118.90
25	RA	1411	C	C6-N1-C1'	-5.38	114.34	120.80
25	RA	2137	C	C6-N1-C1'	-5.38	114.34	120.80
30	RG	177	GLY	C-N-CA	-5.38	108.24	121.70
25	YA	243	U	N3-C2-O2	-5.38	118.43	122.20
22	QV	57	C	N1-C2-O2	5.38	122.13	118.90
25	RA	1901	A	C5-C6-N1	5.38	120.39	117.70
25	RA	2307	G	O4'-C1'-N9	5.38	112.51	108.20
25	RA	2667	C	N3-C2-O2	-5.38	118.13	121.90
1	QA	412	A	P-O3'-C3'	5.38	126.16	119.70
1	XA	1113	C	C6-N1-C2	-5.38	118.15	120.30
25	RA	708	C	C6-N1-C1'	-5.38	114.34	120.80
25	RA	2784	C	N1-C2-O2	5.38	122.13	118.90
25	RA	1920	C	C5-C6-N1	5.38	123.69	121.00
25	YA	721	C	C6-N1-C2	-5.38	118.15	120.30
25	YA	396	G	N7-C8-N9	5.38	115.79	113.10
25	YA	965	C	C5-C6-N1	5.38	123.69	121.00
25	YA	2226	C	N1-C2-O2	5.38	122.12	118.90
1	QA	405	U	N3-C2-O2	-5.37	118.44	122.20
25	RA	1781	C	N1-C2-O2	5.37	122.12	118.90
30	YG	177	GLY	C-N-CA	-5.37	108.27	121.70
1	XA	674	G	N7-C8-N9	5.37	115.78	113.10
1	QA	330	C	N1-C2-O2	5.37	122.12	118.90
25	YA	613	U	C2-N1-C1'	5.37	124.14	117.70
1	XA	1224	G	C4-N9-C1'	-5.37	119.52	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	XV	57	C	N3-C2-O2	-5.37	118.14	121.90
25	RA	721	C	N1-C2-O2	5.37	122.12	118.90
25	RA	1509	C	P-O3'-C3'	5.37	126.14	119.70
1	XA	174	C	C5-C6-N1	5.37	123.68	121.00
1	XA	993	G	C4-C5-N7	5.37	112.95	110.80
25	RA	1786	A	C4-N9-C1'	5.36	135.95	126.30
1	XA	932	C	C6-N1-C2	-5.36	118.15	120.30
25	YA	2128	C	C5-C6-N1	5.36	123.68	121.00
25	RA	880	G	N3-C4-N9	5.36	129.22	126.00
25	RA	974(A)	C	N1-C2-O2	5.36	122.12	118.90
25	YA	1683	C	C6-N1-C2	-5.36	118.16	120.30
25	RA	18	C	C6-N1-C2	-5.36	118.16	120.30
25	RA	2756	U	OP1-P-O3'	5.36	116.99	105.20
1	QA	1054	C	C6-N1-C2	-5.36	118.16	120.30
25	RA	1605	C	C2-N1-C1'	5.36	124.69	118.80
22	XV	33	C	C5-C6-N1	5.36	123.68	121.00
1	QA	623	C	C6-N1-C2	-5.36	118.16	120.30
1	XA	1008	C	C2-N1-C1'	5.36	124.69	118.80
25	YA	529	A	C4-N9-C1'	5.36	135.94	126.30
25	RA	1157	G	C8-N9-C1'	-5.35	120.04	127.00
25	RA	1920	C	N1-C2-O2	5.35	122.11	118.90
1	QA	645	C	N1-C2-O2	5.35	122.11	118.90
1	XA	18	C	C5-C6-N1	5.35	123.68	121.00
25	YA	2137	C	C2-N1-C1'	5.35	124.69	118.80
1	QA	1301	U	C6-N1-C2	-5.35	117.79	121.00
25	RA	1504	C	C6-N1-C1'	-5.35	114.38	120.80
25	YA	1093	G	C4-N9-C1'	5.35	133.46	126.50
25	YA	1496	A	C5-N7-C8	-5.35	101.23	103.90
25	RA	613	U	C2-N1-C1'	5.35	124.11	117.70
25	YA	806	C	C2-N1-C1'	5.35	124.68	118.80
25	RA	1533	C	C5-C6-N1	5.34	123.67	121.00
1	XA	945	G	C8-N9-C1'	-5.34	120.05	127.00
25	YA	2756	U	OP1-P-O3'	5.34	116.95	105.20
25	RA	1430	C	C5-C6-N1	5.34	123.67	121.00
25	RA	1754	C	N3-C2-O2	-5.34	118.16	121.90
25	RA	2321	G	N3-C4-N9	5.34	129.20	126.00
25	YA	2594	C	C5-C6-N1	5.34	123.67	121.00
1	QA	913	A	OP2-P-O3'	5.34	116.94	105.20
25	RA	2205	C	C6-N1-C2	-5.34	118.17	120.30
25	YA	1333	C	N3-C2-O2	-5.34	118.16	121.90
25	YA	1417	C	N1-C2-O2	5.34	122.10	118.90
25	YA	2468	G	O4'-C1'-N9	5.33	112.47	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	RA	198	C	C2-N1-C1'	5.33	124.67	118.80
25	RA	730	C	C6-N1-C2	-5.33	118.17	120.30
25	YA	1314	C	N1-C2-O2	5.33	122.10	118.90
1	QA	1086	U	C5-C6-N1	5.33	125.36	122.70
25	RA	708	C	C6-N1-C2	-5.33	118.17	120.30
25	RA	556	G	C4-N9-C1'	5.33	133.43	126.50
25	RA	1882	C	C6-N1-C1'	-5.33	114.41	120.80
1	XA	1383	C	N1-C2-O2	5.33	122.10	118.90
25	YA	587	C	P-O3'-C3'	5.33	126.09	119.70
1	QA	601	C	C6-N1-C2	-5.33	118.17	120.30
25	RA	806	C	C2-N1-C1'	5.33	124.66	118.80
25	YA	1314	C	C6-N1-C1'	-5.33	114.41	120.80
25	YA	1658	C	C2-N1-C1'	5.33	124.66	118.80
25	YA	1514	U	N3-C2-O2	-5.32	118.47	122.20
22	XV	57	C	N1-C2-O2	5.32	122.09	118.90
25	YA	2474	C	N1-C2-O2	5.32	122.09	118.90
25	YA	2720	U	N1-C2-O2	5.32	126.52	122.80
25	YA	595	C	C5-C6-N1	5.32	123.66	121.00
22	XW	8	U	OP1-P-O3'	5.31	116.89	105.20
25	YA	516	C	C6-N1-C2	-5.31	118.18	120.30
25	YA	2689	U	P-O3'-C3'	5.31	126.07	119.70
26	YB	27	C	C6-N1-C2	-5.31	118.18	120.30
22	QV	57	C	N3-C2-O2	-5.31	118.19	121.90
1	XA	1008	C	N1-C2-O2	5.31	122.08	118.90
25	YA	420	C	C6-N1-C2	-5.31	118.18	120.30
25	YA	654	A	N3-C4-C5	-5.31	123.08	126.80
25	YA	2404	C	N1-C2-O2	5.31	122.08	118.90
1	QA	1502	A	N3-C4-N9	5.30	131.64	127.40
25	RA	1950	G	C6-C5-N7	-5.30	127.22	130.40
25	RA	758	C	C6-N1-C2	-5.30	118.18	120.30
25	YA	2648	C	C5-C6-N1	5.30	123.65	121.00
1	QA	186(A)	C	N1-C2-O2	5.30	122.08	118.90
25	RA	2043	C	C5-C6-N1	5.30	123.65	121.00
22	XV	57	C	C2-N1-C1'	5.30	124.63	118.80
25	RA	392	C	C6-N1-C2	-5.30	118.18	120.30
25	RA	880	G	C6-C5-N7	-5.30	127.22	130.40
25	YA	2350	C	C2-N1-C1'	5.30	124.63	118.80
1	QA	841	U	N1-C2-O2	5.30	126.51	122.80
25	RA	234	C	N3-C2-O2	-5.30	118.19	121.90
1	QA	812	C	OP2-P-O3'	5.29	116.85	105.20
25	RA	1915	U	C2-N1-C1'	5.29	124.05	117.70
25	RA	270(P)	C	N1-C2-O2	5.29	122.08	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	RA	2115	G	C8-N9-C1'	-5.29	120.12	127.00
25	YA	806	C	C5-C6-N1	5.29	123.65	121.00
25	RA	243	U	C2-N1-C1'	5.29	124.05	117.70
25	RA	651	G	C4-N9-C1'	5.29	133.38	126.50
25	RA	1187	G	C6-C5-N7	-5.29	127.23	130.40
22	XV	51	U	N3-C2-O2	-5.29	118.50	122.20
25	RA	57	C	C6-N1-C2	-5.28	118.19	120.30
25	RA	459	U	N1-C2-O2	5.28	126.50	122.80
25	YA	1506	C	N3-C2-O2	-5.28	118.20	121.90
22	QV	57	C	C2-N1-C1'	5.28	124.61	118.80
25	YA	2666	C	C5-C6-N1	5.28	123.64	121.00
1	QA	1502	A	C4-N9-C1'	5.28	135.81	126.30
25	YA	1930	G	OP2-P-O3'	5.28	116.81	105.20
25	YA	2825	C	N1-C2-O2	5.28	122.07	118.90
19	QS	41	VAL	C-N-CD	-5.28	108.99	120.60
1	XA	1347	G	C4-N9-C1'	-5.28	119.64	126.50
1	XA	404	U	N1-C2-O2	5.27	126.49	122.80
1	XA	789	U	C2-N1-C1'	5.27	124.03	117.70
1	QA	543	C	C6-N1-C2	-5.27	118.19	120.30
25	YA	2889	C	N1-C2-O2	5.27	122.06	118.90
1	XA	1224	G	N3-C4-N9	-5.27	122.84	126.00
25	RA	2468	G	C6-C5-N7	-5.27	127.24	130.40
25	RA	672	C	C6-N1-C2	-5.27	118.19	120.30
25	RA	436	C	N1-C2-O2	5.26	122.06	118.90
1	QA	307	C	N3-C2-O2	-5.26	118.22	121.90
25	RA	1947	C	C5-C6-N1	5.26	123.63	121.00
25	RA	650	C	C6-N1-C2	-5.26	118.20	120.30
25	YA	1678	G	N7-C8-N9	5.26	115.73	113.10
25	RA	1660	C	C6-N1-C2	-5.26	118.20	120.30
1	QA	723	U	N1-C2-O2	5.25	126.48	122.80
25	RA	1256	G	N3-C4-N9	5.25	129.15	126.00
25	RA	2321	G	C8-N9-C1'	-5.25	120.17	127.00
25	RA	2498	C	C6-N1-C2	-5.25	118.20	120.30
1	QA	76	G	N3-C4-C5	-5.25	125.97	128.60
1	QA	76	G	N3-C4-N9	5.25	129.15	126.00
1	QA	575	G	N3-C4-N9	-5.25	122.85	126.00
25	YA	1332	G	N3-C4-N9	5.25	129.15	126.00
25	RA	1786	A	N9-C4-C5	-5.25	103.70	105.80
1	XA	330	C	N3-C2-O2	-5.25	118.22	121.90
25	YA	372	G	C4-N9-C1'	-5.25	119.67	126.50
1	QA	455	C	N1-C2-O2	5.25	122.05	118.90
25	RA	1077	A	C2-N3-C4	5.25	113.22	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	455	C	N1-C2-O2	5.25	122.05	118.90
25	RA	2128	C	C6-N1-C2	-5.25	118.20	120.30
1	XA	252	U	N3-C2-O2	-5.25	118.53	122.20
25	YA	265	A	C4-C5-C6	-5.25	114.38	117.00
25	RA	1332	G	N7-C8-N9	5.25	115.72	113.10
25	RA	2063	C	C6-N1-C2	-5.24	118.20	120.30
25	RA	2163	C	C6-N1-C2	-5.24	118.20	120.30
1	XA	703	G	P-O3'-C3'	5.24	125.99	119.70
25	YA	1430	C	C6-N1-C2	-5.24	118.20	120.30
1	QA	789	U	N1-C2-O2	5.24	126.47	122.80
25	YA	333	G	C4-N9-C1'	5.24	133.31	126.50
25	YA	1513	C	C5-C6-N1	5.24	123.62	121.00
1	QA	962	C	C2-N1-C1'	5.24	124.56	118.80
25	RA	1105	U	C2-N1-C1'	5.24	123.98	117.70
25	YA	647	G	C4-N9-C1'	5.24	133.31	126.50
1	QA	91	C	N1-C2-O2	5.23	122.04	118.90
1	XA	398	C	N3-C2-O2	-5.23	118.24	121.90
25	YA	37	C	C6-N1-C2	-5.23	118.21	120.30
25	RA	1775	U	C5-C4-O4	-5.23	122.76	125.90
25	YA	1267	U	N3-C2-O2	-5.23	118.54	122.20
1	XA	1502	A	C8-N9-C1'	-5.23	118.29	127.70
25	RA	2342	C	C5-C6-N1	5.23	123.61	121.00
25	YA	1776	G	N3-C4-N9	5.23	129.14	126.00
25	YA	1819	A	P-O3'-C3'	5.23	125.97	119.70
1	XA	54	C	N1-C2-O2	5.23	122.03	118.90
1	XA	1237	C	C6-N1-C2	-5.23	118.21	120.30
25	YA	2056	G	C4-C5-N7	5.22	112.89	110.80
25	YA	2678	C	C6-N1-C2	-5.22	118.21	120.30
1	XA	1024	G	O5'-P-OP2	-5.22	101.00	105.70
10	XJ	16	LEU	CA-CB-CG	5.22	127.31	115.30
26	YB	60	C	C6-N1-C2	-5.22	118.21	120.30
25	YA	2889	C	C6-N1-C1'	-5.22	114.53	120.80
1	QA	613	C	C6-N1-C2	-5.22	118.21	120.30
1	QA	932	C	N1-C2-O2	5.22	122.03	118.90
25	RA	738	G	C8-N9-C4	-5.22	104.31	106.40
22	QV	49	C	C2-N1-C1'	5.21	124.53	118.80
25	RA	1786	A	C8-N9-C1'	-5.21	118.31	127.70
1	XA	1228	C	C2-N1-C1'	5.21	124.53	118.80
25	YA	1504	C	C2-N1-C1'	5.21	124.53	118.80
25	RA	417	C	C5-C6-N1	5.21	123.61	121.00
26	YB	15	A	OP1-P-O3'	5.21	116.67	105.20
25	YA	1298	C	C2-N1-C1'	5.21	124.53	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	YA	2335	A	O4'-C1'-N9	5.21	112.37	108.20
1	QA	186(F)	C	N1-C2-O2	5.21	122.03	118.90
1	QA	1381	U	N3-C2-O2	-5.21	118.55	122.20
26	RB	15	A	OP1-P-O3'	5.21	116.66	105.20
25	YA	2089	U	C5-C6-N1	5.21	125.31	122.70
1	QA	689	C	C2-N1-C1'	5.21	124.53	118.80
25	RA	1598	C	N3-C2-O2	-5.21	118.25	121.90
25	YA	1793	C	C6-N1-C2	-5.21	118.22	120.30
22	QV	66	C	C6-N1-C1'	-5.21	114.55	120.80
1	QA	960	U	C2-N1-C1'	5.20	123.94	117.70
25	RA	1914	C	C6-N1-C2	-5.20	118.22	120.30
1	XA	381	C	N1-C2-O2	5.20	122.02	118.90
22	XV	66	C	C6-N1-C1'	-5.20	114.56	120.80
25	YA	41	C	C5-C6-N1	5.20	123.60	121.00
25	YA	1437	C	C2-N1-C1'	5.20	124.52	118.80
25	YA	1830	C	C2-N1-C1'	5.20	124.52	118.80
1	QA	1336	C	P-O3'-C3'	5.20	125.94	119.70
25	RA	198	C	C6-N1-C2	-5.20	118.22	120.30
26	RB	60	C	C6-N1-C2	-5.20	118.22	120.30
1	XA	405	U	N1-C2-O2	5.20	126.44	122.80
1	XA	503	C	C6-N1-C2	-5.20	118.22	120.30
25	YA	2739	U	C2-N1-C1'	5.20	123.94	117.70
1	QA	1025	U	OP2-P-O3'	5.19	116.63	105.20
25	YA	1776	G	C8-N9-C1'	-5.19	120.25	127.00
25	RA	589	C	C6-N1-C2	-5.19	118.22	120.30
25	RA	1534	G	N3-C4-N9	5.19	129.11	126.00
25	RA	1725	G	C4-N9-C1'	5.19	133.25	126.50
1	XA	1502	A	N3-C4-N9	5.19	131.55	127.40
25	RA	846	C	C2-N1-C1'	5.19	124.51	118.80
25	YA	2115	G	C2-N3-C4	5.19	114.49	111.90
1	QA	217	C	N1-C2-O2	5.18	122.01	118.90
25	RA	2496	C	C2-N1-C1'	5.18	124.50	118.80
22	XV	49	C	C2-N1-C1'	5.18	124.50	118.80
25	YA	1640	C	N3-C2-O2	-5.18	118.27	121.90
25	YA	1950	G	N7-C8-N9	5.18	115.69	113.10
1	QA	1514	C	C6-N1-C2	-5.18	118.23	120.30
25	RA	669	G	N3-C4-N9	5.18	129.11	126.00
25	YA	1059	G	C4-N9-C1'	5.18	133.23	126.50
1	QA	1066	C	N3-C2-O2	-5.18	118.28	121.90
1	XA	174	C	C6-N1-C2	-5.18	118.23	120.30
1	QA	110	C	N3-C2-O2	-5.17	118.28	121.90
25	RA	2056	G	C6-C5-N7	-5.17	127.30	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	1224	G	C8-N9-C1'	5.17	133.72	127.00
25	YA	243	U	C2-N1-C1'	5.17	123.91	117.70
25	RA	1314	C	C5-C6-N1	5.17	123.58	121.00
25	RA	2103	C	C5-C6-N1	5.17	123.59	121.00
1	XA	972	C	C6-N1-C2	-5.17	118.23	120.30
1	QA	243	A	P-O3'-C3'	5.17	125.90	119.70
25	YA	1256	G	C8-N9-C1'	-5.17	120.28	127.00
25	RA	193	U	C2-N1-C1'	5.17	123.90	117.70
25	RA	2559	C	C2-N1-C1'	5.17	124.48	118.80
25	RA	2642	G	C8-N9-C1'	-5.17	120.28	127.00
1	QA	1086	U	C2-N1-C1'	5.17	123.90	117.70
1	XA	405	U	N3-C2-O2	-5.17	118.58	122.20
1	QA	510	A	O5'-P-OP1	-5.16	101.05	105.70
25	RA	1264	G	C8-N9-C4	-5.16	104.33	106.40
25	YA	183	C	N3-C2-O2	-5.16	118.28	121.90
25	YA	867	C	C6-N1-C1'	-5.16	114.60	120.80
26	YB	43	C	N3-C2-O2	-5.16	118.29	121.90
25	YA	1741	C	C5-C6-N1	5.16	123.58	121.00
1	QA	442	C	N3-C2-O2	-5.16	118.29	121.90
25	YA	1955	U	P-O3'-C3'	5.16	125.89	119.70
25	RA	1313	U	C6-N1-C2	-5.16	117.91	121.00
1	XA	588	G	N3-C4-N9	5.16	129.10	126.00
25	YA	862	G	N3-C4-C5	-5.16	126.02	128.60
25	RA	1372	U	N1-C2-O2	5.15	126.41	122.80
25	RA	1312	U	OP2-P-O3'	5.15	116.54	105.20
1	XA	1414	U	N3-C2-O2	-5.15	118.59	122.20
25	YA	1095	A	N3-C4-C5	-5.15	123.19	126.80
25	YA	198	C	N1-C2-O2	5.15	121.99	118.90
25	RA	654(T)	C	N1-C2-O2	5.15	121.99	118.90
22	XV	49	C	N3-C2-O2	-5.15	118.30	121.90
1	QA	169	C	C6-N1-C2	-5.15	118.24	120.30
25	YA	828	U	C6-N1-C2	-5.15	117.91	121.00
25	YA	2321	G	C8-N9-C4	-5.15	104.34	106.40
25	RA	206	U	N3-C2-O2	-5.15	118.60	122.20
1	XA	690	G	C8-N9-C1'	-5.14	120.31	127.00
25	YA	2723	C	C6-N1-C2	-5.14	118.24	120.30
22	QV	51	U	N3-C2-O2	-5.14	118.60	122.20
22	XW	35	C	C2-N1-C1'	5.14	124.46	118.80
25	YA	1544	C	N1-C2-O2	5.14	121.99	118.90
1	XA	172	A	C8-N9-C4	-5.14	103.74	105.80
25	RA	2702	U	O5'-P-OP2	-5.14	101.08	105.70
25	YA	730	C	N1-C2-O2	5.14	121.98	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	YA	893	C	C6-N1-C1'	-5.14	114.63	120.80
25	YA	2089	U	N3-C2-O2	-5.14	118.60	122.20
1	XA	1200	C	P-O3'-C3'	5.14	125.86	119.70
25	RA	2461	C	C2-N1-C1'	5.14	124.45	118.80
25	YA	105	C	C6-N1-C2	-5.14	118.25	120.30
25	YA	1180	C	C6-N1-C1'	-5.14	114.64	120.80
1	QA	1270	C	N1-C2-O2	5.13	121.98	118.90
25	RA	595	C	C6-N1-C2	-5.13	118.25	120.30
25	YA	2847	U	C2-N1-C1'	5.13	123.86	117.70
25	RA	2307	G	C8-N9-C1'	-5.13	120.33	127.00
26	RB	43	C	N3-C2-O2	-5.13	118.31	121.90
1	XA	945	G	C4-N9-C1'	5.13	133.17	126.50
25	YA	1380	G	O5'-P-OP2	-5.13	101.08	105.70
25	YA	1533	C	C5-C6-N1	5.13	123.56	121.00
25	YA	2350	C	N3-C2-O2	-5.13	118.31	121.90
25	RA	1404	C	C2-N1-C1'	5.13	124.44	118.80
25	YA	2667	C	N1-C2-O2	5.13	121.98	118.90
25	RA	1679	U	N1-C2-O2	5.13	126.39	122.80
1	XA	1362(A)	C	N3-C2-O2	-5.13	118.31	121.90
25	RA	75	G	C4-N9-C1'	5.13	133.16	126.50
25	YA	231	C	C6-N1-C2	-5.13	118.25	120.30
25	YA	613	U	N3-C2-O2	-5.13	118.61	122.20
1	QA	703	G	OP2-P-O3'	5.12	116.47	105.20
25	RA	1430	C	C6-N1-C2	-5.12	118.25	120.30
25	RA	1619	G	C4-C5-N7	5.12	112.85	110.80
1	XA	365	U	C2-N1-C1'	5.12	123.85	117.70
25	YA	1135	C	N1-C2-O2	5.12	121.97	118.90
25	RA	198	C	C5-C6-N1	5.12	123.56	121.00
25	RA	857	C	C5-C6-N1	5.12	123.56	121.00
25	RA	2342	C	N1-C2-O2	5.12	121.97	118.90
25	YA	74	A	O4'-C1'-N9	-5.12	104.10	108.20
22	QV	49	C	N3-C2-O2	-5.12	118.32	121.90
25	RA	365	C	C6-N1-C2	-5.12	118.25	120.30
25	YA	544	C	N1-C2-O2	5.12	121.97	118.90
1	XA	435	C	N1-C2-O2	5.12	121.97	118.90
25	RA	253	C	C6-N1-C2	-5.11	118.25	120.30
25	RA	1741	C	C5-C6-N1	5.11	123.56	121.00
1	XA	993	G	N9-C4-C5	-5.11	103.36	105.40
25	YA	2847	U	N1-C2-O2	5.11	126.38	122.80
22	QV	75	C	N1-C2-O2	5.11	121.97	118.90
25	RA	2226	C	C6-N1-C2	-5.11	118.25	120.30
25	YA	9	U	C5-C6-N1	5.11	125.26	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	YA	2248	C	C6-N1-C2	-5.11	118.25	120.30
25	RA	749	C	C2-N1-C1'	5.11	124.42	118.80
25	RA	1506	C	C2-N1-C1'	5.11	124.42	118.80
25	RA	2785	C	C5-C6-N1	5.11	123.56	121.00
25	YA	1779	U	N3-C2-O2	-5.11	118.62	122.20
1	QA	449	C	C6-N1-C2	-5.11	118.26	120.30
1	QA	485	G	P-O3'-C3'	5.11	125.83	119.70
25	RA	2096	U	C2-N1-C1'	5.11	123.83	117.70
25	YA	1063	G	C6-C5-N7	-5.11	127.34	130.40
25	RA	1819	A	P-O3'-C3'	5.10	125.82	119.70
25	RA	2299	G	C4-N9-C1'	5.10	133.13	126.50
1	XA	1263	C	C2-N1-C1'	5.10	124.41	118.80
22	XV	75	C	N1-C2-O2	5.10	121.96	118.90
1	QA	103	C	N3-C2-O2	-5.10	118.33	121.90
1	QA	337	C	C6-N1-C2	-5.10	118.26	120.30
1	QA	412	A	OP2-P-O3'	5.10	116.42	105.20
1	QA	1290	G	C4-N9-C1'	5.10	133.13	126.50
25	RA	12	U	N1-C2-O2	5.10	126.37	122.80
25	RA	417	C	C6-N1-C2	-5.10	118.26	120.30
25	YA	242	G	OP2-P-O3'	5.10	116.42	105.20
25	YA	1075	C	N1-C2-O2	5.10	121.96	118.90
25	RA	2642	G	C6-C5-N7	-5.10	127.34	130.40
25	YA	417	C	C5-C6-N1	5.09	123.55	121.00
25	YA	2043	C	C6-N1-C2	-5.09	118.26	120.30
25	RA	1817	G	C4-N9-C1'	5.09	133.12	126.50
25	RA	2880	C	N3-C2-O2	-5.09	118.33	121.90
1	XA	217	C	N1-C2-O2	5.09	121.96	118.90
25	YA	2283	C	N1-C2-O2	5.09	121.96	118.90
25	RA	267	C	C5-C6-N1	5.09	123.55	121.00
25	YA	761	A	C5-N7-C8	-5.09	101.36	103.90
25	RA	2164	C	N3-C2-O2	-5.09	118.34	121.90
1	XA	497	U	N1-C2-O2	5.08	126.36	122.80
25	YA	1204	A	OP2-P-O3'	5.08	116.39	105.20
1	QA	1381	U	N1-C2-O2	5.08	126.36	122.80
1	XA	1225	A	N7-C8-N9	5.08	116.34	113.80
25	YA	915	C	C2-N1-C1'	5.08	124.39	118.80
25	YA	1694	C	OP2-P-O3'	5.08	116.38	105.20
25	RA	884	C	C6-N1-C2	-5.08	118.27	120.30
1	QA	525	C	C5-C6-N1	5.08	123.54	121.00
1	XA	588	G	N3-C4-C5	-5.08	126.06	128.60
25	YA	2648	C	C2-N1-C1'	5.08	124.39	118.80
1	QA	308	C	N1-C2-O2	5.08	121.95	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	545	C	C5-C6-N1	5.08	123.54	121.00
1	XA	932	C	C5-C6-N1	5.08	123.54	121.00
1	QA	1502	A	N9-C4-C5	-5.08	103.77	105.80
1	XA	1452	C	N1-C2-O2	5.08	121.94	118.90
25	YA	2292	C	C5-C6-N1	5.08	123.54	121.00
25	RA	1506	C	N3-C2-O2	-5.07	118.35	121.90
25	YA	721	C	N1-C2-O2	5.07	121.94	118.90
25	YA	1950	G	O4'-C1'-N9	5.07	112.26	108.20
25	YA	1786	A	C4-N9-C1'	5.07	135.43	126.30
25	RA	2481	G	OP2-P-O3'	5.07	116.35	105.20
1	XA	974	A	O4'-C1'-N9	5.07	112.26	108.20
25	YA	1210	A	C3'-C2'-C1'	5.07	105.56	101.50
25	YA	2779	U	N3-C2-O2	-5.07	118.65	122.20
25	RA	556	G	C6-C5-N7	-5.07	127.36	130.40
25	YA	1805	U	N3-C2-O2	-5.07	118.65	122.20
25	RA	2342	C	N3-C2-O2	-5.07	118.35	121.90
25	YA	120	U	C6-N1-C1'	-5.07	114.11	121.20
25	YA	1290	C	C6-N1-C2	-5.06	118.27	120.30
25	YA	1831	G	C4-N9-C1'	5.06	133.08	126.50
25	YA	2248	C	C5-C6-N1	5.06	123.53	121.00
25	RA	1267	U	N3-C2-O2	-5.06	118.66	122.20
25	RA	1779	U	N3-C2-O2	-5.06	118.66	122.20
1	QA	1023	G	P-O3'-C3'	5.06	125.77	119.70
1	XA	797	C	C6-N1-C2	-5.06	118.28	120.30
1	QA	528	C	C6-N1-C2	-5.06	118.28	120.30
1	QA	754	C	N1-C2-O2	5.06	121.94	118.90
22	QW	8	U	OP1-P-O3'	5.06	116.33	105.20
1	XA	736	C	C6-N1-C2	-5.06	118.28	120.30
1	XA	1270	C	C5-C6-N1	5.06	123.53	121.00
25	RA	1404	C	C6-N1-C2	-5.06	118.28	120.30
25	YA	1005	C	C6-N1-C1'	-5.06	114.73	120.80
25	YA	2847	U	N3-C2-O2	-5.06	118.66	122.20
25	RA	1402	C	C6-N1-C2	-5.06	118.28	120.30
25	RA	1678	G	N7-C8-N9	5.06	115.63	113.10
25	RA	1694	C	OP2-P-O3'	5.06	116.32	105.20
25	YA	2874	C	N1-C2-O2	5.06	121.93	118.90
25	YA	1924	C	N1-C2-O2	5.05	121.93	118.90
25	RA	2063	C	N1-C2-O2	5.05	121.93	118.90
1	XA	1059	C	C6-N1-C2	-5.05	118.28	120.30
1	QA	690	G	O4'-C1'-N9	5.05	112.24	108.20
1	QA	1414	U	N3-C2-O2	-5.05	118.66	122.20
25	RA	1549	C	C6-N1-C2	-5.05	118.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	RA	2720	U	C2-N1-C1'	5.05	123.76	117.70
25	YA	1849	G	C4-N9-C1'	5.05	133.07	126.50
1	QA	1038	C	N3-C2-O2	-5.05	118.37	121.90
25	YA	1549	C	N3-C2-O2	-5.05	118.37	121.90
1	XA	433	C	N3-C2-O2	-5.04	118.37	121.90
1	XA	723	U	N3-C2-O2	-5.04	118.67	122.20
1	QA	191(B)	G	C5-C6-O6	5.04	131.62	128.60
1	QA	701	C	OP2-P-O3'	5.04	116.29	105.20
22	QW	34	U	C2-N1-C1'	5.04	123.75	117.70
25	RA	867	C	C6-N1-C2	-5.04	118.28	120.30
25	RA	1598	C	C5-C6-N1	5.04	123.52	121.00
25	RA	2394	C	C6-N1-C2	-5.04	118.28	120.30
25	YA	907	U	N3-C2-O2	-5.04	118.67	122.20
25	YA	2685	G	N9-C4-C5	5.04	107.42	105.40
25	RA	1406	U	C5-C6-N1	5.04	125.22	122.70
1	QA	32	A	O5'-P-OP1	-5.04	101.17	105.70
1	XA	891	U	N3-C2-O2	-5.03	118.68	122.20
1	XA	1227	A	N7-C8-N9	5.03	116.32	113.80
25	RA	1762	A	OP2-P-O3'	5.03	116.27	105.20
1	XA	1033	G	N3-C4-N9	5.03	129.02	126.00
25	RA	1180	C	N1-C2-O2	5.03	121.92	118.90
25	RA	2368	C	C6-N1-C2	-5.03	118.29	120.30
25	YA	1950	G	C8-N9-C4	-5.03	104.39	106.40
25	YA	2832	U	OP2-P-O3'	5.03	116.27	105.20
25	YA	1534	G	C2-N3-C4	5.03	114.41	111.90
25	YA	2471	C	C6-N1-C2	-5.03	118.29	120.30
25	RA	404	C	OP2-P-O3'	5.03	116.26	105.20
1	QA	108	G	C4-N9-C1'	5.03	133.03	126.50
25	YA	1598	C	C6-N1-C2	-5.03	118.29	120.30
25	YA	2128	C	C6-N1-C2	-5.03	118.29	120.30
25	YA	2825	C	N3-C2-O2	-5.03	118.38	121.90
28	RE	117	MET	CA-CB-CG	5.02	121.84	113.30
25	RA	1675	C	N3-C2-O2	-5.02	118.38	121.90
25	RA	1804	C	C6-N1-C2	-5.02	118.29	120.30
25	YA	2490	G	C8-N9-C1'	-5.02	120.47	127.00
25	RA	1640	C	C6-N1-C2	-5.02	118.29	120.30
25	RA	1064	C	N1-C2-O2	5.02	121.91	118.90
25	RA	1950	G	C8-N9-C1'	-5.02	120.48	127.00
25	YA	1528	A	N7-C8-N9	5.02	116.31	113.80
28	YE	117	MET	CA-CB-CG	5.02	121.83	113.30
25	RA	2161	C	C5-C6-N1	5.01	123.51	121.00
1	XA	78	G	P-O3'-C3'	5.01	125.72	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	YA	267	C	C5-C6-N1	5.01	123.51	121.00
25	YA	466	A	N7-C8-N9	5.01	116.31	113.80
1	QA	697	U	N3-C2-O2	-5.01	118.69	122.20
25	RA	1370	C	C6-N1-C2	-5.01	118.30	120.30
1	QA	181	G	P-O3'-C3'	5.01	125.71	119.70
25	RA	2785	C	C6-N1-C2	-5.01	118.30	120.30
25	YA	141	A	N7-C8-N9	5.01	116.31	113.80
25	YA	665	C	C6-N1-C2	-5.01	118.30	120.30
25	YA	2471	C	C5-C6-N1	5.01	123.51	121.00
1	QA	545	C	C2-N1-C1'	5.01	124.31	118.80
25	RA	796	C	C5-C6-N1	5.01	123.50	121.00
25	YA	1686	C	C5-C6-N1	5.01	123.50	121.00
25	YA	2889	C	C6-N1-C2	-5.01	118.30	120.30
25	RA	1830	C	N1-C2-O2	5.01	121.91	118.90
25	RA	510	C	N1-C2-O2	5.01	121.90	118.90
1	XA	1285	A	OP2-P-O3'	5.01	116.22	105.20
1	QA	522	C	N1-C2-O2	5.00	121.90	118.90
25	YA	2642	G	C8-N9-C1'	-5.00	120.49	127.00
25	YA	2551	C	N1-C2-O2	5.00	121.90	118.90
1	QA	705	U	C6-N1-C2	-5.00	118.00	121.00
25	RA	1241	A	O4'-C1'-N9	5.00	112.20	108.20

There are no chirality outliers.

All (63) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	QB	15	VAL	Peptide
4	QD	19	LEU	Peptide
12	QL	104	VAL	Peptide
12	QL	47	LYS	Peptide
13	QM	66	LEU	Peptide
50	R4	48	ARG	Peptide
54	R8	28	GLY	Peptide
54	R8	35	GLN	Peptide
54	R8	52	LYS	Peptide
54	R8	62	LEU	Peptide
27	RD	122	ASP	Peptide
27	RD	237	GLU	Peptide
27	RD	33	LEU	Peptide
27	RD	35	LYS	Peptide
28	RE	131	ALA	Peptide
28	RE	17	ASP	Peptide

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Mol	Chain	Res	Type	Group
28	RE	71	GLY	Peptide
30	RG	82	LEU	Peptide
31	RH	7	LEU	Peptide
32	RI	11	ASN	Peptide
32	RI	119	PRO	Peptide
32	RI	131	LYS	Peptide
35	RP	107	LYS	Peptide
37	RR	2	ARG	Peptide
39	RT	123	GLN	Peptide
40	RU	92	ARG	Peptide
40	RU	95	LEU	Peptide
41	RV	44	LYS	Peptide
41	RV	49	THR	Peptide
45	RZ	179	ASP	Peptide
45	RZ	52	SER	Peptide
45	RZ	60	GLU	Peptide
45	RZ	62	PRO	Peptide
4	XD	19	LEU	Peptide
12	XL	104	VAL	Peptide
12	XL	47	LYS	Peptide
50	Y4	48	ARG	Peptide
54	Y8	28	GLY	Peptide
54	Y8	35	GLN	Peptide
54	Y8	52	LYS	Peptide
54	Y8	62	LEU	Peptide
27	YD	122	ASP	Peptide
27	YD	237	GLU	Peptide
27	YD	33	LEU	Peptide
27	YD	35	LYS	Peptide
28	YE	131	ALA	Peptide
28	YE	17	ASP	Peptide
28	YE	71	GLY	Peptide
30	YG	82	LEU	Peptide
31	YH	7	LEU	Peptide
32	YI	11	ASN	Peptide
32	YI	119	PRO	Peptide
32	YI	131	LYS	Peptide
35	YP	107	LYS	Peptide
39	YT	123	GLN	Peptide
40	YU	92	ARG	Peptide
40	YU	95	LEU	Peptide
41	YV	44	LYS	Peptide

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Mol	Chain	Res	Type	Group
41	YV	49	THR	Peptide
45	YZ	179	ASP	Peptide
45	YZ	52	SER	Peptide
45	YZ	60	GLU	Peptide
45	YZ	62	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32244	0	16274	320	0
1	XA	32246	0	16277	343	2
2	QB	1907	0	1958	36	0
2	XB	1915	0	1969	25	0
3	QC	1605	0	1668	17	0
3	XC	1605	0	1668	15	0
4	QD	1703	0	1766	30	0
4	XD	1703	0	1767	29	0
5	QE	1155	0	1213	12	0
5	XE	1155	0	1213	12	0
6	QF	843	0	857	12	0
6	XF	843	0	857	10	0
7	QG	1257	0	1296	18	0
7	XG	1257	0	1296	26	0
8	QH	1108	0	1165	14	0
8	XH	1108	0	1165	15	0
9	QI	1010	0	1037	24	0
9	XI	998	0	1024	25	0
10	QJ	801	0	849	17	0
10	XJ	777	0	816	16	0
11	QK	885	0	904	23	0
11	XK	864	0	881	23	0
12	QL	975	0	1062	16	0
12	XL	956	0	1046	18	0
13	QM	955	0	1021	19	0
13	XM	946	0	1007	20	0
14	QN	492	0	529	8	0
14	XN	492	0	529	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	QO	734	0	771	4	0
15	XO	729	0	768	8	0
16	QP	705	0	725	11	0
16	XP	705	0	725	9	0
17	QQ	834	0	904	14	0
17	XQ	834	0	904	17	0
18	QR	574	0	644	8	0
18	XR	574	0	644	6	0
19	QS	665	0	686	13	0
19	XS	674	0	699	9	0
20	QT	763	0	860	9	0
20	XT	763	0	861	11	0
21	QU	217	0	234	8	0
21	XU	217	0	234	8	0
22	QV	1644	0	836	10	0
22	QW	1640	0	837	57	0
22	XV	1644	0	836	9	0
22	XW	1640	0	837	71	0
23	QX	167	0	86	3	0
23	XX	230	0	120	17	0
24	QY	362	0	183	3	0
24	XY	362	0	184	3	0
25	RA	62071	0	31285	461	0
25	YA	62091	0	31290	472	1
26	RB	2573	0	1306	26	0
26	YB	2573	0	1306	28	1
27	RD	2115	0	2195	49	0
27	YD	2115	0	2195	48	0
28	RE	1568	0	1634	29	0
28	YE	1568	0	1634	33	0
29	RF	1585	0	1632	24	0
29	YF	1585	0	1632	22	0
30	RG	1474	0	1535	26	0
30	YG	1474	0	1535	32	0
31	RH	1336	0	1418	19	0
31	YH	1336	0	1418	20	0
32	RI	1136	0	1223	12	2
32	YI	1136	0	1223	14	0
33	RN	1104	0	1180	9	0
33	YN	1104	0	1180	8	0
34	RO	933	0	996	20	0
34	YO	933	0	996	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	RP	1145	0	1227	25	0
35	YP	1122	0	1204	25	0
36	RQ	1122	0	1179	31	0
36	YQ	1122	0	1179	24	0
37	RR	960	0	1021	14	0
37	YR	960	0	1021	9	0
38	RS	882	0	943	18	0
38	YS	882	0	943	20	0
39	RT	1141	0	1202	23	0
39	YT	1141	0	1202	25	0
40	RU	964	0	1022	33	0
40	YU	964	0	1022	24	0
41	RV	779	0	852	9	0
41	YV	779	0	852	7	4
42	RW	900	0	964	13	1
42	YW	900	0	964	12	0
43	RX	725	0	778	6	0
43	YX	725	0	778	7	0
44	RY	818	0	909	8	4
44	YY	818	0	909	15	1
45	RZ	1461	0	1493	28	0
45	YZ	1461	0	1493	26	0
46	R0	643	0	667	10	0
46	Y0	599	0	617	13	0
47	R1	763	0	848	14	0
47	Y1	729	0	802	10	0
48	R2	581	0	629	9	0
48	Y2	581	0	629	11	4
49	R3	469	0	518	6	0
49	Y3	469	0	518	3	0
50	R4	565	0	557	8	0
50	Y4	565	0	557	10	0
51	R5	459	0	476	6	0
51	Y5	459	0	479	4	4
52	R6	453	0	473	8	0
52	Y6	453	0	473	6	0
53	R7	409	0	454	4	0
53	Y7	418	0	467	5	0
54	R8	517	0	582	14	0
54	Y8	517	0	582	10	0
55	R9	307	0	335	4	0
55	Y9	307	0	335	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	QA	72	0	0	0	0
56	QC	1	0	0	0	0
56	QF	1	0	0	0	0
56	QH	1	0	0	0	0
56	QV	6	0	0	0	0
56	QX	1	0	0	0	0
56	QY	1	0	0	0	0
56	R0	3	0	0	0	0
56	R8	1	0	0	0	0
56	RA	513	0	0	0	0
56	RB	11	0	0	0	0
56	RE	3	0	0	0	0
56	RN	1	0	0	0	0
56	RO	1	0	0	0	0
56	RP	2	0	0	0	0
56	RQ	2	0	0	0	0
56	RR	2	0	0	0	0
56	RT	1	0	0	0	0
56	RY	1	0	0	0	0
56	XA	80	0	0	0	0
56	XC	1	0	0	0	0
56	XE	1	0	0	0	0
56	XL	1	0	0	0	0
56	XM	1	0	0	0	0
56	XQ	1	0	0	0	0
56	XS	1	0	0	0	0
56	XV	8	0	0	0	0
56	XX	1	0	0	0	0
56	Y0	2	0	0	0	0
56	Y5	1	0	0	0	0
56	Y7	1	0	0	0	0
56	Y8	1	0	0	0	0
56	YA	541	0	0	0	0
56	YB	12	0	0	0	0
56	YD	1	0	0	0	0
56	YE	3	0	0	0	0
56	YO	1	0	0	0	0
56	YP	4	0	0	0	0
56	YQ	3	0	0	0	0
56	YX	2	0	0	0	0
56	YY	1	0	0	0	0
57	QD	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	XD	8	0	0	0	0
58	QN	1	0	0	0	0
58	R4	1	0	0	0	0
58	R5	1	0	0	0	0
58	R6	1	0	0	0	0
58	R9	1	0	0	0	0
58	RY	1	0	0	0	0
58	XN	1	0	0	0	0
58	Y4	1	0	0	0	0
58	Y5	1	0	0	0	0
58	Y6	1	0	0	0	0
58	Y9	1	0	0	0	0
58	YY	1	0	0	0	0
All	All	295646	0	199660	2768	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 6.

All (2768) 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)
7:XG:143:ARG:CD	22:XW:42:C:O3'	1.75	1.33
7:QG:143:ARG:HD3	22:QW:42:C:O3'	1.09	1.24
7:QG:143:ARG:CD	22:QW:42:C:O3'	1.88	1.20
23:XX:22:C:H6	23:XX:22:C:H5''	1.06	1.13
11:XK:54:ARG:HH22	22:XW:40:C:H4'	1.12	1.09
11:QK:54:ARG:HH12	22:QW:40:C:H4'	1.01	1.07
7:XG:143:ARG:HD3	22:XW:42:C:O3'	0.90	1.07
25:RA:2135:A:H62	25:RA:2156:G:N2	1.53	1.06
25:RA:2135:A:N6	25:RA:2156:G:H21	1.55	1.05
23:XX:22:C:H5''	23:XX:22:C:C6	1.93	1.04
7:QG:143:ARG:HD3	22:QW:43:G:P	1.98	1.02
7:XG:143:ARG:HD3	22:XW:43:G:P	2.00	1.00
26:RB:8:U:H3	26:RB:112:G:H1	1.00	1.00
1:QA:410:G:N2	1:QA:432:A:H62	1.60	0.99
22:QW:77:A:H8	22:QW:77:A:H5'	1.27	0.97
22:QV:51:U:H3	22:QV:65:G:H1	1.10	0.97
7:XG:143:ARG:HG2	22:XW:42:C:H4'	1.45	0.96
1:XA:1238:A:N6	1:XA:1301:U:H3	1.63	0.96
25:YA:1165:U:H3	25:YA:1184:G:H1	0.99	0.96
26:YB:8:U:H3	26:YB:112:G:H1	1.00	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:QW:77:A:H5'	22:QW:77:A:C8	2.01	0.95
1:QA:410:G:H21	1:QA:432:A:N6	1.66	0.94
22:XV:51:U:H3	22:XV:65:G:H1	1.10	0.94
23:XX:22:C:H6	23:XX:22:C:C5'	1.80	0.93
25:YA:15:G:H1	25:YA:525:U:H3	0.99	0.93
11:QK:54:ARG:NH1	22:QW:40:C:H4'	1.83	0.93
26:YB:22:U:H3	26:YB:61:G:H1	0.95	0.92
1:QA:687:A:H62	1:QA:703:G:N2	1.67	0.91
25:YA:2099:U:H3	25:YA:2190:G:H1	1.14	0.91
7:XG:143:ARG:HD2	22:XW:42:C:O2'	1.71	0.90
26:RB:22:U:H3	26:RB:61:G:H1	0.95	0.90
11:XK:54:ARG:HH22	22:XW:40:C:C4'	1.89	0.85
26:RB:75:G:HO2'	45:RZ:85:HIS:HE2	1.25	0.84
11:XK:54:ARG:NH2	22:XW:40:C:H4'	1.92	0.83
25:RA:1165:U:H3	25:RA:1184:G:H1	1.26	0.83
7:QG:143:ARG:HG2	22:QW:42:C:H4'	1.61	0.82
22:XW:35:C:N4	23:XX:14:A:C6	2.48	0.81
25:YA:2698:U:H3	25:YA:2709:G:H1	1.26	0.81
22:XW:35:C:N4	23:XX:14:A:N6	2.29	0.80
1:XA:1055:A:H62	1:XA:1200:C:H42	1.30	0.79
22:QW:72:C:HO2'	25:RA:1851:U:HO2'	1.16	0.78
25:YA:2343:C:HO2'	25:YA:2373:G:HO2'	1.31	0.78
1:QA:1002:G:H1	1:QA:1038:C:H42	1.32	0.77
25:YA:2245:U:H5'	25:YA:2246:G:H5'	1.67	0.77
1:XA:606:G:H21	1:XA:632:A:H62	1.32	0.76
1:QA:410:G:H21	1:QA:432:A:H62	0.84	0.76
22:XW:77:A:C2	25:YA:2422:A:C2	2.74	0.75
22:XW:77:A:O3'	25:YA:2394:C:O2	2.05	0.74
25:RA:2135:A:H62	25:RA:2156:G:H21	0.78	0.74
1:XA:1127:G:N2	1:XA:1145:C:O2	2.21	0.74
22:XW:20:G:N1	25:YA:2112:G:N2	2.10	0.74
25:RA:883:G:H1	25:RA:893:C:H42	1.35	0.73
1:QA:189:U:O2	17:QQ:63:ARG:NH2	2.22	0.72
1:QA:1422:G:H5''	34:RO:48:PRO:HB3	1.71	0.72
1:XA:69:G:H1	1:XA:99:C:H42	1.36	0.72
47:R1:91:LYS:HE2	47:R1:92:LYS:HE2	1.71	0.71
25:YA:2068:U:H3	25:YA:2430:A:H2	1.37	0.71
1:QA:157:G:H1	1:QA:164:U:H3	1.38	0.71
2:QB:185:ILE:HG22	2:QB:199:TYR:HB2	1.73	0.71
1:QA:687:A:N6	1:QA:703:G:H21	1.88	0.71
25:RA:1055:G:H1	25:RA:1104:C:H42	1.36	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:YA:141:A:H8	25:YA:1595:G:H21	1.40	0.70
28:RE:78:LEU:HG	28:RE:79:ARG:HG2	1.73	0.70
1:QA:687:A:N6	1:QA:703:G:N2	2.40	0.70
22:QW:8:U:N3	22:QW:14:A:C8	2.58	0.70
1:XA:674:G:H2'	1:XA:675:A:H8	1.56	0.70
1:XA:927:G:H1	1:XA:1390:U:H3	1.38	0.70
28:YE:78:LEU:HG	28:YE:79:ARG:HG2	1.73	0.69
25:RA:2118:U:H3	25:RA:2148:G:H4'	1.57	0.69
1:QA:687:A:H62	1:QA:703:G:H21	1.40	0.69
25:RA:1062:G:N2	25:RA:1077:A:N6	2.41	0.69
25:YA:958:U:OP2	36:YQ:14:ARG:NH1	2.25	0.69
22:QW:77:A:O2'	25:RA:2394:C:N3	2.25	0.69
1:XA:1329:A:N7	21:XU:7:ARG:NH2	2.37	0.69
1:XA:1357:A:H61	1:XA:1365:G:H1	1.40	0.69
22:XW:8:U:N3	22:XW:14:A:C8	2.61	0.69
26:YB:114:G:HO2'	38:YS:50:SER:HG	1.34	0.69
40:RU:50:ARG:O	40:RU:54:LYS:NZ	2.26	0.69
25:RA:1309:G:HO2'	25:RA:1611:C:HO2'	1.40	0.68
22:XW:35:C:C4	23:XX:14:A:N6	2.61	0.68
1:QA:1147:C:HO2'	9:QI:5:TYR:HH	1.42	0.68
5:XE:102:ALA:HB1	5:XE:106:PRO:HG2	1.75	0.68
10:XJ:61:GLU:OE1	14:XN:58:LYS:NZ	2.27	0.68
25:YA:602:G:HO2'	25:YA:604:G:HO2'	1.42	0.68
25:YA:1817:G:OP1	27:YD:88:ARG:NH2	2.27	0.68
7:QG:143:ARG:HD2	22:QW:42:C:O2'	1.92	0.68
1:XA:1316:G:H22	1:XA:1319:A:H5''	1.59	0.68
7:XG:143:ARG:HD3	22:XW:42:C:C3'	2.16	0.68
25:YA:888:C:H3'	25:YA:889:C:H4'	1.74	0.68
9:QI:112:LYS:HA	9:QI:119:ALA:HB2	1.76	0.68
5:QE:102:ALA:HB1	5:QE:106:PRO:HG2	1.75	0.67
1:XA:593:G:H1	1:XA:646:U:H3	1.42	0.67
1:XA:1095:U:OP1	1:XA:1108:G:N2	2.25	0.67
1:XA:1238:A:N7	1:XA:1301:U:O4	2.26	0.67
10:QJ:61:GLU:OE1	14:QN:58:LYS:NZ	2.27	0.67
1:XA:1325:C:OP2	21:XU:6:ARG:NH2	2.26	0.67
25:YA:2303:G:N3	30:YG:132:ASN:ND2	2.42	0.67
25:RA:1359:A:H62	25:RA:1372:U:H3	1.42	0.67
40:YU:50:ARG:O	40:YU:54:LYS:NZ	2.26	0.67
7:XG:144:MET:CE	22:XW:31:G:H21	2.07	0.67
27:YD:8:PRO:HB3	27:YD:14:ARG:HB3	1.77	0.67
11:QK:18:ARG:HG2	11:QK:81:ASP:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:QS:67:VAL:HG21	50:R4:58:ARG:HB3	1.77	0.67
25:RA:2096:U:H3	25:RA:2193:G:H1	1.43	0.67
27:RD:8:PRO:HB3	27:RD:14:ARG:HB3	1.77	0.67
50:Y4:16:CYS:SG	50:Y4:17:GLY:N	2.69	0.66
3:QC:172:ARG:HG2	3:QC:174:PRO:HD3	1.78	0.66
25:RA:2068:U:H3	25:RA:2430:A:H2	1.40	0.66
1:QA:339:C:OP2	34:RO:97:ARG:NH1	2.28	0.66
3:XC:172:ARG:HG2	3:XC:174:PRO:HD3	1.78	0.66
25:RA:994:C:OP1	40:RU:53:ARG:NH2	2.28	0.66
25:RA:639:U:H3	25:RA:649:G:H1	1.43	0.66
50:R4:16:CYS:SG	50:R4:17:GLY:N	2.69	0.66
22:XW:77:A:N3	25:YA:2422:A:C2	2.64	0.66
38:YS:20:ARG:NH1	46:Y0:48:GLY:O	2.28	0.66
1:QA:132:C:O3'	20:QT:74:LYS:NZ	2.26	0.66
25:RA:1062:G:N2	25:RA:1077:A:C6	2.64	0.66
40:YU:92:ARG:HD3	40:YU:94:ASN:HB3	1.78	0.66
12:QL:60:LEU:HD12	12:QL:62:SER:H	1.61	0.65
22:QW:34:U:H3'	22:QW:35:C:H5''	1.77	0.65
40:RU:92:ARG:HD3	40:RU:94:ASN:HB3	1.78	0.65
47:R1:83:GLU:HG2	47:R1:85:LEU:H	1.61	0.65
1:QA:8:A:N6	4:QD:205:GLU:O	2.29	0.65
25:RA:2619:C:H5''	28:RE:152:LYS:HA	1.78	0.65
25:YA:2882:A:OP1	37:YR:96:ARG:NH1	2.30	0.65
1:QA:924:C:O2'	1:QA:1502:A:N6	2.30	0.65
7:XG:143:ARG:CD	22:XW:42:C:C3'	2.74	0.65
1:QA:1130:A:O2'	9:QI:3:GLN:NE2	2.30	0.65
22:QW:59:A:O2'	22:QW:60:A:OP1	2.14	0.65
1:XA:261:U:OP2	20:XT:79:ARG:NH2	2.30	0.65
25:RA:83:G:N2	25:RA:103:A:OP2	2.29	0.65
25:RA:2293:C:OP1	38:RS:89:ARG:NH1	2.26	0.65
25:YA:2701:C:H3'	25:YA:2702:U:H5''	1.79	0.65
26:YB:43:C:O2'	30:YG:98:ARG:NH2	2.30	0.65
25:RA:2119:A:N6	25:RA:2170:A:N7	2.44	0.64
2:XB:185:ILE:HG22	2:XB:199:TYR:HB2	1.77	0.64
25:YA:1607:C:N4	25:YA:1622:G:OP2	2.29	0.64
1:QA:403:C:OP2	4:QD:74:GLN:NE2	2.31	0.64
25:RA:2882:A:OP1	37:RR:96:ARG:NH1	2.29	0.64
25:YA:2291:U:H3	25:YA:2341:G:H1	1.44	0.64
40:RU:90:VAL:HG22	41:RV:39:LEU:HD23	1.80	0.64
1:QA:954:G:H21	1:QA:1227:A:H62	1.44	0.64
25:RA:1019:U:H3	25:RA:1142(A):A:H62	1.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:YA:572:A:OP2	41:YV:78:LYS:NZ	2.31	0.64
25:YA:1309:G:HO2'	25:YA:1611:C:HO2'	1.43	0.64
1:XA:1298:C:OP2	7:XG:114:ARG:NH2	2.31	0.64
25:YA:1479:G:N7	25:YA:1510:A:N6	2.45	0.64
25:RA:993:G:OP1	40:RU:50:ARG:NH2	2.29	0.64
25:RA:1111:A:H5'	31:RH:3:ARG:HH21	1.62	0.64
25:RA:1065:U:H3	25:RA:1073:A:H61	1.44	0.64
33:YN:133:GLN:HG2	33:YN:135:PRO:HD3	1.80	0.64
25:RA:1542:G:O6	25:RA:1543:A:N6	2.32	0.63
25:RA:2747:G:H21	25:RA:2757:A:H62	1.46	0.63
12:XL:71:PRO:O	12:XL:102:ARG:NH1	2.32	0.63
15:XO:7:GLU:OE2	15:XO:38:ARG:NH2	2.31	0.63
1:XA:1191:A:OP2	3:XC:3:ASN:ND2	2.32	0.63
3:XC:20:SER:HB2	3:XC:40:ARG:HH22	1.64	0.63
51:R5:20:ARG:HA	51:R5:23:HIS:HD2	1.63	0.63
4:XD:100:ARG:NH2	4:XD:136:PRO:O	2.32	0.63
28:YE:5:LEU:HG	28:YE:49:LEU:HD23	1.81	0.63
28:RE:5:LEU:HG	28:RE:49:LEU:HD23	1.81	0.63
1:XA:606:G:N2	1:XA:632:A:H62	1.97	0.63
1:XA:686:U:H1'	11:XK:42:TRP:HE1	1.63	0.63
25:YA:2314:C:H2'	25:YA:2315:G:H8	1.63	0.63
1:QA:537:G:H5''	12:QL:113:ARG:HH12	1.63	0.63
36:RQ:34:LEU:HD11	36:RQ:129:THR:HB	1.81	0.63
1:XA:950:U:H3	1:XA:1231:G:H1	1.46	0.63
1:XA:1238:A:H62	1:XA:1301:U:H3	0.80	0.63
2:XB:118:LEU:HB3	2:XB:142:LEU:HD12	1.80	0.63
1:XA:708:C:H2'	1:XA:709:G:H8	1.64	0.63
10:XJ:26:ALA:O	10:XJ:84:GLN:NE2	2.32	0.63
16:XP:45:THR:HG22	16:XP:47:ASP:H	1.63	0.63
16:QP:45:THR:HG22	16:QP:47:ASP:H	1.63	0.63
25:RA:1124:C:O2	55:R9:36:GLN:NE2	2.32	0.63
1:XA:842:C:O2'	1:XA:848:C:N4	2.32	0.63
1:XA:1147:C:HO2'	9:XI:5:TYR:HH	1.46	0.63
1:XA:1189:C:OP2	10:XJ:51:ARG:NH2	2.32	0.63
25:YA:884:C:H41	25:YA:886:C:H1'	1.64	0.63
4:QD:100:ARG:NH2	4:QD:136:PRO:O	2.32	0.62
25:YA:2839:G:H1	25:YA:2878:U:H3	1.46	0.62
3:QC:95:THR:HG22	3:QC:97:LYS:H	1.64	0.62
1:XA:80:G:H1	1:XA:89:U:H3	1.46	0.62
3:QC:19:GLU:HG2	3:QC:54:ARG:HE	1.64	0.62
1:XA:266:G:H5'	1:XA:268:C:H41	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:YA:1195:G:O6	35:YP:16:ARG:NH2	2.32	0.62
3:QC:20:SER:HB2	3:QC:40:ARG:HH22	1.64	0.62
10:QJ:51:ARG:O	14:QN:45:ARG:NH1	2.32	0.62
33:RN:133:GLN:HG2	33:RN:135:PRO:HD3	1.80	0.62
41:YV:61:VAL:HG12	41:YV:63:GLY:H	1.64	0.62
1:QA:673:G:O3'	6:QF:87:ARG:NH2	2.32	0.62
25:RA:27:G:N2	25:RA:513:A:OP2	2.32	0.62
1:XA:341:C:H42	1:XA:348:G:H1	1.46	0.62
36:YQ:34:LEU:HD11	36:YQ:129:THR:HB	1.81	0.62
16:QP:4:ILE:HG12	16:QP:21:VAL:HG12	1.82	0.62
41:RV:61:VAL:HG12	41:RV:63:GLY:H	1.64	0.62
1:XA:189:U:O2	17:XQ:63:ARG:NH2	2.32	0.62
1:XA:1249:C:O2'	9:XI:73:GLN:NE2	2.32	0.62
1:XA:1422:G:H5''	34:YO:48:PRO:HB3	1.82	0.62
3:XC:19:GLU:HG2	3:XC:54:ARG:HE	1.64	0.62
25:YA:1728:G:H8	25:YA:1732:A:H62	1.48	0.62
29:YF:116:ASP:OD1	29:YF:119:ARG:NH2	2.33	0.62
25:RA:2303:G:N3	30:RG:132:ASN:ND2	2.48	0.62
1:XA:1130:A:O2'	9:XI:3:GLN:NE2	2.33	0.62
25:YA:259:G:H21	25:YA:621:A:H8	1.48	0.62
25:RA:1607:C:N4	25:RA:1622:G:OP2	2.31	0.62
1:XA:278:G:OP2	17:XQ:92:ARG:NH2	2.31	0.62
11:QK:109:VAL:HG12	18:QR:86:VAL:HA	1.81	0.62
25:RA:2378:A:N1	38:RS:17:ARG:NH1	2.47	0.62
22:XW:59:A:O2'	22:XW:60:A:OP1	2.16	0.61
47:R1:87:PRO:HA	47:R1:90:ILE:HG22	1.82	0.61
1:XA:132:C:O3'	20:XT:74:LYS:NZ	2.29	0.61
2:QB:178:ARG:NH2	2:QB:196:LEU:O	2.32	0.61
35:RP:52:GLU:OE2	54:R8:52:LYS:NZ	2.34	0.61
39:RT:51:ARG:HG2	39:RT:98:LYS:HD2	1.82	0.61
25:YA:2126:A:N6	25:YA:2163:C:O2'	2.31	0.61
1:QA:278:G:OP2	17:QQ:92:ARG:NH2	2.33	0.61
4:QD:62:GLN:HE22	4:QD:65:ARG:HH21	1.48	0.61
25:RA:2296:U:OP2	38:RS:9:ARG:NH1	2.33	0.61
2:XB:178:ARG:NH2	2:XB:196:LEU:O	2.32	0.61
18:QR:32:ARG:HA	18:QR:69:THR:HG21	1.82	0.61
30:RG:37:VAL:HG22	30:RG:159:VAL:HG12	1.83	0.61
22:QW:77:A:H8	22:QW:77:A:C5'	2.08	0.61
25:RA:2734:A:H62	25:RA:2770:G:H21	1.47	0.61
4:XD:62:GLN:HE22	4:XD:65:ARG:HH21	1.48	0.61
10:XJ:49:VAL:HG23	14:XN:41:ARG:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:XR:32:ARG:HA	18:XR:69:THR:HG21	1.82	0.61
47:Y1:83:GLU:HG2	47:Y1:85:LEU:H	1.64	0.61
1:QA:372:C:H42	1:QA:389:A:H62	1.47	0.61
1:XA:544:G:OP1	4:XD:59:ARG:NH2	2.34	0.61
16:XP:4:ILE:HG12	16:XP:21:VAL:HG12	1.82	0.61
51:Y5:20:ARG:HA	51:Y5:23:HIS:HD2	1.63	0.61
10:QJ:49:VAL:HG13	14:QN:41:ARG:HB2	1.83	0.61
25:RA:259:G:H21	25:RA:621:A:H8	1.48	0.61
1:QA:448:A:OP2	1:QA:485:G:N2	2.33	0.61
10:XJ:38:ILE:HD11	10:XJ:71:LEU:HD23	1.82	0.61
25:YA:1666:G:N3	34:YO:3:GLN:NE2	2.48	0.61
39:YT:51:ARG:HG2	39:YT:98:LYS:HD2	1.82	0.61
1:QA:806:C:H2'	1:QA:807:A:H8	1.66	0.61
29:RF:116:ASP:OD1	29:RF:119:ARG:NH2	2.33	0.61
25:YA:1055:G:H1	25:YA:1104:C:H42	1.49	0.61
31:RH:46:GLU:OE1	31:RH:51:ARG:NH1	2.34	0.60
1:XA:664:G:H22	1:XA:741:G:H1	1.49	0.60
1:XA:1125:U:OP2	1:XA:1145:C:N4	2.34	0.60
1:XA:1305:G:N2	1:XA:1332:A:OP2	2.33	0.60
3:XC:95:THR:HG22	3:XC:97:LYS:H	1.64	0.60
22:QW:20:G:O6	25:RA:2112:G:C2	2.55	0.60
25:RA:2788:C:O2'	25:RA:2809:A:N3	2.33	0.60
9:XI:21:PRO:HA	9:XI:59:PHE:HA	1.83	0.60
1:QA:34:C:H2'	1:QA:35:G:H8	1.67	0.60
1:QA:664:G:H22	1:QA:741:G:H1	1.48	0.60
1:QA:979:C:O2	14:QN:19:ARG:NE	2.34	0.60
25:RA:2292:C:OP1	38:RS:17:ARG:NH2	2.34	0.60
29:RF:116:ASP:OD2	35:RP:1:MET:N	2.30	0.60
9:QI:28:VAL:HG22	9:QI:63:ILE:HB	1.83	0.60
22:QW:77:A:N1	54:R8:31:HIS:CE1	2.70	0.60
25:RA:1056:G:H21	25:RA:1103:A:H62	1.49	0.60
1:XA:1356:G:H2'	1:XA:1357:A:H8	1.65	0.60
10:XJ:7:LYS:HB2	10:XJ:97:GLU:HB2	1.82	0.60
25:YA:83:G:N2	25:YA:103:A:OP2	2.25	0.60
28:YE:201:THR:HG22	28:YE:203:LYS:H	1.66	0.60
28:RE:201:THR:HG22	28:RE:203:LYS:H	1.66	0.60
10:QJ:3:LYS:N	10:QJ:74:ILE:O	2.35	0.60
25:RA:2784:C:O2'	28:RE:37:ARG:NH1	2.34	0.60
1:XA:1351:U:H3	1:XA:1371:G:H1	1.49	0.60
1:QA:1306:A:N6	1:QA:1331:G:O2'	2.34	0.60
22:QW:15:G:H2'	22:QW:60:A:N1	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:RA:94:G:N3	48:R2:47:ASN:ND2	2.49	0.60
25:RA:1817:G:OP1	27:RD:88:ARG:NH2	2.34	0.60
1:XA:1034:G:N2	1:XA:1035:A:N7	2.49	0.60
11:XK:83:ILE:HG12	11:XK:109:VAL:HB	1.83	0.60
31:YH:46:GLU:OE1	31:YH:51:ARG:NH1	2.34	0.60
35:YP:62:LEU:HD12	54:Y8:30:ARG:HH21	1.65	0.60
28:YE:24:THR:HG21	28:YE:188:VAL:HG11	1.84	0.60
45:YZ:7:ALA:HB2	45:YZ:59:LEU:HB3	1.83	0.60
25:RA:587:C:OP2	35:RP:21:ARG:NH1	2.34	0.60
25:YA:676:A:H8	25:YA:2069:G:H21	1.49	0.60
25:RA:987:G:O2'	25:RA:1000:A:N3	2.33	0.60
35:RP:58:THR:O	35:RP:61:ARG:NH2	2.35	0.60
45:RZ:163:LEU:HD13	45:RZ:167:PRO:HD3	1.84	0.60
25:YA:1365:A:O2'	47:Y1:11:ARG:NH2	2.34	0.60
45:YZ:163:LEU:HD22	45:YZ:167:PRO:HG3	1.84	0.60
25:YA:2845:G:H2'	25:YA:2846:G:H8	1.67	0.59
9:QI:128:ARG:NH2	22:QV:34:U:OP2	2.35	0.59
10:QJ:4:ILE:HG12	10:QJ:100:THR:HG22	1.84	0.59
25:RA:631:A:OP1	54:R8:46:ARG:NH2	2.36	0.59
43:RX:53:LYS:NZ	43:RX:55:ASN:OD1	2.36	0.59
1:XA:148:G:H2'	1:XA:149:A:H8	1.67	0.59
12:XL:60:LEU:HD12	12:XL:62:SER:H	1.67	0.59
30:YG:37:VAL:HG22	30:YG:159:VAL:HG12	1.83	0.59
1:QA:674:G:H2'	1:QA:675:A:H8	1.67	0.59
17:QQ:66:SER:O	17:QQ:70:ARG:NH1	2.35	0.59
25:YA:27:G:N2	25:YA:513:A:OP2	2.35	0.59
1:QA:544:G:OP1	4:QD:59:ARG:NH2	2.36	0.59
2:QB:47:THR:HA	2:QB:202:PRO:HG2	1.85	0.59
19:QS:40:ILE:HG13	19:QS:44:MET:HG3	1.84	0.59
25:YA:1316:U:H2'	25:YA:1317:A:H8	1.67	0.59
25:YA:1858:G:O2'	25:YA:1884:A:N6	2.35	0.59
43:YX:53:LYS:NZ	43:YX:55:ASN:OD1	2.36	0.59
1:QA:134:A:H61	16:QP:25:ARG:HH12	1.51	0.59
25:RA:1270:C:H5''	25:RA:1271:G:H5'	1.85	0.59
25:RA:2701:C:H3'	25:RA:2702:U:H5''	1.84	0.59
36:RQ:48:GLU:OE2	36:RQ:51:ARG:NH2	2.35	0.59
45:RZ:7:ALA:HB2	45:RZ:59:LEU:HB3	1.83	0.59
1:XA:924:C:O2'	1:XA:1502:A:N6	2.34	0.59
17:XQ:66:SER:O	17:XQ:70:ARG:NH1	2.35	0.59
25:YA:270(U):C:H2'	25:YA:270(V):G:H8	1.68	0.59
25:RA:2597:G:H5'	27:RD:243:GLY:HA3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:YA:300:A:OP1	44:YY:86:ARG:NH2	2.36	0.59
46:Y0:70:GLN:OE1	46:Y0:80:HIS:NE2	2.34	0.59
25:RA:1510:A:O2'	25:RA:1511:A:N7	2.36	0.59
33:RN:58:ASP:N	33:RN:58:ASP:OD1	2.36	0.59
1:XA:1296:C:OP1	13:XM:44:ARG:NH2	2.35	0.59
8:QH:10:LEU:HD22	8:QH:83:ILE:HD11	1.84	0.59
28:RE:24:THR:HG21	28:RE:188:VAL:HG11	1.84	0.59
18:XR:86:VAL:HG12	18:XR:87:ARG:HG2	1.85	0.59
25:YA:665:C:H2'	25:YA:666:G:H8	1.67	0.59
36:YQ:48:GLU:OE2	36:YQ:51:ARG:NH2	2.35	0.59
1:QA:1073:U:O2	2:QB:104:ASN:ND2	2.35	0.59
22:QW:77:A:C2	25:RA:2421:G:C6	2.91	0.59
25:RA:630:G:N2	25:RA:633:A:OP2	2.34	0.59
25:RA:2494:G:OP1	46:R0:3:HIS:N	2.36	0.59
44:YY:47:LYS:NZ	44:YY:48:ALA:O	2.35	0.59
25:RA:557:U:H2'	25:RA:558:G:H8	1.68	0.58
30:RG:29:TRP:O	30:RG:33:ARG:NH1	2.36	0.58
40:RU:95:LEU:HD13	41:RV:4:ILE:HD12	1.85	0.58
41:RV:24:LYS:HA	41:RV:92:THR:HG23	1.85	0.58
27:YD:168:ARG:HG2	27:YD:173:VAL:HG12	1.85	0.58
45:YZ:163:LEU:HD13	45:YZ:167:PRO:HD3	1.84	0.58
55:R9:27:CYS:SG	55:R9:28:GLU:N	2.76	0.58
1:XA:673:G:H2'	1:XA:674:G:C8	2.37	0.58
1:QA:261:U:OP2	20:QT:79:ARG:NH2	2.36	0.58
1:QA:979:C:OP1	1:QA:1223:C:N4	2.36	0.58
1:QA:1245:A:OP2	21:QU:9:ARG:NH2	2.33	0.58
35:RP:62:LEU:HD12	54:R8:30:ARG:HH21	1.68	0.58
45:RZ:163:LEU:HD22	45:RZ:167:PRO:HG3	1.84	0.58
25:YA:1651:G:OP1	37:YR:40:LYS:NZ	2.34	0.58
35:YP:68:GLN:HG2	54:Y8:12:LYS:HG2	1.85	0.58
41:YV:24:LYS:HA	41:YV:92:THR:HG23	1.85	0.58
1:QA:1104:G:O2'	2:QB:111:ARG:NH1	2.36	0.58
1:QA:1305:G:N2	1:QA:1332:A:OP2	2.36	0.58
25:RA:1567:A:O2'	27:RD:63:ARG:NH2	2.37	0.58
30:RG:40:ASN:ND2	30:RG:90:LEU:O	2.36	0.58
8:XH:34:GLU:OE1	8:XH:37:ARG:NH2	2.37	0.58
25:YA:1971:A:OP2	27:YD:242:ARG:NH2	2.36	0.58
25:RA:467:G:HO2'	25:RA:796:C:HO2'	1.49	0.58
26:RB:111:U:H2'	26:RB:112:G:H8	1.68	0.58
55:R9:25:VAL:HB	55:R9:34:GLN:HB2	1.85	0.58
13:XM:3:ARG:HH12	30:YG:113:ARG:HH21	1.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:Y9:27:CYS:SG	55:Y9:28:GLU:N	2.76	0.58
1:QA:552:U:H2'	1:QA:553:A:H8	1.68	0.58
25:RA:26:G:H1'	25:RA:515:A:H61	1.68	0.58
25:RA:1228:G:OP2	40:RU:16:LYS:NZ	2.37	0.58
25:RA:2540:C:O2'	25:RA:2740:A:N3	2.35	0.58
27:RD:168:ARG:HG2	27:RD:173:VAL:HG12	1.85	0.58
28:RE:50:GLY:HA2	28:RE:77:ILE:HA	1.86	0.58
22:XW:5:G:H2'	22:XW:6:G:H8	1.69	0.58
25:YA:2508:G:H1	25:YA:2580:U:H3	1.49	0.58
30:YG:40:ASN:ND2	30:YG:90:LEU:O	2.36	0.58
37:YR:86:ARG:NH2	37:YR:118:GLU:OXT	2.37	0.58
18:QR:86:VAL:HG12	18:QR:87:ARG:HG2	1.85	0.58
1:XA:411:A:OP1	4:XD:30:LYS:NZ	2.37	0.58
1:XA:1347:G:N2	1:XA:1374:A:OP2	2.37	0.58
26:YB:111:U:H2'	26:YB:112:G:H8	1.68	0.58
11:QK:86:GLY:O	11:QK:91:ARG:NH1	2.37	0.58
1:XA:701:C:O2	1:XA:703:G:N1	2.37	0.58
8:XH:10:LEU:HD22	8:XH:83:ILE:HD11	1.84	0.58
23:XX:23:A:H8	23:XX:23:A:H3'	1.69	0.58
25:YA:861:A:N3	26:YB:79:C:O2'	2.37	0.58
1:QA:673:G:H2'	1:QA:674:G:C8	2.39	0.58
30:RG:108:ASN:HA	50:R4:37:SER:HB3	1.86	0.58
25:YA:631:A:OP1	54:Y8:46:ARG:NH2	2.37	0.58
25:YA:2033:A:O2'	25:YA:2035:G:OP2	2.21	0.58
27:YD:77:ALA:HB3	27:YD:117:VAL:HG13	1.86	0.58
1:QA:593:G:H1	1:QA:646:U:H3	1.51	0.58
1:QA:1104:G:H4'	2:QB:111:ARG:HD2	1.85	0.58
25:RA:662:G:OP1	35:RP:15:ARG:NH1	2.36	0.58
26:RB:22:U:O2	26:RB:61:G:N2	2.32	0.58
46:R0:27:GLU:HG3	46:R0:68:GLU:HA	1.86	0.58
23:XX:22:C:C6	23:XX:22:C:C5'	2.70	0.58
25:YA:857:C:OP2	46:Y0:77:ARG:NH2	2.37	0.58
25:YA:1212:G:O2'	25:YA:1236:G:N2	2.33	0.58
25:YA:1689:A:H62	25:YA:1698:A:H2	1.52	0.58
30:YG:29:TRP:O	30:YG:33:ARG:NH1	2.36	0.58
44:YY:102:CYS:SG	44:YY:103:GLY:N	2.77	0.58
1:QA:689:C:H3'	1:QA:690:G:H21	1.67	0.57
37:RR:86:ARG:NH2	37:RR:118:GLU:OXT	2.38	0.57
1:XA:545:C:OP1	4:XD:61:LYS:NZ	2.37	0.57
22:XW:8:U:H4'	22:XW:9:G:OP1	2.04	0.57
36:YQ:66:ILE:HA	36:YQ:104:PHE:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:QS:50:ALA:HA	19:QS:58:VAL:O	2.04	0.57
25:RA:1666:G:N3	34:RO:3:GLN:NE2	2.52	0.57
1:XA:1227:A:OP1	19:XS:80:TYR:OH	2.19	0.57
1:QA:272:C:H2'	1:QA:273:A:H8	1.68	0.57
1:QA:490:G:OP2	4:QD:132:ARG:NH2	2.37	0.57
8:QH:34:GLU:OE1	8:QH:37:ARG:NH2	2.37	0.57
27:RD:146:GLU:HB2	27:RD:189:CYS:HB3	1.86	0.57
36:RQ:66:ILE:HA	36:RQ:104:PHE:HA	1.86	0.57
1:XA:403:C:OP2	4:XD:74:GLN:NE2	2.37	0.57
1:XA:913:A:OP1	12:XL:46:LYS:NZ	2.36	0.57
19:XS:50:ALA:HB1	19:XS:57:HIS:HB3	1.86	0.57
25:YA:793:A:OP2	25:YA:2071:A:O2'	2.21	0.57
27:YD:143:HIS:ND1	27:YD:194:GLY:O	2.37	0.57
55:Y9:25:VAL:HB	55:Y9:34:GLN:HB2	1.85	0.57
1:XA:486:U:H2'	1:XA:487:A:H8	1.69	0.57
1:XA:1286:A:H2'	1:XA:1287:A:H4'	1.87	0.57
25:YA:2030:A:H4'	25:YA:2031:A:H8	1.69	0.57
25:YA:2102:U:H3	25:YA:2187:G:H1	1.52	0.57
28:YE:50:GLY:HA2	28:YE:77:ILE:HA	1.86	0.57
1:QA:405:U:O4	4:QD:2:GLY:N	2.37	0.57
1:XA:1244:C:H42	1:XA:1293:G:H1	1.52	0.57
25:YA:918:A:N3	26:YB:80:U:O2'	2.35	0.57
25:YA:2822:G:OP1	28:YE:159:HIS:NE2	2.38	0.57
1:QA:1129:C:N4	1:QA:1133:G:O6	2.37	0.57
44:RY:102:CYS:SG	44:RY:103:GLY:N	2.77	0.57
49:R3:15:TYR:O	49:R3:20:LYS:NZ	2.38	0.57
1:XA:159:G:H21	1:XA:161:A:H8	1.52	0.57
1:QA:562:C:H1'	12:QL:15:ARG:HD2	1.86	0.57
1:QA:1249:C:O2'	9:QI:73:GLN:NE2	2.38	0.57
1:QA:1325:C:H4'	21:QU:17:THR:HG21	1.87	0.57
28:RE:9:VAL:HB	28:RE:25:VAL:HG23	1.87	0.57
25:YA:468:G:OP2	53:Y7:37:LYS:NZ	2.37	0.57
25:YA:768:G:O2'	25:YA:1379:A:N6	2.37	0.57
25:YA:2100:G:H1	25:YA:2189:U:H3	1.53	0.57
25:YA:2313:C:H5''	30:YG:91:ARG:HD3	1.87	0.57
27:YD:146:GLU:HB2	27:YD:189:CYS:HB3	1.86	0.57
40:YU:58:ARG:HH11	40:YU:93:LYS:HE2	1.70	0.57
25:RA:998:C:OP2	40:RU:58:ARG:NH1	2.33	0.57
1:XA:1484:C:HO2'	25:YA:1960:A:HO2'	1.52	0.57
25:YA:521:G:H2'	25:YA:522:G:H8	1.70	0.57
45:YZ:52:SER:O	45:YZ:54:HIS:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1397:C:N3	23:QX:22:C:C5	2.73	0.57
25:RA:815:C:OP2	41:RV:83:ARG:NH1	2.38	0.57
1:XA:1123:A:H4'	10:XJ:36:GLY:HA3	1.86	0.57
25:YA:2646:C:OP2	25:YA:2732:G:O2'	2.20	0.57
25:YA:2680:C:H5'	28:YE:189:PRO:HA	1.87	0.57
25:YA:2729:G:H1'	28:YE:187:ALA:HB2	1.87	0.57
28:YE:9:VAL:HB	28:YE:25:VAL:HG23	1.87	0.57
2:QB:51:LEU:HD23	2:QB:201:ILE:HD12	1.87	0.56
35:RP:68:GLN:HG2	54:R8:12:LYS:HG2	1.86	0.56
47:R1:80:LEU:HD12	47:R1:81:LYS:HG2	1.87	0.56
25:YA:58:G:H5'	43:YX:74:PRO:HB3	1.86	0.56
25:YA:2597:G:H5'	27:YD:243:GLY:HA3	1.86	0.56
36:YQ:77:LYS:NZ	36:YQ:80:GLU:OE2	2.30	0.56
25:RA:2680:C:OP2	28:RE:111:ARG:NH2	2.36	0.56
27:RD:77:ALA:HB3	27:RD:117:VAL:HG13	1.86	0.56
1:XA:356:A:N3	1:XA:368:U:O2'	2.34	0.56
1:XA:1128:C:OP1	9:XI:66:ARG:NH2	2.38	0.56
3:XC:19:GLU:O	3:XC:40:ARG:NH2	2.38	0.56
22:XW:15:G:H2'	22:XW:60:A:N1	2.19	0.56
25:YA:2741:A:H5''	55:Y9:22:ARG:HH12	1.70	0.56
19:QS:50:ALA:HB1	19:QS:57:HIS:HB3	1.88	0.56
25:RA:919:G:N2	25:RA:2269:A:OP2	2.37	0.56
25:RA:1092:C:N4	25:RA:1099:G:O6	2.39	0.56
25:RA:1694:C:O2	25:RA:1695:G:N2	2.39	0.56
26:RB:37:C:O2	38:RS:95:HIS:NE2	2.38	0.56
40:RU:58:ARG:HH11	40:RU:93:LYS:HE2	1.70	0.56
47:R1:52:ARG:HH11	47:R1:57:GLU:HB2	1.71	0.56
2:XB:77:ALA:HB2	2:XB:211:ILE:HD13	1.88	0.56
25:YA:1228:G:OP2	40:YU:16:LYS:NZ	2.38	0.56
37:YR:88:ARG:NH2	37:YR:89:ASP:OD1	2.38	0.56
50:Y4:56:VAL:HG23	50:Y4:58:ARG:HG3	1.88	0.56
1:QA:56:U:H2'	1:QA:57:G:H8	1.70	0.56
25:RA:907:U:O2'	36:RQ:101:ARG:NH2	2.37	0.56
25:RA:2851:A:O2'	37:RR:64:ARG:NH2	2.38	0.56
7:XG:144:MET:HE1	22:XW:31:G:H21	1.69	0.56
12:XL:114:LYS:O	12:XL:117:ARG:NH1	2.38	0.56
25:YA:996:A:OP2	40:YU:92:ARG:NH2	2.39	0.56
25:YA:1857:G:O2'	25:YA:1885:A:N6	2.38	0.56
36:YQ:81:VAL:O	36:YQ:82:ARG:NE	2.36	0.56
25:RA:288:C:H2'	25:RA:289:A:H8	1.71	0.56
26:RB:42:C:O2	30:RG:93:THR:N	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:128:G:O2'	17:XQ:3:LYS:NZ	2.36	0.56
25:YA:1220:A:OP2	40:YU:19:LYS:NZ	2.34	0.56
1:QA:1484:C:HO2'	25:RA:1960:A:HO2'	1.53	0.56
3:QC:19:GLU:O	3:QC:40:ARG:NH2	2.38	0.56
22:QW:40:C:H2'	22:QW:41:C:H6	1.70	0.56
25:RA:2112:G:O6	25:RA:2169:A:N6	2.38	0.56
27:RD:36:PRO:HB2	27:RD:61:LEU:HD12	1.87	0.56
1:XA:1224:G:O2'	1:XA:1322:C:OP2	2.23	0.56
1:XA:1522:U:H2'	1:XA:1523:G:H8	1.71	0.56
13:XM:14:ARG:NH2	13:XM:16:ASP:OD2	2.38	0.56
22:XW:40:C:H2'	22:XW:41:C:H6	1.71	0.56
25:YA:527:C:N4	25:YA:2779:U:OP2	2.37	0.56
25:YA:662:G:OP1	35:YP:15:ARG:NH1	2.39	0.56
25:YA:1196:C:HO2'	25:YA:1228:G:HO2'	1.50	0.56
35:YP:52:GLU:OE2	54:Y8:52:LYS:NZ	2.38	0.56
54:Y8:29:LYS:O	54:Y8:31:HIS:N	2.39	0.56
1:QA:606:G:H22	1:QA:631:G:H5'	1.70	0.56
36:RQ:81:VAL:O	36:RQ:82:ARG:NE	2.36	0.56
30:YG:59:GLU:OE1	30:YG:153:ARG:NH2	2.39	0.56
30:YG:65:GLY:HA2	50:Y4:7:PRO:HG2	1.88	0.56
49:Y3:15:TYR:O	49:Y3:20:LYS:NZ	2.38	0.56
1:QA:464:G:N2	1:QA:467:G:N7	2.53	0.56
25:RA:321:G:O2'	25:RA:340:A:N3	2.36	0.56
25:RA:458:G:N2	25:RA:470:A:OP2	2.39	0.56
25:RA:527:C:N4	25:RA:2779:U:OP2	2.39	0.56
37:RR:104:ARG:HG3	37:RR:107:ASP:HB3	1.87	0.56
50:R4:56:VAL:HG23	50:R4:58:ARG:HG3	1.88	0.56
7:XG:94:ARG:NH1	7:XG:98:SER:OG	2.39	0.56
1:QA:244:U:OP2	17:QQ:100:LYS:NZ	2.38	0.56
1:QA:439:A:OP2	1:QA:493:G:N1	2.39	0.56
1:QA:707:C:OP1	11:QK:85:ARG:NH1	2.36	0.56
1:QA:827:U:O2	1:QA:874:G:N2	2.39	0.56
13:QM:14:ARG:NH2	13:QM:16:ASP:OD2	2.39	0.56
22:QW:8:U:H4'	22:QW:9:G:OP1	2.05	0.56
25:RA:1062:G:C2	25:RA:1077:A:N6	2.74	0.56
25:RA:2123:G:H2'	25:RA:2124:G:H8	1.71	0.56
25:RA:2503:A:O2'	25:RA:2505:G:OP2	2.22	0.56
25:RA:2848:G:O2'	25:RA:2867:G:N2	2.38	0.56
46:Y0:27:GLU:HG3	46:Y0:68:GLU:HA	1.87	0.56
7:QG:86:GLN:OE1	22:QW:32:G:N2	2.31	0.56
25:RA:1041:C:H2'	25:RA:1042:G:H8	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:RA:2102:U:H3	25:RA:2187:G:H1	1.54	0.56
1:XA:8:A:N6	4:XD:205:GLU:O	2.39	0.56
24:XY:37:A:O2'	25:YA:1913:A:N1	2.37	0.56
2:QB:209:ARG:HD3	2:QB:240:GLN:HE22	1.71	0.55
7:QG:94:ARG:NH1	7:QG:98:SER:OG	2.39	0.55
25:RA:955:C:OP1	36:RQ:85:LYS:NZ	2.35	0.55
25:RA:2245:U:H5''	25:RA:2246:G:H5'	1.88	0.55
1:XA:1077:G:N2	1:XA:1080:A:OP2	2.32	0.55
25:YA:1791:A:N6	25:YA:1828:G:O2'	2.36	0.55
25:YA:2619:C:H5''	28:YE:152:LYS:HA	1.87	0.55
35:YP:101:VAL:HB	35:YP:106:LEU:HB2	1.88	0.55
1:QA:581:G:O3'	15:QO:64:ARG:NH2	2.39	0.55
1:QA:1261:A:H62	1:QA:1274:G:H21	1.54	0.55
25:RA:956:G:OP2	36:RQ:14:ARG:NH2	2.37	0.55
25:RA:2816:C:O2	25:RA:2883:A:O2'	2.25	0.55
27:YD:17:THR:HB	27:YD:205:VAL:H	1.72	0.55
32:YI:3:VAL:HG12	32:YI:38:LEU:HA	1.88	0.55
28:RE:36:ARG:NH1	28:RE:85:ASN:OD1	2.39	0.55
1:XA:34:C:H2'	1:XA:35:G:H8	1.71	0.55
22:XW:77:A:C4	25:YA:2422:A:C2	2.94	0.55
23:XX:22:C:C6	23:XX:22:C:C4'	2.90	0.55
25:YA:1215:G:H1	25:YA:1234:U:H3	1.55	0.55
25:YA:1667:G:O2'	25:YA:1991:U:O4	2.23	0.55
1:QA:1502:A:H2	1:QA:1505:G:H1	1.53	0.55
22:QW:8:U:C2	22:QW:14:A:N7	2.74	0.55
25:RA:2285:C:OP1	52:R6:29:ASN:ND2	2.39	0.55
25:YA:467:G:N7	53:Y7:39:ARG:NH2	2.54	0.55
6:QF:47:ARG:NH2	6:QF:57:GLN:OE1	2.39	0.55
25:YA:1065:U:H3	25:YA:1073:A:H61	1.55	0.55
25:YA:1682:G:OP2	25:YA:1699:G:N2	2.40	0.55
25:YA:1889:A:N3	25:YA:2086:U:O2'	2.38	0.55
27:YD:36:PRO:HB2	27:YD:61:LEU:HD12	1.88	0.55
2:QB:77:ALA:HB2	2:QB:211:ILE:HD13	1.88	0.55
10:QJ:6:ILE:HA	10:QJ:97:GLU:O	2.07	0.55
25:RA:1689:A:H62	25:RA:1698:A:H2	1.53	0.55
32:RI:3:VAL:HG12	32:RI:38:LEU:HA	1.88	0.55
52:R6:10:LEU:HD13	52:R6:19:ARG:HG2	1.88	0.55
1:XA:1055:A:H62	1:XA:1200:C:N4	2.04	0.55
11:XK:34:ASP:OD1	11:XK:38:ASN:N	2.39	0.55
25:YA:1827:C:OP2	27:YD:222:ARG:NH1	2.40	0.55
25:YA:1906:G:N2	25:YA:1925:C:O2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:Y6:10:LEU:HD13	52:Y6:19:ARG:HG2	1.88	0.55
1:QA:297:G:N2	1:QA:300:A:OP2	2.33	0.55
25:RA:2576:G:O2'	25:RA:2579:C:OP2	2.25	0.55
1:XA:244:U:OP2	17:XQ:100:LYS:NZ	2.40	0.55
1:XA:811:C:O2'	1:XA:901:A:N1	2.40	0.55
1:XA:1372:U:H5''	9:XI:71:SER:HB3	1.89	0.55
25:YA:1062:G:H2'	25:YA:1063:G:H8	1.71	0.55
25:YA:1124:C:O2	55:Y9:36:GLN:NE2	2.39	0.55
25:YA:1666:G:HO2'	34:YO:6:THR:HG1	1.51	0.55
30:YG:114:ILE:HB	30:YG:117:PHE:HB2	1.88	0.55
5:QE:91:LEU:HG	5:QE:120:THR:HG22	1.89	0.55
25:RA:2729:G:H1'	28:RE:187:ALA:HB2	1.88	0.55
30:RG:114:ILE:HB	30:RG:117:PHE:HB2	1.88	0.55
48:R2:23:LYS:NZ	48:R2:27:GLU:OE2	2.40	0.55
1:XA:1036:G:N7	1:XA:1037:C:N4	2.55	0.55
7:XG:147:ALA:HB2	22:XW:42:C:H5'	1.89	0.55
25:YA:297:C:OP1	44:YY:87:LYS:NZ	2.32	0.55
26:YB:11:C:OP2	46:Y0:72:ARG:NH2	2.40	0.55
35:YP:135:LEU:HG	35:YP:139:LYS:HE2	1.89	0.55
25:RA:270(T):G:H5''	47:R1:97:LEU:HD22	1.89	0.55
25:RA:332:A:O2'	25:RA:334:C:OP2	2.20	0.55
25:RA:2683:C:OP1	39:RT:53:ARG:NH2	2.30	0.55
22:XW:8:U:C2	22:XW:14:A:N7	2.75	0.55
36:RQ:77:LYS:NZ	36:RQ:80:GLU:OE2	2.30	0.55
1:XA:272:C:H2'	1:XA:273:A:H8	1.71	0.55
25:YA:363(A):A:H2'	25:YA:363(B):G:H8	1.72	0.55
28:YE:36:ARG:NH1	28:YE:85:ASN:OD1	2.39	0.55
1:QA:963:G:H1	1:QA:972:C:H42	1.54	0.54
1:QA:1129:C:N4	1:QA:1142:G:O6	2.30	0.54
4:QD:119:GLN:OE1	4:QD:123:HIS:ND1	2.41	0.54
38:RS:15:ARG:NE	38:RS:88:ASP:OD1	2.40	0.54
45:RZ:48:PHE:HA	45:RZ:51:ALA:HB3	1.89	0.54
19:XS:32:LYS:HA	19:XS:50:ALA:HB3	1.90	0.54
25:YA:296:C:O3'	44:YY:95:LYS:NZ	2.41	0.54
25:YA:581:C:H2'	25:YA:582:G:H8	1.72	0.54
1:QA:587:G:N2	1:QA:754:C:OP2	2.40	0.54
37:RR:103:ARG:NH1	42:RW:40:ASN:OD1	2.36	0.54
1:XA:1264:C:H2'	1:XA:1265:G:H8	1.71	0.54
1:XA:1321:C:H5''	1:XA:1322:C:H5''	1.90	0.54
1:XA:1401:G:O6	1:XA:1504:G:N2	2.40	0.54
3:XC:70:VAL:HG12	3:XC:72:LYS:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:XF:47:ARG:NH2	6:XF:57:GLN:OE1	2.39	0.54
19:XS:22:LEU:HD21	19:XS:29:ARG:HG2	1.89	0.54
22:XW:17:C:OP1	22:XW:61:U:O2'	2.25	0.54
25:YA:2354:G:H4'	46:Y0:35:ASN:HD22	1.71	0.54
45:YZ:48:PHE:HA	45:YZ:51:ALA:HB3	1.89	0.54
1:QA:742:G:OP2	15:QO:35:ARG:NH2	2.40	0.54
1:QA:1099:G:OP1	2:QB:96:ARG:NH2	2.40	0.54
1:QA:1227:A:OP1	19:QS:80:TYR:OH	2.22	0.54
25:RA:17:G:H4'	40:RU:25:TRP:HE1	1.72	0.54
25:RA:958:U:OP2	36:RQ:14:ARG:NH1	2.41	0.54
25:RA:1568:G:H5''	27:RD:61:LEU:HD23	1.89	0.54
29:RF:143:ALA:HB1	29:RF:148:LEU:HB2	1.89	0.54
36:RQ:28:ALA:N	36:RQ:105:GLU:OE2	2.41	0.54
1:XA:316:G:OP2	1:XA:351:G:O2'	2.21	0.54
1:XA:689:C:OP2	11:XK:55:LYS:NZ	2.39	0.54
11:XK:86:GLY:O	11:XK:91:ARG:NH1	2.37	0.54
25:YA:675:A:OP1	29:YF:63:LYS:NZ	2.32	0.54
26:YB:116:G:H5'	38:YS:55:ALA:HA	1.88	0.54
25:RA:1678:G:N2	25:RA:1990:C:O2	2.39	0.54
30:RG:59:GLU:OE1	30:RG:153:ARG:NH2	2.39	0.54
25:YA:414:C:O2	25:YA:1864:U:O2'	2.24	0.54
36:YQ:28:ALA:N	36:YQ:105:GLU:OE2	2.41	0.54
40:YU:95:LEU:HD13	41:YV:4:ILE:HD12	1.88	0.54
44:YY:11:ASP:OD1	44:YY:11:ASP:N	2.40	0.54
25:RA:906:G:O3'	36:RQ:67:ARG:NH2	2.41	0.54
1:XA:559:A:OP1	5:XE:126:ARG:NH2	2.41	0.54
34:YO:23:ARG:NH2	34:YO:28:SER:O	2.41	0.54
25:RA:1341:U:OP2	25:RA:1394:U:O2'	2.20	0.54
2:XB:69:LEU:HB3	2:XB:162:ILE:HG22	1.90	0.54
11:XK:54:ARG:NH2	22:XW:40:C:O2'	2.41	0.54
25:YA:546:C:OP1	25:YA:547:A:N6	2.40	0.54
25:YA:987:G:O2'	25:YA:1000:A:N3	2.38	0.54
3:QC:108:ASN:HD21	3:QC:144:SER:HB2	1.73	0.54
6:QF:9:VAL:HB	6:QF:87:ARG:HB2	1.90	0.54
25:RA:589:C:H2'	25:RA:590:A:H8	1.73	0.54
30:RG:55:LYS:NZ	30:RG:59:GLU:OE2	2.40	0.54
45:RZ:5:LEU:H	45:RZ:59:LEU:HA	1.72	0.54
1:XA:581:G:OP1	15:XO:65:ARG:NH1	2.41	0.54
1:XA:971:G:N2	1:XA:1363:A:OP2	2.35	0.54
5:XE:91:LEU:HG	5:XE:120:THR:HG22	1.89	0.54
38:YS:15:ARG:NE	38:YS:88:ASP:OD1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:RA:768:G:O2'	25:RA:1379:A:N6	2.41	0.54
32:RI:99:GLU:OE2	32:RI:103:ARG:NH2	2.40	0.54
36:RQ:31:ASP:OD1	36:RQ:134:ARG:NH1	2.41	0.54
1:XA:452:A:H62	1:XA:480:U:H3	1.56	0.54
16:XP:23:ASP:OD2	16:XP:25:ARG:NH2	2.41	0.54
25:YA:814:C:O2'	25:YA:1225:C:N3	2.40	0.54
25:YA:971:C:O2'	25:YA:983:A:N3	2.35	0.54
27:YD:122:ASP:OD1	27:YD:122:ASP:N	2.36	0.54
29:YF:31:HIS:NE2	29:YF:35:GLU:OE2	2.41	0.54
1:QA:545:C:H5'	4:QD:72:GLU:HG3	1.90	0.54
1:QA:1343:G:H4'	9:QI:122:ALA:HB3	1.89	0.54
13:QM:93:ARG:NH1	25:RA:888:C:OP1	2.41	0.54
25:RA:2133:G:H1'	25:RA:2158:A:H61	1.73	0.54
31:RH:88:LEU:HA	31:RH:130:ARG:HA	1.90	0.54
1:XA:618:C:H5''	1:XA:619:U:H5''	1.89	0.54
25:YA:1405:U:H2'	25:YA:1406:U:H6	1.73	0.54
29:YF:143:ALA:HB1	29:YF:148:LEU:HB2	1.89	0.54
36:YQ:31:ASP:OD1	36:YQ:134:ARG:NH1	2.41	0.54
1:QA:1119:C:H2'	1:QA:1120:G:H8	1.72	0.54
45:RZ:52:SER:O	45:RZ:54:HIS:N	2.37	0.54
25:YA:783:A:H8	25:YA:784:A:H4'	1.73	0.54
30:YG:55:LYS:NZ	30:YG:59:GLU:OE2	2.40	0.54
32:YI:99:GLU:OE2	32:YI:103:ARG:NH2	2.40	0.54
1:QA:1512:U:H3	1:QA:1523:G:H1	1.55	0.53
13:QM:86:CYS:SG	13:QM:87:TYR:N	2.81	0.53
25:RA:746:A:O2'	25:RA:2611:U:O2'	2.22	0.53
29:RF:198:ALA:HA	29:RF:201:VAL:HG12	1.90	0.53
37:RR:51:LEU:HD22	37:RR:66:VAL:HG13	1.91	0.53
1:XA:191:G:O2'	20:XT:101:GLY:O	2.25	0.53
3:XC:108:ASN:HD21	3:XC:144:SER:HB2	1.73	0.53
13:XM:19:LEU:HD21	13:XM:56:LEU:HD11	1.88	0.53
43:YX:6:ASP:OD2	48:Y2:29:LYS:NZ	2.39	0.53
1:QA:421:U:O4	3:QC:127:ARG:NH1	2.42	0.53
1:QA:1359:C:OP1	14:QN:22:THR:OG1	2.22	0.53
1:QA:1522:U:H2'	1:QA:1523:G:H8	1.73	0.53
10:QJ:28:ARG:NH2	10:QJ:34:VAL:O	2.41	0.53
22:QW:4:G:H2'	22:QW:5:G:C8	2.43	0.53
25:RA:521:G:H2'	25:RA:522:G:H8	1.73	0.53
29:RF:31:HIS:NE2	29:RF:35:GLU:OE2	2.41	0.53
39:RT:124:ASP:O	39:RT:128:GLU:N	2.39	0.53
1:XA:582:U:OP2	1:XA:758:G:N1	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:XD:119:GLN:OE1	4:XD:123:HIS:ND1	2.41	0.53
25:YA:629:G:N3	25:YA:639:U:O2'	2.41	0.53
25:YA:2105:C:H2'	25:YA:2106:G:H8	1.74	0.53
29:YF:198:ALA:HA	29:YF:201:VAL:HG12	1.90	0.53
39:YT:16:ARG:HH21	39:YT:19:LEU:HD21	1.73	0.53
2:QB:118:LEU:HB3	2:QB:142:LEU:HD12	1.90	0.53
25:RA:270(N):G:OP1	32:RI:57:ARG:NH1	2.41	0.53
25:RA:820:A:N3	25:RA:943:U:O2'	2.38	0.53
27:RD:17:THR:HB	27:RD:205:VAL:H	1.72	0.53
27:RD:182:LEU:H	27:RD:272:ALA:HB3	1.74	0.53
1:XA:28:G:O2'	1:XA:296:U:OP1	2.26	0.53
12:XL:56:ALA:HB2	12:XL:70:ILE:HD11	1.90	0.53
42:YW:22:ASP:OD1	42:YW:25:ARG:NH1	2.30	0.53
45:YZ:5:LEU:H	45:YZ:59:LEU:HA	1.72	0.53
1:QA:139:G:H2'	1:QA:140:A:H8	1.73	0.53
1:QA:1279:A:O2'	1:QA:1281:U:OP2	2.26	0.53
2:QB:74:LYS:NZ	2:QB:205:ASP:O	2.41	0.53
25:RA:2104:G:H1	25:RA:2185:C:H42	1.56	0.53
25:RA:2258:C:O2'	25:RA:2427:C:OP2	2.26	0.53
34:RO:23:ARG:NH2	34:RO:28:SER:O	2.41	0.53
1:XA:619:U:N3	4:XD:134:ASP:OD1	2.35	0.53
23:XX:22:C:C6	23:XX:22:C:C3'	2.91	0.53
26:YB:7:G:N3	38:YS:38:GLN:NE2	2.52	0.53
27:YD:151:LYS:O	27:YD:154:LYS:NZ	2.42	0.53
31:YH:88:LEU:HA	31:YH:130:ARG:HA	1.90	0.53
43:YX:72:LYS:NZ	43:YX:75:ASP:OD1	2.40	0.53
48:Y2:23:LYS:NZ	48:Y2:27:GLU:OE2	2.40	0.53
27:RD:143:HIS:ND1	27:RD:194:GLY:O	2.37	0.53
30:RG:71:THR:N	30:RG:89:GLY:O	2.41	0.53
2:XB:72:GLY:HA3	2:XB:81:VAL:HG21	1.91	0.53
2:XB:82:ARG:NH1	2:XB:92:TYR:OH	2.41	0.53
10:XJ:51:ARG:O	14:XN:45:ARG:NH1	2.42	0.53
25:YA:993:G:OP1	40:YU:50:ARG:NH2	2.33	0.53
30:YG:71:THR:N	30:YG:89:GLY:O	2.41	0.53
30:YG:97:ASP:H	30:YG:100:TRP:HD1	1.55	0.53
3:QC:70:VAL:HG12	3:QC:72:LYS:H	1.72	0.53
6:QF:5:GLU:HB3	6:QF:62:TRP:HE1	1.73	0.53
25:RA:1614:A:N1	42:RW:91:GLY:HA2	2.23	0.53
25:RA:1652:A:OP1	37:RR:8:ARG:NH1	2.41	0.53
43:RX:72:LYS:NZ	43:RX:75:ASP:OD1	2.40	0.53
1:XA:8:A:N6	4:XD:208:SER:O	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:548:G:OP1	4:XD:73:ARG:NH2	2.41	0.53
1:XA:1343:G:H4'	9:XI:122:ALA:HB3	1.90	0.53
2:XB:84:GLU:OE1	2:XB:87:ARG:NH2	2.32	0.53
6:XF:9:VAL:HB	6:XF:87:ARG:HB2	1.90	0.53
25:YA:1270:C:H5''	25:YA:1271:G:H5'	1.89	0.53
1:QA:662:G:O2'	1:QA:836:G:OP1	2.27	0.53
4:QD:127:THR:HA	4:QD:132:ARG:HA	1.90	0.53
25:RA:593:G:H4'	54:R8:61:LEU:HD13	1.91	0.53
25:RA:2638:G:OP1	28:RE:82:ARG:NH2	2.41	0.53
27:RD:151:LYS:O	27:RD:154:LYS:NZ	2.42	0.53
1:XA:21:G:H2'	1:XA:22:G:H8	1.74	0.53
1:XA:1229:A:OP2	13:XM:114:ARG:NH1	2.39	0.53
25:YA:249:C:O2	54:Y8:12:LYS:NZ	2.32	0.53
32:YI:79:ILE:N	32:YI:141:LYS:O	2.42	0.53
47:Y1:52:ARG:HH11	47:Y1:57:GLU:HB2	1.74	0.53
5:XE:12:LEU:HB3	5:XE:31:LEU:HB3	1.91	0.53
22:XW:4:G:H2'	22:XW:5:G:H8	1.74	0.53
23:XX:23:A:H3'	23:XX:23:A:C8	2.44	0.53
47:Y1:80:LEU:HD12	47:Y1:81:LYS:HG2	1.89	0.53
1:QA:624:C:H2'	1:QA:625:G:H8	1.74	0.53
25:RA:1262:A:OP2	42:RW:97:LYS:NZ	2.42	0.53
26:RB:8:U:O4	26:RB:112:G:O6	2.27	0.53
1:XA:993:G:O2'	1:XA:994:A:N7	2.39	0.53
25:YA:1191:G:OP1	35:YP:18:ARG:NH2	2.42	0.53
26:YB:8:U:O4	26:YB:112:G:O6	2.27	0.53
38:YS:20:ARG:NH2	46:Y0:51:VAL:O	2.39	0.53
16:QP:23:ASP:OD2	16:QP:25:ARG:NH2	2.41	0.53
25:RA:141:A:H8	25:RA:1595:G:H21	1.56	0.53
25:RA:242:G:H2'	54:R8:5:LYS:HA	1.91	0.53
25:RA:581:C:H2'	25:RA:582:G:H8	1.74	0.53
25:RA:1818:U:OP2	27:RD:157:ARG:NE	2.41	0.53
25:RA:1824:G:N3	27:RD:254:THR:OG1	2.42	0.53
38:RS:31:SER:O	38:RS:97:ARG:NH1	2.39	0.53
44:RY:47:LYS:NZ	44:RY:48:ALA:O	2.35	0.53
47:R1:51:VAL:HG11	47:R1:74:VAL:HG21	1.90	0.53
1:XA:23:C:OP2	1:XA:561:U:N3	2.39	0.53
6:XF:5:GLU:HB3	6:XF:62:TRP:HE1	1.73	0.53
25:YA:745:G:O6	25:YA:746:A:N6	2.41	0.53
31:YH:8:PRO:HG2	31:YH:69:ARG:HE	1.75	0.53
1:QA:279:A:OP2	17:QQ:95:TYR:OH	2.25	0.52
1:QA:1095:U:OP2	1:QA:1108:G:N1	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:QW:17:C:OP1	22:QW:61:U:O2'	2.24	0.52
25:RA:71:A:H62	25:RA:114:U:H1'	1.74	0.52
25:RA:674:G:H1'	29:RF:74:ARG:HD3	1.91	0.52
40:RU:28:ARG:NH1	40:RU:38:THR:OG1	2.41	0.52
1:QA:1356:G:H2'	1:QA:1357:A:C8	2.44	0.52
2:QB:48:MET:HA	2:QB:51:LEU:HD12	1.91	0.52
25:RA:184:C:O2'	25:RA:217:G:N3	2.37	0.52
26:RB:8:U:O2	26:RB:112:G:N2	2.37	0.52
1:XA:414:A:OP2	1:XA:428:G:N2	2.32	0.52
22:XW:28:U:H2'	22:XW:29:C:H6	1.73	0.52
25:YA:523:C:O2	25:YA:553:U:O2'	2.27	0.52
25:YA:2361:A:O5'	54:Y8:27:THR:OG1	2.27	0.52
34:YO:87:ILE:HD12	34:YO:91:LEU:HA	1.91	0.52
40:YU:28:ARG:NH1	40:YU:38:THR:OG1	2.41	0.52
1:QA:1141:C:H2'	1:QA:1142:G:H8	1.75	0.52
13:QM:58:GLU:O	13:QM:62:ASN:HB2	2.09	0.52
25:RA:523:C:O2	25:RA:553:U:O2'	2.26	0.52
25:YA:2328:A:H2'	25:YA:2329:G:C8	2.44	0.52
1:QA:1414:U:H2'	1:QA:1415:G:H8	1.75	0.52
1:XA:279:A:OP2	17:XQ:95:TYR:OH	2.24	0.52
12:XL:27:LEU:O	12:XL:33:ARG:NH2	2.40	0.52
25:YA:321:G:O2'	25:YA:340:A:N3	2.41	0.52
25:YA:815:C:OP2	41:YV:83:ARG:NH1	2.43	0.52
25:YA:1918:A:O2'	25:YA:1920:C:N4	2.43	0.52
25:YA:2212:A:H1'	25:YA:2215:G:C4	2.45	0.52
29:YF:32:LEU:HD11	29:YF:105:VAL:HG13	1.91	0.52
45:YZ:10:ARG:NH2	45:YZ:37:VAL:O	2.43	0.52
1:QA:1286:A:H2'	1:QA:1287:A:H4'	1.91	0.52
9:QI:63:ILE:HG21	9:QI:77:ILE:HG12	1.90	0.52
22:QW:57:C:C6	25:RA:2169:A:N7	2.78	0.52
25:RA:1165:U:O4	25:RA:1184:G:O6	2.28	0.52
8:XH:106:GLY:O	8:XH:122:ARG:NH2	2.43	0.52
25:YA:1266:G:O2'	25:YA:2012:G:O6	2.23	0.52
47:Y1:90:ILE:HD12	47:Y1:94:LEU:HD12	1.92	0.52
9:QI:42:ARG:NH1	9:QI:71:SER:OG	2.43	0.52
29:RF:32:LEU:HD11	29:RF:105:VAL:HG13	1.91	0.52
30:RG:97:ASP:H	30:RG:100:TRP:HD1	1.55	0.52
39:RT:16:ARG:HH21	39:RT:19:LEU:HD21	1.73	0.52
54:R8:29:LYS:O	54:R8:31:HIS:N	2.39	0.52
10:XJ:9:ARG:HB2	10:XJ:95:GLU:HB3	1.92	0.52
25:YA:2784:C:O2'	28:YE:37:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:YD:62:TYR:HA	27:YD:87:ASN:HD21	1.74	0.52
31:YH:52:VAL:O	31:YH:65:HIS:NE2	2.34	0.52
36:YQ:111:GLU:OE1	36:YQ:133:ARG:NH2	2.43	0.52
1:QA:475:G:H2'	1:QA:476:G:H8	1.75	0.52
1:QA:948:C:H2'	1:QA:949:A:H8	1.75	0.52
11:QK:34:ASP:OD1	11:QK:38:ASN:N	2.43	0.52
25:RA:2199:A:OP1	47:R1:50:ARG:NH2	2.38	0.52
44:RY:11:ASP:N	44:RY:11:ASP:OD1	2.40	0.52
1:XA:1356:G:H2'	1:XA:1357:A:C8	2.45	0.52
22:XW:71:G:H21	25:YA:1851:U:H5'	1.75	0.52
1:QA:227:G:N2	16:QP:62:VAL:O	2.35	0.52
2:QB:61:LEU:HG	2:QB:66:GLY:HA3	1.90	0.52
25:RA:2845:G:H2'	25:RA:2846:G:H8	1.74	0.52
27:RD:62:TYR:HA	27:RD:87:ASN:HD21	1.74	0.52
34:RO:87:ILE:HD12	34:RO:91:LEU:HA	1.91	0.52
1:XA:401:C:O2'	1:XA:621:A:N3	2.33	0.52
4:XD:127:THR:HA	4:XD:132:ARG:HA	1.90	0.52
25:YA:1479:G:H1	25:YA:1514:U:H3	1.58	0.52
1:QA:713:G:H2'	1:QA:714:G:C8	2.45	0.52
22:QW:5:G:H2'	22:QW:6:G:C8	2.45	0.52
25:RA:900:A:H3'	25:RA:901:A:H8	1.73	0.52
25:RA:2808:U:H2'	25:RA:2809:A:H8	1.75	0.52
27:RD:35:LYS:HZ1	27:RD:63:ARG:HB3	1.75	0.52
1:XA:405:U:O4	4:XD:2:GLY:N	2.43	0.52
25:YA:270(A):A:N3	25:YA:365:C:O2'	2.39	0.52
25:YA:630:G:N2	25:YA:633:A:OP2	2.34	0.52
25:YA:2123:G:H1	25:YA:2175:C:H42	1.56	0.52
1:QA:159:G:N2	1:QA:162:A:OP2	2.43	0.52
1:QA:1327:C:OP2	21:QU:12:LYS:NZ	2.41	0.52
22:QW:57:C:C6	25:RA:2169:A:C8	2.97	0.52
25:RA:2228:G:OP1	27:RD:261:LYS:NZ	2.36	0.52
25:RA:2293:C:O2'	38:RS:93:LYS:NZ	2.43	0.52
25:RA:2328:A:H2'	25:RA:2329:G:C8	2.45	0.52
22:XW:4:G:H2'	22:XW:5:G:C8	2.44	0.52
25:YA:1062:G:H2'	25:YA:1063:G:C8	2.44	0.52
25:YA:2081:C:H2'	25:YA:2082:A:H8	1.74	0.52
34:YO:68:GLU:HG3	34:YO:78:ARG:HD3	1.92	0.52
38:YS:32:LEU:O	38:YS:62:LYS:NZ	2.33	0.52
1:QA:148:G:H2'	1:QA:149:A:H8	1.76	0.51
22:QW:28:U:H2'	22:QW:29:C:H6	1.75	0.51
25:RA:138:G:N2	43:RX:44:GLU:OE1	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:RA:2354:G:H4'	46:R0:35:ASN:HD22	1.74	0.51
31:RH:8:PRO:HG2	31:RH:69:ARG:HE	1.75	0.51
36:RQ:111:GLU:OE1	36:RQ:133:ARG:NH2	2.43	0.51
40:RU:88:ILE:HG23	40:RU:90:VAL:HG23	1.91	0.51
1:XA:35:G:O2'	12:XL:118:SER:O	2.23	0.51
25:YA:486:C:O2'	42:YW:60:ASN:ND2	2.41	0.51
31:YH:153:LYS:HB3	31:YH:161:GLY:HA2	1.91	0.51
48:Y2:22:GLU:OE2	48:Y2:68:ARG:NH2	2.43	0.51
1:QA:656:C:O2	15:QO:28:GLN:NE2	2.43	0.51
1:QA:1432:G:OP1	39:RT:108:ARG:N	2.42	0.51
7:QG:143:ARG:HD2	22:QW:42:C:O3'	2.01	0.51
25:RA:577:G:O2'	25:RA:1254:A:OP1	2.27	0.51
1:XA:1397:C:H5'	23:XX:23:A:O2'	2.10	0.51
25:YA:1681:G:O2'	25:YA:1762:A:O2'	2.29	0.51
25:YA:1728:G:N2	25:YA:1730:U:OP2	2.43	0.51
27:YD:182:LEU:H	27:YD:272:ALA:HB3	1.74	0.51
25:RA:602:G:HO2'	25:RA:604:G:HO2'	1.57	0.51
25:RA:676:A:H8	25:RA:2069:G:H21	1.58	0.51
25:RA:1799:G:N2	25:RA:1818:U:O2'	2.43	0.51
9:XI:47:LEU:HD12	9:XI:50:LEU:HD12	1.92	0.51
22:XW:5:G:H2'	22:XW:6:G:C8	2.44	0.51
37:YR:51:LEU:HD22	37:YR:66:VAL:HG13	1.92	0.51
1:QA:972:C:H4'	10:QJ:57:LYS:HB2	1.91	0.51
9:QI:5:TYR:HE1	9:QI:16:ARG:HB2	1.75	0.51
25:RA:996:A:OP2	40:RU:92:ARG:NH2	2.43	0.51
31:RH:153:LYS:HB3	31:RH:161:GLY:HA2	1.91	0.51
1:QA:21:G:H2'	1:QA:22:G:C8	2.45	0.51
1:QA:1080:A:H5'	5:QE:14:ARG:NH2	2.25	0.51
1:XA:631:G:H3'	1:XA:632:A:H8	1.75	0.51
1:XA:692:U:OP1	11:XK:124:LYS:NZ	2.37	0.51
1:XA:707:C:H4'	11:XK:20:TYR:HD2	1.76	0.51
1:XA:1414:U:H2'	1:XA:1415:G:H8	1.75	0.51
4:XD:14:ARG:HE	4:XD:40:PRO:HD2	1.75	0.51
25:YA:288:C:H2'	25:YA:289:A:H8	1.75	0.51
25:YA:2688:U:OP1	25:YA:2713:A:N6	2.40	0.51
34:YO:7:TYR:HE1	34:YO:44:LYS:HG3	1.76	0.51
40:YU:88:ILE:HG23	40:YU:90:VAL:HG23	1.92	0.51
1:QA:401:C:O2'	1:QA:621:A:N3	2.41	0.51
24:QY:37:A:O2'	25:RA:1913:A:N1	2.42	0.51
25:RA:585:G:H21	25:RA:1254:A:H62	1.58	0.51
29:RF:63:LYS:HE2	29:RF:67:GLN:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:392:G:HO2'	1:XA:483:C:HO2'	1.56	0.51
1:XA:1226:C:O2'	13:XM:111:LYS:NZ	2.43	0.51
29:YF:63:LYS:HE2	29:YF:67:GLN:HB2	1.92	0.51
30:YG:142:PRO:HB2	50:Y4:31:ILE:HG21	1.92	0.51
45:YZ:4:ARG:HG2	45:YZ:58:VAL:HB	1.93	0.51
10:QJ:24:VAL:HG21	10:QJ:37:PRO:HG3	1.93	0.51
25:RA:1316:U:H2'	25:RA:1317:A:H8	1.76	0.51
1:XA:490:G:OP2	4:XD:132:ARG:NH2	2.44	0.51
25:YA:500:G:N1	25:YA:503:A:OP2	2.43	0.51
25:YA:1566:A:OP1	27:YD:211:ARG:NE	2.40	0.51
25:YA:2788:C:O2'	25:YA:2809:A:N3	2.40	0.51
39:YT:124:ASP:O	39:YT:128:GLU:N	2.39	0.51
22:QW:5:G:H2'	22:QW:6:G:H8	1.74	0.51
25:RA:665:C:H2'	25:RA:666:G:H8	1.75	0.51
1:XA:927:G:N2	1:XA:1390:U:O2	2.38	0.51
1:XA:1342:C:H4'	9:XI:125:TYR:HB3	1.92	0.51
12:XL:32:PHE:HB3	12:XL:84:LEU:HD11	1.92	0.51
13:XM:3:ARG:HA	13:XM:9:ILE:HG21	1.92	0.51
13:XM:47:ASP:OD1	13:XM:47:ASP:N	2.43	0.51
25:YA:2315:G:OP1	30:YG:36:LYS:NZ	2.43	0.51
25:RA:831:G:O2'	35:RP:38:GLN:OE1	2.27	0.51
25:RA:2844:G:H3'	25:RA:2845:G:H8	1.76	0.51
32:RI:79:ILE:N	32:RI:141:LYS:O	2.42	0.51
25:YA:878:A:N6	25:YA:899:A:O2'	2.43	0.51
25:YA:942:G:OP2	35:YP:39:LYS:NZ	2.34	0.51
25:YA:1382:G:O3'	25:YA:1573:G:N2	2.43	0.51
36:YQ:58:PHE:HD2	36:YQ:61:GLY:HA3	1.76	0.51
1:QA:110:C:O2'	16:QP:25:ARG:O	2.26	0.51
1:QA:714:G:H2'	1:QA:715:A:C8	2.46	0.51
31:RH:52:VAL:O	31:RH:65:HIS:NE2	2.34	0.51
42:RW:111:HIS:CD2	42:RW:113:LYS:H	2.29	0.51
45:RZ:10:ARG:NH2	45:RZ:37:VAL:O	2.43	0.51
23:XX:23:A:C8	23:XX:23:A:C3'	2.93	0.51
25:YA:870:A:OP1	36:YQ:6:ARG:NH2	2.38	0.51
33:YN:58:ASP:OD1	33:YN:58:ASP:N	2.36	0.51
4:QD:14:ARG:HE	4:QD:40:PRO:HD2	1.75	0.50
13:QM:16:ASP:N	13:QM:16:ASP:OD1	2.42	0.50
19:QS:3:ARG:HE	19:QS:7:LYS:HE2	1.76	0.50
25:RA:13:A:O2'	25:RA:15:G:N7	2.43	0.50
34:RO:68:GLU:HG3	34:RO:78:ARG:HD3	1.92	0.50
42:RW:22:ASP:OD1	42:RW:25:ARG:NH1	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:RZ:4:ARG:HG2	45:RZ:58:VAL:HB	1.93	0.50
25:YA:1316:U:H2'	25:YA:1317:A:C8	2.46	0.50
25:YA:2008:C:H2'	25:YA:2009:G:H8	1.77	0.50
25:YA:2076:U:OP2	25:YA:2238:G:N2	2.43	0.50
35:YP:65:ARG:O	35:YP:68:GLN:NE2	2.44	0.50
42:YW:111:HIS:CD2	42:YW:113:LYS:H	2.29	0.50
1:QA:1077:G:N2	1:QA:1080:A:OP2	2.36	0.50
1:QA:1142:G:H3'	1:QA:1143:G:H8	1.76	0.50
4:QD:102:ASP:OD1	4:QD:102:ASP:N	2.43	0.50
11:QK:58:PRO:HB2	11:QK:93:GLN:HG3	1.94	0.50
25:RA:1365:A:O2'	47:R1:11:ARG:NH2	2.39	0.50
45:RZ:30:ASN:OD1	45:RZ:33:LEU:N	2.44	0.50
1:XA:514:C:H2'	1:XA:515:G:H8	1.76	0.50
22:XW:34:U:H3'	22:XW:35:C:H5''	1.92	0.50
25:YA:688:U:H2'	25:YA:689:A:H8	1.76	0.50
1:QA:12:U:H3	1:QA:22:G:H1	1.60	0.50
1:QA:35:G:O2'	12:QL:118:SER:O	2.21	0.50
1:QA:156:G:H2'	1:QA:157:G:H8	1.75	0.50
1:QA:411:A:H62	1:QA:413:G:H21	1.57	0.50
2:QB:69:LEU:O	2:QB:162:ILE:HA	2.10	0.50
25:RA:39:C:O2	29:RF:46:ARG:NH2	2.45	0.50
34:RO:7:TYR:HE1	34:RO:44:LYS:HG3	1.75	0.50
50:R4:47:GLN:HG2	50:R4:49:PHE:HB3	1.93	0.50
4:XD:102:ASP:N	4:XD:102:ASP:OD1	2.43	0.50
7:XG:143:ARG:HD2	22:XW:42:C:O3'	1.96	0.50
10:XJ:34:VAL:HG22	10:XJ:74:ILE:HG22	1.93	0.50
22:XW:52:C:H2'	22:XW:53:G:C8	2.46	0.50
25:YA:67:U:H3	25:YA:74:A:H2	1.58	0.50
25:YA:1403:C:H5''	25:YA:1471:A:H1'	1.93	0.50
25:RA:819:A:OP2	25:RA:1187:G:N2	2.32	0.50
25:RA:1056:G:H5''	25:RA:1057:A:H5'	1.93	0.50
25:RA:1751:C:HO2'	25:RA:2861:G:HO2'	1.58	0.50
25:RA:1826:G:O2'	27:RD:242:ARG:NH2	2.44	0.50
33:RN:96:GLU:HB2	33:RN:122:VAL:HG12	1.94	0.50
48:R2:22:GLU:OE2	48:R2:68:ARG:NH2	2.43	0.50
25:YA:338:G:OP1	44:YY:4:LYS:NZ	2.42	0.50
25:YA:1341:U:OP2	25:YA:1394:U:O2'	2.23	0.50
26:YB:9:G:OP1	38:YS:15:ARG:NH1	2.38	0.50
39:YT:66:VAL:HA	39:YT:71:GLY:HA2	1.93	0.50
45:YZ:30:ASN:OD1	45:YZ:33:LEU:N	2.45	0.50
1:QA:877:C:H2'	1:QA:878:G:H8	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:RA:144:C:H2'	25:RA:145:G:H8	1.76	0.50
25:RA:572:A:OP2	41:RV:78:LYS:NZ	2.36	0.50
25:RA:1266:G:O2'	25:RA:2012:G:O6	2.26	0.50
25:RA:2291:U:OP1	25:RA:2380:C:O2'	2.29	0.50
1:XA:676:A:H1'	11:XK:115:PRO:HB3	1.94	0.50
25:YA:1980:G:O2'	25:YA:1982:C:OP2	2.21	0.50
25:YA:2130:U:H2'	25:YA:2131:G:C8	2.47	0.50
25:YA:2676:C:O2	25:YA:2732:G:N2	2.41	0.50
1:QA:501:C:OP1	12:QL:117:ARG:NH2	2.45	0.50
1:QA:1007:C:H42	1:QA:1022:G:H1	1.58	0.50
1:QA:1304:G:N2	1:QA:1334:G:O6	2.44	0.50
12:QL:117:ARG:HB2	12:QL:122:THR:HB	1.92	0.50
36:RQ:58:PHE:HD2	36:RQ:61:GLY:HA3	1.76	0.50
1:XA:426:G:OP1	4:XD:38:TYR:OH	2.28	0.50
25:YA:458:G:N2	25:YA:470:A:OP2	2.44	0.50
1:QA:348:G:H2'	1:QA:349:A:H8	1.77	0.50
2:QB:109:SER:O	2:QB:113:HIS:ND1	2.36	0.50
5:QE:12:LEU:HB3	5:QE:31:LEU:HB3	1.91	0.50
21:QU:9:ARG:HD3	21:QU:22:ARG:HD2	1.94	0.50
22:QW:9:G:H5''	22:QW:10:G:OP2	2.12	0.50
30:RG:47:LYS:HD3	30:RG:81:LYS:HB2	1.93	0.50
39:RT:50:ILE:HD11	39:RT:100:TYR:HA	1.93	0.50
45:RZ:97:GLU:HG2	45:RZ:125:LEU:HD11	1.94	0.50
25:YA:529:A:H4'	25:YA:530:G:H5'	1.94	0.50
25:YA:578:A:OP1	25:YA:1255:U:O2'	2.29	0.50
25:YA:1795:C:O2	27:YD:255:LYS:NZ	2.35	0.50
25:YA:2809:A:H2'	25:YA:2810:A:C8	2.47	0.50
26:YB:22:U:O2	26:YB:61:G:N2	2.32	0.50
1:QA:382:A:H2'	1:QA:383:A:C8	2.47	0.50
25:RA:2291:U:O2'	25:RA:2374:C:O2	2.28	0.50
25:RA:2508:G:HO2'	25:RA:2554:U:HO2'	1.60	0.50
21:XU:9:ARG:HD3	21:XU:22:ARG:HD2	1.94	0.50
25:YA:679:C:H2'	25:YA:680:G:H8	1.76	0.50
1:QA:1100:C:OP2	2:QB:96:ARG:NE	2.38	0.50
2:QB:74:LYS:HZ3	2:QB:166:ASP:HB2	1.77	0.50
11:QK:20:TYR:HE1	11:QK:83:ILE:HD12	1.76	0.50
22:QW:8:U:O2	22:QW:14:A:N7	2.45	0.50
25:RA:442:G:H1'	29:RF:48:THR:HG21	1.94	0.50
25:RA:1212:G:O2'	25:RA:1236:G:N2	2.35	0.50
25:RA:1264:G:OP1	51:R5:19:ARG:NH2	2.29	0.50
26:RB:33:G:OP2	30:RG:96:ARG:NH2	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:474:G:H2'	1:XA:475:G:C8	2.47	0.50
1:XA:675:A:H1'	11:XK:116:HIS:CD2	2.46	0.50
1:XA:742:G:OP2	15:XO:35:ARG:NH2	2.43	0.50
1:XA:1178:G:OP2	9:XI:93:ARG:NH2	2.37	0.50
25:YA:2839:G:O6	25:YA:2878:U:O4	2.30	0.50
1:QA:137:C:H2'	1:QA:138:G:H8	1.76	0.49
1:QA:1281:U:H5''	1:QA:1282:C:H5	1.77	0.49
25:RA:281:G:H21	25:RA:359:A:H62	1.59	0.49
1:XA:443:C:H42	1:XA:491:G:H1	1.59	0.49
1:XA:1350:A:O2'	7:XG:33:ASP:OD1	2.27	0.49
2:XB:91:PRO:HG3	2:XB:154:LEU:HB2	1.94	0.49
25:YA:2845:G:OP1	39:YT:56:GLY:N	2.45	0.49
25:YA:2853:C:H2'	25:YA:2854:G:H8	1.77	0.49
50:Y4:47:GLN:HG2	50:Y4:49:PHE:HB3	1.93	0.49
1:QA:452:A:O2'	1:QA:453:A:O4'	2.30	0.49
1:QA:559:A:OP1	5:QE:126:ARG:NH2	2.44	0.49
1:QA:1244:C:H2'	1:QA:1245:A:H8	1.77	0.49
1:QA:1251:A:H2'	1:QA:1252:A:C8	2.47	0.49
22:QW:4:G:H2'	22:QW:5:G:H8	1.75	0.49
25:RA:2384:G:OP2	46:R0:55:ARG:NH2	2.39	0.49
1:XA:489:C:H2'	1:XA:490:G:H8	1.76	0.49
1:XA:714:G:H2'	1:XA:715:A:C8	2.46	0.49
1:XA:806:C:H2'	1:XA:807:A:H8	1.77	0.49
1:XA:925:G:H1	1:XA:1391:U:H3	1.60	0.49
1:XA:1492:A:H5''	12:XL:47:LYS:HB3	1.95	0.49
22:XW:11:A:H2'	22:XW:12:G:C8	2.47	0.49
23:XX:22:C:C6	23:XX:22:C:H3'	2.47	0.49
25:YA:776:G:N7	25:YA:793:A:O2'	2.46	0.49
25:YA:819:A:OP2	25:YA:1187:G:N2	2.34	0.49
25:YA:1230:C:H2'	25:YA:1231:G:H8	1.76	0.49
1:QA:356:A:N3	1:QA:368:U:O2'	2.42	0.49
1:QA:628:G:H2'	1:QA:629:G:C8	2.47	0.49
1:QA:1510:U:H2'	1:QA:1511:G:C8	2.47	0.49
2:QB:71:VAL:HA	2:QB:93:VAL:HB	1.94	0.49
9:QI:104:ARG:NH1	9:QI:105:ASP:O	2.45	0.49
25:RA:2612:C:OP2	51:R5:2:ALA:N	2.44	0.49
1:XA:715:A:H2'	1:XA:716:A:C8	2.47	0.49
22:XW:10:G:H2'	22:XW:11:A:C8	2.47	0.49
25:YA:1454:U:O2'	25:YA:1455:G:N7	2.42	0.49
1:QA:824:C:H2'	1:QA:825:G:H8	1.78	0.49
5:QE:105:VAL:HG21	5:QE:128:PRO:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:QW:77:A:N6	25:RA:2422:A:O4'	2.45	0.49
25:RA:863:A:H2'	25:RA:864:G:H8	1.77	0.49
25:RA:1315:C:O2'	25:RA:1392:A:N3	2.39	0.49
1:XA:1287:A:H2'	1:XA:1288:A:C8	2.47	0.49
23:XX:22:C:H6	23:XX:22:C:C4'	2.23	0.49
25:YA:28:A:N6	25:YA:512:G:O2'	2.45	0.49
25:YA:1263:U:H5''	51:Y5:16:ARG:HD3	1.94	0.49
25:YA:2781:A:H5''	25:YA:2782:G:H5'	1.93	0.49
32:YI:27:ARG:HD2	47:Y1:71:TYR:HE2	1.77	0.49
32:YI:78:THR:HG22	32:YI:141:LYS:HE3	1.95	0.49
35:YP:106:LEU:HD21	35:YP:112:LEU:HD13	1.94	0.49
47:Y1:65:SER:HG	47:Y1:66:HIS:HD1	1.59	0.49
1:QA:1151:A:H2'	1:QA:1152:A:H8	1.78	0.49
1:QA:1298:C:OP2	7:QG:114:ARG:NH2	2.39	0.49
2:QB:69:LEU:HB3	2:QB:162:ILE:HG22	1.93	0.49
13:QM:49:THR:HG22	13:QM:51:ALA:H	1.77	0.49
25:RA:2685:G:P	39:RT:51:ARG:HH22	2.36	0.49
32:RI:78:THR:HG22	32:RI:141:LYS:HE3	1.95	0.49
1:XA:749:C:H2'	1:XA:750:G:H8	1.78	0.49
1:XA:765:G:N2	1:XA:813:U:OP2	2.46	0.49
25:YA:13:A:O2'	25:YA:15:G:N7	2.45	0.49
25:YA:458:G:O2'	25:YA:469:G:O6	2.31	0.49
25:YA:1657:C:H4'	28:YE:133:LYS:HB3	1.94	0.49
25:YA:2845:G:H2'	25:YA:2846:G:C8	2.47	0.49
33:YN:96:GLU:HB2	33:YN:122:VAL:HG12	1.94	0.49
1:QA:579:G:H5'	1:QA:728:A:H1'	1.93	0.49
25:RA:1649:G:O2'	37:RR:107:ASP:OD1	2.21	0.49
25:RA:2011:U:OP2	42:RW:16:LYS:NZ	2.35	0.49
28:RE:16:ARG:NH2	28:RE:171:GLU:OE2	2.42	0.49
4:XD:98:GLU:HA	4:XD:103:ASN:HD22	1.77	0.49
7:XG:88:PRO:HG2	7:XG:152:ALA:HB2	1.95	0.49
25:YA:184:C:O2'	25:YA:217:G:N3	2.40	0.49
25:YA:558:G:H2'	25:YA:559:G:H8	1.77	0.49
25:YA:574:C:N3	28:YE:145:LYS:NZ	2.44	0.49
46:Y0:46:LYS:HD2	46:Y0:78:TYR:HE1	1.78	0.49
1:QA:452:A:H62	1:QA:480:U:H3	1.60	0.49
1:QA:790:A:OP1	22:QV:39:A:O2'	2.23	0.49
1:QA:953:G:N7	13:QM:104:ARG:NH2	2.61	0.49
1:QA:1074:G:O2'	2:QB:103:THR:OG1	2.27	0.49
1:QA:1261:A:H62	1:QA:1274:G:N2	2.10	0.49
1:QA:1391:U:H2'	1:QA:1392:G:H8	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:QH:106:GLY:O	8:QH:122:ARG:NH2	2.43	0.49
25:RA:709:U:H2'	25:RA:710:G:H8	1.78	0.49
25:RA:2392:A:H2	25:RA:2424:C:H42	1.61	0.49
25:RA:2676:C:O2	25:RA:2732:G:N2	2.36	0.49
38:RS:32:LEU:O	38:RS:62:LYS:NZ	2.33	0.49
1:XA:269:C:H2'	1:XA:270:A:C8	2.47	0.49
1:XA:1251:A:H2'	1:XA:1252:A:C8	2.48	0.49
11:XK:86:GLY:N	11:XK:112:THR:OG1	2.41	0.49
25:YA:2099:U:O4	25:YA:2190:G:O6	2.30	0.49
39:YT:50:ILE:HD11	39:YT:100:TYR:HA	1.93	0.49
40:YU:98:LEU:O	40:YU:102:GLU:N	2.46	0.49
1:QA:1060:C:H2'	1:QA:1061:G:H8	1.77	0.49
1:QA:1329:A:N7	21:QU:7:ARG:NH2	2.60	0.49
22:QW:77:A:C2	54:R8:31:HIS:CE1	3.01	0.49
25:RA:1184:G:P	49:R3:29:ARG:HH12	2.35	0.49
25:RA:1827:C:OP2	27:RD:222:ARG:NH1	2.44	0.49
25:RA:2618:G:H21	28:RE:150:VAL:HG21	1.78	0.49
39:RT:66:VAL:HA	39:RT:71:GLY:HA2	1.93	0.49
1:XA:1071:C:H2'	1:XA:1072:G:H8	1.78	0.49
1:XA:1414:U:O2	1:XA:1487:G:N2	2.45	0.49
25:YA:1858:G:H2'	25:YA:1883:G:H22	1.78	0.49
25:YA:2327:A:H2'	25:YA:2328:A:C8	2.47	0.49
33:YN:30:ILE:HG23	33:YN:52:VAL:HG11	1.95	0.49
8:QH:51:VAL:HG21	8:QH:60:ARG:HG3	1.95	0.49
25:RA:270(U):C:H2'	25:RA:270(V):G:H8	1.77	0.49
25:RA:2707:G:H2'	25:RA:2708:G:H8	1.77	0.49
27:RD:13:ARG:NH1	27:RD:16:MET:SD	2.86	0.49
43:RX:26:TYR:HD2	43:RX:89:ILE:HD12	1.78	0.49
1:XA:161:A:H2'	1:XA:162:A:H8	1.77	0.49
1:XA:522:C:H41	12:XL:53:ARG:NH2	2.10	0.49
2:XB:87:ARG:NH1	2:XB:220:ASP:OD1	2.45	0.49
22:XW:49:C:N3	22:XW:60:A:H1'	2.27	0.49
25:YA:546:C:H3'	25:YA:547:A:C8	2.48	0.49
25:YA:1438:U:H2'	25:YA:1439:A:H8	1.78	0.49
25:YA:2135:A:H62	25:YA:2156:G:H21	1.61	0.49
30:YG:47:LYS:HD3	30:YG:81:LYS:HB2	1.93	0.49
45:YZ:97:GLU:HG2	45:YZ:125:LEU:HD11	1.94	0.49
1:QA:254:G:O2'	17:QQ:16:GLN:O	2.30	0.49
2:QB:132:LYS:HA	2:QB:135:GLN:HB2	1.95	0.49
25:RA:1022:G:N2	25:RA:1023:U:O4	2.46	0.49
25:RA:2314:C:H2'	25:RA:2315:G:H8	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:RA:2515:C:H2'	25:RA:2516:G:H8	1.77	0.49
25:RA:2579:C:H4'	28:RE:134:ILE:HG12	1.94	0.49
1:XA:167:G:H2'	1:XA:168:G:C8	2.48	0.49
1:XA:1328:C:OP1	21:XU:21:TYR:OH	2.24	0.49
22:XW:8:U:O2	22:XW:14:A:N7	2.46	0.49
25:YA:834:C:H2'	25:YA:835:A:H8	1.78	0.49
26:YB:8:U:O2	26:YB:112:G:N2	2.37	0.49
1:QA:745:C:OP1	1:QA:851:G:O2'	2.27	0.48
1:QA:1124:G:H3'	1:QA:1145:C:N4	2.28	0.48
35:RP:115:LEU:HA	35:RP:134:ALA:HB2	1.96	0.48
44:RY:15:VAL:HG21	44:RY:42:VAL:HG11	1.95	0.48
1:XA:1151:A:H2'	1:XA:1152:A:H8	1.78	0.48
1:XA:1259:C:H42	1:XA:1276:G:H1	1.60	0.48
7:XG:143:ARG:CG	22:XW:42:C:H4'	2.30	0.48
25:YA:2421:G:N7	54:Y8:31:HIS:NE2	2.60	0.48
27:YD:148:GLU:OE1	27:YD:151:LYS:NZ	2.45	0.48
1:QA:1244:C:H2'	1:QA:1245:A:C8	2.48	0.48
1:QA:1352:C:OP1	21:QU:3:LYS:NZ	2.33	0.48
7:QG:88:PRO:HG2	7:QG:152:ALA:HB2	1.94	0.48
7:QG:150:ALA:HB1	11:QK:57:THR:HG21	1.96	0.48
22:QW:2:G:H2'	22:QW:3:C:C6	2.48	0.48
25:RA:500:G:N1	25:RA:503:A:OP2	2.45	0.48
1:XA:1175:G:H2'	1:XA:1176:A:C8	2.48	0.48
5:XE:105:VAL:HG21	5:XE:128:PRO:HB3	1.95	0.48
25:YA:857:C:H42	25:YA:920:G:H1	1.61	0.48
27:YD:13:ARG:NH1	27:YD:16:MET:SD	2.86	0.48
32:YI:93:THR:HA	32:YI:119:PRO:HB3	1.96	0.48
34:YO:28:SER:OG	34:YO:29:ASN:N	2.46	0.48
1:QA:260:G:OP2	20:QT:83:ARG:NH1	2.46	0.48
25:RA:244:A:H4'	35:RP:74:GLU:HB2	1.95	0.48
31:RH:164:TYR:HB2	31:RH:167:GLU:HB2	1.95	0.48
32:RI:65:ALA:O	32:RI:69:LYS:N	2.46	0.48
9:XI:112:LYS:HA	9:XI:119:ALA:HB2	1.96	0.48
13:XM:23:TYR:N	13:XM:67:GLU:OE2	2.46	0.48
1:QA:426:G:OP1	4:QD:38:TYR:OH	2.28	0.48
22:QW:11:A:H2'	22:QW:12:G:C8	2.49	0.48
25:RA:679:C:H2'	25:RA:680:G:H8	1.79	0.48
25:RA:2010:G:H5''	42:RW:42:ARG:HB2	1.95	0.48
25:RA:2134:A:H2'	25:RA:2135:A:H8	1.78	0.48
34:RO:28:SER:OG	34:RO:29:ASN:N	2.46	0.48
42:RW:111:HIS:HD2	42:RW:113:LYS:H	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:1000:A:H2'	1:XA:1001:G:H8	1.78	0.48
1:XA:1308:U:H2'	1:XA:1309:G:H8	1.78	0.48
2:XB:80:ILE:HD11	2:XB:208:ILE:HG23	1.94	0.48
3:XC:152:ILE:HG12	3:XC:167:TRP:HD1	1.78	0.48
22:XV:51:U:O4	22:XV:65:G:O6	2.31	0.48
25:YA:955:C:OP1	36:YQ:85:LYS:NZ	2.39	0.48
25:YA:1600:C:OP1	43:YX:58:HIS:NE2	2.44	0.48
30:YG:161:THR:HG22	30:YG:163:ALA:H	1.77	0.48
1:QA:1228:C:OP2	13:QM:108:ARG:NH2	2.46	0.48
4:QD:98:GLU:HA	4:QD:103:ASN:HD22	1.77	0.48
9:QI:15:ALA:HA	9:QI:64:THR:O	2.13	0.48
22:QW:52:C:H2'	22:QW:53:G:C8	2.49	0.48
25:RA:918:A:N3	26:RB:80:U:O2'	2.39	0.48
25:RA:1433:U:H3	25:RA:1560:G:H1	1.62	0.48
26:RB:22:U:O4	26:RB:61:G:O6	2.32	0.48
32:RI:13:GLY:HA3	32:RI:17:GLN:HG2	1.96	0.48
1:XA:522:C:H41	12:XL:53:ARG:HH22	1.61	0.48
1:XA:1386:G:H2'	1:XA:1387:G:H8	1.77	0.48
14:YN:45:ARG:HE	14:YN:49:HIS:CE1	2.32	0.48
25:YA:71:A:N3	25:YA:73:A:N6	2.62	0.48
25:YA:787:U:H5''	25:YA:788:A:H5'	1.95	0.48
28:YE:25:VAL:HG21	39:YT:8:LYS:HG2	1.95	0.48
31:YH:164:TYR:HB2	31:YH:167:GLU:HB2	1.95	0.48
35:YP:121:LYS:HD3	35:YP:122:PRO:HD2	1.96	0.48
42:YW:111:HIS:HD2	42:YW:113:LYS:H	1.61	0.48
27:RD:122:ASP:N	27:RD:122:ASP:OD1	2.36	0.48
31:RH:9:ILE:HD13	31:RH:49:VAL:HG12	1.96	0.48
1:XA:1101:A:N6	2:XB:176:GLU:OE2	2.46	0.48
13:XM:49:THR:HG22	13:XM:51:ALA:H	1.78	0.48
25:YA:380:U:H2'	25:YA:381:G:H8	1.77	0.48
25:YA:2285:C:OP1	52:Y6:29:ASN:ND2	2.46	0.48
37:YR:104:ARG:HG3	37:YR:107:ASP:HB3	1.95	0.48
44:YY:15:VAL:HG21	44:YY:42:VAL:HG11	1.95	0.48
1:QA:707:C:H4'	11:QK:20:TYR:CD2	2.49	0.48
9:QI:121:ARG:NH1	9:QI:122:ALA:O	2.47	0.48
12:QL:53:ARG:HH12	12:QL:92:ASP:HB2	1.78	0.48
25:RA:557:U:H2'	25:RA:558:G:C8	2.48	0.48
25:RA:1333:C:H2'	25:RA:1334:G:H8	1.79	0.48
25:RA:2195:C:H2'	25:RA:2196:C:H6	1.79	0.48
25:RA:2361:A:O5'	54:R8:27:THR:OG1	2.32	0.48
25:RA:2611:U:C4	51:R5:3:LYS:HG3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:RD:27:THR:HG21	27:RD:81:ALA:HB1	1.95	0.48
1:XA:235:C:H2'	1:XA:236:G:H8	1.77	0.48
26:YB:22:U:O4	26:YB:61:G:O6	2.32	0.48
1:QA:59:A:H3'	1:QA:331:G:H22	1.79	0.48
1:QA:368:U:OP1	32:YI:91:SER:OG	2.27	0.48
1:QA:689:C:OP1	11:QK:27:ASN:ND2	2.44	0.48
1:QA:1172:C:H2'	1:QA:1173:G:C8	2.49	0.48
25:RA:2033:A:O2'	25:RA:2035:G:OP2	2.29	0.48
30:RG:161:THR:HG22	30:RG:163:ALA:H	1.77	0.48
22:XW:36:A:H2'	22:XW:37:U:C6	2.49	0.48
25:YA:1299:G:H21	25:YA:1641:A:H62	1.61	0.48
28:YE:74:PRO:HG2	28:YE:77:ILE:HG22	1.96	0.48
14:QN:45:ARG:HE	14:QN:49:HIS:CE1	2.32	0.48
25:RA:1568:G:OP1	27:RD:63:ARG:NH1	2.31	0.48
25:RA:2030:A:H4'	25:RA:2031:A:H8	1.79	0.48
25:RA:2674:G:H5''	34:RO:26:LYS:HE2	1.95	0.48
1:XA:573:A:N3	1:XA:883:C:O2'	2.41	0.48
1:XA:790:A:OP1	22:XV:39:A:O2'	2.26	0.48
9:XI:28:VAL:HG22	9:XI:63:ILE:HB	1.94	0.48
25:YA:589:C:H2'	25:YA:590:A:C8	2.49	0.48
25:YA:1068:G:O2'	25:YA:1096:A:N3	2.47	0.48
25:YA:2503:A:O2'	25:YA:2505:G:OP2	2.24	0.48
31:YH:9:ILE:HD13	31:YH:49:VAL:HG12	1.96	0.48
38:YS:26:LEU:HB3	38:YS:87:PHE:HA	1.96	0.48
2:QB:91:PRO:HG3	2:QB:154:LEU:HB2	1.96	0.48
12:QL:32:PHE:HE1	12:QL:86:ARG:HG3	1.78	0.48
22:QW:77:A:N1	54:R8:31:HIS:NE2	2.62	0.48
25:RA:177:G:H3'	25:RA:178:G:H8	1.79	0.48
25:RA:1184:G:OP1	49:R3:29:ARG:NH1	2.47	0.48
32:RI:93:THR:HA	32:RI:119:PRO:HB3	1.95	0.48
36:RQ:39:PRO:HB3	36:RQ:99:PRO:HD3	1.96	0.48
38:RS:25:ARG:NH1	38:RS:42:ASP:OD2	2.47	0.48
1:XA:781:A:O2'	1:XA:1522:U:O2	2.29	0.48
1:XA:1357:A:N6	1:XA:1365:G:H1	2.10	0.48
25:YA:840:C:OP2	25:YA:932:G:N2	2.40	0.48
25:YA:1131:G:C2	33:YN:75:TYR:HB2	2.48	0.48
25:YA:1231:G:H2'	25:YA:1232:G:H8	1.78	0.48
25:YA:1571:A:H2'	25:YA:1572:A:C8	2.49	0.48
27:YD:27:THR:HG21	27:YD:81:ALA:HB1	1.95	0.48
31:YH:43:VAL:HG22	31:YH:52:VAL:HG22	1.96	0.48
1:QA:1071:C:H2'	1:QA:1072:G:H8	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1492:A:H5''	12:QL:47:LYS:HB3	1.95	0.47
3:QC:152:ILE:HG12	3:QC:167:TRP:HD1	1.78	0.47
25:RA:851:U:H2'	25:RA:852:G:H8	1.79	0.47
25:RA:996:A:H4'	40:RU:92:ARG:HG2	1.95	0.47
25:RA:2212:A:H1'	25:RA:2215:G:C5	2.49	0.47
37:RR:3:HIS:O	37:RR:5:LYS:N	2.47	0.47
47:R1:52:ARG:NH2	47:R1:55:GLY:O	2.47	0.47
1:XA:1288:A:N3	1:XA:1352:C:O2'	2.37	0.47
8:XH:49:GLU:OE2	8:XH:62:TYR:OH	2.29	0.47
11:XK:54:ARG:HH22	22:XW:40:C:C3'	2.25	0.47
25:YA:694:U:O4	25:YA:768:G:O6	2.32	0.47
25:YA:831:G:O2'	35:YP:38:GLN:OE1	2.28	0.47
25:YA:1113:U:H2'	25:YA:1114:G:H8	1.78	0.47
25:YA:2211:G:H21	25:YA:2212:A:H2	1.62	0.47
1:QA:1347:G:N2	1:QA:1374:A:OP2	2.31	0.47
22:QV:51:U:O4	22:QV:65:G:O6	2.31	0.47
22:QW:32:G:H3'	22:QW:33:C:O4'	2.13	0.47
25:RA:414:C:H2'	25:RA:415:A:H8	1.79	0.47
25:RA:495:G:H21	42:RW:61:ASN:HD21	1.62	0.47
25:RA:2845:G:H2'	25:RA:2846:G:C8	2.49	0.47
35:RP:101:VAL:HB	35:RP:106:LEU:HB2	1.96	0.47
37:RR:88:ARG:NH2	37:RR:89:ASP:OD1	2.47	0.47
1:XA:321:A:N6	1:XA:329:A:OP2	2.47	0.47
1:XA:748:C:H1'	1:XA:749:C:H5	1.79	0.47
3:XC:9:GLY:HA3	14:XN:49:HIS:HA	1.95	0.47
6:XF:36:ARG:NH2	6:XF:66:GLU:OE1	2.47	0.47
9:XI:13:ALA:HB2	9:XI:68:GLY:HA3	1.95	0.47
25:YA:2339:G:H2'	25:YA:2340:G:H8	1.78	0.47
25:YA:2707:G:H2'	25:YA:2708:G:H8	1.79	0.47
30:YG:63:ILE:HG22	30:YG:143:GLU:HB2	1.96	0.47
37:YR:3:HIS:O	37:YR:5:LYS:N	2.47	0.47
38:YS:25:ARG:NH1	38:YS:42:ASP:OD2	2.47	0.47
43:YX:26:TYR:HD2	43:YX:89:ILE:HD12	1.78	0.47
47:Y1:87:PRO:HA	47:Y1:90:ILE:HG22	1.95	0.47
25:RA:709:U:H2'	25:RA:710:G:C8	2.50	0.47
1:XA:948:C:H2'	1:XA:949:A:H8	1.79	0.47
13:XM:99:ARG:HB2	13:XM:101:GLN:HE22	1.78	0.47
25:YA:890:A:H2'	25:YA:892:G:H8	1.79	0.47
25:YA:1262:A:OP2	42:YW:97:LYS:NZ	2.47	0.47
25:YA:1264:G:OP1	51:Y5:19:ARG:NH2	2.29	0.47
25:YA:1510:A:O2'	25:YA:1512:G:N7	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:YA:1592:C:H2'	25:YA:1593:G:H8	1.80	0.47
30:YG:105:LYS:HD3	50:Y4:26:SER:HB2	1.95	0.47
45:YZ:5:LEU:HD11	45:YZ:44:PHE:HA	1.97	0.47
1:QA:765:G:N2	1:QA:813:U:OP2	2.43	0.47
1:QA:1191:A:OP2	3:QC:3:ASN:ND2	2.47	0.47
1:QA:1273:G:H3'	1:QA:1274:G:H8	1.79	0.47
22:QW:36:A:H2'	22:QW:37:U:C6	2.50	0.47
25:RA:10:G:N2	25:RA:2802:G:OP1	2.37	0.47
25:RA:237:C:O2	25:RA:609:A:O2'	2.32	0.47
25:RA:358:U:H2'	25:RA:359:A:H8	1.79	0.47
25:RA:1638:C:O2	25:RA:2698:U:O2'	2.31	0.47
25:RA:2150:U:H2'	25:RA:2151:G:H8	1.79	0.47
45:RZ:5:LEU:HD11	45:RZ:44:PHE:HA	1.97	0.47
1:XA:1375:A:H4'	7:XG:29:LYS:HD3	1.97	0.47
22:XW:10:G:H2'	22:XW:11:A:H8	1.79	0.47
25:YA:589:C:H2'	25:YA:590:A:H8	1.78	0.47
25:YA:782:A:O2'	27:YD:225:ALA:O	2.32	0.47
25:YA:1508:A:O2'	25:YA:1509:C:O4'	2.31	0.47
38:YS:12:PHE:O	38:YS:16:ASN:ND2	2.48	0.47
1:QA:985:C:H2'	1:QA:986:A:H8	1.78	0.47
1:QA:1222:G:OP1	19:QS:78:ARG:NH1	2.34	0.47
4:QD:60:GLU:HG2	4:QD:202:LEU:HB2	1.95	0.47
52:R6:10:LEU:HG	52:R6:54:ILE:HG13	1.97	0.47
1:XA:67:C:H2'	1:XA:68:G:C8	2.49	0.47
1:XA:377:G:H2'	1:XA:378:G:H8	1.79	0.47
8:XH:51:VAL:HG21	8:XH:60:ARG:HG3	1.95	0.47
11:XK:34:ASP:OD1	11:XK:37:GLY:N	2.48	0.47
22:XW:8:U:H2'	22:XW:13:C:H41	1.80	0.47
22:XW:68:C:H2'	22:XW:69:C:C6	2.49	0.47
25:YA:1535:U:H3	25:YA:1537:C:H1'	1.78	0.47
25:YA:2100:G:H2'	25:YA:2101:G:H8	1.79	0.47
32:YI:13:GLY:HA3	32:YI:17:GLN:HG2	1.95	0.47
1:QA:148:G:H2'	1:QA:149:A:C8	2.49	0.47
1:QA:1175:G:H2'	1:QA:1176:A:C8	2.49	0.47
4:QD:166:LYS:HG2	27:YD:135:PHE:HZ	1.78	0.47
25:RA:1791:A:N6	25:RA:1828:G:O2'	2.39	0.47
25:RA:2327:A:H2'	25:RA:2328:A:C8	2.49	0.47
27:RD:153:ALA:O	27:RD:157:ARG:NH1	2.48	0.47
31:RH:12:PRO:HG2	31:RH:13:LYS:HG2	1.97	0.47
36:RQ:71:ASP:OD1	36:RQ:71:ASP:N	2.45	0.47
38:RS:12:PHE:O	38:RS:16:ASN:ND2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:RT:50:ILE:HG13	39:RT:99:LEU:HD12	1.97	0.47
1:XA:1004:A:O5'	1:XA:1025:U:N3	2.43	0.47
1:XA:1235:U:H5''	21:XU:3:LYS:HD2	1.95	0.47
25:YA:2637:U:H5''	28:YE:82:ARG:NH1	2.30	0.47
34:YO:104:ARG:NH1	34:YO:121:VAL:O	2.47	0.47
1:QA:62:U:H3	1:QA:105:G:H1	1.62	0.47
1:QA:1013:G:N2	1:QA:1016:A:OP2	2.43	0.47
1:QA:1172:C:H2'	1:QA:1173:G:H8	1.78	0.47
1:QA:1309:G:OP1	13:QM:88:ARG:NH2	2.48	0.47
1:QA:1340:A:OP1	22:QW:36:A:H5'	2.15	0.47
1:QA:1354:C:H2'	1:QA:1355:G:H8	1.80	0.47
3:QC:20:SER:OG	3:QC:22:TRP:NE1	2.48	0.47
22:QW:77:A:C8	22:QW:77:A:C5'	2.85	0.47
25:RA:942:G:OP2	35:RP:39:LYS:NZ	2.37	0.47
25:RA:1140:C:OP2	33:RN:66:LYS:NZ	2.39	0.47
25:RA:1582:C:H2'	25:RA:1583:A:H8	1.80	0.47
25:RA:1662:C:O2'	25:RA:2687:U:OP1	2.30	0.47
25:RA:2047:U:H2'	25:RA:2048:G:H8	1.79	0.47
27:RD:25:THR:HG22	27:RD:82:ILE:H	1.80	0.47
31:RH:43:VAL:HG22	31:RH:52:VAL:HG22	1.96	0.47
1:XA:243:A:H4'	1:XA:244:U:H3'	1.96	0.47
1:XA:477:G:H2'	1:XA:478:A:H8	1.80	0.47
1:XA:510:A:OP2	4:XD:49:ARG:NH2	2.43	0.47
2:XB:168:THR:HA	2:XB:171:ALA:HB2	1.96	0.47
4:XD:60:GLU:HG2	4:XD:202:LEU:HB2	1.95	0.47
25:YA:270(R):G:H2'	25:YA:270(S):G:C8	2.50	0.47
25:YA:301:G:OP2	44:YY:84:ARG:NH2	2.41	0.47
25:YA:863:A:H2'	25:YA:864:G:H8	1.79	0.47
25:YA:1087:G:C4	25:YA:1089:G:H1'	2.50	0.47
25:YA:2848:G:C8	39:YT:97:ALA:HB2	2.50	0.47
31:YH:106:THR:HG22	31:YH:112:PRO:HB3	1.97	0.47
36:YQ:39:PRO:HB3	36:YQ:99:PRO:HD3	1.96	0.47
1:QA:973:G:H3'	1:QA:974:A:H5''	1.97	0.47
1:QA:1386:G:H2'	1:QA:1387:G:H8	1.80	0.47
7:QG:86:GLN:CD	22:QW:32:G:H21	2.17	0.47
22:QW:8:U:H2'	22:QW:13:C:H41	1.80	0.47
24:QY:28:G:H1	24:QY:42:C:H42	1.63	0.47
25:RA:994:C:OP2	40:RU:54:LYS:NZ	2.39	0.47
25:RA:1296:G:OP1	25:RA:2709:G:O2'	2.24	0.47
33:RN:30:ILE:HG23	33:RN:52:VAL:HG11	1.95	0.47
2:XB:32:ILE:HD11	2:XB:40:HIS:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:YA:581:C:H2'	25:YA:582:G:C8	2.50	0.47
25:YA:2581:G:OP2	25:YA:2581:G:N2	2.44	0.47
27:YD:25:THR:HG22	27:YD:82:ILE:H	1.80	0.47
1:QA:677:U:O2	1:QA:777:A:O2'	2.31	0.47
6:QF:36:ARG:NH2	6:QF:66:GLU:OE1	2.47	0.47
13:QM:13:LYS:HA	13:QM:44:ARG:HD2	1.97	0.47
13:QM:99:ARG:HB2	13:QM:101:GLN:HE22	1.79	0.47
25:RA:439:G:H2'	25:RA:440:G:C8	2.50	0.47
25:RA:587:C:OP1	35:RP:21:ARG:NH2	2.42	0.47
17:XQ:43:LEU:HD12	17:XQ:68:ARG:HG3	1.97	0.47
25:YA:1174:A:H2'	25:YA:1175:U:H4'	1.97	0.47
25:YA:2228:G:OP1	27:YD:261:LYS:NZ	2.36	0.47
27:YD:153:ALA:O	27:YD:157:ARG:NH1	2.48	0.47
1:QA:28:G:O2'	1:QA:296:U:OP1	2.30	0.47
1:QA:1342:C:H4'	9:QI:125:TYR:HB3	1.97	0.47
1:QA:1422:G:H2'	1:QA:1423:G:H8	1.80	0.47
1:QA:1454:G:H2'	1:QA:1455:G:H8	1.79	0.47
13:QM:3:ARG:HA	13:QM:9:ILE:HG21	1.97	0.47
28:RE:13:ARG:HA	28:RE:22:PRO:HA	1.97	0.47
40:RU:52:ARG:HH11	40:RU:55:ARG:HH21	1.63	0.47
41:RV:51:VAL:HG12	41:RV:53:GLU:H	1.80	0.47
1:XA:56:U:H2'	1:XA:57:G:H8	1.79	0.47
1:XA:254:G:O2'	17:XQ:16:GLN:O	2.32	0.47
1:XA:628:G:H2'	1:XA:629:G:C8	2.50	0.47
8:XH:112:LEU:HD23	8:XH:133:LEU:HA	1.97	0.47
13:XM:89:GLY:O	13:XM:93:ARG:N	2.48	0.47
25:YA:244:A:H4'	35:YP:74:GLU:HB2	1.97	0.47
25:YA:635:C:O2'	25:YA:639:U:OP1	2.33	0.47
25:YA:1530:G:O6	25:YA:1542:G:N2	2.47	0.47
25:YA:1791:A:H3'	25:YA:1792:G:H8	1.79	0.47
1:QA:45:U:H2'	1:QA:46:G:C8	2.50	0.46
1:QA:1061:G:OP1	10:QJ:59:SER:OG	2.27	0.46
2:QB:15:VAL:H	2:QB:16:HIS:CD2	2.33	0.46
25:RA:581:C:H2'	25:RA:582:G:C8	2.49	0.46
25:RA:822:U:H2'	25:RA:823:G:H8	1.80	0.46
25:RA:1114:G:H2'	25:RA:1115:G:C8	2.50	0.46
25:RA:2467:C:N4	25:RA:2484:G:O6	2.48	0.46
25:RA:2500:U:O2'	25:RA:2504:U:OP1	2.24	0.46
29:RF:195:ASP:OD1	29:RF:195:ASP:N	2.46	0.46
37:RR:38:VAL:HG22	37:RR:112:ALA:HB2	1.96	0.46
38:RS:26:LEU:HB3	38:RS:87:PHE:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:RU:98:LEU:O	40:RU:102:GLU:N	2.45	0.46
1:XA:178:C:H2'	1:XA:179:A:H8	1.79	0.46
1:XA:708:C:OP1	11:XK:85:ARG:NH2	2.43	0.46
1:XA:1250:A:N3	1:XA:1370:G:O2'	2.39	0.46
22:XV:57:C:N4	30:YG:83:ARG:HH12	2.13	0.46
1:QA:539:A:H2'	1:QA:540:G:C8	2.51	0.46
1:QA:1326:C:OP1	21:QU:17:THR:OG1	2.31	0.46
2:QB:189:ASP:N	2:QB:189:ASP:OD1	2.48	0.46
4:QD:107:ARG:NH1	6:XF:17:SER:OG	2.48	0.46
22:QW:1:C:H42	22:QW:73:A:H61	1.63	0.46
25:RA:270(G):C:H42	25:RA:270(S):G:H1	1.61	0.46
25:RA:807:U:O2'	25:RA:2060:A:N1	2.42	0.46
25:RA:1636:C:H2'	25:RA:1637:A:C8	2.50	0.46
25:RA:1753:G:N2	25:RA:1756:G:OP2	2.47	0.46
25:RA:2020:A:H5'	51:R5:12:SER:HB3	1.96	0.46
33:RN:47:ALA:O	33:RN:119:ARG:NH1	2.45	0.46
1:XA:1060:C:H2'	1:XA:1061:G:H8	1.80	0.46
13:XM:16:ASP:OD1	13:XM:16:ASP:N	2.47	0.46
25:YA:694:U:H3	25:YA:768:G:H1	1.62	0.46
26:YB:60:C:H2'	26:YB:61:G:H8	1.80	0.46
29:YF:195:ASP:N	29:YF:195:ASP:OD1	2.46	0.46
40:YU:52:ARG:HH11	40:YU:55:ARG:HH21	1.63	0.46
1:QA:501:C:H2'	1:QA:502:G:C8	2.50	0.46
1:QA:514:C:H2'	1:QA:515:G:H8	1.80	0.46
1:QA:1412:C:H2'	1:QA:1413:A:C8	2.50	0.46
21:QU:6:ARG:HE	21:QU:15:ARG:HH21	1.63	0.46
25:RA:693:C:O2'	25:RA:1353:A:N3	2.37	0.46
1:XA:352:C:O2'	1:XA:354:G:OP1	2.26	0.46
1:XA:376:G:H5''	16:XP:5:ARG:HD2	1.97	0.46
1:XA:380:G:N2	1:XA:383:A:OP2	2.36	0.46
1:XA:601:C:H2'	1:XA:602:A:H8	1.80	0.46
1:XA:713:G:H2'	1:XA:714:G:C8	2.50	0.46
1:XA:1391:U:H2'	1:XA:1392:G:H8	1.80	0.46
22:XW:32:G:H3'	22:XW:33:C:O4'	2.15	0.46
25:YA:1799:G:N2	25:YA:1818:U:O2'	2.48	0.46
25:YA:1826:G:O2'	27:YD:242:ARG:NH2	2.48	0.46
25:YA:2071:A:H2'	25:YA:2072:G:H8	1.81	0.46
25:YA:2293:C:O2'	38:YS:93:LYS:NZ	2.47	0.46
25:YA:2377:A:O2'	38:YS:111:GLU:O	2.30	0.46
25:YA:2632:A:HO2'	25:YA:2811:G:HO2'	1.64	0.46
31:YH:12:PRO:HG2	31:YH:13:LYS:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:YZ:17:ALA:O	45:YZ:21:ALA:N	2.45	0.46
1:QA:369:C:OP2	1:QA:388:G:N1	2.41	0.46
1:QA:715:A:H2'	1:QA:716:A:C8	2.49	0.46
22:QW:49:C:N3	22:QW:60:A:H1'	2.30	0.46
25:RA:782:A:O2'	27:RD:225:ALA:O	2.31	0.46
25:RA:922:U:H2'	25:RA:923:C:C6	2.51	0.46
25:RA:1363:C:O2'	25:RA:1809:A:N3	2.42	0.46
25:RA:1598:C:O3'	43:RX:35:THR:OG1	2.32	0.46
25:RA:2734:A:H62	25:RA:2770:G:N2	2.12	0.46
26:RB:33:G:H5'	30:RG:2:PRO:HG3	1.98	0.46
42:RW:25:ARG:NH2	42:RW:74:ALA:O	2.31	0.46
1:XA:452:A:O2'	1:XA:453:A:O4'	2.31	0.46
7:XG:73:MET:HG2	7:XG:90:GLU:HA	1.97	0.46
12:XL:45:PRO:HB3	12:XL:92:ASP:HB3	1.97	0.46
25:YA:1815:A:OP2	27:YD:54:ARG:NH1	2.46	0.46
25:YA:2816:C:O2	25:YA:2883:A:O2'	2.29	0.46
32:YI:2:LYS:HA	32:YI:20:ASP:HA	1.98	0.46
39:YT:18:ASP:N	39:YT:18:ASP:OD1	2.45	0.46
1:QA:128:G:O2'	17:QQ:3:LYS:NZ	2.43	0.46
1:QA:1367:C:OP2	9:QI:112:LYS:NZ	2.48	0.46
9:QI:29:ASN:HD21	9:QI:65:VAL:HB	1.78	0.46
10:QJ:78:ASN:HB2	10:QJ:81:THR:HG23	1.98	0.46
13:QM:40:ASN:HB3	13:QM:43:THR:HG23	1.98	0.46
28:RE:74:PRO:HG2	28:RE:77:ILE:HG22	1.96	0.46
30:RG:63:ILE:HG22	30:RG:143:GLU:HB2	1.96	0.46
1:XA:656:C:O2	15:XO:28:GLN:NE2	2.44	0.46
1:XA:1393:U:HO2'	1:XA:1501:C:HO2'	1.59	0.46
19:XS:27:GLU:OE2	19:XS:29:ARG:NH2	2.42	0.46
22:XW:77:A:C2	25:YA:2422:A:N1	2.82	0.46
30:YG:173:LEU:O	30:YG:178:PHE:N	2.46	0.46
37:YR:79:LEU:HD12	37:YR:83:ILE:HB	1.97	0.46
48:Y2:4:SER:OG	48:Y2:5:GLU:N	2.48	0.46
1:QA:45:U:H3	1:QA:396:G:H1	1.63	0.46
1:QA:178:C:H2'	1:QA:179:A:H8	1.80	0.46
1:QA:501:C:H2'	1:QA:502:G:H8	1.79	0.46
1:QA:985:C:H2'	1:QA:986:A:C8	2.50	0.46
19:QS:10:PHE:HE2	19:QS:16:LEU:HB2	1.80	0.46
25:RA:78:A:H2'	25:RA:79:G:H8	1.80	0.46
25:RA:261:G:O2'	25:RA:609(A):G:O2'	2.32	0.46
25:RA:890:A:H2'	25:RA:892:G:H8	1.81	0.46
25:RA:1061:U:OP2	25:RA:1070:A:O2'	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:RA:1971:A:OP2	27:RD:242:ARG:NH2	2.45	0.46
25:RA:2547:U:O2	34:RO:23:ARG:NH2	2.49	0.46
26:RB:60:C:H2'	26:RB:61:G:H8	1.80	0.46
28:RE:143:ASN:HB2	28:RE:147:PRO:HD2	1.98	0.46
34:RO:19:ILE:HG22	34:RO:43:VAL:HA	1.98	0.46
35:RP:47:ASP:OD2	35:RP:50:ARG:NH2	2.49	0.46
1:XA:1127:G:H21	1:XA:1147:C:H41	1.64	0.46
1:XA:1287:A:H2	1:XA:1353:G:H1'	1.80	0.46
1:XA:1317:C:O2	19:XS:37:ARG:NH1	2.49	0.46
1:XA:1427:U:H2'	1:XA:1428:A:C8	2.49	0.46
8:XH:82:HIS:N	8:XH:138:TRP:OXT	2.49	0.46
21:XU:6:ARG:HE	21:XU:15:ARG:HH21	1.64	0.46
25:YA:297:C:H5''	44:YY:87:LYS:HG3	1.97	0.46
25:YA:1085:A:H2'	25:YA:1086:A:C4	2.51	0.46
25:YA:1779:U:OP2	25:YA:1784:A:N6	2.40	0.46
25:YA:2105:C:H2'	25:YA:2106:G:C8	2.50	0.46
32:YI:79:ILE:HB	32:YI:142:VAL:HA	1.98	0.46
47:Y1:60:PHE:HB3	47:Y1:62:VAL:HG13	1.98	0.46
1:QA:642:A:N3	8:QH:113:SER:OG	2.41	0.46
1:QA:748:C:H1'	1:QA:749:C:H5	1.81	0.46
1:QA:925:G:H1	1:QA:1391:U:H3	1.62	0.46
2:QB:15:VAL:HG21	2:QB:209:ARG:HG3	1.97	0.46
8:QH:82:HIS:N	8:QH:138:TRP:OXT	2.49	0.46
25:RA:300:A:OP1	44:RY:86:ARG:NH2	2.49	0.46
25:RA:589:C:H2'	25:RA:590:A:C8	2.51	0.46
25:RA:629:G:N3	25:RA:639:U:O2'	2.47	0.46
38:RS:40:ILE:HA	38:RS:47:THR:HA	1.98	0.46
1:XA:156:G:H2'	1:XA:157:G:H8	1.81	0.46
1:XA:979:C:OP1	1:XA:1223:C:N4	2.48	0.46
25:YA:674:G:H1'	29:YF:74:ARG:HD3	1.96	0.46
25:YA:1176:G:O2'	25:YA:1178:C:N4	2.49	0.46
25:YA:1841:U:H2'	25:YA:1842:G:H8	1.79	0.46
25:YA:1939:U:OP1	25:YA:2604:U:O2'	2.31	0.46
28:YE:13:ARG:HA	28:YE:22:PRO:HA	1.97	0.46
49:Y3:39:ASP:OD1	49:Y3:44:ARG:NH2	2.46	0.46
1:QA:56:U:H2'	1:QA:57:G:C8	2.50	0.46
1:QA:166:G:H2'	1:QA:167:G:H8	1.81	0.46
1:QA:352:C:O2'	1:QA:354:G:OP1	2.22	0.46
1:QA:539:A:H2'	1:QA:540:G:H8	1.81	0.46
17:QQ:43:LEU:HD12	17:QQ:68:ARG:HG3	1.96	0.46
17:QQ:83:ASP:N	17:QQ:83:ASP:OD1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:RA:579:G:O2'	25:RA:2019:A:OP1	2.34	0.46
25:RA:2495:G:H5''	36:RQ:81:VAL:HG12	1.98	0.46
34:RO:2:ILE:HB	34:RO:33:ALA:HB3	1.98	0.46
44:RY:14:LEU:HB2	44:RY:75:ILE:HD11	1.98	0.46
45:RZ:30:ASN:HB3	45:RZ:90:VAL:HB	1.98	0.46
25:YA:24:G:O2'	42:YW:78:GLU:O	2.32	0.46
25:YA:1111:A:OP1	31:YH:3:ARG:NH2	2.49	0.46
25:YA:1184:G:P	49:Y3:29:ARG:HH12	2.38	0.46
25:YA:1731:G:H2'	25:YA:1732:A:H8	1.81	0.46
25:YA:1782:C:O2	25:YA:2608:G:O2'	2.28	0.46
25:YA:2737:G:H2'	25:YA:2738:A:C8	2.51	0.46
26:YB:113:C:O2'	38:YS:47:THR:N	2.49	0.46
45:YZ:30:ASN:HB3	45:YZ:90:VAL:HB	1.98	0.46
1:QA:309:G:H2'	1:QA:310:G:H8	1.80	0.46
1:QA:360:A:H2'	1:QA:361:G:C8	2.51	0.46
1:QA:864:A:H2'	1:QA:865:A:C8	2.51	0.46
2:QB:32:ILE:HD11	2:QB:40:HIS:HB3	1.96	0.46
5:QE:101:ILE:O	5:QE:120:THR:OG1	2.31	0.46
25:RA:345:A:N3	25:RA:347:A:N6	2.63	0.46
25:RA:1114:G:H2'	25:RA:1115:G:H8	1.81	0.46
25:RA:2081:C:H2'	25:RA:2082:A:H8	1.81	0.46
28:RE:105:THR:HB	28:RE:197:ILE:HG23	1.98	0.46
34:RO:104:ARG:NH1	34:RO:121:VAL:O	2.47	0.46
53:R7:13:ALA:HB2	53:R7:46:VAL:HG11	1.97	0.46
22:XW:9:G:H5''	22:XW:10:G:OP2	2.16	0.46
25:YA:1568:G:H5''	27:YD:61:LEU:HD23	1.98	0.46
25:YA:1818:U:OP2	27:YD:157:ARG:NE	2.48	0.46
25:YA:2185:C:H2'	25:YA:2186:G:H8	1.80	0.46
25:YA:2328:A:H2'	25:YA:2329:G:H8	1.80	0.46
25:YA:2467:C:O2	36:YQ:124:LYS:NZ	2.33	0.46
29:YF:34:TRP:CE3	35:YP:8:PRO:HB3	2.51	0.46
38:YS:31:SER:O	38:YS:97:ARG:NH1	2.39	0.46
41:YV:51:VAL:HG12	41:YV:53:GLU:H	1.80	0.46
52:Y6:10:LEU:HG	52:Y6:54:ILE:HG13	1.97	0.46
1:QA:1443:G:N2	25:RA:2864:G:OP1	2.45	0.46
5:QE:75:THR:OG1	5:QE:76:ILE:N	2.49	0.46
8:QH:112:LEU:HD23	8:QH:133:LEU:HA	1.97	0.46
31:RH:12:PRO:HB3	31:RH:48:GLY:HA2	1.98	0.46
34:RO:104:ARG:HH11	34:RO:121:VAL:HG12	1.81	0.46
48:R2:4:SER:OG	48:R2:5:GLU:N	2.48	0.46
1:XA:911:U:OP2	12:XL:97:ARG:NH2	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:XC:20:SER:OG	3:XC:22:TRP:NE1	2.48	0.46
10:XJ:78:ASN:O	10:XJ:81:THR:OG1	2.25	0.46
25:YA:1078:U:H1'	25:YA:1088:A:H2	1.81	0.46
25:YA:2692:C:H1'	25:YA:2847:U:H1'	1.97	0.46
31:YH:54:ARG:NH2	31:YH:57:ASP:OD1	2.48	0.46
34:YO:107:ARG:NH1	39:YT:36:GLU:OE1	2.49	0.46
1:QA:1096:C:H2'	1:QA:1097:C:H6	1.81	0.45
1:QA:1287:A:H2	1:QA:1353:G:H1'	1.81	0.45
1:QA:1435:G:H2'	1:QA:1436:U:C6	2.51	0.45
7:QG:73:MET:HG2	7:QG:90:GLU:HA	1.98	0.45
25:RA:770:G:OP1	53:R7:8:ASN:ND2	2.39	0.45
25:RA:949:C:H2'	25:RA:950:G:H8	1.81	0.45
27:RD:148:GLU:HB2	27:RD:151:LYS:HD2	1.99	0.45
29:RF:28:ILE:HG22	29:RF:112:MET:HB3	1.98	0.45
51:R5:41:PRO:O	51:R5:44:THR:OG1	2.34	0.45
1:XA:662:G:H2'	1:XA:663:A:C8	2.51	0.45
1:XA:1096:C:H2'	1:XA:1097:C:H6	1.81	0.45
1:XA:1329:A:H5''	13:XM:26:GLY:H	1.81	0.45
2:XB:132:LYS:HA	2:XB:135:GLN:HB2	1.98	0.45
22:XW:35:C:C5	23:XX:14:A:N6	2.84	0.45
25:YA:2282:G:H21	25:YA:2390:U:H3	1.64	0.45
25:YA:2529:G:H5''	25:YA:2530:A:H5''	1.97	0.45
27:YD:148:GLU:HB2	27:YD:151:LYS:HD2	1.98	0.45
31:YH:12:PRO:HB3	31:YH:48:GLY:HA2	1.98	0.45
35:YP:122:PRO:HB3	35:YP:141:ALA:HB1	1.99	0.45
1:QA:62:U:O2'	1:QA:379:C:O2	2.33	0.45
1:QA:376:G:O3'	16:QP:5:ARG:NH1	2.43	0.45
1:QA:677:U:H3	1:QA:713:G:H22	1.65	0.45
13:QM:47:ASP:OD1	13:QM:47:ASP:N	2.41	0.45
28:RE:92:THR:HG23	28:RE:94:GLU:H	1.82	0.45
29:RF:178:PRO:HB3	29:RF:198:ALA:HB2	1.98	0.45
37:RR:12:ARG:O	37:RR:17:ARG:NH2	2.49	0.45
20:XT:89:ARG:HH21	20:XT:104:LEU:HD21	1.82	0.45
22:XV:35:C:H2'	22:XV:36:A:H8	1.81	0.45
25:YA:657:U:H2'	25:YA:658:C:H6	1.82	0.45
25:YA:1059:G:O6	25:YA:1079:C:N4	2.47	0.45
25:YA:1204:A:H1'	25:YA:1206:G:C8	2.52	0.45
26:YB:33:G:H5'	30:YG:2:PRO:HG3	1.97	0.45
29:YF:116:ASP:OD2	35:YP:1:MET:N	2.39	0.45
39:YT:50:ILE:HG13	39:YT:99:LEU:HD12	1.97	0.45
40:YU:91:ASP:O	40:YU:95:LEU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:YY:17:SER:HG	44:YY:71:LYS:HZ2	1.62	0.45
25:RA:15:G:H1	25:RA:525:U:H3	1.63	0.45
25:RA:380:U:H2'	25:RA:381:G:H8	1.82	0.45
25:RA:469:G:O6	53:R7:39:ARG:NH1	2.49	0.45
25:RA:675:A:N3	25:RA:2443:C:O2'	2.38	0.45
25:RA:1695:G:N7	27:RD:14:ARG:NH2	2.64	0.45
25:RA:1962:C:O2'	25:RA:1964:G:OP2	2.31	0.45
25:RA:2630:G:H2'	25:RA:2631:G:H8	1.80	0.45
1:XA:22:G:H2'	1:XA:23:C:C6	2.51	0.45
1:XA:971:G:H5''	1:XA:972:C:H5''	1.97	0.45
1:XA:1292:U:H2'	1:XA:1293:G:C8	2.50	0.45
1:XA:1355:G:H2'	1:XA:1356:G:H8	1.81	0.45
1:XA:1507:A:H2'	1:XA:1508:G:C8	2.52	0.45
1:XA:1510:U:H2'	1:XA:1511:G:C8	2.51	0.45
22:XW:2:G:H2'	22:XW:3:C:C6	2.51	0.45
25:YA:1031:G:O2'	55:Y9:7:VAL:O	2.32	0.45
25:YA:2329:G:H2'	25:YA:2330:G:C8	2.52	0.45
25:YA:2387:U:O2'	46:Y0:19:LYS:NZ	2.49	0.45
33:YN:47:ALA:O	33:YN:119:ARG:NH1	2.45	0.45
38:YS:40:ILE:HA	38:YS:47:THR:HA	1.98	0.45
1:QA:191:G:O2'	20:QT:101:GLY:O	2.35	0.45
1:QA:684:A:O2'	11:QK:39:PRO:O	2.32	0.45
20:QT:49:ALA:HA	20:QT:52:ALA:HB3	1.98	0.45
25:RA:583:G:H5''	40:RU:10:ARG:NH1	2.31	0.45
25:RA:1156:A:P	40:RU:55:ARG:HH11	2.40	0.45
45:RZ:120:ILE:H	45:RZ:172:ALA:HA	1.82	0.45
1:XA:1352:C:OP1	21:XU:3:LYS:NZ	2.32	0.45
25:YA:392:C:H5''	25:YA:409:C:H5''	1.98	0.45
25:YA:1754:C:P	39:YT:96:ARG:HH12	2.40	0.45
32:YI:65:ALA:O	32:YI:69:LYS:N	2.46	0.45
36:YQ:71:ASP:OD1	36:YQ:71:ASP:N	2.45	0.45
1:QA:34:C:H2'	1:QA:35:G:C8	2.49	0.45
1:QA:718:G:O6	18:QR:74:ARG:NH1	2.50	0.45
1:QA:864:A:O2'	1:QA:1078:U:O4	2.29	0.45
8:QH:49:GLU:OE2	8:QH:62:TYR:OH	2.29	0.45
25:RA:1041:C:H2'	25:RA:1042:G:C8	2.51	0.45
25:RA:1316:U:H2'	25:RA:1317:A:C8	2.51	0.45
25:RA:2683:C:H5''	39:RT:53:ARG:HH12	1.81	0.45
50:R4:28:LYS:HB2	50:R4:31:ILE:HD11	1.98	0.45
1:XA:116:A:H61	1:XA:313:A:H1'	1.81	0.45
1:XA:1169:A:H2'	1:XA:1170:A:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:XI:26:VAL:HG22	9:XI:61:ALA:HB3	1.97	0.45
24:XY:28:G:H1	24:XY:42:C:H42	1.63	0.45
11:QK:22:HIS:HB3	11:QK:29:ILE:HG23	1.97	0.45
25:RA:18:C:O2'	25:RA:553:U:OP1	2.34	0.45
25:RA:255:A:O2'	25:RA:384:U:OP1	2.27	0.45
25:RA:392:C:H5''	25:RA:409:C:H5''	1.97	0.45
25:RA:629:G:H1'	25:RA:639:U:H1'	1.98	0.45
25:RA:1657:C:H2'	25:RA:1658:C:H6	1.82	0.45
25:RA:2006:C:O2'	25:RA:2823:A:N3	2.49	0.45
30:RG:16:ARG:NH2	30:RG:28:VAL:O	2.49	0.45
31:RH:54:ARG:NH2	31:RH:57:ASP:OD1	2.48	0.45
40:RU:91:ASP:O	40:RU:95:LEU:N	2.49	0.45
50:R4:51:ASP:N	50:R4:51:ASP:OD1	2.49	0.45
1:XA:529:G:O6	12:XL:49:ASN:ND2	2.43	0.45
1:XA:1219:U:OP1	14:XN:19:ARG:NH2	2.41	0.45
3:XC:59:ARG:HH12	3:XC:97:LYS:HE3	1.82	0.45
8:XH:104:ARG:HD2	8:XH:138:TRP:CD2	2.52	0.45
25:YA:172:C:H2'	25:YA:173:G:H8	1.82	0.45
25:YA:532:A:N1	25:YA:2035:G:N2	2.64	0.45
29:YF:40:GLN:HE22	29:YF:182:ASN:HB2	1.82	0.45
34:YO:2:ILE:HB	34:YO:33:ALA:HB3	1.98	0.45
34:YO:104:ARG:HH11	34:YO:121:VAL:HG12	1.81	0.45
50:Y4:28:LYS:HB2	50:Y4:31:ILE:HD11	1.98	0.45
1:QA:1128:C:H1'	1:QA:1146:A:H61	1.82	0.45
1:QA:1308:U:OP2	13:QM:101:GLN:NE2	2.50	0.45
1:QA:1397:C:N3	23:QX:22:C:H5	2.15	0.45
5:QE:143:ARG:NE	8:QH:77:GLU:OE2	2.47	0.45
44:RY:29:GLU:HB3	44:RY:38:ILE:HD12	1.99	0.45
1:XA:269:C:H2'	1:XA:270:A:H8	1.82	0.45
1:XA:532:A:H2	1:XA:1206:G:H21	1.62	0.45
12:XL:28:LYS:HB2	12:XL:28:LYS:HE3	1.70	0.45
25:YA:767:U:H2'	25:YA:768:G:H8	1.81	0.45
25:YA:852:G:H2'	25:YA:853:G:H8	1.82	0.45
25:YA:1638:C:O2	25:YA:2698:U:O2'	2.31	0.45
25:YA:1761:C:H42	25:YA:1762:A:H62	1.65	0.45
30:YG:16:ARG:NH2	30:YG:28:VAL:O	2.49	0.45
30:YG:49:ASP:OD2	30:YG:51:ARG:NH2	2.49	0.45
45:YZ:102:LEU:HD23	45:YZ:137:ILE:HB	1.99	0.45
1:QA:21:G:H2'	1:QA:22:G:H8	1.81	0.45
1:QA:444:C:H2'	1:QA:445:G:H8	1.82	0.45
1:QA:736:C:O2'	6:QF:90:VAL:O	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:923:A:O2'	1:QA:1399:C:OP2	2.28	0.45
9:QI:13:ALA:HB2	9:QI:68:GLY:HA3	1.99	0.45
25:RA:110:G:H2'	25:RA:111:A:H8	1.80	0.45
25:RA:911:A:H2'	36:RQ:9:TYR:HE2	1.82	0.45
25:RA:1152:C:H4'	40:RU:77:SER:HA	1.98	0.45
25:RA:2632:A:O2'	25:RA:2811:G:O2'	2.23	0.45
28:RE:51:PHE:HD2	28:RE:52:LEU:HG	1.82	0.45
31:RH:106:THR:HG22	31:RH:112:PRO:HB3	1.97	0.45
32:RI:79:ILE:HB	32:RI:142:VAL:HA	1.98	0.45
46:R0:32:ARG:N	46:R0:35:ASN:OD1	2.49	0.45
1:XA:745:C:OP1	1:XA:851:G:O2'	2.34	0.45
1:XA:1254:C:H2'	1:XA:1255:G:C8	2.52	0.45
1:XA:1264:C:H2'	1:XA:1265:G:C8	2.52	0.45
7:XG:86:GLN:OE1	22:XW:32:G:N2	2.43	0.45
8:XH:91:ARG:NE	17:XQ:32:TYR:O	2.34	0.45
13:XM:14:ARG:HG2	13:XM:44:ARG:NH1	2.32	0.45
25:YA:414:C:H2'	25:YA:415:A:C8	2.51	0.45
25:YA:463:G:N2	25:YA:466:A:OP2	2.42	0.45
25:YA:1000:A:OP2	25:YA:1154:G:N1	2.30	0.45
48:Y2:66:GLU:HA	48:Y2:69:ARG:HH21	1.82	0.45
1:QA:359:U:H2'	1:QA:360:A:H8	1.81	0.45
1:QA:376:G:H5''	16:QP:5:ARG:HB2	1.99	0.45
1:QA:618:C:H5'	1:QA:619:U:H5''	1.99	0.45
1:QA:811:C:O2'	1:QA:901:A:N1	2.49	0.45
1:QA:835:U:H3	1:QA:851:G:H1	1.65	0.45
8:QH:104:ARG:HD2	8:QH:138:TRP:CD2	2.52	0.45
22:QW:77:A:N3	25:RA:2421:G:C6	2.85	0.45
5:XE:75:THR:OG1	5:XE:76:ILE:N	2.50	0.45
8:XH:17:THR:O	8:XH:78:GLN:NE2	2.50	0.45
15:XO:17:ARG:HH12	15:XO:77:ARG:NH1	2.14	0.45
16:XP:67:THR:O	16:XP:71:ARG:N	2.50	0.45
22:XV:44:A:H2'	22:XV:45:A:C8	2.52	0.45
25:YA:172:C:H2'	25:YA:173:G:C8	2.52	0.45
25:YA:1657:C:H2'	25:YA:1658:C:C6	2.52	0.45
25:YA:2314:C:H5'	30:YG:38:VAL:HG11	1.98	0.45
27:YD:52:ARG:H	27:YD:52:ARG:HG2	1.56	0.45
28:YE:143:ASN:HB2	28:YE:147:PRO:HD2	1.98	0.45
29:YF:28:ILE:HG22	29:YF:112:MET:HB3	1.98	0.45
29:YF:117:ARG:HH21	29:YF:187:VAL:HA	1.82	0.45
30:YG:166:ASP:OD1	30:YG:166:ASP:N	2.49	0.45
11:QK:21:ILE:HB	11:QK:84:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:RA:1083:U:H2'	25:RA:1085:A:H5'	1.99	0.45
25:RA:1490:A:O2'	27:RD:99:ASP:OD1	2.35	0.45
25:RA:1588:C:H2'	25:RA:1589:C:H6	1.82	0.45
34:RO:64:ARG:HB2	34:RO:83:ALA:HB3	1.99	0.45
1:XA:636:U:H5'	17:XQ:2:PRO:HG3	1.98	0.45
1:XA:1293:G:H2'	1:XA:1294:G:C8	2.51	0.45
25:YA:629:G:H1'	25:YA:639:U:H1'	1.99	0.45
25:YA:639:U:H3	25:YA:649:G:H1	1.65	0.45
25:YA:664:C:OP1	35:YP:18:ARG:NH1	2.50	0.45
25:YA:1539:G:H2'	25:YA:1540:G:H8	1.82	0.45
28:YE:159:HIS:HE1	28:YE:162:ALA:HB3	1.82	0.45
45:YZ:120:ILE:H	45:YZ:172:ALA:HA	1.82	0.45
1:QA:67:C:H2'	1:QA:68:G:C8	2.51	0.44
1:QA:429:U:OP2	4:QD:36:ARG:NH2	2.51	0.44
1:QA:969:A:N6	9:QI:128:ARG:O	2.51	0.44
2:QB:167:PRO:HG2	2:QB:192:SER:HB3	1.98	0.44
3:QC:59:ARG:HH12	3:QC:97:LYS:HE3	1.82	0.44
20:QT:89:ARG:HH21	20:QT:104:LEU:HD21	1.82	0.44
22:QV:35:C:H2'	22:QV:36:A:H8	1.81	0.44
25:RA:873:G:O3'	36:RQ:63:LYS:NZ	2.47	0.44
25:RA:1665:A:N1	25:RA:1996:C:N4	2.65	0.44
26:RB:42:C:H5''	30:RG:69:ALA:HB2	1.99	0.44
30:RG:49:ASP:OD2	30:RG:51:ARG:NH2	2.49	0.44
39:RT:20:PRO:HD2	39:RT:86:ILE:HG23	1.99	0.44
1:XA:943:U:H1'	9:XI:124:GLN:HE22	1.82	0.44
1:XA:1004:A:P	1:XA:1025:U:H3	2.40	0.44
5:XE:101:ILE:O	5:XE:120:THR:OG1	2.31	0.44
20:XT:49:ALA:HA	20:XT:52:ALA:HB3	1.98	0.44
25:YA:995:C:O2	33:YN:3:THR:OG1	2.32	0.44
25:YA:1297:C:H2'	25:YA:1298:C:H6	1.83	0.44
25:YA:1657:C:OP1	28:YE:136:ARG:N	2.50	0.44
25:YA:2576:G:O2'	25:YA:2579:C:OP2	2.27	0.44
29:YF:178:PRO:HB3	29:YF:198:ALA:HB2	1.98	0.44
39:YT:128:GLU:O	39:YT:132:LYS:N	2.49	0.44
17:QQ:22:LEU:HD11	17:QQ:39:SER:HB2	1.99	0.44
18:QR:58:LEU:HD23	18:QR:62:GLU:HB3	1.99	0.44
25:RA:38:A:N3	29:RF:48:THR:OG1	2.45	0.44
25:RA:746:A:HO2'	25:RA:2611:U:HO2'	1.62	0.44
25:RA:910:A:H62	36:RQ:12:GLN:HA	1.82	0.44
25:RA:1590:U:H2'	25:RA:1591:G:H8	1.82	0.44
25:RA:2502:G:H5''	25:RA:2503:A:H5''	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:RA:2730:C:O2'	28:RE:168:MET:O	2.34	0.44
32:RI:88:ILE:HB	32:RI:121:LYS:HG3	1.99	0.44
35:RP:65:ARG:O	35:RP:68:GLN:NE2	2.51	0.44
38:RS:3:ARG:HE	38:RS:4:LEU:HD13	1.82	0.44
39:RT:39:ARG:HH22	39:RT:41:ARG:HD3	1.82	0.44
39:RT:128:GLU:O	39:RT:132:LYS:N	2.49	0.44
49:R3:39:ASP:OD1	49:R3:44:ARG:NH2	2.46	0.44
1:XA:684:A:O2'	11:XK:39:PRO:O	2.33	0.44
1:XA:718:G:O6	18:XR:74:ARG:NH1	2.50	0.44
1:XA:1326:C:OP1	21:XU:12:LYS:NZ	2.47	0.44
1:XA:1343:G:H1'	9:XI:121:ARG:NH1	2.32	0.44
1:XA:1367:C:OP1	9:XI:115:GLY:N	2.46	0.44
9:XI:42:ARG:NH2	9:XI:75:ASP:OD2	2.47	0.44
25:YA:385:C:O2'	25:YA:388:G:N2	2.50	0.44
25:YA:469:G:O6	53:Y7:39:ARG:NH1	2.51	0.44
25:YA:2502:G:H5''	25:YA:2503:A:H5''	1.99	0.44
44:YY:14:LEU:HB2	44:YY:75:ILE:HD11	1.98	0.44
1:QA:1443:G:C6	39:RT:118:ARG:HB2	2.52	0.44
4:QD:15:GLU:OE2	4:QD:59:ARG:NH1	2.50	0.44
4:QD:57:ARG:NH2	4:QD:205:GLU:OE2	2.49	0.44
7:QG:147:ALA:HB1	22:QW:41:C:O3'	2.17	0.44
25:RA:463:G:N2	25:RA:466:A:OP2	2.40	0.44
25:RA:616:A:C5	29:RF:180:GLY:HA3	2.53	0.44
25:RA:971:C:O2'	25:RA:983:A:N3	2.40	0.44
25:RA:2747:G:OP1	31:RH:138:LYS:NZ	2.42	0.44
29:RF:117:ARG:HH21	29:RF:187:VAL:HA	1.82	0.44
4:XD:15:GLU:OE2	4:XD:59:ARG:NH1	2.50	0.44
25:YA:593:G:H2'	25:YA:594:U:C6	2.52	0.44
25:YA:1341:U:OP1	25:YA:1397:U:N3	2.45	0.44
25:YA:1657:C:H2'	25:YA:1658:C:H6	1.80	0.44
34:YO:19:ILE:HG22	34:YO:43:VAL:HA	1.98	0.44
1:QA:337:C:H2'	1:QA:338:A:H8	1.82	0.44
1:QA:370:C:H2'	1:QA:371:G:C8	2.52	0.44
1:QA:662:G:H2'	1:QA:663:A:C8	2.53	0.44
1:QA:946:A:H2'	1:QA:947:G:C8	2.52	0.44
2:QB:231:GLU:HA	2:QB:232:PRO:HD3	1.87	0.44
7:QG:143:ARG:CD	22:QW:42:C:C3'	2.92	0.44
22:QV:44:A:H2'	22:QV:45:A:C8	2.52	0.44
1:XA:34:C:H2'	1:XA:35:G:C8	2.51	0.44
1:XA:545:C:O2'	1:XA:549:C:OP1	2.30	0.44
11:XK:57:THR:HG22	11:XK:59:TYR:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:XQ:22:LEU:HD11	17:XQ:39:SER:HB2	1.99	0.44
22:XW:20:G:H3'	22:XW:21:U:C5	2.51	0.44
25:YA:657:U:H2'	25:YA:658:C:C6	2.53	0.44
25:YA:1061:U:H4'	25:YA:1070:A:H1'	1.98	0.44
25:YA:1224:G:N2	25:YA:1227:A:OP2	2.48	0.44
25:YA:2103:C:H2'	25:YA:2104:G:C8	2.52	0.44
25:YA:2115:G:O2'	25:YA:2166:G:OP1	2.30	0.44
28:YE:105:THR:HB	28:YE:197:ILE:HG23	1.98	0.44
24:QY:28:G:H2'	24:QY:29:G:H8	1.82	0.44
25:RA:220:G:O2'	25:RA:233:A:N3	2.43	0.44
25:RA:1405:U:H2'	25:RA:1406:U:H6	1.81	0.44
25:RA:1815:A:OP2	27:RD:54:ARG:NH1	2.49	0.44
25:RA:2285:C:OP2	52:R6:6:ARG:NH1	2.50	0.44
25:RA:2329:G:H2'	25:RA:2330:G:H8	1.83	0.44
32:RI:2:LYS:HA	32:RI:20:ASP:HA	1.98	0.44
1:XA:59:A:H5''	1:XA:60:A:H5''	1.98	0.44
1:XA:148:G:H2'	1:XA:149:A:C8	2.50	0.44
1:XA:1291:G:O2'	9:XI:38:GLN:OE1	2.34	0.44
1:XA:1391:U:H2'	1:XA:1392:G:C8	2.53	0.44
10:XJ:45:ARG:HB3	10:XJ:65:LEU:HB3	1.99	0.44
14:YN:29:ARG:HD3	14:YN:40:CYS:HB2	2.00	0.44
24:XY:28:G:H2'	24:XY:29:G:H8	1.82	0.44
25:YA:272:G:H2'	25:YA:273:G:H8	1.81	0.44
25:YA:989:G:OP1	25:YA:1157:G:O2'	2.34	0.44
25:YA:1353:A:H2'	25:YA:1354:A:C8	2.52	0.44
25:YA:2246:G:H2'	25:YA:2247:A:H8	1.83	0.44
26:YB:28:C:OP2	38:YS:33:LYS:HB2	2.18	0.44
1:QA:687:A:N6	1:QA:703:G:C2	2.85	0.44
1:QA:1397:C:O2	23:QX:22:C:C4	2.71	0.44
12:QL:67:THR:OG1	12:QL:95:GLY:O	2.34	0.44
22:QW:23:G:C2	22:QW:24:C:C5	3.06	0.44
25:RA:389:G:H1	35:RP:70:GLN:HB3	1.83	0.44
25:RA:583:G:H5''	40:RU:10:ARG:HH12	1.82	0.44
25:RA:1332:G:H8	25:RA:1332:G:H2'	1.64	0.44
25:RA:2791:C:OP1	25:RA:2893:G:N2	2.50	0.44
28:RE:2:LYS:NZ	28:RE:100:GLU:OE2	2.37	0.44
30:RG:67:LYS:HD2	30:RG:68:PRO:HD2	2.00	0.44
45:RZ:102:LEU:HD11	45:RZ:124:ILE:HG13	1.99	0.44
1:XA:985:C:H2'	1:XA:986:A:H8	1.83	0.44
17:XQ:83:ASP:N	17:XQ:83:ASP:OD1	2.49	0.44
25:YA:220:G:O2'	25:YA:233:A:N3	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:YA:949:C:H2'	25:YA:950:G:H8	1.83	0.44
25:YA:2096:U:H2'	25:YA:2097:C:H6	1.83	0.44
25:YA:2306:C:N4	30:YG:42:GLY:O	2.51	0.44
25:YA:2314:C:H2'	25:YA:2315:G:C8	2.48	0.44
34:YO:104:ARG:NH2	39:YT:43:GLN:OE1	2.33	0.44
1:QA:337:C:H2'	1:QA:338:A:C8	2.53	0.44
9:QI:16:ARG:O	9:QI:63:ILE:HA	2.17	0.44
25:RA:654(A):G:H22	25:RA:654(T):C:H42	1.65	0.44
25:RA:1782:C:O2	25:RA:2608:G:O2'	2.28	0.44
25:RA:1789:A:P	27:RD:222:ARG:HE	2.40	0.44
25:RA:2328:A:H2'	25:RA:2329:G:H8	1.81	0.44
36:RQ:24:GLY:HA2	36:RQ:67:ARG:HH21	1.83	0.44
1:XA:21:G:H2'	1:XA:22:G:C8	2.52	0.44
1:XA:45:U:H2'	1:XA:46:G:C8	2.52	0.44
1:XA:411:A:C4	1:XA:413:G:H1'	2.53	0.44
1:XA:578:C:O2'	1:XA:728:A:N3	2.41	0.44
1:XA:735:C:H2'	1:XA:736:C:H6	1.83	0.44
1:XA:1003:G:N2	1:XA:1004:A:O2'	2.50	0.44
1:XA:1062:U:H2'	1:XA:1063:C:C6	2.53	0.44
1:XA:1308:U:H2'	1:XA:1309:G:C8	2.52	0.44
22:XW:25:U:H2'	22:XW:26:C:C6	2.53	0.44
25:YA:996:A:H5'	40:YU:92:ARG:NH1	2.32	0.44
25:YA:1412:A:H2'	25:YA:1413:G:C8	2.53	0.44
25:YA:1464:C:HO2'	25:YA:1528:A:H8	1.63	0.44
25:YA:1853:A:H2'	25:YA:1854:A:H8	1.83	0.44
39:YT:20:PRO:HD2	39:YT:86:ILE:HG23	1.99	0.44
39:YT:39:ARG:HH22	39:YT:41:ARG:HD3	1.82	0.44
1:QA:45:U:H2'	1:QA:46:G:H8	1.82	0.44
1:QA:1010:G:H2'	1:QA:1011:G:H8	1.83	0.44
1:QA:1022:G:H2'	1:QA:1023:G:C8	2.53	0.44
1:QA:1141:C:H2'	1:QA:1142:G:C8	2.51	0.44
1:QA:1512:U:H2'	1:QA:1513:A:C8	2.53	0.44
25:RA:270(R):G:H2'	25:RA:270(S):G:C8	2.53	0.44
25:RA:631:A:P	54:R8:46:ARG:HH22	2.40	0.44
25:RA:1230:C:H2'	25:RA:1231:G:H8	1.83	0.44
25:RA:2396:G:OP1	47:R1:25:LYS:NZ	2.35	0.44
1:XA:1126:U:H1'	1:XA:1280:A:C5	2.53	0.44
1:XA:1412:C:H2'	1:XA:1413:A:C8	2.52	0.44
1:XA:1484:C:O2'	25:YA:1960:A:O2'	2.25	0.44
5:XE:78:HIS:CE1	8:XH:104:ARG:HH21	2.36	0.44
25:YA:1423:G:H2'	25:YA:1424:G:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:YA:1693:U:O2	27:YD:14:ARG:NH1	2.50	0.44
25:YA:2146:C:H4'	25:YA:2147:G:C8	2.53	0.44
28:YE:92:THR:HG23	28:YE:94:GLU:H	1.82	0.44
43:YX:11:PRO:HD3	48:Y2:37:PHE:CD1	2.53	0.44
45:YZ:166:SER:HB2	45:YZ:168:GLU:N	2.33	0.44
1:QA:1318:A:H4'	19:QS:11:VAL:HG11	2.00	0.44
2:QB:163:PHE:HA	2:QB:185:ILE:O	2.18	0.44
25:RA:270(S):G:H2'	25:RA:270(T):G:H8	1.83	0.44
25:RA:840:C:H2'	25:RA:841:A:H8	1.82	0.44
25:RA:996:A:H5'	40:RU:92:ARG:NH1	2.32	0.44
25:RA:1473:G:H1	25:RA:1520:U:H3	1.66	0.44
25:RA:2102:U:H2'	25:RA:2103:C:H6	1.83	0.44
25:RA:2105:C:H2'	25:RA:2106:G:C8	2.53	0.44
27:RD:25:THR:OG1	27:RD:26:LYS:N	2.50	0.44
39:RT:3:ARG:HB2	39:RT:6:LEU:HB3	2.00	0.44
1:XA:1435:G:H2'	1:XA:1436:U:C6	2.52	0.44
22:XW:52:C:O2	22:XW:65:G:N2	2.51	0.44
25:YA:336:C:O2'	44:YY:35:TYR:OH	2.36	0.44
25:YA:431:U:H2'	25:YA:432:A:H8	1.83	0.44
25:YA:1153:C:H5'	40:YU:76:TYR:HE2	1.83	0.44
25:YA:2291:U:H2'	25:YA:2292:C:C6	2.53	0.44
25:RA:570:G:H2'	25:RA:2030:A:C5	2.53	0.43
25:RA:578:A:OP1	25:RA:1255:U:O2'	2.33	0.43
25:RA:628:G:H5''	54:R8:18:ALA:HB2	1.99	0.43
25:RA:946:G:O6	25:RA:972:G:N2	2.50	0.43
25:RA:2514:U:H3	25:RA:2570:G:H1	1.65	0.43
30:RG:173:LEU:O	30:RG:178:PHE:N	2.46	0.43
45:RZ:102:LEU:HD23	45:RZ:137:ILE:HB	1.99	0.43
45:RZ:166:SER:HB2	45:RZ:168:GLU:N	2.33	0.43
1:XA:606:G:H21	1:XA:632:A:N6	2.08	0.43
1:XA:1255:G:O2'	1:XA:1258:G:N3	2.39	0.43
1:XA:1299:A:H2'	1:XA:1301:U:H1'	2.00	0.43
8:XH:121:ASP:OD1	8:XH:121:ASP:N	2.51	0.43
25:YA:594:U:H3	25:YA:663:G:H1	1.66	0.43
25:YA:598:G:H5'	35:YP:11:GLY:HA3	2.00	0.43
25:YA:746:A:O2'	25:YA:2611:U:O2'	2.32	0.43
25:YA:822:U:H2'	25:YA:823:G:H8	1.83	0.43
25:YA:1019:U:H3	25:YA:1142(A):A:H62	1.65	0.43
25:YA:2515:C:H2'	25:YA:2516:G:H8	1.83	0.43
25:YA:2521:C:O2'	25:YA:2564:A:N3	2.44	0.43
40:YU:49:HIS:O	40:YU:53:ARG:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1308:U:H2'	1:QA:1309:G:H8	1.84	0.43
1:QA:1355:G:H2'	1:QA:1356:G:C8	2.53	0.43
9:QI:113:LYS:HB2	9:QI:119:ALA:HA	1.99	0.43
14:QN:29:ARG:HD3	14:QN:40:CYS:HB2	2.00	0.43
25:RA:139:G:H1'	25:RA:140:A:H2	1.84	0.43
25:RA:1113:U:H2'	25:RA:1114:G:C8	2.53	0.43
25:RA:1176:G:OP1	25:RA:1178:C:N4	2.51	0.43
25:RA:1353:A:H2'	25:RA:1354:A:C8	2.53	0.43
25:RA:1853:A:N3	25:RA:2233:U:O2'	2.43	0.43
25:RA:2146:C:H4'	25:RA:2147:G:C8	2.53	0.43
25:RA:2489:G:N2	25:RA:2491:U:O4	2.47	0.43
33:RN:6:PRO:HG3	33:RN:41:ASP:HB2	2.00	0.43
1:XA:134:A:H61	16:XP:25:ARG:HH12	1.66	0.43
1:XA:376:G:H5''	16:XP:5:ARG:HB2	1.99	0.43
1:XA:390:C:H2'	1:XA:391:G:C8	2.53	0.43
1:XA:407:G:H2'	1:XA:408:A:H8	1.83	0.43
1:XA:902:G:H2'	1:XA:903:G:H8	1.82	0.43
1:XA:1427:U:H2'	1:XA:1428:A:H8	1.84	0.43
18:XR:58:LEU:HD23	18:XR:62:GLU:HB3	1.99	0.43
20:XT:26:ASN:HB2	20:XT:71:THR:HG23	2.00	0.43
25:YA:270(H):C:H2'	25:YA:270(I):G:C8	2.53	0.43
25:YA:573:G:N1	25:YA:2031:A:OP2	2.29	0.43
25:YA:2278:A:OP2	46:Y0:12:ASN:ND2	2.47	0.43
28:YE:16:ARG:NH2	28:YE:171:GLU:OE2	2.42	0.43
28:YE:51:PHE:HD2	28:YE:52:LEU:HG	1.82	0.43
1:QA:407:G:H2'	1:QA:408:A:C8	2.53	0.43
1:QA:543:C:OP2	4:QD:10:ARG:NH1	2.52	0.43
1:QA:782:A:H62	1:QA:800:G:H21	1.66	0.43
20:QT:26:ASN:HB2	20:QT:71:THR:HG23	2.00	0.43
25:RA:65:C:H1'	25:RA:456:C:H42	1.84	0.43
25:RA:1153:C:H5'	40:RU:76:TYR:HE2	1.83	0.43
28:RE:144:ARG:HB3	28:RE:145:LYS:H	1.66	0.43
36:RQ:17:LEU:HD23	36:RQ:39:PRO:HB2	2.00	0.43
1:XA:1119:C:H2'	1:XA:1120:G:H8	1.84	0.43
2:XB:101:MET:HA	2:XB:108:ILE:HG13	1.99	0.43
7:XG:147:ALA:HB1	22:XW:41:C:O3'	2.17	0.43
11:XK:21:ILE:HG13	11:XK:30:VAL:HG12	1.99	0.43
25:YA:493:G:H4'	42:YW:8:ARG:HB2	2.01	0.43
25:YA:601:C:O2'	25:YA:605:C:OP1	2.36	0.43
25:YA:1055:G:H22	25:YA:1104:C:H42	1.66	0.43
25:YA:2131:G:N2	25:YA:2158:A:N7	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:YA:2329:G:H2'	25:YA:2330:G:H8	1.82	0.43
29:YF:149:ASP:OD1	29:YF:149:ASP:N	2.51	0.43
42:YW:86:LEU:HD22	42:YW:96:ILE:HD11	2.00	0.43
44:YY:29:GLU:HB3	44:YY:38:ILE:HD12	1.99	0.43
45:YZ:102:LEU:HD11	45:YZ:124:ILE:HG13	1.99	0.43
1:QA:544:G:OP2	4:QD:66:ARG:NH2	2.52	0.43
1:QA:578:C:O2'	1:QA:728:A:N3	2.44	0.43
4:QD:205:GLU:HA	4:QD:208:SER:HB2	2.01	0.43
8:QH:17:THR:O	8:QH:78:GLN:NE2	2.50	0.43
9:QI:111:ARG:HH22	10:QJ:62:HIS:CE1	2.35	0.43
17:QQ:45:HIS:CD2	17:QQ:47:PRO:HG3	2.53	0.43
20:QT:29:LYS:O	20:QT:33:ILE:HG12	2.19	0.43
22:QW:15:G:N2	22:QW:60:A:N7	2.66	0.43
25:RA:270(H):C:H2'	25:RA:270(I):G:H8	1.84	0.43
25:RA:1543:A:O2'	25:RA:1545:A:OP2	2.31	0.43
25:RA:1844:C:H2'	25:RA:1845:G:H8	1.82	0.43
26:RB:23:G:H2'	26:RB:24:G:C5	2.54	0.43
27:RD:52:ARG:H	27:RD:52:ARG:HG2	1.56	0.43
48:R2:66:GLU:HA	48:R2:69:ARG:HH21	1.82	0.43
1:XA:686:U:H2'	1:XA:687:A:C8	2.54	0.43
1:XA:718:G:H5'	11:XK:117:ASN:ND2	2.33	0.43
1:XA:1129:C:OP1	9:XI:62:TYR:OH	2.33	0.43
1:XA:1342:C:H2'	1:XA:1343:G:C8	2.54	0.43
4:XD:23:GLY:N	4:XD:26:CYS:SG	2.74	0.43
25:YA:142:G:H2'	25:YA:143:C:H6	1.82	0.43
25:YA:1636:C:H2'	25:YA:1637:A:C8	2.52	0.43
25:YA:2805:G:H2'	25:YA:2807:G:C8	2.54	0.43
32:YI:88:ILE:HB	32:YI:121:LYS:HG3	1.99	0.43
34:YO:64:ARG:HB2	34:YO:83:ALA:HB3	1.99	0.43
25:RA:299:A:N3	25:RA:319:C:O2'	2.43	0.43
25:RA:1664:A:H61	25:RA:1996:C:N4	2.16	0.43
25:RA:1791:A:H4'	27:RD:206:LEU:HB2	2.00	0.43
26:RB:56:G:H5'	30:RG:27:ASN:ND2	2.34	0.43
1:XA:195:A:H4'	20:XT:68:LYS:HE3	2.00	0.43
1:XA:359:U:H2'	1:XA:360:A:C8	2.54	0.43
12:XL:44:THR:HA	12:XL:45:PRO:HD3	1.78	0.43
25:YA:270(I):G:H1	25:YA:270(Q):C:H42	1.64	0.43
25:YA:694:U:OP1	27:YD:59:LYS:NZ	2.39	0.43
25:YA:863:A:H2'	25:YA:864:G:C8	2.53	0.43
32:YI:20:ASP:OD1	32:YI:20:ASP:N	2.51	0.43
8:QH:121:ASP:N	8:QH:121:ASP:OD1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:RA:1061:U:H5''	25:RA:1070:A:H1'	2.00	0.43
25:RA:1423:G:H2'	25:RA:1424:G:H8	1.83	0.43
25:RA:2041:U:H2'	25:RA:2042:A:H8	1.83	0.43
25:RA:2626:C:H2'	25:RA:2627:G:H8	1.84	0.43
30:RG:166:ASP:OD1	30:RG:166:ASP:N	2.49	0.43
39:RT:16:ARG:NH2	39:RT:18:ASP:OD2	2.52	0.43
40:RU:49:HIS:O	40:RU:53:ARG:N	2.50	0.43
1:XA:1151:A:H2'	1:XA:1152:A:C8	2.53	0.43
1:XA:1408:A:O2'	25:YA:1916:A:N1	2.49	0.43
1:XA:1441:G:H21	1:XA:1460:A:H62	1.67	0.43
1:XA:1512:U:H2'	1:XA:1513:A:H8	1.84	0.43
17:XQ:45:HIS:CD2	17:XQ:47:PRO:HG3	2.53	0.43
20:XT:29:LYS:O	20:XT:33:ILE:HG12	2.19	0.43
25:YA:363(B):G:H2'	25:YA:363(C):G:C8	2.54	0.43
25:YA:2853:C:H2'	25:YA:2854:G:C8	2.53	0.43
27:YD:25:THR:OG1	27:YD:26:LYS:N	2.50	0.43
29:YF:70:THR:HG23	29:YF:72:ARG:H	1.83	0.43
30:YG:67:LYS:HD2	30:YG:68:PRO:HD2	2.00	0.43
33:YN:6:PRO:HG3	33:YN:41:ASP:HB2	2.00	0.43
53:Y7:5:TRP:NE1	53:Y7:7:PRO:HG3	2.34	0.43
1:QA:1427:U:H2'	1:QA:1428:A:H8	1.84	0.43
4:QD:23:GLY:N	4:QD:26:CYS:SG	2.74	0.43
9:QI:128:ARG:NH1	22:QV:36:A:OP2	2.52	0.43
25:RA:263:C:H2'	25:RA:264:C:O4'	2.18	0.43
25:RA:389:G:N1	35:RP:70:GLN:HB3	2.33	0.43
25:RA:964:C:O2'	25:RA:2273:A:N3	2.42	0.43
25:RA:1952:A:N3	25:RA:2560:C:O2'	2.42	0.43
25:RA:2074:U:H2'	25:RA:2075:U:C6	2.54	0.43
29:RF:40:GLN:HE22	29:RF:182:ASN:HB2	1.82	0.43
45:RZ:114:GLY:HA3	45:RZ:177:PRO:HG3	2.00	0.43
48:R2:14:ARG:NH1	48:R2:66:GLU:OE1	2.52	0.43
1:XA:17:U:H2'	1:XA:18:C:C6	2.54	0.43
1:XA:164:U:H2'	1:XA:165:C:C6	2.54	0.43
1:XA:552:U:H2'	1:XA:553:A:H8	1.82	0.43
1:XA:627:G:H2'	1:XA:628:G:H8	1.82	0.43
1:XA:973:G:H3'	1:XA:974:A:H5''	1.99	0.43
1:XA:1268:A:H2'	1:XA:1269:A:C8	2.54	0.43
1:XA:1355:G:H2'	1:XA:1356:G:C8	2.53	0.43
1:XA:1469:G:H2'	1:XA:1470:G:H8	1.83	0.43
3:XC:17:ASP:O	3:XC:54:ARG:NH2	2.52	0.43
12:XL:70:ILE:HG12	12:XL:100:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:XQ:43:LEU:HD23	17:XQ:43:LEU:HA	1.86	0.43
25:YA:441:U:O2	29:YF:46:ARG:NH2	2.50	0.43
25:YA:764:A:H5'	27:YD:210:GLY:HA3	2.00	0.43
25:YA:1113:U:H2'	25:YA:1114:G:C8	2.53	0.43
25:YA:1266:G:O6	42:YW:13:SER:OG	2.26	0.43
25:YA:1652:A:OP1	37:YR:8:ARG:NH1	2.50	0.43
27:YD:85:ASP:OD2	27:YD:88:ARG:NH1	2.42	0.43
29:YF:161:GLU:OE1	29:YF:164:ARG:NH2	2.52	0.43
1:QA:501:C:H1'	1:QA:549:C:H1'	2.01	0.43
1:QA:806:C:H2'	1:QA:807:A:C8	2.51	0.43
1:QA:1002:G:H2'	1:QA:1003:G:H8	1.82	0.43
16:QP:67:THR:O	16:QP:71:ARG:N	2.50	0.43
25:RA:460:A:H62	25:RA:469:G:H21	1.66	0.43
25:RA:1972:A:H2'	25:RA:1973:G:H8	1.83	0.43
36:RQ:80:GLU:HB2	46:R0:7:LEU:HG	2.00	0.43
45:RZ:109:ALA:HB3	45:RZ:143:GLY:HA2	2.01	0.43
46:R0:70:GLN:OE1	46:R0:80:HIS:NE2	2.51	0.43
1:XA:376:G:H2'	1:XA:377:G:H8	1.83	0.43
1:XA:377:G:H2'	1:XA:378:G:C8	2.54	0.43
1:XA:1512:U:H2'	1:XA:1513:A:C8	2.54	0.43
13:XM:91:ARG:HB2	13:XM:98:VAL:HG22	2.00	0.43
25:YA:358:U:H2'	25:YA:359:A:H8	1.83	0.43
25:YA:1666:G:O2'	34:YO:6:THR:OG1	2.31	0.43
25:YA:1748:G:H2'	25:YA:1749:A:H8	1.84	0.43
25:YA:2351:G:O6	54:Y8:42:ARG:NH2	2.40	0.43
26:YB:23:G:H2'	26:YB:24:G:C5	2.54	0.43
31:YH:86:GLU:HB2	31:YH:165:ALA:H	1.84	0.43
40:YU:39:LEU:HD23	40:YU:39:LEU:HA	1.89	0.43
45:YZ:148:ASP:N	45:YZ:148:ASP:OD1	2.52	0.43
46:Y0:23:VAL:HG13	46:Y0:38:VAL:HG22	2.01	0.43
1:QA:370:C:H2'	1:QA:371:G:H8	1.83	0.43
1:QA:1112:C:H1'	3:QC:179:ARG:HH11	1.84	0.43
1:QA:1316:G:H4'	14:QN:18:VAL:HG11	2.01	0.43
1:QA:1427:U:H2'	1:QA:1428:A:C8	2.53	0.43
13:QM:57:ARG:O	13:QM:61:GLU:HG2	2.18	0.43
25:RA:86:C:H4'	25:RA:104:U:H1'	2.01	0.43
25:RA:532:A:N1	25:RA:2035:G:N2	2.66	0.43
25:RA:2517:C:N3	25:RA:2542:A:N6	2.66	0.43
29:RF:70:THR:HG23	29:RF:72:ARG:H	1.83	0.43
1:XA:337:C:H2'	1:XA:338:A:H8	1.84	0.43
1:XA:707:C:H4'	11:XK:20:TYR:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:1404:C:H2'	1:XA:1405:G:C8	2.54	0.43
4:XD:72:GLU:OE1	4:XD:207:TYR:OH	2.37	0.43
9:XI:46:ALA:HA	9:XI:78:LYS:HB2	2.00	0.43
18:XR:47:THR:O	18:XR:83:GLU:N	2.50	0.43
22:XV:20:G:H3'	22:XV:21:U:C2	2.54	0.43
25:YA:142:G:H2'	25:YA:143:C:C6	2.53	0.43
25:YA:226:G:H2'	25:YA:227:A:C8	2.54	0.43
25:YA:579:G:O2'	25:YA:2019:A:OP1	2.36	0.43
36:YQ:17:LEU:HD23	36:YQ:39:PRO:HB2	2.00	0.43
39:YT:3:ARG:HB2	39:YT:6:LEU:HB3	2.00	0.43
39:YT:62:THR:HG22	39:YT:75:ILE:HG12	2.00	0.43
1:QA:17:U:H2'	1:QA:18:C:C6	2.54	0.43
1:QA:51:A:N7	1:QA:114:U:O2'	2.52	0.43
1:QA:378:G:O6	1:QA:386:C:N4	2.52	0.43
1:QA:427:U:OP2	1:QA:428:G:O2'	2.37	0.43
1:QA:444:C:H2'	1:QA:445:G:C8	2.54	0.43
1:QA:1100:C:HO2'	1:QA:1102:A:P	2.42	0.43
2:QB:67:THR:HG21	2:QB:155:LEU:HD11	2.01	0.43
25:RA:265:A:N6	25:RA:427:U:O2'	2.52	0.43
25:RA:1204:A:H1'	25:RA:1206:G:C8	2.53	0.43
25:RA:1231:G:H2'	25:RA:1232:G:H8	1.84	0.43
35:RP:9:ASN:OD1	35:RP:9:ASN:N	2.51	0.43
1:XA:376:G:H1	1:XA:387:U:H3	1.67	0.43
1:XA:579:G:O2'	15:XO:54:ARG:NE	2.43	0.43
22:XW:10:G:C6	22:XW:27:G:C5	3.07	0.43
22:XW:72:C:H1'	25:YA:1851:U:O2'	2.18	0.43
25:YA:1550:C:H2'	25:YA:1551:C:H6	1.84	0.43
36:YQ:21:THR:HB	36:YQ:22:LYS:H	1.54	0.43
39:YT:16:ARG:NH2	39:YT:18:ASP:OD2	2.52	0.43
1:QA:1119:C:OP2	9:QI:9:ARG:NH2	2.52	0.42
20:QT:30:LYS:HG3	20:QT:34:LYS:HE3	2.00	0.42
25:RA:582:G:OP1	40:RU:14:HIS:ND1	2.49	0.42
25:RA:2839:G:H5'	37:RR:46:GLY:HA2	2.00	0.42
1:XA:309:G:H2'	1:XA:310:G:H8	1.84	0.42
1:XA:977:A:O2'	1:XA:979:C:OP2	2.34	0.42
6:XF:15:ASP:N	6:XF:15:ASP:OD1	2.52	0.42
12:XL:53:ARG:HB3	12:XL:69:TYR:HE1	1.83	0.42
20:XT:30:LYS:HG3	20:XT:34:LYS:HE3	2.00	0.42
25:YA:78:A:H2'	25:YA:79:G:H8	1.83	0.42
25:YA:271:G:H2'	25:YA:272:G:H8	1.84	0.42
25:YA:2246:G:H2'	25:YA:2247:A:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:YA:2446:G:N2	25:YA:2449:U:O2	2.45	0.42
36:YQ:24:GLY:HA2	36:YQ:67:ARG:HH21	1.83	0.42
1:QA:186(B):C:H2'	1:QA:186(C):G:H8	1.84	0.42
1:QA:475:G:H2'	1:QA:476:G:C8	2.54	0.42
1:QA:627:G:H2'	1:QA:628:G:H8	1.84	0.42
1:QA:988:G:H2'	1:QA:989:C:O4'	2.19	0.42
3:QC:17:ASP:O	3:QC:54:ARG:NH2	2.52	0.42
15:QO:24:SER:OG	15:QO:25:THR:N	2.52	0.42
22:QW:41:C:H2'	22:QW:42:C:C6	2.54	0.42
25:RA:270(I):G:H2'	25:RA:270(J):G:C8	2.53	0.42
25:RA:1191:G:OP1	35:RP:18:ARG:NH2	2.49	0.42
25:RA:1600:C:OP1	43:RX:58:HIS:NE2	2.44	0.42
25:RA:2183:C:H2'	25:RA:2184:G:C8	2.54	0.42
26:RB:49:C:OP2	38:RS:30:ARG:NH1	2.51	0.42
28:RE:159:HIS:HE1	28:RE:162:ALA:HB3	1.82	0.42
36:RQ:32:TYR:CE1	36:RQ:133:ARG:HG3	2.54	0.42
4:XD:173:TRP:CD2	4:XD:189:PRO:HB3	2.54	0.42
15:XO:79:ARG:HA	15:XO:82:ILE:HG12	2.00	0.42
25:YA:823:G:H2'	25:YA:824:A:H8	1.84	0.42
25:YA:1270:C:O2'	25:YA:1648:C:OP2	2.26	0.42
25:YA:2074:U:H2'	25:YA:2075:U:C6	2.54	0.42
25:YA:2590:A:H2'	25:YA:2591:C:H6	1.84	0.42
36:YQ:32:TYR:CE1	36:YQ:133:ARG:HG3	2.54	0.42
1:QA:927:G:H1	1:QA:1390:U:H3	1.67	0.42
1:QA:1352:C:H2'	1:QA:1353:G:C8	2.54	0.42
2:QB:192:SER:OG	2:QB:193:ASP:N	2.52	0.42
22:QV:59:A:O2'	22:QV:61:U:OP2	2.23	0.42
25:RA:530:G:O2'	25:RA:532:A:N7	2.52	0.42
25:RA:2443:C:H2'	25:RA:2444:G:H8	1.84	0.42
25:RA:2576:G:N2	25:RA:2576:G:OP2	2.52	0.42
45:RZ:17:ALA:O	45:RZ:21:ALA:N	2.45	0.42
1:XA:1218:C:H2'	1:XA:1219:U:C6	2.53	0.42
25:YA:17:G:H4'	40:YU:25:TRP:HE1	1.82	0.42
25:YA:238:C:O2'	25:YA:608:A:N3	2.43	0.42
25:YA:411:G:OP2	25:YA:2406:U:O2'	2.29	0.42
25:YA:672:C:OP1	25:YA:801:G:N2	2.49	0.42
25:YA:1022:G:N2	25:YA:1023:U:O4	2.48	0.42
25:YA:1789:A:P	27:YD:222:ARG:HE	2.42	0.42
25:YA:2469:A:O2'	36:YQ:56:ARG:HG2	2.19	0.42
25:YA:2618:G:H21	28:YE:150:VAL:HG21	1.84	0.42
25:YA:2751:G:C2	31:YH:3:ARG:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:YF:28:ILE:H	29:YF:28:ILE:HG13	1.70	0.42
29:YF:77:ASP:OD1	29:YF:77:ASP:N	2.42	0.42
36:YQ:74:TYR:HD2	36:YQ:91:GLU:HB3	1.84	0.42
40:YU:90:VAL:HG12	40:YU:91:ASP:H	1.84	0.42
45:YZ:70:LEU:HG	45:YZ:91:LEU:HD21	2.01	0.42
1:QA:359:U:H2'	1:QA:360:A:C8	2.54	0.42
1:QA:738:C:OP1	6:QF:4:TYR:OH	2.31	0.42
1:QA:1391:U:H2'	1:QA:1392:G:C8	2.54	0.42
1:QA:1525:G:H2'	1:QA:1526:G:H8	1.84	0.42
4:QD:72:GLU:OE1	4:QD:207:TYR:OH	2.37	0.42
4:QD:173:TRP:CD2	4:QD:189:PRO:HB3	2.54	0.42
12:QL:58:VAL:O	12:QL:65:GLU:HA	2.19	0.42
25:RA:172:C:H2'	25:RA:173:G:H8	1.84	0.42
25:RA:639:U:H2'	25:RA:640:C:C6	2.55	0.42
25:RA:1021:A:H62	25:RA:1141:U:H3	1.67	0.42
25:RA:2836:U:H2'	25:RA:2837:G:C8	2.55	0.42
27:RD:259:THR:OG1	27:RD:259:THR:O	2.37	0.42
29:RF:161:GLU:OE1	29:RF:164:ARG:NH2	2.52	0.42
40:RU:90:VAL:HG12	40:RU:91:ASP:H	1.84	0.42
1:XA:131:C:H2'	1:XA:132:C:H6	1.84	0.42
1:XA:265:G:H4'	17:XQ:66:SER:HA	2.01	0.42
1:XA:382:A:H2'	1:XA:383:A:H8	1.83	0.42
1:XA:448:A:OP2	1:XA:485:G:N2	2.45	0.42
25:YA:685:A:OP1	25:YA:686:G:N2	2.51	0.42
25:YA:807:U:OP2	35:YP:41:ARG:NH1	2.52	0.42
25:YA:2011:U:OP2	42:YW:16:LYS:NZ	2.37	0.42
25:YA:2795:G:H21	25:YA:2801:A:N6	2.17	0.42
35:YP:18:ARG:HE	35:YP:27:HIS:HE1	1.68	0.42
1:QA:114:U:H2'	1:QA:115:G:C8	2.54	0.42
1:QA:559:A:H4'	1:QA:560:U:H3'	2.00	0.42
10:QJ:5:ARG:HH21	10:QJ:99:LYS:HD2	1.84	0.42
11:QK:21:ILE:HG13	11:QK:30:VAL:HG12	2.00	0.42
25:RA:210:C:H2'	25:RA:211:A:C8	2.54	0.42
25:RA:407:G:H2'	25:RA:408:G:C8	2.54	0.42
25:RA:828:U:H4'	25:RA:831:G:C6	2.55	0.42
25:RA:949:C:H2'	25:RA:950:G:C8	2.54	0.42
25:RA:1939:U:OP1	25:RA:2604:U:O2'	2.36	0.42
25:RA:2250:G:C4	36:RQ:82:ARG:HG3	2.55	0.42
36:RQ:74:TYR:HD2	36:RQ:91:GLU:HB3	1.85	0.42
41:RV:43:GLU:HG3	41:RV:44:LYS:H	1.84	0.42
47:R1:65:SER:HG	47:R1:66:HIS:HD1	1.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:R6:37:ARG:HA	52:R6:48:VAL:HA	2.01	0.42
1:XA:56:U:H2'	1:XA:57:G:C8	2.54	0.42
1:XA:129(A):G:H4'	1:XA:130:A:H5''	2.01	0.42
1:XA:599:C:O2'	8:XH:129:VAL:O	2.29	0.42
25:YA:151:C:H2'	25:YA:152:G:H8	1.84	0.42
25:YA:581:C:OP1	40:YU:31:SER:OG	2.31	0.42
25:YA:820:A:N3	25:YA:943:U:O2'	2.46	0.42
25:YA:1311:G:H21	25:YA:1603:A:H62	1.67	0.42
25:YA:2753:A:O2'	55:Y9:15:LYS:NZ	2.52	0.42
28:YE:2:LYS:NZ	28:YE:100:GLU:OE2	2.37	0.42
1:QA:636:U:H5'	17:QQ:2:PRO:HG3	2.01	0.42
1:QA:737:A:H2'	1:QA:738:C:C6	2.55	0.42
19:QS:10:PHE:CD1	19:QS:38:SER:HB2	2.55	0.42
25:RA:1416:G:H2'	25:RA:1417:C:C6	2.55	0.42
25:RA:1812:A:H4'	27:RD:46:GLN:HE22	1.85	0.42
25:RA:2250:G:C5	36:RQ:82:ARG:HG3	2.55	0.42
25:RA:2590:A:H2'	25:RA:2591:C:H6	1.85	0.42
32:RI:27:ARG:HB2	47:R1:71:TYR:HE2	1.84	0.42
39:RT:62:THR:HG22	39:RT:75:ILE:HG12	2.00	0.42
1:XA:884:U:H4'	1:XA:885:G:H5''	2.00	0.42
1:XA:1028(A):C:N3	1:XA:1028(B):C:N4	2.68	0.42
1:XA:1322:C:H5'	13:XM:100:GLY:HA3	2.02	0.42
25:YA:15:G:O6	25:YA:525:U:O4	2.38	0.42
26:YB:89:G:H2'	26:YB:89(A):A:C8	2.55	0.42
34:YO:76:ALA:HB3	39:YT:75:ILE:HD12	2.01	0.42
38:YS:3:ARG:HE	38:YS:4:LEU:HD13	1.82	0.42
48:Y2:14:ARG:NH1	48:Y2:66:GLU:OE1	2.52	0.42
1:QA:516:U:O2'	1:QA:519:C:N3	2.53	0.42
1:QA:1224:G:O2'	1:QA:1322:C:OP2	2.38	0.42
3:QC:23:TYR:CD2	10:QJ:95:GLU:HB2	2.55	0.42
4:QD:173:TRP:CD1	4:QD:174:LEU:HG	2.55	0.42
25:RA:576:U:H2'	25:RA:577:G:C8	2.54	0.42
25:RA:729:G:C5	27:RD:208:LYS:HB2	2.54	0.42
25:RA:1011:G:OP1	40:RU:66:ASN:ND2	2.53	0.42
25:RA:1795:C:O2	27:RD:255:LYS:NZ	2.41	0.42
25:RA:1969:A:O2'	25:RA:1972:A:N3	2.37	0.42
25:RA:2747:G:N2	25:RA:2757:A:H62	2.14	0.42
26:RB:44:G:H1'	26:RB:47:C:H42	1.84	0.42
45:RZ:145:GLU:HG3	45:RZ:146:ILE:HG12	2.02	0.42
1:XA:104:G:H2'	1:XA:105:G:H8	1.85	0.42
1:XA:130:A:O2'	1:XA:131:C:O5'	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:255:G:OP1	17:XQ:69:LYS:NZ	2.52	0.42
25:YA:244:A:O2'	35:YP:74:GLU:N	2.45	0.42
25:YA:1824:G:N3	27:YD:254:THR:OG1	2.53	0.42
45:YZ:114:GLY:HA3	45:YZ:177:PRO:HG3	2.00	0.42
1:QA:301:G:H2'	1:QA:302:G:H8	1.83	0.42
1:QA:999:U:H2'	1:QA:1000:A:C8	2.55	0.42
1:QA:1118:C:H1'	1:QA:1179:A:C4	2.54	0.42
1:QA:1356:G:H2'	1:QA:1357:A:H8	1.85	0.42
11:QK:38:ASN:HA	11:QK:39:PRO:HD3	1.93	0.42
19:QS:10:PHE:CE2	19:QS:16:LEU:HB2	2.54	0.42
25:RA:580:C:OP2	40:RU:33:ARG:NH2	2.53	0.42
25:RA:999:U:H2'	25:RA:1000:A:H8	1.85	0.42
25:RA:1326:U:HO2'	25:RA:2010:G:HO2'	1.68	0.42
25:RA:1454:U:O2'	25:RA:1455:G:N7	2.48	0.42
25:RA:1782:C:H1'	25:RA:2609:U:H5''	2.02	0.42
25:RA:2105:C:H2'	25:RA:2106:G:H8	1.84	0.42
25:RA:2387:U:O2'	46:R0:41:ARG:NH2	2.52	0.42
25:RA:2537:U:H2'	25:RA:2538:C:C6	2.54	0.42
25:RA:2809:A:H2'	25:RA:2810:A:C8	2.54	0.42
34:RO:80:ASP:OD2	39:RT:64:ARG:NH2	2.52	0.42
39:RT:62:THR:HG22	39:RT:75:ILE:HG23	2.02	0.42
46:R0:46:LYS:HD2	46:R0:78:TYR:HE1	1.85	0.42
1:XA:337:C:H2'	1:XA:338:A:C8	2.55	0.42
1:XA:403:C:H2'	1:XA:404:U:H6	1.84	0.42
1:XA:486:U:H2'	1:XA:487:A:C8	2.52	0.42
1:XA:1053:G:N7	1:XA:1199:U:H2'	2.35	0.42
2:XB:33:TYR:HB2	2:XB:43:ASP:HB2	2.02	0.42
2:XB:95:GLN:HG3	2:XB:147:LYS:HG2	2.02	0.42
22:XW:19:G:H1'	22:XW:59:A:C2	2.55	0.42
22:XW:52:C:H2'	22:XW:53:G:H8	1.85	0.42
25:YA:363(B):G:H2'	25:YA:363(C):G:H8	1.85	0.42
25:YA:483:A:O2'	44:YY:49:VAL:O	2.28	0.42
25:YA:2712:U:H1'	25:YA:2712(A):A:C8	2.55	0.42
35:YP:6:LEU:HD23	35:YP:6:LEU:HA	1.84	0.42
45:YZ:4:ARG:HA	45:YZ:59:LEU:H	1.85	0.42
45:YZ:109:ALA:HB3	45:YZ:143:GLY:HA2	2.01	0.42
52:Y6:37:ARG:HA	52:Y6:48:VAL:HA	2.01	0.42
1:QA:1213:A:N6	1:QA:1215:G:N3	2.68	0.42
1:QA:1469:G:H2'	1:QA:1470:G:H8	1.85	0.42
12:QL:28:LYS:HB2	12:QL:28:LYS:HE3	1.68	0.42
13:QM:84:ILE:HD12	13:QM:84:ILE:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:QV:15:G:H1	22:QV:49:C:H5	1.68	0.42
25:RA:2630:G:H2'	25:RA:2631:G:C8	2.55	0.42
26:RB:86:G:H2'	26:RB:87:G:C8	2.55	0.42
33:RN:60:ILE:H	33:RN:60:ILE:HG13	1.63	0.42
1:XA:339:C:OP1	34:YO:13:ASN:ND2	2.52	0.42
1:XA:814:A:OP2	1:XA:816:A:N6	2.43	0.42
1:XA:962:C:H2'	1:XA:963:G:H8	1.85	0.42
1:XA:1452:C:H4'	1:XA:1453:G:H5'	2.01	0.42
19:XS:33:THR:OG1	19:XS:34:TRP:N	2.53	0.42
25:YA:640:C:H2'	25:YA:641:C:C6	2.55	0.42
25:YA:1568:G:OP1	27:YD:63:ARG:NH1	2.41	0.42
25:YA:2111:C:H2'	25:YA:2118:U:H4'	2.01	0.42
27:YD:142:VAL:HG23	27:YD:193:VAL:HA	2.02	0.42
53:Y7:10:ARG:HE	53:Y7:14:LYS:HD2	1.84	0.42
1:QA:1512:U:H2'	1:QA:1513:A:H8	1.85	0.42
3:QC:153:VAL:HG22	3:QC:198:VAL:HG22	2.02	0.42
3:QC:189:ALA:HB3	3:QC:196:LEU:HB2	2.02	0.42
7:QG:26:PHE:HD1	7:QG:101:LEU:HD22	1.85	0.42
10:QJ:45:ARG:HB3	10:QJ:65:LEU:HB3	2.01	0.42
25:RA:407:G:H2'	25:RA:408:G:H8	1.85	0.42
25:RA:635:C:O2'	25:RA:639:U:OP1	2.35	0.42
25:RA:659:C:H2'	25:RA:660:G:H8	1.84	0.42
25:RA:2086:U:H2'	25:RA:2087:G:C8	2.55	0.42
25:RA:2109:U:H2'	25:RA:2110:G:C8	2.55	0.42
25:RA:2737:G:H2'	25:RA:2738:A:C8	2.55	0.42
27:RD:142:VAL:HG23	27:RD:193:VAL:HA	2.02	0.42
27:RD:254:THR:OG1	27:RD:254:THR:O	2.37	0.42
31:RH:86:GLU:HB2	31:RH:165:ALA:H	1.84	0.42
48:R2:45:SER:O	48:R2:46:GLN:NE2	2.53	0.42
1:XA:1243:C:H42	1:XA:1294:G:H1	1.68	0.42
4:XD:205:GLU:HA	4:XD:208:SER:HB2	2.01	0.42
22:XV:15:G:H1	22:XV:49:C:H5	1.68	0.42
22:XW:1:C:H42	22:XW:73:A:H61	1.68	0.42
22:XW:72:C:HO2'	25:YA:1851:U:HO2'	0.43	0.42
25:YA:94:G:N3	48:Y2:47:ASN:ND2	2.68	0.42
25:YA:270:A:OP2	25:YA:270(Y):G:N1	2.53	0.42
25:YA:605:C:OP1	29:YF:104:LYS:NZ	2.53	0.42
25:YA:729:G:C5	27:YD:208:LYS:HB2	2.55	0.42
25:YA:1853:A:H2'	25:YA:1854:A:C8	2.54	0.42
25:YA:2030:A:H4'	25:YA:2031:A:C8	2.53	0.42
25:YA:2405:G:O2'	25:YA:2411:A:N6	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:YA:2495:G:H5''	36:YQ:81:VAL:HG12	2.01	0.42
35:YP:7:ARG:HA	35:YP:8:PRO:HD2	1.90	0.42
39:YT:123:GLN:O	39:YT:125:ARG:N	2.53	0.42
45:YZ:14:LYS:HA	45:YZ:15:PRO:HD3	1.86	0.42
51:Y5:41:PRO:O	51:Y5:44:THR:OG1	2.34	0.42
1:QA:1015:A:H2'	1:QA:1016:A:C8	2.55	0.41
1:QA:1366:C:O2'	10:QJ:60:ARG:NH2	2.49	0.41
12:QL:32:PHE:HA	12:QL:85:ILE:O	2.20	0.41
19:QS:18:LYS:HG2	19:QS:31:ILE:HD12	2.02	0.41
22:QW:57:C:C5	25:RA:2169:A:N7	2.88	0.41
25:RA:323:G:HO2'	25:RA:1205:U:H3	1.68	0.41
25:RA:458:G:O2'	25:RA:469:G:O6	2.35	0.41
25:RA:1592:C:H2'	25:RA:1593:G:H8	1.85	0.41
36:RQ:28:ALA:HB3	36:RQ:67:ARG:HH12	1.84	0.41
40:RU:10:ARG:HH11	40:RU:10:ARG:HD2	1.71	0.41
1:XA:60:A:N7	1:XA:108:G:O2'	2.53	0.41
1:XA:382:A:H2'	1:XA:383:A:C8	2.55	0.41
1:XA:429:U:H1'	1:XA:430:A:H5''	2.02	0.41
1:XA:611:A:H61	1:XA:629:G:H1	1.67	0.41
1:XA:762:C:H2'	1:XA:763:G:H8	1.85	0.41
15:XO:24:SER:OG	15:XO:25:THR:N	2.53	0.41
22:XW:23:G:C2	22:XW:24:C:C5	3.08	0.41
25:YA:323:G:HO2'	25:YA:1205:U:H3	1.68	0.41
25:YA:1844:C:H2'	25:YA:1845:G:H8	1.85	0.41
25:YA:2126:A:H61	25:YA:2163:C:HO2'	1.65	0.41
26:YB:86:G:H2'	26:YB:87:G:C8	2.55	0.41
27:YD:245:PRO:HA	27:YD:246:PRO:HD3	1.88	0.41
41:YV:43:GLU:HG3	41:YV:44:LYS:H	1.84	0.41
45:YZ:145:GLU:HG3	45:YZ:146:ILE:HG12	2.02	0.41
1:QA:362:G:OP2	12:QL:34:ARG:NH2	2.51	0.41
11:QK:103:LEU:HD13	11:QK:103:LEU:HA	1.91	0.41
22:QV:20:G:H3'	22:QV:21:U:C2	2.54	0.41
25:RA:774:A:O2'	25:RA:777:A:N3	2.46	0.41
25:RA:1796:U:H2'	25:RA:1797:C:H6	1.86	0.41
27:RD:85:ASP:OD2	27:RD:88:ARG:NH1	2.42	0.41
28:RE:104:VAL:HG11	28:RE:188:VAL:HG23	2.02	0.41
29:RF:149:ASP:OD1	29:RF:149:ASP:N	2.52	0.41
34:RO:17:ARG:HE	34:RO:47:ILE:HD13	1.86	0.41
39:RT:123:GLN:O	39:RT:125:ARG:N	2.52	0.41
45:RZ:4:ARG:HA	45:RZ:59:LEU:H	1.85	0.41
45:RZ:70:LEU:HG	45:RZ:91:LEU:HD21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:657:G:H2'	1:XA:658:G:H8	1.85	0.41
1:XA:940:C:H2'	1:XA:941:G:C8	2.54	0.41
1:XA:1122:U:O4	1:XA:1123:A:N6	2.53	0.41
5:XE:98:THR:HB	5:XE:117:ASP:HB3	2.02	0.41
7:XG:26:PHE:HD1	7:XG:101:LEU:HD22	1.85	0.41
25:YA:814:C:H1'	25:YA:1226:G:H21	1.86	0.41
25:YA:1141:U:H1'	25:YA:1142(A):A:C6	2.55	0.41
25:YA:1486:A:H2'	25:YA:1487:G:H8	1.83	0.41
46:Y0:39:ARG:NH1	46:Y0:58:THR:OG1	2.53	0.41
48:Y2:45:SER:O	48:Y2:46:GLN:NE2	2.53	0.41
1:QA:958:A:H2'	1:QA:959:A:C8	2.56	0.41
2:QB:174:VAL:HG11	2:QB:196:LEU:HD13	2.02	0.41
5:QE:98:THR:HB	5:QE:117:ASP:HB3	2.02	0.41
8:QH:100:ILE:HA	8:QH:101:PRO:HD3	1.90	0.41
18:QR:74:ARG:HD3	18:QR:81:PHE:HA	2.01	0.41
25:RA:2102:U:H2'	25:RA:2103:C:C6	2.54	0.41
25:RA:2635:C:H5''	28:RE:78:LEU:HA	2.02	0.41
26:RB:89:G:H2'	26:RB:89(A):A:C8	2.54	0.41
30:RG:142:PRO:HB2	50:R4:31:ILE:HG21	2.02	0.41
38:RS:6:ALA:HA	38:RS:9:ARG:HB3	2.02	0.41
39:RT:18:ASP:OD1	39:RT:18:ASP:N	2.44	0.41
42:RW:76:VAL:HG22	42:RW:103:ILE:HA	2.03	0.41
1:XA:191:G:C4	20:XT:105:SER:HB3	2.56	0.41
1:XA:227:G:N2	16:XP:62:VAL:O	2.44	0.41
1:XA:1323:G:H2'	1:XA:1324:A:C8	2.55	0.41
1:XA:1351:U:O2	1:XA:1371:G:N2	2.42	0.41
1:XA:1393:U:O2'	1:XA:1501:C:O2'	2.35	0.41
7:XG:126:ASP:O	7:XG:131:LYS:N	2.50	0.41
22:XV:59:A:O2'	22:XV:61:U:OP2	2.23	0.41
25:YA:668:G:H2'	25:YA:670:A:H62	1.84	0.41
25:YA:864:G:H2'	25:YA:865:C:C6	2.54	0.41
25:YA:2193:G:H2'	25:YA:2194:G:H8	1.84	0.41
36:YQ:28:ALA:HB3	36:YQ:67:ARG:HH12	1.84	0.41
52:Y6:23:THR:OG1	52:Y6:24:GLU:N	2.51	0.41
1:QA:255:G:P	17:QQ:69:LYS:HZ3	2.44	0.41
1:QA:373:A:H2'	1:QA:374:A:H8	1.84	0.41
11:QK:62:GLN:HG3	11:QK:97:ALA:HB2	2.03	0.41
25:RA:620:G:H4'	25:RA:621:A:H5''	2.03	0.41
25:RA:659:C:H2'	25:RA:660:G:C8	2.56	0.41
25:RA:848:G:H2'	25:RA:849:A:C8	2.55	0.41
25:RA:2197:U:H1'	25:RA:2198:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:RB:48:A:OP2	38:RS:30:ARG:NH2	2.53	0.41
27:RD:136:ILE:O	27:RD:168:ARG:NH2	2.54	0.41
29:RF:157:VAL:HB	29:RF:194:MET:HB3	2.02	0.41
35:RP:6:LEU:HD23	35:RP:6:LEU:HA	1.84	0.41
37:RR:45:ARG:HA	37:RR:95:THR:HG21	2.02	0.41
1:XA:97:U:H2'	1:XA:99:C:C6	2.56	0.41
1:XA:1432:G:OP1	39:YT:108:ARG:N	2.48	0.41
2:XB:84:GLU:OE2	2:XB:233:SER:OG	2.37	0.41
4:XD:57:ARG:NH2	4:XD:205:GLU:OE2	2.49	0.41
13:XM:15:VAL:HG22	13:XM:45:VAL:HB	2.01	0.41
18:XR:74:ARG:HD3	18:XR:81:PHE:HA	2.01	0.41
19:XS:12:ASP:OD2	19:XS:35:SER:OG	2.33	0.41
25:YA:1165:U:H2'	25:YA:1166:C:C6	2.55	0.41
25:YA:2031:A:N3	25:YA:2455:G:O2'	2.43	0.41
25:YA:2047:U:H2'	25:YA:2048:G:H8	1.85	0.41
25:YA:2195:C:H2'	25:YA:2196:C:H6	1.86	0.41
25:YA:2199:A:OP1	47:Y1:50:ARG:NH2	2.53	0.41
30:YG:107:LEU:HD23	30:YG:111:LEU:HD12	2.02	0.41
40:YU:10:ARG:HH11	40:YU:10:ARG:HD2	1.71	0.41
45:YZ:53:ILE:HG22	45:YZ:71:VAL:HG13	2.02	0.41
1:QA:398:C:H2'	1:QA:399:G:H8	1.85	0.41
1:QA:1080:A:H5'	5:QE:14:ARG:HH21	1.85	0.41
1:QA:1348:U:H4'	9:QI:120:ARG:HD2	2.02	0.41
2:QB:58:ILE:HD11	2:QB:185:ILE:HD13	2.01	0.41
22:QW:52:C:O2	22:QW:65:G:N2	2.54	0.41
25:RA:208:C:H2'	25:RA:209:C:H6	1.85	0.41
25:RA:618:G:OP2	29:RF:106:ARG:NH1	2.47	0.41
25:RA:1525:G:H2'	25:RA:1526:G:C8	2.56	0.41
25:RA:2103:C:H2'	25:RA:2104:G:C8	2.56	0.41
36:RQ:13:GLN:O	36:RQ:72:LYS:NZ	2.46	0.41
36:RQ:62:GLY:HA2	45:RZ:116:VAL:HG21	2.00	0.41
42:RW:86:LEU:HD22	42:RW:96:ILE:HD11	2.00	0.41
1:XA:127:G:O2'	17:XQ:2:PRO:O	2.38	0.41
2:XB:130:ARG:HA	2:XB:131:PRO:HD3	1.87	0.41
2:XB:231:GLU:HG3	2:XB:233:SER:H	1.86	0.41
9:XI:10:ARG:HH21	9:XI:107:ARG:HE	1.68	0.41
22:XW:10:G:N2	22:XW:27:G:H1'	2.35	0.41
25:YA:52:A:OP2	25:YA:117:G:N1	2.48	0.41
25:YA:710:G:H2'	25:YA:711:G:C8	2.56	0.41
25:YA:840:C:H2'	25:YA:841:A:C8	2.55	0.41
25:YA:998:C:OP2	40:YU:58:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:YA:1678:G:N2	25:YA:1989:G:H22	2.18	0.41
25:YA:2198:A:OP1	32:YI:33:ARG:NH2	2.52	0.41
25:YA:2291:U:O2'	25:YA:2374:C:O2	2.38	0.41
25:YA:2740:A:H2'	25:YA:2741:A:C8	2.55	0.41
26:YB:3:C:H2'	26:YB:4:C:H6	1.84	0.41
1:QA:287:U:H2'	1:QA:288:A:C8	2.55	0.41
1:QA:601:C:H2'	1:QA:602:A:C8	2.55	0.41
6:QF:12:PRO:HG3	6:QF:57:GLN:HG3	2.03	0.41
6:QF:15:ASP:OD1	6:QF:15:ASP:N	2.52	0.41
6:QF:60:PHE:HE2	18:QR:78:LEU:HD21	1.85	0.41
18:QR:47:THR:O	18:QR:83:GLU:N	2.50	0.41
25:RA:1403:C:H5''	25:RA:1471:A:H1'	2.02	0.41
25:RA:2692:C:H2'	25:RA:2693:A:H8	1.86	0.41
28:RE:105:THR:HA	28:RE:166:THR:HA	2.02	0.41
45:RZ:123:ASP:OD1	45:RZ:123:ASP:N	2.52	0.41
3:XC:153:VAL:HG22	3:XC:198:VAL:HG22	2.02	0.41
4:XD:155:LEU:HD23	4:XD:155:LEU:HA	1.86	0.41
8:XH:97:VAL:HG21	8:XH:128:GLY:HA2	2.03	0.41
9:XI:8:GLY:HA2	9:XI:79:LEU:HD12	2.03	0.41
11:XK:20:TYR:HE1	11:XK:83:ILE:HD12	1.86	0.41
25:YA:562:U:H6	25:YA:562:U:H2'	1.73	0.41
26:YB:44:G:H1'	26:YB:47:C:H42	1.84	0.41
50:Y4:51:ASP:OD1	50:Y4:51:ASP:N	2.49	0.41
1:QA:362:G:O3'	12:QL:33:ARG:NH1	2.54	0.41
1:QA:688:G:H2'	1:QA:689:C:H6	1.86	0.41
1:QA:920:U:H2'	1:QA:921:U:C6	2.55	0.41
1:QA:1095:U:P	1:QA:1108:G:H1	2.41	0.41
1:QA:1355:G:H2'	1:QA:1356:G:H8	1.84	0.41
25:RA:740:U:H2'	25:RA:741:G:C8	2.56	0.41
25:RA:840:C:H2'	25:RA:841:A:C8	2.56	0.41
25:RA:1297:C:H2'	25:RA:1298:C:H6	1.86	0.41
25:RA:2291:U:H2'	25:RA:2292:C:C6	2.56	0.41
27:RD:92:ILE:HD12	27:RD:104:TYR:CD2	2.56	0.41
30:RG:107:LEU:HD23	30:RG:111:LEU:HD12	2.03	0.41
1:XA:477:G:H2'	1:XA:478:A:C8	2.56	0.41
1:XA:736:C:H2'	1:XA:737:A:C8	2.55	0.41
1:XA:908:A:H2'	1:XA:909:A:H8	1.86	0.41
7:XG:46:ALA:O	7:XG:50:ILE:HG12	2.21	0.41
13:XM:4:ILE:H	13:XM:9:ILE:HG22	1.85	0.41
25:YA:484:C:H2'	25:YA:485:C:H6	1.85	0.41
25:YA:513:A:O2'	25:YA:1217:C:OP1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:YA:679:C:H2'	25:YA:680:G:C8	2.55	0.41
25:YA:1059:G:C6	25:YA:1060:U:H1'	2.56	0.41
26:YB:5:C:O2'	26:YB:27:C:O2	2.39	0.41
28:YE:12:THR:OG1	28:YE:13:ARG:N	2.54	0.41
28:YE:18:ASP:HB3	39:YT:82:LEU:HD11	2.02	0.41
30:YG:37:VAL:HG23	30:YG:99:MET:HE3	2.02	0.41
39:YT:27:THR:HB	39:YT:90:GLN:HB3	2.03	0.41
1:QA:255:G:OP1	17:QQ:69:LYS:NZ	2.52	0.41
1:QA:692:U:OP2	11:QK:26:ASN:ND2	2.43	0.41
1:QA:881:G:P	12:QL:12:ARG:HH22	2.43	0.41
1:QA:978:A:O2'	1:QA:1322:C:N3	2.52	0.41
1:QA:1342:C:H2'	1:QA:1343:G:H8	1.86	0.41
7:QG:126:ASP:O	7:QG:131:LYS:N	2.50	0.41
25:RA:117:G:OP2	25:RA:119:A:O2'	2.28	0.41
25:RA:1149:G:H2'	25:RA:1150:C:C6	2.55	0.41
25:RA:1666:G:O2'	34:RO:6:THR:OG1	2.29	0.41
26:RB:52:A:O2'	26:RB:53:A:N7	2.53	0.41
52:R6:23:THR:OG1	52:R6:24:GLU:N	2.51	0.41
54:R8:61:LEU:HD23	54:R8:61:LEU:HA	1.90	0.41
1:XA:832:C:N4	1:XA:855:G:O6	2.54	0.41
7:XG:15:ASP:H	7:XG:20:ASP:H	1.69	0.41
25:YA:363(A):A:H2'	25:YA:363(B):G:C8	2.55	0.41
25:YA:414:C:H2'	25:YA:415:A:H8	1.84	0.41
25:YA:1296:G:OP1	25:YA:2709:G:O2'	2.28	0.41
25:YA:1882:C:H3'	25:YA:1883:G:H8	1.86	0.41
27:YD:44:ASN:HB3	27:YD:49:ILE:HA	2.03	0.41
39:YT:62:THR:HG22	39:YT:75:ILE:HG23	2.02	0.41
1:QA:411:A:C5	1:QA:413:G:H1'	2.56	0.41
1:QA:430:A:P	4:QD:8:VAL:H	2.43	0.41
1:QA:711:G:H2'	1:QA:712:A:C8	2.56	0.41
1:QA:745:C:H2'	1:QA:746:A:C8	2.56	0.41
1:QA:1016:A:HO2'	1:QA:1217:C:HO2'	1.65	0.41
1:QA:1268:A:H2'	1:QA:1269:A:C8	2.55	0.41
6:QF:41:GLU:HB3	6:QF:62:TRP:HE3	1.86	0.41
7:QG:46:ALA:O	7:QG:50:ILE:HG12	2.21	0.41
8:QH:97:VAL:HG21	8:QH:128:GLY:HA2	2.03	0.41
11:QK:20:TYR:CD1	11:QK:83:ILE:HB	2.56	0.41
13:QM:15:VAL:HG22	13:QM:45:VAL:HB	2.02	0.41
22:QW:14:A:C4	22:QW:23:G:C2	3.09	0.41
25:RA:24:G:O2'	42:RW:78:GLU:O	2.39	0.41
25:RA:180:G:O2'	25:RA:181:A:N7	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:RA:521:G:H2'	25:RA:522:G:C8	2.56	0.41
25:RA:544:C:H3'	25:RA:545:G:H8	1.86	0.41
25:RA:807:U:OP2	35:RP:41:ARG:NH1	2.54	0.41
25:RA:1359:A:N6	25:RA:1372:U:H3	2.15	0.41
25:RA:1399:C:H2'	25:RA:1400:G:H8	1.85	0.41
25:RA:1657:C:H2'	25:RA:1658:C:C6	2.56	0.41
25:RA:1858:G:O2'	25:RA:1884:A:N6	2.54	0.41
25:RA:2246:G:H2'	25:RA:2247:A:C8	2.56	0.41
25:RA:2572:A:OP1	25:RA:2574:G:O2'	2.30	0.41
25:RA:2751:G:N7	31:RH:2:SER:HB3	2.36	0.41
26:RB:5:C:O2'	26:RB:27:C:O2	2.38	0.41
27:RD:24:ILE:HD11	27:RD:91:ARG:HD2	2.03	0.41
31:RH:102:ALA:HA	31:RH:117:PRO:HD3	2.03	0.41
35:RP:122:PRO:HB3	35:RP:141:ALA:HB1	2.02	0.41
40:RU:92:ARG:NH1	40:RU:94:ASN:HD22	2.19	0.41
40:RU:92:ARG:HD2	41:RV:11:GLN:HB2	2.03	0.41
45:RZ:53:ILE:HG22	45:RZ:71:VAL:HG13	2.02	0.41
1:XA:201:C:H42	1:XA:216:G:H1	1.68	0.41
1:XA:359:U:H2'	1:XA:360:A:H8	1.85	0.41
1:XA:537:G:H2'	1:XA:538:G:H8	1.86	0.41
1:XA:707:C:H2'	1:XA:708:C:C6	2.56	0.41
1:XA:736:C:O2'	6:XF:90:VAL:O	2.33	0.41
1:XA:972:C:H4'	10:XJ:57:LYS:HB2	2.02	0.41
1:XA:985:C:H2'	1:XA:986:A:C8	2.56	0.41
1:XA:1124:G:H3'	1:XA:1145:C:H41	1.86	0.41
1:XA:1241:G:H2'	1:XA:1242:C:C6	2.56	0.41
1:XA:1288:A:N1	1:XA:1371:G:H1'	2.36	0.41
1:XA:1443:G:N2	25:YA:2864:G:OP1	2.38	0.41
2:XB:48:MET:HA	2:XB:51:LEU:HD12	2.02	0.41
3:XC:135:LYS:HE2	5:XE:53:LEU:HD11	2.03	0.41
4:XD:173:TRP:CD1	4:XD:174:LEU:HG	2.55	0.41
5:XE:7:GLU:OE1	5:XE:37:ARG:NE	2.46	0.41
6:XF:41:GLU:HB3	6:XF:62:TRP:HE3	1.86	0.41
10:XJ:28:ARG:NH2	10:XJ:34:VAL:O	2.53	0.41
25:YA:247:G:H4'	25:YA:386:G:C5	2.56	0.41
25:YA:1035:U:OP1	31:YH:59:ARG:NH1	2.53	0.41
25:YA:2154:G:H2'	25:YA:2155:G:H8	1.86	0.41
25:YA:2674:G:H2'	25:YA:2675:A:C8	2.56	0.41
25:YA:2836:U:H2'	25:YA:2837:G:C8	2.55	0.41
27:YD:50:THR:OG1	27:YD:51:VAL:N	2.53	0.41
28:YE:104:VAL:HG11	28:YE:188:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:YE:105:THR:HA	28:YE:166:THR:HA	2.02	0.41
35:YP:58:THR:O	35:YP:61:ARG:NH2	2.49	0.41
38:YS:6:ALA:HA	38:YS:9:ARG:HB3	2.02	0.41
16:QP:4:ILE:HB	16:QP:66:PRO:HB3	2.03	0.41
25:RA:2707:G:H2'	25:RA:2708:G:C8	2.54	0.41
26:RB:3:C:H2'	26:RB:4:C:H6	1.84	0.41
27:RD:50:THR:OG1	27:RD:51:VAL:N	2.53	0.41
29:RF:34:TRP:CE3	35:RP:8:PRO:HB3	2.56	0.41
31:RH:124:GLU:HB3	31:RH:132:ARG:HG3	2.03	0.41
48:R2:18:PRO:HA	48:R2:21:LEU:HD12	2.02	0.41
1:XA:22:G:H4'	1:XA:885:G:C8	2.56	0.41
1:XA:41:G:H2'	1:XA:42:G:H8	1.86	0.41
1:XA:728:A:H2'	1:XA:729:A:H8	1.86	0.41
1:XA:1513:A:H2'	1:XA:1514:C:C6	2.56	0.41
2:XB:177:ALA:HB1	2:XB:182:ILE:HB	2.03	0.41
2:XB:189:ASP:OD1	2:XB:189:ASP:N	2.54	0.41
5:XE:81:GLU:HG2	5:XE:90:VAL:HG22	2.03	0.41
22:XW:14:A:C4	22:XW:23:G:C2	3.09	0.41
25:YA:363(C):G:H2'	25:YA:363(D):G:C8	2.56	0.41
25:YA:519:U:H2'	25:YA:520:G:H8	1.86	0.41
25:YA:576:U:H2'	25:YA:577:G:C8	2.56	0.41
25:YA:675:A:N3	25:YA:2443:C:O2'	2.45	0.41
25:YA:704:G:H1'	25:YA:727:A:H61	1.85	0.41
25:YA:1130:U:N3	25:YA:2025:C:OP1	2.52	0.41
25:YA:1230:C:H2'	25:YA:1231:G:C8	2.55	0.41
25:YA:1252:G:N2	40:YU:37:GLU:OE2	2.40	0.41
25:YA:1419:A:H62	25:YA:1578:U:H3	1.69	0.41
25:YA:2086:U:H2'	25:YA:2087:G:C8	2.56	0.41
25:YA:2096:U:H2'	25:YA:2097:C:C6	2.56	0.41
25:YA:2666:C:O2	31:YH:152:ARG:NH1	2.54	0.41
34:YO:2:ILE:O	34:YO:33:ALA:N	2.54	0.41
1:QA:398:C:H2'	1:QA:399:G:C8	2.57	0.40
1:QA:1454:G:H2'	1:QA:1455:G:C8	2.55	0.40
2:QB:130:ARG:HA	2:QB:131:PRO:HD3	1.91	0.40
11:QK:18:ARG:HA	11:QK:81:ASP:H	1.86	0.40
25:RA:467:G:O2'	25:RA:796:C:O2'	2.24	0.40
25:RA:582:G:H2'	25:RA:583:G:H8	1.85	0.40
25:RA:823:G:H2'	25:RA:824:A:H8	1.86	0.40
25:RA:1085:A:O2'	25:RA:1086:A:O5'	2.38	0.40
25:RA:2637:U:H5''	28:RE:82:ARG:NH1	2.35	0.40
25:RA:2703:C:H2'	25:RA:2704:C:H6	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:RA:2737:G:H2'	25:RA:2738:A:H8	1.86	0.40
25:RA:2756:U:OP2	55:R9:19:ARG:NE	2.43	0.40
27:RD:44:ASN:HB3	27:RD:49:ILE:HA	2.03	0.40
33:RN:54:VAL:HB	33:RN:122:VAL:HG22	2.03	0.40
46:R0:18:ALA:O	46:R0:20:ARG:NH1	2.50	0.40
48:R2:51:ARG:HH11	48:R2:55:ARG:NH2	2.19	0.40
52:R6:38:LYS:HB2	52:R6:49:HIS:CE1	2.57	0.40
1:XA:114:U:H2'	1:XA:115:G:C8	2.55	0.40
1:XA:192:U:H2'	1:XA:193:C:C6	2.56	0.40
1:XA:1129:C:N4	1:XA:1133:G:O6	2.55	0.40
1:XA:1311:G:H5''	50:Y4:61:ARG:NH2	2.36	0.40
6:XF:6:VAL:HB	6:XF:63:TYR:HB2	2.02	0.40
20:XT:55:ILE:HD13	20:XT:55:ILE:HA	1.93	0.40
25:YA:710:G:H2'	25:YA:711:G:H8	1.84	0.40
25:YA:1400:G:H2'	25:YA:1401:G:C8	2.57	0.40
25:YA:1822:G:O3'	27:YD:54:ARG:NH2	2.54	0.40
25:YA:2572:A:H2'	28:YE:144:ARG:HD3	2.02	0.40
31:YH:55:PRO:HG2	31:YH:61:HIS:CE1	2.56	0.40
40:YU:92:ARG:NH1	40:YU:94:ASN:HD22	2.19	0.40
48:Y2:18:PRO:HA	48:Y2:21:LEU:HD12	2.02	0.40
52:Y6:38:LYS:HB2	52:Y6:49:HIS:CE1	2.57	0.40
1:QA:328:C:H4'	1:QA:329:A:H5'	2.04	0.40
16:QP:21:VAL:HG23	16:QP:34:GLU:H	1.85	0.40
25:RA:310:A:H1'	25:RA:311:A:H2'	2.03	0.40
25:RA:586:A:H5'	29:RF:89:VAL:HG21	2.03	0.40
25:RA:710:G:H2'	25:RA:711:G:H8	1.86	0.40
25:RA:1065:U:H1'	25:RA:1074:G:H22	1.86	0.40
30:RG:37:VAL:HG23	30:RG:99:MET:HE3	2.04	0.40
34:RO:104:ARG:NH2	39:RT:43:GLN:OE1	2.37	0.40
35:RP:106:LEU:HD21	35:RP:112:LEU:HD13	2.03	0.40
45:RZ:57:ILE:O	45:RZ:69:THR:OG1	2.37	0.40
47:R1:60:PHE:HB3	47:R1:62:VAL:HG13	2.02	0.40
52:R6:34:LEU:HD23	52:R6:34:LEU:HA	1.91	0.40
1:XA:131:C:O2'	1:XA:262:A:N3	2.46	0.40
1:XA:652:U:O4	1:XA:752:G:O2'	2.26	0.40
10:XJ:42:THR:HG21	10:XJ:66:ARG:HE	1.86	0.40
19:XS:41:VAL:H	19:XS:44:MET:HE3	1.87	0.40
22:XW:35:C:H41	23:XX:14:A:N6	2.13	0.40
25:YA:691:C:H2'	25:YA:692:C:H6	1.86	0.40
25:YA:1614:A:H62	42:YW:93:ALA:HB2	1.86	0.40
25:YA:2041:U:H2'	25:YA:2042:A:H8	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:YA:2212:A:H1'	25:YA:2215:G:C5	2.56	0.40
42:YW:71:VAL:HA	42:YW:107:LEU:HD23	2.04	0.40
45:YZ:144:LEU:HD21	45:YZ:149:SER:HA	2.04	0.40
1:QA:575:G:N2	1:QA:576:G:N7	2.63	0.40
1:QA:684:A:H1'	11:QK:39:PRO:HD2	2.04	0.40
1:QA:701:C:O2	1:QA:703:G:N1	2.54	0.40
2:QB:6:THR:OG1	2:QB:7:VAL:N	2.55	0.40
10:QJ:38:ILE:HD11	10:QJ:71:LEU:HD23	2.04	0.40
19:QS:33:THR:OG1	19:QS:34:TRP:N	2.53	0.40
25:RA:373:U:H2'	25:RA:374:A:H8	1.86	0.40
25:RA:1771:C:H2'	25:RA:1772:G:C8	2.56	0.40
25:RA:2784:C:H2'	25:RA:2785:C:H6	1.85	0.40
36:RQ:55:VAL:HG13	45:RZ:178:GLU:HB3	2.03	0.40
49:R3:31:LEU:HD23	49:R3:31:LEU:HA	1.91	0.40
53:R7:5:TRP:NE1	53:R7:7:PRO:HG3	2.36	0.40
1:XA:430:A:P	4:XD:8:VAL:H	2.44	0.40
1:XA:440:A:H3'	1:XA:442:C:H6	1.86	0.40
1:XA:626:U:H2'	1:XA:627:G:H8	1.87	0.40
1:XA:1157:A:H62	1:XA:1178:G:N2	2.18	0.40
2:XB:144:ARG:HD3	2:XB:145:LEU:HD22	2.04	0.40
8:XH:100:ILE:HA	8:XH:101:PRO:HD3	1.90	0.40
16:XP:21:VAL:HG23	16:XP:34:GLU:H	1.85	0.40
22:XW:33:C:H5'	22:XW:34:U:OP2	2.21	0.40
25:YA:557:U:H2'	25:YA:558:G:C8	2.57	0.40
25:YA:902:C:H2'	25:YA:903:C:C6	2.57	0.40
26:YB:105:G:H2'	26:YB:106:G:H8	1.86	0.40
27:YD:136:ILE:O	27:YD:168:ARG:NH2	2.54	0.40
30:YG:39:ILE:HG12	30:YG:157:ILE:HG12	2.04	0.40
31:YH:137:ASP:HB3	31:YH:140:LYS:HB3	2.03	0.40
46:Y0:46:LYS:HB2	46:Y0:78:TYR:CD1	2.55	0.40
1:QA:1002:G:H2'	1:QA:1003:G:C8	2.56	0.40
1:QA:1329:A:H5''	13:QM:26:GLY:H	1.86	0.40
1:QA:1435:G:H2'	1:QA:1436:U:H6	1.86	0.40
6:QF:6:VAL:HB	6:QF:63:TYR:HB2	2.02	0.40
25:RA:483:A:O2'	44:RY:49:VAL:O	2.31	0.40
25:RA:892:G:H2'	25:RA:893:C:H6	1.87	0.40
25:RA:2123:G:H2'	25:RA:2124:G:C8	2.52	0.40
25:RA:2341:G:H2'	25:RA:2342:C:C6	2.56	0.40
25:RA:2693:A:H2'	25:RA:2694:G:H8	1.86	0.40
26:RB:105:G:H2'	26:RB:106:G:H8	1.86	0.40
34:RO:76:ALA:HB3	39:RT:75:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:R3:18:ASP:N	49:R3:18:ASP:OD1	2.55	0.40
1:XA:782:A:H62	1:XA:800:G:H21	1.69	0.40
1:XA:1061:G:OP1	10:XJ:59:SER:OG	2.39	0.40
1:XA:1342:C:H2'	1:XA:1343:G:H8	1.86	0.40
13:XM:3:ARG:NH2	50:Y4:34:GLU:OE2	2.54	0.40
25:YA:270(U):C:H2'	25:YA:270(V):G:C8	2.53	0.40
25:YA:593:G:H4'	54:Y8:61:LEU:HD13	2.03	0.40
25:YA:852:G:H2'	25:YA:853:G:C8	2.56	0.40
25:YA:2086:U:OP2	27:YD:263:ARG:NE	2.45	0.40
25:YA:2185:C:H2'	25:YA:2186:G:C8	2.55	0.40
25:YA:2312:U:O2'	30:YG:71:THR:OG1	2.29	0.40
25:YA:2450:A:H62	25:YA:2501:C:N4	2.19	0.40
26:YB:7:G:H4'	38:YS:29:PHE:CG	2.56	0.40
27:YD:92:ILE:HD12	27:YD:104:TYR:CD2	2.56	0.40
31:YH:124:GLU:HB3	31:YH:132:ARG:HG3	2.03	0.40
36:YQ:4:PRO:HG3	36:YQ:69:PHE:HE2	1.87	0.40
48:Y2:51:ARG:HH11	48:Y2:55:ARG:NH2	2.19	0.40
1:QA:407:G:OP1	4:QD:115:ARG:NH1	2.55	0.40
1:QA:1342:C:H2'	1:QA:1343:G:C8	2.56	0.40
4:QD:116:GLN:HE21	4:QD:157:LEU:HD21	1.87	0.40
5:QE:11:ILE:HD13	5:QE:105:VAL:HA	2.03	0.40
25:RA:1590:U:H2'	25:RA:1591:G:C8	2.56	0.40
25:RA:2696:U:H2'	25:RA:2697:G:C8	2.55	0.40
25:RA:2784:C:H2'	25:RA:2785:C:C6	2.55	0.40
25:RA:2812:G:H2'	25:RA:2813:A:H8	1.87	0.40
27:RD:121:PRO:HB3	27:RD:135:PHE:CE2	2.57	0.40
31:RH:55:PRO:HG2	31:RH:61:HIS:CE1	2.56	0.40
35:RP:121:LYS:HD3	35:RP:122:PRO:HD2	2.02	0.40
38:RS:18:ILE:HD13	38:RS:18:ILE:HA	1.93	0.40
40:RU:61:TRP:HB3	40:RU:93:LYS:O	2.22	0.40
1:XA:59:A:H3'	1:XA:331:G:H22	1.87	0.40
1:XA:673:G:O3'	6:XF:87:ARG:NH2	2.55	0.40
1:XA:1147:C:O2'	9:XI:5:TYR:OH	2.23	0.40
1:XA:1256:A:H4'	1:XA:1258:G:C4	2.57	0.40
7:XG:144:MET:HE2	22:XW:31:G:H21	1.84	0.40
7:XG:147:ALA:HB3	22:XW:41:C:O2'	2.21	0.40
9:XI:5:TYR:CE1	9:XI:16:ARG:HB2	2.56	0.40
25:YA:78:A:H2'	25:YA:79:G:C8	2.56	0.40
25:YA:1051:G:H1	25:YA:1108:U:H3	1.70	0.40
25:YA:2258:C:O2'	25:YA:2427:C:OP2	2.38	0.40
25:YA:2575:C:H5'	28:YE:144:ARG:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:YB:44:G:H1'	26:YB:47:C:N4	2.37	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)
25:YA:1411:C:O2'	26:YB:53:A:O2'[1_655]	1.11	1.09
32:RI:87:LYS:NZ	1:XA:359:U:OP1[4_555]	1.48	0.72
41:YV:49:THR:O	51:Y5:59:GLU:OE2[4_445]	1.56	0.64
44:RY:21:LYS:NZ	48:Y2:71:ASN:CB[3_555]	1.64	0.56
44:RY:19:LYS:O	48:Y2:71:ASN:ND2[3_555]	1.71	0.49
41:YV:49:THR:OG1	51:Y5:60:VAL:O[4_445]	1.86	0.34
44:RY:19:LYS:C	48:Y2:71:ASN:ND2[3_555]	1.88	0.32
32:RI:89:TYR:O	1:XA:357:G:O2'[4_555]	1.91	0.29
44:RY:19:LYS:CA	48:Y2:71:ASN:ND2[3_555]	1.97	0.23
42:RW:63:ASP:OD1	44:YY:92:ASN:ND2[3_555]	2.03	0.17
41:YV:51:VAL:O	51:Y5:59:GLU:CD[4_445]	2.03	0.17
41:YV:51:VAL:O	51:Y5:59:GLU:CG[4_445]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	233/256 (91%)	207 (89%)	25 (11%)	1 (0%)	30	62
2	XB	234/256 (91%)	208 (89%)	26 (11%)	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%)	190 (92%)	16 (8%)	0	100	100
4	XD	206/209 (99%)	190 (92%)	16 (8%)	0	100	100
5	QE	149/162 (92%)	144 (97%)	4 (3%)	1 (1%)	19	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	XE	149/162 (92%)	144 (97%)	4 (3%)	1 (1%)	19	51
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%)	149 (97%)	4 (3%)	0	100	100
7	XG	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
8	QH	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
8	XH	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
9	QI	125/128 (98%)	115 (92%)	10 (8%)	0	100	100
9	XI	124/128 (97%)	114 (92%)	10 (8%)	0	100	100
10	QJ	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
10	XJ	94/105 (90%)	83 (88%)	11 (12%)	0	100	100
11	QK	117/129 (91%)	106 (91%)	11 (9%)	0	100	100
11	XK	114/129 (88%)	109 (96%)	5 (4%)	0	100	100
12	QL	123/132 (93%)	106 (86%)	17 (14%)	0	100	100
12	XL	120/132 (91%)	106 (88%)	13 (11%)	1 (1%)	16	49
13	QM	118/126 (94%)	99 (84%)	18 (15%)	1 (1%)	16	49
13	XM	117/126 (93%)	98 (84%)	19 (16%)	0	100	100
14	QN	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	7	36
14	XN	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	7	36
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%)	80 (98%)	2 (2%)	0	100	100
16	XP	82/88 (93%)	80 (98%)	2 (2%)	0	100	100
17	QQ	98/105 (93%)	95 (97%)	3 (3%)	0	100	100
17	XQ	98/105 (93%)	95 (97%)	3 (3%)	0	100	100
18	QR	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
18	XR	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
19	QS	81/93 (87%)	69 (85%)	12 (15%)	0	100	100
19	XS	82/93 (88%)	67 (82%)	15 (18%)	0	100	100
20	QT	97/106 (92%)	86 (89%)	11 (11%)	0	100	100
20	XT	97/106 (92%)	86 (89%)	11 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	QU	23/27 (85%)	20 (87%)	3 (13%)	0	100	100
21	XU	23/27 (85%)	20 (87%)	3 (13%)	0	100	100
27	RD	270/276 (98%)	247 (92%)	22 (8%)	1 (0%)	30	62
27	YD	270/276 (98%)	247 (92%)	22 (8%)	1 (0%)	30	62
28	RE	203/206 (98%)	165 (81%)	36 (18%)	2 (1%)	13	44
28	YE	203/206 (98%)	165 (81%)	36 (18%)	2 (1%)	13	44
29	RF	200/210 (95%)	181 (90%)	19 (10%)	0	100	100
29	YF	200/210 (95%)	181 (90%)	19 (10%)	0	100	100
30	RG	179/182 (98%)	148 (83%)	30 (17%)	1 (1%)	22	54
30	YG	179/182 (98%)	148 (83%)	30 (17%)	1 (1%)	22	54
31	RH	172/180 (96%)	151 (88%)	17 (10%)	4 (2%)	5	32
31	YH	172/180 (96%)	151 (88%)	17 (10%)	4 (2%)	5	32
32	RI	144/148 (97%)	124 (86%)	18 (12%)	2 (1%)	9	39
32	YI	144/148 (97%)	124 (86%)	18 (12%)	2 (1%)	9	39
33	RN	136/140 (97%)	119 (88%)	16 (12%)	1 (1%)	19	51
33	YN	136/140 (97%)	119 (88%)	16 (12%)	1 (1%)	19	51
34	RO	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
34	YO	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
35	RP	148/150 (99%)	117 (79%)	30 (20%)	1 (1%)	19	51
35	YP	145/150 (97%)	113 (78%)	31 (21%)	1 (1%)	19	51
36	RQ	139/141 (99%)	114 (82%)	24 (17%)	1 (1%)	19	51
36	YQ	139/141 (99%)	114 (82%)	24 (17%)	1 (1%)	19	51
37	RR	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	14	46
37	YR	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	14	46
38	RS	109/112 (97%)	93 (85%)	16 (15%)	0	100	100
38	YS	109/112 (97%)	93 (85%)	16 (15%)	0	100	100
39	RT	135/146 (92%)	119 (88%)	14 (10%)	2 (2%)	8	38
39	YT	135/146 (92%)	119 (88%)	14 (10%)	2 (2%)	8	38
40	RU	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	14	46
40	YU	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	14	46
41	RV	99/101 (98%)	89 (90%)	10 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	YV	99/101 (98%)	89 (90%)	10 (10%)	0	100	100
42	RW	111/113 (98%)	102 (92%)	9 (8%)	0	100	100
42	YW	111/113 (98%)	102 (92%)	9 (8%)	0	100	100
43	RX	90/96 (94%)	87 (97%)	3 (3%)	0	100	100
43	YX	90/96 (94%)	87 (97%)	3 (3%)	0	100	100
44	RY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
44	YY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
45	RZ	181/206 (88%)	150 (83%)	29 (16%)	2 (1%)	12	43
45	YZ	181/206 (88%)	149 (82%)	30 (17%)	2 (1%)	12	43
46	R0	79/85 (93%)	74 (94%)	5 (6%)	0	100	100
46	Y0	73/85 (86%)	67 (92%)	6 (8%)	0	100	100
47	R1	95/98 (97%)	83 (87%)	12 (13%)	0	100	100
47	Y1	91/98 (93%)	77 (85%)	14 (15%)	0	100	100
48	R2	67/72 (93%)	64 (96%)	2 (3%)	1 (2%)	8	38
48	Y2	67/72 (93%)	64 (96%)	2 (3%)	1 (2%)	8	38
49	R3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
49	Y3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
50	R4	67/71 (94%)	55 (82%)	11 (16%)	1 (2%)	8	38
50	Y4	67/71 (94%)	55 (82%)	11 (16%)	1 (2%)	8	38
51	R5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
51	Y5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
52	R6	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
52	Y6	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
53	R7	45/49 (92%)	45 (100%)	0	0	100	100
53	Y7	46/49 (94%)	46 (100%)	0	0	100	100
54	R8	62/65 (95%)	47 (76%)	13 (21%)	2 (3%)	3	27
54	Y8	62/65 (95%)	47 (76%)	13 (21%)	2 (3%)	3	27
55	R9	35/37 (95%)	35 (100%)	0	0	100	100
55	Y9	35/37 (95%)	35 (100%)	0	0	100	100
All	All	11452/12128 (94%)	10311 (90%)	1088 (10%)	53 (0%)	25	57

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
39	RT	124	ASP
45	RZ	53	ILE
39	YT	124	ASP
45	YZ	53	ILE
14	QN	17	LYS
32	RI	15	VAL
35	RP	108	LYS
39	RT	123	GLN
54	R8	29	LYS
12	XL	105	TYR
14	XN	17	LYS
32	YI	15	VAL
35	YP	108	LYS
39	YT	123	GLN
54	Y8	29	LYS
30	RG	81	LYS
31	RH	86	GLU
33	RN	22	THR
54	R8	30	ARG
30	YG	81	LYS
31	YH	86	GLU
33	YN	22	THR
54	Y8	30	ARG
31	RH	87	LEU
40	RU	93	LYS
31	YH	87	LEU
37	YR	4	LEU
40	YU	93	LYS
13	QM	14	ARG
27	RD	243	GLY
28	RE	19	ARG
31	RH	12	PRO
36	RQ	78	PRO
37	RR	4	LEU
48	R2	70	GLN
50	R4	47	GLN
27	YD	243	GLY
28	YE	19	ARG
31	YH	12	PRO
36	YQ	78	PRO
48	Y2	70	GLN
50	Y4	47	GLN
2	QB	208	ILE

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Mol	Chain	Res	Type
28	RE	132	HIS
31	RH	152	ARG
28	YE	132	HIS
31	YH	152	ARG
32	RI	16	GLY
32	YI	16	GLY
5	QE	74	GLY
45	RZ	166	SER
5	XE	74	GLY
45	YZ	166	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	203/220 (92%)	202 (100%)	1 (0%)	86	92
2	XB	204/220 (93%)	201 (98%)	3 (2%)	60	75
3	QC	159/188 (85%)	158 (99%)	1 (1%)	84	90
3	XC	159/188 (85%)	158 (99%)	1 (1%)	84	90
4	QD	180/181 (99%)	179 (99%)	1 (1%)	84	90
4	XD	180/181 (99%)	179 (99%)	1 (1%)	84	90
5	QE	116/123 (94%)	115 (99%)	1 (1%)	75	84
5	XE	116/123 (94%)	115 (99%)	1 (1%)	75	84
6	QF	90/90 (100%)	89 (99%)	1 (1%)	70	80
6	XF	90/90 (100%)	89 (99%)	1 (1%)	70	80
7	QG	126/127 (99%)	126 (100%)	0	100	100
7	XG	126/127 (99%)	126 (100%)	0	100	100
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%)	50	69
9	XI	97/99 (98%)	97 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	48 (98%)	1 (2%)	50	69
14	XN	49/50 (98%)	48 (98%)	1 (2%)	50	69
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%)	62	76
16	XP	72/74 (97%)	71 (99%)	1 (1%)	62	76
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%)	71 (99%)	1 (1%)	62	76
19	XS	73/80 (91%)	72 (99%)	1 (1%)	62	76
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
27	RD	214/218 (98%)	212 (99%)	2 (1%)	75	84
27	YD	214/218 (98%)	212 (99%)	2 (1%)	75	84
28	RE	165/166 (99%)	165 (100%)	0	100	100
28	YE	165/166 (99%)	165 (100%)	0	100	100
29	RF	161/166 (97%)	159 (99%)	2 (1%)	67	79
29	YF	161/166 (97%)	159 (99%)	2 (1%)	67	79
30	RG	155/156 (99%)	153 (99%)	2 (1%)	65	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	YG	155/156 (99%)	153 (99%)	2 (1%)	65	77
31	RH	145/148 (98%)	141 (97%)	4 (3%)	38	60
31	YH	145/148 (98%)	141 (97%)	4 (3%)	38	60
32	RI	122/124 (98%)	122 (100%)	0	100	100
32	YI	122/124 (98%)	122 (100%)	0	100	100
33	RN	117/119 (98%)	116 (99%)	1 (1%)	75	84
33	YN	117/119 (98%)	116 (99%)	1 (1%)	75	84
34	RO	100/100 (100%)	98 (98%)	2 (2%)	50	69
34	YO	100/100 (100%)	98 (98%)	2 (2%)	50	69
35	RP	116/116 (100%)	114 (98%)	2 (2%)	56	73
35	YP	114/116 (98%)	113 (99%)	1 (1%)	75	84
36	RQ	111/111 (100%)	111 (100%)	0	100	100
36	YQ	111/111 (100%)	111 (100%)	0	100	100
37	RR	100/101 (99%)	100 (100%)	0	100	100
37	YR	100/101 (99%)	100 (100%)	0	100	100
38	RS	87/88 (99%)	86 (99%)	1 (1%)	70	80
38	YS	87/88 (99%)	86 (99%)	1 (1%)	70	80
39	RT	120/127 (94%)	119 (99%)	1 (1%)	79	85
39	YT	120/127 (94%)	119 (99%)	1 (1%)	79	85
40	RU	93/94 (99%)	93 (100%)	0	100	100
40	YU	93/94 (99%)	93 (100%)	0	100	100
41	RV	82/82 (100%)	82 (100%)	0	100	100
41	YV	82/82 (100%)	82 (100%)	0	100	100
42	RW	92/92 (100%)	90 (98%)	2 (2%)	47	66
42	YW	92/92 (100%)	90 (98%)	2 (2%)	47	66
43	RX	74/78 (95%)	74 (100%)	0	100	100
43	YX	74/78 (95%)	74 (100%)	0	100	100
44	RY	88/91 (97%)	88 (100%)	0	100	100
44	YY	88/91 (97%)	88 (100%)	0	100	100
45	RZ	162/179 (90%)	161 (99%)	1 (1%)	84	90
45	YZ	162/179 (90%)	161 (99%)	1 (1%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	R0	65/67 (97%)	64 (98%)	1 (2%)	60	75
46	Y0	61/67 (91%)	60 (98%)	1 (2%)	58	74
47	R1	82/83 (99%)	82 (100%)	0	100	100
47	Y1	78/83 (94%)	78 (100%)	0	100	100
48	R2	64/67 (96%)	64 (100%)	0	100	100
48	Y2	64/67 (96%)	64 (100%)	0	100	100
49	R3	51/52 (98%)	50 (98%)	1 (2%)	50	69
49	Y3	51/52 (98%)	50 (98%)	1 (2%)	50	69
50	R4	62/63 (98%)	61 (98%)	1 (2%)	58	74
50	Y4	62/63 (98%)	61 (98%)	1 (2%)	58	74
51	R5	51/52 (98%)	51 (100%)	0	100	100
51	Y5	51/52 (98%)	51 (100%)	0	100	100
52	R6	51/52 (98%)	51 (100%)	0	100	100
52	Y6	51/52 (98%)	51 (100%)	0	100	100
53	R7	40/42 (95%)	40 (100%)	0	100	100
53	Y7	41/42 (98%)	41 (100%)	0	100	100
54	R8	54/55 (98%)	54 (100%)	0	100	100
54	Y8	54/55 (98%)	54 (100%)	0	100	100
55	R9	34/34 (100%)	34 (100%)	0	100	100
55	Y9	34/34 (100%)	34 (100%)	0	100	100
All	All	9687/10066 (96%)	9622 (99%)	65 (1%)	81	88

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	QB	30	ARG
3	QC	165	THR
4	QD	119	GLN
5	QE	73	ASN
6	QF	80	ARG
9	QI	10	ARG
9	QI	111	ARG
14	QN	45	ARG
16	QP	67	THR
19	QS	41	VAL

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Mol	Chain	Res	Type
27	RD	33	LEU
27	RD	273	ARG
29	RF	38	ARG
29	RF	44	ARG
30	RG	33	ARG
30	RG	40	ASN
31	RH	23	ARG
31	RH	69	ARG
31	RH	149	ARG
31	RH	152	ARG
33	RN	115	ARG
34	RO	7	TYR
34	RO	97	ARG
35	RP	58	THR
35	RP	125	VAL
38	RS	3	ARG
39	RT	38	ASN
42	RW	15	ARG
42	RW	40	ASN
45	RZ	34	ASN
46	R0	14	ARG
49	R3	30	ARG
50	R4	56	VAL
2	XB	30	ARG
2	XB	64	ARG
2	XB	144	ARG
3	XC	165	THR
4	XD	119	GLN
5	XE	73	ASN
6	XF	80	ARG
14	XN	45	ARG
16	XP	67	THR
19	XS	39	THR
27	YD	33	LEU
27	YD	273	ARG
29	YF	38	ARG
29	YF	44	ARG
30	YG	33	ARG
30	YG	40	ASN
31	YH	23	ARG
31	YH	69	ARG
31	YH	149	ARG

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Mol	Chain	Res	Type
31	YH	152	ARG
33	YN	115	ARG
34	YO	7	TYR
34	YO	97	ARG
35	YP	58	THR
38	YS	3	ARG
39	YT	38	ASN
42	YW	15	ARG
42	YW	40	ASN
45	YZ	34	ASN
46	Y0	43	THR
49	Y3	30	ARG
50	Y4	56	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
2	QB	16	HIS
3	QC	37	GLN
5	QE	73	ASN
6	QF	7	ASN
7	QG	28	ASN
7	QG	68	ASN
9	QI	3	GLN
9	QI	73	GLN
10	QJ	62	HIS
14	QN	49	HIS
28	RE	159	HIS
29	RF	40	GLN
31	RH	147	ASN
34	RO	3	GLN
35	RP	27	HIS
37	RR	71	GLN
39	RT	38	ASN
40	RU	94	ASN
42	RW	61	ASN
42	RW	111	HIS
45	RZ	32	HIS
46	R0	3	HIS
48	R2	46	GLN
48	R2	47	ASN
51	R5	23	HIS

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Mol	Chain	Res	Type
2	XB	40	HIS
5	XE	73	ASN
6	XF	7	ASN
7	XG	28	ASN
7	XG	68	ASN
9	XI	73	GLN
9	XI	124	GLN
14	XN	49	HIS
29	YF	40	GLN
31	YH	147	ASN
35	YP	27	HIS
39	YT	38	ASN
40	YU	94	ASN
42	YW	61	ASN
42	YW	62	HIS
42	YW	111	HIS
43	YX	41	ASN
45	YZ	32	HIS
45	YZ	34	ASN
51	Y5	23	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1508 (99%)	297 (19%)	32 (2%)
1	XA	1498/1508 (99%)	282 (18%)	27 (1%)
22	QV	76/77 (98%)	15 (19%)	2 (2%)
22	QW	76/77 (98%)	33 (43%)	2 (2%)
22	XV	76/77 (98%)	15 (19%)	2 (2%)
22	XW	76/77 (98%)	34 (44%)	2 (2%)
23	QX	7/25 (28%)	0	0
23	XX	10/25 (40%)	2 (20%)	0
24	QY	16/17 (94%)	4 (25%)	0
24	XY	16/17 (94%)	4 (25%)	0
25	RA	2879/2915 (98%)	613 (21%)	41 (1%)
25	YA	2880/2915 (98%)	609 (21%)	41 (1%)
26	RB	119/122 (97%)	24 (20%)	0
26	YB	119/122 (97%)	24 (20%)	0
All	All	9346/9482 (98%)	1956 (20%)	149 (1%)

All (1956) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	32	A
1	QA	39	G
1	QA	41	G
1	QA	47	C
1	QA	48	C
1	QA	50	A
1	QA	51	A
1	QA	54	C
1	QA	64	G
1	QA	65	U
1	QA	66	G
1	QA	76	G
1	QA	81	G
1	QA	90	C
1	QA	91	C
1	QA	95	G
1	QA	101	A
1	QA	108	G
1	QA	116	A
1	QA	120	A
1	QA	121	C
1	QA	122	G
1	QA	129(A)	G
1	QA	131	C
1	QA	144	G
1	QA	146	G
1	QA	159	G
1	QA	162	A
1	QA	163	C
1	QA	169	C
1	QA	173	U
1	QA	174	C
1	QA	182	U
1	QA	190	G
1	QA	191(A)	G
1	QA	195	A
1	QA	197	A
1	QA	208	U
1	QA	209	U
1	QA	210	U
1	QA	216	G
1	QA	244	U

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Mol	Chain	Res	Type
1	QA	247	G
1	QA	251	G
1	QA	262	A
1	QA	263	A
1	QA	267	C
1	QA	269	C
1	QA	279	A
1	QA	281	G
1	QA	289	G
1	QA	301	G
1	QA	306	G
1	QA	321	A
1	QA	328	C
1	QA	329	A
1	QA	332	G
1	QA	343	U
1	QA	344	A
1	QA	345	C
1	QA	346	G
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	390	C
1	QA	397	A
1	QA	398	C
1	QA	406	G
1	QA	410	G
1	QA	411	A
1	QA	412	A
1	QA	413	G
1	QA	421	U
1	QA	422	C
1	QA	423	G
1	QA	424	G
1	QA	429	U
1	QA	435	C

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Mol	Chain	Res	Type
1	QA	442	C
1	QA	465	A
1	QA	466	C
1	QA	482	A
1	QA	485	G
1	QA	486	U
1	QA	496	A
1	QA	497	U
1	QA	505	G
1	QA	509	A
1	QA	510	A
1	QA	511	C
1	QA	518	C
1	QA	521	G
1	QA	527	G
1	QA	532	A
1	QA	533	A
1	QA	534	U
1	QA	539	A
1	QA	545	C
1	QA	547	A
1	QA	559	A
1	QA	565	U
1	QA	566	G
1	QA	568	G
1	QA	572	A
1	QA	573	A
1	QA	576	G
1	QA	577	G
1	QA	596	C
1	QA	618	C
1	QA	630	G
1	QA	631	G
1	QA	633	G
1	QA	652	U
1	QA	653	A
1	QA	665	A
1	QA	688	G
1	QA	702	A
1	QA	703	G
1	QA	704	A
1	QA	717	C

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Mol	Chain	Res	Type
1	QA	723	U
1	QA	731	G
1	QA	748	C
1	QA	749	C
1	QA	754	C
1	QA	755	G
1	QA	760	G
1	QA	777	A
1	QA	781	A
1	QA	792	A
1	QA	793	U
1	QA	794	A
1	QA	813	U
1	QA	817	C
1	QA	818	G
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	885	G
1	QA	902	G
1	QA	914	A
1	QA	922	G
1	QA	926	G
1	QA	927	G
1	QA	934	C
1	QA	935	A
1	QA	936	C
1	QA	960	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

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Mol	Chain	Res	Type
1	QA	977	A
1	QA	981	U
1	QA	982	U
1	QA	983	A
1	QA	990	C
1	QA	991	U
1	QA	992	U
1	QA	993	G
1	QA	994	A
1	QA	995	C
1	QA	1004	A
1	QA	1006	C
1	QA	1008	C
1	QA	1009	G
1	QA	1020	U
1	QA	1021	G
1	QA	1024	G
1	QA	1025	U
1	QA	1028	C
1	QA	1028(A)	C
1	QA	1028(B)	C
1	QA	1029	G
1	QA	1030	C
1	QA	1031	G
1	QA	1032	A
1	QA	1032(A)	G
1	QA	1034	G
1	QA	1040	U
1	QA	1044	A
1	QA	1046	A
1	QA	1050	G
1	QA	1053	G
1	QA	1054	C
1	QA	1055	A
1	QA	1066	C
1	QA	1078	U
1	QA	1081	G
1	QA	1086	U
1	QA	1094	G
1	QA	1095	U
1	QA	1100	C
1	QA	1101	A

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Mol	Chain	Res	Type
1	QA	1108	G
1	QA	1124	G
1	QA	1125	U
1	QA	1126	U
1	QA	1130	A
1	QA	1131	G
1	QA	1136	U
1	QA	1137	C
1	QA	1138	G
1	QA	1139	G
1	QA	1146	A
1	QA	1157	A
1	QA	1158	C
1	QA	1159	U
1	QA	1161	C
1	QA	1171	G
1	QA	1176	A
1	QA	1178	G
1	QA	1181	G
1	QA	1183	A
1	QA	1184	G
1	QA	1187	G
1	QA	1196	U
1	QA	1197	G
1	QA	1201	A
1	QA	1202	G
1	QA	1211	U
1	QA	1212	U
1	QA	1213	A
1	QA	1225	A
1	QA	1226	C
1	QA	1228	C
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

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Mol	Chain	Res	Type
1	QA	1282	C
1	QA	1285	A
1	QA	1286	A
1	QA	1287	A
1	QA	1298	C
1	QA	1299	A
1	QA	1300	G
1	QA	1301	U
1	QA	1303	C
1	QA	1305	G
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	1362(A)	C
1	QA	1363	A
1	QA	1368	G
1	QA	1370	G
1	QA	1397	C
1	QA	1398	A
1	QA	1401	G
1	QA	1419	G
1	QA	1442	G
1	QA	1446	A
1	QA	1447	G
1	QA	1452	C
1	QA	1453	G
1	QA	1492	A
1	QA	1497	G
1	QA	1499	A
1	QA	1503	A
1	QA	1506	U
1	QA	1517	G
1	QA	1519	A
1	QA	1520	G

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Mol	Chain	Res	Type
1	QA	1529	G
1	QA	1530	G
22	QV	7	G
22	QV	8	U
22	QV	13	C
22	QV	18	U
22	QV	20	G
22	QV	21	U
22	QV	22	A
22	QV	36	A
22	QV	48	U
22	QV	49	C
22	QV	50	G
22	QV	53	G
22	QV	54	G
22	QV	55	U
22	QV	77	A
22	QW	8	U
22	QW	9	G
22	QW	13	C
22	QW	14	A
22	QW	18	U
22	QW	19	G
22	QW	20	G
22	QW	21	U
22	QW	27	G
22	QW	32	G
22	QW	33	C
22	QW	34	U
22	QW	35	C
22	QW	36	A
22	QW	38	A
22	QW	39	A
22	QW	43	G
22	QW	46	G
22	QW	47	G
22	QW	48	U
22	QW	49	C
22	QW	50	G
22	QW	56	U
22	QW	57	C
22	QW	58	A

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Mol	Chain	Res	Type
22	QW	59	A
22	QW	60	A
22	QW	61	U
22	QW	62	C
22	QW	67	C
22	QW	74	A
22	QW	75	C
22	QW	77	A
24	QY	30	G
24	QY	36	A
24	QY	37	A
24	QY	43	C
25	RA	11	G
25	RA	14	A
25	RA	15	G
25	RA	27	G
25	RA	34	C
25	RA	35	G
25	RA	46	C
25	RA	51	G
25	RA	55	G
25	RA	61	G
25	RA	64	A
25	RA	72	U
25	RA	73	A
25	RA	74	A
25	RA	75	G
25	RA	95	G
25	RA	101	G
25	RA	102	G
25	RA	103	A
25	RA	118	A
25	RA	120	U
25	RA	125	G
25	RA	131	G
25	RA	161	U
25	RA	177	G
25	RA	196	A
25	RA	199	A
25	RA	201	C
25	RA	204	A
25	RA	205	G

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Mol	Chain	Res	Type
25	RA	215	G
25	RA	216	A
25	RA	221	A
25	RA	222	A
25	RA	223	A
25	RA	228	A
25	RA	229	A
25	RA	230	U
25	RA	242	G
25	RA	243	U
25	RA	248	G
25	RA	249	C
25	RA	252	G
25	RA	264	C
25	RA	265	A
25	RA	266	G
25	RA	267	C
25	RA	269	U
25	RA	270(L)	U
25	RA	270(M)	U
25	RA	270(N)	G
25	RA	270(P)	C
25	RA	271(C)	U
25	RA	271	G
25	RA	275	G
25	RA	276	A
25	RA	277	C
25	RA	278	A
25	RA	294	A
25	RA	299	A
25	RA	311	A
25	RA	323	G
25	RA	324	A
25	RA	327	G
25	RA	329	G
25	RA	330	A
25	RA	346	A
25	RA	352	G
25	RA	362	U
25	RA	364	C
25	RA	371	A
25	RA	372	G

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Mol	Chain	Res	Type
25	RA	386	G
25	RA	387	U
25	RA	395	U
25	RA	405	U
25	RA	411	G
25	RA	412	A
25	RA	428	A
25	RA	435	C
25	RA	444	C
25	RA	448	U
25	RA	451	C
25	RA	456	C
25	RA	457	A
25	RA	458	G
25	RA	464	U
25	RA	467	G
25	RA	470	A
25	RA	481	G
25	RA	504	U
25	RA	505	A
25	RA	508	G
25	RA	509	C
25	RA	513	A
25	RA	527	C
25	RA	529	A
25	RA	530	G
25	RA	531	C
25	RA	532	A
25	RA	533	G
25	RA	537	C
25	RA	539	G
25	RA	540	G
25	RA	546	C
25	RA	547	A
25	RA	554	U
25	RA	563	G
25	RA	571	A
25	RA	573	G
25	RA	575	A
25	RA	603	A
25	RA	607	U
25	RA	614	U

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Mol	Chain	Res	Type
25	RA	615	G
25	RA	617	G
25	RA	621	A
25	RA	622	G
25	RA	627	A
25	RA	631	A
25	RA	634	C
25	RA	637	A
25	RA	638	G
25	RA	645	C
25	RA	646	A
25	RA	651	G
25	RA	654	A
25	RA	654(A)	G
25	RA	654(B)	C
25	RA	668	G
25	RA	669	G
25	RA	670	A
25	RA	686	G
25	RA	702	G
25	RA	717	G
25	RA	722	A
25	RA	730	C
25	RA	738	G
25	RA	740	U
25	RA	748	G
25	RA	765	G
25	RA	775	G
25	RA	776	G
25	RA	782	A
25	RA	784	A
25	RA	785	G
25	RA	790	C
25	RA	800	A
25	RA	805	G
25	RA	812	C
25	RA	819	A
25	RA	827	U
25	RA	828	U
25	RA	830	G
25	RA	846	C
25	RA	847	U

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Mol	Chain	Res	Type
25	RA	856	C
25	RA	857	C
25	RA	859	G
25	RA	860	U
25	RA	881	G
25	RA	882	G
25	RA	884	C
25	RA	886	C
25	RA	888	C
25	RA	889	C
25	RA	890	A
25	RA	896	A
25	RA	897	C
25	RA	900	A
25	RA	901	A
25	RA	907	U
25	RA	910	A
25	RA	914	C
25	RA	915	C
25	RA	917	A
25	RA	919	G
25	RA	932	G
25	RA	938	G
25	RA	941	A
25	RA	945	A
25	RA	946	G
25	RA	953	A
25	RA	959	A
25	RA	961	C
25	RA	973	A
25	RA	974	G
25	RA	974(A)	C
25	RA	975	G
25	RA	980	A
25	RA	983	A
25	RA	989	G
25	RA	996	A
25	RA	1003	G
25	RA	1005	C
25	RA	1010	A
25	RA	1012	U
25	RA	1013	C

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Mol	Chain	Res	Type
25	RA	1015	G
25	RA	1017	G
25	RA	1020	A
25	RA	1022	G
25	RA	1023	U
25	RA	1025	G
25	RA	1026	U
25	RA	1027	A
25	RA	1033	U
25	RA	1044	G
25	RA	1045	A
25	RA	1046	A
25	RA	1050	A
25	RA	1054	A
25	RA	1055	G
25	RA	1060	U
25	RA	1061	U
25	RA	1066	U
25	RA	1067	A
25	RA	1068	G
25	RA	1070	A
25	RA	1071	G
25	RA	1076	C
25	RA	1077	A
25	RA	1078	U
25	RA	1079	C
25	RA	1080	C
25	RA	1082	U
25	RA	1083	U
25	RA	1084	A
25	RA	1085	A
25	RA	1086	A
25	RA	1087	G
25	RA	1088	A
25	RA	1090	U
25	RA	1091	G
25	RA	1093	G
25	RA	1096	A
25	RA	1099	G
25	RA	1103	A
25	RA	1110	G
25	RA	1111	A

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Mol	Chain	Res	Type
25	RA	1112	G
25	RA	1126	A
25	RA	1128	A
25	RA	1129	A
25	RA	1130	U
25	RA	1135	C
25	RA	1136	G
25	RA	1139	G
25	RA	1141	U
25	RA	1142	U
25	RA	1142(A)	A
25	RA	1151	G
25	RA	1155	A
25	RA	1170	G
25	RA	1173	G
25	RA	1174	A
25	RA	1175	U
25	RA	1176	G
25	RA	1178	C
25	RA	1179	C
25	RA	1195	G
25	RA	1204	A
25	RA	1205	U
25	RA	1206	G
25	RA	1210	A
25	RA	1211	U
25	RA	1220	A
25	RA	1236	G
25	RA	1238	G
25	RA	1247	A
25	RA	1253	A
25	RA	1256	G
25	RA	1265	A
25	RA	1272	A
25	RA	1273	U
25	RA	1288	U
25	RA	1300	U
25	RA	1301	A
25	RA	1309	G
25	RA	1312	U
25	RA	1313	U
25	RA	1314	C

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Mol	Chain	Res	Type
25	RA	1319	G
25	RA	1321	A
25	RA	1325	G
25	RA	1329	U
25	RA	1330	C
25	RA	1341	U
25	RA	1349	A
25	RA	1352	U
25	RA	1365	A
25	RA	1368	G
25	RA	1370	C
25	RA	1378	A
25	RA	1379	A
25	RA	1380	G
25	RA	1384	A
25	RA	1385	G
25	RA	1391	U
25	RA	1395	A
25	RA	1407	C
25	RA	1411	C
25	RA	1414	G
25	RA	1416	G
25	RA	1419	A
25	RA	1420	U
25	RA	1421	G
25	RA	1428	C
25	RA	1444(A)	A
25	RA	1445	C
25	RA	1449	A
25	RA	1449(A)	G
25	RA	1455	G
25	RA	1458	C
25	RA	1460	A
25	RA	1461	G
25	RA	1471	A
25	RA	1474	C
25	RA	1479	G
25	RA	1482	U
25	RA	1483	G
25	RA	1485	G
25	RA	1487	G
25	RA	1493	C

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Mol	Chain	Res	Type
25	RA	1494	A
25	RA	1497	U
25	RA	1505	C
25	RA	1506	C
25	RA	1507	A
25	RA	1508	A
25	RA	1510	A
25	RA	1511	A
25	RA	1514	U
25	RA	1515	C
25	RA	1528	A
25	RA	1534	G
25	RA	1535	U
25	RA	1536	A
25	RA	1537	C
25	RA	1538	G
25	RA	1543	A
25	RA	1544	C
25	RA	1545	A
25	RA	1547	C
25	RA	1554	A
25	RA	1558	A
25	RA	1559	G
25	RA	1560	G
25	RA	1566	A
25	RA	1569	A
25	RA	1578	U
25	RA	1579	A
25	RA	1585	C
25	RA	1586	A
25	RA	1598	C
25	RA	1608	A
25	RA	1610	A
25	RA	1616	A
25	RA	1617	C
25	RA	1639	U
25	RA	1640	C
25	RA	1648	C
25	RA	1651	G
25	RA	1660	C
25	RA	1674	G
25	RA	1695	G

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Mol	Chain	Res	Type
25	RA	1703	G
25	RA	1725	G
25	RA	1728	G
25	RA	1729	A
25	RA	1730	U
25	RA	1733	G
25	RA	1742	C
25	RA	1743	G
25	RA	1756	G
25	RA	1762	A
25	RA	1763	G
25	RA	1764	G
25	RA	1773	A
25	RA	1774	C
25	RA	1776	G
25	RA	1780	A
25	RA	1781	C
25	RA	1782	C
25	RA	1784	A
25	RA	1791	A
25	RA	1800	C
25	RA	1801	G
25	RA	1802	A
25	RA	1811	G
25	RA	1815	A
25	RA	1816	G
25	RA	1820	U
25	RA	1828	G
25	RA	1829	A
25	RA	1835	G
25	RA	1847	A
25	RA	1858	G
25	RA	1860	G
25	RA	1869	G
25	RA	1870	C
25	RA	1872	A
25	RA	1878	G
25	RA	1882	C
25	RA	1885	A
25	RA	1888	G
25	RA	1889	A
25	RA	1905	C

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Mol	Chain	Res	Type
25	RA	1906	G
25	RA	1913	A
25	RA	1927	A
25	RA	1929	G
25	RA	1930	G
25	RA	1931	U
25	RA	1936	A
25	RA	1938	A
25	RA	1939	U
25	RA	1940	U
25	RA	1955	U
25	RA	1963	U
25	RA	1965	C
25	RA	1967	C
25	RA	1969	A
25	RA	1970	A
25	RA	1971	A
25	RA	1972	A
25	RA	1991	U
25	RA	1992	G
25	RA	1993	U
25	RA	1996	C
25	RA	2013	A
25	RA	2020	A
25	RA	2023	G
25	RA	2030	A
25	RA	2031	A
25	RA	2032	G
25	RA	2033	A
25	RA	2034	U
25	RA	2043	C
25	RA	2052	G
25	RA	2055	C
25	RA	2056	G
25	RA	2059	A
25	RA	2060	A
25	RA	2061	G
25	RA	2062	A
25	RA	2063	C
25	RA	2069	G
25	RA	2093	G
25	RA	2107	C

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Mol	Chain	Res	Type
25	RA	2111	C
25	RA	2112	G
25	RA	2113	U
25	RA	2114	A
25	RA	2115	G
25	RA	2116	G
25	RA	2117	A
25	RA	2126	A
25	RA	2127	G
25	RA	2128	C
25	RA	2131	G
25	RA	2132	U
25	RA	2133	G
25	RA	2135	A
25	RA	2136	C
25	RA	2146	C
25	RA	2147	G
25	RA	2148	G
25	RA	2152	G
25	RA	2166	G
25	RA	2168	G
25	RA	2170	A
25	RA	2173	A
25	RA	2190	G
25	RA	2198	A
25	RA	2210	G
25	RA	2211	G
25	RA	2212	A
25	RA	2213	U
25	RA	2215	G
25	RA	2225	A
25	RA	2238	G
25	RA	2239	G
25	RA	2243	U
25	RA	2249	U
25	RA	2266	A
25	RA	2275	C
25	RA	2278	A
25	RA	2280	G
25	RA	2283	C
25	RA	2287	A
25	RA	2288	A

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Mol	Chain	Res	Type
25	RA	2307	G
25	RA	2308	G
25	RA	2311	A
25	RA	2312	U
25	RA	2319	G
25	RA	2320	A
25	RA	2325	G
25	RA	2334	G
25	RA	2336	A
25	RA	2345	G
25	RA	2346	A
25	RA	2347	C
25	RA	2350	C
25	RA	2354	G
25	RA	2358	G
25	RA	2383	G
25	RA	2385	C
25	RA	2392	A
25	RA	2394	C
25	RA	2402	C
25	RA	2403	C
25	RA	2406	U
25	RA	2410	G
25	RA	2423	U
25	RA	2425	A
25	RA	2427	C
25	RA	2429	G
25	RA	2430	A
25	RA	2435	A
25	RA	2439	A
25	RA	2440	C
25	RA	2441	C
25	RA	2445	G
25	RA	2448	A
25	RA	2469	A
25	RA	2470	G
25	RA	2474	C
25	RA	2475	C
25	RA	2480	C
25	RA	2482	G
25	RA	2494	G
25	RA	2502	G

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Mol	Chain	Res	Type
25	RA	2503	A
25	RA	2505	G
25	RA	2519	U
25	RA	2529	G
25	RA	2542	A
25	RA	2543	G
25	RA	2553	G
25	RA	2554	U
25	RA	2562	U
25	RA	2566	A
25	RA	2567	G
25	RA	2569	G
25	RA	2572	A
25	RA	2578	G
25	RA	2582	G
25	RA	2585	U
25	RA	2586	C
25	RA	2602	A
25	RA	2609	U
25	RA	2610	C
25	RA	2611	U
25	RA	2612	C
25	RA	2615	U
25	RA	2619	C
25	RA	2623	G
25	RA	2629	A
25	RA	2642	G
25	RA	2646	C
25	RA	2655	G
25	RA	2665	A
25	RA	2673	G
25	RA	2682	U
25	RA	2689	U
25	RA	2690	C
25	RA	2691	C
25	RA	2702	U
25	RA	2712	U
25	RA	2712(A)	A
25	RA	2713	A
25	RA	2714	G
25	RA	2718	G
25	RA	2726	U

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Mol	Chain	Res	Type
25	RA	2733	A
25	RA	2739	U
25	RA	2744	G
25	RA	2748	A
25	RA	2751	G
25	RA	2752	C
25	RA	2758	A
25	RA	2761	G
25	RA	2764	A
25	RA	2765	A
25	RA	2766	G
25	RA	2777	G
25	RA	2778	A
25	RA	2779	U
25	RA	2780	G
25	RA	2789	C
25	RA	2790	A
25	RA	2791	C
25	RA	2797	U
25	RA	2802	G
25	RA	2807	G
25	RA	2818	G
25	RA	2820	A
25	RA	2821	A
25	RA	2823	A
25	RA	2833	G
25	RA	2834	G
25	RA	2835	A
25	RA	2839	G
25	RA	2849	U
25	RA	2867	G
25	RA	2868	A
25	RA	2872	G
25	RA	2879	C
25	RA	2892	A
25	RA	2893	G
25	RA	2894	G
26	RB	2	C
26	RB	8	U
26	RB	13	A
26	RB	15	A
26	RB	16	G

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Mol	Chain	Res	Type
26	RB	22	U
26	RB	25	A
26	RB	26	A
26	RB	27	C
26	RB	32	C
26	RB	35	U
26	RB	41	U
26	RB	42	C
26	RB	45	A
26	RB	66	A
26	RB	67	G
26	RB	73	A
26	RB	81	G
26	RB	87	G
26	RB	89	G
26	RB	101	A
26	RB	108	C
26	RB	109	G
26	RB	118	G
1	XA	6	G
1	XA	32	A
1	XA	39	G
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	77	C
1	XA	78	G
1	XA	79	G
1	XA	89	U
1	XA	90	C
1	XA	91	C
1	XA	92	G
1	XA	93	U
1	XA	95	G
1	XA	108	G
1	XA	116	A
1	XA	121	C

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Mol	Chain	Res	Type
1	XA	129(A)	G
1	XA	131	C
1	XA	144	G
1	XA	147	G
1	XA	159	G
1	XA	163	C
1	XA	172	A
1	XA	174	C
1	XA	182	U
1	XA	190	G
1	XA	195	A
1	XA	197	A
1	XA	201	C
1	XA	208	U
1	XA	209	U
1	XA	210	U
1	XA	216	G
1	XA	244	U
1	XA	245	C
1	XA	247	G
1	XA	251	G
1	XA	262	A
1	XA	267	C
1	XA	270	A
1	XA	279	A
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	343	U
1	XA	344	A
1	XA	345	C
1	XA	346	G
1	XA	347	U
1	XA	352	C
1	XA	353	A
1	XA	354	G
1	XA	356	A
1	XA	367	U
1	XA	372	C

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Mol	Chain	Res	Type
1	XA	373	A
1	XA	384	G
1	XA	388	G
1	XA	390	C
1	XA	397	A
1	XA	398	C
1	XA	406	G
1	XA	412	A
1	XA	413	G
1	XA	414	A
1	XA	421	U
1	XA	422	C
1	XA	423	G
1	XA	424	G
1	XA	428	G
1	XA	429	U
1	XA	439	A
1	XA	442	C
1	XA	446	G
1	XA	458	C
1	XA	466	C
1	XA	485	G
1	XA	486	U
1	XA	496	A
1	XA	497	U
1	XA	509	A
1	XA	510	A
1	XA	511	C
1	XA	517	G
1	XA	518	C
1	XA	521	G
1	XA	527	G
1	XA	531	U
1	XA	532	A
1	XA	533	A
1	XA	545	C
1	XA	547	A
1	XA	548	G
1	XA	559	A
1	XA	561	U
1	XA	564	C
1	XA	568	G

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Mol	Chain	Res	Type
1	XA	572	A
1	XA	573	A
1	XA	576	G
1	XA	577	G
1	XA	618	C
1	XA	630	G
1	XA	631	G
1	XA	632	A
1	XA	653	A
1	XA	665	A
1	XA	686	U
1	XA	688	G
1	XA	702	A
1	XA	703	G
1	XA	704	A
1	XA	717	C
1	XA	718	G
1	XA	721	G
1	XA	723	U
1	XA	731	G
1	XA	748	C
1	XA	749	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	841	U
1	XA	843	U
1	XA	848	C
1	XA	853	G
1	XA	859	A
1	XA	864	A
1	XA	871	U

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Mol	Chain	Res	Type
1	XA	872	A
1	XA	876	G
1	XA	889	A
1	XA	902	G
1	XA	914	A
1	XA	916	G
1	XA	919	A
1	XA	927	G
1	XA	934	C
1	XA	935	A
1	XA	942	G
1	XA	960	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	1001	G
1	XA	1003	G
1	XA	1004	A
1	XA	1005	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	1032(A)	G
1	XA	1053	G
1	XA	1054	C
1	XA	1055	A
1	XA	1056	U
1	XA	1064	G
1	XA	1066	C

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Mol	Chain	Res	Type
1	XA	1081	G
1	XA	1094	G
1	XA	1101	A
1	XA	1108	G
1	XA	1113	C
1	XA	1124	G
1	XA	1125	U
1	XA	1126	U
1	XA	1127	G
1	XA	1130	A
1	XA	1131	G
1	XA	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	1171	G
1	XA	1176	A
1	XA	1177	G
1	XA	1178	G
1	XA	1179	A
1	XA	1180	A
1	XA	1181	G
1	XA	1182	G
1	XA	1183	A
1	XA	1184	G
1	XA	1187	G
1	XA	1189	C
1	XA	1190	G
1	XA	1196	U
1	XA	1201	A
1	XA	1212	U
1	XA	1214	C
1	XA	1227	A
1	XA	1238	A
1	XA	1240	U
1	XA	1241	G

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Mol	Chain	Res	Type
1	XA	1256	A
1	XA	1257	U
1	XA	1258	G
1	XA	1263	C
1	XA	1270	C
1	XA	1273	G
1	XA	1280	A
1	XA	1281	U
1	XA	1282	C
1	XA	1286	A
1	XA	1287	A
1	XA	1297	C
1	XA	1300	G
1	XA	1301	U
1	XA	1302	U
1	XA	1303	C
1	XA	1305	G
1	XA	1319	A
1	XA	1320	C
1	XA	1321	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	1370	G
1	XA	1379	G
1	XA	1397	C
1	XA	1419	G
1	XA	1442	G
1	XA	1443	G
1	XA	1452	C
1	XA	1453	G
1	XA	1454	G
1	XA	1487	G
1	XA	1492	A
1	XA	1497	G
1	XA	1499	A
1	XA	1502	A
1	XA	1503	A

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Mol	Chain	Res	Type
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	7	G
22	XV	8	U
22	XV	13	C
22	XV	18	U
22	XV	20	G
22	XV	21	U
22	XV	22	A
22	XV	36	A
22	XV	48	U
22	XV	49	C
22	XV	50	G
22	XV	53	G
22	XV	54	G
22	XV	55	U
22	XV	77	A
22	XW	8	U
22	XW	9	G
22	XW	10	G
22	XW	13	C
22	XW	14	A
22	XW	18	U
22	XW	19	G
22	XW	20	G
22	XW	21	U
22	XW	23	G
22	XW	27	G
22	XW	32	G
22	XW	33	C
22	XW	34	U
22	XW	35	C
22	XW	36	A
22	XW	38	A
22	XW	39	A
22	XW	43	G
22	XW	46	G

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Mol	Chain	Res	Type
22	XW	47	G
22	XW	48	U
22	XW	49	C
22	XW	50	G
22	XW	56	U
22	XW	57	C
22	XW	58	A
22	XW	59	A
22	XW	60	A
22	XW	61	U
22	XW	62	C
22	XW	74	A
22	XW	75	C
22	XW	77	A
23	XX	14	A
23	XX	23	A
24	XY	30	G
24	XY	36	A
24	XY	37	A
24	XY	43	C
25	YA	10	G
25	YA	12	U
25	YA	34	C
25	YA	35	G
25	YA	46	C
25	YA	51	G
25	YA	55	G
25	YA	61	G
25	YA	72	U
25	YA	73	A
25	YA	74	A
25	YA	75	G
25	YA	95	G
25	YA	96	G
25	YA	101	G
25	YA	102	G
25	YA	103	A
25	YA	118	A
25	YA	120	U
25	YA	125	G
25	YA	131	G
25	YA	138	G

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Mol	Chain	Res	Type
25	YA	149	A
25	YA	161	U
25	YA	162	U
25	YA	181	A
25	YA	196	A
25	YA	199	A
25	YA	204	A
25	YA	215	G
25	YA	216	A
25	YA	221	A
25	YA	222	A
25	YA	223	A
25	YA	226	G
25	YA	228	A
25	YA	229	A
25	YA	230	U
25	YA	232	G
25	YA	233	A
25	YA	241	A
25	YA	242	G
25	YA	243	U
25	YA	248	G
25	YA	252	G
25	YA	264	C
25	YA	265	A
25	YA	266	G
25	YA	270(K)	C
25	YA	270(L)	U
25	YA	270(M)	U
25	YA	270(N)	G
25	YA	270(P)	C
25	YA	271(B)	G
25	YA	271(C)	U
25	YA	271	G
25	YA	274	G
25	YA	275	G
25	YA	276	A
25	YA	278	A
25	YA	279	C
25	YA	299	A
25	YA	300	A
25	YA	311	A

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Mol	Chain	Res	Type
25	YA	323	G
25	YA	324	A
25	YA	329	G
25	YA	330	A
25	YA	332	A
25	YA	342	G
25	YA	352	G
25	YA	363	G
25	YA	371	A
25	YA	372	G
25	YA	386	G
25	YA	387	U
25	YA	405	U
25	YA	406	G
25	YA	407	G
25	YA	411	G
25	YA	412	A
25	YA	428	A
25	YA	443	A
25	YA	444	C
25	YA	448	U
25	YA	451	C
25	YA	456	C
25	YA	457	A
25	YA	458	G
25	YA	467	G
25	YA	470	A
25	YA	473	G
25	YA	481	G
25	YA	496	G
25	YA	504	U
25	YA	505	A
25	YA	508	G
25	YA	509	C
25	YA	512	G
25	YA	530	G
25	YA	531	C
25	YA	532	A
25	YA	533	G
25	YA	537	C
25	YA	539	G
25	YA	540	G

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Mol	Chain	Res	Type
25	YA	546	C
25	YA	547	A
25	YA	549	G
25	YA	563	G
25	YA	571	A
25	YA	573	G
25	YA	575	A
25	YA	588	U
25	YA	603	A
25	YA	607	U
25	YA	614	U
25	YA	615	G
25	YA	617	G
25	YA	621	A
25	YA	622	G
25	YA	627	A
25	YA	631	A
25	YA	634	C
25	YA	637	A
25	YA	638	G
25	YA	645	C
25	YA	646	A
25	YA	651	G
25	YA	654(A)	G
25	YA	654(B)	C
25	YA	670	A
25	YA	686	G
25	YA	695	G
25	YA	704	G
25	YA	717	G
25	YA	722	A
25	YA	730	C
25	YA	734	A
25	YA	765	G
25	YA	782	A
25	YA	784	A
25	YA	785	G
25	YA	790	C
25	YA	792	G
25	YA	793	A
25	YA	800	A
25	YA	805	G

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Mol	Chain	Res	Type
25	YA	812	C
25	YA	819	A
25	YA	827	U
25	YA	828	U
25	YA	830	G
25	YA	831	G
25	YA	847	U
25	YA	856	C
25	YA	857	C
25	YA	860	U
25	YA	865	C
25	YA	866	A
25	YA	884	C
25	YA	885	C
25	YA	886	C
25	YA	888	C
25	YA	889	C
25	YA	896	A
25	YA	897	C
25	YA	900	A
25	YA	901	A
25	YA	902	C
25	YA	906	G
25	YA	907	U
25	YA	910	A
25	YA	914	C
25	YA	917	A
25	YA	918	A
25	YA	932	G
25	YA	941	A
25	YA	945	A
25	YA	946	G
25	YA	957	A
25	YA	959	A
25	YA	961	C
25	YA	973	A
25	YA	974	G
25	YA	974(A)	C
25	YA	980	A
25	YA	983	A
25	YA	989	G
25	YA	990	A

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Mol	Chain	Res	Type
25	YA	996	A
25	YA	1003	G
25	YA	1005	C
25	YA	1008	C
25	YA	1011	G
25	YA	1012	U
25	YA	1013	C
25	YA	1015	G
25	YA	1020	A
25	YA	1022	G
25	YA	1023	U
25	YA	1025	G
25	YA	1026	U
25	YA	1027	A
25	YA	1033	U
25	YA	1046	A
25	YA	1047	G
25	YA	1050	A
25	YA	1054	A
25	YA	1059	G
25	YA	1060	U
25	YA	1061	U
25	YA	1062	G
25	YA	1066	U
25	YA	1067	A
25	YA	1068	G
25	YA	1070	A
25	YA	1071	G
25	YA	1073	A
25	YA	1076	C
25	YA	1077	A
25	YA	1078	U
25	YA	1079	C
25	YA	1082	U
25	YA	1083	U
25	YA	1084	A
25	YA	1085	A
25	YA	1086	A
25	YA	1088	A
25	YA	1089	G
25	YA	1090	U
25	YA	1095	A

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Mol	Chain	Res	Type
25	YA	1096	A
25	YA	1097	U
25	YA	1103	A
25	YA	1104	C
25	YA	1105	U
25	YA	1106	G
25	YA	1109	C
25	YA	1110	G
25	YA	1111	A
25	YA	1122	G
25	YA	1126	A
25	YA	1128	A
25	YA	1129	A
25	YA	1130	U
25	YA	1131	G
25	YA	1135	C
25	YA	1136	G
25	YA	1139	G
25	YA	1142	U
25	YA	1142(A)	A
25	YA	1151	G
25	YA	1155	A
25	YA	1156	A
25	YA	1170	G
25	YA	1173	G
25	YA	1174	A
25	YA	1175	U
25	YA	1176	G
25	YA	1177	A
25	YA	1179	C
25	YA	1195	G
25	YA	1204	A
25	YA	1205	U
25	YA	1206	G
25	YA	1211	U
25	YA	1220	A
25	YA	1236	G
25	YA	1238	G
25	YA	1244	G
25	YA	1247	A
25	YA	1248	G
25	YA	1252	G

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Mol	Chain	Res	Type
25	YA	1253	A
25	YA	1256	G
25	YA	1265	A
25	YA	1272	A
25	YA	1273	U
25	YA	1300	U
25	YA	1301	A
25	YA	1329	U
25	YA	1330	C
25	YA	1341	U
25	YA	1349	A
25	YA	1352	U
25	YA	1359	A
25	YA	1360	A
25	YA	1365	A
25	YA	1368	G
25	YA	1378	A
25	YA	1379	A
25	YA	1380	G
25	YA	1384	A
25	YA	1385	G
25	YA	1392	A
25	YA	1407	C
25	YA	1411	C
25	YA	1416	G
25	YA	1419	A
25	YA	1420	U
25	YA	1428	C
25	YA	1444(A)	A
25	YA	1445	C
25	YA	1449	A
25	YA	1449(A)	G
25	YA	1455	G
25	YA	1458	C
25	YA	1460	A
25	YA	1461	G
25	YA	1467	C
25	YA	1471	A
25	YA	1478	G
25	YA	1482	U
25	YA	1483	G
25	YA	1486	A

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Mol	Chain	Res	Type
25	YA	1493	C
25	YA	1496	A
25	YA	1497	U
25	YA	1507	A
25	YA	1508	A
25	YA	1510	A
25	YA	1511	A
25	YA	1522	G
25	YA	1533	C
25	YA	1534	G
25	YA	1535	U
25	YA	1536	A
25	YA	1537	C
25	YA	1538	G
25	YA	1540	G
25	YA	1543	A
25	YA	1544	C
25	YA	1545	A
25	YA	1554	A
25	YA	1558	A
25	YA	1559	G
25	YA	1567	A
25	YA	1569	A
25	YA	1578	U
25	YA	1579	A
25	YA	1581	G
25	YA	1585	C
25	YA	1586	A
25	YA	1591	G
25	YA	1592	C
25	YA	1598	C
25	YA	1608	A
25	YA	1609	A
25	YA	1615	C
25	YA	1617	C
25	YA	1618	A
25	YA	1634	A
25	YA	1639	U
25	YA	1640	C
25	YA	1648	C
25	YA	1660	C
25	YA	1665	A

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Mol	Chain	Res	Type
25	YA	1674	G
25	YA	1695	G
25	YA	1698	A
25	YA	1699	G
25	YA	1703	G
25	YA	1718	G
25	YA	1725	G
25	YA	1728	G
25	YA	1729	A
25	YA	1730	U
25	YA	1731	G
25	YA	1742	C
25	YA	1743	G
25	YA	1756	G
25	YA	1763	G
25	YA	1764	G
25	YA	1769	G
25	YA	1773	A
25	YA	1779	U
25	YA	1780	A
25	YA	1781	C
25	YA	1791	A
25	YA	1800	C
25	YA	1801	G
25	YA	1802	A
25	YA	1811	G
25	YA	1815	A
25	YA	1816	G
25	YA	1820	U
25	YA	1828	G
25	YA	1829	A
25	YA	1835	G
25	YA	1836	C
25	YA	1847	A
25	YA	1848	A
25	YA	1858	G
25	YA	1869	G
25	YA	1872	A
25	YA	1878	G
25	YA	1882	C
25	YA	1885	A
25	YA	1888	G

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Mol	Chain	Res	Type
25	YA	1889	A
25	YA	1900	A
25	YA	1903	G
25	YA	1906	G
25	YA	1913	A
25	YA	1919	A
25	YA	1930	G
25	YA	1936	A
25	YA	1938	A
25	YA	1939	U
25	YA	1940	U
25	YA	1955	U
25	YA	1956	U
25	YA	1960	A
25	YA	1963	U
25	YA	1966	A
25	YA	1967	C
25	YA	1969	A
25	YA	1970	A
25	YA	1971	A
25	YA	1972	A
25	YA	1982	C
25	YA	1992	G
25	YA	1993	U
25	YA	2020	A
25	YA	2021	C
25	YA	2023	G
25	YA	2030	A
25	YA	2031	A
25	YA	2032	G
25	YA	2033	A
25	YA	2034	U
25	YA	2043	C
25	YA	2052	G
25	YA	2054	A
25	YA	2055	C
25	YA	2056	G
25	YA	2059	A
25	YA	2060	A
25	YA	2061	G
25	YA	2062	A
25	YA	2069	G

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Mol	Chain	Res	Type
25	YA	2093	G
25	YA	2099	U
25	YA	2111	C
25	YA	2112	G
25	YA	2113	U
25	YA	2114	A
25	YA	2115	G
25	YA	2116	G
25	YA	2120	G
25	YA	2126	A
25	YA	2127	G
25	YA	2128	C
25	YA	2131	G
25	YA	2132	U
25	YA	2133	G
25	YA	2135	A
25	YA	2146	C
25	YA	2147	G
25	YA	2148	G
25	YA	2158	A
25	YA	2165	G
25	YA	2166	G
25	YA	2167	U
25	YA	2169	A
25	YA	2173	A
25	YA	2178	C
25	YA	2190	G
25	YA	2191	G
25	YA	2193	G
25	YA	2198	A
25	YA	2199	A
25	YA	2210	G
25	YA	2211	G
25	YA	2212	A
25	YA	2215	G
25	YA	2225	A
25	YA	2238	G
25	YA	2239	G
25	YA	2243	U
25	YA	2249	U
25	YA	2266	A
25	YA	2269	A

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Mol	Chain	Res	Type
25	YA	2275	C
25	YA	2278	A
25	YA	2280	G
25	YA	2283	C
25	YA	2287	A
25	YA	2288	A
25	YA	2299	G
25	YA	2307	G
25	YA	2308	G
25	YA	2309	A
25	YA	2311	A
25	YA	2312	U
25	YA	2319	G
25	YA	2320	A
25	YA	2325	G
25	YA	2335	A
25	YA	2336	A
25	YA	2342	C
25	YA	2345	G
25	YA	2346	A
25	YA	2347	C
25	YA	2350	C
25	YA	2383	G
25	YA	2385	C
25	YA	2392	A
25	YA	2394	C
25	YA	2396	G
25	YA	2402	C
25	YA	2403	C
25	YA	2406	U
25	YA	2410	G
25	YA	2423	U
25	YA	2424	C
25	YA	2425	A
25	YA	2427	C
25	YA	2428	G
25	YA	2429	G
25	YA	2430	A
25	YA	2435	A
25	YA	2439	A
25	YA	2440	C
25	YA	2441	C

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Mol	Chain	Res	Type
25	YA	2447	G
25	YA	2448	A
25	YA	2469	A
25	YA	2471	C
25	YA	2484	G
25	YA	2494	G
25	YA	2502	G
25	YA	2504	U
25	YA	2505	G
25	YA	2518	A
25	YA	2524	G
25	YA	2529	G
25	YA	2554	U
25	YA	2562	U
25	YA	2566	A
25	YA	2567	G
25	YA	2572	A
25	YA	2573	C
25	YA	2576	G
25	YA	2577	A
25	YA	2578	G
25	YA	2602	A
25	YA	2609	U
25	YA	2611	U
25	YA	2612	C
25	YA	2619	C
25	YA	2621	A
25	YA	2629	A
25	YA	2632	A
25	YA	2642	G
25	YA	2646	C
25	YA	2655	G
25	YA	2656	U
25	YA	2665	A
25	YA	2666	C
25	YA	2673	G
25	YA	2682	U
25	YA	2689	U
25	YA	2690	C
25	YA	2691	C
25	YA	2702	U
25	YA	2712(A)	A

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Mol	Chain	Res	Type
25	YA	2713	A
25	YA	2714	G
25	YA	2718	G
25	YA	2726	U
25	YA	2733	A
25	YA	2739	U
25	YA	2744	G
25	YA	2751	G
25	YA	2752	C
25	YA	2759	G
25	YA	2762	G
25	YA	2765	A
25	YA	2766	G
25	YA	2771	C
25	YA	2778	A
25	YA	2779	U
25	YA	2790	A
25	YA	2791	C
25	YA	2792	G
25	YA	2794	C
25	YA	2797	U
25	YA	2798	C
25	YA	2801	A
25	YA	2807	G
25	YA	2808	U
25	YA	2818	G
25	YA	2820	A
25	YA	2821	A
25	YA	2823	A
25	YA	2830	G
25	YA	2833	G
25	YA	2834	G
25	YA	2835	A
25	YA	2836	U
25	YA	2872	G
25	YA	2876	G
25	YA	2879	C
25	YA	2880	C
25	YA	2891	G
25	YA	2892	A
25	YA	2893	G
26	YB	2	C

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Mol	Chain	Res	Type
26	YB	8	U
26	YB	13	A
26	YB	15	A
26	YB	16	G
26	YB	22	U
26	YB	25	A
26	YB	26	A
26	YB	27	C
26	YB	32	C
26	YB	35	U
26	YB	41	U
26	YB	42	C
26	YB	45	A
26	YB	66	A
26	YB	67	G
26	YB	73	A
26	YB	81	G
26	YB	87	G
26	YB	89	G
26	YB	101	A
26	YB	108	C
26	YB	109	G
26	YB	118	G

All (149) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
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	266	G
1	QA	328	C
1	QA	410	G
1	QA	412	A
1	QA	481	G
1	QA	484	G
1	QA	485	G
1	QA	509	A
1	QA	533	A

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Mol	Chain	Res	Type
1	QA	687	A
1	QA	701	C
1	QA	703	G
1	QA	753	A
1	QA	812	C
1	QA	913	A
1	QA	992	U
1	QA	1027	C
1	QA	1182	G
1	QA	1200	C
1	QA	1285	A
1	QA	1298	C
1	QA	1336	C
1	QA	1346	A
1	QA	1347	G
1	QA	1498	U
1	QA	1528	U
22	QV	35	C
22	QV	53	G
22	QW	8	U
22	QW	59	A
25	RA	99	U
25	RA	102	G
25	RA	221	A
25	RA	222	A
25	RA	227	A
25	RA	228	A
25	RA	229	A
25	RA	242	G
25	RA	271(B)	G
25	RA	404	C
25	RA	503	A
25	RA	512	G
25	RA	637	A
25	RA	846	C
25	RA	856	C
25	RA	859	G
25	RA	974(A)	C
25	RA	1012	U
25	RA	1022	G
25	RA	1026	U
25	RA	1045	A

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Mol	Chain	Res	Type
25	RA	1078	U
25	RA	1085	A
25	RA	1178	C
25	RA	1204	A
25	RA	1210	A
25	RA	1312	U
25	RA	1427	A
25	RA	1558	A
25	RA	1694	C
25	RA	1819	A
25	RA	1992	G
25	RA	2126	A
25	RA	2210	G
25	RA	2439	A
25	RA	2481	G
25	RA	2518	A
25	RA	2689	U
25	RA	2712	U
25	RA	2776	A
25	RA	2867	G
1	XA	31	G
1	XA	60	A
1	XA	78	G
1	XA	89	U
1	XA	115	G
1	XA	181	G
1	XA	243	A
1	XA	244	U
1	XA	250	A
1	XA	266	G
1	XA	328	C
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	812	C
1	XA	913	A
1	XA	992	U
1	XA	1027	C
1	XA	1200	C

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Mol	Chain	Res	Type
1	XA	1285	A
1	XA	1336	C
1	XA	1346	A
1	XA	1498	U
1	XA	1503	A
22	XV	35	C
22	XV	53	G
22	XW	8	U
22	XW	59	A
25	YA	99	U
25	YA	102	G
25	YA	221	A
25	YA	222	A
25	YA	229	A
25	YA	242	G
25	YA	271(B)	G
25	YA	404	C
25	YA	587	C
25	YA	637	A
25	YA	846	C
25	YA	856	C
25	YA	859	G
25	YA	1012	U
25	YA	1022	G
25	YA	1026	U
25	YA	1045	A
25	YA	1078	U
25	YA	1085	A
25	YA	1109	C
25	YA	1178	C
25	YA	1210	A
25	YA	1379	A
25	YA	1427	A
25	YA	1460	A
25	YA	1509	C
25	YA	1558	A
25	YA	1694	C
25	YA	1698	A
25	YA	1819	A
25	YA	1929	G
25	YA	1955	U
25	YA	1992	G

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Mol	Chain	Res	Type
25	YA	2126	A
25	YA	2406	U
25	YA	2439	A
25	YA	2610	C
25	YA	2655	G
25	YA	2681	C
25	YA	2689	U
25	YA	2832	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1306 ligands modelled in this entry, 1304 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	$\# Z > 2$
57	SF4	QD	301	4	0,12,12	-	-	-		
57	SF4	XD	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
57	SF4	QD	301	4	-	-	0/6/5/5

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	QA	1500/1508 (99%)	-0.13	16 (1%) 77 60	65, 113, 205, 388	0
1	XA	1500/1508 (99%)	-0.15	8 (0%) 87 72	59, 117, 222, 400	0
2	QB	235/256 (91%)	0.37	6 (2%) 57 41	103, 168, 244, 304	0
2	XB	236/256 (92%)	0.11	4 (1%) 69 50	93, 161, 229, 286	0
3	QC	205/239 (85%)	0.06	2 (0%) 79 62	111, 157, 211, 257	0
3	XC	205/239 (85%)	0.11	5 (2%) 59 44	91, 139, 206, 284	0
4	QD	208/209 (99%)	0.20	2 (0%) 79 62	63, 127, 183, 212	0
4	XD	208/209 (99%)	0.49	11 (5%) 33 26	73, 112, 164, 213	0
5	QE	151/162 (93%)	0.20	2 (1%) 74 56	83, 122, 165, 211	0
5	XE	151/162 (93%)	0.22	10 (6%) 26 21	69, 114, 158, 241	0
6	QF	101/101 (100%)	0.18	0 100 100	74, 119, 160, 190	0
6	XF	101/101 (100%)	0.22	3 (2%) 52 38	82, 126, 163, 232	0
7	QG	155/156 (99%)	0.10	3 (1%) 66 48	94, 134, 191, 284	0
7	XG	155/156 (99%)	0.25	4 (2%) 57 41	108, 158, 205, 249	0
8	QH	137/138 (99%)	0.04	2 (1%) 71 53	84, 127, 162, 189	0
8	XH	137/138 (99%)	0.19	3 (2%) 62 45	90, 123, 161, 180	0
9	QI	127/128 (99%)	0.40	13 (10%) 13 14	97, 156, 212, 304	0
9	XI	126/128 (98%)	0.30	11 (8%) 17 15	113, 173, 215, 258	0
10	QJ	99/105 (94%)	0.77	14 (14%) 7 10	130, 171, 227, 269	0
10	XJ	96/105 (91%)	0.39	4 (4%) 41 31	109, 175, 232, 260	0
11	QK	119/129 (92%)	0.23	4 (3%) 48 35	79, 120, 201, 273	0
11	XK	116/129 (89%)	0.24	1 (0%) 81 64	88, 126, 195, 263	0
12	QL	125/132 (94%)	0.94	15 (12%) 10 12	80, 116, 169, 249	0
12	XL	122/132 (92%)	0.55	14 (11%) 11 13	61, 99, 141, 240	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	120/126 (95%)	0.52	9 (7%) 22 18	97, 145, 199, 267	0
13	XM	119/126 (94%)	0.31	6 (5%) 35 27	101, 153, 216, 284	0
14	QN	60/61 (98%)	0.34	1 (1%) 69 50	107, 144, 190, 207	0
14	XN	60/61 (98%)	0.46	2 (3%) 49 36	102, 134, 173, 189	0
15	QO	88/89 (98%)	-0.07	0 100 100	67, 111, 147, 159	0
15	XO	87/89 (97%)	0.17	3 (3%) 48 35	80, 108, 156, 178	0
16	QP	84/88 (95%)	0.16	2 (2%) 59 44	94, 114, 160, 233	0
16	XP	84/88 (95%)	0.24	1 (1%) 76 57	87, 123, 161, 256	0
17	QQ	100/105 (95%)	0.11	1 (1%) 79 62	79, 113, 152, 230	0
17	XQ	100/105 (95%)	0.47	10 (10%) 14 14	85, 119, 164, 246	0
18	QR	70/88 (79%)	0.01	2 (2%) 54 39	72, 117, 168, 230	0
18	XR	70/88 (79%)	0.25	2 (2%) 54 39	83, 123, 187, 211	0
19	QS	83/93 (89%)	0.63	12 (14%) 7 10	107, 168, 223, 268	0
19	XS	84/93 (90%)	0.51	4 (4%) 36 28	102, 150, 205, 256	0
20	QT	99/106 (93%)	0.69	11 (11%) 12 13	72, 122, 187, 203	0
20	XT	99/106 (93%)	0.58	11 (11%) 12 13	92, 140, 202, 263	0
21	QU	25/27 (92%)	0.35	1 (4%) 43 32	107, 134, 199, 206	0
21	XU	25/27 (92%)	0.03	0 100 100	123, 145, 194, 197	0
22	QV	77/77 (100%)	0.17	2 (2%) 57 41	84, 123, 169, 246	0
22	QW	77/77 (100%)	1.20	10 (12%) 9 11	139, 313, 405, 436	0
22	XV	77/77 (100%)	0.05	2 (2%) 57 41	86, 119, 171, 232	0
22	XW	77/77 (100%)	0.82	5 (6%) 26 21	135, 350, 419, 437	0
23	QX	8/25 (32%)	0.79	1 (12%) 9 12	87, 89, 104, 143	0
23	XX	11/25 (44%)	0.89	1 (9%) 16 15	80, 88, 175, 184	0
24	QY	17/17 (100%)	-0.07	0 100 100	111, 139, 243, 275	0
24	XY	17/17 (100%)	0.01	0 100 100	105, 141, 239, 250	0
25	RA	2882/2915 (98%)	-0.14	25 (0%) 81 64	50, 90, 246, 448	0
25	YA	2883/2915 (98%)	-0.08	26 (0%) 81 64	45, 86, 245, 477	0
26	RB	120/122 (98%)	-0.20	1 (0%) 82 66	93, 129, 176, 215	0
26	YB	120/122 (98%)	-0.01	1 (0%) 82 66	107, 175, 227, 258	0
27	RD	272/276 (98%)	0.76	27 (9%) 14 14	50, 83, 132, 208	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	YD	272/276 (98%)	0.55	16 (5%) 29 23	46, 82, 130, 294	0
28	RE	205/206 (99%)	0.33	7 (3%) 48 35	62, 102, 184, 262	0
28	YE	205/206 (99%)	0.59	18 (8%) 17 15	49, 103, 190, 326	0
29	RF	202/210 (96%)	0.54	11 (5%) 32 25	62, 103, 184, 233	0
29	YF	202/210 (96%)	0.20	7 (3%) 47 35	52, 92, 151, 220	0
30	RG	181/182 (99%)	0.17	4 (2%) 62 45	82, 137, 185, 287	0
30	YG	181/182 (99%)	0.34	2 (1%) 77 60	105, 165, 210, 256	0
31	RH	174/180 (96%)	0.23	1 (0%) 85 70	106, 176, 240, 355	0
31	YH	174/180 (96%)	0.65	8 (4%) 38 29	73, 130, 181, 270	0
32	RI	146/148 (98%)	0.57	11 (7%) 22 18	77, 144, 201, 258	0
32	YI	146/148 (98%)	0.46	8 (5%) 32 24	81, 142, 198, 251	0
33	RN	138/140 (98%)	0.54	8 (5%) 30 24	66, 108, 161, 194	0
33	YN	138/140 (98%)	0.52	9 (6%) 26 21	73, 109, 169, 195	0
34	RO	122/122 (100%)	0.24	4 (3%) 49 36	57, 99, 135, 164	0
34	YO	122/122 (100%)	0.13	3 (2%) 58 43	61, 91, 122, 142	0
35	RP	150/150 (100%)	0.61	9 (6%) 29 23	62, 112, 181, 243	0
35	YP	147/150 (98%)	0.36	7 (4%) 36 28	57, 103, 159, 195	0
36	RQ	141/141 (100%)	0.57	14 (9%) 14 14	70, 115, 185, 274	0
36	YQ	141/141 (100%)	0.61	13 (9%) 16 15	67, 113, 187, 294	0
37	RR	117/118 (99%)	0.09	5 (4%) 40 31	51, 93, 127, 246	0
37	YR	117/118 (99%)	0.40	5 (4%) 40 31	64, 94, 134, 214	0
38	RS	111/112 (99%)	0.23	2 (1%) 67 49	81, 133, 200, 253	0
38	YS	111/112 (99%)	0.87	10 (9%) 17 15	124, 175, 247, 333	0
39	RT	137/146 (93%)	0.32	2 (1%) 71 53	70, 111, 197, 271	0
39	YT	137/146 (93%)	0.43	9 (6%) 26 21	64, 109, 192, 233	0
40	RU	117/118 (99%)	0.60	6 (5%) 34 27	60, 103, 181, 251	0
40	YU	117/118 (99%)	0.64	7 (5%) 29 23	53, 93, 159, 213	0
41	RV	101/101 (100%)	0.55	6 (5%) 29 23	69, 122, 185, 288	0
41	YV	101/101 (100%)	0.45	3 (2%) 52 38	59, 113, 178, 321	0
42	RW	113/113 (100%)	0.21	5 (4%) 39 30	53, 81, 146, 249	0
42	YW	113/113 (100%)	0.24	4 (3%) 47 35	54, 81, 135, 258	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	RX	92/96 (95%)	0.35	4 (4%) 40 31	62, 96, 137, 202	0
43	YX	92/96 (95%)	0.09	0 100 100	50, 84, 128, 162	0
44	RY	107/110 (97%)	0.63	8 (7%) 22 18	77, 119, 185, 233	0
44	YY	107/110 (97%)	0.30	2 (1%) 66 48	62, 105, 157, 191	0
45	RZ	183/206 (88%)	0.13	0 100 100	107, 155, 233, 281	0
45	YZ	183/206 (88%)	0.11	2 (1%) 77 60	103, 168, 229, 303	0
46	R0	81/85 (95%)	0.39	5 (6%) 28 22	71, 104, 139, 233	0
46	Y0	75/85 (88%)	0.20	2 (2%) 56 41	80, 119, 149, 184	0
47	R1	97/98 (98%)	0.53	6 (6%) 28 22	61, 93, 187, 254	0
47	Y1	93/98 (94%)	0.67	8 (8%) 18 15	55, 94, 158, 196	0
48	R2	69/72 (95%)	0.54	4 (5%) 30 24	67, 120, 196, 265	0
48	Y2	69/72 (95%)	0.11	3 (4%) 40 31	60, 94, 173, 360	0
49	R3	59/60 (98%)	-0.03	0 100 100	64, 106, 171, 193	0
49	Y3	59/60 (98%)	0.15	1 (1%) 69 50	79, 106, 171, 207	0
50	R4	69/71 (97%)	0.29	0 100 100	118, 170, 258, 325	0
50	Y4	69/71 (97%)	0.27	1 (1%) 73 55	149, 197, 246, 317	0
51	R5	59/60 (98%)	0.14	1 (1%) 69 50	63, 96, 179, 245	0
51	Y5	59/60 (98%)	0.16	1 (1%) 69 50	63, 98, 192, 287	0
52	R6	53/54 (98%)	0.53	1 (1%) 66 48	136, 156, 204, 236	0
52	Y6	53/54 (98%)	0.45	0 100 100	129, 168, 237, 253	0
53	R7	47/49 (95%)	0.46	2 (4%) 40 31	48, 77, 119, 190	0
53	Y7	48/49 (97%)	0.30	3 (6%) 27 22	47, 68, 135, 168	0
54	R8	64/65 (98%)	0.89	5 (7%) 20 17	59, 98, 156, 238	0
54	Y8	64/65 (98%)	0.84	8 (12%) 9 12	67, 96, 145, 265	0
55	R9	37/37 (100%)	0.10	0 100 100	118, 151, 203, 237	0
55	Y9	37/37 (100%)	0.22	1 (2%) 56 41	118, 137, 202, 214	0
All	All	21014/21610 (97%)	0.16	628 (2%) 52 38	45, 114, 216, 477	0

All (628) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	RD	2	ALA	8.3
12	XL	28	LYS	7.4

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Mol	Chain	Res	Type	RSRZ
20	QT	9	ASN	7.4
35	RP	13	ASN	7.1
20	XT	9	ASN	6.7
27	YD	34	VAL	6.7
46	R0	4	LYS	6.2
13	QM	102	ARG	6.1
19	QS	83	HIS	5.8
46	R0	3	HIS	5.8
27	RD	5	LYS	5.7
13	QM	120	LYS	5.7
12	QL	19	ARG	5.6
10	XJ	54	PHE	5.5
27	YD	2	ALA	5.4
36	YQ	80	GLU	5.1
47	Y1	27	GLU	4.9
39	YT	106	SER	4.8
10	QJ	58	ASP	4.8
47	Y1	26	ARG	4.7
27	RD	33	LEU	4.7
32	RI	20	ASP	4.7
12	XL	16	GLU	4.7
22	XW	47	G	4.6
12	QL	18	VAL	4.6
36	YQ	90	VAL	4.6
10	QJ	55	LYS	4.6
27	RD	34	VAL	4.5
10	QJ	54	PHE	4.5
27	RD	40	THR	4.5
22	QW	47	G	4.4
20	XT	18	GLN	4.4
13	QM	117	VAL	4.4
36	RQ	90	VAL	4.3
27	RD	44	ASN	4.3
9	QI	126	SER	4.3
22	XW	1	C	4.3
13	QM	106	ASN	4.2
9	XI	126	SER	4.1
9	XI	110	GLU	4.1
27	YD	33	LEU	4.1
35	RP	15	ARG	4.1
12	QL	16	GLU	4.1
48	R2	52	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
12	QL	27	LEU	4.1
10	XJ	55	LYS	4.0
53	R7	1	MET	4.0
29	RF	78	ILE	4.0
44	RY	107	ASP	4.0
20	QT	15	ARG	3.9
42	YW	92	ARG	3.9
35	RP	74	GLU	3.9
13	QM	121	LYS	3.9
12	XL	27	LEU	3.9
38	YS	22	GLY	3.9
23	XX	23	A	3.9
42	RW	92	ARG	3.8
12	XL	13	LYS	3.8
38	YS	86	ALA	3.8
9	XI	127	LYS	3.8
9	QI	125	TYR	3.8
4	XD	24	GLU	3.8
20	QT	11	SER	3.8
27	RD	38	LYS	3.7
10	QJ	46	ARG	3.7
12	QL	28	LYS	3.7
41	YV	36	PRO	3.7
22	QW	1	C	3.7
19	QS	78	ARG	3.7
28	YE	127	ASP	3.7
12	XL	26	ALA	3.7
35	YP	61	ARG	3.7
20	QT	14	LYS	3.7
40	YU	97	ASP	3.6
20	XT	23	ARG	3.6
35	RP	61	ARG	3.6
27	RD	25	THR	3.6
39	YT	104	ASN	3.6
36	YQ	83	MET	3.6
44	RY	58	GLY	3.6
3	XC	62	ASP	3.6
12	XL	8	ASN	3.6
11	XK	87	THR	3.5
2	QB	231	GLU	3.5
42	RW	90	ARG	3.5
27	YD	240	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
2	QB	215	LEU	3.5
47	Y1	91	LYS	3.5
38	YS	43	GLU	3.5
9	XI	124	GLN	3.5
19	QS	76	PRO	3.5
14	XN	2	ALA	3.4
13	XM	120	LYS	3.4
37	RR	9	LYS	3.4
36	RQ	80	GLU	3.4
12	QL	21	LYS	3.4
54	R8	3	LYS	3.4
15	XO	50	HIS	3.4
21	QU	2	GLY	3.4
25	YA	1762	A	3.4
12	XL	7	ILE	3.3
33	YN	109	LYS	3.3
25	RA	2506	U	3.3
25	YA	2506	U	3.3
5	XE	11	ILE	3.3
20	QT	20	LEU	3.3
7	XG	146	GLU	3.3
39	YT	69	GLY	3.3
33	RN	12	ARG	3.3
17	XQ	30	PRO	3.3
28	YE	114	ALA	3.3
17	XQ	96	GLU	3.3
23	QX	22	C	3.3
37	YR	102	GLU	3.3
27	YD	203	ASN	3.2
27	RD	28	GLU	3.2
32	YI	121	LYS	3.2
35	RP	27	HIS	3.2
29	YF	70	THR	3.2
31	YH	18	GLU	3.2
1	XA	5	U	3.2
20	QT	25	ARG	3.2
25	RA	1762	A	3.2
47	R1	92	LYS	3.2
35	YP	24	GLY	3.2
53	Y7	1	MET	3.2
19	XS	74	PHE	3.2
25	YA	2602	A	3.1

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Mol	Chain	Res	Type	RSRZ
29	RF	72	ARG	3.1
13	QM	103	THR	3.1
19	XS	79	THR	3.1
33	RN	133	GLN	3.1
7	XG	5	ARG	3.1
29	RF	62	ARG	3.1
35	YP	13	ASN	3.1
9	QI	127	LYS	3.1
31	YH	155	SER	3.1
35	YP	65	ARG	3.1
9	QI	106	ALA	3.1
11	QK	127	LYS	3.1
9	QI	128	ARG	3.1
29	YF	131	GLY	3.1
27	RD	240	ALA	3.1
29	YF	47	GLY	3.1
42	RW	78	GLU	3.1
51	Y5	2	ALA	3.1
29	YF	69	HIS	3.1
31	YH	3	ARG	3.1
41	RV	26	ASP	3.0
1	QA	966	G	3.0
19	QS	80	TYR	3.0
29	RF	133	ASN	3.0
10	QJ	47	PHE	3.0
25	RA	2602	A	3.0
25	YA	2142	C	3.0
29	YF	56	GLU	3.0
42	YW	93	ALA	3.0
27	RD	22	SER	3.0
8	XH	102	ARG	3.0
32	YI	1	MET	3.0
38	RS	110	LEU	3.0
27	RD	176	ARG	3.0
20	XT	24	LEU	3.0
46	R0	5	LYS	3.0
28	RE	130	GLY	3.0
9	XI	118	LYS	3.0
11	QK	11	LYS	3.0
27	RD	35	LYS	3.0
47	Y1	22	GLY	3.0
22	QV	77	A	3.0

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Mol	Chain	Res	Type	RSRZ
48	R2	43	GLN	3.0
20	QT	29	LYS	3.0
16	XP	25	ARG	3.0
38	YS	37	ALA	3.0
25	RA	1099	G	2.9
25	RA	2062	A	2.9
12	QL	22	SER	2.9
25	YA	1659	U	2.9
17	XQ	38	ARG	2.9
32	YI	82	ARG	2.9
40	RU	7	GLY	2.9
15	XO	48	LYS	2.9
8	XH	25	ASP	2.9
27	RD	200	ASP	2.9
17	XQ	68	ARG	2.9
10	QJ	62	HIS	2.9
22	XV	1	C	2.9
25	YA	1660	C	2.9
9	QI	124	GLN	2.9
29	RF	56	GLU	2.9
39	RT	106	SER	2.9
27	YD	38	LYS	2.9
3	XC	15	THR	2.9
10	QJ	48	THR	2.9
33	YN	93	THR	2.9
25	YA	1678	G	2.9
5	XE	18	ARG	2.9
39	YT	8	LYS	2.9
31	YH	150	ALA	2.9
47	R1	95	LEU	2.9
22	QV	1	C	2.9
25	YA	1656	C	2.9
12	XL	15	ARG	2.9
19	QS	81	ARG	2.9
9	QI	115	GLY	2.8
3	QC	3	ASN	2.8
39	YT	109	GLU	2.8
37	YR	7	GLY	2.8
43	RX	69	TYR	2.8
32	YI	143	SER	2.8
32	YI	118	LYS	2.8
36	YQ	86	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
36	YQ	88	GLY	2.8
12	QL	15	ARG	2.8
25	RA	2142	C	2.8
18	XR	82	THR	2.8
25	RA	214	G	2.8
12	QL	17	LYS	2.8
20	QT	21	LYS	2.8
27	YD	97	TYR	2.8
30	RG	97	ASP	2.8
41	YV	38	LEU	2.8
30	RG	28	VAL	2.8
35	RP	38	GLN	2.8
2	QB	152	PHE	2.8
19	QS	41	VAL	2.8
32	RI	16	GLY	2.8
32	RI	84	GLY	2.8
42	RW	91	GLY	2.8
53	Y7	48	LYS	2.8
25	RA	34	C	2.7
47	R1	98	LEU	2.7
40	YU	91	ASP	2.7
9	XI	121	ARG	2.7
17	XQ	101	ARG	2.7
5	XE	21	ALA	2.7
4	XD	154	ASN	2.7
20	XT	14	LYS	2.7
36	RQ	83	MET	2.7
19	QS	79	THR	2.7
33	YN	61	ARG	2.7
28	YE	118	LYS	2.7
29	RF	131	GLY	2.7
19	QS	40	ILE	2.7
39	YT	1	MET	2.7
36	YQ	104	PHE	2.7
27	YD	91	ARG	2.7
36	RQ	87	LYS	2.7
41	YV	37	VAL	2.7
25	YA	744	G	2.7
44	RY	33	LYS	2.7
47	Y1	11	ARG	2.7
12	QL	14	GLY	2.7
26	RB	1	U	2.7

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Mol	Chain	Res	Type	RSRZ
27	RD	12	SER	2.7
40	YU	95	LEU	2.7
43	RX	66	LEU	2.7
12	XL	19	ARG	2.7
10	QJ	56	HIS	2.7
33	YN	53	VAL	2.7
28	RE	20	ALA	2.7
28	YE	205	ALA	2.7
51	R5	2	ALA	2.7
34	RO	34	THR	2.7
31	YH	4	ILE	2.7
13	XM	94	ARG	2.7
37	RR	2	ARG	2.7
28	YE	25	VAL	2.6
25	YA	2031	A	2.6
48	Y2	11	GLU	2.6
33	YN	138	LEU	2.6
1	QA	570	G	2.6
25	YA	745	G	2.6
54	Y8	52	LYS	2.6
4	XD	31	CYS	2.6
20	XT	20	LEU	2.6
53	Y7	36	GLN	2.6
12	QL	105	TYR	2.6
25	RA	6	A	2.6
1	QA	1124	G	2.6
5	QE	24	ARG	2.6
5	XE	24	ARG	2.6
20	XT	25	ARG	2.6
28	RE	152	LYS	2.6
39	YT	11	GLU	2.6
25	RA	2140	C	2.6
25	YA	1273	U	2.6
40	RU	97	ASP	2.6
36	RQ	79	LEU	2.6
20	XT	21	LYS	2.6
28	YE	130	GLY	2.6
9	XI	123	PRO	2.6
41	RV	28	GLU	2.6
1	QA	64	G	2.6
12	QL	26	ALA	2.6
25	YA	270(Y)	G	2.6

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Mol	Chain	Res	Type	RSRZ
25	YA	363	G	2.6
1	QA	1126	U	2.6
10	QJ	50	ILE	2.6
34	RO	74	GLY	2.6
10	QJ	61	GLU	2.6
41	RV	33	VAL	2.6
27	YD	200	ASP	2.6
27	RD	273	ARG	2.6
36	YQ	91	GLU	2.5
2	QB	168	THR	2.5
22	QW	32	G	2.5
25	RA	2141	G	2.5
2	QB	195	ASP	2.5
46	Y0	9	SER	2.5
27	YD	35	LYS	2.5
31	YH	153	LYS	2.5
31	YH	152	ARG	2.5
48	Y2	7	ARG	2.5
1	XA	334	C	2.5
22	XW	66	C	2.5
19	QS	82	GLY	2.5
1	XA	631	G	2.5
22	XV	77	A	2.5
25	RA	1847	A	2.5
32	RI	38	LEU	2.5
20	QT	17	ARG	2.5
46	R0	53	MET	2.5
28	YE	186	GLY	2.5
25	YA	889	C	2.5
34	RO	120	GLU	2.5
7	QG	32	ARG	2.5
7	QG	2	ALA	2.5
22	QW	6	G	2.5
25	YA	275	G	2.5
36	RQ	105	GLU	2.5
42	YW	90	ARG	2.5
28	YE	90	THR	2.5
36	YQ	21	THR	2.5
25	RA	1053	C	2.5
9	XI	115	GLY	2.5
18	QR	84	LYS	2.5
33	YN	29	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
20	QT	24	LEU	2.5
32	RI	12	LEU	2.5
33	YN	134	ARG	2.5
37	YR	8	ARG	2.5
39	YT	6	LEU	2.5
10	QJ	49	VAL	2.5
12	XL	18	VAL	2.5
30	RG	2	PRO	2.5
44	RY	29	GLU	2.5
7	QG	152	ALA	2.4
25	RA	2611	U	2.4
9	XI	122	ALA	2.4
29	RF	70	THR	2.4
20	XT	22	ARG	2.4
28	YE	111	ARG	2.4
25	YA	1661	G	2.4
33	RN	1	MET	2.4
12	QL	48	PRO	2.4
4	XD	163	GLU	2.4
4	XD	208	SER	2.4
5	XE	81	GLU	2.4
27	RD	26	LYS	2.4
36	YQ	79	LEU	2.4
27	RD	238	GLY	2.4
47	Y1	9	GLY	2.4
19	QS	10	PHE	2.4
43	RX	55	ASN	2.4
47	R1	91	LYS	2.4
48	Y2	72	ALA	2.4
17	XQ	91	ARG	2.4
25	YA	2688	U	2.4
19	XS	63	THR	2.4
41	RV	35	LEU	2.4
1	QA	346	G	2.4
39	RT	69	GLY	2.4
55	Y9	37	GLY	2.4
25	YA	34	C	2.4
4	XD	150	GLU	2.4
30	RG	75	LYS	2.4
14	QN	2	ALA	2.4
28	RE	187	ALA	2.4
13	QM	94	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
9	QI	109	VAL	2.4
32	RI	18	VAL	2.4
37	RR	73	VAL	2.4
38	YS	82	ILE	2.4
29	YF	66	PRO	2.4
4	XD	60	GLU	2.4
17	QQ	24	GLU	2.4
1	QA	1202	G	2.4
39	YT	112	ARG	2.4
36	RQ	81	VAL	2.3
41	RV	45	THR	2.3
32	RI	80	PRO	2.3
11	QK	128	ALA	2.3
27	RD	195	ALA	2.3
35	RP	31	ALA	2.3
44	YY	78	ALA	2.3
20	QT	16	HIS	2.3
28	YE	72	VAL	2.3
40	RU	105	VAL	2.3
12	XL	6	THR	2.3
27	RD	259	THR	2.3
29	RF	85	GLY	2.3
28	YE	113	PHE	2.3
47	Y1	92	LYS	2.3
54	Y8	29	LYS	2.3
1	QA	811	C	2.3
6	XF	53	ALA	2.3
29	RF	81	PRO	2.3
22	QW	66	C	2.3
1	QA	965	A	2.3
2	QB	172	ILE	2.3
20	XT	11	SER	2.3
27	RD	4	LYS	2.3
28	YE	203	LYS	2.3
1	QA	1281	U	2.3
27	YD	259	THR	2.3
32	YI	84	GLY	2.3
36	YQ	75	THR	2.3
13	XM	87	TYR	2.3
29	RF	140	LEU	2.3
4	QD	24	GLU	2.3
8	QH	99	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
9	QI	38	GLN	2.3
33	RN	46	VAL	2.3
49	Y3	59	VAL	2.3
1	QA	280	C	2.3
22	XW	75	C	2.3
25	RA	2146	C	2.3
35	RP	28	GLY	2.3
12	QL	64	TYR	2.3
1	QA	975	A	2.3
20	XT	15	ARG	2.3
25	YA	1677	A	2.3
13	XM	90	LEU	2.3
28	YE	77	ILE	2.3
42	RW	94	ASP	2.3
54	Y8	46	ARG	2.3
35	YP	62	LEU	2.3
12	XL	5	PRO	2.3
54	R8	63	PRO	2.3
13	XM	8	GLU	2.3
17	XQ	90	ILE	2.3
22	QW	4	G	2.3
22	QW	12	G	2.3
25	RA	1098	A	2.3
25	YA	2062	A	2.3
27	RD	237	GLU	2.3
1	QA	82	U	2.3
28	YE	132	HIS	2.3
36	RQ	65	PHE	2.3
17	XQ	93	GLN	2.3
37	YR	2	ARG	2.3
28	YE	153	GLY	2.3
46	R0	6	GLY	2.3
48	R2	44	LEU	2.3
34	YO	81	ASP	2.3
36	RQ	25	ASP	2.3
28	YE	131	ALA	2.3
12	XL	17	LYS	2.2
32	RI	1	MET	2.2
32	RI	2	LYS	2.2
5	XE	83	GLU	2.2
40	YU	90	VAL	2.2
54	R8	54	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
10	XJ	62	HIS	2.2
14	XN	29	ARG	2.2
1	XA	60	A	2.2
3	XC	165	THR	2.2
27	YD	12	SER	2.2
31	YH	154	PRO	2.2
15	XO	60	VAL	2.2
4	XD	81	GLU	2.2
5	XE	152	ARG	2.2
33	YN	68	GLU	2.2
45	YZ	181	GLU	2.2
34	YO	91	LEU	2.2
3	QC	160	ALA	2.2
33	RN	13	TRP	2.2
29	YF	89	VAL	2.2
1	XA	968	A	2.2
25	YA	270(O)	U	2.2
26	YB	1	U	2.2
27	YD	176	ARG	2.2
33	YN	96	GLU	2.2
17	XQ	95	TYR	2.2
25	RA	1068	G	2.2
40	RU	96	ALA	2.2
9	QI	123	PRO	2.2
12	QL	5	PRO	2.2
33	RN	14	VAL	2.2
40	RU	36	ARG	2.2
4	XD	156	GLU	2.2
5	XE	50	GLU	2.2
47	R1	27	GLU	2.2
36	YQ	87	LYS	2.2
38	YS	108	GLY	2.2
5	QE	13	ILE	2.2
19	XS	78	ARG	2.2
19	QS	53	ASN	2.2
28	RE	17	ASP	2.2
25	RA	101	G	2.2
8	XH	99	GLU	2.2
18	QR	46	GLU	2.2
47	R1	93	GLU	2.2
48	R2	31	GLU	2.2
27	RD	59	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
36	YQ	84	GLY	2.2
9	XI	117	HIS	2.2
10	XJ	23	ILE	2.2
38	YS	18	ILE	2.2
4	QD	49	ARG	2.2
10	QJ	85	LEU	2.2
25	RA	1937	A	2.2
25	RA	2015	A	2.2
37	YR	15	SER	2.2
9	QI	118	LYS	2.1
27	YD	5	LYS	2.1
27	RD	23	GLU	2.1
42	YW	78	GLU	2.1
13	XM	85	GLY	2.1
29	RF	59	TYR	2.1
32	YI	133	HIS	2.1
7	XG	147	ALA	2.1
9	XI	120	ARG	2.1
35	RP	62	LEU	2.1
32	RI	134	PRO	2.1
54	Y8	63	PRO	2.1
27	RD	20	ASP	2.1
46	Y0	53	MET	2.1
28	YE	151	TYR	2.1
36	RQ	33	GLY	2.1
4	XD	48	ALA	2.1
22	QW	75	C	2.1
36	RQ	76	LYS	2.1
38	RS	59	LYS	2.1
44	RY	47	LYS	2.1
27	YD	25	THR	2.1
5	XE	10	MET	2.1
31	RH	155	SER	2.1
38	YS	88	ASP	2.1
54	Y8	56	GLU	2.1
17	XQ	36	ILE	2.1
44	RY	10	GLY	2.1
1	QA	963	G	2.1
22	QW	9	G	2.1
25	YA	2578	G	2.1
35	YP	71	VAL	2.1
40	RU	98	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
12	XL	47	LYS	2.1
19	QS	32	LYS	2.1
27	RD	68	LYS	2.1
1	QA	242	C	2.1
1	XA	311	C	2.1
13	QM	116	THR	2.1
25	RA	2145	C	2.1
11	QK	129	SER	2.1
30	YG	164	GLU	2.1
32	RI	42	SER	2.1
34	YO	45	GLU	2.1
36	RQ	89	ASN	2.1
36	RQ	104	PHE	2.1
38	YS	2	ALA	2.1
2	XB	15	VAL	2.1
2	XB	138	LEU	2.1
30	YG	36	LYS	2.1
27	YD	40	THR	2.1
34	RO	1	MET	2.1
43	RX	3	THR	2.1
2	XB	96	ARG	2.1
22	XW	2	G	2.1
25	YA	2141	G	2.1
44	RY	50	ARG	2.1
5	XE	111	GLU	2.1
44	RY	64	GLU	2.1
22	QW	38	A	2.1
47	Y1	36	GLY	2.1
1	QA	63	C	2.1
1	XA	280	C	2.1
25	RA	1761	C	2.1
25	YA	2143	C	2.1
28	RE	116	VAL	2.1
36	RQ	130	LYS	2.1
38	YS	44	LYS	2.1
52	R6	5	VAL	2.1
41	RV	36	PRO	2.1
16	QP	26	ARG	2.1
37	RR	103	ARG	2.1
3	XC	32	LEU	2.1
6	XF	54	LYS	2.1
28	YE	133	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
50	Y4	25	TYR	2.1
6	XF	55	ASP	2.0
36	YQ	135	ASP	2.0
16	QP	76	GLN	2.0
33	RN	8	GLN	2.0
25	RA	1093	G	2.0
25	YA	2003	G	2.0
54	R8	53	PRO	2.0
1	XA	63	C	2.0
27	RD	27	THR	2.0
4	XD	130	GLY	2.0
9	QI	96	LEU	2.0
10	QJ	71	LEU	2.0
35	YP	64	LYS	2.0
9	QI	110	GLU	2.0
40	YU	89	GLU	2.0
40	YU	108	GLU	2.0
10	QJ	68	HIS	2.0
53	R7	36	GLN	2.0
54	Y8	35	GLN	2.0
7	XG	4	ARG	2.0
2	XB	214	ILE	2.0
54	Y8	53	PRO	2.0
13	QM	2	ALA	2.0
54	R8	45	GLY	2.0
54	Y8	45	GLY	2.0
18	XR	46	GLU	2.0
37	RR	102	GLU	2.0
45	YZ	169	GLU	2.0
25	RA	654(S)	G	2.0
25	RA	2789	C	2.0
40	YU	69	CYS	2.0
3	XC	28	GLN	2.0
8	QH	52	ASP	2.0
28	RE	54	GLN	2.0
44	YY	107	ASP	2.0
32	YI	119	PRO	2.0
33	RN	137	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3392	1/1	0.09	0.19	124,124,124,124	0
56	MG	XS	101	1/1	0.19	0.11	125,125,125,125	0
56	MG	YA	3357	1/1	0.20	0.14	204,204,204,204	0
56	MG	YA	3294	1/1	0.24	0.27	99,99,99,99	0
56	MG	YA	3173	1/1	0.29	0.23	78,78,78,78	0
56	MG	XV	108	1/1	0.36	0.13	130,130,130,130	0
56	MG	RA	3212	1/1	0.37	0.24	81,81,81,81	0
56	MG	RB	207	1/1	0.40	0.14	94,94,94,94	0
56	MG	RA	3337	1/1	0.41	0.24	85,85,85,85	0
56	MG	RA	3467	1/1	0.42	0.12	99,99,99,99	0
56	MG	YX	102	1/1	0.42	0.33	63,63,63,63	0
56	MG	RA	3430	1/1	0.43	0.12	171,171,171,171	0
56	MG	RA	3002	1/1	0.44	0.26	70,70,70,70	0
56	MG	QA	1668	1/1	0.46	0.23	84,84,84,84	0
56	MG	RA	3213	1/1	0.47	0.45	39,39,39,39	0
56	MG	YA	3184	1/1	0.47	0.17	66,66,66,66	0
56	MG	YA	3451	1/1	0.48	0.15	100,100,100,100	0
56	MG	YA	3361	1/1	0.49	0.12	83,83,83,83	0
56	MG	YB	207	1/1	0.49	0.13	113,113,113,113	0
56	MG	YA	3358	1/1	0.49	0.12	91,91,91,91	0
56	MG	YA	3266	1/1	0.50	0.18	96,96,96,96	0
56	MG	XA	1662	1/1	0.50	0.14	107,107,107,107	0
56	MG	XA	1665	1/1	0.50	0.07	118,118,118,118	0
56	MG	YA	3449	1/1	0.51	0.09	89,89,89,89	0
56	MG	RA	3202	1/1	0.51	0.21	52,52,52,52	0
56	MG	RA	3318	1/1	0.52	0.13	53,53,53,53	0
56	MG	RA	3453	1/1	0.52	0.10	268,268,268,268	0
56	MG	QA	1624	1/1	0.53	0.17	72,72,72,72	0
56	MG	RA	3472	1/1	0.53	0.10	84,84,84,84	0
56	MG	RA	3485	1/1	0.53	0.22	73,73,73,73	0
56	MG	RA	3308	1/1	0.53	0.15	70,70,70,70	0
56	MG	YA	3319	1/1	0.54	0.20	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3425	1/1	0.54	0.23	64,64,64,64	0
56	MG	YA	3471	1/1	0.55	0.14	78,78,78,78	0
56	MG	RA	3209	1/1	0.55	0.25	80,80,80,80	0
56	MG	RA	3357	1/1	0.55	0.17	80,80,80,80	0
56	MG	RA	3442	1/1	0.56	0.15	70,70,70,70	0
56	MG	YA	3485	1/1	0.56	0.07	94,94,94,94	0
56	MG	YA	3345	1/1	0.56	0.13	104,104,104,104	0
56	MG	XM	201	1/1	0.56	0.12	110,110,110,110	0
56	MG	YA	3456	1/1	0.57	0.29	84,84,84,84	0
56	MG	YA	3331	1/1	0.58	0.23	62,62,62,62	0
56	MG	YD	301	1/1	0.58	0.29	52,52,52,52	0
56	MG	RA	3322	1/1	0.58	0.20	74,74,74,74	0
56	MG	XA	1661	1/1	0.59	0.14	78,78,78,78	0
56	MG	RA	3108	1/1	0.59	0.21	52,52,52,52	0
58	ZN	R5	501	1/1	0.59	0.25	247,247,247,247	0
56	MG	RA	3283	1/1	0.60	0.22	69,69,69,69	0
56	MG	RA	3363	1/1	0.60	0.19	70,70,70,70	0
56	MG	RA	3287	1/1	0.60	0.25	102,102,102,102	0
56	MG	RA	3272	1/1	0.60	0.21	50,50,50,50	0
56	MG	QA	1638	1/1	0.61	0.32	62,62,62,62	0
56	MG	QA	1650	1/1	0.61	0.33	76,76,76,76	0
56	MG	YA	3212	1/1	0.61	0.22	72,72,72,72	0
56	MG	RA	3478	1/1	0.61	0.10	94,94,94,94	0
56	MG	RA	3304	1/1	0.61	0.27	71,71,71,71	0
56	MG	YA	3397	1/1	0.61	0.10	75,75,75,75	0
56	MG	RB	206	1/1	0.61	0.17	87,87,87,87	0
56	MG	RA	3098	1/1	0.61	0.20	44,44,44,44	0
56	MG	RA	3366	1/1	0.62	0.15	95,95,95,95	0
56	MG	YA	3512	1/1	0.62	0.24	82,82,82,82	0
56	MG	RA	3355	1/1	0.62	0.09	103,103,103,103	0
56	MG	YA	3254	1/1	0.62	0.25	51,51,51,51	0
56	MG	YQ	203	1/1	0.62	0.13	82,82,82,82	0
56	MG	RB	205	1/1	0.62	0.23	85,85,85,85	0
56	MG	YA	3353	1/1	0.62	0.23	78,78,78,78	0
56	MG	RA	3460	1/1	0.63	0.11	65,65,65,65	0
56	MG	YA	3085	1/1	0.63	0.24	28,28,28,28	0
56	MG	YA	3309	1/1	0.63	0.11	99,99,99,99	0
56	MG	YA	3534	1/1	0.63	0.14	89,89,89,89	0
56	MG	QA	1664	1/1	0.63	0.29	84,84,84,84	0
56	MG	YB	209	1/1	0.63	0.10	75,75,75,75	0
56	MG	RA	3125	1/1	0.63	0.15	80,80,80,80	0
56	MG	YA	3195	1/1	0.63	0.31	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3215	1/1	0.63	0.24	65,65,65,65	0
56	MG	Y8	101	1/1	0.63	0.23	74,74,74,74	0
56	MG	XA	1637	1/1	0.63	0.24	145,145,145,145	0
56	MG	YA	3320	1/1	0.64	0.18	85,85,85,85	0
56	MG	RA	3512	1/1	0.64	0.25	64,64,64,64	0
56	MG	RA	3374	1/1	0.64	0.13	73,73,73,73	0
56	MG	YA	3350	1/1	0.64	0.18	76,76,76,76	0
56	MG	RA	3505	1/1	0.64	0.32	67,67,67,67	0
56	MG	RA	3465	1/1	0.65	0.17	89,89,89,89	0
56	MG	YA	3077	1/1	0.65	0.14	52,52,52,52	0
56	MG	XA	1633	1/1	0.65	0.15	70,70,70,70	0
56	MG	RA	3409	1/1	0.65	0.57	81,81,81,81	0
56	MG	YA	3292	1/1	0.65	0.15	57,57,57,57	0
56	MG	YA	3346	1/1	0.65	0.09	82,82,82,82	0
56	MG	RA	3452	1/1	0.65	0.14	67,67,67,67	0
58	ZN	YY	202	1/1	0.65	0.28	234,234,234,234	0
56	MG	YA	3409	1/1	0.66	0.29	43,43,43,43	0
56	MG	YA	3414	1/1	0.66	0.16	67,67,67,67	0
56	MG	XA	1628	1/1	0.66	0.17	61,61,61,61	0
56	MG	RA	3282	1/1	0.66	0.14	100,100,100,100	0
56	MG	RA	3342	1/1	0.66	0.08	100,100,100,100	0
56	MG	RA	3353	1/1	0.66	0.11	74,74,74,74	0
56	MG	YA	3002	1/1	0.67	0.22	85,85,85,85	0
56	MG	QC	301	1/1	0.67	0.15	159,159,159,159	0
56	MG	RA	3470	1/1	0.67	0.25	92,92,92,92	0
56	MG	YA	3508	1/1	0.67	0.14	69,69,69,69	0
56	MG	QA	1670	1/1	0.67	0.12	86,86,86,86	0
56	MG	YA	3375	1/1	0.67	0.22	81,81,81,81	0
56	MG	YB	201	1/1	0.67	0.11	69,69,69,69	0
56	MG	RA	3418	1/1	0.67	0.19	65,65,65,65	0
56	MG	XA	1678	1/1	0.67	0.23	71,71,71,71	0
56	MG	YA	3334	1/1	0.67	0.07	67,67,67,67	0
56	MG	YA	3336	1/1	0.67	0.20	45,45,45,45	0
56	MG	YA	3419	1/1	0.67	0.16	79,79,79,79	0
56	MG	XA	1627	1/1	0.67	0.14	43,43,43,43	0
56	MG	RA	3421	1/1	0.67	0.07	98,98,98,98	0
56	MG	RA	3316	1/1	0.67	0.23	59,59,59,59	0
56	MG	QA	1661	1/1	0.68	0.14	50,50,50,50	0
56	MG	YA	3228	1/1	0.68	0.26	77,77,77,77	0
56	MG	YA	3520	1/1	0.68	0.42	48,48,48,48	0
56	MG	YA	3344	1/1	0.68	0.25	73,73,73,73	0
56	MG	QX	101	1/1	0.68	0.11	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3406	1/1	0.68	0.17	56,56,56,56	0
56	MG	YA	3155	1/1	0.68	0.16	60,60,60,60	0
56	MG	YA	3444	1/1	0.68	0.19	86,86,86,86	0
56	MG	RT	201	1/1	0.68	0.14	64,64,64,64	0
56	MG	YA	3179	1/1	0.68	0.13	96,96,96,96	0
56	MG	RA	3473	1/1	0.68	0.11	82,82,82,82	0
56	MG	YA	3194	1/1	0.68	0.22	28,28,28,28	0
56	MG	XX	101	1/1	0.68	0.16	81,81,81,81	0
56	MG	RA	3275	1/1	0.69	0.25	49,49,49,49	0
56	MG	YA	3394	1/1	0.69	0.22	80,80,80,80	0
56	MG	YA	3165	1/1	0.69	0.11	68,68,68,68	0
56	MG	RA	3006	1/1	0.69	0.14	54,54,54,54	0
56	MG	YA	3035	1/1	0.69	0.20	35,35,35,35	0
56	MG	YA	3182	1/1	0.69	0.11	85,85,85,85	0
56	MG	YA	3074	1/1	0.69	0.26	75,75,75,75	0
56	MG	XV	101	1/1	0.69	0.17	50,50,50,50	0
56	MG	RA	3321	1/1	0.69	0.17	73,73,73,73	0
56	MG	YA	3116	1/1	0.69	0.28	41,41,41,41	0
56	MG	YA	3362	1/1	0.69	0.14	70,70,70,70	0
56	MG	YA	3219	1/1	0.69	0.16	30,30,30,30	0
56	MG	YA	3390	1/1	0.69	0.20	63,63,63,63	0
56	MG	RA	3499	1/1	0.70	0.19	70,70,70,70	0
56	MG	RA	3179	1/1	0.70	0.23	84,84,84,84	0
56	MG	RA	3345	1/1	0.70	0.20	90,90,90,90	0
56	MG	YA	3203	1/1	0.70	0.12	100,100,100,100	0
56	MG	RB	202	1/1	0.70	0.11	76,76,76,76	0
56	MG	RA	3320	1/1	0.70	0.15	74,74,74,74	0
56	MG	RA	3134	1/1	0.70	0.17	30,30,30,30	0
56	MG	RA	3159	1/1	0.70	0.12	46,46,46,46	0
56	MG	YA	3470	1/1	0.70	0.14	106,106,106,106	0
56	MG	YA	3262	1/1	0.70	0.20	77,77,77,77	0
58	ZN	R4	500	1/1	0.70	0.21	241,241,241,241	0
56	MG	RA	3216	1/1	0.70	0.27	88,88,88,88	0
56	MG	YA	3288	1/1	0.70	0.25	81,81,81,81	0
56	MG	YA	3284	1/1	0.71	0.18	51,51,51,51	0
56	MG	RA	3147	1/1	0.71	0.13	85,85,85,85	0
56	MG	YA	3291	1/1	0.71	0.26	37,37,37,37	0
56	MG	YA	3118	1/1	0.71	0.14	46,46,46,46	0
56	MG	RA	3007	1/1	0.71	0.15	84,84,84,84	0
56	MG	RA	3348	1/1	0.71	0.16	87,87,87,87	0
56	MG	YA	3169	1/1	0.71	0.25	74,74,74,74	0
56	MG	YB	210	1/1	0.71	0.10	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3222	1/1	0.71	0.14	73,73,73,73	0
56	MG	YA	3450	1/1	0.71	0.14	90,90,90,90	0
56	MG	YA	3330	1/1	0.71	0.12	68,68,68,68	0
56	MG	YA	3364	1/1	0.71	0.21	68,68,68,68	0
56	MG	RB	201	1/1	0.71	0.14	68,68,68,68	0
56	MG	RA	3208	1/1	0.71	0.16	43,43,43,43	0
56	MG	RA	3341	1/1	0.71	0.15	85,85,85,85	0
56	MG	YA	3403	1/1	0.72	0.12	64,64,64,64	0
56	MG	YA	3312	1/1	0.72	0.33	76,76,76,76	0
56	MG	RA	3156	1/1	0.72	0.11	44,44,44,44	0
56	MG	YA	3006	1/1	0.72	0.24	49,49,49,49	0
56	MG	YA	3322	1/1	0.72	0.10	94,94,94,94	0
56	MG	RA	3117	1/1	0.72	0.13	39,39,39,39	0
56	MG	YA	3172	1/1	0.72	0.16	54,54,54,54	0
56	MG	RA	3085	1/1	0.72	0.21	26,26,26,26	0
56	MG	YA	3174	1/1	0.72	0.09	76,76,76,76	0
56	MG	YA	3130	1/1	0.72	0.26	68,68,68,68	0
56	MG	YA	3463	1/1	0.72	0.13	110,110,110,110	0
56	MG	YA	3299	1/1	0.72	0.23	104,104,104,104	0
56	MG	YA	3131	1/1	0.72	0.13	86,86,86,86	0
56	MG	YA	3348	1/1	0.72	0.12	61,61,61,61	0
56	MG	YA	3489	1/1	0.72	0.23	102,102,102,102	0
56	MG	RA	3356	1/1	0.73	0.09	45,45,45,45	0
56	MG	YA	3491	1/1	0.73	0.15	76,76,76,76	0
56	MG	YA	3501	1/1	0.73	0.07	85,85,85,85	0
56	MG	YP	204	1/1	0.73	0.22	55,55,55,55	0
56	MG	YA	3149	1/1	0.73	0.27	88,88,88,88	0
56	MG	YA	3183	1/1	0.73	0.19	44,44,44,44	0
56	MG	RA	3324	1/1	0.73	0.16	91,91,91,91	0
56	MG	YA	3373	1/1	0.73	0.20	62,62,62,62	0
56	MG	YA	3481	1/1	0.73	0.23	87,87,87,87	0
56	MG	RA	3438	1/1	0.73	0.19	74,74,74,74	0
56	MG	YA	3301	1/1	0.74	0.17	60,60,60,60	0
56	MG	QV	106	1/1	0.74	0.32	95,95,95,95	0
56	MG	RA	3186	1/1	0.74	0.15	84,84,84,84	0
56	MG	YA	3264	1/1	0.74	0.35	82,82,82,82	0
56	MG	RA	3279	1/1	0.74	0.27	69,69,69,69	0
56	MG	RA	3488	1/1	0.74	0.17	66,66,66,66	0
56	MG	RA	3246	1/1	0.74	0.26	57,57,57,57	0
56	MG	RA	3450	1/1	0.74	0.12	79,79,79,79	0
56	MG	YA	3213	1/1	0.74	0.11	70,70,70,70	0
56	MG	YA	3422	1/1	0.74	0.23	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3495	1/1	0.74	0.16	74,74,74,74	0
56	MG	XA	1666	1/1	0.74	0.11	45,45,45,45	0
56	MG	YA	3370	1/1	0.74	0.18	55,55,55,55	0
56	MG	RA	3365	1/1	0.74	0.19	70,70,70,70	0
56	MG	RA	3251	1/1	0.75	0.21	43,43,43,43	0
56	MG	YA	3170	1/1	0.75	0.21	43,43,43,43	0
56	MG	RA	3458	1/1	0.75	0.10	64,64,64,64	0
56	MG	RA	3325	1/1	0.75	0.13	66,66,66,66	0
56	MG	YA	3311	1/1	0.75	0.17	48,48,48,48	0
56	MG	YA	3229	1/1	0.75	0.14	75,75,75,75	0
56	MG	YA	3098	1/1	0.75	0.31	34,34,34,34	0
56	MG	YA	3360	1/1	0.75	0.17	81,81,81,81	0
56	MG	RA	3175	1/1	0.75	0.10	56,56,56,56	0
56	MG	QA	1616	1/1	0.75	0.15	72,72,72,72	0
56	MG	YA	3326	1/1	0.75	0.13	52,52,52,52	0
56	MG	YA	3369	1/1	0.75	0.15	45,45,45,45	0
56	MG	YE	303	1/1	0.75	0.10	61,61,61,61	0
56	MG	RA	3138	1/1	0.75	0.19	40,40,40,40	0
56	MG	XA	1648	1/1	0.75	0.09	68,68,68,68	0
56	MG	RA	3089	1/1	0.75	0.27	28,28,28,28	0
56	MG	YA	3383	1/1	0.75	0.13	59,59,59,59	0
58	ZN	RY	202	1/1	0.75	0.25	226,226,226,226	0
56	MG	YA	3386	1/1	0.75	0.14	68,68,68,68	0
56	MG	RA	3121	1/1	0.75	0.18	37,37,37,37	0
56	MG	RA	3082	1/1	0.75	0.21	28,28,28,28	0
58	ZN	Y5	501	1/1	0.75	0.28	124,124,124,124	0
56	MG	YA	3376	1/1	0.76	0.10	141,141,141,141	0
56	MG	YA	3201	1/1	0.76	0.11	62,62,62,62	0
56	MG	YA	3537	1/1	0.76	0.19	63,63,63,63	0
56	MG	YA	3384	1/1	0.76	0.28	68,68,68,68	0
56	MG	YA	3453	1/1	0.76	0.18	80,80,80,80	0
56	MG	YA	3352	1/1	0.76	0.08	106,106,106,106	0
56	MG	YA	3283	1/1	0.76	0.18	80,80,80,80	0
56	MG	RA	3255	1/1	0.76	0.18	72,72,72,72	0
56	MG	RA	3314	1/1	0.76	0.17	56,56,56,56	0
56	MG	YA	3477	1/1	0.76	0.17	58,58,58,58	0
56	MG	YA	3137	1/1	0.76	0.12	73,73,73,73	0
56	MG	YA	3217	1/1	0.76	0.12	61,61,61,61	0
56	MG	Y7	101	1/1	0.76	0.17	82,82,82,82	0
56	MG	RA	3233	1/1	0.76	0.27	44,44,44,44	0
56	MG	RA	3377	1/1	0.76	0.15	81,81,81,81	0
56	MG	YA	3158	1/1	0.76	0.19	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RB	204	1/1	0.76	0.09	73,73,73,73	0
56	MG	RA	3317	1/1	0.76	0.24	65,65,65,65	0
56	MG	XA	1635	1/1	0.76	0.21	66,66,66,66	0
56	MG	RA	3471	1/1	0.77	0.19	65,65,65,65	0
56	MG	YA	3399	1/1	0.77	0.09	88,88,88,88	0
56	MG	YA	3461	1/1	0.77	0.16	76,76,76,76	0
56	MG	RA	3378	1/1	0.77	0.10	58,58,58,58	0
56	MG	YA	3407	1/1	0.77	0.18	72,72,72,72	0
56	MG	YA	3140	1/1	0.77	0.22	83,83,83,83	0
56	MG	RA	3201	1/1	0.77	0.16	89,89,89,89	0
56	MG	YA	3418	1/1	0.77	0.20	73,73,73,73	0
56	MG	RA	3227	1/1	0.77	0.12	50,50,50,50	0
56	MG	RA	3443	1/1	0.77	0.12	87,87,87,87	0
56	MG	YA	3306	1/1	0.77	0.23	102,102,102,102	0
56	MG	YA	3443	1/1	0.77	0.13	69,69,69,69	0
56	MG	YA	3269	1/1	0.77	0.13	46,46,46,46	0
56	MG	YA	3446	1/1	0.77	0.18	70,70,70,70	0
56	MG	YA	3342	1/1	0.77	0.16	49,49,49,49	0
56	MG	QA	1653	1/1	0.77	0.11	130,130,130,130	0
56	MG	RA	3280	1/1	0.77	0.30	73,73,73,73	0
56	MG	YA	3324	1/1	0.78	0.21	59,59,59,59	0
56	MG	QA	1649	1/1	0.78	0.07	62,62,62,62	0
56	MG	RA	3008	1/1	0.78	0.26	86,86,86,86	0
56	MG	RA	3047	1/1	0.78	0.12	71,71,71,71	0
56	MG	RA	3241	1/1	0.78	0.40	64,64,64,64	0
56	MG	RA	3153	1/1	0.78	0.10	38,38,38,38	0
56	MG	RA	3154	1/1	0.78	0.22	38,38,38,38	0
56	MG	RA	3292	1/1	0.78	0.17	56,56,56,56	0
56	MG	YA	3293	1/1	0.78	0.22	65,65,65,65	0
56	MG	RA	3294	1/1	0.78	0.27	63,63,63,63	0
56	MG	YA	3047	1/1	0.78	0.24	31,31,31,31	0
56	MG	YA	3166	1/1	0.78	0.38	64,64,64,64	0
56	MG	YQ	201	1/1	0.78	0.12	72,72,72,72	0
56	MG	YA	3303	1/1	0.78	0.23	50,50,50,50	0
56	MG	XA	1663	1/1	0.78	0.14	64,64,64,64	0
56	MG	Y0	102	1/1	0.78	0.09	51,51,51,51	0
56	MG	YA	3227	1/1	0.78	0.20	49,49,49,49	0
56	MG	RA	3065	1/1	0.78	0.12	36,36,36,36	0
56	MG	RA	3260	1/1	0.78	0.21	45,45,45,45	0
56	MG	RA	3218	1/1	0.78	0.14	67,67,67,67	0
56	MG	YA	3111	1/1	0.78	0.13	39,39,39,39	0
56	MG	YA	3497	1/1	0.78	0.21	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	XA	1679	1/1	0.78	0.14	86,86,86,86	0
56	MG	RA	3211	1/1	0.79	0.16	69,69,69,69	0
56	MG	XE	201	1/1	0.79	0.14	80,80,80,80	0
56	MG	RA	3457	1/1	0.79	0.10	97,97,97,97	0
56	MG	YA	3523	1/1	0.79	0.19	21,21,21,21	0
56	MG	RA	3495	1/1	0.79	0.24	15,15,15,15	0
56	MG	RA	3326	1/1	0.79	0.14	75,75,75,75	0
56	MG	RA	3334	1/1	0.79	0.09	58,58,58,58	0
56	MG	YB	205	1/1	0.79	0.15	76,76,76,76	0
56	MG	YA	3132	1/1	0.79	0.13	55,55,55,55	0
56	MG	RA	3300	1/1	0.79	0.17	68,68,68,68	0
56	MG	YA	3382	1/1	0.79	0.26	98,98,98,98	0
56	MG	YB	212	1/1	0.79	0.07	99,99,99,99	0
56	MG	RA	3266	1/1	0.79	0.16	52,52,52,52	0
56	MG	YA	3338	1/1	0.79	0.24	84,84,84,84	0
56	MG	RA	3009	1/1	0.79	0.19	38,38,38,38	0
56	MG	YA	3020	1/1	0.79	0.11	30,30,30,30	0
56	MG	YA	3026	1/1	0.79	0.27	55,55,55,55	0
56	MG	RA	3344	1/1	0.79	0.16	58,58,58,58	0
56	MG	Y0	101	1/1	0.79	0.19	54,54,54,54	0
56	MG	RA	3231	1/1	0.79	0.16	31,31,31,31	0
56	MG	RA	3087	1/1	0.79	0.23	64,64,64,64	0
56	MG	YA	3402	1/1	0.79	0.11	69,69,69,69	0
56	MG	RA	3352	1/1	0.79	0.17	75,75,75,75	0
56	MG	RO	201	1/1	0.79	0.29	79,79,79,79	0
56	MG	YA	3232	1/1	0.79	0.20	56,56,56,56	0
56	MG	YA	3249	1/1	0.79	0.26	64,64,64,64	0
56	MG	YA	3315	1/1	0.79	0.16	77,77,77,77	0
56	MG	RA	3029	1/1	0.80	0.22	26,26,26,26	0
56	MG	YA	3286	1/1	0.80	0.09	55,55,55,55	0
56	MG	YA	3143	1/1	0.80	0.12	77,77,77,77	0
56	MG	YA	3028	1/1	0.80	0.29	23,23,23,23	0
56	MG	XA	1675	1/1	0.80	0.13	82,82,82,82	0
56	MG	YA	3156	1/1	0.80	0.15	60,60,60,60	0
56	MG	RA	3237	1/1	0.80	0.28	62,62,62,62	0
56	MG	YA	3161	1/1	0.80	0.16	56,56,56,56	0
56	MG	QV	101	1/1	0.80	0.22	45,45,45,45	0
56	MG	YA	3224	1/1	0.80	0.13	52,52,52,52	0
56	MG	YA	3398	1/1	0.80	0.25	78,78,78,78	0
56	MG	XA	1680	1/1	0.80	0.17	44,44,44,44	0
56	MG	RA	3177	1/1	0.80	0.12	74,74,74,74	0
56	MG	RA	3391	1/1	0.80	0.31	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3393	1/1	0.80	0.14	69,69,69,69	0
56	MG	RA	3463	1/1	0.80	0.07	72,72,72,72	0
56	MG	XA	1650	1/1	0.80	0.17	114,114,114,114	0
56	MG	YA	3178	1/1	0.80	0.18	39,39,39,39	0
56	MG	RA	3394	1/1	0.80	0.09	53,53,53,53	0
56	MG	YA	3421	1/1	0.80	0.12	56,56,56,56	0
56	MG	RE	303	1/1	0.80	0.09	87,87,87,87	0
56	MG	RA	3400	1/1	0.80	0.10	85,85,85,85	0
56	MG	RP	202	1/1	0.80	0.29	56,56,56,56	0
56	MG	YA	3396	1/1	0.81	0.30	74,74,74,74	0
56	MG	RA	3313	1/1	0.81	0.16	63,63,63,63	0
56	MG	YA	3494	1/1	0.81	0.11	102,102,102,102	0
56	MG	YA	3171	1/1	0.81	0.26	44,44,44,44	0
56	MG	RA	3024	1/1	0.81	0.30	15,15,15,15	0
56	MG	RA	3351	1/1	0.81	0.20	63,63,63,63	0
56	MG	QA	1657	1/1	0.81	0.12	67,67,67,67	0
56	MG	YA	3404	1/1	0.81	0.15	73,73,73,73	0
56	MG	YA	3514	1/1	0.81	0.12	47,47,47,47	0
56	MG	XA	1668	1/1	0.81	0.24	95,95,95,95	0
56	MG	RA	3448	1/1	0.81	0.17	71,71,71,71	0
56	MG	RA	3329	1/1	0.81	0.09	76,76,76,76	0
56	MG	RA	3451	1/1	0.81	0.18	56,56,56,56	0
56	MG	RA	3293	1/1	0.81	0.16	70,70,70,70	0
56	MG	YB	204	1/1	0.81	0.07	118,118,118,118	0
56	MG	RY	201	1/1	0.81	0.22	67,67,67,67	0
56	MG	R0	102	1/1	0.81	0.10	54,54,54,54	0
56	MG	YA	3199	1/1	0.81	0.11	39,39,39,39	0
56	MG	R8	101	1/1	0.81	0.24	61,61,61,61	0
56	MG	YA	3305	1/1	0.81	0.15	41,41,41,41	0
56	MG	YA	3135	1/1	0.81	0.17	43,43,43,43	0
56	MG	QA	1648	1/1	0.81	0.11	55,55,55,55	0
56	MG	RA	3405	1/1	0.81	0.20	55,55,55,55	0
56	MG	RA	3500	1/1	0.81	0.12	35,35,35,35	0
56	MG	YA	3146	1/1	0.81	0.12	67,67,67,67	0
56	MG	RA	3338	1/1	0.81	0.22	57,57,57,57	0
56	MG	YA	3004	1/1	0.81	0.12	56,56,56,56	0
56	MG	YA	3005	1/1	0.81	0.12	55,55,55,55	0
56	MG	YA	3464	1/1	0.81	0.18	56,56,56,56	0
56	MG	RA	3507	1/1	0.81	0.15	63,63,63,63	0
56	MG	RA	3133	1/1	0.81	0.14	92,92,92,92	0
56	MG	QA	1671	1/1	0.81	0.20	55,55,55,55	0
56	MG	YA	3480	1/1	0.81	0.10	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	QA	1647	1/1	0.81	0.15	45,45,45,45	0
56	MG	YA	3033	1/1	0.81	0.20	41,41,41,41	0
56	MG	RA	3439	1/1	0.82	0.18	84,84,84,84	0
56	MG	RA	3261	1/1	0.82	0.13	63,63,63,63	0
56	MG	YA	3238	1/1	0.82	0.15	77,77,77,77	0
56	MG	YA	3439	1/1	0.82	0.09	70,70,70,70	0
56	MG	RA	3361	1/1	0.82	0.09	72,72,72,72	0
56	MG	YA	3177	1/1	0.82	0.23	63,63,63,63	0
56	MG	RA	3398	1/1	0.82	0.11	50,50,50,50	0
56	MG	RA	3242	1/1	0.82	0.23	71,71,71,71	0
56	MG	RA	3332	1/1	0.82	0.13	58,58,58,58	0
56	MG	YA	3328	1/1	0.82	0.09	72,72,72,72	0
56	MG	RA	3305	1/1	0.82	0.20	66,66,66,66	0
56	MG	YB	208	1/1	0.82	0.10	122,122,122,122	0
56	MG	YA	3455	1/1	0.82	0.14	66,66,66,66	0
56	MG	YA	3276	1/1	0.82	0.17	75,75,75,75	0
56	MG	QA	1603	1/1	0.82	0.21	34,34,34,34	0
56	MG	RA	3412	1/1	0.82	0.12	69,69,69,69	0
56	MG	XA	1676	1/1	0.82	0.12	99,99,99,99	0
56	MG	RA	3161	1/1	0.82	0.15	88,88,88,88	0
56	MG	XA	1611	1/1	0.82	0.15	34,34,34,34	0
56	MG	YA	3054	1/1	0.82	0.12	49,49,49,49	0
56	MG	YA	3059	1/1	0.82	0.23	40,40,40,40	0
56	MG	RA	3420	1/1	0.82	0.10	52,52,52,52	0
56	MG	RA	3039	1/1	0.82	0.14	27,27,27,27	0
56	MG	RA	3425	1/1	0.82	0.08	61,61,61,61	0
56	MG	YA	3302	1/1	0.82	0.18	109,109,109,109	0
56	MG	YA	3222	1/1	0.82	0.08	42,42,42,42	0
56	MG	RA	3379	1/1	0.82	0.14	84,84,84,84	0
56	MG	RA	3187	1/1	0.82	0.13	77,77,77,77	0
56	MG	YA	3499	1/1	0.82	0.10	64,64,64,64	0
56	MG	YA	3113	1/1	0.82	0.13	33,33,33,33	0
56	MG	RA	3370	1/1	0.83	0.11	56,56,56,56	0
56	MG	RA	3158	1/1	0.83	0.29	51,51,51,51	0
56	MG	RA	3375	1/1	0.83	0.14	52,52,52,52	0
56	MG	RN	201	1/1	0.83	0.38	80,80,80,80	0
56	MG	YA	3259	1/1	0.83	0.16	56,56,56,56	0
56	MG	RA	3127	1/1	0.83	0.17	56,56,56,56	0
56	MG	RA	3433	1/1	0.83	0.14	66,66,66,66	0
56	MG	RA	3092	1/1	0.83	0.14	22,22,22,22	0
56	MG	YA	3105	1/1	0.83	0.08	60,60,60,60	0
56	MG	YA	3271	1/1	0.83	0.40	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3172	1/1	0.83	0.20	59,59,59,59	0
56	MG	RA	3093	1/1	0.83	0.21	19,19,19,19	0
56	MG	YA	3180	1/1	0.83	0.10	45,45,45,45	0
56	MG	RA	3486	1/1	0.83	0.14	74,74,74,74	0
56	MG	RA	3214	1/1	0.83	0.26	72,72,72,72	0
56	MG	YA	3426	1/1	0.83	0.28	78,78,78,78	0
56	MG	RA	3445	1/1	0.83	0.09	47,47,47,47	0
56	MG	YA	3186	1/1	0.83	0.11	53,53,53,53	0
56	MG	RA	3296	1/1	0.83	0.19	66,66,66,66	0
56	MG	RA	3080	1/1	0.83	0.14	43,43,43,43	0
56	MG	RA	3145	1/1	0.83	0.11	40,40,40,40	0
56	MG	QA	1602	1/1	0.83	0.20	36,36,36,36	0
56	MG	RA	3058	1/1	0.83	0.26	72,72,72,72	0
56	MG	YA	3205	1/1	0.83	0.15	48,48,48,48	0
56	MG	YA	3018	1/1	0.83	0.26	14,14,14,14	0
56	MG	RA	3513	1/1	0.83	0.22	58,58,58,58	0
56	MG	YA	3148	1/1	0.83	0.19	51,51,51,51	0
56	MG	YA	3377	1/1	0.83	0.11	57,57,57,57	0
56	MG	RA	3061	1/1	0.83	0.42	26,26,26,26	0
56	MG	YA	3467	1/1	0.83	0.10	92,92,92,92	0
56	MG	QA	1611	1/1	0.83	0.19	35,35,35,35	0
56	MG	RA	3413	1/1	0.83	0.13	41,41,41,41	0
56	MG	YA	3475	1/1	0.83	0.23	66,66,66,66	0
56	MG	RA	3203	1/1	0.83	0.14	63,63,63,63	0
56	MG	YA	3040	1/1	0.83	0.12	61,61,61,61	0
56	MG	YA	3045	1/1	0.83	0.11	59,59,59,59	0
56	MG	YA	3230	1/1	0.83	0.15	70,70,70,70	0
56	MG	RA	3422	1/1	0.84	0.09	55,55,55,55	0
56	MG	YA	3168	1/1	0.84	0.11	68,68,68,68	0
56	MG	YA	3270	1/1	0.84	0.23	39,39,39,39	0
56	MG	XA	1634	1/1	0.84	0.22	59,59,59,59	0
56	MG	YA	3029	1/1	0.84	0.16	27,27,27,27	0
56	MG	RA	3041	1/1	0.84	0.13	37,37,37,37	0
56	MG	RA	3328	1/1	0.84	0.19	65,65,65,65	0
56	MG	XA	1639	1/1	0.84	0.20	38,38,38,38	0
56	MG	XA	1640	1/1	0.84	0.11	48,48,48,48	0
56	MG	RA	3367	1/1	0.84	0.33	119,119,119,119	0
56	MG	YA	3486	1/1	0.84	0.12	58,58,58,58	0
56	MG	YA	3051	1/1	0.84	0.19	31,31,31,31	0
56	MG	RA	3249	1/1	0.84	0.12	76,76,76,76	0
56	MG	XA	1654	1/1	0.84	0.12	54,54,54,54	0
56	MG	YA	3296	1/1	0.84	0.18	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3180	1/1	0.84	0.09	68,68,68,68	0
56	MG	RA	3441	1/1	0.84	0.20	87,87,87,87	0
56	MG	RA	3298	1/1	0.84	0.22	53,53,53,53	0
56	MG	YA	3093	1/1	0.84	0.17	47,47,47,47	0
56	MG	RA	3336	1/1	0.84	0.21	71,71,71,71	0
56	MG	YA	3100	1/1	0.84	0.17	44,44,44,44	0
56	MG	RA	3131	1/1	0.84	0.14	25,25,25,25	0
56	MG	RA	3132	1/1	0.84	0.17	50,50,50,50	0
56	MG	YA	3527	1/1	0.84	0.16	24,24,24,24	0
56	MG	RA	3381	1/1	0.84	0.24	77,77,77,77	0
56	MG	RA	3191	1/1	0.84	0.11	54,54,54,54	0
56	MG	YA	3538	1/1	0.84	0.24	45,45,45,45	0
56	MG	YA	3318	1/1	0.84	0.14	43,43,43,43	0
56	MG	RA	3306	1/1	0.84	0.17	31,31,31,31	0
56	MG	YA	3121	1/1	0.84	0.16	30,30,30,30	0
56	MG	YA	3216	1/1	0.84	0.11	49,49,49,49	0
56	MG	RA	3265	1/1	0.84	0.16	47,47,47,47	0
56	MG	QA	1631	1/1	0.84	0.09	123,123,123,123	0
56	MG	RA	3270	1/1	0.84	0.13	86,86,86,86	0
56	MG	RA	3223	1/1	0.84	0.17	52,52,52,52	0
56	MG	YA	3226	1/1	0.84	0.09	44,44,44,44	0
56	MG	YA	3332	1/1	0.84	0.14	47,47,47,47	0
56	MG	QA	1654	1/1	0.84	0.08	62,62,62,62	0
56	MG	RA	3407	1/1	0.84	0.11	54,54,54,54	0
56	MG	RA	3229	1/1	0.84	0.27	52,52,52,52	0
56	MG	RA	3469	1/1	0.84	0.24	85,85,85,85	0
56	MG	RA	3059	1/1	0.84	0.15	95,95,95,95	0
56	MG	RA	3164	1/1	0.84	0.12	60,60,60,60	0
56	MG	XA	1606	1/1	0.84	0.29	41,41,41,41	0
56	MG	YA	3347	1/1	0.84	0.19	47,47,47,47	0
56	MG	QA	1626	1/1	0.84	0.13	51,51,51,51	0
56	MG	YA	3013	1/1	0.84	0.22	29,29,29,29	0
56	MG	QY	101	1/1	0.84	0.15	60,60,60,60	0
56	MG	YA	3460	1/1	0.84	0.05	84,84,84,84	0
56	MG	RA	3149	1/1	0.84	0.23	62,62,62,62	0
56	MG	YA	3335	1/1	0.85	0.20	46,46,46,46	0
56	MG	RA	3088	1/1	0.85	0.19	22,22,22,22	0
56	MG	RA	3170	1/1	0.85	0.07	43,43,43,43	0
56	MG	YA	3340	1/1	0.85	0.15	78,78,78,78	0
56	MG	RA	3432	1/1	0.85	0.08	57,57,57,57	0
56	MG	YA	3001	1/1	0.85	0.21	52,52,52,52	0
56	MG	R0	103	1/1	0.85	0.15	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3506	1/1	0.85	0.15	70,70,70,70	0
56	MG	YA	3413	1/1	0.85	0.11	53,53,53,53	0
56	MG	YA	3003	1/1	0.85	0.29	17,17,17,17	0
56	MG	YA	3214	1/1	0.85	0.26	60,60,60,60	0
56	MG	RA	3049	1/1	0.85	0.17	20,20,20,20	0
56	MG	RA	3455	1/1	0.85	0.09	55,55,55,55	0
56	MG	RA	3484	1/1	0.85	0.09	84,84,84,84	0
56	MG	YA	3298	1/1	0.85	0.26	57,57,57,57	0
56	MG	YA	3008	1/1	0.85	0.27	18,18,18,18	0
56	MG	RA	3312	1/1	0.85	0.14	60,60,60,60	0
56	MG	YA	3225	1/1	0.85	0.12	35,35,35,35	0
56	MG	YA	3016	1/1	0.85	0.22	24,24,24,24	0
56	MG	YA	3017	1/1	0.85	0.25	16,16,16,16	0
56	MG	YA	3363	1/1	0.85	0.10	85,85,85,85	0
56	MG	YA	3115	1/1	0.85	0.14	43,43,43,43	0
56	MG	YA	3368	1/1	0.85	0.14	53,53,53,53	0
56	MG	RA	3173	1/1	0.85	0.11	51,51,51,51	0
56	MG	YA	3117	1/1	0.85	0.15	37,37,37,37	0
56	MG	XA	1630	1/1	0.85	0.08	41,41,41,41	0
56	MG	YA	3374	1/1	0.85	0.08	48,48,48,48	0
56	MG	YP	203	1/1	0.85	0.23	70,70,70,70	0
56	MG	QV	105	1/1	0.85	0.22	65,65,65,65	0
56	MG	YA	3243	1/1	0.85	0.21	51,51,51,51	0
56	MG	YA	3247	1/1	0.85	0.14	24,24,24,24	0
56	MG	RB	211	1/1	0.85	0.09	83,83,83,83	0
56	MG	QA	1615	1/1	0.85	0.09	43,43,43,43	0
56	MG	YA	3030	1/1	0.85	0.36	28,28,28,28	0
56	MG	XA	1636	1/1	0.85	0.09	93,93,93,93	0
56	MG	RA	3372	1/1	0.85	0.17	68,68,68,68	0
56	MG	RA	3373	1/1	0.85	0.11	63,63,63,63	0
56	MG	YA	3187	1/1	0.85	0.09	39,39,39,39	0
56	MG	YA	3141	1/1	0.85	0.21	60,60,60,60	0
56	MG	RA	3291	1/1	0.85	0.13	75,75,75,75	0
56	MG	YA	3487	1/1	0.85	0.11	58,58,58,58	0
58	ZN	Y6	101	1/1	0.85	0.16	233,233,233,233	0
56	MG	XA	1608	1/1	0.86	0.07	78,78,78,78	0
56	MG	RA	3396	1/1	0.86	0.12	50,50,50,50	0
56	MG	XA	1612	1/1	0.86	0.15	41,41,41,41	0
56	MG	YA	3351	1/1	0.86	0.27	62,62,62,62	0
56	MG	YA	3114	1/1	0.86	0.19	66,66,66,66	0
56	MG	XA	1620	1/1	0.86	0.17	29,29,29,29	0
56	MG	XA	1671	1/1	0.86	0.17	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	XA	1623	1/1	0.86	0.12	77,77,77,77	0
56	MG	RA	3474	1/1	0.86	0.12	46,46,46,46	0
56	MG	YA	3308	1/1	0.86	0.20	77,77,77,77	0
56	MG	RA	3128	1/1	0.86	0.08	58,58,58,58	0
56	MG	YA	3435	1/1	0.86	0.13	37,37,37,37	0
56	MG	YA	3436	1/1	0.86	0.13	60,60,60,60	0
56	MG	YA	3128	1/1	0.86	0.14	64,64,64,64	0
56	MG	RA	3482	1/1	0.86	0.21	65,65,65,65	0
56	MG	RA	3050	1/1	0.86	0.25	20,20,20,20	0
56	MG	RA	3116	1/1	0.86	0.09	71,71,71,71	0
56	MG	RA	3051	1/1	0.86	0.11	38,38,38,38	0
56	MG	YA	3372	1/1	0.86	0.14	74,74,74,74	0
56	MG	YA	3257	1/1	0.86	0.21	38,38,38,38	0
56	MG	RA	3339	1/1	0.86	0.21	34,34,34,34	0
56	MG	RA	3461	1/1	0.86	0.11	67,67,67,67	0
56	MG	RA	3020	1/1	0.86	0.34	29,29,29,29	0
56	MG	QA	1644	1/1	0.86	0.09	58,58,58,58	0
56	MG	YA	3380	1/1	0.86	0.15	65,65,65,65	0
56	MG	XA	1644	1/1	0.86	0.13	64,64,64,64	0
56	MG	XA	1645	1/1	0.86	0.09	57,57,57,57	0
56	MG	RA	3141	1/1	0.86	0.17	55,55,55,55	0
56	MG	YA	3468	1/1	0.86	0.21	50,50,50,50	0
56	MG	RA	3382	1/1	0.86	0.20	61,61,61,61	0
56	MG	RA	3126	1/1	0.86	0.17	32,32,32,32	0
56	MG	YA	3157	1/1	0.86	0.10	71,71,71,71	0
56	MG	YA	3393	1/1	0.86	0.10	46,46,46,46	0
56	MG	RA	3331	1/1	0.86	0.14	65,65,65,65	0
56	MG	RA	3040	1/1	0.86	0.15	25,25,25,25	0
56	MG	YA	3341	1/1	0.86	0.16	92,92,92,92	0
56	MG	YA	3101	1/1	0.86	0.08	63,63,63,63	0
56	MG	YA	3218	1/1	0.86	0.10	62,62,62,62	0
56	MG	YA	3104	1/1	0.86	0.24	42,42,42,42	0
56	MG	YA	3221	1/1	0.86	0.12	51,51,51,51	0
56	MG	RA	3183	1/1	0.87	0.10	43,43,43,43	0
56	MG	YA	3185	1/1	0.87	0.10	49,49,49,49	0
56	MG	YA	3261	1/1	0.87	0.24	56,56,56,56	0
56	MG	YA	3483	1/1	0.87	0.15	66,66,66,66	0
56	MG	RA	3490	1/1	0.87	0.13	33,33,33,33	0
56	MG	YA	3263	1/1	0.87	0.17	43,43,43,43	0
56	MG	RA	3267	1/1	0.87	0.25	55,55,55,55	0
56	MG	YA	3488	1/1	0.87	0.18	87,87,87,87	0
56	MG	RA	3167	1/1	0.87	0.12	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3414	1/1	0.87	0.14	67,67,67,67	0
56	MG	YA	3196	1/1	0.87	0.09	48,48,48,48	0
56	MG	YA	3038	1/1	0.87	0.16	25,25,25,25	0
56	MG	RA	3271	1/1	0.87	0.15	77,77,77,77	0
56	MG	YA	3343	1/1	0.87	0.09	44,44,44,44	0
56	MG	YA	3278	1/1	0.87	0.11	105,105,105,105	0
56	MG	YA	3504	1/1	0.87	0.18	53,53,53,53	0
56	MG	RA	3376	1/1	0.87	0.10	79,79,79,79	0
56	MG	RA	3168	1/1	0.87	0.13	63,63,63,63	0
56	MG	YA	3510	1/1	0.87	0.13	71,71,71,71	0
56	MG	YA	3211	1/1	0.87	0.08	45,45,45,45	0
56	MG	QA	1663	1/1	0.87	0.19	58,58,58,58	0
56	MG	RA	3197	1/1	0.87	0.20	44,44,44,44	0
56	MG	RA	3466	1/1	0.87	0.10	57,57,57,57	0
56	MG	YA	3525	1/1	0.87	0.26	15,15,15,15	0
56	MG	QV	104	1/1	0.87	0.17	116,116,116,116	0
56	MG	YA	3532	1/1	0.87	0.17	50,50,50,50	0
56	MG	QA	1635	1/1	0.87	0.10	64,64,64,64	0
56	MG	RA	3385	1/1	0.87	0.06	61,61,61,61	0
56	MG	YA	3427	1/1	0.87	0.17	53,53,53,53	0
56	MG	YA	3541	1/1	0.87	0.14	35,35,35,35	0
56	MG	YA	3429	1/1	0.87	0.25	58,58,58,58	0
56	MG	RA	3053	1/1	0.87	0.15	32,32,32,32	0
56	MG	YA	3359	1/1	0.87	0.18	56,56,56,56	0
56	MG	YB	206	1/1	0.87	0.10	49,49,49,49	0
56	MG	YA	3220	1/1	0.87	0.11	41,41,41,41	0
56	MG	RB	208	1/1	0.87	0.12	65,65,65,65	0
56	MG	RA	3259	1/1	0.87	0.17	69,69,69,69	0
56	MG	RA	3290	1/1	0.87	0.15	60,60,60,60	0
56	MG	YB	211	1/1	0.87	0.09	71,71,71,71	0
56	MG	YA	3447	1/1	0.87	0.16	64,64,64,64	0
56	MG	YA	3103	1/1	0.87	0.17	40,40,40,40	0
56	MG	YE	302	1/1	0.87	0.25	83,83,83,83	0
56	MG	RA	3364	1/1	0.87	0.09	93,93,93,93	0
56	MG	XA	1647	1/1	0.87	0.09	66,66,66,66	0
56	MG	YA	3452	1/1	0.87	0.12	78,78,78,78	0
56	MG	RA	3113	1/1	0.87	0.14	87,87,87,87	0
56	MG	YA	3007	1/1	0.87	0.16	39,39,39,39	0
56	MG	RA	3479	1/1	0.87	0.09	56,56,56,56	0
56	MG	XA	1653	1/1	0.87	0.23	51,51,51,51	0
56	MG	YA	3317	1/1	0.87	0.11	49,49,49,49	0
56	MG	RA	3068	1/1	0.87	0.15	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	XA	1659	1/1	0.87	0.22	71,71,71,71	0
56	MG	YA	3378	1/1	0.87	0.14	67,67,67,67	0
56	MG	RA	3340	1/1	0.87	0.08	53,53,53,53	0
56	MG	YA	3469	1/1	0.87	0.17	90,90,90,90	0
56	MG	RA	3368	1/1	0.87	0.10	27,27,27,27	0
56	MG	RA	3076	1/1	0.87	0.28	35,35,35,35	0
56	MG	YA	3256	1/1	0.87	0.22	34,34,34,34	0
56	MG	RA	3392	1/1	0.88	0.17	32,32,32,32	0
56	MG	YA	3204	1/1	0.88	0.24	61,61,61,61	0
56	MG	YA	3274	1/1	0.88	0.31	65,65,65,65	0
56	MG	RA	3178	1/1	0.88	0.11	63,63,63,63	0
56	MG	YA	3210	1/1	0.88	0.40	60,60,60,60	0
56	MG	XV	106	1/1	0.88	0.29	70,70,70,70	0
56	MG	YA	3070	1/1	0.88	0.13	47,47,47,47	0
56	MG	YA	3152	1/1	0.88	0.18	60,60,60,60	0
56	MG	RA	3307	1/1	0.88	0.07	83,83,83,83	0
56	MG	YA	3075	1/1	0.88	0.15	12,12,12,12	0
56	MG	RA	3026	1/1	0.88	0.20	24,24,24,24	0
56	MG	RA	3289	1/1	0.88	0.13	70,70,70,70	0
56	MG	YA	3086	1/1	0.88	0.20	28,28,28,28	0
56	MG	YA	3516	1/1	0.88	0.09	30,30,30,30	0
56	MG	YA	3356	1/1	0.88	0.25	53,53,53,53	0
56	MG	YA	3295	1/1	0.88	0.09	67,67,67,67	0
56	MG	RA	3447	1/1	0.88	0.13	49,49,49,49	0
56	MG	RA	3165	1/1	0.88	0.18	42,42,42,42	0
56	MG	YA	3528	1/1	0.88	0.10	54,54,54,54	0
56	MG	RR	202	1/1	0.88	0.15	80,80,80,80	0
56	MG	YA	3440	1/1	0.88	0.12	56,56,56,56	0
56	MG	XA	1649	1/1	0.88	0.11	67,67,67,67	0
56	MG	QA	1646	1/1	0.88	0.11	60,60,60,60	0
56	MG	YA	3445	1/1	0.88	0.12	71,71,71,71	0
56	MG	QA	1601	1/1	0.88	0.21	47,47,47,47	0
56	MG	QA	1667	1/1	0.88	0.20	52,52,52,52	0
56	MG	QA	1623	1/1	0.88	0.12	37,37,37,37	0
56	MG	RA	3295	1/1	0.88	0.17	53,53,53,53	0
56	MG	RA	3192	1/1	0.88	0.14	49,49,49,49	0
56	MG	XA	1607	1/1	0.88	0.16	64,64,64,64	0
56	MG	RA	3297	1/1	0.88	0.15	50,50,50,50	0
56	MG	YA	3313	1/1	0.88	0.24	60,60,60,60	0
56	MG	YA	3242	1/1	0.88	0.08	50,50,50,50	0
56	MG	YA	3025	1/1	0.88	0.09	38,38,38,38	0
56	MG	RA	3504	1/1	0.88	0.14	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3349	1/1	0.88	0.14	70,70,70,70	0
56	MG	YA	3251	1/1	0.88	0.38	56,56,56,56	0
56	MG	YO	201	1/1	0.88	0.28	52,52,52,52	0
56	MG	RA	3140	1/1	0.88	0.15	50,50,50,50	0
56	MG	YA	3255	1/1	0.88	0.15	46,46,46,46	0
56	MG	YA	3129	1/1	0.88	0.09	51,51,51,51	0
56	MG	RA	3299	1/1	0.88	0.20	76,76,76,76	0
56	MG	YA	3387	1/1	0.88	0.14	58,58,58,58	0
56	MG	RA	3198	1/1	0.88	0.14	66,66,66,66	0
56	MG	RA	3303	1/1	0.88	0.16	62,62,62,62	0
56	MG	RA	3111	1/1	0.88	0.24	26,26,26,26	0
56	MG	YA	3333	1/1	0.88	0.26	36,36,36,36	0
56	MG	YA	3482	1/1	0.88	0.13	67,67,67,67	0
56	MG	RA	3070	1/1	0.88	0.10	27,27,27,27	0
56	MG	YA	3198	1/1	0.88	0.11	70,70,70,70	0
56	MG	RA	3389	1/1	0.88	0.19	104,104,104,104	0
56	MG	RA	3359	1/1	0.88	0.27	37,37,37,37	0
56	MG	YA	3401	1/1	0.88	0.15	62,62,62,62	0
56	MG	RA	3309	1/1	0.89	0.29	63,63,63,63	0
56	MG	YA	3511	1/1	0.89	0.17	67,67,67,67	0
56	MG	RA	3195	1/1	0.89	0.09	36,36,36,36	0
56	MG	RA	3501	1/1	0.89	0.09	58,58,58,58	0
56	MG	RA	3054	1/1	0.89	0.09	42,42,42,42	0
56	MG	QA	1655	1/1	0.89	0.13	51,51,51,51	0
56	MG	YA	3202	1/1	0.89	0.11	73,73,73,73	0
56	MG	RA	3181	1/1	0.89	0.10	47,47,47,47	0
56	MG	YA	3087	1/1	0.89	0.11	24,24,24,24	0
56	MG	YA	3089	1/1	0.89	0.16	42,42,42,42	0
56	MG	RA	3101	1/1	0.89	0.10	37,37,37,37	0
56	MG	RA	3274	1/1	0.89	0.07	74,74,74,74	0
56	MG	YA	3099	1/1	0.89	0.19	16,16,16,16	0
56	MG	RA	3319	1/1	0.89	0.11	44,44,44,44	0
56	MG	RA	3016	1/1	0.89	0.14	24,24,24,24	0
56	MG	YA	3215	1/1	0.89	0.12	69,69,69,69	0
56	MG	YA	3391	1/1	0.89	0.10	46,46,46,46	0
56	MG	YA	3102	1/1	0.89	0.14	18,18,18,18	0
56	MG	YA	3167	1/1	0.89	0.08	66,66,66,66	0
56	MG	RA	3205	1/1	0.89	0.12	49,49,49,49	0
56	MG	YA	3022	1/1	0.89	0.16	20,20,20,20	0
56	MG	RA	3256	1/1	0.89	0.23	61,61,61,61	0
56	MG	RA	3323	1/1	0.89	0.15	57,57,57,57	0
56	MG	YA	3472	1/1	0.89	0.11	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3281	1/1	0.89	0.28	57,57,57,57	0
56	MG	RA	3480	1/1	0.89	0.09	44,44,44,44	0
56	MG	RA	3258	1/1	0.89	0.19	106,106,106,106	0
56	MG	YA	3176	1/1	0.89	0.11	65,65,65,65	0
56	MG	RA	3135	1/1	0.89	0.23	52,52,52,52	0
56	MG	YA	3034	1/1	0.89	0.23	35,35,35,35	0
56	MG	RA	3189	1/1	0.89	0.38	75,75,75,75	0
56	MG	RA	3419	1/1	0.89	0.07	65,65,65,65	0
56	MG	YA	3355	1/1	0.89	0.17	51,51,51,51	0
56	MG	RP	201	1/1	0.89	0.08	46,46,46,46	0
56	MG	RA	3288	1/1	0.89	0.11	59,59,59,59	0
56	MG	YA	3304	1/1	0.89	0.09	57,57,57,57	0
56	MG	YA	3239	1/1	0.89	0.30	48,48,48,48	0
56	MG	YA	3240	1/1	0.89	0.12	36,36,36,36	0
56	MG	RA	3137	1/1	0.89	0.14	84,84,84,84	0
56	MG	RA	3494	1/1	0.89	0.14	45,45,45,45	0
56	MG	RA	3119	1/1	0.89	0.12	41,41,41,41	0
56	MG	YA	3058	1/1	0.89	0.12	49,49,49,49	0
56	MG	R0	101	1/1	0.89	0.43	70,70,70,70	0
56	MG	YA	3253	1/1	0.89	0.22	67,67,67,67	0
56	MG	RA	3395	1/1	0.90	0.10	55,55,55,55	0
56	MG	RA	3169	1/1	0.90	0.11	21,21,21,21	0
56	MG	RB	210	1/1	0.90	0.10	78,78,78,78	0
56	MG	RA	3273	1/1	0.90	0.24	51,51,51,51	0
56	MG	RE	302	1/1	0.90	0.09	84,84,84,84	0
56	MG	RA	3244	1/1	0.90	0.10	33,33,33,33	0
56	MG	RA	3444	1/1	0.90	0.17	73,73,73,73	0
56	MG	RA	3199	1/1	0.90	0.11	44,44,44,44	0
56	MG	RA	3347	1/1	0.90	0.21	33,33,33,33	0
56	MG	RA	3247	1/1	0.90	0.17	55,55,55,55	0
56	MG	QA	1605	1/1	0.90	0.30	35,35,35,35	0
56	MG	YA	3522	1/1	0.90	0.20	27,27,27,27	0
56	MG	RA	3184	1/1	0.90	0.14	51,51,51,51	0
56	MG	RA	3221	1/1	0.90	0.06	58,58,58,58	0
56	MG	QA	1636	1/1	0.90	0.10	39,39,39,39	0
56	MG	RA	3204	1/1	0.90	0.14	50,50,50,50	0
56	MG	RA	3456	1/1	0.90	0.10	51,51,51,51	0
56	MG	RA	3144	1/1	0.90	0.08	53,53,53,53	0
56	MG	XA	1605	1/1	0.90	0.17	34,34,34,34	0
56	MG	QA	1620	1/1	0.90	0.08	85,85,85,85	0
56	MG	XA	1667	1/1	0.90	0.20	48,48,48,48	0
56	MG	YA	3188	1/1	0.90	0.15	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3323	1/1	0.90	0.13	48,48,48,48	0
56	MG	YA	3381	1/1	0.90	0.13	55,55,55,55	0
56	MG	RA	3384	1/1	0.90	0.12	43,43,43,43	0
56	MG	RA	3230	1/1	0.90	0.14	44,44,44,44	0
56	MG	RA	3001	1/1	0.90	0.18	28,28,28,28	0
56	MG	YA	3465	1/1	0.90	0.14	88,88,88,88	0
56	MG	YA	3329	1/1	0.90	0.17	54,54,54,54	0
56	MG	RA	3508	1/1	0.90	0.16	33,33,33,33	0
56	MG	XA	1677	1/1	0.90	0.09	62,62,62,62	0
56	MG	YA	3139	1/1	0.90	0.12	36,36,36,36	0
56	MG	XA	1617	1/1	0.90	0.16	22,22,22,22	0
56	MG	XA	1618	1/1	0.90	0.10	45,45,45,45	0
56	MG	RA	3426	1/1	0.90	0.13	49,49,49,49	0
56	MG	YP	201	1/1	0.90	0.42	68,68,68,68	0
56	MG	YP	202	1/1	0.90	0.13	76,76,76,76	0
56	MG	RA	3427	1/1	0.90	0.22	58,58,58,58	0
56	MG	YA	3479	1/1	0.90	0.20	84,84,84,84	0
56	MG	YA	3206	1/1	0.90	0.06	41,41,41,41	0
56	MG	XL	201	1/1	0.90	0.17	74,74,74,74	0
56	MG	YA	3062	1/1	0.90	0.13	23,23,23,23	0
56	MG	YY	201	1/1	0.90	0.27	66,66,66,66	0
56	MG	XA	1624	1/1	0.90	0.19	58,58,58,58	0
56	MG	YA	3153	1/1	0.90	0.26	59,59,59,59	0
56	MG	XQ	201	1/1	0.90	0.08	108,108,108,108	0
56	MG	RA	3031	1/1	0.90	0.22	30,30,30,30	0
56	MG	RA	3235	1/1	0.90	0.15	44,44,44,44	0
56	MG	YA	3290	1/1	0.90	0.17	57,57,57,57	0
56	MG	RA	3012	1/1	0.90	0.17	24,24,24,24	0
56	MG	YA	3159	1/1	0.90	0.14	39,39,39,39	0
58	ZN	Y4	500	1/1	0.90	0.15	242,242,242,242	0
56	MG	RA	3436	1/1	0.90	0.13	41,41,41,41	0
56	MG	QA	1632	1/1	0.90	0.25	27,27,27,27	0
56	MG	RA	3033	1/1	0.91	0.15	20,20,20,20	0
56	MG	RA	3038	1/1	0.91	0.15	22,22,22,22	0
56	MG	YA	3389	1/1	0.91	0.10	57,57,57,57	0
56	MG	RA	3207	1/1	0.91	0.08	47,47,47,47	0
56	MG	RB	203	1/1	0.91	0.07	64,64,64,64	0
56	MG	XV	102	1/1	0.91	0.08	53,53,53,53	0
56	MG	YA	3236	1/1	0.91	0.16	60,60,60,60	0
56	MG	YA	3492	1/1	0.91	0.12	76,76,76,76	0
56	MG	YA	3237	1/1	0.91	0.21	47,47,47,47	0
56	MG	YA	3395	1/1	0.91	0.29	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	XA	1629	1/1	0.91	0.06	51,51,51,51	0
56	MG	RA	3060	1/1	0.91	0.27	16,16,16,16	0
56	MG	YA	3500	1/1	0.91	0.12	103,103,103,103	0
56	MG	YA	3094	1/1	0.91	0.11	43,43,43,43	0
56	MG	YA	3503	1/1	0.91	0.29	52,52,52,52	0
56	MG	RA	3182	1/1	0.91	0.14	69,69,69,69	0
56	MG	YA	3400	1/1	0.91	0.11	67,67,67,67	0
56	MG	YA	3507	1/1	0.91	0.09	61,61,61,61	0
56	MG	RA	3096	1/1	0.91	0.14	60,60,60,60	0
56	MG	YA	3244	1/1	0.91	0.18	45,45,45,45	0
56	MG	RA	3434	1/1	0.91	0.14	38,38,38,38	0
56	MG	RA	3435	1/1	0.91	0.06	61,61,61,61	0
56	MG	QA	1627	1/1	0.91	0.14	35,35,35,35	0
56	MG	RA	3437	1/1	0.91	0.21	64,64,64,64	0
56	MG	RA	3018	1/1	0.91	0.19	14,14,14,14	0
56	MG	XA	1642	1/1	0.91	0.13	71,71,71,71	0
56	MG	XA	1643	1/1	0.91	0.07	73,73,73,73	0
56	MG	RA	3107	1/1	0.91	0.12	26,26,26,26	0
56	MG	QA	1610	1/1	0.91	0.16	19,19,19,19	0
56	MG	YA	3260	1/1	0.91	0.22	51,51,51,51	0
56	MG	RA	3284	1/1	0.91	0.11	53,53,53,53	0
56	MG	RA	3402	1/1	0.91	0.20	64,64,64,64	0
56	MG	YA	3535	1/1	0.91	0.22	52,52,52,52	0
56	MG	RA	3045	1/1	0.91	0.18	24,24,24,24	0
56	MG	RQ	202	1/1	0.91	0.08	74,74,74,74	0
56	MG	YA	3193	1/1	0.91	0.26	42,42,42,42	0
56	MG	RA	3022	1/1	0.91	0.10	27,27,27,27	0
56	MG	YA	3123	1/1	0.91	0.15	75,75,75,75	0
56	MG	YA	3124	1/1	0.91	0.13	48,48,48,48	0
56	MG	YA	3126	1/1	0.91	0.10	43,43,43,43	0
56	MG	RA	3220	1/1	0.91	0.08	63,63,63,63	0
56	MG	QA	1652	1/1	0.91	0.06	45,45,45,45	0
56	MG	YA	3280	1/1	0.91	0.14	72,72,72,72	0
56	MG	QA	1662	1/1	0.91	0.20	41,41,41,41	0
56	MG	RA	3491	1/1	0.91	0.09	39,39,39,39	0
56	MG	QA	1618	1/1	0.91	0.25	67,67,67,67	0
56	MG	YA	3134	1/1	0.91	0.08	60,60,60,60	0
56	MG	RA	3263	1/1	0.91	0.16	43,43,43,43	0
56	MG	YA	3208	1/1	0.91	0.10	67,67,67,67	0
56	MG	XA	1604	1/1	0.91	0.15	64,64,64,64	0
56	MG	RA	3030	1/1	0.91	0.27	8,8,8,8	0
56	MG	RA	3454	1/1	0.91	0.08	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3367	1/1	0.91	0.11	51,51,51,51	0
56	MG	RA	3122	1/1	0.91	0.14	34,34,34,34	0
56	MG	YA	3142	1/1	0.91	0.14	32,32,32,32	0
56	MG	YA	3297	1/1	0.91	0.15	51,51,51,51	0
56	MG	YA	3046	1/1	0.91	0.19	20,20,20,20	0
56	MG	RA	3502	1/1	0.91	0.08	43,43,43,43	0
56	MG	YA	3300	1/1	0.91	0.17	91,91,91,91	0
56	MG	RA	3380	1/1	0.91	0.18	57,57,57,57	0
56	MG	RA	3148	1/1	0.91	0.20	36,36,36,36	0
56	MG	XA	1615	1/1	0.91	0.12	25,25,25,25	0
56	MG	QA	1641	1/1	0.91	0.10	37,37,37,37	0
56	MG	YA	3061	1/1	0.91	0.15	22,22,22,22	0
56	MG	YA	3478	1/1	0.91	0.19	74,74,74,74	0
58	ZN	R6	101	1/1	0.91	0.13	213,213,213,213	0
56	MG	RA	3459	1/1	0.91	0.11	53,53,53,53	0
56	MG	RA	3423	1/1	0.91	0.12	57,57,57,57	0
56	MG	YA	3072	1/1	0.91	0.15	3,3,3,3	0
56	MG	XA	1622	1/1	0.91	0.07	53,53,53,53	0
56	MG	RA	3066	1/1	0.92	0.20	29,29,29,29	0
56	MG	RA	3174	1/1	0.92	0.06	40,40,40,40	0
56	MG	YA	3272	1/1	0.92	0.14	33,33,33,33	0
56	MG	RA	3401	1/1	0.92	0.08	41,41,41,41	0
56	MG	YA	3056	1/1	0.92	0.23	28,28,28,28	0
56	MG	YA	3277	1/1	0.92	0.12	38,38,38,38	0
56	MG	XA	1631	1/1	0.92	0.13	38,38,38,38	0
56	MG	RA	3067	1/1	0.92	0.13	28,28,28,28	0
56	MG	RA	3124	1/1	0.92	0.09	36,36,36,36	0
56	MG	YA	3509	1/1	0.92	0.09	54,54,54,54	0
56	MG	RA	3302	1/1	0.92	0.10	46,46,46,46	0
56	MG	YA	3069	1/1	0.92	0.15	68,68,68,68	0
56	MG	YA	3287	1/1	0.92	0.18	59,59,59,59	0
56	MG	RA	3052	1/1	0.92	0.09	41,41,41,41	0
56	MG	RA	3240	1/1	0.92	0.10	47,47,47,47	0
56	MG	YA	3519	1/1	0.92	0.11	34,34,34,34	0
56	MG	YA	3073	1/1	0.92	0.09	39,39,39,39	0
56	MG	YA	3437	1/1	0.92	0.04	60,60,60,60	0
56	MG	YA	3438	1/1	0.92	0.14	56,56,56,56	0
56	MG	RQ	201	1/1	0.92	0.23	74,74,74,74	0
56	MG	RA	3371	1/1	0.92	0.14	82,82,82,82	0
56	MG	YA	3076	1/1	0.92	0.09	20,20,20,20	0
56	MG	YA	3531	1/1	0.92	0.05	23,23,23,23	0
56	MG	RR	201	1/1	0.92	0.08	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3081	1/1	0.92	0.08	42,42,42,42	0
56	MG	RA	3097	1/1	0.92	0.16	36,36,36,36	0
56	MG	QA	1608	1/1	0.92	0.10	35,35,35,35	0
56	MG	YA	3448	1/1	0.92	0.30	67,67,67,67	0
56	MG	YA	3164	1/1	0.92	0.14	46,46,46,46	0
56	MG	RA	3100	1/1	0.92	0.10	23,23,23,23	0
56	MG	XA	1646	1/1	0.92	0.12	29,29,29,29	0
56	MG	RA	3496	1/1	0.92	0.14	26,26,26,26	0
56	MG	YA	3371	1/1	0.92	0.24	59,59,59,59	0
56	MG	RA	3130	1/1	0.92	0.18	47,47,47,47	0
56	MG	YA	3097	1/1	0.92	0.23	21,21,21,21	0
56	MG	RA	3071	1/1	0.92	0.07	37,37,37,37	0
56	MG	RA	3013	1/1	0.92	0.15	25,25,25,25	0
56	MG	XA	1652	1/1	0.92	0.07	68,68,68,68	0
56	MG	RA	3056	1/1	0.92	0.13	62,62,62,62	0
56	MG	RA	3285	1/1	0.92	0.13	60,60,60,60	0
56	MG	RA	3315	1/1	0.92	0.19	40,40,40,40	0
56	MG	YA	3241	1/1	0.92	0.23	31,31,31,31	0
56	MG	YA	3019	1/1	0.92	0.29	34,34,34,34	0
56	MG	XA	1660	1/1	0.92	0.14	55,55,55,55	0
56	MG	RA	3163	1/1	0.92	0.07	38,38,38,38	0
56	MG	YA	3023	1/1	0.92	0.20	24,24,24,24	0
56	MG	RA	3003	1/1	0.92	0.18	39,39,39,39	0
56	MG	YA	3388	1/1	0.92	0.10	46,46,46,46	0
56	MG	YQ	202	1/1	0.92	0.17	108,108,108,108	0
56	MG	RA	3350	1/1	0.92	0.15	61,61,61,61	0
56	MG	QA	1621	1/1	0.92	0.08	47,47,47,47	0
56	MG	QA	1617	1/1	0.92	0.08	42,42,42,42	0
56	MG	QA	1659	1/1	0.92	0.11	67,67,67,67	0
56	MG	RA	3139	1/1	0.92	0.16	23,23,23,23	0
56	MG	YA	3122	1/1	0.92	0.11	26,26,26,26	0
56	MG	XA	1670	1/1	0.92	0.07	36,36,36,36	0
56	MG	RA	3262	1/1	0.92	0.09	61,61,61,61	0
56	MG	YA	3036	1/1	0.92	0.20	16,16,16,16	0
56	MG	QA	1606	1/1	0.92	0.10	49,49,49,49	0
56	MG	RA	3120	1/1	0.92	0.09	55,55,55,55	0
56	MG	YA	3043	1/1	0.92	0.17	42,42,42,42	0
56	MG	RA	3200	1/1	0.92	0.12	43,43,43,43	0
56	MG	YA	3268	1/1	0.92	0.05	44,44,44,44	0
56	MG	RA	3476	1/1	0.92	0.16	73,73,73,73	0
56	MG	QA	1633	1/1	0.93	0.06	63,63,63,63	0
56	MG	XA	1614	1/1	0.93	0.12	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3410	1/1	0.93	0.12	49,49,49,49	0
56	MG	YA	3385	1/1	0.93	0.11	46,46,46,46	0
56	MG	RA	3245	1/1	0.93	0.17	35,35,35,35	0
56	MG	YA	3063	1/1	0.93	0.09	34,34,34,34	0
56	MG	YA	3067	1/1	0.93	0.19	31,31,31,31	0
56	MG	YA	3068	1/1	0.93	0.12	29,29,29,29	0
56	MG	XC	301	1/1	0.93	0.10	112,112,112,112	0
56	MG	YA	3314	1/1	0.93	0.10	53,53,53,53	0
56	MG	YA	3231	1/1	0.93	0.14	40,40,40,40	0
56	MG	YA	3316	1/1	0.93	0.14	52,52,52,52	0
56	MG	RA	3276	1/1	0.93	0.07	60,60,60,60	0
56	MG	YA	3498	1/1	0.93	0.17	52,52,52,52	0
56	MG	RA	3277	1/1	0.93	0.19	39,39,39,39	0
56	MG	RA	3415	1/1	0.93	0.14	50,50,50,50	0
56	MG	YA	3163	1/1	0.93	0.05	60,60,60,60	0
56	MG	YA	3502	1/1	0.93	0.12	54,54,54,54	0
56	MG	RA	3416	1/1	0.93	0.08	38,38,38,38	0
56	MG	RA	3511	1/1	0.93	0.08	80,80,80,80	0
56	MG	RA	3023	1/1	0.93	0.09	30,30,30,30	0
56	MG	RA	3196	1/1	0.93	0.07	44,44,44,44	0
56	MG	YA	3079	1/1	0.93	0.28	23,23,23,23	0
56	MG	RA	3248	1/1	0.93	0.10	87,87,87,87	0
56	MG	YA	3082	1/1	0.93	0.13	31,31,31,31	0
56	MG	RA	3217	1/1	0.93	0.09	87,87,87,87	0
56	MG	RA	3105	1/1	0.93	0.10	48,48,48,48	0
56	MG	YA	3513	1/1	0.93	0.08	95,95,95,95	0
56	MG	XA	1632	1/1	0.93	0.11	51,51,51,51	0
56	MG	RA	3042	1/1	0.93	0.10	54,54,54,54	0
56	MG	YA	3175	1/1	0.93	0.08	33,33,33,33	0
56	MG	RA	3424	1/1	0.93	0.18	58,58,58,58	0
56	MG	YA	3420	1/1	0.93	0.15	55,55,55,55	0
56	MG	RA	3150	1/1	0.93	0.07	31,31,31,31	0
56	MG	RA	3468	1/1	0.93	0.24	54,54,54,54	0
56	MG	YA	3526	1/1	0.93	0.19	13,13,13,13	0
56	MG	RA	3286	1/1	0.93	0.28	54,54,54,54	0
56	MG	RB	209	1/1	0.93	0.08	87,87,87,87	0
56	MG	QA	1604	1/1	0.93	0.11	20,20,20,20	0
56	MG	YA	3428	1/1	0.93	0.11	32,32,32,32	0
56	MG	RA	3428	1/1	0.93	0.19	46,46,46,46	0
56	MG	YA	3431	1/1	0.93	0.11	55,55,55,55	0
56	MG	YA	3432	1/1	0.93	0.08	44,44,44,44	0
56	MG	RE	301	1/1	0.93	0.08	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3539	1/1	0.93	0.17	53,53,53,53	0
56	MG	RA	3429	1/1	0.93	0.14	80,80,80,80	0
56	MG	RA	3109	1/1	0.93	0.11	50,50,50,50	0
56	MG	RA	3225	1/1	0.93	0.11	17,17,17,17	0
56	MG	YA	3106	1/1	0.93	0.18	31,31,31,31	0
56	MG	YA	3190	1/1	0.93	0.21	54,54,54,54	0
56	MG	QA	1642	1/1	0.93	0.17	40,40,40,40	0
56	MG	QA	1672	1/1	0.93	0.06	75,75,75,75	0
56	MG	QA	1609	1/1	0.93	0.10	24,24,24,24	0
56	MG	RA	3354	1/1	0.93	0.09	54,54,54,54	0
56	MG	RA	3481	1/1	0.93	0.11	58,58,58,58	0
56	MG	RA	3264	1/1	0.93	0.19	41,41,41,41	0
56	MG	YA	3281	1/1	0.93	0.14	35,35,35,35	0
56	MG	RA	3483	1/1	0.93	0.09	70,70,70,70	0
56	MG	XA	1657	1/1	0.93	0.11	55,55,55,55	0
56	MG	RA	3091	1/1	0.93	0.20	18,18,18,18	0
56	MG	RA	3118	1/1	0.93	0.17	33,33,33,33	0
56	MG	RA	3014	1/1	0.93	0.12	17,17,17,17	0
56	MG	YA	3365	1/1	0.93	0.08	53,53,53,53	0
56	MG	YA	3458	1/1	0.93	0.09	54,54,54,54	0
56	MG	YA	3459	1/1	0.93	0.13	48,48,48,48	0
56	MG	YA	3366	1/1	0.93	0.18	49,49,49,49	0
56	MG	RA	3487	1/1	0.93	0.15	48,48,48,48	0
56	MG	YA	3037	1/1	0.93	0.19	20,20,20,20	0
56	MG	QA	1665	1/1	0.93	0.05	42,42,42,42	0
56	MG	YA	3039	1/1	0.93	0.17	16,16,16,16	0
56	MG	RA	3362	1/1	0.93	0.10	37,37,37,37	0
56	MG	Y5	502	1/1	0.93	0.07	40,40,40,40	0
56	MG	XA	1603	1/1	0.93	0.14	16,16,16,16	0
56	MG	RA	3327	1/1	0.93	0.15	84,84,84,84	0
56	MG	QV	103	1/1	0.93	0.09	49,49,49,49	0
56	MG	QA	1637	1/1	0.93	0.17	55,55,55,55	0
56	MG	YA	3050	1/1	0.93	0.18	23,23,23,23	0
56	MG	RA	3330	1/1	0.93	0.12	54,54,54,54	0
58	ZN	R9	101	1/1	0.93	0.27	122,122,122,122	0
56	MG	RA	3498	1/1	0.93	0.08	29,29,29,29	0
56	MG	YA	3379	1/1	0.93	0.20	45,45,45,45	0
56	MG	YA	3055	1/1	0.93	0.10	26,26,26,26	0
56	MG	RA	3074	1/1	0.93	0.07	56,56,56,56	0
58	ZN	Y9	101	1/1	0.93	0.19	197,197,197,197	0
56	MG	RA	3160	1/1	0.94	0.10	45,45,45,45	0
56	MG	QA	1613	1/1	0.94	0.06	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3028	1/1	0.94	0.06	20,20,20,20	0
56	MG	YA	3307	1/1	0.94	0.24	55,55,55,55	0
56	MG	QA	1622	1/1	0.94	0.13	51,51,51,51	0
56	MG	YA	3442	1/1	0.94	0.06	68,68,68,68	0
56	MG	YA	3192	1/1	0.94	0.08	56,56,56,56	0
56	MG	YA	3310	1/1	0.94	0.13	31,31,31,31	0
56	MG	YA	3517	1/1	0.94	0.11	53,53,53,53	0
56	MG	XA	1619	1/1	0.94	0.11	48,48,48,48	0
56	MG	RA	3239	1/1	0.94	0.24	50,50,50,50	0
56	MG	RA	3073	1/1	0.94	0.13	30,30,30,30	0
56	MG	RA	3449	1/1	0.94	0.07	59,59,59,59	0
56	MG	YA	3524	1/1	0.94	0.23	7,7,7,7	0
56	MG	YA	3197	1/1	0.94	0.05	119,119,119,119	0
56	MG	RA	3417	1/1	0.94	0.13	63,63,63,63	0
56	MG	YA	3258	1/1	0.94	0.13	30,30,30,30	0
56	MG	YA	3084	1/1	0.94	0.09	22,22,22,22	0
56	MG	YA	3529	1/1	0.94	0.10	46,46,46,46	0
56	MG	QA	1628	1/1	0.94	0.10	44,44,44,44	0
56	MG	RA	3044	1/1	0.94	0.22	18,18,18,18	0
56	MG	YA	3321	1/1	0.94	0.10	51,51,51,51	0
56	MG	RA	3243	1/1	0.94	0.21	54,54,54,54	0
56	MG	YA	3150	1/1	0.94	0.07	51,51,51,51	0
56	MG	QA	1629	1/1	0.94	0.05	60,60,60,60	0
56	MG	YA	3325	1/1	0.94	0.06	56,56,56,56	0
56	MG	YA	3540	1/1	0.94	0.11	29,29,29,29	0
56	MG	YA	3462	1/1	0.94	0.08	78,78,78,78	0
56	MG	YA	3092	1/1	0.94	0.21	21,21,21,21	0
56	MG	YB	202	1/1	0.94	0.07	50,50,50,50	0
56	MG	YB	203	1/1	0.94	0.07	75,75,75,75	0
56	MG	YA	3154	1/1	0.94	0.17	40,40,40,40	0
56	MG	RA	3032	1/1	0.94	0.18	30,30,30,30	0
56	MG	YA	3466	1/1	0.94	0.08	36,36,36,36	0
56	MG	RA	3386	1/1	0.94	0.06	43,43,43,43	0
56	MG	RA	3492	1/1	0.94	0.10	21,21,21,21	0
56	MG	RA	3084	1/1	0.94	0.08	51,51,51,51	0
56	MG	RA	3106	1/1	0.94	0.19	31,31,31,31	0
56	MG	RA	3219	1/1	0.94	0.07	49,49,49,49	0
56	MG	RA	3048	1/1	0.94	0.07	24,24,24,24	0
56	MG	RA	3086	1/1	0.94	0.13	28,28,28,28	0
56	MG	YA	3337	1/1	0.94	0.07	45,45,45,45	0
56	MG	YA	3279	1/1	0.94	0.25	56,56,56,56	0
56	MG	RA	3462	1/1	0.94	0.07	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3253	1/1	0.94	0.16	58,58,58,58	0
56	MG	YA	3282	1/1	0.94	0.24	33,33,33,33	0
56	MG	RA	3335	1/1	0.94	0.06	51,51,51,51	0
56	MG	YA	3049	1/1	0.94	0.18	21,21,21,21	0
56	MG	YA	3484	1/1	0.94	0.07	40,40,40,40	0
56	MG	YA	3285	1/1	0.94	0.14	30,30,30,30	0
56	MG	YA	3109	1/1	0.94	0.15	45,45,45,45	0
56	MG	RA	3503	1/1	0.94	0.06	56,56,56,56	0
56	MG	XV	104	1/1	0.94	0.05	65,65,65,65	0
56	MG	RA	3176	1/1	0.94	0.15	51,51,51,51	0
56	MG	RA	3399	1/1	0.94	0.07	60,60,60,60	0
56	MG	RA	3004	1/1	0.94	0.15	28,28,28,28	0
56	MG	RA	3110	1/1	0.94	0.10	42,42,42,42	0
56	MG	RA	3509	1/1	0.94	0.21	7,7,7,7	0
56	MG	RA	3034	1/1	0.94	0.20	23,23,23,23	0
56	MG	YA	3424	1/1	0.94	0.13	49,49,49,49	0
56	MG	XA	1651	1/1	0.94	0.07	52,52,52,52	0
56	MG	YA	3235	1/1	0.94	0.12	57,57,57,57	0
56	MG	RA	3228	1/1	0.94	0.17	32,32,32,32	0
56	MG	YA	3064	1/1	0.94	0.08	41,41,41,41	0
56	MG	RA	3112	1/1	0.94	0.08	28,28,28,28	0
56	MG	QA	1669	1/1	0.94	0.06	56,56,56,56	0
56	MG	XA	1656	1/1	0.94	0.07	45,45,45,45	0
56	MG	RA	3343	1/1	0.94	0.14	36,36,36,36	0
56	MG	QF	201	1/1	0.95	0.07	55,55,55,55	0
56	MG	RA	3075	1/1	0.95	0.09	39,39,39,39	0
56	MG	RA	3232	1/1	0.95	0.13	30,30,30,30	0
56	MG	RA	3185	1/1	0.95	0.09	60,60,60,60	0
56	MG	RA	3210	1/1	0.95	0.15	55,55,55,55	0
56	MG	RA	3236	1/1	0.95	0.22	23,23,23,23	0
56	MG	YA	3248	1/1	0.95	0.13	20,20,20,20	0
56	MG	YA	3066	1/1	0.95	0.10	22,22,22,22	0
56	MG	YA	3521	1/1	0.95	0.15	13,13,13,13	0
56	MG	RA	3035	1/1	0.95	0.12	27,27,27,27	0
56	MG	RA	3238	1/1	0.95	0.10	57,57,57,57	0
56	MG	YA	3189	1/1	0.95	0.05	42,42,42,42	0
56	MG	RA	3094	1/1	0.95	0.21	21,21,21,21	0
56	MG	XA	1658	1/1	0.95	0.06	58,58,58,58	0
56	MG	YA	3071	1/1	0.95	0.11	92,92,92,92	0
56	MG	YA	3009	1/1	0.95	0.07	37,37,37,37	0
56	MG	RA	3268	1/1	0.95	0.16	48,48,48,48	0
56	MG	YA	3138	1/1	0.95	0.08	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3037	1/1	0.95	0.07	9,9,9,9	0
56	MG	YA	3533	1/1	0.95	0.26	73,73,73,73	0
56	MG	QA	1639	1/1	0.95	0.05	46,46,46,46	0
56	MG	RA	3489	1/1	0.95	0.18	70,70,70,70	0
56	MG	RA	3171	1/1	0.95	0.12	39,39,39,39	0
56	MG	XA	1664	1/1	0.95	0.14	31,31,31,31	0
56	MG	YA	3145	1/1	0.95	0.07	32,32,32,32	0
56	MG	YA	3327	1/1	0.95	0.06	20,20,20,20	0
56	MG	XA	1625	1/1	0.95	0.06	55,55,55,55	0
56	MG	XA	1626	1/1	0.95	0.07	30,30,30,30	0
56	MG	YA	3024	1/1	0.95	0.16	14,14,14,14	0
56	MG	RA	3194	1/1	0.95	0.23	59,59,59,59	0
56	MG	YA	3273	1/1	0.95	0.14	28,28,28,28	0
56	MG	YA	3151	1/1	0.95	0.07	37,37,37,37	0
56	MG	RA	3358	1/1	0.95	0.06	38,38,38,38	0
56	MG	RA	3493	1/1	0.95	0.18	70,70,70,70	0
56	MG	QA	1651	1/1	0.95	0.08	45,45,45,45	0
56	MG	YA	3474	1/1	0.95	0.10	41,41,41,41	0
56	MG	XA	1673	1/1	0.95	0.05	36,36,36,36	0
56	MG	XA	1674	1/1	0.95	0.07	93,93,93,93	0
56	MG	RA	3099	1/1	0.95	0.10	30,30,30,30	0
56	MG	RA	3155	1/1	0.95	0.08	48,48,48,48	0
56	MG	RA	3019	1/1	0.95	0.09	29,29,29,29	0
56	MG	YA	3160	1/1	0.95	0.06	73,73,73,73	0
56	MG	RA	3333	1/1	0.95	0.17	37,37,37,37	0
56	MG	RA	3278	1/1	0.95	0.22	41,41,41,41	0
56	MG	RA	3157	1/1	0.95	0.08	26,26,26,26	0
56	MG	YA	3410	1/1	0.95	0.11	76,76,76,76	0
56	MG	YA	3411	1/1	0.95	0.07	57,57,57,57	0
56	MG	YA	3412	1/1	0.95	0.27	55,55,55,55	0
56	MG	QA	1625	1/1	0.95	0.07	43,43,43,43	0
56	MG	YA	3289	1/1	0.95	0.08	50,50,50,50	0
56	MG	YA	3415	1/1	0.95	0.09	43,43,43,43	0
56	MG	YA	3349	1/1	0.95	0.16	54,54,54,54	0
56	MG	RA	3021	1/1	0.95	0.06	29,29,29,29	0
56	MG	QA	1630	1/1	0.95	0.07	42,42,42,42	0
56	MG	XA	1641	1/1	0.95	0.06	54,54,54,54	0
56	MG	RA	3311	1/1	0.95	0.14	63,63,63,63	0
56	MG	YA	3423	1/1	0.95	0.08	91,91,91,91	0
56	MG	YA	3107	1/1	0.95	0.10	55,55,55,55	0
56	MG	RA	3506	1/1	0.95	0.15	46,46,46,46	0
56	MG	QA	1614	1/1	0.95	0.06	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3112	1/1	0.95	0.14	18,18,18,18	0
56	MG	YA	3233	1/1	0.95	0.14	64,64,64,64	0
56	MG	RA	3162	1/1	0.95	0.12	49,49,49,49	0
56	MG	YA	3052	1/1	0.95	0.11	30,30,30,30	0
56	MG	RA	3090	1/1	0.95	0.08	31,31,31,31	0
56	MG	RA	3475	1/1	0.95	0.14	44,44,44,44	0
56	MG	XV	107	1/1	0.95	0.07	23,23,23,23	0
56	MG	YA	3207	1/1	0.96	0.20	54,54,54,54	0
56	MG	RA	3146	1/1	0.96	0.19	40,40,40,40	0
56	MG	YA	3095	1/1	0.96	0.08	24,24,24,24	0
56	MG	YA	3518	1/1	0.96	0.15	32,32,32,32	0
56	MG	RA	3010	1/1	0.96	0.06	29,29,29,29	0
56	MG	RA	3129	1/1	0.96	0.10	46,46,46,46	0
56	MG	YA	3275	1/1	0.96	0.24	33,33,33,33	0
56	MG	RA	3011	1/1	0.96	0.08	42,42,42,42	0
56	MG	YA	3041	1/1	0.96	0.08	21,21,21,21	0
56	MG	XV	105	1/1	0.96	0.10	42,42,42,42	0
56	MG	RA	3115	1/1	0.96	0.07	45,45,45,45	0
56	MG	XA	1655	1/1	0.96	0.09	31,31,31,31	0
56	MG	XA	1621	1/1	0.96	0.09	48,48,48,48	0
56	MG	RA	3224	1/1	0.96	0.05	40,40,40,40	0
56	MG	RA	3269	1/1	0.96	0.17	65,65,65,65	0
56	MG	QA	1658	1/1	0.96	0.09	80,80,80,80	0
56	MG	RA	3369	1/1	0.96	0.13	40,40,40,40	0
56	MG	RA	3005	1/1	0.96	0.21	27,27,27,27	0
56	MG	RA	3497	1/1	0.96	0.26	21,21,21,21	0
56	MG	RA	3188	1/1	0.96	0.08	45,45,45,45	0
56	MG	QA	1645	1/1	0.96	0.09	51,51,51,51	0
56	MG	RA	3346	1/1	0.96	0.06	46,46,46,46	0
56	MG	RA	3250	1/1	0.96	0.15	47,47,47,47	0
56	MG	YA	3011	1/1	0.96	0.06	25,25,25,25	0
56	MG	YA	3406	1/1	0.96	0.06	29,29,29,29	0
56	MG	YA	3473	1/1	0.96	0.09	65,65,65,65	0
56	MG	YA	3012	1/1	0.96	0.12	22,22,22,22	0
56	MG	YA	3119	1/1	0.96	0.19	44,44,44,44	0
56	MG	RA	3408	1/1	0.96	0.08	61,61,61,61	0
56	MG	YA	3065	1/1	0.96	0.22	21,21,21,21	0
56	MG	YA	3014	1/1	0.96	0.19	27,27,27,27	0
56	MG	YA	3354	1/1	0.96	0.23	43,43,43,43	0
56	MG	QA	1607	1/1	0.96	0.07	37,37,37,37	0
56	MG	YA	3125	1/1	0.96	0.18	23,23,23,23	0
56	MG	XA	1669	1/1	0.96	0.12	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3017	1/1	0.96	0.13	20,20,20,20	0
56	MG	RA	3411	1/1	0.96	0.05	42,42,42,42	0
56	MG	RA	3254	1/1	0.96	0.18	27,27,27,27	0
56	MG	YE	301	1/1	0.96	0.10	37,37,37,37	0
56	MG	YA	3021	1/1	0.96	0.12	20,20,20,20	0
56	MG	RA	3193	1/1	0.96	0.07	54,54,54,54	0
56	MG	YA	3133	1/1	0.96	0.09	27,27,27,27	0
56	MG	YA	3490	1/1	0.96	0.10	52,52,52,52	0
56	MG	QA	1643	1/1	0.96	0.09	58,58,58,58	0
56	MG	RA	3446	1/1	0.96	0.38	55,55,55,55	0
56	MG	YA	3493	1/1	0.96	0.07	102,102,102,102	0
56	MG	YA	3191	1/1	0.96	0.09	93,93,93,93	0
56	MG	RA	3510	1/1	0.96	0.06	21,21,21,21	0
56	MG	YA	3496	1/1	0.96	0.12	59,59,59,59	0
56	MG	RA	3257	1/1	0.96	0.10	39,39,39,39	0
56	MG	YA	3430	1/1	0.96	0.07	65,65,65,65	0
56	MG	YA	3027	1/1	0.96	0.07	28,28,28,28	0
56	MG	YA	3080	1/1	0.96	0.18	21,21,21,21	0
56	MG	RA	3062	1/1	0.96	0.05	36,36,36,36	0
56	MG	RA	3078	1/1	0.96	0.12	42,42,42,42	0
56	MG	RA	3383	1/1	0.96	0.16	32,32,32,32	0
56	MG	YA	3144	1/1	0.96	0.18	41,41,41,41	0
56	MG	YA	3505	1/1	0.96	0.09	105,105,105,105	0
56	MG	YA	3200	1/1	0.96	0.08	55,55,55,55	0
56	MG	YA	3031	1/1	0.96	0.07	24,24,24,24	0
56	MG	YA	3441	1/1	0.96	0.05	77,77,77,77	0
56	MG	YA	3032	1/1	0.96	0.13	24,24,24,24	0
56	MG	QA	1612	1/1	0.96	0.04	34,34,34,34	0
56	MG	RA	3081	1/1	0.96	0.09	16,16,16,16	0
56	MG	RA	3095	1/1	0.96	0.09	42,42,42,42	0
56	MG	RA	3310	1/1	0.96	0.07	38,38,38,38	0
56	MG	RA	3440	1/1	0.97	0.06	64,64,64,64	0
56	MG	YA	3267	1/1	0.97	0.12	23,23,23,23	0
56	MG	RA	3143	1/1	0.97	0.08	56,56,56,56	0
56	MG	YA	3078	1/1	0.97	0.06	41,41,41,41	0
56	MG	YA	3530	1/1	0.97	0.04	52,52,52,52	0
56	MG	RA	3055	1/1	0.97	0.05	46,46,46,46	0
56	MG	YA	3476	1/1	0.97	0.11	49,49,49,49	0
56	MG	YA	3127	1/1	0.97	0.15	38,38,38,38	0
56	MG	RA	3360	1/1	0.97	0.18	45,45,45,45	0
56	MG	RA	3036	1/1	0.97	0.06	24,24,24,24	0
56	MG	RA	3057	1/1	0.97	0.12	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	RA	3226	1/1	0.97	0.12	10,10,10,10	0
56	MG	YA	3223	1/1	0.97	0.09	43,43,43,43	0
56	MG	RA	3166	1/1	0.97	0.04	39,39,39,39	0
56	MG	QA	1660	1/1	0.97	0.04	80,80,80,80	0
56	MG	QA	1619	1/1	0.97	0.07	53,53,53,53	0
56	MG	YA	3088	1/1	0.97	0.06	38,38,38,38	0
56	MG	YA	3433	1/1	0.97	0.15	50,50,50,50	0
56	MG	YA	3434	1/1	0.97	0.04	64,64,64,64	0
56	MG	YA	3136	1/1	0.97	0.07	53,53,53,53	0
56	MG	QA	1634	1/1	0.97	0.09	57,57,57,57	0
56	MG	YA	3048	1/1	0.97	0.05	19,19,19,19	0
56	MG	RA	3103	1/1	0.97	0.05	45,45,45,45	0
56	MG	XA	1638	1/1	0.97	0.03	69,69,69,69	0
56	MG	RA	3190	1/1	0.97	0.03	47,47,47,47	0
56	MG	RA	3397	1/1	0.97	0.07	57,57,57,57	0
56	MG	YA	3053	1/1	0.97	0.14	9,9,9,9	0
56	MG	YA	3015	1/1	0.97	0.08	18,18,18,18	0
56	MG	RA	3152	1/1	0.97	0.21	38,38,38,38	0
56	MG	RA	3301	1/1	0.97	0.18	49,49,49,49	0
56	MG	YA	3147	1/1	0.97	0.04	51,51,51,51	0
56	MG	YA	3057	1/1	0.97	0.13	20,20,20,20	0
56	MG	RA	3234	1/1	0.97	0.11	32,32,32,32	0
56	MG	XA	1609	1/1	0.97	0.09	82,82,82,82	0
56	MG	RA	3104	1/1	0.97	0.11	62,62,62,62	0
56	MG	RA	3025	1/1	0.97	0.08	22,22,22,22	0
56	MG	RA	3403	1/1	0.97	0.09	41,41,41,41	0
56	MG	YA	3108	1/1	0.97	0.05	27,27,27,27	0
56	MG	YA	3454	1/1	0.97	0.13	49,49,49,49	0
56	MG	YX	101	1/1	0.97	0.15	118,118,118,118	0
56	MG	YA	3250	1/1	0.97	0.17	16,16,16,16	0
56	MG	RA	3431	1/1	0.97	0.04	38,38,38,38	0
56	MG	YA	3457	1/1	0.97	0.06	104,104,104,104	0
56	MG	YA	3252	1/1	0.97	0.24	22,22,22,22	0
56	MG	XA	1616	1/1	0.97	0.05	35,35,35,35	0
56	MG	RA	3404	1/1	0.97	0.06	50,50,50,50	0
56	MG	YA	3515	1/1	0.97	0.07	48,48,48,48	0
57	SF4	QD	301	8/8	0.97	0.08	78,114,135,135	0
56	MG	RA	3136	1/1	0.97	0.09	54,54,54,54	0
56	MG	RA	3077	1/1	0.97	0.09	23,23,23,23	0
56	MG	RA	3464	1/1	0.97	0.09	72,72,72,72	0
56	MG	RA	3015	1/1	0.97	0.06	20,20,20,20	0
56	MG	XV	103	1/1	0.97	0.08	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3209	1/1	0.97	0.06	48,48,48,48	0
56	MG	RA	3027	1/1	0.97	0.12	20,20,20,20	0
56	MG	RA	3043	1/1	0.97	0.09	15,15,15,15	0
56	MG	QA	1656	1/1	0.97	0.05	46,46,46,46	0
56	MG	RA	3142	1/1	0.97	0.14	38,38,38,38	0
56	MG	RA	3206	1/1	0.98	0.04	39,39,39,39	0
56	MG	YA	3096	1/1	0.98	0.03	39,39,39,39	0
56	MG	YA	3416	1/1	0.98	0.05	70,70,70,70	0
56	MG	YA	3417	1/1	0.98	0.06	63,63,63,63	0
56	MG	RA	3102	1/1	0.98	0.09	18,18,18,18	0
56	MG	XA	1610	1/1	0.98	0.07	40,40,40,40	0
56	MG	RA	3063	1/1	0.98	0.07	25,25,25,25	0
56	MG	YA	3234	1/1	0.98	0.07	63,63,63,63	0
56	MG	YA	3265	1/1	0.98	0.09	26,26,26,26	0
56	MG	RA	3114	1/1	0.98	0.06	42,42,42,42	0
56	MG	YA	3181	1/1	0.98	0.07	24,24,24,24	0
56	MG	YA	3010	1/1	0.98	0.09	24,24,24,24	0
56	MG	XA	1613	1/1	0.98	0.06	40,40,40,40	0
56	MG	RA	3069	1/1	0.98	0.06	28,28,28,28	0
56	MG	RA	3064	1/1	0.98	0.09	24,24,24,24	0
56	MG	RA	3151	1/1	0.98	0.06	31,31,31,31	0
56	MG	QA	1666	1/1	0.98	0.05	48,48,48,48	0
56	MG	XA	1672	1/1	0.98	0.04	44,44,44,44	0
56	MG	RA	3079	1/1	0.98	0.07	24,24,24,24	0
56	MG	YA	3245	1/1	0.98	0.24	8,8,8,8	0
56	MG	YA	3083	1/1	0.98	0.07	29,29,29,29	0
56	MG	XA	1601	1/1	0.98	0.18	28,28,28,28	0
56	MG	YA	3339	1/1	0.98	0.12	20,20,20,20	0
56	MG	XA	1602	1/1	0.98	0.04	56,56,56,56	0
57	SF4	XD	301	8/8	0.98	0.09	64,81,107,108	0
56	MG	RA	3072	1/1	0.98	0.09	23,23,23,23	0
56	MG	QV	102	1/1	0.98	0.07	63,63,63,63	0
56	MG	YA	3405	1/1	0.98	0.08	27,27,27,27	0
56	MG	YA	3042	1/1	0.98	0.09	38,38,38,38	0
56	MG	RA	3388	1/1	0.98	0.06	26,26,26,26	0
56	MG	YA	3091	1/1	0.98	0.06	34,34,34,34	0
56	MG	YA	3044	1/1	0.98	0.15	28,28,28,28	0
56	MG	QH	201	1/1	0.98	0.16	64,64,64,64	0
56	MG	YA	3120	1/1	0.98	0.06	35,35,35,35	0
56	MG	RA	3083	1/1	0.98	0.12	42,42,42,42	0
56	MG	RA	3123	1/1	0.99	0.04	25,25,25,25	0
56	MG	QA	1640	1/1	0.99	0.05	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	YA	3246	1/1	0.99	0.07	24,24,24,24	0
56	MG	YA	3090	1/1	0.99	0.03	40,40,40,40	0
58	ZN	QN	101	1/1	0.99	0.05	104,104,104,104	0
56	MG	RA	3477	1/1	0.99	0.13	74,74,74,74	0
56	MG	YA	3110	1/1	0.99	0.04	30,30,30,30	0
56	MG	YA	3536	1/1	0.99	0.09	52,52,52,52	0
56	MG	RA	3387	1/1	0.99	0.04	38,38,38,38	0
56	MG	YA	3162	1/1	0.99	0.04	32,32,32,32	0
58	ZN	XN	101	1/1	0.99	0.04	111,111,111,111	0
56	MG	YA	3408	1/1	0.99	0.05	27,27,27,27	0
56	MG	YA	3060	1/1	0.99	0.04	22,22,22,22	0
56	MG	RA	3046	1/1	0.99	0.05	13,13,13,13	0
56	MG	RA	3252	1/1	0.99	0.19	19,19,19,19	0
56	MG	RA	3390	1/1	0.99	0.04	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.