



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:17 AM UTC

PDB ID : 8FON / pdb_00008fon
Title : Crystal structure of tRNA^{Lys}(SUU) bound to AUA codon in the ribosomal P site
Authors : Nguyen, H.A.; Hoffer, E.D.; Maehigashi, T.; Fagan, C.E.; Dunham, C.M.
Deposited on : 2023-01-02
Resolution : 3.64 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

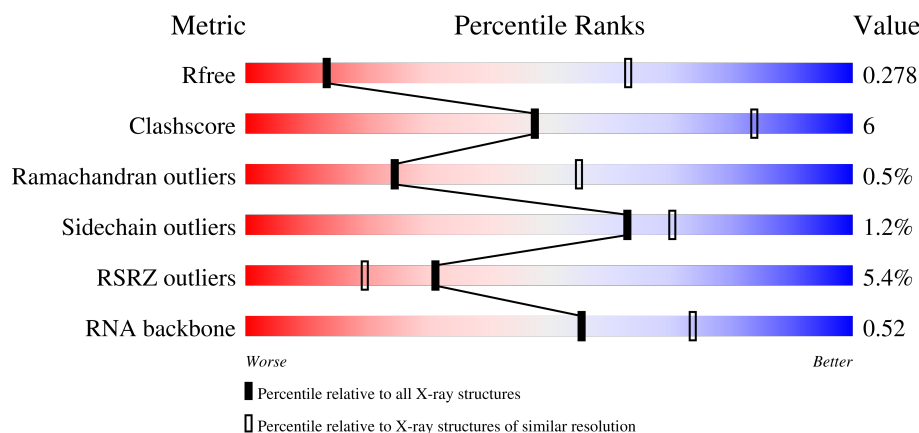
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

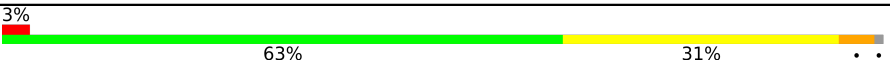
The reported resolution of this entry is 3.64 Å.

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.



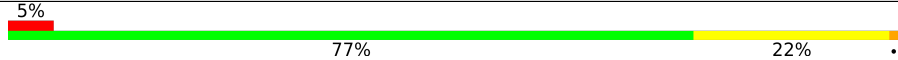
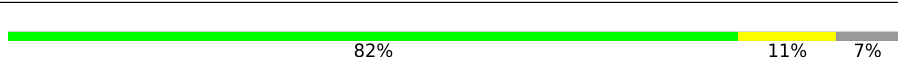
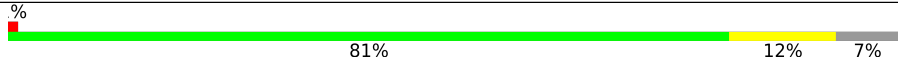
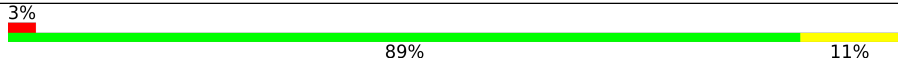
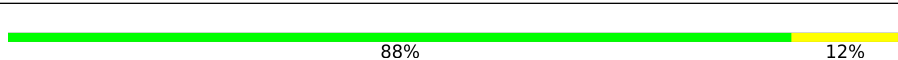
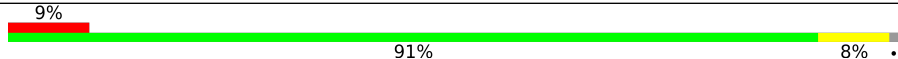
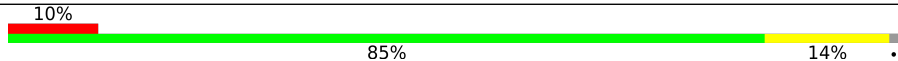
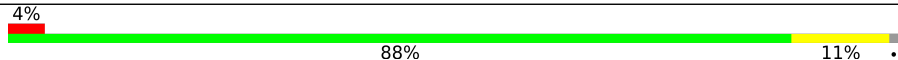
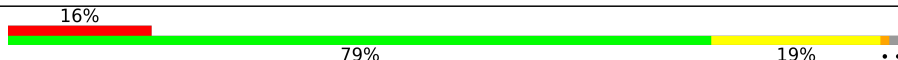
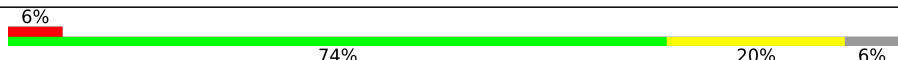
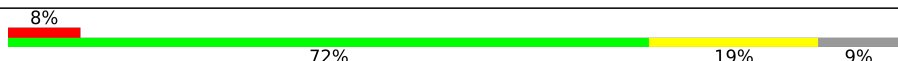
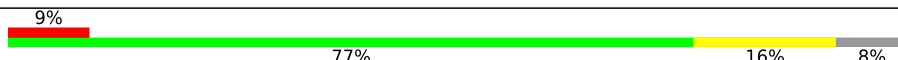
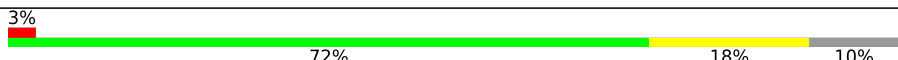
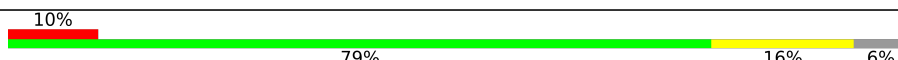
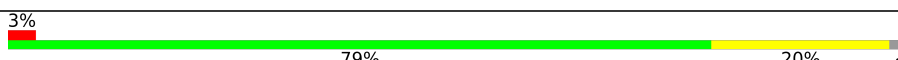
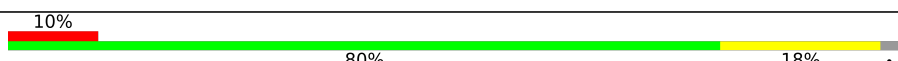
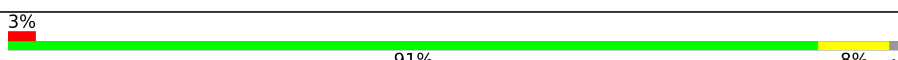
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1132 (3.76-3.52)
Clashscore	190562	1014 (3.74-3.54)
Ramachandran outliers	187476	1123 (3.76-3.52)
Sidechain outliers	187428	1121 (3.76-3.52)
RSRZ outliers	180081	1130 (3.76-3.52)
RNA backbone	3983	1026 (4.22-3.06)

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	1522	
1	XA	1522	
2	QB	256	
2	XB	256	

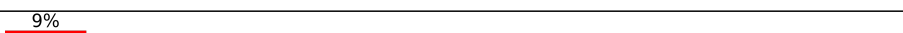
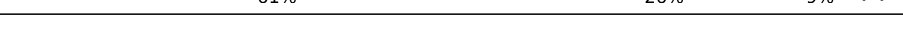
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Mol	Chain	Length	Quality of chain
3	QC	239	
3	XC	239	
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	131	
12	XL	131	
13	QM	126	
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	76	
22	XV	76	
23	QX	23	
23	XX	23	
24	R0	85	
24	Y0	85	
25	R1	98	
25	Y1	98	
26	R2	72	
26	Y2	72	
27	R3	60	
27	Y3	60	

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Mol	Chain	Length	Quality of chain
28	R4	71	83% 14% .
28	Y4	71	4% 82% 14% ..
29	R5	60	7% 92% 7% .
29	Y5	60	2% 90% 8% .
30	R6	54	15% 81% 17% .
30	Y6	54	9% 80% 19% .
31	R7	49	4% 84% 12% .
31	Y7	49	4% 90% 8% .
32	R8	65	5% 52% 31% 15% .
32	Y8	65	6% 77% 22% .
33	R9	37	24% 81% 19%
33	Y9	37	5% 73% 27%
34	RA	2915	5% 65% 29% ..
34	YA	2915	5% 65% 29% ..
35	RB	122	73% 24% ..
35	YB	122	7% 73% 23% ..
36	RD	276	4% 79% 19% .
36	YD	276	2% 83% 15% .
37	RE	206	12% 78% 20% .
37	YE	206	14% 87% 11% .
38	RF	210	10% 80% 16% .
38	YF	210	8% 86% 10% .
39	RG	182	4% 70% 26% ...
39	YG	182	5% 70% 27% ...
40	RH	180	14% 67% 26% ...

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Mol	Chain	Length	Quality of chain
40	YH	180	
41	RI	148	
41	YI	148	
42	RN	140	
42	YN	140	
43	RO	122	
43	YO	122	
44	RP	150	
44	YP	150	
45	RQ	141	
45	YQ	141	
46	RR	118	
46	YR	118	
47	RS	112	
47	YS	112	
48	RT	146	
48	YT	146	
49	RU	118	
49	YU	118	
50	RV	101	
50	YV	101	
51	RW	113	
51	YW	113	
52	RX	96	
52	YX	96	

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Mol	Chain	Length	Quality of chain
53	RY	110	
53	YY	110	
54	RZ	206	
54	YZ	206	
55	XY	17	
56	Z6	3	
56	Z8	3	

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 292577 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QA	1500	Total	C	N	O	P	0	0	0
			32247	14353	5981	10414	1499			
1	XA	1511	Total	C	N	O	P	0	0	0
			32471	14454	6014	10493	1510			

- 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			
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			

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

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	QU	25	Total	C	N	O	0	0	0
			217	134	52	31			
21	XU	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 22 is a RNA chain called P-site tRNA^{Lys}(SUU).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	74	Total	C	N	O	P	0	0	0
			1584	710	278	523	73			
22	XV	74	Total	C	N	O	P	0	0	0
			1584	710	278	523	73			

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	3	Total	C	N	O	P	0	0	0
			65	29	12	21	3			
23	XX	23	Total	C	N	O	P	0	0	0
			499	223	96	157	23			

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	R0	76	Total	C	N	O	S	0	0	0
			603	372	128	102	1			
24	Y0	75	Total	C	N	O	S	0	0	0
			599	370	127	101	1			

- Molecule 25 is a protein called 50S ribosomal protein L28.

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

- Molecule 26 is a protein called 50S ribosomal protein L29.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Y2	68	Total	C	N	O	S	0	0	0
			575	355	117	102	1			

- Molecule 27 is a protein called 50S ribosomal protein L30.

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

- Molecule 28 is a protein called 50S ribosomal protein L31.

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

- Molecule 29 is a protein called 50S ribosomal protein L32.

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

- Molecule 30 is a protein called 50S ribosomal protein L33.

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

- Molecule 31 is a protein called 50S ribosomal protein L34.

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

- Molecule 32 is a protein called 50S ribosomal protein L35.

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

- Molecule 33 is a protein called 50S ribosomal protein L36.

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

- Molecule 34 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	RA	2881	Total	C	N	O	P	0	0	0
			62051	27618	11609	19944	2880			
34	YA	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			

- Molecule 35 is a RNA chain called 5S rRNA.

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

- Molecule 36 is a protein called 50S ribosomal protein L2.

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

- Molecule 37 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	RE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
37	YE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 38 is a protein called 50S ribosomal protein L4.

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

- Molecule 39 is a protein called 50S ribosomal protein L5.

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

- Molecule 40 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	RH	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
40	YH	173	Total	C	N	O	S	0	0	0
			1330	845	250	234	1			

- Molecule 41 is a protein called 50S ribosomal protein L9.

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

- Molecule 42 is a protein called 50S ribosomal protein L13.

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

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

- Molecule 43 is a protein called 50S ribosomal protein L14.

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

- Molecule 44 is a protein called 50S ribosomal protein L15.

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

- Molecule 45 is a protein called 50S ribosomal protein L16.

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

- Molecule 46 is a protein called 50S ribosomal protein L17.

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

- Molecule 47 is a protein called 50S ribosomal protein L18.

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

- Molecule 48 is a protein called 50S ribosomal protein L19.

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

- Molecule 49 is a protein called 50S ribosomal protein L20.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L22.

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

- Molecule 52 is a protein called 50S ribosomal protein L23.

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

- Molecule 53 is a protein called 50S ribosomal protein L24.

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

- Molecule 54 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	RZ	203	Total	C	N	O	S	0	0	0
			1601	1020	283	295	3			
54	YZ	203	Total	C	N	O	S	0	0	0
			1601	1020	283	295	3			

- Molecule 55 is a RNA chain called A-site ASL⁺Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	XY	17	Total	C	N	O	P	0	0	0
			362	163	68	115	16			

- Molecule 56 is a RNA chain called CC-puro.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	Z6	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			
56	Z8	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	73	Total	Mg	0	0
			73	73		
57	QF	1	Total	Mg	0	0
			1	1		
57	QH	1	Total	Mg	0	0
			1	1		
57	QJ	1	Total	Mg	0	0
			1	1		
57	QM	1	Total	Mg	0	0
			1	1		
57	QV	1	Total	Mg	0	0
			1	1		

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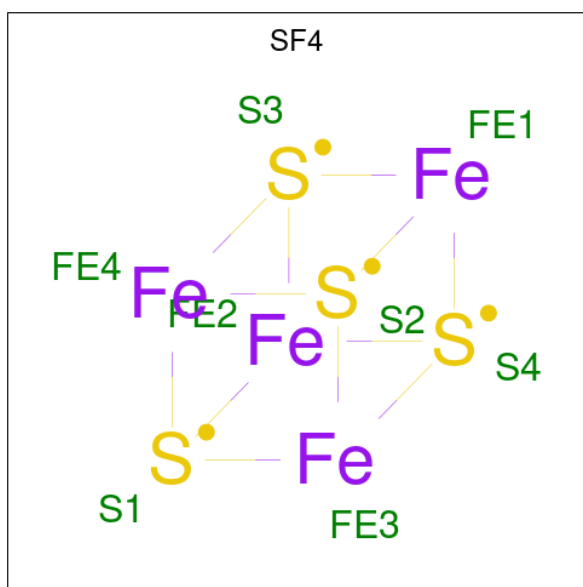
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	R0	1	Total 1	Mg 1	0	0
57	R1	1	Total 1	Mg 1	0	0
57	R3	1	Total 1	Mg 1	0	0
57	RA	483	Total 483	Mg 483	0	0
57	RB	7	Total 7	Mg 7	0	0
57	RE	4	Total 4	Mg 4	0	0
57	RN	1	Total 1	Mg 1	0	0
57	RO	1	Total 1	Mg 1	0	0
57	RP	3	Total 3	Mg 3	0	0
57	RQ	3	Total 3	Mg 3	0	0
57	RR	1	Total 1	Mg 1	0	0
57	RT	1	Total 1	Mg 1	0	0
57	RY	1	Total 1	Mg 1	0	0
57	XA	73	Total 73	Mg 73	0	0
57	XE	1	Total 1	Mg 1	0	0
57	XK	1	Total 1	Mg 1	0	0
57	XL	1	Total 1	Mg 1	0	0
57	XM	1	Total 1	Mg 1	0	0
57	XQ	1	Total 1	Mg 1	0	0
57	XS	1	Total 1	Mg 1	0	0
57	Y0	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	Y1	1	Total 1	Mg 1	0	0
57	Y7	1	Total 1	Mg 1	0	0
57	Y8	1	Total 1	Mg 1	0	0
57	YA	538	Total 538	Mg 538	0	0
57	YB	13	Total 13	Mg 13	0	0
57	YD	3	Total 3	Mg 3	0	0
57	YE	4	Total 4	Mg 4	0	0
57	YN	1	Total 1	Mg 1	0	0
57	YO	1	Total 1	Mg 1	0	0
57	YP	1	Total 1	Mg 1	0	0
57	YQ	3	Total 3	Mg 3	0	0
57	YR	2	Total 2	Mg 2	0	0
57	YX	2	Total 2	Mg 2	0	0
57	YY	1	Total 1	Mg 1	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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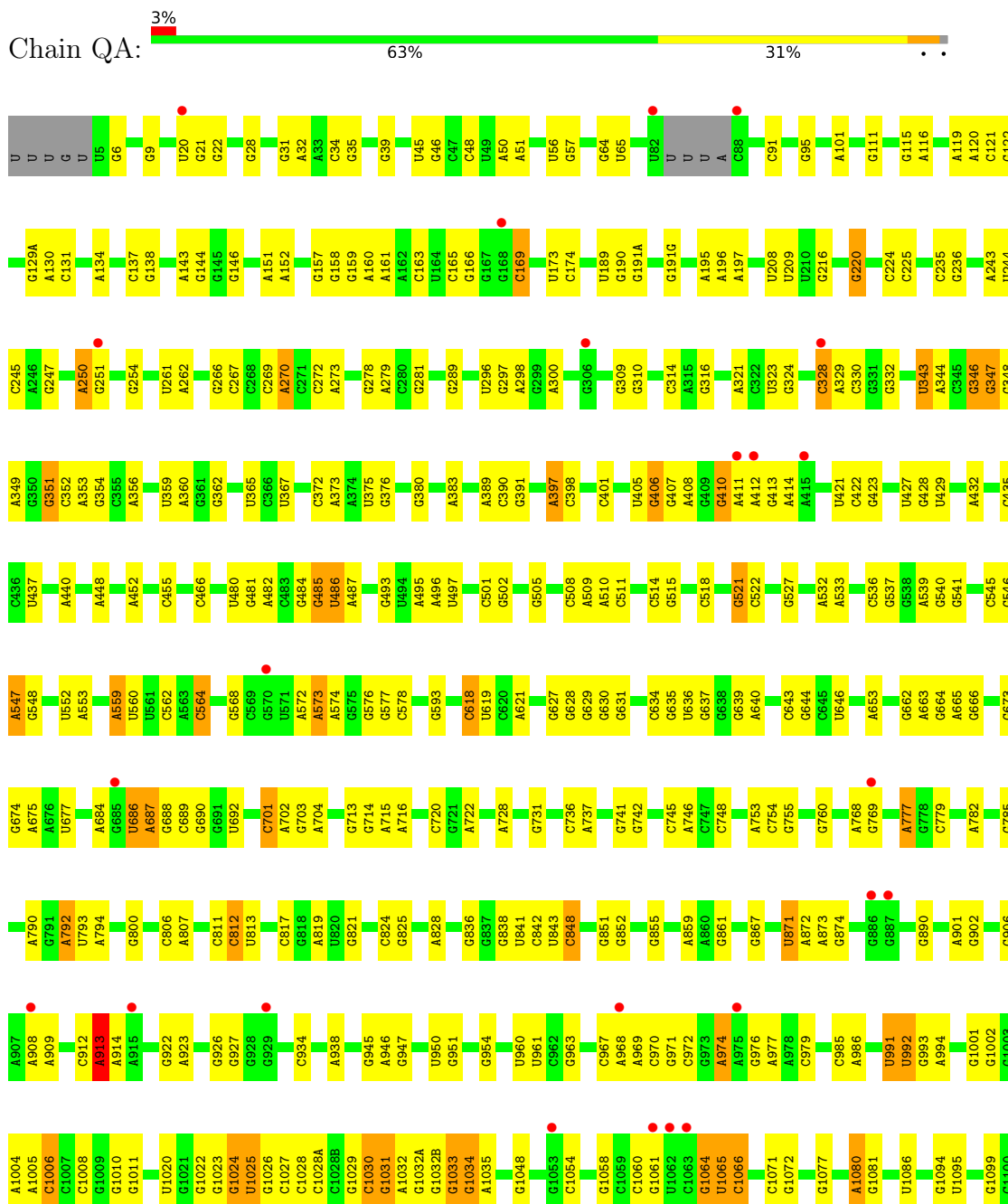
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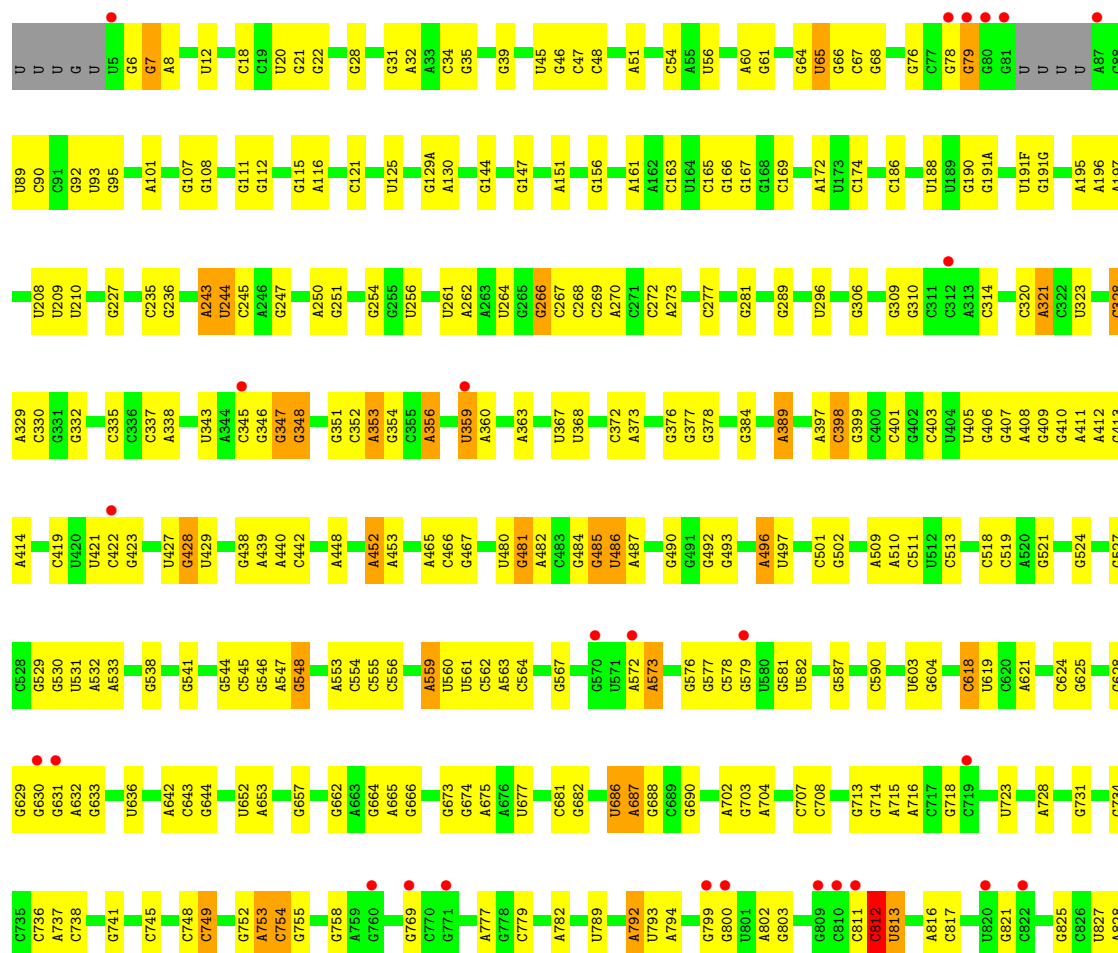
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	Y9	1	Total 1	Zn 1	0	0
59	YY	1	Total 1	Zn 1	0	0

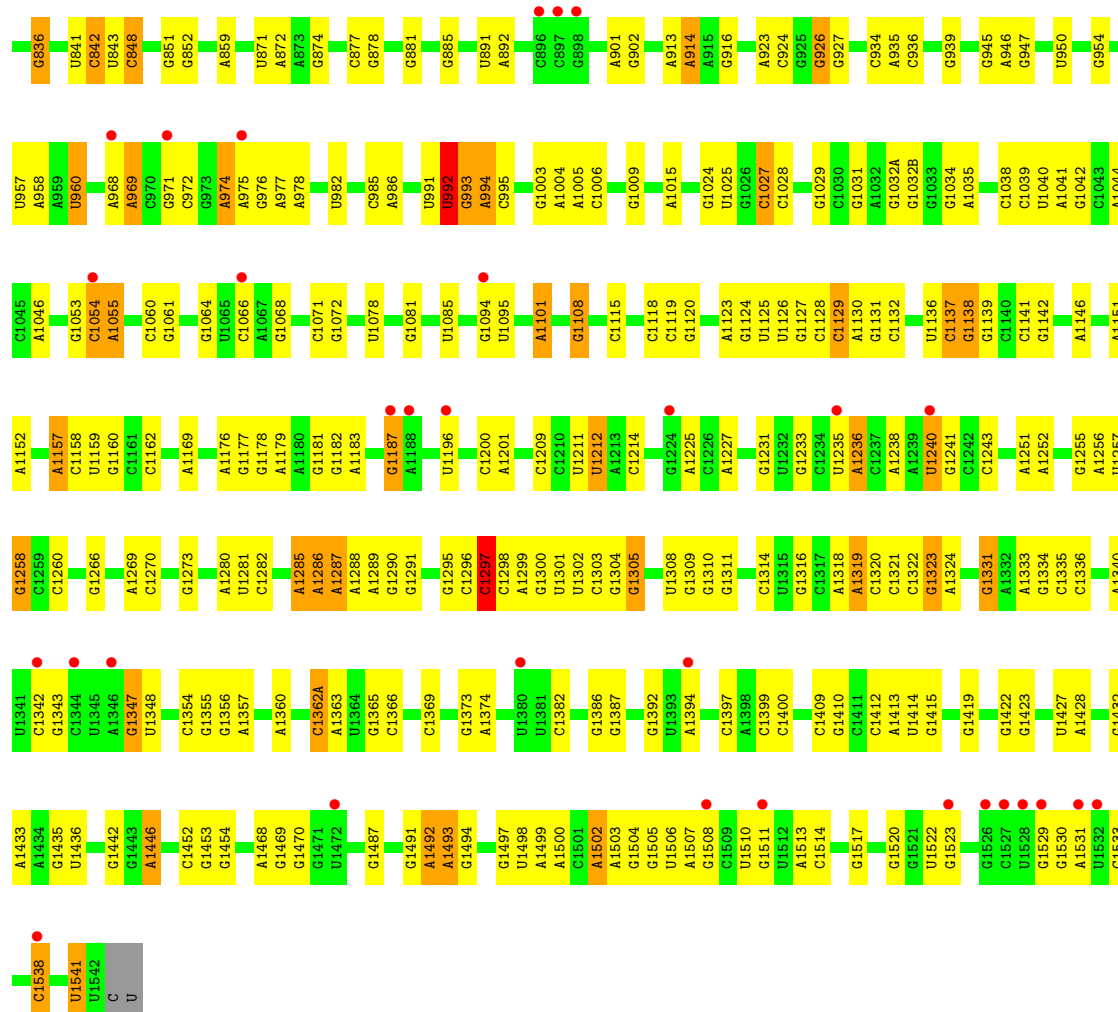
3 Residue-property plots

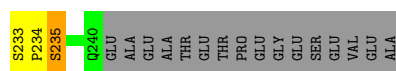
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

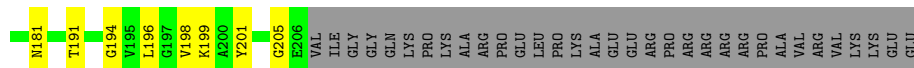
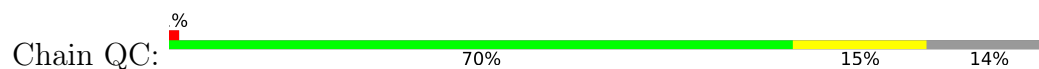




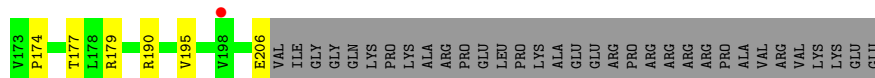
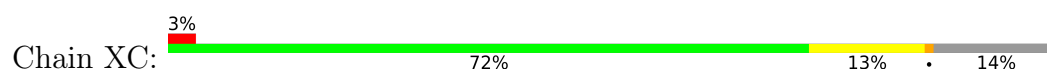




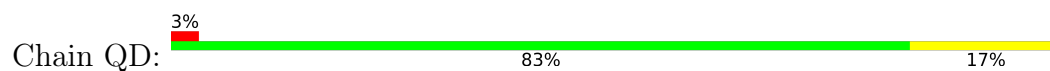
- Molecule 3: 30S ribosomal protein S3



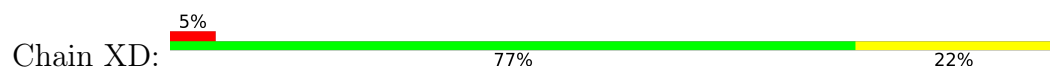
- Molecule 3: 30S ribosomal protein S3



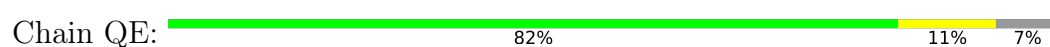
- Molecule 4: 30S ribosomal protein S4

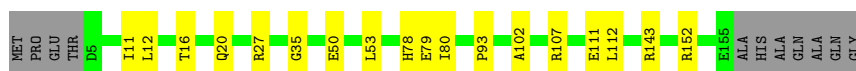


- Molecule 4: 30S ribosomal protein S4

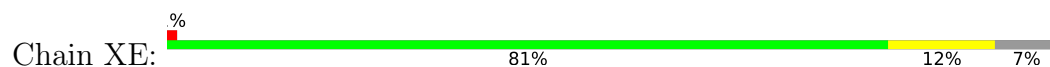


- Molecule 5: 30S ribosomal protein S5

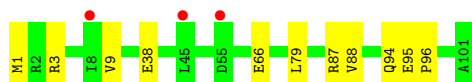
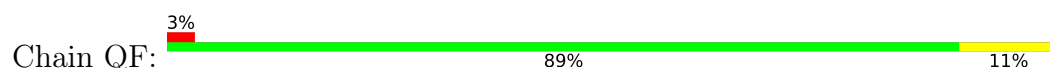




- Molecule 5: 30S ribosomal protein S5



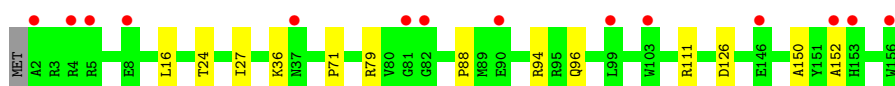
- Molecule 6: 30S ribosomal protein S6



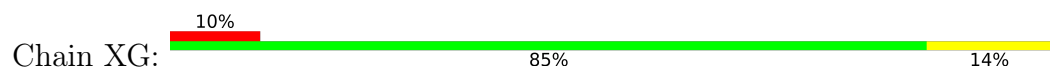
- Molecule 6: 30S ribosomal protein S6



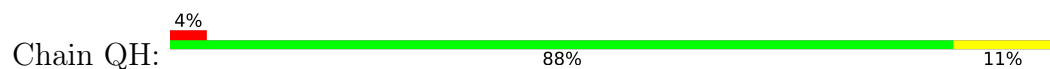
- Molecule 7: 30S ribosomal protein S7



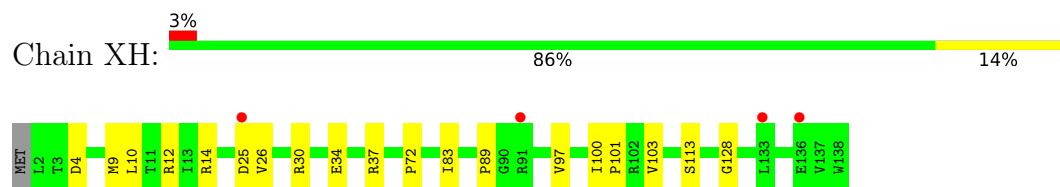
- Molecule 7: 30S ribosomal protein S7



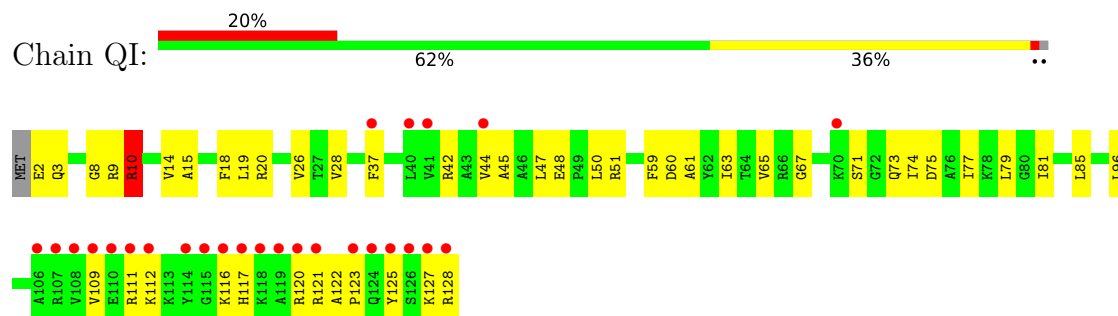
- Molecule 8: 30S ribosomal protein S8



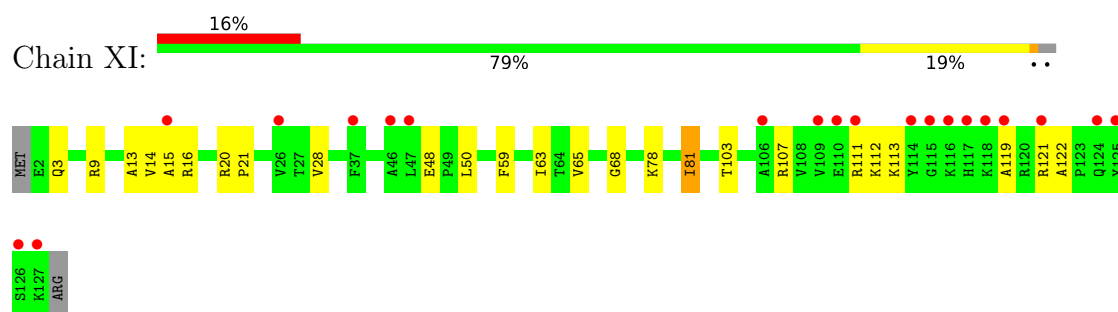
- Molecule 8: 30S ribosomal protein S8



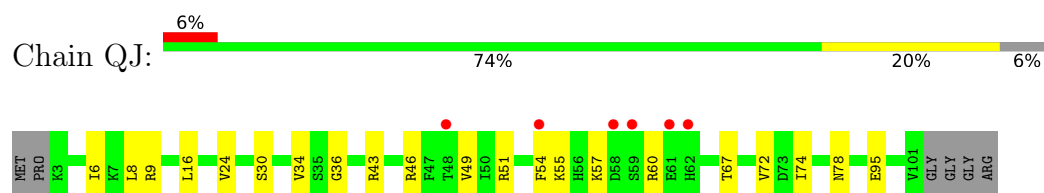
- Molecule 9: 30S ribosomal protein S9



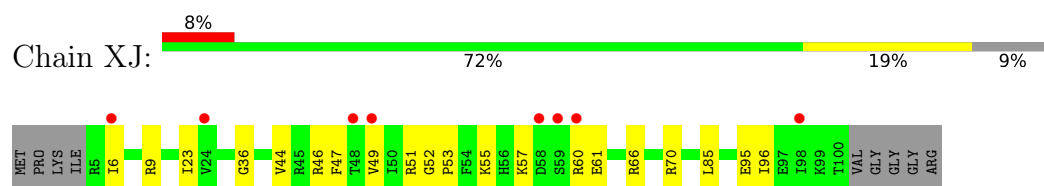
- Molecule 9: 30S ribosomal protein S9



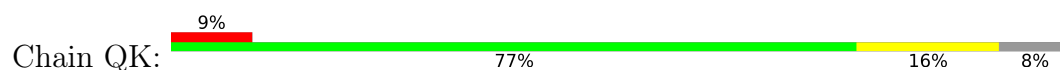
- Molecule 10: 30S ribosomal protein S10

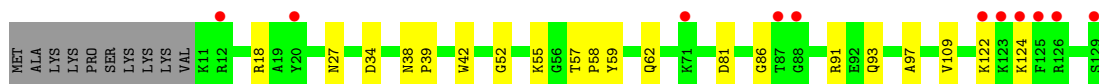


- Molecule 10: 30S ribosomal protein S10

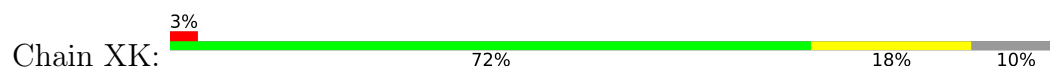


- Molecule 11: 30S ribosomal protein S11

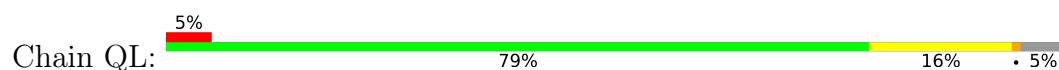




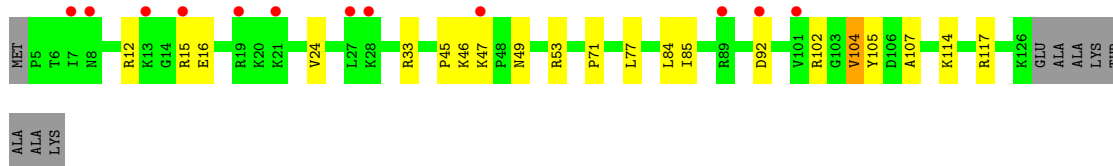
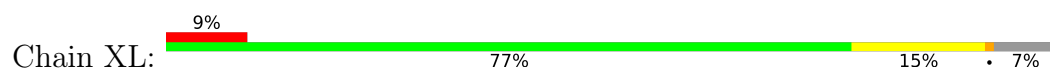
- Molecule 11: 30S ribosomal protein S11



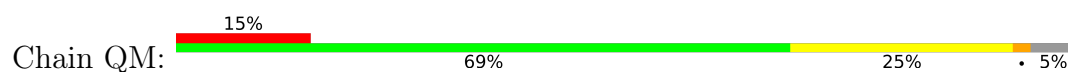
- Molecule 12: 30S ribosomal protein S12



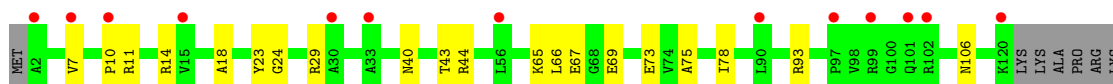
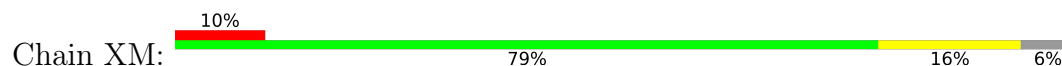
- Molecule 12: 30S ribosomal protein S12



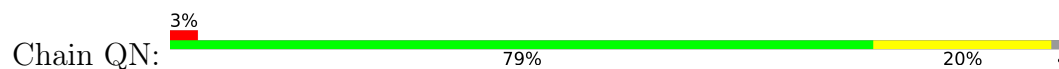
- Molecule 13: 30S ribosomal protein S13

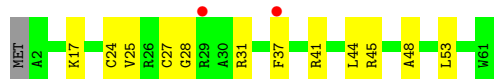


- Molecule 13: 30S ribosomal protein S13

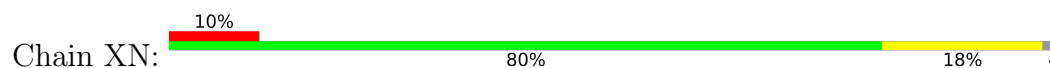


- Molecule 14: 30S ribosomal protein S14 type Z

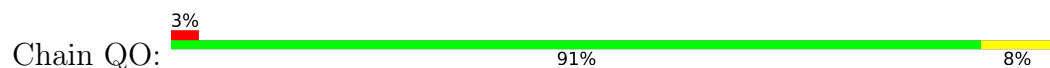




- Molecule 14: 30S ribosomal protein S14 type Z



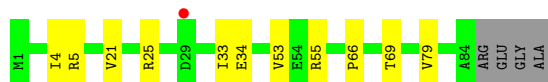
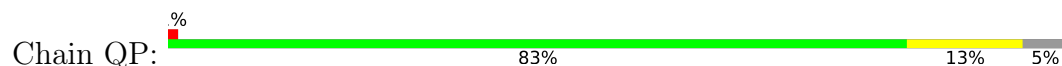
- Molecule 15: 30S ribosomal protein S15



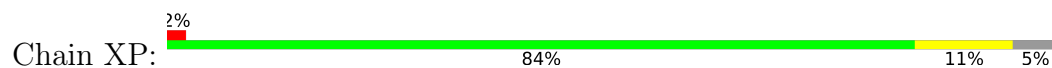
- Molecule 15: 30S ribosomal protein S15



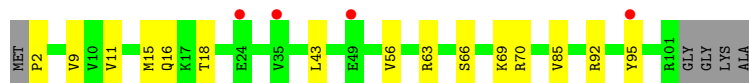
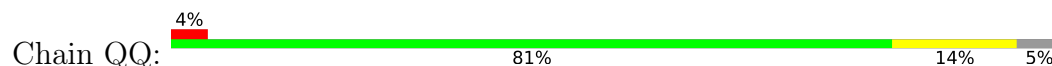
- Molecule 16: 30S ribosomal protein S16



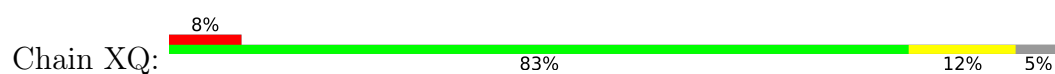
- Molecule 16: 30S ribosomal protein S16



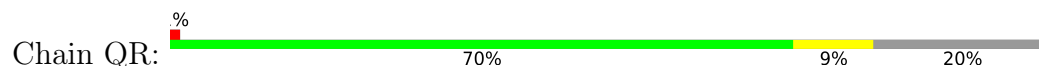
- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17



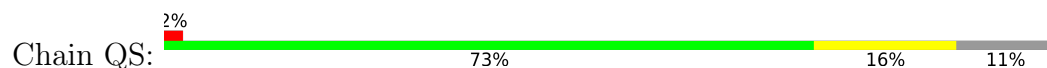
- Molecule 18: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S18



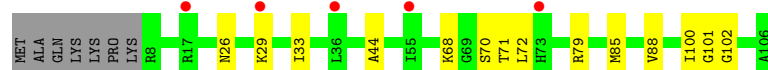
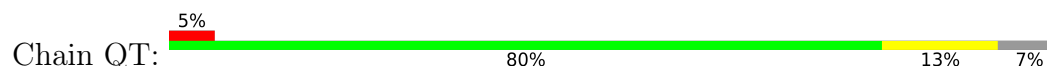
- Molecule 19: 30S ribosomal protein S19



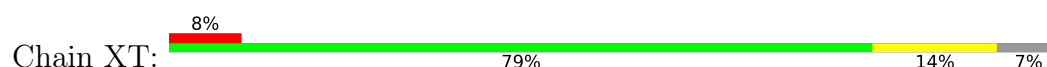
- Molecule 19: 30S ribosomal protein S19



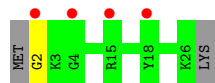
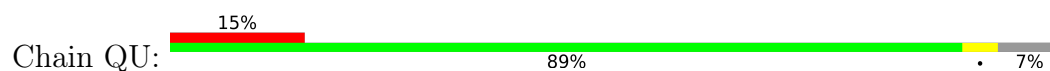
- Molecule 20: 30S ribosomal protein S20



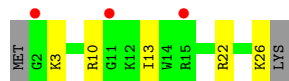
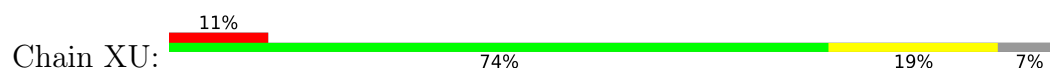
- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein Thx



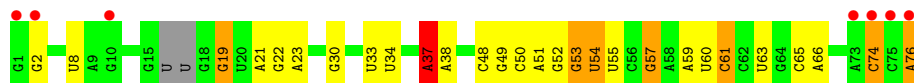
- Molecule 21: 30S ribosomal protein Thx



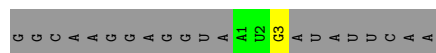
- Molecule 22: P-site tRNA^{Lys}(SUU)



- Molecule 22: P-site tRNA^{Lys}(SUU)



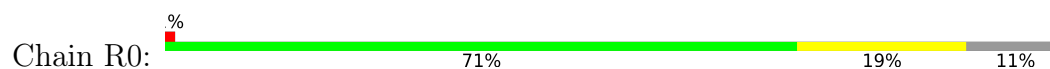
- Molecule 23: mRNA



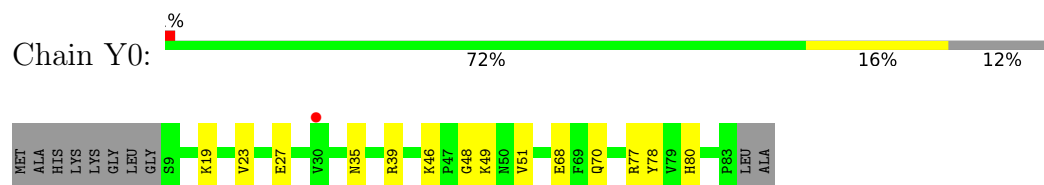
- Molecule 23: mRNA



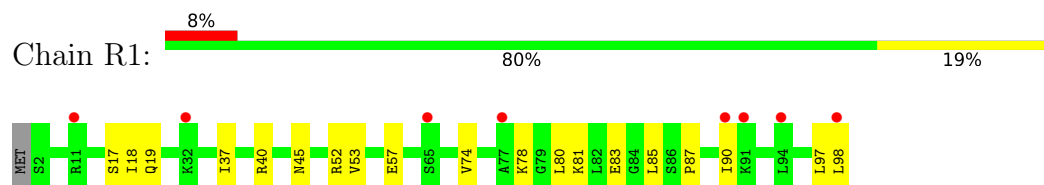
- Molecule 24: 50S ribosomal protein L27



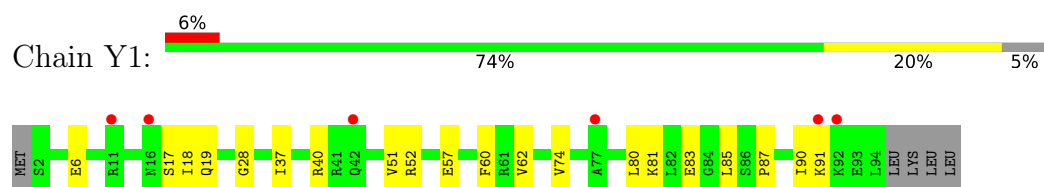
- Molecule 24: 50S ribosomal protein L27



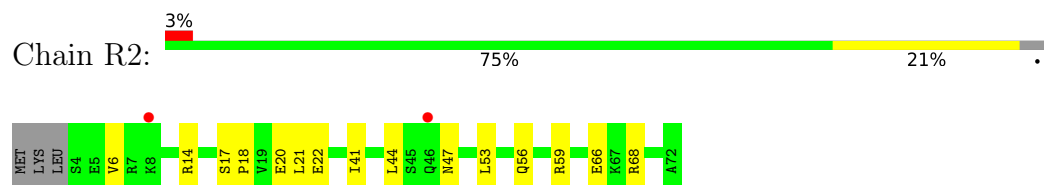
- Molecule 25: 50S ribosomal protein L28



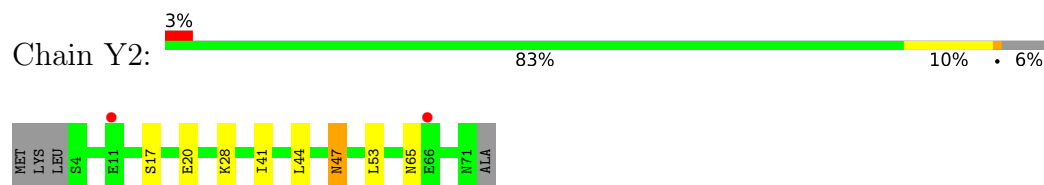
- Molecule 25: 50S ribosomal protein L28



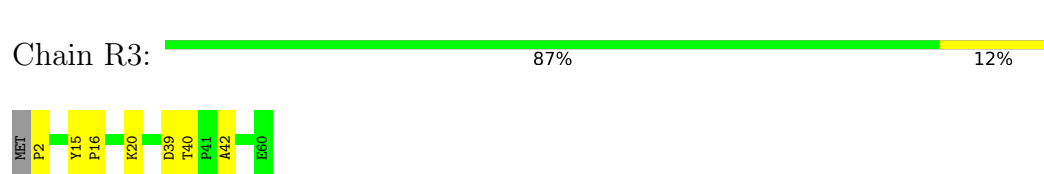
- Molecule 26: 50S ribosomal protein L29



- Molecule 26: 50S ribosomal protein L29



- Molecule 27: 50S ribosomal protein L30

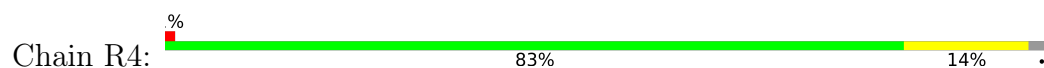


- Molecule 27: 50S ribosomal protein L30

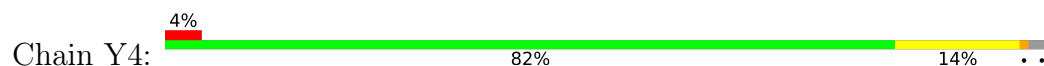




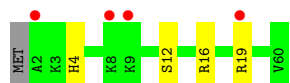
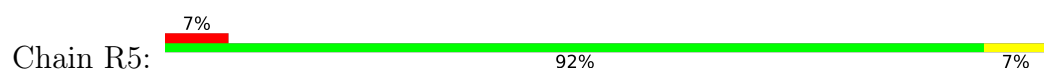
- Molecule 28: 50S ribosomal protein L31



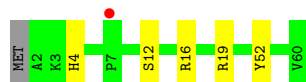
- Molecule 28: 50S ribosomal protein L31



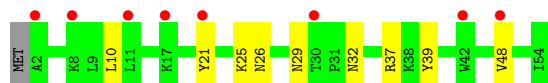
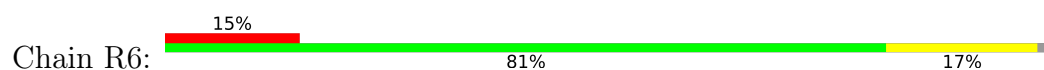
- Molecule 29: 50S ribosomal protein L32



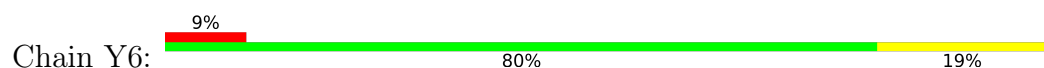
- Molecule 29: 50S ribosomal protein L32



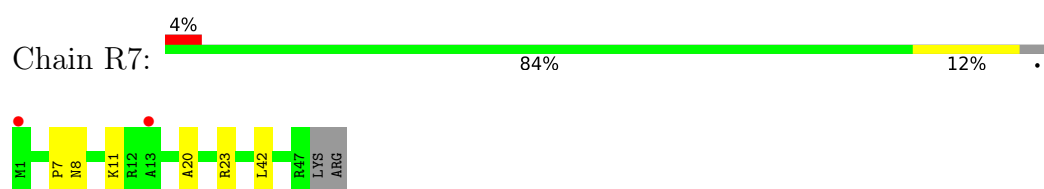
- Molecule 30: 50S ribosomal protein L33



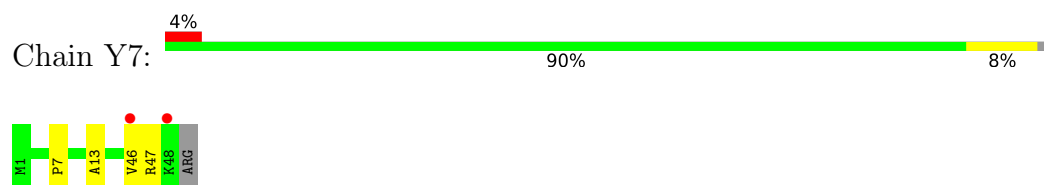
- Molecule 30: 50S ribosomal protein L33



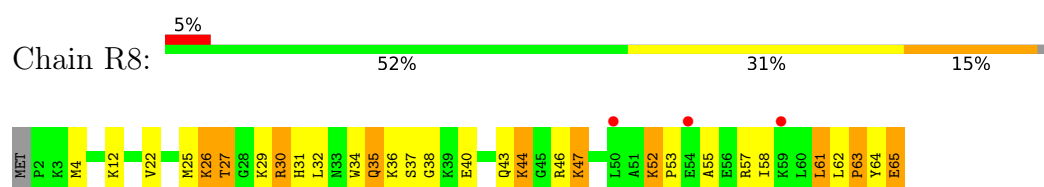
- Molecule 31: 50S ribosomal protein L34



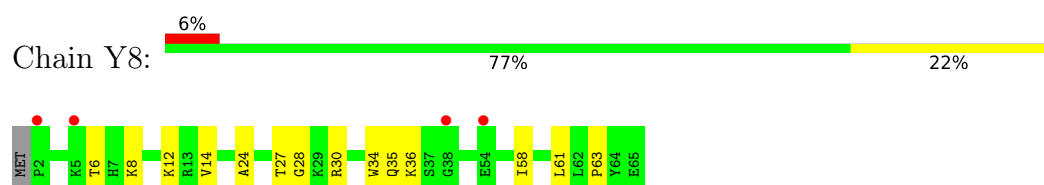
- Molecule 31: 50S ribosomal protein L34



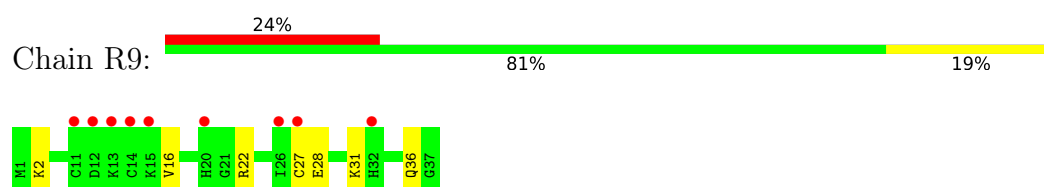
- Molecule 32: 50S ribosomal protein L35



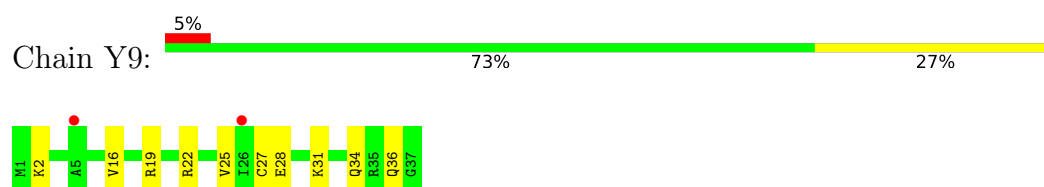
- Molecule 32: 50S ribosomal protein L35



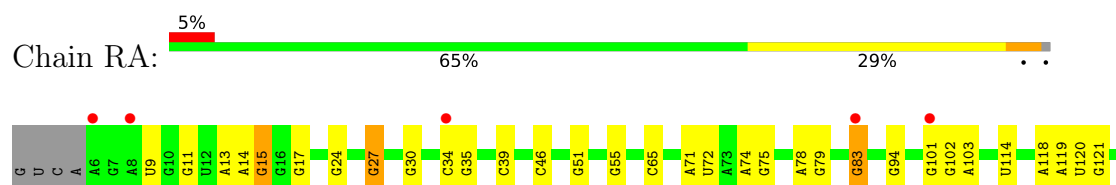
- Molecule 33: 50S ribosomal protein L36

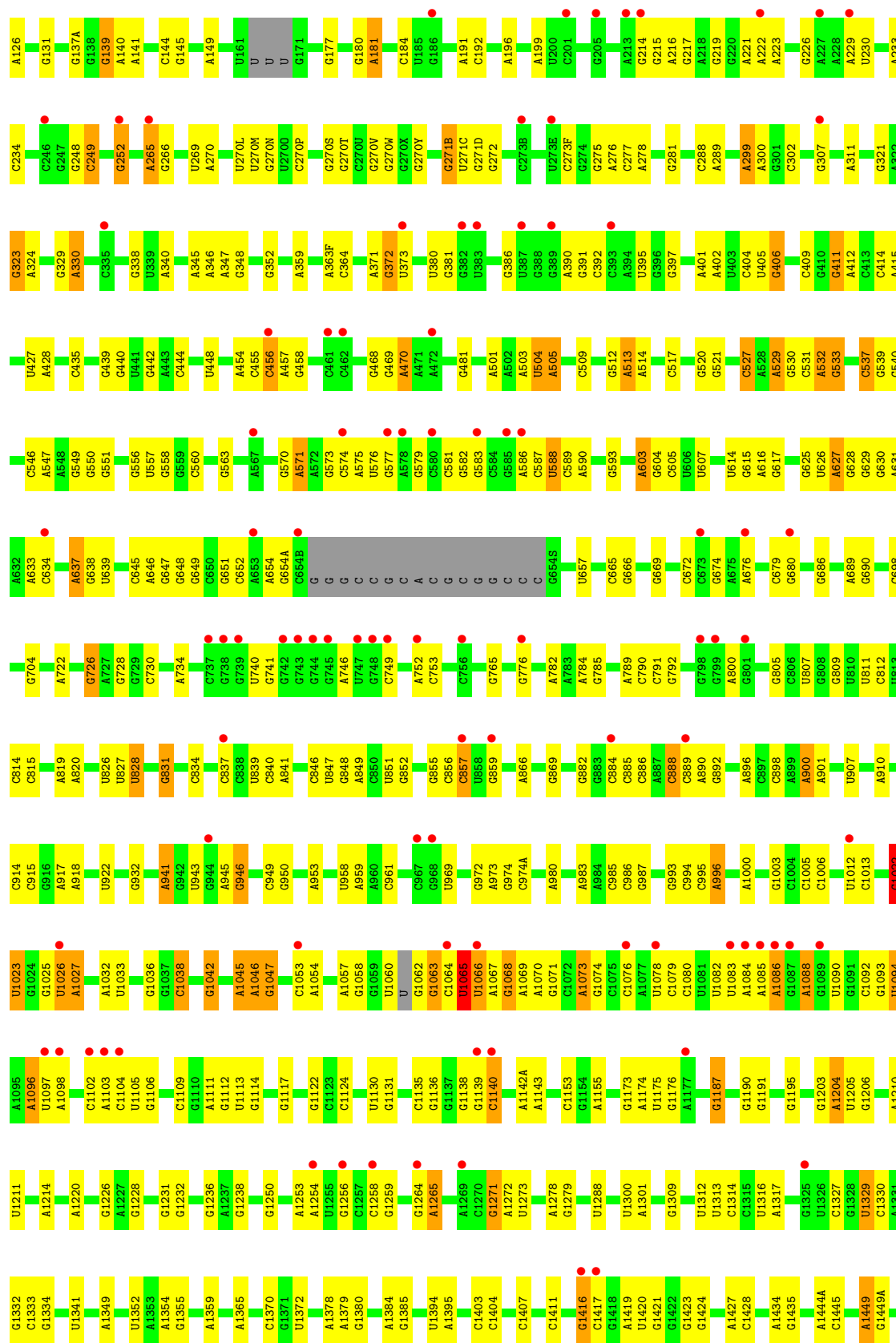


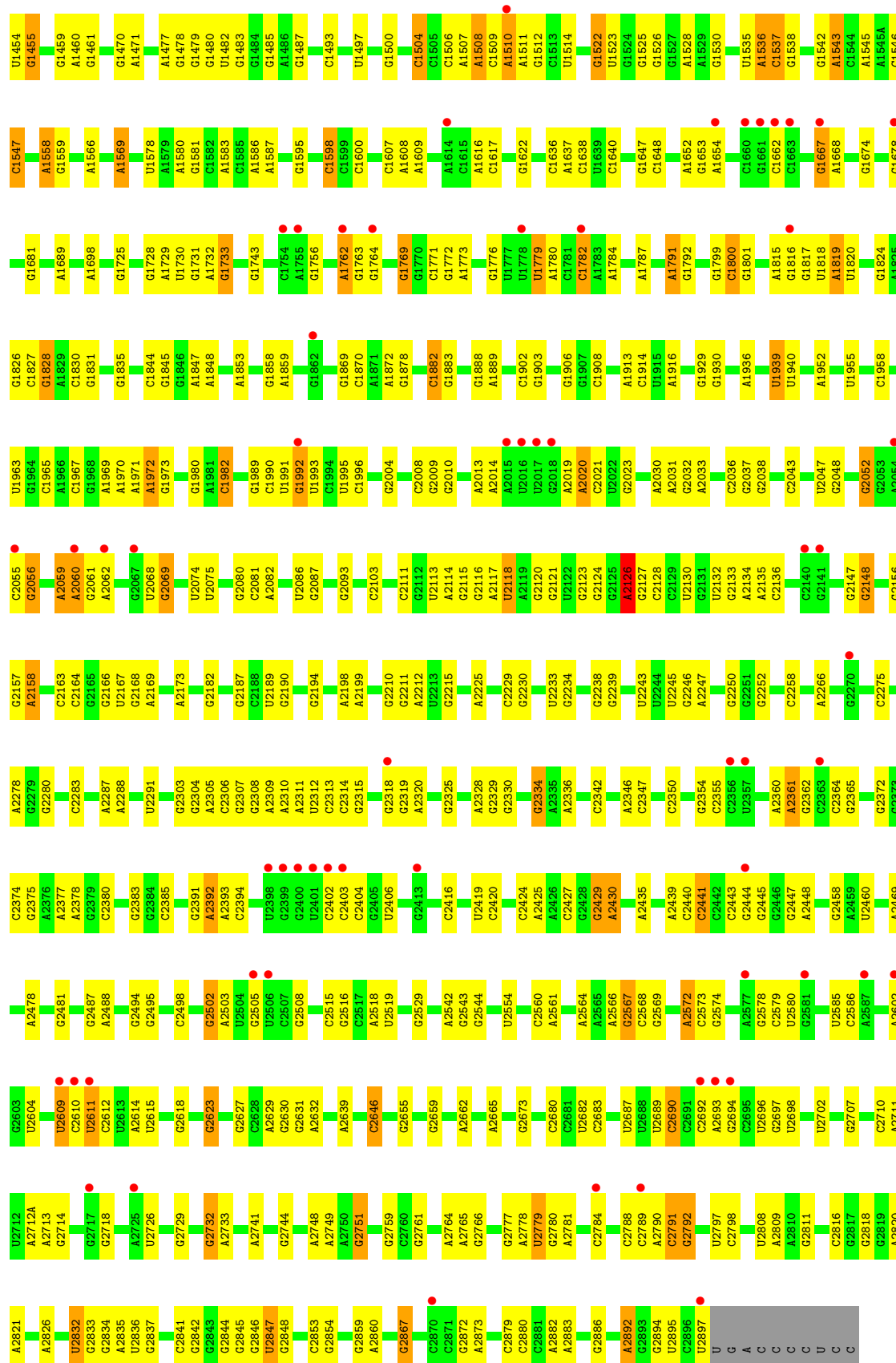
- Molecule 33: 50S ribosomal protein L36

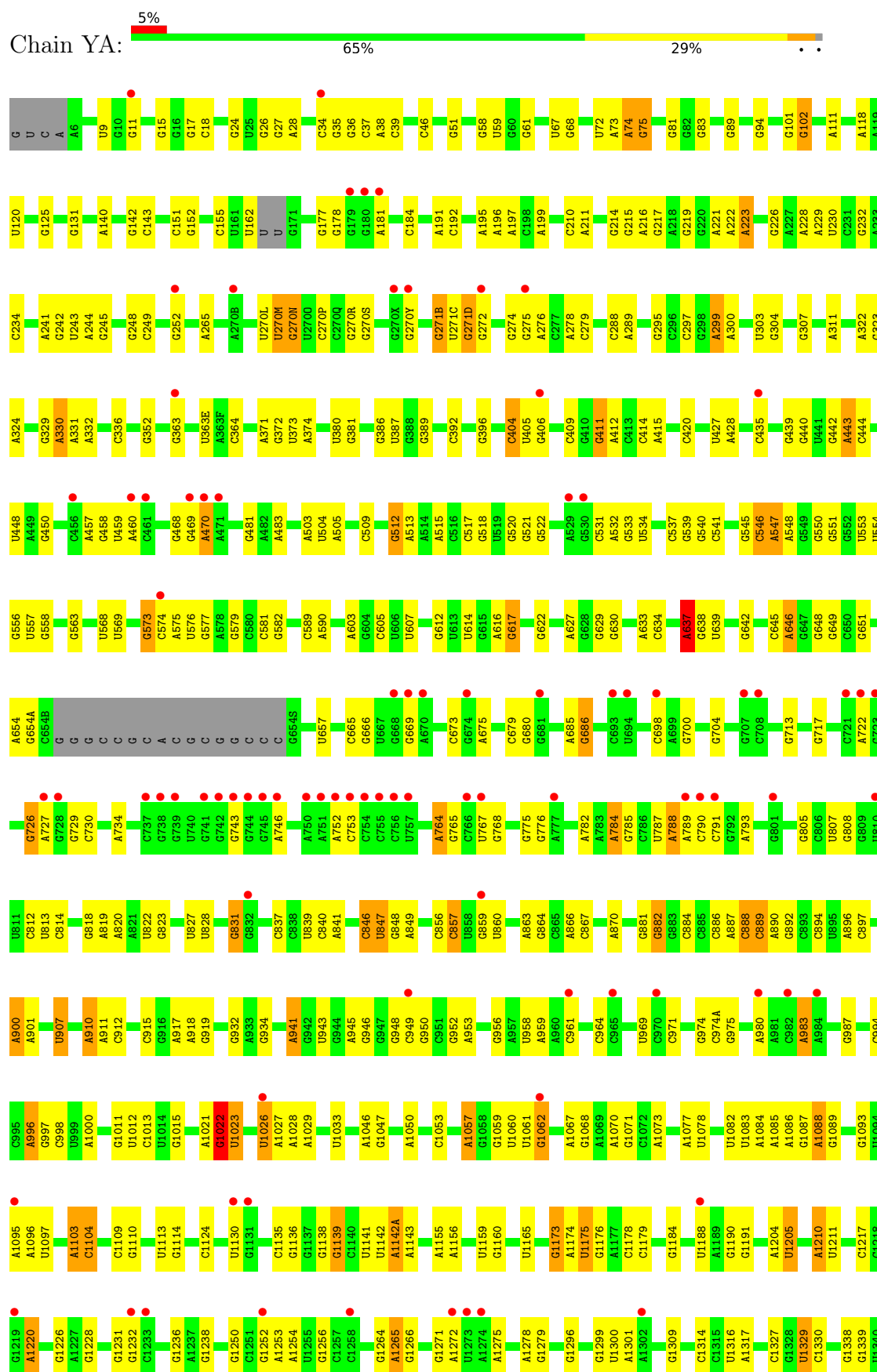


- Molecule 34: 23S rRNA

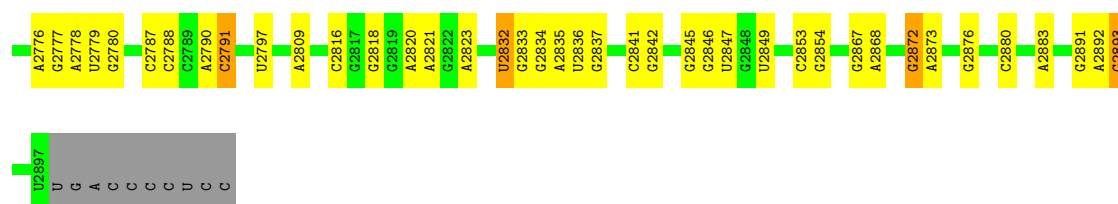




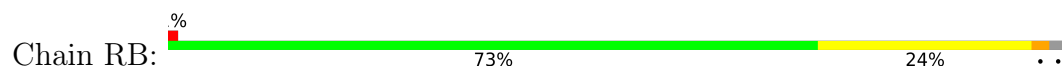




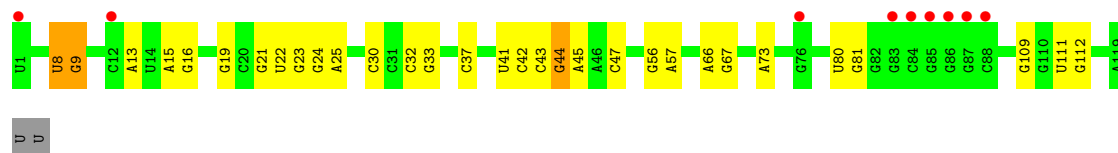
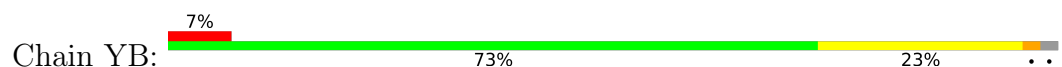
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U2682	G2567	G2447	G2344	A2042	G1817	A1689	G1568	A1449	A1353
U2688	C2571	A2448	G2345	U2047	U1819	C1694	A1569	G1449A	A1354
U2689	A2572	A2449	A2346	G2048	G1824	G1695	A1570	U1454	A1359
C2690	C2573	A2451	C2347	A2051	A1825	A1698	A1572	G1455	
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C2692	C2575	A2453	A2351	G2056	G1827	G1728	G1585	A1461	G1368
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	A2577	G2455	G2353	G2056	A1829	U1730	G1591	C1471	G1372
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	C2581	G2470	G2365	C2063	A1847	A1608	C1607	G1483	G1385
U2702	U2585	G2481	G2374	G2069	A1853	A1749	A1609	G1487	
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G2708	G2590	G2494	G2384	A2071	A1859	A1755	A1611	G1492	A1393
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A2713	U2604	C2499	C2389	G2080	G1878		G1627	U1406	
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	U2609	U2504	G2397	U2086	G1888	U1774	A1510	A1409	
G2730	C2610	G2505	C2403	G2087	A1889	U1775	G1512	G1410	
G2731	U2611	C2404	G2405	G2093	G1903	A1784	G1522	C1411	
G2732	C2612	U2406	G2406	U2096	G1906	A1784	A1528	G1416	
A2733	U2615	G2407	C2417	G2099	G1913	A1784	A1529	G1417	
G2737	G2618	G2410	C2179	U2100	A1918	A1784	C1533	A1418	
A2738	C2619	A2411	U2180	G2100	A1919	A1784	G1534	U1419	
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C2742	G2627	U2423	C2183	G2111	A1928	A1784	G1537	G1422	
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G2766		C2442	G2215	G2127	A1936	A1784	A1545	A1434	
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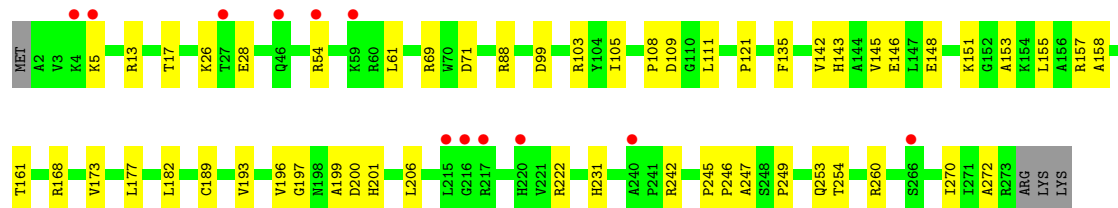
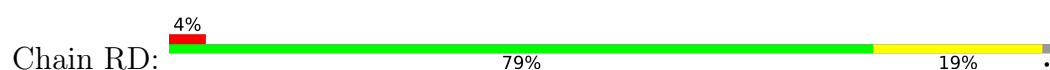
- Molecule 35: 5S rRNA



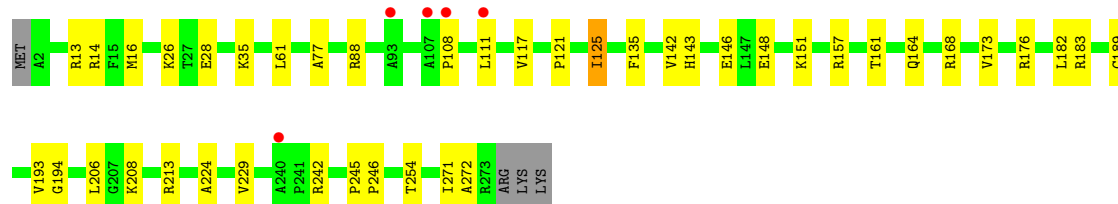
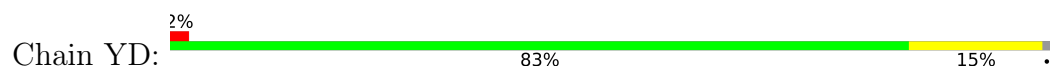
- Molecule 35: 5S rRNA



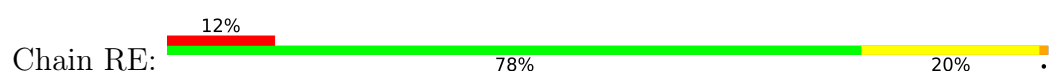
- Molecule 36: 50S ribosomal protein L2

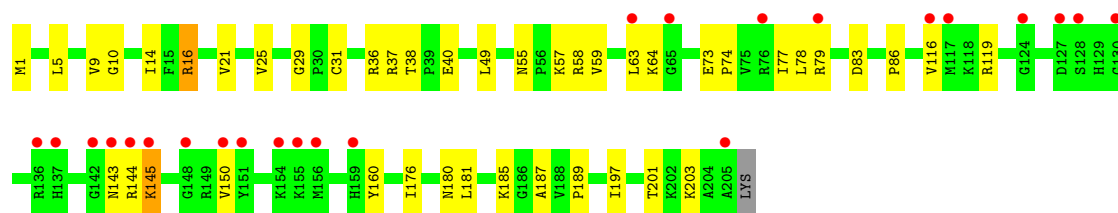


- Molecule 36: 50S ribosomal protein L2

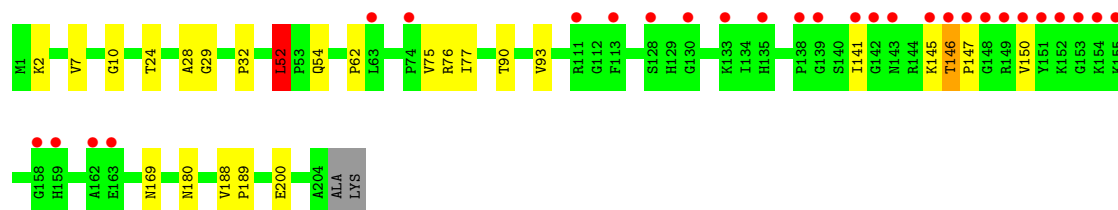
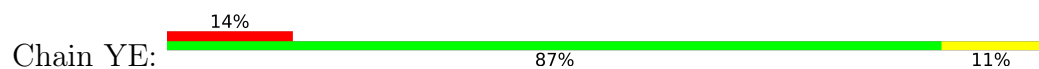


- Molecule 37: 50S ribosomal protein L3

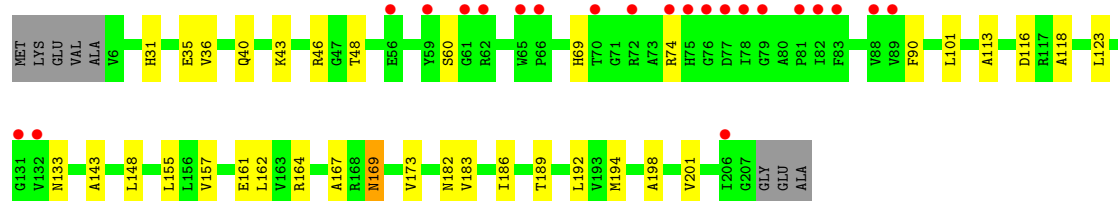
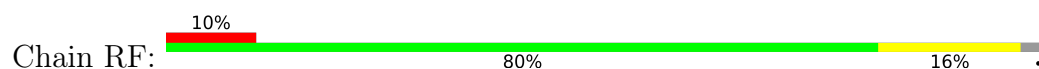




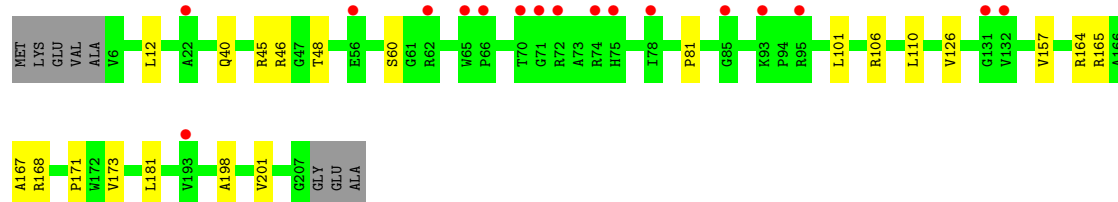
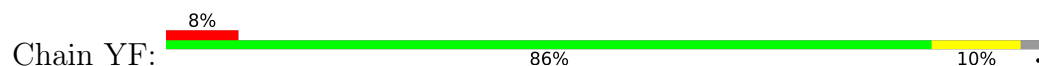
• Molecule 37: 50S ribosomal protein L3



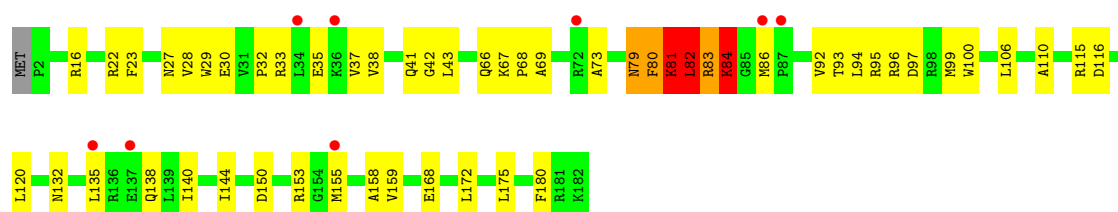
• Molecule 38: 50S ribosomal protein L4



• Molecule 38: 50S ribosomal protein L4

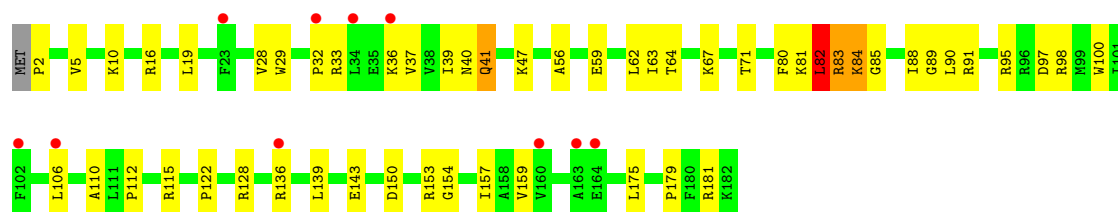


• Molecule 39: 50S ribosomal protein L5



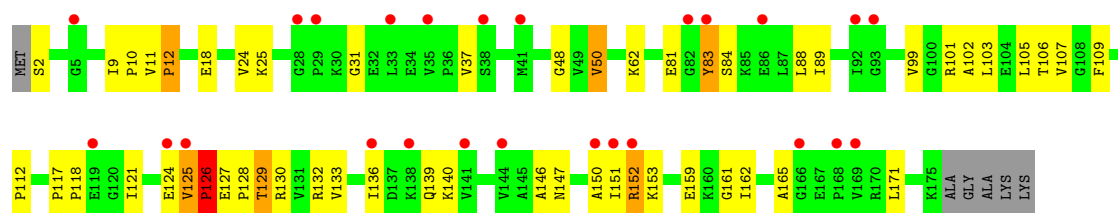
- Molecule 39: 50S ribosomal protein L5

Chain YG:  5% 70% 27% ..



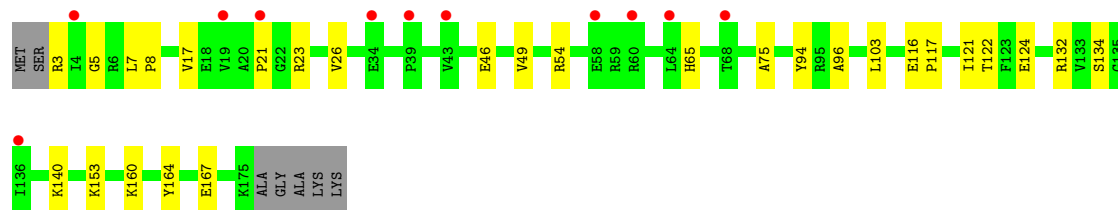
- Molecule 40: 50S ribosomal protein L6

Chain RH:  14% 67% 26% ..



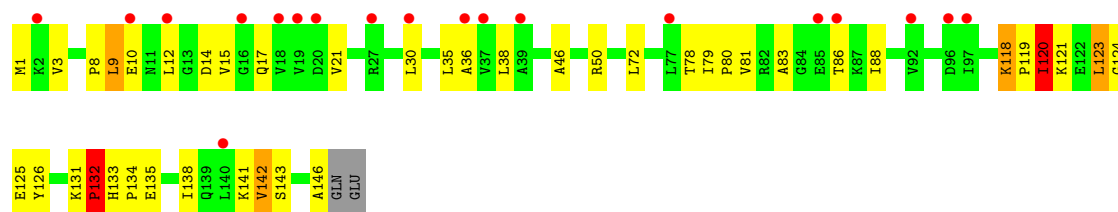
- Molecule 40: 50S ribosomal protein L6

Chain YH:  6% 81% 16% .



- Molecule 41: 50S ribosomal protein L9

Chain RI:  13% 70% 24% ..

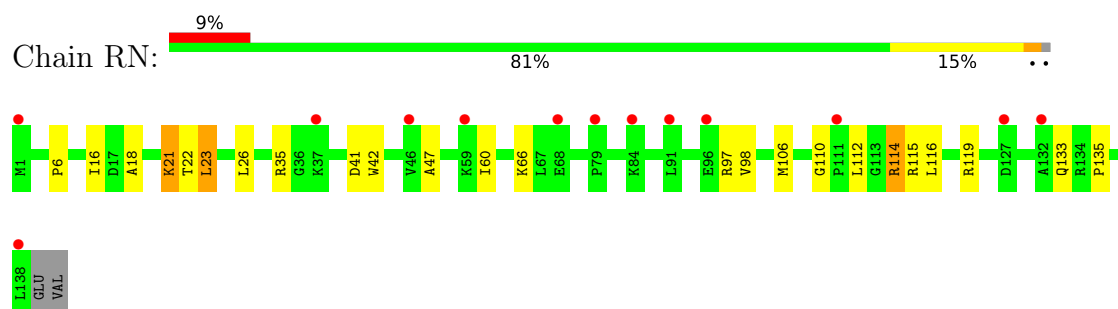


- Molecule 41: 50S ribosomal protein L9

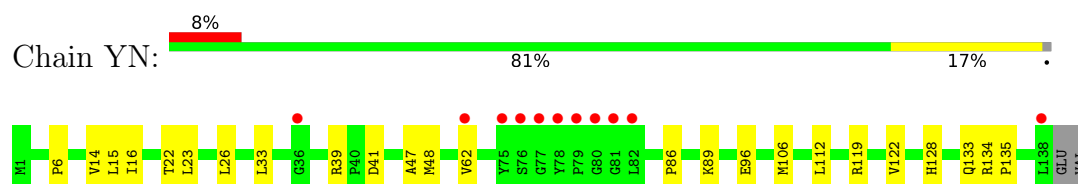
Chain YI:  2% 78% 14% 5% ..



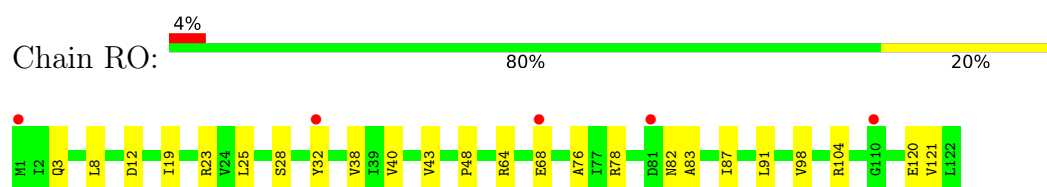
- Molecule 42: 50S ribosomal protein L13



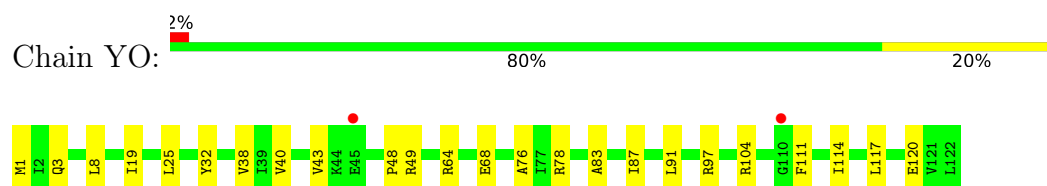
- Molecule 42: 50S ribosomal protein L13



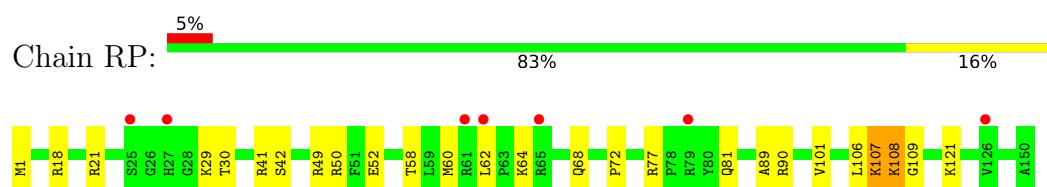
- Molecule 43: 50S ribosomal protein L14



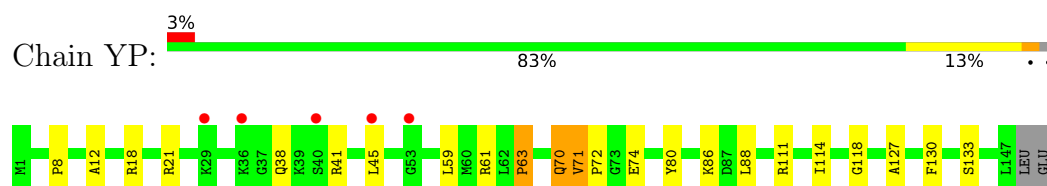
- Molecule 43: 50S ribosomal protein L14



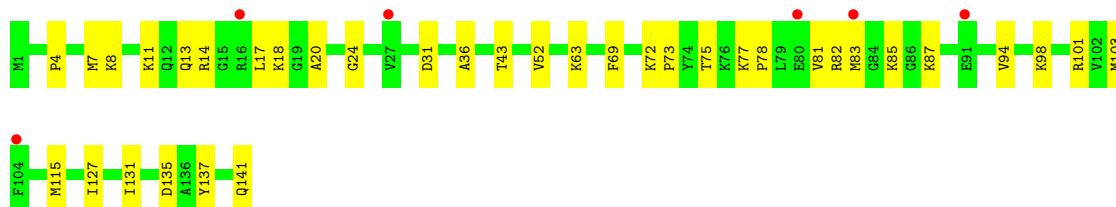
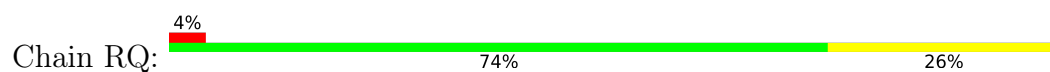
- Molecule 44: 50S ribosomal protein L15



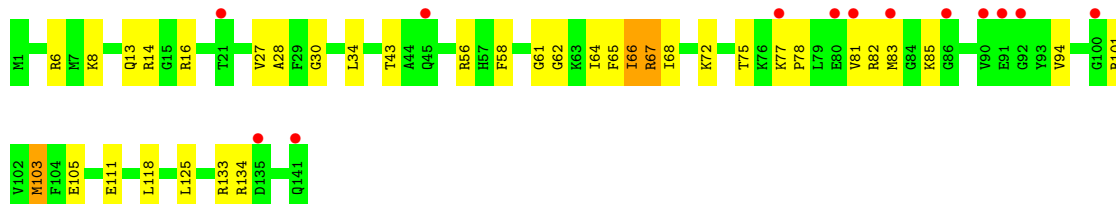
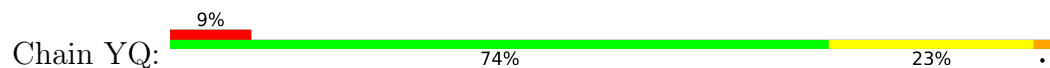
- Molecule 44: 50S ribosomal protein L15



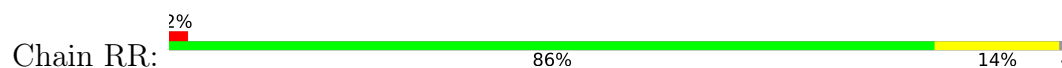
- Molecule 45: 50S ribosomal protein L16



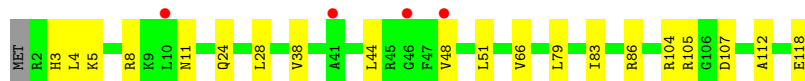
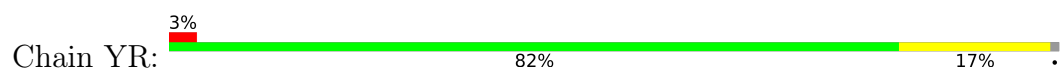
- Molecule 45: 50S ribosomal protein L16



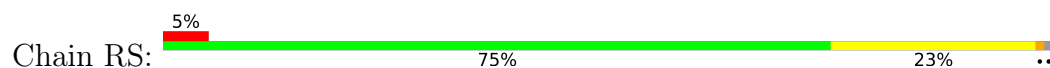
- Molecule 46: 50S ribosomal protein L17



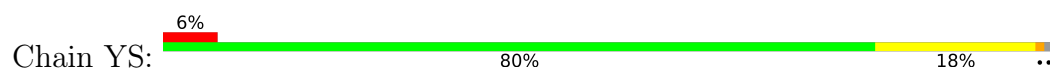
- Molecule 46: 50S ribosomal protein L17



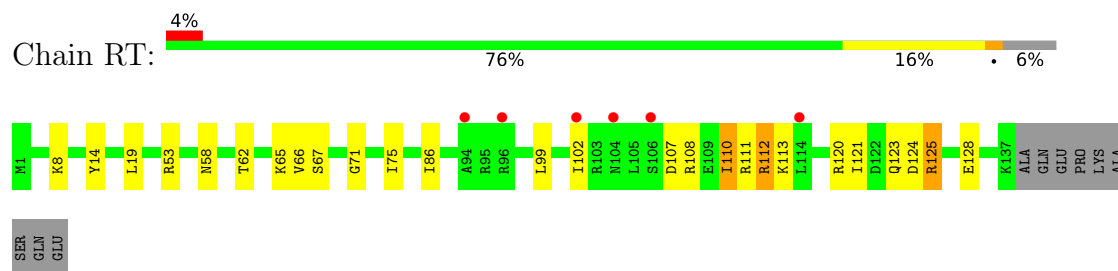
- Molecule 47: 50S ribosomal protein L18



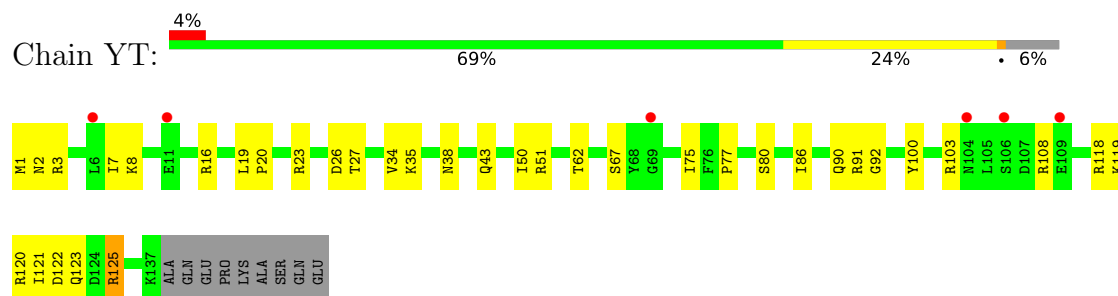
- Molecule 47: 50S ribosomal protein L18



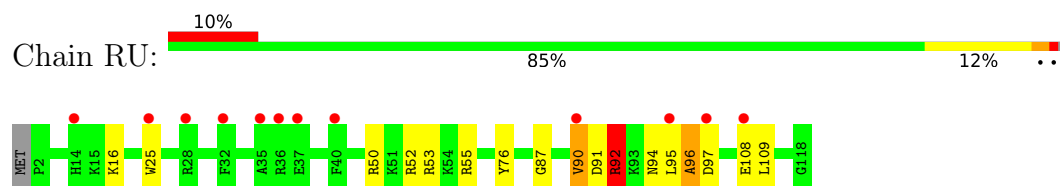
- Molecule 48: 50S ribosomal protein L19



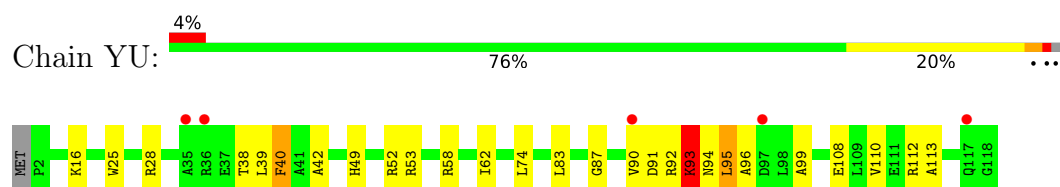
- Molecule 48: 50S ribosomal protein L19



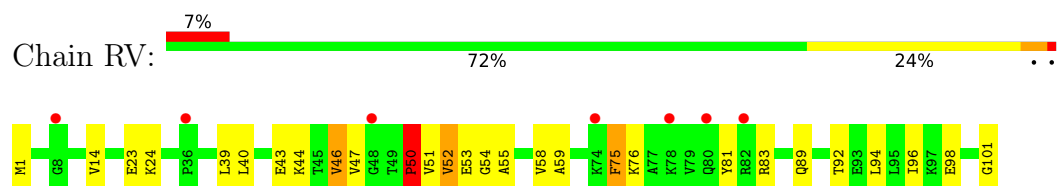
- Molecule 49: 50S ribosomal protein L20



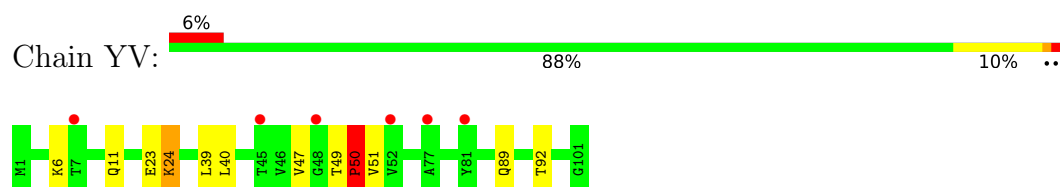
- Molecule 49: 50S ribosomal protein L20



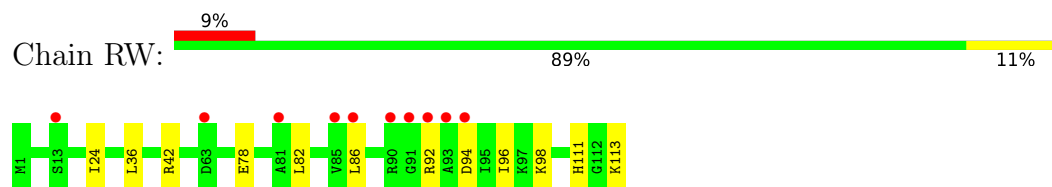
- Molecule 50: 50S ribosomal protein L21



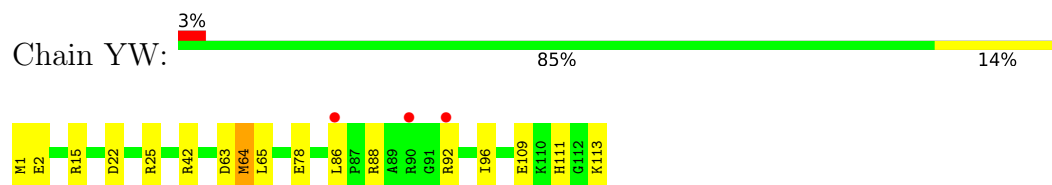
- Molecule 50: 50S ribosomal protein L21



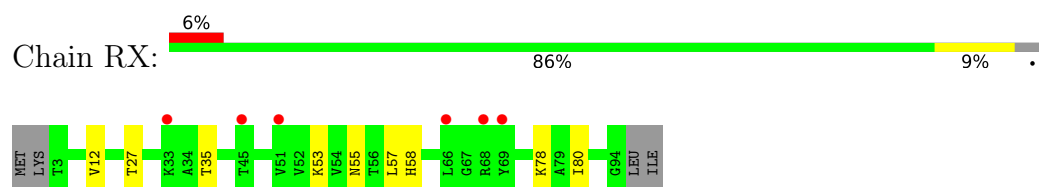
- Molecule 51: 50S ribosomal protein L22



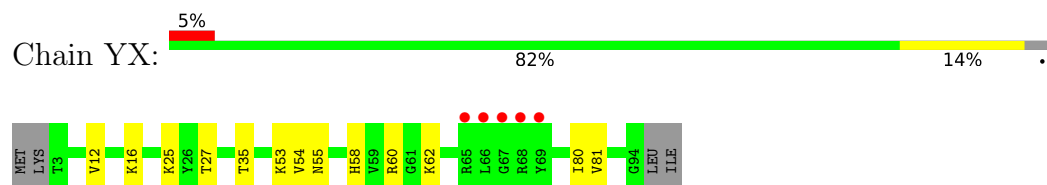
- Molecule 51: 50S ribosomal protein L22



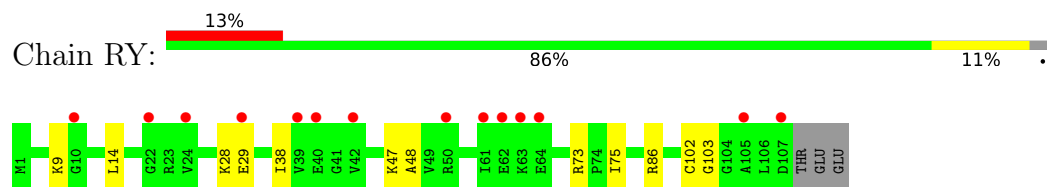
- Molecule 52: 50S ribosomal protein L23



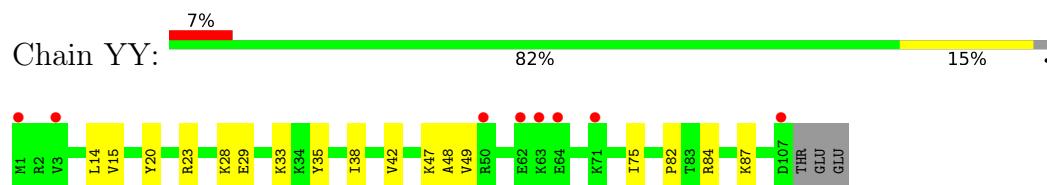
- Molecule 52: 50S ribosomal protein L23



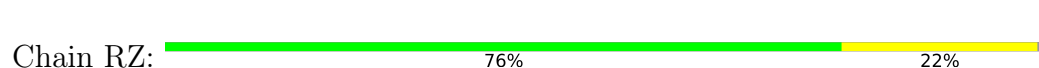
- Molecule 53: 50S ribosomal protein L24

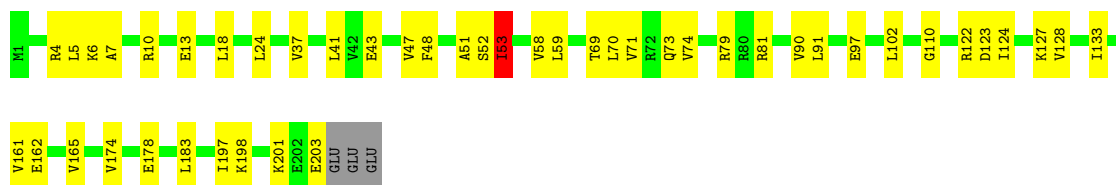


- Molecule 53: 50S ribosomal protein L24

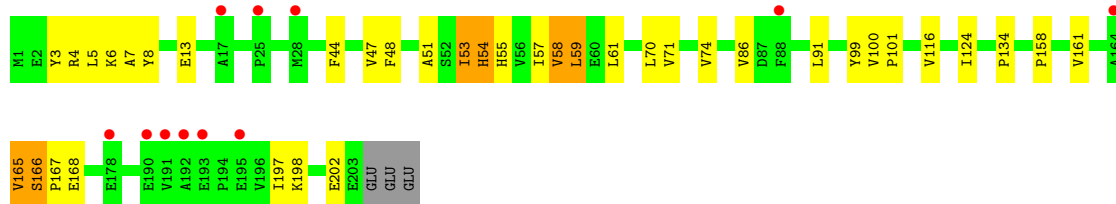
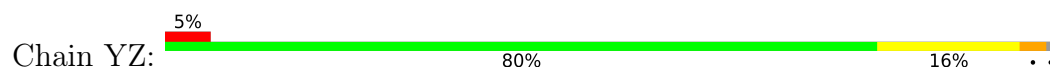


- Molecule 54: 50S ribosomal protein L25

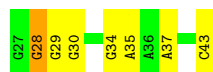




- Molecule 54: 50S ribosomal protein L25



- Molecule 55: A-site ASL^{Phe}



- Molecule 56: CC-puro



- Molecule 56: CC-puro



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.56Å 447.23Å 618.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	174.01 – 3.64 174.01 – 3.64	Depositor EDS
% Data completeness (in resolution range)	95.7 (174.01-3.64) 95.7 (174.01-3.64)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.232 , 0.278 0.232 , 0.278	Depositor DCC
R_{free} test set	32021 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å ²)	105.8	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 127.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	292577	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% 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: MNU, SF4, MG, ZN, T6A, PPU

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	0.18	0/36098	0.39	11/56341 (0.0%)
1	XA	0.18	0/36346	0.39	8/56725 (0.0%)
2	QB	0.26	0/1942	0.58	2/2619 (0.1%)
2	XB	0.23	0/1950	0.57	4/2630 (0.2%)
3	QC	0.23	0/1629	0.50	0/2195
3	XC	0.24	0/1629	0.54	0/2195
4	QD	0.19	0/1733	0.48	0/2318
4	XD	0.26	0/1733	0.56	0/2318
5	QE	0.20	0/1171	0.49	0/1576
5	XE	0.20	0/1171	0.50	0/1576
6	QF	0.18	0/856	0.44	0/1154
6	XF	0.18	0/856	0.44	0/1154
7	QG	0.20	0/1276	0.48	0/1709
7	XG	0.23	0/1276	0.55	0/1709
8	QH	0.17	0/1128	0.45	0/1517
8	XH	0.18	0/1128	0.46	0/1517
9	QI	0.52	3/1029 (0.3%)	0.72	0/1379
9	XI	0.27	0/1017	0.61	0/1365
10	QJ	0.21	0/814	0.53	0/1095
10	XJ	0.21	0/790	0.55	0/1063
11	QK	0.16	0/900	0.41	0/1213
11	XK	0.18	0/879	0.42	0/1187
12	QL	0.28	0/991	0.55	0/1327
12	XL	0.30	0/972	0.59	0/1301
13	QM	0.28	0/965	0.62	0/1292
13	XM	0.25	0/956	0.71	2/1281 (0.2%)
14	QN	0.27	0/501	0.63	0/664
14	XN	0.25	0/501	0.67	0/664
15	QO	0.19	0/745	0.45	0/992
15	XO	0.18	0/740	0.43	0/987
16	QP	0.18	0/721	0.47	0/970
16	XP	0.18	0/721	0.51	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.16	0/847	0.43	0/1131
17	XQ	0.19	0/847	0.45	0/1131
18	QR	0.20	0/579	0.52	0/768
18	XR	0.19	0/579	0.48	0/768
19	QS	0.21	0/680	0.54	0/915
19	XS	0.21	0/689	0.57	0/926
20	QT	0.24	0/765	0.59	0/1007
20	XT	0.25	0/765	0.60	0/1007
21	QU	0.18	0/221	0.42	0/288
21	XU	0.16	0/221	0.42	0/288
22	QV	0.26	0/1706	0.47	1/2652 (0.0%)
22	XV	0.23	0/1706	0.48	2/2652 (0.1%)
23	QX	0.26	0/72	0.56	0/110
23	XX	0.18	0/560	0.42	0/872
24	R0	0.18	0/611	0.45	0/814
24	Y0	0.17	0/607	0.41	0/809
25	R1	0.21	0/770	0.56	0/1022
25	Y1	0.20	0/736	0.51	0/978
26	R2	0.21	0/583	0.53	0/771
26	Y2	0.25	0/577	0.55	0/764
27	R3	0.19	0/474	0.49	0/635
27	Y3	0.44	0/474	0.71	0/635
28	R4	0.27	0/578	0.68	0/776
28	Y4	0.22	0/578	0.65	0/776
29	R5	0.18	0/473	0.45	0/639
29	Y5	0.17	0/473	0.45	0/639
30	R6	0.17	0/460	0.50	0/613
30	Y6	0.15	0/460	0.41	0/613
31	R7	0.17	0/417	0.47	0/550
31	Y7	0.18	0/426	0.47	0/561
32	R8	0.55	0/525	0.95	1/691 (0.1%)
32	Y8	0.19	0/525	0.45	0/691
33	R9	0.15	0/310	0.41	0/407
33	Y9	0.15	0/310	0.41	0/407
34	RA	0.19	0/69498	0.40	7/108491 (0.0%)
34	YA	0.19	0/69543	0.40	11/108563 (0.0%)
35	RB	0.19	0/2878	0.37	0/4490
35	YB	0.20	0/2878	0.38	0/4490
36	RD	0.25	0/2165	0.53	1/2919 (0.0%)
36	YD	0.24	0/2165	0.50	0/2919
37	RE	0.35	0/1601	0.73	2/2160 (0.1%)
37	YE	0.27	0/1596	0.56	0/2153
38	RF	0.23	0/1620	0.59	0/2194

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YF	0.22	0/1620	0.56	0/2194
39	RG	0.30	0/1499	0.66	2/2016 (0.1%)
39	YG	0.33	0/1499	0.64	0/2016
40	RH	0.42	0/1362	0.81	5/1841 (0.3%)
40	YH	0.18	0/1356	0.45	0/1833
41	RI	0.45	0/1151	0.81	3/1558 (0.2%)
41	YI	0.54	1/1151 (0.1%)	0.95	2/1558 (0.1%)
42	RN	0.27	0/1131	0.58	0/1525
42	YN	0.20	0/1131	0.52	0/1525
43	RO	0.18	0/943	0.44	0/1269
43	YO	0.17	0/943	0.43	0/1269
44	RP	0.29	0/1162	0.70	0/1544
44	YP	0.26	0/1139	0.59	0/1514
45	RQ	0.28	0/1143	0.63	0/1527
45	YQ	0.32	0/1143	0.65	0/1527
46	RR	0.21	0/974	0.60	0/1302
46	YR	0.22	0/974	0.59	0/1302
47	RS	0.31	0/892	0.76	2/1187 (0.2%)
47	YS	0.30	0/892	0.69	0/1187
48	RT	0.29	0/1155	0.63	1/1542 (0.1%)
48	YT	0.26	0/1155	0.59	0/1542
49	RU	0.28	0/982	0.68	5/1306 (0.4%)
49	YU	0.33	0/982	0.76	4/1306 (0.3%)
50	RV	0.35	0/790	0.76	3/1057 (0.3%)
50	YV	0.33	0/790	0.76	3/1057 (0.3%)
51	RW	0.20	0/911	0.52	0/1220
51	YW	0.25	0/911	0.57	0/1220
52	RX	0.18	0/739	0.48	0/993
52	YX	0.18	0/739	0.48	0/993
53	RY	0.17	0/831	0.43	0/1108
53	YY	0.17	0/831	0.44	0/1108
54	RZ	0.27	0/1634	0.65	2/2216 (0.1%)
54	YZ	0.32	0/1634	0.60	0/2216
55	XY	0.16	0/405	0.37	0/630
56	Z6	0.25	0/40	0.37	0/60
56	Z8	0.23	0/40	0.38	0/60
All	All	0.21	4/316386 (0.0%)	0.45	84/473016 (0.0%)

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
27	Y3	0	1
37	YE	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	YI	133	HIS	C-N	13.24	1.50	1.33
9	QI	10	ARG	CA-CB	7.23	1.66	1.53
9	QI	10	ARG	CZ-NH1	6.47	1.41	1.32
9	QI	10	ARG	NE-CZ	5.20	1.38	1.33

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	YI	133	HIS	CA-C-N	17.93	138.27	120.52
41	YI	133	HIS	C-N-CA	17.93	138.27	120.52
22	XV	53	G	OP1-P-O3'	-11.34	73.97	108.00
49	YU	40	PHE	N-CA-CB	7.19	122.11	110.40
49	RU	96	ALA	N-CA-C	-6.80	103.89	111.71
40	RH	128	PRO	CA-C-N	6.67	134.27	121.54
40	RH	128	PRO	C-N-CA	6.67	134.27	121.54
49	RU	92	ARG	CA-C-N	6.62	134.19	121.54
49	RU	92	ARG	C-N-CA	6.62	134.19	121.54
34	YA	271(B)	G	P-O3'-C3'	6.54	127.55	119.70
41	RI	132	PRO	N-CA-C	-6.33	99.43	112.47
40	RH	128	PRO	CA-C-O	-6.33	114.46	121.23
13	XM	11	ARG	CA-C-N	6.12	133.23	121.54
13	XM	11	ARG	C-N-CA	6.12	133.23	121.54
34	YA	2712	U	P-O3'-C3'	6.08	126.99	119.70
32	R8	63	PRO	N-CA-C	-6.07	105.27	113.40
1	XA	812	C	P-O3'-C3'	5.98	129.17	120.20
50	RV	50	PRO	N-CA-CB	-5.95	97.00	103.25
41	RI	120	ILE	CA-C-N	5.93	132.86	121.54
41	RI	120	ILE	C-N-CA	5.93	132.86	121.54
49	YU	40	PHE	CA-CB-CG	5.90	119.70	113.80
39	RG	115	ARG	CA-C-N	5.85	132.71	121.54
39	RG	115	ARG	C-N-CA	5.85	132.71	121.54
49	YU	39	LEU	CA-C-N	-5.79	111.00	121.14
49	YU	39	LEU	C-N-CA	-5.79	111.00	121.14
40	RH	126	PRO	N-CA-CB	-5.75	97.21	103.25
34	RA	271(B)	G	P-O3'-C3'	5.71	126.56	119.70
2	XB	235	SER	CA-C-N	-5.70	113.62	122.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	XB	235	SER	C-N-CA	-5.70	113.62	122.16
34	RA	2832	U	P-O3'-C3'	5.60	128.60	120.20
40	RH	128	PRO	O-C-N	5.59	129.44	123.01
22	XV	53	G	OP2-P-O3'	-5.54	91.39	108.00
34	RA	1065	U	P-O3'-C3'	5.52	128.48	120.20
50	YV	49	THR	CA-C-N	5.48	126.69	119.84
50	YV	49	THR	C-N-CA	5.48	126.69	119.84
22	QV	53	G	C4'-C3'-O3'	5.47	121.21	113.00
36	RD	197	GLY	CA-C-O	-5.46	117.91	122.33
1	QA	1297	C	P-O3'-C3'	5.39	128.29	120.20
1	QA	1065	U	P-O3'-C3'	5.38	128.27	120.20
50	YV	50	PRO	N-CA-CB	-5.38	97.60	103.25
1	QA	328	C	P-O3'-C3'	5.37	128.26	120.20
49	RU	90	VAL	CA-C-N	5.37	131.79	121.54
49	RU	90	VAL	C-N-CA	5.37	131.79	121.54
1	XA	812	C	C2'-C3'-O3'	5.30	117.45	109.50
37	RE	116	VAL	CA-C-N	5.29	131.64	121.54
37	RE	116	VAL	C-N-CA	5.29	131.64	121.54
50	RV	52	VAL	N-CA-C	-5.26	106.08	112.76
1	XA	481	G	C2'-C3'-O3'	5.23	121.55	113.70
54	RZ	201	LYS	CA-CB-CG	5.23	124.56	114.10
1	QA	1528	U	P-O3'-C3'	5.22	128.03	120.20
2	QB	154	LEU	CA-C-N	5.22	131.52	121.54
2	QB	154	LEU	C-N-CA	5.22	131.52	121.54
34	RA	1022	G	P-O3'-C3'	5.21	128.02	120.20
1	QA	250	A	P-O3'-C3'	5.20	128.00	120.20
34	YA	1558	A	P-O3'-C3'	5.20	127.99	120.20
1	XA	992	U	P-O3'-C3'	5.18	127.97	120.20
34	YA	2832	U	P-O3'-C3'	5.17	127.96	120.20
34	YA	846	C	P-O3'-C3'	5.17	127.95	120.20
1	QA	792	A	P-O3'-C3'	5.16	127.95	120.20
1	QA	992	U	P-O3'-C3'	5.16	127.94	120.20
1	QA	913	A	P-O3'-C3'	5.16	127.94	120.20
1	QA	1498	U	P-O3'-C3'	5.16	127.94	120.20
34	RA	2126	A	P-O3'-C3'	5.16	127.93	120.20
34	YA	271(B)	G	OP2-P-O3'	5.15	116.53	105.20
34	YA	1022	G	P-O3'-C3'	5.15	127.92	120.20
34	YA	1026	U	P-O3'-C3'	5.12	127.88	120.20
1	XA	1027	C	P-O3'-C3'	5.12	127.87	120.20
48	RT	110	ILE	N-CA-C	-5.10	104.71	111.09
1	XA	687	A	P-O3'-C3'	5.10	127.85	120.20
34	RA	1558	A	P-O3'-C3'	5.09	127.84	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	XB	233	SER	CA-C-N	5.08	126.19	119.84
2	XB	233	SER	C-N-CA	5.08	126.19	119.84
1	XA	328	C	P-O3'-C3'	5.08	127.82	120.20
54	RZ	201	LYS	N-CA-C	-5.07	107.26	112.93
1	XA	1297	C	P-O3'-C3'	5.06	127.80	120.20
1	QA	1285	A	P-O3'-C3'	5.06	127.79	120.20
1	QA	812	C	P-O3'-C3'	5.05	127.78	120.20
34	RA	637	A	P-O3'-C3'	5.05	127.78	120.20
34	YA	2681	C	P-O3'-C3'	5.04	127.77	120.20
50	RV	50	PRO	CA-N-CD	-5.03	104.95	112.00
47	RS	42	ASP	CA-C-N	5.02	131.13	121.54
47	RS	42	ASP	C-N-CA	5.02	131.13	121.54
34	YA	404	C	P-O3'-C3'	5.01	127.72	120.20
34	YA	637	A	P-O3'-C3'	5.00	127.71	120.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	Y3	34	GLU	Mainchain
37	YE	146	THR	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	32247	0	16278	255	0
1	XA	32471	0	16395	254	0
2	QB	1907	0	1958	21	0
2	XB	1915	0	1969	20	0
3	QC	1605	0	1668	30	0
3	XC	1605	0	1668	21	0
4	QD	1703	0	1767	20	0
4	XD	1703	0	1767	48	0
5	QE	1155	0	1213	13	0
5	XE	1155	0	1213	12	0
6	QF	843	0	857	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	XF	843	0	857	9	0
7	QG	1257	0	1296	11	0
7	XG	1257	0	1296	13	0
8	QH	1108	0	1165	13	0
8	XH	1108	0	1165	12	0
9	QI	1010	0	1037	31	0
9	XI	998	0	1024	16	0
10	QJ	801	0	849	15	0
10	XJ	777	0	816	14	0
11	QK	885	0	904	16	0
11	XK	864	0	881	16	0
12	QL	975	0	1062	20	0
12	XL	956	0	1046	25	0
13	QM	955	0	1021	31	0
13	XM	946	0	1008	14	0
14	QN	492	0	531	8	0
14	XN	492	0	529	8	0
15	QO	734	0	771	4	0
15	XO	729	0	768	6	0
16	QP	705	0	725	8	0
16	XP	705	0	725	8	0
17	QQ	834	0	904	10	0
17	XQ	834	0	904	9	0
18	QR	574	0	644	6	0
18	XR	574	0	644	11	0
19	QS	665	0	686	13	0
19	XS	674	0	699	11	0
20	QT	763	0	861	11	0
20	XT	763	0	861	9	0
21	QU	217	0	234	1	0
21	XU	217	0	234	5	0
22	QV	1584	0	808	13	0
22	XV	1584	0	808	13	0
23	QX	65	0	33	1	0
23	XX	499	0	249	6	0
24	R0	603	0	620	12	0
24	Y0	599	0	617	11	0
25	R1	763	0	848	12	0
25	Y1	729	0	802	11	0
26	R2	581	0	629	8	0
26	Y2	575	0	624	7	0
27	R3	469	0	518	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	Y3	469	0	518	22	0
28	R4	565	0	557	6	0
28	Y4	565	0	559	7	0
29	R5	459	0	478	4	0
29	Y5	459	0	477	6	0
30	R6	453	0	477	5	0
30	Y6	453	0	476	6	0
31	R7	409	0	454	4	0
31	Y7	418	0	467	3	0
32	R8	517	0	582	50	0
32	Y8	517	0	582	10	0
33	R9	307	0	337	5	0
33	Y9	307	0	336	8	0
34	RA	62051	0	31279	384	0
34	YA	62091	0	31298	433	0
35	RB	2573	0	1306	16	0
35	YB	2573	0	1306	11	0
36	RD	2115	0	2195	43	0
36	YD	2115	0	2195	37	0
37	RE	1568	0	1634	29	0
37	YE	1563	0	1629	21	0
38	RF	1585	0	1632	23	0
38	YF	1585	0	1632	16	0
39	RG	1474	0	1535	51	0
39	YG	1474	0	1535	45	0
40	RH	1336	0	1418	48	0
40	YH	1330	0	1413	16	0
41	RI	1136	0	1223	32	0
41	YI	1136	0	1223	55	0
42	RN	1104	0	1180	30	0
42	YN	1104	0	1180	13	0
43	RO	933	0	996	17	0
43	YO	933	0	996	19	0
44	RP	1145	0	1228	41	0
44	YP	1122	0	1204	22	0
45	RQ	1122	0	1179	25	0
45	YQ	1122	0	1179	31	0
46	RR	960	0	1021	11	0
46	YR	960	0	1021	11	0
47	RS	882	0	943	20	0
47	YS	882	0	943	18	0
48	RT	1141	0	1202	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	YT	1141	0	1202	32	0
49	RU	964	0	1022	27	0
49	YU	964	0	1022	50	0
50	RV	779	0	852	32	0
50	YV	779	0	852	16	0
51	RW	900	0	964	9	0
51	YW	900	0	964	24	0
52	RX	725	0	778	6	0
52	YX	725	0	778	10	0
53	RY	818	0	910	8	0
53	YY	818	0	911	12	0
54	RZ	1601	0	1630	32	0
54	YZ	1601	0	1630	30	0
55	XY	362	0	186	4	0
56	Z6	74	0	51	0	0
56	Z8	74	0	51	2	0
57	QA	73	0	0	0	0
57	QF	1	0	0	0	0
57	QH	1	0	0	0	0
57	QJ	1	0	0	0	0
57	QM	1	0	0	0	0
57	QV	1	0	0	0	0
57	R0	1	0	0	0	0
57	R1	1	0	0	0	0
57	R3	1	0	0	0	0
57	RA	483	0	0	0	0
57	RB	7	0	0	0	0
57	RE	4	0	0	0	0
57	RN	1	0	0	0	0
57	RO	1	0	0	0	0
57	RP	3	0	0	0	0
57	RQ	3	0	0	0	0
57	RR	1	0	0	0	0
57	RT	1	0	0	0	0
57	RY	1	0	0	0	0
57	XA	73	0	0	0	0
57	XE	1	0	0	0	0
57	XK	1	0	0	0	0
57	XL	1	0	0	0	0
57	XM	1	0	0	0	0
57	XQ	1	0	0	0	0
57	XS	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	Y0	2	0	0	0	0
57	Y1	1	0	0	0	0
57	Y7	1	0	0	0	0
57	Y8	1	0	0	0	0
57	YA	538	0	0	0	0
57	YB	13	0	0	0	0
57	YD	3	0	0	0	0
57	YE	4	0	0	0	0
57	YN	1	0	0	0	0
57	YO	1	0	0	0	0
57	YP	1	0	0	0	0
57	YQ	3	0	0	0	0
57	YR	2	0	0	0	0
57	YX	2	0	0	0	0
57	YY	1	0	0	0	0
58	QD	8	0	0	0	0
58	XD	8	0	0	0	0
59	QN	1	0	0	0	0
59	R4	1	0	0	0	0
59	R5	1	0	0	0	0
59	R6	1	0	0	0	0
59	R9	1	0	0	0	0
59	RY	1	0	0	0	0
59	XN	1	0	0	0	0
59	Y4	1	0	0	0	0
59	Y5	1	0	0	0	0
59	Y6	1	0	0	0	0
59	Y9	1	0	0	0	0
59	YY	1	0	0	0	0
All	All	292577	0	198284	2634	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (2634) 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)
51:YW:1:MET:HG3	51:YW:64:MET:CE	1.51	1.41
50:YV:40:LEU:CD2	50:YV:47:VAL:HG12	1.52	1.40
4:XD:19:LEU:CD2	4:XD:197:PRO:HG3	1.59	1.33
1:QA:1189:C:H5''	3:QC:5:ILE:CD1	1.56	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:YI:61:ARG:HB2	41:YI:133:HIS:CE1	1.73	1.23
51:YW:1:MET:C	51:YW:64:MET:HE1	1.60	1.23
13:QM:24:GLY:HA3	13:QM:66:LEU:CD2	1.71	1.18
42:RN:112:LEU:O	42:RN:116:LEU:HD12	1.41	1.17
41:YI:14:ASP:OD1	41:YI:17:GLN:HG2	1.45	1.16
51:YW:1:MET:CG	51:YW:64:MET:HE3	1.75	1.16
49:RU:92:ARG:HG2	49:RU:95:LEU:CD2	1.77	1.14
41:YI:61:ARG:CB	41:YI:133:HIS:CE1	2.29	1.14
2:XB:212:GLN:CD	2:XB:235:SER:HB3	1.71	1.14
36:RD:121:PRO:HB3	36:RD:135:PHE:CE2	1.82	1.13
41:YI:92:VAL:O	41:YI:120:ILE:HG22	1.46	1.13
2:XB:212:GLN:NE2	2:XB:235:SER:HB3	1.65	1.11
51:YW:1:MET:CG	51:YW:64:MET:CE	2.28	1.11
36:RD:121:PRO:HB3	36:RD:135:PHE:HE2	1.14	1.11
42:RN:23:LEU:HD12	42:RN:60:ILE:CD1	1.81	1.10
12:XL:46:LYS:HG2	12:XL:47:LYS:H	1.05	1.09
48:YT:120:ARG:HA	48:YT:123:GLN:HG3	1.30	1.09
4:XD:19:LEU:HD21	4:XD:197:PRO:HG3	1.34	1.08
34:YA:997:G:OP1	49:YU:93:LYS:HB2	1.50	1.08
41:YI:61:ARG:HB2	41:YI:133:HIS:HE1	1.06	1.08
41:RI:123:LEU:HD12	41:RI:123:LEU:H	1.16	1.08
41:YI:118:LYS:HB3	41:YI:119:PRO:HD3	1.36	1.05
50:RV:52:VAL:HG21	50:RV:55:ALA:HB3	1.36	1.05
41:YI:92:VAL:HB	41:YI:120:ILE:CG2	1.86	1.04
13:QM:24:GLY:HA3	13:QM:66:LEU:HD22	1.04	1.04
44:RP:101:VAL:HB	44:RP:106:LEU:HB3	1.40	1.04
50:YV:40:LEU:HD22	50:YV:47:VAL:HG12	1.39	1.04
48:RT:107:ASP:O	48:RT:110:ILE:HG22	1.58	1.03
1:QA:1189:C:H5''	3:QC:5:ILE:HD12	1.37	1.03
34:RA:2361:A:H5''	34:RA:2361:A:H8	1.24	1.02
41:YI:92:VAL:HB	41:YI:120:ILE:HG23	1.40	1.02
51:YW:1:MET:C	51:YW:64:MET:CE	2.33	1.01
34:YA:996:A:O2'	49:YU:92:ARG:HD2	1.60	1.01
49:RU:91:ASP:HA	49:RU:95:LEU:HB2	1.43	1.01
41:YI:118:LYS:HB3	41:YI:119:PRO:CD	1.90	1.01
51:YW:2:GLU:N	51:YW:64:MET:HE1	1.74	1.00
42:RN:23:LEU:CD1	42:RN:60:ILE:HD12	1.92	1.00
42:RN:23:LEU:HD12	42:RN:60:ILE:HD12	1.00	1.00
41:YI:120:ILE:HD11	41:YI:126:TYR:CE2	1.96	1.00
2:XB:212:GLN:CD	2:XB:235:SER:CB	2.34	1.00
32:R8:61:LEU:HD12	34:RA:593:G:H4'	1.45	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:2135:A:H62	34:RA:2156:G:N2	1.61	0.99
34:YA:997:G:H5'	49:YU:92:ARG:HB2	1.45	0.98
35:RB:8:U:H3	35:RB:112:G:H1	1.03	0.98
32:R8:61:LEU:CD1	34:RA:593:G:H4'	1.94	0.98
49:YU:92:ARG:NH1	49:YU:95:LEU:CD1	2.26	0.97
39:RG:83:ARG:HB3	39:RG:83:ARG:HH11	1.24	0.97
4:XD:19:LEU:HD22	4:XD:197:PRO:HG3	1.44	0.97
41:YI:120:ILE:HD11	41:YI:126:TYR:CD2	2.00	0.97
4:XD:19:LEU:HD21	4:XD:197:PRO:CG	1.95	0.96
32:R8:25:MET:CE	44:RP:64:LYS:HD2	1.95	0.96
32:R8:27:THR:HG23	34:RA:2392:A:O2'	1.64	0.96
4:XD:19:LEU:CD2	4:XD:197:PRO:CG	2.43	0.95
41:RI:132:PRO:HD2	41:RI:134:PRO:O	1.63	0.95
13:QM:24:GLY:CA	13:QM:66:LEU:HD22	1.96	0.95
50:YV:40:LEU:HD23	50:YV:47:VAL:HG12	1.49	0.95
34:RA:2135:A:N6	34:RA:2156:G:H21	1.63	0.94
34:YA:1359:A:H62	34:YA:1372:U:H3	0.99	0.94
41:YI:133:HIS:HB3	41:YI:134:PRO:HD3	1.48	0.94
50:YV:40:LEU:CD2	50:YV:47:VAL:CG1	2.46	0.93
34:YA:2096:U:H3	34:YA:2193:G:H1	1.15	0.93
12:XL:84:LEU:CB	12:XL:104:VAL:HG11	1.98	0.93
51:YW:1:MET:CB	51:YW:64:MET:HE2	1.99	0.93
34:YA:997:G:OP1	49:YU:93:LYS:HE2	1.68	0.93
39:YG:84:LYS:HA	39:YG:84:LYS:NZ	1.85	0.92
41:RI:120:ILE:HD11	41:RI:126:TYR:CE2	2.05	0.91
40:RH:9:ILE:CG2	40:RH:10:PRO:CD	2.48	0.91
45:YQ:27:VAL:HA	45:YQ:105:GLU:OE2	1.69	0.91
4:XD:31:CYS:O	4:XD:31:CYS:SG	2.29	0.91
41:YI:61:ARG:HB3	41:YI:133:HIS:CE1	2.06	0.90
40:RH:9:ILE:CG2	40:RH:10:PRO:HD2	2.02	0.90
27:Y3:5:LYS:HA	27:Y3:36:VAL:HG12	1.49	0.90
32:R8:61:LEU:HD11	34:RA:593:G:O2'	1.72	0.90
27:Y3:5:LYS:HB2	27:Y3:36:VAL:CG1	2.01	0.90
41:YI:133:HIS:CB	41:YI:134:PRO:CD	2.50	0.90
50:RV:52:VAL:HG23	50:RV:55:ALA:H	1.36	0.89
51:YW:1:MET:HB3	51:YW:64:MET:HE2	1.51	0.89
41:YI:9:LEU:H	41:YI:9:LEU:HD12	1.37	0.89
34:YA:1359:A:N6	34:YA:1372:U:H3	1.70	0.89
32:R8:57:ARG:O	32:R8:61:LEU:CD2	2.21	0.89
34:RA:2808:U:C2	34:RA:2892:A:N6	2.41	0.89
45:RQ:36:ALA:HB2	45:RQ:103:MET:HE2	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:1357:A:H61	1:XA:1365:G:H1	1.20	0.89
34:YA:2099:U:H3	34:YA:2190:G:H1	1.16	0.89
37:YE:28:ALA:O	37:YE:93:VAL:CG1	2.20	0.89
37:YE:28:ALA:O	37:YE:93:VAL:HG13	1.74	0.88
32:R8:52:LYS:H	32:R8:53:PRO:CD	1.85	0.88
48:YT:119:LYS:O	48:YT:123:GLN:HG3	1.74	0.88
12:XL:46:LYS:HG2	12:XL:47:LYS:N	1.84	0.87
40:RH:12:PRO:HG3	40:RH:48:GLY:HA2	1.54	0.87
41:YI:133:HIS:CB	41:YI:134:PRO:HD3	2.03	0.87
48:YT:120:ARG:HA	48:YT:123:GLN:CG	2.04	0.87
40:RH:9:ILE:HG22	40:RH:10:PRO:HD2	1.57	0.87
44:RP:107:LYS:HB3	44:RP:107:LYS:HZ3	1.39	0.87
1:QA:1189:C:C5'	3:QC:5:ILE:CD1	2.49	0.87
1:QA:1189:C:H5''	3:QC:5:ILE:HD13	1.53	0.86
27:Y3:5:LYS:HB2	27:Y3:36:VAL:HG12	1.57	0.86
39:YG:84:LYS:HA	39:YG:84:LYS:HZ2	1.39	0.86
39:RG:84:LYS:HA	39:RG:84:LYS:CE	2.03	0.86
45:YQ:27:VAL:HG13	45:YQ:105:GLU:OE2	1.76	0.85
51:YW:1:MET:HG3	51:YW:64:MET:HE3	0.87	0.85
34:RA:2135:A:H62	34:RA:2156:G:H21	0.88	0.85
54:YZ:7:ALA:HB2	54:YZ:59:LEU:HD12	1.57	0.85
49:RU:92:ARG:HG2	49:RU:95:LEU:HD21	1.59	0.84
44:RP:101:VAL:CB	44:RP:106:LEU:HB3	2.05	0.84
13:QM:66:LEU:HD23	13:QM:70:LEU:HD22	1.59	0.84
27:Y3:5:LYS:CA	27:Y3:36:VAL:HG12	2.08	0.83
12:XL:84:LEU:HB3	12:XL:104:VAL:HG11	1.60	0.83
39:RG:83:ARG:HH11	39:RG:83:ARG:CB	1.92	0.83
35:YB:8:U:H3	35:YB:112:G:H1	1.23	0.83
49:YU:92:ARG:HH12	49:YU:95:LEU:HG	1.41	0.83
32:R8:57:ARG:O	32:R8:61:LEU:HD23	1.78	0.83
32:R8:52:LYS:N	32:R8:53:PRO:CD	2.42	0.83
39:RG:84:LYS:HA	39:RG:84:LYS:HE3	1.59	0.83
4:XD:19:LEU:HD11	4:XD:63:LYS:HG3	1.61	0.83
41:YI:8:PRO:HG3	41:YI:14:ASP:HA	1.61	0.82
32:R8:25:MET:HE2	44:RP:64:LYS:HD2	1.60	0.82
49:YU:87:GLY:O	50:YV:50:PRO:HD3	1.79	0.82
41:RI:86:THR:HA	41:RI:123:LEU:HD13	1.62	0.82
48:YT:120:ARG:CA	48:YT:123:GLN:HG3	2.10	0.82
13:QM:24:GLY:CA	13:QM:66:LEU:CD2	2.57	0.82
51:YW:1:MET:CB	51:YW:64:MET:CE	2.58	0.81
49:YU:92:ARG:HH12	49:YU:95:LEU:CD1	1.94	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:RP:101:VAL:HB	44:RP:106:LEU:CB	2.11	0.81
12:XL:84:LEU:HB2	12:XL:104:VAL:HG11	1.61	0.80
34:YA:2069:G:N2	34:YA:2443:C:C2	2.49	0.80
45:YQ:27:VAL:CA	45:YQ:105:GLU:OE2	2.28	0.80
32:R8:52:LYS:N	32:R8:53:PRO:HD2	1.97	0.80
40:RH:9:ILE:HG22	40:RH:10:PRO:CD	2.10	0.80
27:Y3:5:LYS:CB	27:Y3:36:VAL:HG12	2.12	0.80
49:YU:92:ARG:HH11	49:YU:95:LEU:HD12	1.46	0.80
40:RH:9:ILE:HG23	40:RH:10:PRO:CD	2.11	0.80
34:YA:2308:G:N1	39:YG:80:PHE:HZ	1.78	0.80
54:RZ:48:PHE:HA	54:RZ:51:ALA:HB3	1.62	0.80
49:YU:92:ARG:HH12	49:YU:95:LEU:CG	1.95	0.79
34:RA:2361:A:H5''	34:RA:2361:A:C8	2.15	0.79
49:YU:92:ARG:NH1	49:YU:95:LEU:HD12	1.97	0.79
22:XV:54:U:H5''	54:YZ:202:GLU:HA	1.65	0.79
48:YT:119:LYS:O	48:YT:123:GLN:CG	2.31	0.79
50:RV:44:LYS:O	50:RV:46:VAL:HG12	1.82	0.79
41:YI:61:ARG:CB	41:YI:133:HIS:HE1	1.79	0.78
41:YI:118:LYS:CB	41:YI:119:PRO:CD	2.60	0.78
40:RH:12:PRO:HG3	40:RH:48:GLY:CA	2.14	0.77
36:YD:121:PRO:HB3	36:YD:135:PHE:CD2	2.19	0.77
37:RE:55:ASN:OD1	37:RE:58:ARG:HD2	1.84	0.77
41:RI:123:LEU:H	41:RI:123:LEU:CD1	1.93	0.77
36:YD:121:PRO:HB3	36:YD:135:PHE:CE2	2.18	0.77
34:YA:2304:G:H22	34:YA:2312:U:H3	1.33	0.77
42:RN:115:ARG:HG2	42:RN:115:ARG:HH11	1.50	0.77
50:YV:40:LEU:HD21	50:YV:47:VAL:HG12	1.65	0.77
48:RT:121:ILE:O	48:RT:125:ARG:HG2	1.84	0.76
41:YI:131:LYS:HB3	41:YI:135:GLU:HA	1.66	0.76
54:YZ:53:ILE:HG22	54:YZ:71:VAL:HG13	1.66	0.76
1:XA:452:A:H62	1:XA:480:U:H3	1.33	0.76
39:RG:81:LYS:HE3	39:RG:83:ARG:HD2	1.68	0.76
37:RE:16:ARG:HG3	37:RE:16:ARG:O	1.86	0.76
48:RT:120:ARG:HG2	48:RT:123:GLN:OE1	1.84	0.76
54:YZ:124:ILE:HD11	54:YZ:165:VAL:HG11	1.66	0.76
41:RI:83:ALA:HB1	41:RI:123:LEU:HD21	1.68	0.76
27:Y3:37:LEU:HD12	27:Y3:37:LEU:N	2.01	0.76
41:YI:65:ALA:CB	41:YI:132:PRO:HG2	2.16	0.76
34:RA:2245:U:H5'	34:RA:2246:G:H5'	1.68	0.75
34:YA:411:G:N2	44:YP:71:VAL:HG11	2.01	0.75
49:YU:87:GLY:O	50:YV:50:PRO:CD	2.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:RU:92:ARG:HG2	49:RU:95:LEU:HD23	1.67	0.75
42:RN:23:LEU:HD11	42:RN:98:VAL:HG22	1.69	0.75
13:QM:66:LEU:CD2	13:QM:70:LEU:HD22	2.17	0.74
48:RT:112:ARG:HH11	48:RT:112:ARG:HG3	1.51	0.74
39:YG:82:LEU:HD11	39:YG:88:ILE:HD13	1.67	0.74
41:YI:14:ASP:OD1	41:YI:17:GLN:CG	2.32	0.74
1:QA:440:A:H62	1:QA:493:G:H21	1.36	0.74
34:YA:2406:U:C4	44:YP:72:PRO:HD2	2.22	0.74
49:RU:87:GLY:O	50:RV:50:PRO:HD2	1.88	0.74
45:YQ:27:VAL:CG1	45:YQ:105:GLU:OE2	2.36	0.74
40:RH:147:ASN:O	40:RH:151:ILE:HG13	1.87	0.74
50:YV:40:LEU:HD22	50:YV:47:VAL:CG1	2.16	0.74
44:RP:101:VAL:HB	44:RP:106:LEU:HD23	1.70	0.73
40:RH:9:ILE:HG21	40:RH:50:VAL:H	1.54	0.73
41:RI:132:PRO:CD	41:RI:134:PRO:O	2.35	0.73
49:RU:92:ARG:CG	49:RU:95:LEU:CD2	2.63	0.73
26:Y2:47:ASN:HD22	34:YA:94:G:H21	1.37	0.72
34:YA:2245:U:H5'	34:YA:2246:G:H5'	1.70	0.72
41:YI:132:PRO:HD2	41:YI:134:PRO:O	1.89	0.72
34:RA:2508:G:H1	34:RA:2580:U:H3	1.37	0.72
50:RV:52:VAL:HG21	50:RV:55:ALA:CB	2.15	0.72
34:YA:2069:G:C2	34:YA:2443:C:C2	2.78	0.72
48:YT:120:ARG:HG2	48:YT:123:GLN:OE1	1.89	0.72
22:QV:52:G:H21	54:RZ:198:LYS:HE3	1.54	0.72
42:RN:112:LEU:C	42:RN:116:LEU:HD12	2.13	0.72
34:YA:2406:U:H2'	34:YA:2406:U:OP2	1.90	0.71
34:YA:2308:G:N1	39:YG:80:PHE:CZ	2.59	0.71
39:YG:47:LYS:HD2	39:YG:81:LYS:HB2	1.73	0.71
51:YW:2:GLU:CA	51:YW:64:MET:HE1	2.20	0.71
1:XA:1357:A:N6	1:XA:1365:G:H1	1.88	0.71
12:XL:46:LYS:CG	12:XL:47:LYS:H	1.93	0.71
50:RV:51:VAL:HG12	50:RV:53:GLU:H	1.56	0.71
34:RA:2808:U:N3	34:RA:2892:A:N6	2.39	0.71
41:YI:9:LEU:HD12	41:YI:9:LEU:N	2.06	0.71
42:RN:112:LEU:O	42:RN:116:LEU:CD1	2.31	0.71
47:YS:74:ALA:HB1	47:YS:107:GLU:HB3	1.73	0.71
32:R8:37:SER:O	32:R8:40:GLU:N	2.21	0.70
48:RT:102:ILE:HB	48:RT:110:ILE:HD13	1.74	0.70
4:XD:19:LEU:HD22	4:XD:197:PRO:CG	2.18	0.70
54:YZ:48:PHE:HA	54:YZ:51:ALA:HB3	1.73	0.70
32:R8:25:MET:HE2	44:RP:64:LYS:HB2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RB:80:U:H2'	35:RB:81:G:H21	1.55	0.70
22:QV:34:MNU:HN3	23:QX:3:G:H1	1.37	0.70
32:R8:25:MET:HE1	44:RP:64:LYS:HD2	1.72	0.70
50:RV:52:VAL:CG2	50:RV:55:ALA:HB3	2.18	0.70
19:XS:19:VAL:HG11	19:XS:44:MET:HG2	1.73	0.70
35:YB:80:U:H2'	35:YB:81:G:H21	1.57	0.70
2:XB:212:GLN:CD	2:XB:235:SER:HB2	2.15	0.70
34:YA:996:A:O2'	49:YU:92:ARG:CD	2.37	0.70
49:YU:91:ASP:O	49:YU:95:LEU:HB2	1.92	0.70
32:R8:35:GLN:OE1	32:R8:35:GLN:HA	1.91	0.69
27:Y3:2:PRO:HA	27:Y3:39:ASP:HB3	1.73	0.69
12:QL:117:ARG:HB2	12:QL:122:THR:HB	1.75	0.69
1:XA:664:G:H22	1:XA:741:G:H1	1.41	0.69
41:RI:8:PRO:HD3	41:RI:15:VAL:HG22	1.73	0.69
41:YI:65:ALA:HB1	41:YI:132:PRO:HG2	1.73	0.69
1:XA:438:G:H21	1:XA:496:A:H62	1.40	0.69
47:YS:74:ALA:CB	47:YS:107:GLU:HB3	2.23	0.69
49:YU:95:LEU:HD11	50:YV:11:GLN:HB2	1.73	0.69
34:RA:1038:C:H42	34:RA:1117:G:H1	1.41	0.69
2:QB:231:GLU:HG3	2:QB:232:PRO:HD2	1.75	0.68
27:Y3:3:ARG:CB	27:Y3:60:GLU:OXT	2.41	0.68
41:YI:92:VAL:O	41:YI:120:ILE:CG2	2.36	0.68
22:XV:74:C:H42	34:YA:2252:G:H1	1.40	0.68
36:RD:109:ASP:N	36:RD:196:VAL:O	2.27	0.68
41:RI:120:ILE:CD1	41:RI:126:TYR:CE2	2.76	0.68
49:YU:92:ARG:NH1	49:YU:95:LEU:HG	2.07	0.68
32:R8:30:ARG:NH2	44:RP:62:LEU:HD12	2.08	0.68
42:RN:114:ARG:HB3	42:RN:114:ARG:HH11	1.57	0.68
1:QA:1492:A:OP2	12:QL:47:LYS:HE2	1.93	0.68
44:RP:107:LYS:HB3	44:RP:107:LYS:NZ	2.08	0.68
4:XD:17:VAL:C	4:XD:33:MET:HE1	2.18	0.68
34:YA:997:G:OP1	49:YU:93:LYS:CE	2.42	0.68
25:Y1:83:GLU:HG2	25:Y1:85:LEU:H	1.58	0.67
34:RA:1062:G:H22	34:RA:1088:A:H62	1.42	0.67
41:YI:14:ASP:OD1	41:YI:14:ASP:N	2.24	0.67
41:YI:133:HIS:HB2	41:YI:134:PRO:CD	2.25	0.67
1:XA:827:U:O2	1:XA:874:G:N2	2.27	0.67
35:YB:30:C:H1'	35:YB:57:A:H61	1.60	0.67
44:RP:101:VAL:HB	44:RP:106:LEU:CD2	2.25	0.67
50:RV:52:VAL:CG2	50:RV:55:ALA:H	2.08	0.67
34:RA:2361:A:H8	34:RA:2361:A:C5'	2.04	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:RG:83:ARG:HB3	39:RG:83:ARG:NH1	2.06	0.67
3:XC:81:GLY:O	3:XC:85:ARG:HG2	1.95	0.66
29:R5:19:ARG:NH2	34:RA:1264:G:OP1	2.29	0.66
54:RZ:4:ARG:HG2	54:RZ:58:VAL:HB	1.78	0.66
34:YA:67:U:H3	34:YA:74:A:H2	1.41	0.66
32:R8:27:THR:CG2	34:RA:2392:A:O2'	2.41	0.66
41:RI:83:ALA:CB	41:RI:123:LEU:HD21	2.26	0.66
1:XA:111:G:H1	1:XA:330:C:H41	1.44	0.66
1:XA:954:G:H21	1:XA:1227:A:H62	1.44	0.66
4:XD:19:LEU:CD1	4:XD:63:LYS:HG3	2.25	0.66
40:RH:12:PRO:CG	40:RH:48:GLY:HA2	2.26	0.66
4:XD:18:LYS:HB3	4:XD:33:MET:SD	2.36	0.66
32:Y8:14:VAL:HG23	32:Y8:24:ALA:HB2	1.77	0.66
24:R0:27:GLU:HG3	24:R0:68:GLU:HA	1.77	0.66
36:RD:121:PRO:CB	36:RD:135:PHE:HE2	2.01	0.66
1:QA:689:C:H3'	1:QA:690:G:H21	1.60	0.65
1:QA:1322:C:OP2	19:QS:78:ARG:NH1	2.29	0.65
24:Y0:27:GLU:HG3	24:Y0:68:GLU:HA	1.77	0.65
34:YA:1995:U:O2	43:YO:3:GLN:NE2	2.29	0.65
1:QA:1322:C:OP2	19:QS:78:ARG:NH2	2.29	0.65
42:RN:110:GLY:O	42:RN:114:ARG:NH1	2.29	0.65
47:RS:10:ARG:NH1	47:RS:91:PRO:O	2.29	0.65
32:R8:30:ARG:HH21	44:RP:62:LEU:HD12	1.62	0.65
40:RH:9:ILE:HD12	40:RH:50:VAL:O	1.96	0.65
34:YA:1568:G:H5''	36:YD:61:LEU:HD23	1.78	0.65
32:R8:52:LYS:HZ2	34:RA:834:C:H4'	1.62	0.65
40:RH:9:ILE:HG23	40:RH:10:PRO:HD3	1.77	0.65
11:QK:18:ARG:HG2	11:QK:81:ASP:HB2	1.77	0.65
13:QM:80:ARG:HH12	13:QM:84:ILE:HD13	1.61	0.65
54:YZ:54:HIS:ND1	54:YZ:101:PRO:HG3	2.11	0.65
34:RA:855:G:H1	34:RA:922:U:H3	1.45	0.65
25:Y1:18:ILE:HG12	25:Y1:37:ILE:HG12	1.79	0.65
49:YU:92:ARG:NH1	49:YU:95:LEU:HD11	2.10	0.65
1:QA:664:G:H22	1:QA:741:G:H1	1.43	0.65
51:YW:1:MET:O	51:YW:64:MET:HE1	1.96	0.65
9:XI:3:GLN:HG2	9:XI:20:ARG:HB2	1.79	0.64
54:YZ:54:HIS:HB3	54:YZ:101:PRO:HD3	1.80	0.64
34:RA:2751:G:N7	40:RH:2:SER:N	2.45	0.64
1:XA:686:U:H1'	11:XK:42:TRP:HE1	1.62	0.64
1:QA:1066:C:N4	1:QA:1191:A:N6	2.46	0.64
13:XM:14:ARG:H	13:XM:44:ARG:HG3	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:RG:84:LYS:HE3	39:RG:84:LYS:CA	2.28	0.64
1:QA:686:U:H1'	11:QK:42:TRP:HE1	1.62	0.64
17:QQ:66:SER:O	17:QQ:70:ARG:NH1	2.31	0.64
32:R8:61:LEU:HD13	34:RA:593:G:H4'	1.79	0.64
1:XA:950:U:H3	1:XA:1231:G:H1	1.46	0.64
32:R8:30:ARG:HG3	32:R8:30:ARG:O	1.97	0.64
1:XA:1502:A:H2	1:XA:1505:G:H1	1.46	0.64
1:QA:1492:A:OP2	12:QL:47:LYS:CE	2.46	0.64
19:QS:19:VAL:HG21	19:QS:44:MET:HG2	1.80	0.64
2:XB:212:GLN:OE1	2:XB:235:SER:CB	2.46	0.64
4:XD:20:TYR:CE1	4:XD:106:TYR:OH	2.51	0.64
41:YI:61:ARG:CB	41:YI:133:HIS:ND1	2.61	0.64
1:QA:152:A:H62	1:QA:169:C:H42	1.44	0.64
4:XD:19:LEU:HD11	4:XD:63:LYS:CG	2.28	0.64
1:QA:1086:U:H3	1:QA:1099:G:H22	1.46	0.63
34:RA:1678:G:N2	34:RA:1990:C:O2	2.31	0.63
1:QA:1322:C:H6	1:QA:1322:C:OP1	1.80	0.63
3:XC:20:SER:HB2	3:XC:40:ARG:HH22	1.62	0.63
36:YD:182:LEU:H	36:YD:272:ALA:HB3	1.63	0.63
49:YU:92:ARG:NH1	49:YU:95:LEU:CG	2.59	0.63
19:XS:41:VAL:HG12	19:XS:43:GLU:H	1.63	0.63
32:R8:12:LYS:HG2	44:RP:68:GLN:HG2	1.79	0.63
4:QD:62:GLN:HE22	4:QD:65:ARG:HH21	1.47	0.63
41:YI:91:SER:HB2	41:YI:119:PRO:HB2	1.79	0.63
32:R8:40:GLU:O	32:R8:44:LYS:HD3	1.99	0.63
1:XA:545:C:OP1	4:XD:61:LYS:NZ	2.32	0.63
49:YU:92:ARG:HG3	49:YU:92:ARG:O	1.98	0.63
25:R1:83:GLU:HG2	25:R1:85:LEU:H	1.62	0.63
1:XA:1422:G:H5''	43:YO:48:PRO:HB3	1.80	0.63
42:YN:133:GLN:HG2	42:YN:135:PRO:HD3	1.80	0.63
1:QA:674:G:H2'	1:QA:675:A:H8	1.64	0.63
34:RA:2393:A:C8	34:RA:2393:A:H5''	2.34	0.63
17:XQ:66:SER:O	17:XQ:70:ARG:NH1	2.32	0.63
41:YI:133:HIS:HB2	41:YI:134:PRO:HD2	1.80	0.63
48:YT:51:ARG:HH21	48:YT:62:THR:HG21	1.63	0.63
3:QC:114:PRO:O	3:QC:118:GLN:HB2	1.99	0.62
1:QA:1189:C:H5''	3:QC:5:ILE:HD11	1.73	0.62
34:RA:2360:A:H8	34:RA:2360:A:O5'	1.81	0.62
1:XA:439:A:OP2	1:XA:493:G:N1	2.31	0.62
41:YI:117:GLU:OE1	41:YI:117:GLU:N	2.19	0.62
22:QV:74:C:H42	34:RA:2252:G:H1	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:R5:16:ARG:NH2	34:RA:517:C:OP1	2.33	0.62
9:XI:121:ARG:NH1	9:XI:122:ALA:O	2.33	0.62
34:RA:2068:U:H3	34:RA:2430:A:H2	1.47	0.62
34:YA:996:A:H4'	49:YU:92:ARG:NE	2.14	0.62
41:RI:79:ILE:HG22	41:RI:79:ILE:O	2.00	0.62
34:YA:1250:G:OP2	44:YP:18:ARG:NH2	2.32	0.62
34:YA:2443:C:H2'	34:YA:2444:G:H8	1.65	0.62
34:YA:2392:A:H1'	44:YP:61:ARG:HE	1.64	0.62
54:YZ:124:ILE:CD1	54:YZ:165:VAL:HG11	2.29	0.62
10:XJ:6:ILE:HD11	10:XJ:96:ILE:HB	1.81	0.62
54:YZ:166:SER:HB3	54:YZ:168:GLU:H	1.65	0.62
1:QA:1422:G:H5''	43:RO:48:PRO:HB3	1.81	0.62
36:YD:125:ILE:HD13	36:YD:125:ILE:N	2.16	0.61
1:QA:1222:G:H5''	19:QS:78:ARG:HE	1.64	0.61
9:QI:8:GLY:HA2	9:QI:79:LEU:HD23	1.83	0.61
36:RD:161:THR:O	36:RD:196:VAL:HG23	2.00	0.61
1:XA:562:C:H1'	12:XL:15:ARG:HD2	1.82	0.61
34:YA:300:A:OP2	53:YY:84:ARG:NH2	2.34	0.61
14:QN:24:CYS:HB3	14:QN:28:GLY:H	1.65	0.61
34:RA:676:A:H8	34:RA:2069:G:H21	1.47	0.61
34:YA:83:G:H1	34:YA:102:G:HO2'	1.48	0.61
34:YA:2406:U:O4	44:YP:70:GLN:NE2	2.34	0.61
32:R8:52:LYS:H	32:R8:53:PRO:HD3	1.61	0.61
34:RA:27:G:N2	34:RA:513:A:OP2	2.32	0.61
16:XP:53:VAL:HG13	16:XP:79:VAL:HG12	1.82	0.61
10:QJ:24:VAL:HG21	10:QJ:36:GLY:HA2	1.81	0.61
32:R8:25:MET:HE2	44:RP:64:LYS:CD	2.29	0.61
42:YN:15:LEU:HD22	42:YN:134:ARG:HD2	1.83	0.61
42:RN:114:ARG:HH11	42:RN:114:ARG:CG	2.13	0.61
34:YA:997:G:OP1	49:YU:93:LYS:CB	2.39	0.61
1:QA:410:G:H21	1:QA:432:A:H62	1.49	0.61
34:RA:1652:A:OP1	46:RR:8:ARG:NH1	2.34	0.61
42:RN:23:LEU:CD1	42:RN:60:ILE:CD1	2.66	0.60
34:YA:2731:G:OP1	37:YE:169:ASN:ND2	2.34	0.60
41:YI:120:ILE:HG23	41:YI:120:ILE:O	2.00	0.60
12:QL:36:VAL:HG22	12:QL:82:VAL:HG22	1.83	0.60
34:RA:2618:G:H21	37:RE:150:VAL:HG21	1.66	0.60
15:XO:54:ARG:HG2	15:XO:58:MET:HE2	1.83	0.60
6:QF:3:ARG:NH1	6:QF:38:GLU:OE2	2.34	0.60
34:RA:1187:G:H5'	50:RV:81:TYR:HE1	1.66	0.60
1:XA:674:G:H2'	1:XA:675:A:H8	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:YD:125:ILE:O	36:YD:125:ILE:HG22	2.00	0.60
28:R4:16:CYS:SG	28:R4:17:GLY:N	2.74	0.60
34:RA:1069:A:H2'	34:RA:1073:A:H62	1.67	0.60
26:Y2:47:ASN:ND2	34:YA:94:G:N3	2.50	0.60
1:QA:1522:U:H2'	1:QA:1523:G:H8	1.66	0.60
41:RI:131:LYS:HG3	41:RI:135:GLU:OE1	2.02	0.60
4:QD:57:ARG:HB3	4:QD:206:PHE:HB2	1.83	0.60
34:RA:1902:C:OP1	36:RD:242:ARG:NH1	2.34	0.60
37:YE:28:ALA:O	37:YE:93:VAL:HG12	1.99	0.60
34:RA:321:G:O2'	34:RA:340:A:N3	2.34	0.60
53:RY:9:LYS:NZ	53:RY:28:LYS:O	2.35	0.60
5:XE:102:ALA:HB1	5:XE:106:PRO:HG2	1.83	0.60
34:YA:2069:G:N2	34:YA:2443:C:O2	2.34	0.60
34:RA:2759:G:H21	40:RH:139:GLN:HE21	1.49	0.60
37:YE:29:GLY:CA	37:YE:180:ASN:HB3	2.31	0.59
1:QA:1066:C:H42	1:QA:1191:A:N6	2.00	0.59
40:RH:118:PRO:HG2	40:RH:121:ILE:HD13	1.83	0.59
46:RR:86:ARG:NH2	46:RR:118:GLU:OXT	2.35	0.59
34:YA:994:C:OP1	49:YU:53:ARG:NH2	2.35	0.59
39:YG:84:LYS:HA	39:YG:84:LYS:HZ3	1.68	0.59
43:YO:104:ARG:HH21	48:YT:34:VAL:HG11	1.68	0.59
34:RA:1779:U:OP2	34:RA:1784:A:N6	2.32	0.59
34:RA:2303:G:N3	39:RG:132:ASN:ND2	2.50	0.59
24:Y0:39:ARG:HH21	34:YA:2355:C:H1'	1.65	0.59
34:YA:1728:G:H8	34:YA:1732:A:H62	1.48	0.59
34:YA:2287:A:H62	34:YA:2344:U:H3	1.50	0.59
34:RA:2759:G:H21	40:RH:139:GLN:NE2	2.00	0.59
36:RD:108:PRO:HA	36:RD:196:VAL:O	2.03	0.59
39:RG:150:ASP:HB3	39:RG:153:ARG:HH22	1.67	0.59
1:XA:8:A:N6	4:XD:205:GLU:O	2.35	0.59
51:YW:1:MET:O	51:YW:64:MET:CE	2.49	0.59
34:RA:1047:G:H21	34:RA:1111:A:H62	1.50	0.59
28:Y4:53:GLU:OE2	28:Y4:60:GLN:NE2	2.35	0.59
35:YB:111:U:H2'	35:YB:112:G:H8	1.68	0.59
1:QA:1251:A:N3	1:QA:1369:C:O2'	2.35	0.59
14:QN:24:CYS:SG	14:QN:25:VAL:N	2.76	0.59
34:RA:571:A:H5'	34:RA:2030:A:H62	1.67	0.59
37:RE:5:LEU:HG	37:RE:49:LEU:HD23	1.82	0.59
54:RZ:47:VAL:O	54:RZ:51:ALA:N	2.33	0.59
1:QA:111:G:H1	1:QA:330:C:H41	1.50	0.59
34:RA:2130:U:O2	34:RA:2158:A:N6	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:RT:112:ARG:HH11	48:RT:112:ARG:CG	2.16	0.59
34:YA:1165:U:H3	34:YA:1184:G:H1	1.50	0.59
39:YG:82:LEU:CD1	39:YG:88:ILE:HD13	2.33	0.59
1:QA:1190:G:OP2	3:QC:5:ILE:HD12	2.02	0.59
1:QA:1077:G:N2	1:QA:1080:A:OP2	2.36	0.59
37:RE:78:LEU:HG	37:RE:79:ARG:HG2	1.84	0.59
43:RO:68:GLU:OE2	43:RO:78:ARG:NH1	2.36	0.59
48:RT:125:ARG:O	48:RT:128:GLU:N	2.36	0.59
50:RV:46:VAL:O	50:RV:46:VAL:HG22	2.01	0.59
8:XH:12:ARG:NH1	8:XH:25:ASP:O	2.34	0.59
18:XR:32:ARG:HA	18:XR:69:THR:HG21	1.85	0.59
41:YI:61:ARG:HB3	41:YI:133:HIS:ND1	2.18	0.59
54:RZ:5:LEU:H	54:RZ:59:LEU:HA	1.67	0.59
54:RZ:127:LYS:HB3	54:RZ:162:GLU:HB2	1.84	0.59
3:XC:88:ARG:HG2	3:XC:101:LEU:HD13	1.85	0.59
1:QA:278:G:OP2	17:QQ:92:ARG:NH2	2.37	0.58
1:QA:1199:U:O2'	1:QA:1202:G:OP1	2.21	0.58
4:QD:18:LYS:NZ	4:QD:26:CYS:SG	2.76	0.58
32:R8:43:GLN:NE2	34:RA:2365:G:O6	2.35	0.58
35:RB:48:A:OP2	47:RS:30:ARG:NH2	2.36	0.58
12:XL:33:ARG:H	12:XL:85:ILE:HG22	1.67	0.58
34:RA:1859:A:N6	34:RA:1883:G:O2'	2.37	0.58
1:XA:403:C:OP2	4:XD:74:GLN:NE2	2.33	0.58
1:XA:544:G:OP1	4:XD:59:ARG:NH2	2.36	0.58
1:XA:825:G:O2'	8:XH:12:ARG:NH2	2.34	0.58
28:Y4:56:VAL:HG11	28:Y4:58:ARG:HE	1.68	0.58
39:YG:63:ILE:HG13	39:YG:64:THR:HG23	1.85	0.58
34:RA:11:G:H22	34:RA:2627:G:H5''	1.68	0.58
38:RF:157:VAL:HB	38:RF:194:MET:HG2	1.84	0.58
1:XA:261:U:OP2	20:XT:79:ARG:NH2	2.36	0.58
8:XH:10:LEU:HD22	8:XH:83:ILE:HD11	1.85	0.58
32:Y8:30:ARG:HH21	44:YP:63:PRO:HB2	1.68	0.58
34:YA:997:G:C5'	49:YU:92:ARG:HB2	2.27	0.58
43:YO:104:ARG:NH2	48:YT:43:GLN:OE1	2.37	0.58
34:RA:1817:G:OP1	36:RD:88:ARG:NH2	2.35	0.58
34:RA:2788:C:O2'	34:RA:2809:A:N3	2.35	0.58
40:RH:83:TYR:HD2	40:RH:83:TYR:O	1.86	0.58
54:RZ:7:ALA:HB2	54:RZ:59:LEU:HB3	1.84	0.58
1:XA:1119:C:H2'	1:XA:1120:G:H8	1.69	0.58
11:XK:62:GLN:HB3	11:XK:93:GLN:HG3	1.85	0.58
34:YA:1359:A:N7	34:YA:1372:U:O4	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YB:9:G:OP1	47:YS:15:ARG:NH1	2.37	0.58
1:QA:316:G:OP2	1:QA:351:G:O2'	2.22	0.58
9:QI:47:LEU:HD22	9:QI:50:LEU:HD22	1.84	0.58
34:RA:307:G:H21	34:RA:330:A:H62	1.50	0.58
34:RA:2848:G:O2'	34:RA:2867:G:N2	2.36	0.58
25:Y1:87:PRO:HA	25:Y1:90:ILE:HG22	1.85	0.58
34:YA:1830:C:H2'	34:YA:1831:G:H8	1.69	0.58
34:YA:2069:G:C2	34:YA:2443:C:O2	2.56	0.58
45:YQ:28:ALA:N	45:YQ:105:GLU:OE2	2.37	0.58
1:QA:437:U:H3	1:QA:495:A:H62	1.51	0.58
34:RA:2784:C:O2'	37:RE:37:ARG:NH1	2.36	0.58
43:YO:3:GLN:HE21	43:YO:32:TYR:HE1	1.51	0.58
1:QA:945:G:N2	1:QA:1334:G:O2'	2.36	0.58
19:QS:53:ASN:HB2	19:QS:77:THR:HG22	1.85	0.58
49:RU:95:LEU:HD22	49:RU:95:LEU:N	2.18	0.58
53:RY:47:LYS:NZ	53:RY:48:ALA:O	2.36	0.58
34:YA:698:C:O2'	34:YA:734:A:N6	2.36	0.58
34:RA:2729:G:H1'	37:RE:187:ALA:HB2	1.86	0.58
35:RB:43:C:O2	39:RG:95:ARG:NH1	2.36	0.58
45:YQ:67:ARG:HD2	45:YQ:105:GLU:OE1	2.03	0.58
1:QA:1366:C:O2'	10:QJ:60:ARG:NH2	2.36	0.58
32:R8:52:LYS:H	32:R8:53:PRO:HD2	1.58	0.58
32:R8:61:LEU:CD1	34:RA:593:G:C4'	2.78	0.58
39:RG:73:ALA:HB2	39:RG:82:LEU:HD21	1.85	0.58
1:XA:452:A:O2'	16:XP:72:ARG:NH1	2.37	0.58
9:QI:3:GLN:NE2	9:QI:18:PHE:CG	2.72	0.58
36:RD:168:ARG:HG2	36:RD:173:VAL:HG12	1.85	0.58
1:XA:12:U:H3	1:XA:22:G:H1	1.52	0.58
34:YA:1327:C:O2'	46:YR:105:ARG:NH1	2.37	0.58
34:RA:527:C:N4	34:RA:2779:U:OP2	2.37	0.57
1:XA:926:G:O2'	23:XX:-3:A:N1	2.37	0.57
1:XA:1266:G:N2	1:XA:1269:A:OP2	2.35	0.57
14:YN:55:GLY:O	14:YN:57:ARG:NH1	2.36	0.57
1:QA:1502:A:H2	1:QA:1505:G:H22	1.52	0.57
42:RN:18:ALA:HA	42:RN:21:LYS:HE3	1.86	0.57
27:Y3:3:ARG:HB3	27:Y3:60:GLU:OXT	2.03	0.57
33:Y9:36:GLN:NE2	34:YA:1124:C:O2	2.38	0.57
34:YA:1454:U:O2'	34:YA:1455:G:N7	2.33	0.57
41:YI:65:ALA:HB2	41:YI:132:PRO:HG2	1.85	0.57
9:XI:48:GLU:HB2	9:XI:78:LYS:HE3	1.87	0.57
41:YI:133:HIS:CB	41:YI:134:PRO:HD2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:2572:A:H5''	34:RA:2574:G:H4'	1.87	0.57
38:RF:133:ASN:H	38:RF:162:LEU:HD13	1.69	0.57
1:QA:559:A:H4'	1:QA:560:U:H3'	1.86	0.57
39:RG:66:GLN:NE2	39:RG:93:THR:O	2.38	0.57
40:RH:9:ILE:HG23	40:RH:50:VAL:O	2.05	0.57
54:RZ:110:GLY:HA3	54:RZ:174:VAL:HG11	1.85	0.57
34:RA:300:A:OP1	53:RY:86:ARG:NH2	2.38	0.57
34:YA:1859:A:N6	34:YA:1883:G:O2'	2.38	0.57
49:YU:92:ARG:HH11	49:YU:92:ARG:HG2	1.70	0.57
2:QB:178:ARG:NH2	2:QB:196:LEU:O	2.38	0.57
34:RA:141:A:H8	34:RA:1595:G:H21	1.51	0.57
34:RA:2816:C:O2	34:RA:2883:A:O2'	2.23	0.57
43:RO:68:GLU:HG3	43:RO:78:ARG:HD2	1.87	0.57
1:XA:553:A:H5''	12:XL:24:VAL:HG21	1.86	0.57
2:XB:223:ILE:HG13	2:XB:229:VAL:HG22	1.86	0.57
19:XS:50:ALA:HB1	19:XS:57:HIS:HB3	1.86	0.57
34:YA:589:C:H2'	34:YA:590:A:H8	1.69	0.57
34:YA:1510:A:O2'	34:YA:1512:G:N7	2.37	0.57
34:YA:1817:G:OP1	36:YD:88:ARG:NH2	2.37	0.57
39:YG:36:LYS:HE2	39:YG:95:ARG:HH22	1.70	0.57
39:YG:41:GLN:HE21	39:YG:90:LEU:HD12	1.69	0.57
42:RN:115:ARG:HG2	42:RN:115:ARG:NH1	2.16	0.57
1:XA:1295:G:O2'	13:XM:14:ARG:NH1	2.38	0.57
34:YA:2406:U:N3	44:YP:72:PRO:HD2	2.19	0.57
44:YP:18:ARG:HH21	44:YP:21:ARG:HE	1.53	0.57
1:QA:1306:A:N6	1:QA:1331:G:O2'	2.37	0.57
34:RA:458:G:N2	34:RA:470:A:OP2	2.37	0.57
34:RA:2882:A:OP1	46:RR:96:ARG:NH1	2.36	0.57
1:XA:1286:A:H5''	21:XU:26:LYS:HD2	1.87	0.57
7:XG:30:ILE:HD12	7:XG:32:ARG:HH12	1.70	0.57
34:YA:2107:C:O2	34:YA:2182:G:N2	2.38	0.57
1:QA:811:C:O2'	1:QA:901:A:N1	2.38	0.57
13:QM:49:THR:HG22	13:QM:51:ALA:H	1.70	0.57
13:QM:97:PRO:HB2	13:QM:101:GLN:HG3	1.85	0.57
34:RA:674:G:H1'	38:RF:74:ARG:HD3	1.86	0.57
34:RA:1327:C:O2'	46:RR:105:ARG:NH1	2.37	0.57
36:RD:108:PRO:C	36:RD:196:VAL:O	2.47	0.57
42:RN:114:ARG:HH11	42:RN:114:ARG:CB	2.17	0.57
34:YA:2470:G:H5'	45:YQ:56:ARG:HH21	1.70	0.57
53:YY:47:LYS:NZ	53:YY:48:ALA:O	2.38	0.57
1:QA:254:G:O2'	17:QQ:16:GLN:O	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:QB:98:LEU:HB2	2:QB:101:MET:HE2	1.86	0.56
20:QT:44:ALA:HB2	20:QT:88:VAL:HG23	1.86	0.56
22:QV:63:U:OP1	24:R0:11:ARG:NH1	2.37	0.56
34:RA:665:C:H2'	34:RA:666:G:H8	1.70	0.56
45:RQ:36:ALA:HB2	45:RQ:103:MET:CE	2.31	0.56
1:XA:227:G:N2	16:XP:62:VAL:O	2.37	0.56
4:XD:4:TYR:OH	4:XD:10:ARG:NH2	2.38	0.56
34:YA:998:C:OP2	49:YU:58:ARG:NH1	2.38	0.56
34:YA:2030:A:H4'	34:YA:2031:A:H8	1.70	0.56
1:QA:406:G:H21	4:QD:119:GLN:HE22	1.51	0.56
34:RA:2361:A:C8	34:RA:2361:A:C5'	2.85	0.56
36:RD:71:ASP:HB2	36:RD:103:ARG:HH12	1.69	0.56
39:RG:116:ASP:OD1	39:RG:116:ASP:O	2.22	0.56
48:RT:111:ARG:C	48:RT:113:LYS:H	2.14	0.56
2:XB:68:ILE:HG12	2:XB:161:ALA:HB3	1.87	0.56
25:Y1:80:LEU:HD12	25:Y1:81:LYS:HG2	1.87	0.56
47:YS:78:LEU:HD21	47:YS:108:GLY:HA3	1.87	0.56
1:QA:440:A:H62	1:QA:493:G:N2	2.01	0.56
1:QA:1321:C:H5''	1:QA:1322:C:H5''	1.87	0.56
32:R8:58:ILE:HG22	44:RP:49:ARG:HH11	1.71	0.56
34:RA:184:C:O2'	34:RA:217:G:N3	2.36	0.56
34:RA:807:U:O2'	34:RA:2060:A:N1	2.37	0.56
34:RA:2334:G:H5'	47:RS:9:ARG:HG2	1.86	0.56
50:RV:76:LYS:H	50:RV:81:TYR:HB3	1.71	0.56
54:RZ:10:ARG:NH2	54:RZ:37:VAL:O	2.39	0.56
1:XA:64:G:H5''	1:XA:65:U:H5'	1.88	0.56
1:XA:538:G:H5''	12:XL:114:LYS:HB2	1.87	0.56
12:XL:71:PRO:O	12:XL:102:ARG:NH1	2.38	0.56
34:YA:392:C:H5''	34:YA:409:C:H5''	1.87	0.56
34:YA:2876:G:H5'	48:YT:2:ASN:HB3	1.88	0.56
44:YP:127:ALA:HB3	44:YP:130:PHE:HE1	1.69	0.56
45:YQ:43:THR:HG22	45:YQ:94:VAL:HG12	1.86	0.56
37:YE:29:GLY:HA2	37:YE:180:ASN:HB3	1.87	0.56
39:YG:136:ARG:HA	39:YG:154:GLY:HA3	1.88	0.56
33:R9:36:GLN:NE2	34:RA:1124:C:O2	2.39	0.56
11:XK:57:THR:HG22	11:XK:59:TYR:H	1.69	0.56
39:YG:10:LYS:NZ	39:YG:175:LEU:O	2.38	0.56
1:QA:35:G:N3	12:QL:118:SER:OG	2.39	0.56
50:RV:23:GLU:OE2	50:RV:89:GLN:NE2	2.39	0.56
34:YA:888:C:H3'	34:YA:889:C:H4'	1.87	0.56
39:YG:29:TRP:O	39:YG:33:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1137:C:O2	1:QA:1138:G:N2	2.39	0.56
39:RG:80:PHE:CD1	39:RG:80:PHE:N	2.73	0.56
51:RW:82:LEU:HB2	51:RW:98:LYS:HB2	1.88	0.56
1:XA:79:G:H1	1:XA:90:C:H42	1.53	0.56
1:XA:971:G:N2	1:XA:1363:A:OP2	2.38	0.56
41:YI:133:HIS:HB3	41:YI:134:PRO:CD	2.21	0.56
49:YU:94:ASN:C	49:YU:96:ALA:H	2.13	0.56
1:QA:1031:G:H2'	1:QA:1032:A:H8	1.70	0.56
1:QA:1119:C:OP2	9:QI:9:ARG:NH2	2.39	0.56
13:QM:24:GLY:HA3	13:QM:66:LEU:HD21	1.80	0.56
38:RF:161:GLU:OE1	38:RF:164:ARG:NH2	2.39	0.56
1:XA:1321:C:H5''	1:XA:1322:C:H2'	1.88	0.56
1:XA:1347:G:N2	1:XA:1374:A:OP2	2.39	0.56
22:XV:63:U:O2	54:YZ:198:LYS:NZ	2.38	0.56
1:QA:1414:U:H2'	1:QA:1415:G:H8	1.69	0.56
9:QI:121:ARG:NH1	9:QI:122:ALA:O	2.39	0.56
31:R7:7:PRO:HB2	34:RA:1309:G:H4'	1.88	0.56
34:RA:814:C:H1'	34:RA:1226:G:H21	1.71	0.56
34:RA:1359:A:H62	34:RA:1372:U:H3	1.53	0.56
54:RZ:5:LEU:HD12	54:RZ:43:GLU:HB3	1.87	0.56
1:XA:1179:A:H4'	9:XI:103:THR:HA	1.87	0.56
1:XA:1356:G:H2'	1:XA:1357:A:H8	1.71	0.56
16:XP:45:THR:HG22	16:XP:47:ASP:H	1.71	0.56
45:YQ:8:LYS:HA	54:YZ:197:ILE:HB	1.88	0.56
25:R1:18:ILE:HG12	25:R1:37:ILE:HG12	1.88	0.56
9:XI:111:ARG:O	9:XI:113:LYS:NZ	2.38	0.56
32:Y8:8:LYS:NZ	34:YA:245:G:O6	2.39	0.56
34:YA:2602:A:N6	56:Z8:76:PPU:OP2	2.39	0.56
50:YV:47:VAL:HG23	50:YV:47:VAL:O	2.04	0.56
50:RV:47:VAL:O	50:RV:47:VAL:HG22	2.05	0.55
4:XD:20:TYR:O	4:XD:20:TYR:CD1	2.59	0.55
43:YO:76:ALA:HB3	48:YT:75:ILE:HD12	1.87	0.55
17:QQ:9:VAL:HG22	17:QQ:56:VAL:HG22	1.87	0.55
34:YA:729:G:C6	34:YA:1775:U:C4	2.93	0.55
35:YB:43:C:H4'	39:YG:98:ARG:HH12	1.69	0.55
36:YD:168:ARG:HG2	36:YD:173:VAL:HG12	1.88	0.55
2:QB:231:GLU:HG3	2:QB:232:PRO:CD	2.36	0.55
34:RA:1800:C:H42	34:RA:1817:G:N2	2.05	0.55
34:RA:1992:G:N2	34:RA:1996:C:O2'	2.40	0.55
40:RH:83:TYR:N	40:RH:83:TYR:CD2	2.72	0.55
49:RU:90:VAL:HG22	50:RV:39:LEU:HD12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:26:G:H1'	34:YA:515:A:H61	1.70	0.55
34:YA:336:C:O2'	53:YY:35:TYR:OH	2.24	0.55
34:YA:807:U:O2'	34:YA:2060:A:N1	2.39	0.55
49:YU:90:VAL:HG22	50:YV:39:LEU:HD12	1.88	0.55
1:QA:1261:A:H62	1:QA:1274:G:H21	1.53	0.55
1:XA:1055:A:H8	1:XA:1055:A:O5'	1.89	0.55
4:XD:73:ARG:O	4:XD:77:ASN:ND2	2.39	0.55
24:Y0:51:VAL:O	47:YS:20:ARG:NH2	2.38	0.55
39:YG:97:ASP:H	39:YG:100:TRP:HD1	1.54	0.55
1:QA:261:U:OP2	20:QT:79:ARG:NH2	2.39	0.55
34:RA:2126:A:N6	34:RA:2163:C:O2'	2.39	0.55
39:RG:83:ARG:HH11	39:RG:83:ARG:CG	2.20	0.55
49:RU:87:GLY:O	50:RV:50:PRO:CD	2.53	0.55
1:XA:34:C:H2'	1:XA:35:G:H8	1.72	0.55
1:XA:1119:C:OP2	9:XI:9:ARG:NH2	2.39	0.55
41:YI:130:TYR:O	41:YI:136:VAL:HG13	2.06	0.55
53:YY:15:VAL:HG21	53:YY:42:VAL:HG11	1.87	0.55
34:RA:1546:C:H5'	34:RA:1547:C:H5'	1.88	0.55
34:RA:2502:G:H5''	34:RA:2503:A:H5''	1.88	0.55
39:RG:95:ARG:HB3	39:RG:96:ARG:HG2	1.87	0.55
40:RH:107:VAL:O	40:RH:152:ARG:NH1	2.39	0.55
34:YA:2183:C:H2'	34:YA:2184:G:H8	1.71	0.55
40:YH:96:ALA:HB1	40:YH:103:LEU:HD11	1.88	0.55
9:QI:9:ARG:HG2	9:QI:14:VAL:HG12	1.88	0.55
34:RA:1329:U:H5''	34:RA:1330:C:H5	1.72	0.55
34:RA:1818:U:H2'	36:RD:157:ARG:HG2	1.89	0.55
1:XA:643:C:H2'	1:XA:644:G:H8	1.71	0.55
1:XA:1503:A:C4	1:XA:1531:A:C2	2.95	0.55
9:XI:13:ALA:HB2	9:XI:68:GLY:HA3	1.88	0.55
10:XJ:44:VAL:HG22	10:XJ:66:ARG:HG2	1.88	0.55
34:YA:2680:C:H5'	37:YE:189:PRO:HA	1.88	0.55
1:QA:954:G:H21	1:QA:1227:A:H62	1.55	0.55
34:RA:900:A:H3'	34:RA:901:A:H8	1.72	0.55
35:RB:44:G:H1'	35:RB:47:C:H42	1.71	0.55
24:Y0:77:ARG:NH2	34:YA:857:C:OP2	2.39	0.55
45:YQ:30:GLY:O	45:YQ:134:ARG:NH2	2.38	0.55
1:QA:677:U:H3	1:QA:713:G:H22	1.55	0.55
1:QA:974:A:N3	14:QN:31:ARG:NH1	2.55	0.55
34:RA:1800:C:H42	34:RA:1817:G:H22	1.54	0.55
40:RH:121:ILE:HD11	40:RH:140:LYS:HB3	1.88	0.55
43:RO:23:ARG:NH2	43:RO:28:SER:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:RS:23:ARG:NH1	47:RS:85:VAL:O	2.40	0.55
54:RZ:52:SER:O	54:RZ:52:SER:OG	2.17	0.55
1:XA:20:U:O2'	1:XA:573:A:N6	2.40	0.55
22:XV:19:G:N3	22:XV:57:G:N2	2.54	0.55
34:YA:581:C:H2'	34:YA:582:G:H8	1.72	0.55
34:YA:958:U:OP2	45:YQ:14:ARG:NH1	2.39	0.55
34:YA:1939:U:OP1	34:YA:2604:U:O2'	2.24	0.55
34:YA:2446:G:N2	34:YA:2449:U:O2	2.40	0.55
42:YN:16:ILE:HG21	42:YN:26:LEU:HD11	1.89	0.55
1:QA:152:A:H62	1:QA:169:C:N4	2.04	0.55
10:QJ:51:ARG:O	14:QN:45:ARG:NH1	2.39	0.55
34:RA:65:C:H1'	34:RA:456:C:H42	1.71	0.55
34:RA:1140:C:OP2	42:RN:66:LYS:NZ	2.39	0.55
47:RS:71:ARG:NH1	47:RS:75:GLU:OE2	2.40	0.55
34:YA:793:A:OP2	34:YA:2071:A:O2'	2.25	0.55
35:YB:33:G:H5'	39:YG:2:PRO:HG3	1.89	0.55
1:QA:720:C:O2	18:QR:71:LYS:NZ	2.34	0.54
1:QA:1028(A):C:H42	1:QA:1032(B):G:H1	1.55	0.54
13:QM:68:GLY:O	39:RG:116:ASP:HB2	2.06	0.54
34:RA:1607:C:N4	34:RA:1622:G:OP2	2.36	0.54
34:RA:2306:C:N4	39:RG:42:GLY:O	2.40	0.54
1:XA:254:G:O2'	17:XQ:16:GLN:O	2.24	0.54
1:XA:587:G:N2	1:XA:754:C:OP2	2.38	0.54
1:XA:618:C:H5'	1:XA:619:U:H5''	1.88	0.54
33:Y9:2:LYS:NZ	33:Y9:31:LYS:O	2.38	0.54
34:YA:2111:C:H5	34:YA:2145:C:H42	1.55	0.54
34:YA:2115:G:N2	34:YA:2165:G:N7	2.56	0.54
54:YZ:7:ALA:HB2	54:YZ:59:LEU:CD1	2.34	0.54
22:QV:19:G:N3	22:QV:57:G:N2	2.55	0.54
34:RA:137(A):G:O6	34:RA:139:G:O2'	2.21	0.54
50:RV:58:VAL:HB	50:RV:98:GLU:HB2	1.88	0.54
28:Y4:42:PHE:HE2	39:YG:179:PRO:HB2	1.73	0.54
34:YA:2150:U:H2'	34:YA:2151:G:H8	1.73	0.54
41:YI:120:ILE:C	41:YI:120:ILE:HD12	2.32	0.54
1:QA:825:G:O2'	8:QH:12:ARG:NH2	2.37	0.54
10:QJ:54:PHE:HB2	10:QJ:55:LYS:HD3	1.87	0.54
32:R8:34:TRP:HB3	34:RA:2420:C:OP1	2.06	0.54
34:RA:392:C:H5''	34:RA:409:C:H5''	1.88	0.54
22:QV:65:C:H2'	22:QV:66:A:H8	1.73	0.54
32:R8:57:ARG:O	32:R8:61:LEU:HD21	2.07	0.54
34:YA:288:C:H2'	34:YA:289:A:H8	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:1600:C:OP1	52:YX:58:HIS:NE2	2.38	0.54
39:YG:84:LYS:HG3	39:YG:84:LYS:O	2.08	0.54
54:YZ:3:TYR:HB2	54:YZ:57:ILE:HG13	1.89	0.54
13:QM:80:ARG:NH1	13:QM:80:ARG:O	2.39	0.54
18:QR:70:ILE:O	18:QR:74:ARG:HB2	2.07	0.54
7:XG:15:ASP:HB3	7:XG:19:GLY:H	1.73	0.54
9:XI:112:LYS:HA	9:XI:119:ALA:HB2	1.88	0.54
34:RA:2318:G:N2	34:RA:2318:G:OP2	2.41	0.54
38:RF:116:ASP:OD2	44:RP:1:MET:N	2.40	0.54
40:RH:109:PHE:CE1	40:RH:152:ARG:HD2	2.42	0.54
20:XT:71:THR:OG1	20:XT:72:LEU:N	2.39	0.54
25:Y1:52:ARG:HH11	25:Y1:57:GLU:HB2	1.73	0.54
27:Y3:3:ARG:HG2	27:Y3:60:GLU:OXT	2.08	0.54
28:Y4:16:CYS:SG	28:Y4:17:GLY:N	2.81	0.54
34:YA:2688:U:OP1	34:YA:2713:A:N6	2.40	0.54
1:QA:1190:G:OP1	3:QC:5:ILE:HB	2.07	0.54
8:QH:4:ASP:HB2	8:QH:89:PRO:HG3	1.90	0.54
9:QI:44:VAL:O	9:QI:51:ARG:NH2	2.41	0.54
30:R6:26:ASN:ND2	30:R6:29:ASN:OD1	2.40	0.54
39:RG:32:PRO:HB2	39:RG:172:LEU:HD13	1.89	0.54
24:Y0:48:GLY:O	47:YS:20:ARG:NH1	2.40	0.54
54:YZ:158:PRO:HG2	54:YZ:161:VAL:HG21	1.89	0.54
1:QA:1296:C:OP1	13:QM:44:ARG:NH2	2.41	0.54
4:QD:166:LYS:HA	4:QD:178:VAL:HG21	1.90	0.54
10:QJ:49:VAL:HG23	14:QN:41:ARG:HB2	1.90	0.54
11:QK:52:GLY:H	11:QK:55:LYS:HE2	1.73	0.54
34:YA:882:G:H22	34:YA:894:C:H42	1.55	0.54
1:QA:405:U:O4	4:QD:2:GLY:N	2.41	0.54
34:RA:987:G:O2'	34:RA:1000:A:N3	2.39	0.54
34:RA:996:A:H4'	49:RU:92:ARG:HE	1.72	0.54
34:RA:1102:C:H2'	34:RA:1103:A:H8	1.72	0.54
34:RA:2328:A:H2'	34:RA:2329:G:C8	2.43	0.54
41:RI:86:THR:HA	41:RI:123:LEU:CD1	2.37	0.54
1:XA:992:U:H3	1:XA:1044:A:H62	1.54	0.54
32:Y8:27:THR:HG22	44:YP:63:PRO:HD3	1.90	0.54
33:Y9:27:CYS:SG	33:Y9:28:GLU:N	2.81	0.54
34:RA:603:A:N1	34:RA:625:G:O2'	2.39	0.54
34:RA:994:C:OP1	49:RU:53:ARG:NH2	2.41	0.54
34:RA:2120:G:N2	34:RA:2121:G:O6	2.41	0.54
34:RA:2134:A:N7	34:RA:2157:G:O2'	2.41	0.54
35:RB:30:C:H1'	35:RB:57:A:H61	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:RD:158:ALA:O	36:RD:196:VAL:HG21	2.08	0.54
34:YA:1359:A:N6	34:YA:1372:U:N3	2.40	0.54
34:YA:1816:G:O6	36:YD:35:LYS:NZ	2.40	0.54
37:YE:52:LEU:HD13	37:YE:52:LEU:N	2.23	0.54
1:QA:643:C:H2'	1:QA:644:G:H8	1.73	0.53
19:QS:50:ALA:HB1	19:QS:57:HIS:HB3	1.90	0.53
32:R8:61:LEU:HD12	34:RA:593:G:C4'	2.29	0.53
10:XJ:49:VAL:HG23	14:XN:41:ARG:HB2	1.90	0.53
24:Y0:70:GLN:OE1	24:Y0:80:HIS:NE2	2.40	0.53
34:YA:996:A:HO2'	49:YU:92:ARG:HD2	1.67	0.53
34:YA:1479:G:N7	34:YA:1510:A:N6	2.56	0.53
34:YA:2122:U:H2'	34:YA:2123:G:H8	1.72	0.53
24:R0:48:GLY:O	47:RS:20:ARG:NH1	2.40	0.53
1:XA:1538:C:H42	23:XX:-11:A:H61	1.55	0.53
34:YA:1385:G:O2'	34:YA:1396:U:O2	2.26	0.53
39:YG:83:ARG:C	39:YG:85:GLY:H	2.17	0.53
40:YH:94:TYR:OH	40:YH:160:LYS:NZ	2.42	0.53
49:YU:87:GLY:O	50:YV:50:PRO:HD2	2.09	0.53
49:YU:108:GLU:OE2	49:YU:112:ARG:NH1	2.41	0.53
1:XA:1034:G:H2'	1:XA:1035:A:H8	1.72	0.53
1:XA:1432:G:O2'	1:XA:1468:A:N6	2.41	0.53
11:XK:34:ASP:OD1	11:XK:38:ASN:N	2.39	0.53
34:YA:2120:G:H21	34:YA:2179:C:H41	1.55	0.53
2:QB:88:ALA:HB2	2:QB:219:VAL:HG13	1.91	0.53
27:R3:15:TYR:O	27:R3:20:LYS:NZ	2.41	0.53
40:RH:125:VAL:O	40:RH:125:VAL:HG12	2.07	0.53
6:XF:94:GLN:OE1	18:XR:32:ARG:NH1	2.40	0.53
34:YA:1338:G:N7	52:YX:62:LYS:NZ	2.53	0.53
34:YA:2071:A:H2'	34:YA:2072:G:H8	1.73	0.53
40:YH:124:GLU:HB2	40:YH:132:ARG:HB3	1.90	0.53
1:QA:768:A:N3	1:QA:1512:U:O2'	2.42	0.53
26:R2:47:ASN:ND2	34:RA:94:G:N3	2.56	0.53
32:R8:58:ILE:HA	32:R8:61:LEU:HD21	1.91	0.53
34:RA:577:G:O2'	34:RA:1254:A:OP1	2.26	0.53
48:RT:124:ASP:OD1	48:RT:124:ASP:N	2.42	0.53
1:XA:974:A:OP2	14:XN:41:ARG:NH1	2.41	0.53
1:XA:1015:A:OP1	19:XS:14:HIS:NE2	2.42	0.53
38:YF:101:LEU:O	38:YF:106:ARG:NH1	2.41	0.53
50:YV:23:GLU:OE2	50:YV:89:GLN:NE2	2.41	0.53
1:QA:1373:G:H5'	7:QG:36:LYS:HG2	1.91	0.53
15:QO:39:LEU:HD11	15:QO:52:SER:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:RF:143:ALA:HB1	38:RF:148:LEU:HB2	1.90	0.53
44:RP:101:VAL:CB	44:RP:106:LEU:HD23	2.38	0.53
48:RT:19:LEU:HD22	48:RT:86:ILE:HG22	1.90	0.53
53:RY:29:GLU:HB3	53:RY:38:ILE:HD12	1.90	0.53
13:XM:24:GLY:O	13:XM:29:ARG:NH2	2.42	0.53
29:Y5:12:SER:HB3	34:YA:2020:A:H5'	1.90	0.53
30:Y6:26:ASN:ND2	30:Y6:29:ASN:OD1	2.40	0.53
33:Y9:2:LYS:HB2	33:Y9:34:GLN:HG2	1.91	0.53
34:YA:629:G:N3	34:YA:639:U:O2'	2.41	0.53
34:YA:2743:C:O2'	40:YH:153:LYS:NZ	2.41	0.53
51:YW:1:MET:CG	51:YW:64:MET:HE2	2.20	0.53
9:QI:65:VAL:HG21	9:QI:73:GLN:HG3	1.91	0.53
34:RA:65:C:O2'	34:RA:456:C:N3	2.39	0.53
34:RA:372:G:N2	34:RA:401:A:OP2	2.39	0.53
37:RE:64:LYS:O	37:RE:73:GLU:OE2	2.27	0.53
42:YN:86:PRO:HD2	42:YN:89:LYS:HE2	1.91	0.53
1:QA:1032(B):G:O6	1:QA:1034:G:N2	2.41	0.53
1:QA:1305:G:N2	1:QA:1332:A:OP2	2.41	0.53
4:QD:140:VAL:HG11	4:QD:146:ILE:HD11	1.90	0.53
16:QP:4:ILE:HG12	16:QP:21:VAL:HG12	1.89	0.53
1:XA:993:G:O2'	1:XA:994:A:N7	2.38	0.53
4:XD:20:TYR:HE1	4:XD:106:TYR:OH	1.89	0.53
25:Y1:19:GLN:HG3	34:YA:2080:G:H5'	1.90	0.53
34:RA:625:G:O6	44:RP:107:LYS:HD3	2.09	0.53
34:RA:1939:U:OP1	34:RA:2604:U:O2'	2.26	0.53
37:RE:1:MET:N	37:RE:83:ASP:O	2.42	0.53
39:RG:35:GLU:HA	39:RG:99:MET:HE1	1.90	0.53
1:XA:842:C:O2'	1:XA:848:C:N4	2.42	0.53
13:XM:10:PRO:HB2	13:XM:18:ALA:HB1	1.90	0.53
55:XY:37:A:O2'	34:YA:1913:A:N1	2.42	0.53
54:YZ:53:ILE:HD11	54:YZ:99:TYR:HB2	1.91	0.53
10:QJ:9:ARG:HB2	10:QJ:95:GLU:HB2	1.91	0.53
13:QM:65:LYS:O	13:QM:66:LEU:HG	2.09	0.53
32:R8:61:LEU:CD1	34:RA:593:G:O2'	2.51	0.53
34:RA:1094:U:OP1	34:RA:1096:A:N6	2.42	0.53
34:RA:2392:A:H1'	44:RP:60:MET:HG2	1.90	0.53
37:RE:9:VAL:HB	37:RE:25:VAL:HG23	1.91	0.53
52:RX:53:LYS:NZ	52:RX:55:ASN:OD1	2.42	0.53
4:XD:105:VAL:HG23	4:XD:117:ALA:HB1	1.91	0.53
7:XG:88:PRO:HG2	7:XG:152:ALA:HB2	1.91	0.53
38:YF:165:ARG:HG2	38:YF:168:ARG:HH12	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:YI:118:LYS:HB3	41:YI:119:PRO:HD2	1.87	0.53
49:YU:92:ARG:HH11	49:YU:92:ARG:CG	2.22	0.53
51:YW:64:MET:HA	51:YW:109:GLU:OE2	2.09	0.53
1:QA:20:U:O2'	1:QA:573:A:N6	2.41	0.52
13:QM:15:VAL:HA	13:QM:18:ALA:HB3	1.91	0.52
26:R2:22:GLU:OE2	26:R2:68:ARG:NH2	2.42	0.52
34:RA:820:A:N3	34:RA:943:U:O2'	2.40	0.52
54:RZ:6:LYS:HD2	54:RZ:43:GLU:HG3	1.90	0.52
1:XA:811:C:O2'	1:XA:901:A:N1	2.42	0.52
27:Y3:5:LYS:HA	27:Y3:36:VAL:CG1	2.30	0.52
48:YT:16:ARG:HH21	48:YT:19:LEU:HD21	1.73	0.52
48:YT:118:ARG:HA	48:YT:121:ILE:HB	1.91	0.52
49:YU:49:HIS:HA	49:YU:52:ARG:HB3	1.91	0.52
1:QA:1321:C:O2	19:QS:36:ARG:NH2	2.42	0.52
45:RQ:81:VAL:O	45:RQ:82:ARG:NE	2.39	0.52
48:RT:62:THR:HG22	48:RT:75:ILE:HG12	1.91	0.52
50:RV:24:LYS:HA	50:RV:92:THR:HG23	1.92	0.52
32:Y8:58:ILE:HG12	44:YP:59:LEU:HD12	1.91	0.52
1:QA:1119:C:H2'	1:QA:1120:G:H8	1.74	0.52
1:QA:1141:C:H2'	1:QA:1142:G:H8	1.73	0.52
24:R0:38:VAL:HG21	24:R0:45:PHE:HD2	1.74	0.52
43:RO:19:ILE:HG22	43:RO:43:VAL:HA	1.92	0.52
1:XA:21:G:H21	1:XA:914:A:H62	1.56	0.52
34:YA:458:G:N2	34:YA:470:A:OP2	2.42	0.52
34:YA:2392:A:H2	34:YA:2424:C:H42	1.57	0.52
39:YG:39:ILE:HG12	39:YG:157:ILE:HG12	1.90	0.52
43:YO:64:ARG:HB2	43:YO:83:ALA:HB3	1.91	0.52
7:QG:16:LEU:HD11	9:QI:45:ALA:HB2	1.91	0.52
34:RA:1250:G:OP2	44:RP:18:ARG:NH2	2.42	0.52
34:RA:2258:C:O2'	34:RA:2427:C:OP2	2.25	0.52
47:RS:26:LEU:HB2	47:RS:87:PHE:HA	1.90	0.52
1:XA:1095:U:OP1	1:XA:1108:G:N2	2.37	0.52
1:XA:1240:U:H3	7:XG:32:ARG:HD2	1.74	0.52
1:XA:1360:A:OP2	14:XN:35:ARG:NH2	2.42	0.52
34:YA:89:G:OP1	53:YY:33:LYS:NZ	2.41	0.52
34:YA:820:A:N3	34:YA:943:U:O2'	2.38	0.52
34:YA:2010:G:H5''	51:YW:42:ARG:HB2	1.92	0.52
1:QA:297:G:N2	1:QA:300:A:OP2	2.42	0.52
1:XA:619:U:N3	4:XD:134:ASP:OD1	2.38	0.52
1:XA:957:U:H4'	19:XS:79:THR:HG23	1.90	0.52
3:XC:172:ARG:HG2	3:XC:174:PRO:HD3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:XH:4:ASP:HB2	8:XH:89:PRO:HG3	1.91	0.52
16:QP:4:ILE:HB	16:QP:66:PRO:HB3	1.91	0.52
34:RA:2683:C:OP1	48:RT:53:ARG:NH2	2.39	0.52
48:RT:121:ILE:O	48:RT:125:ARG:CG	2.55	0.52
1:XA:129(A):G:N2	1:XA:188:U:O2'	2.43	0.52
1:XA:414:A:OP2	1:XA:428:G:N2	2.43	0.52
34:YA:1664:A:H61	34:YA:1996:C:N4	2.08	0.52
1:QA:501:C:H2'	1:QA:502:G:H8	1.75	0.52
9:QI:10:ARG:HH12	9:QI:79:LEU:HD22	1.73	0.52
9:QI:109:VAL:O	9:QI:111:ARG:NH2	2.42	0.52
28:R4:14:ILE:HB	28:R4:22:ILE:HB	1.90	0.52
34:RA:530:G:O2'	34:RA:532:A:N7	2.43	0.52
34:RA:1791:A:H4'	36:RD:206:LEU:HB2	1.91	0.52
22:XV:52:G:H21	54:YZ:198:LYS:HE3	1.75	0.52
27:Y3:3:ARG:HG3	27:Y3:59:VAL:HB	1.90	0.52
37:YE:10:GLY:HA3	48:YT:8:LYS:HD3	1.90	0.52
9:QI:19:LEU:HD11	9:QI:81:ILE:HD13	1.92	0.52
13:QM:93:ARG:NH1	34:RA:888:C:OP2	2.43	0.52
42:RN:133:GLN:HG2	42:RN:135:PRO:HD3	1.92	0.52
1:XA:713:G:H2'	1:XA:714:G:C8	2.45	0.52
1:XA:945:G:N2	1:XA:1334:G:O2'	2.43	0.52
1:XA:1522:U:H2'	1:XA:1523:G:H8	1.74	0.52
2:XB:67:THR:HG21	2:XB:155:LEU:HG	1.92	0.52
22:XV:65:C:H2'	22:XV:66:A:H8	1.75	0.52
32:Y8:6:THR:HG22	32:Y8:63:PRO:HD2	1.90	0.52
34:YA:746:A:O2'	34:YA:2611:U:O2'	2.26	0.52
36:YD:146:GLU:HB2	36:YD:189:CYS:HB3	1.91	0.52
41:YI:13:GLY:HA3	41:YI:17:GLN:HB2	1.92	0.52
5:QE:152:ARG:NH1	8:QH:42:GLU:O	2.43	0.52
37:RE:5:LEU:HD23	37:RE:197:ILE:HG22	1.92	0.52
40:RH:9:ILE:HG23	40:RH:10:PRO:HD2	1.75	0.52
40:RH:153:LYS:HG2	40:RH:161:GLY:HA2	1.92	0.52
43:RO:8:LEU:HD13	43:RO:82:ASN:HB3	1.91	0.52
47:RS:95:HIS:HA	47:RS:99:LYS:HE3	1.92	0.52
48:RT:65:LYS:HE3	48:RT:67:SER:HB2	1.92	0.52
49:RU:92:ARG:NH2	49:RU:94:ASN:OD1	2.43	0.52
1:XA:1235:U:H5''	21:XU:3:LYS:HD2	1.90	0.52
22:XV:76:A:OP1	34:YA:2439:A:N6	2.42	0.52
35:YB:44:G:H1'	35:YB:47:C:H42	1.74	0.52
1:QA:401:C:O2'	1:QA:621:A:N3	2.37	0.52
1:QA:972:C:OP2	10:QJ:57:LYS:NZ	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:QF:79:LEU:HB3	6:QF:88:VAL:HG21	1.92	0.52
25:R1:52:ARG:HH11	25:R1:57:GLU:HB2	1.75	0.52
34:RA:996:A:OP2	49:RU:92:ARG:NH2	2.42	0.52
1:XA:673:G:H2'	1:XA:674:G:C8	2.44	0.52
1:XA:1071:C:H2'	1:XA:1072:G:H8	1.74	0.52
1:XA:1236:A:H4'	1:XA:1304:G:H4'	1.92	0.52
51:YW:88:ARG:HB2	51:YW:92:ARG:HB3	1.91	0.52
1:QA:684:A:O2'	11:QK:39:PRO:O	2.27	0.51
9:QI:48:GLU:OE2	9:QI:51:ARG:NH2	2.42	0.51
16:QP:53:VAL:HG13	16:QP:79:VAL:HG22	1.91	0.51
42:RN:47:ALA:O	42:RN:119:ARG:NH1	2.40	0.51
43:RO:3:GLN:HE21	43:RO:32:TYR:HE1	1.59	0.51
50:RV:51:VAL:C	50:RV:53:GLU:H	2.18	0.51
1:XA:745:C:OP1	1:XA:851:G:O2'	2.28	0.51
27:Y3:51:ALA:HA	27:Y3:54:VAL:HG12	1.92	0.51
34:YA:1689:A:H62	34:YA:1698:A:H2	1.57	0.51
34:YA:2008:C:H2'	34:YA:2009:G:H8	1.76	0.51
36:YD:148:GLU:OE1	36:YD:151:LYS:NZ	2.38	0.51
7:QG:150:ALA:HB1	11:QK:57:THR:HG21	1.92	0.51
16:QP:21:VAL:HG23	16:QP:33:ILE:HB	1.92	0.51
34:RA:890:A:H2'	34:RA:892:G:H8	1.75	0.51
4:XD:17:VAL:CA	4:XD:33:MET:HE1	2.39	0.51
9:XI:21:PRO:HA	9:XI:59:PHE:HA	1.91	0.51
14:YN:29:ARG:HG2	14:YN:31:ARG:H	1.74	0.51
34:YA:442:G:H1'	38:YF:48:THR:HG21	1.91	0.51
34:YA:1022:G:N2	34:YA:1023:U:O4	2.43	0.51
43:YO:19:ILE:HG22	43:YO:43:VAL:HA	1.93	0.51
1:QA:1382:C:O2'	7:QG:79:ARG:NH1	2.43	0.51
27:R3:2:PRO:HD2	27:R3:39:ASP:HB3	1.92	0.51
30:R6:25:LYS:NZ	30:R6:32:ASN:O	2.35	0.51
34:RA:537:C:OP1	34:RA:995:C:N4	2.36	0.51
34:RA:589:C:H2'	34:RA:590:A:H8	1.74	0.51
36:RD:69:ARG:HD3	36:RD:105:ILE:HD13	1.91	0.51
1:XA:1314:C:N4	19:XS:2:PRO:O	2.44	0.51
2:XB:69:LEU:HB3	2:XB:162:ILE:HG22	1.92	0.51
19:XS:29:ARG:HH21	19:XS:30:LEU:HD23	1.75	0.51
34:YA:581:C:H2'	34:YA:582:G:C8	2.46	0.51
34:YA:2069:G:C2	34:YA:2443:C:N3	2.78	0.51
1:QA:343:U:O2	1:QA:346:G:N2	2.31	0.51
1:QA:1304:G:OP1	21:QU:2:GLY:N	2.43	0.51
34:RA:144:C:H2'	34:RA:145:G:H8	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:RE:63:LEU:O	37:RE:73:GLU:OE2	2.27	0.51
43:RO:64:ARG:HB2	43:RO:83:ALA:HB3	1.92	0.51
45:RQ:13:GLN:O	45:RQ:72:LYS:NZ	2.42	0.51
8:XH:9:MET:HG3	8:XH:26:VAL:HG11	1.92	0.51
9:XI:15:ALA:HA	9:XI:65:VAL:HG22	1.92	0.51
29:Y5:16:ARG:NH2	34:YA:517:C:OP1	2.42	0.51
32:Y8:28:GLY:O	32:Y8:36:LYS:NZ	2.41	0.51
34:YA:612:G:N2	34:YA:616:A:O2'	2.43	0.51
34:YA:637:A:OP1	44:YP:133:SER:OG	2.27	0.51
34:YA:964:C:O2'	34:YA:2273:A:N3	2.40	0.51
34:YA:2328:A:H2'	34:YA:2329:G:C8	2.46	0.51
34:YA:2788:C:O2'	34:YA:2809:A:N3	2.39	0.51
34:RA:2632:A:HO2'	34:RA:2811:G:HO2'	1.55	0.51
45:RQ:141:GLN:NE2	54:RZ:123:ASP:OD1	2.43	0.51
1:XA:1414:U:H2'	1:XA:1415:G:H8	1.74	0.51
11:XK:62:GLN:OE1	11:XK:93:GLN:NE2	2.40	0.51
20:XT:56:MET:HE2	20:XT:88:VAL:HG21	1.93	0.51
23:XX:-12:C:H2'	23:XX:-11:A:H8	1.75	0.51
34:YA:2033:A:O2'	34:YA:2035:G:OP2	2.24	0.51
34:YA:2816:C:O2	34:YA:2883:A:O2'	2.26	0.51
34:RA:1047:G:H21	34:RA:1111:A:N6	2.08	0.51
34:RA:1333:C:H2'	34:RA:1334:G:H8	1.76	0.51
34:RA:1454:U:O2'	34:RA:1455:G:N7	2.40	0.51
40:RH:124:GLU:HB3	40:RH:132:ARG:HB2	1.91	0.51
26:Y2:47:ASN:HD22	34:YA:94:G:N2	2.06	0.51
42:YN:96:GLU:HB2	42:YN:122:VAL:HG12	1.93	0.51
49:YU:96:ALA:O	49:YU:99:ALA:HB3	2.11	0.51
54:YZ:53:ILE:C	54:YZ:55:HIS:H	2.19	0.51
1:QA:514:C:H2'	1:QA:515:G:H8	1.76	0.51
3:QC:153:VAL:HG22	3:QC:198:VAL:HG22	1.92	0.51
8:QH:10:LEU:HD22	8:QH:83:ILE:HD11	1.93	0.51
10:QJ:43:ARG:HB2	10:QJ:67:THR:HB	1.92	0.51
34:RA:252:G:OP2	44:RP:50:ARG:NH1	2.43	0.51
34:RA:1536:A:OP2	34:RA:1537:C:N4	2.43	0.51
34:RA:2515:C:H2'	34:RA:2516:G:H8	1.75	0.51
34:RA:2682:U:O3'	48:RT:58:ASN:ND2	2.44	0.51
34:RA:2845:G:H2'	34:RA:2846:G:H8	1.76	0.51
39:RG:27:ASN:HB3	39:RG:30:GLU:HG3	1.93	0.51
34:YA:1930:G:N2	34:YA:1969:A:OP2	2.35	0.51
45:YQ:81:VAL:O	45:YQ:82:ARG:NE	2.40	0.51
1:QA:235:C:H2'	1:QA:236:G:H8	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:R9:27:CYS:SG	33:R9:28:GLU:N	2.83	0.51
34:RA:1228:G:OP2	49:RU:16:LYS:NZ	2.40	0.51
34:RA:1689:A:H62	34:RA:1698:A:H2	1.58	0.51
34:RA:2393:A:H5''	34:RA:2393:A:H8	1.74	0.51
1:XA:978:A:OP2	1:XA:1362(A):C:N4	2.36	0.51
34:YA:184:C:O2'	34:YA:217:G:N3	2.43	0.51
34:YA:1652:A:OP1	46:YR:8:ARG:NH1	2.43	0.51
34:YA:2258:C:O2'	34:YA:2427:C:OP2	2.27	0.51
34:YA:2293:C:O2'	47:YS:93:LYS:NZ	2.42	0.51
32:R8:12:LYS:NZ	34:RA:249:C:O2	2.40	0.51
1:XA:1305:G:H22	1:XA:1331:G:H2'	1.74	0.51
1:QA:689:C:OP1	11:QK:27:ASN:ND2	2.40	0.51
34:RA:1047:G:N2	34:RA:1111:A:H62	2.08	0.51
34:RA:1500:G:N2	36:RD:99:ASP:O	2.43	0.51
46:RR:51:LEU:HD22	46:RR:66:VAL:HG13	1.92	0.51
1:XA:407:G:H2'	1:XA:408:A:H8	1.74	0.51
4:XD:80:GLU:OE1	4:XD:84:LYS:NZ	2.43	0.51
19:XS:36:ARG:NH2	19:XS:72:GLY:O	2.44	0.51
34:YA:1693:U:O2	36:YD:14:ARG:NH1	2.44	0.51
1:QA:165:C:H2'	1:QA:166:G:H8	1.76	0.50
1:QA:191(G):G:O2'	20:QT:101:GLY:O	2.29	0.50
1:QA:1010:G:H2'	1:QA:1011:G:H8	1.75	0.50
34:RA:557:U:H2'	34:RA:558:G:H8	1.76	0.50
34:RA:1542:G:O6	34:RA:1543:A:N6	2.43	0.50
34:RA:2059:A:HO2'	38:RF:69:HIS:HD1	1.58	0.50
51:RW:86:LEU:HD22	51:RW:96:ILE:HD11	1.93	0.50
34:YA:223:A:O2'	34:YA:420:C:O2	2.28	0.50
34:YA:1341:U:OP2	34:YA:1394:U:O2'	2.26	0.50
34:YA:1667:G:O2'	34:YA:1991:U:O4	2.29	0.50
34:YA:1799:G:O2'	36:YD:183:ARG:NH1	2.44	0.50
46:YR:86:ARG:NH2	46:YR:118:GLU:OXT	2.38	0.50
1:QA:1347:G:N2	1:QA:1374:A:OP2	2.39	0.50
3:QC:34:LEU:HD13	14:QN:25:VAL:HG11	1.94	0.50
26:R2:41:ILE:HD11	26:R2:44:LEU:HD12	1.92	0.50
32:R8:4:MET:HE2	34:RA:666:G:H1'	1.92	0.50
37:RE:14:ILE:HG23	48:RT:14:TYR:HE2	1.76	0.50
40:RH:88:LEU:HA	40:RH:130:ARG:HA	1.92	0.50
1:QA:56:U:H2'	1:QA:57:G:H8	1.76	0.50
4:QD:129:ASN:HD21	4:QD:144:ASP:HA	1.76	0.50
10:QJ:6:ILE:HG23	10:QJ:72:VAL:HB	1.93	0.50
11:QK:57:THR:HG22	11:QK:59:TYR:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:QK:109:VAL:HG12	18:QR:86:VAL:HA	1.94	0.50
34:RA:1022:G:N2	34:RA:1023:U:O4	2.41	0.50
34:RA:2680:C:H5'	37:RE:189:PRO:HA	1.93	0.50
13:XM:69:GLU:HG2	28:Y4:50:VAL:HG21	1.93	0.50
34:YA:244:A:H4'	44:YP:74:GLU:HB2	1.92	0.50
34:YA:1316:U:H2'	34:YA:1317:A:H8	1.76	0.50
41:YI:24:GLY:O	41:YI:28:ASN:HB2	2.11	0.50
1:QA:954:G:O6	13:QM:104:ARG:NH1	2.44	0.50
1:QA:1229:A:OP1	13:QM:114:ARG:NH1	2.44	0.50
8:QH:12:ARG:NH1	8:QH:25:ASP:O	2.39	0.50
25:R1:98:LEU:O	34:RA:269:U:O2'	2.30	0.50
32:R8:46:ARG:NH2	34:RA:631:A:OP1	2.45	0.50
34:RA:826:U:OP1	34:RA:2429:G:OP1	2.30	0.50
1:XA:7:G:O2'	5:XE:120:THR:O	2.30	0.50
1:XA:191(F):U:H2'	1:XA:191(G):G:H8	1.77	0.50
1:XA:993:G:H2'	1:XA:995:C:H41	1.76	0.50
2:XB:32:ILE:HD11	2:XB:40:HIS:HB3	1.92	0.50
4:XD:98:GLU:HA	4:XD:103:ASN:HD22	1.75	0.50
34:YA:2515:C:H2'	34:YA:2516:G:H8	1.76	0.50
39:YG:122:PRO:HD3	39:YG:181:ARG:HB2	1.94	0.50
41:YI:130:TYR:O	41:YI:136:VAL:CG1	2.59	0.50
44:YP:38:GLN:HG3	44:YP:45:LEU:HD23	1.94	0.50
37:RE:31:CYS:HB3	37:RE:49:LEU:HG	1.93	0.50
39:RG:37:VAL:HG22	39:RG:159:VAL:HG23	1.93	0.50
41:RI:3:VAL:HG12	41:RI:38:LEU:HA	1.94	0.50
1:XA:1356:G:H2'	1:XA:1357:A:C8	2.46	0.50
9:XI:9:ARG:HG2	9:XI:14:VAL:HG12	1.94	0.50
27:Y3:5:LYS:HE3	27:Y3:34:GLU:OE2	2.10	0.50
35:YB:37:C:O2	47:YS:95:HIS:NE2	2.42	0.50
38:YF:164:ARG:O	38:YF:168:ARG:HB2	2.11	0.50
54:YZ:53:ILE:C	54:YZ:53:ILE:HD12	2.36	0.50
38:RF:36:VAL:HG22	38:RF:101:LEU:HD21	1.94	0.50
45:RQ:63:LYS:HA	54:RZ:178:GLU:HG2	1.92	0.50
1:XA:924:C:O2'	1:XA:1502:A:N6	2.43	0.50
1:QA:427:U:O2'	1:QA:541:G:OP1	2.28	0.50
1:QA:1497:G:H1'	1:QA:1518:A:H2	1.76	0.50
15:QO:16:ALA:HB1	15:QO:21:ASP:HB3	1.93	0.50
20:QT:85:MET:HA	20:QT:88:VAL:HG12	1.94	0.50
34:RA:581:C:H2'	34:RA:582:G:H8	1.77	0.50
34:RA:1139:G:O2'	34:RA:1143:A:N1	2.41	0.50
38:RF:155:LEU:HB2	38:RF:189:THR:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:RN:114:ARG:NH1	42:RN:114:ARG:CG	2.73	0.50
1:XA:1251:A:N3	1:XA:1369:C:O2'	2.36	0.50
1:XA:1347:G:H5''	9:XI:107:ARG:HB2	1.94	0.50
1:XA:1432:G:OP1	48:YT:108:ARG:N	2.44	0.50
25:Y1:51:VAL:HG11	25:Y1:74:VAL:HG21	1.94	0.50
34:YA:630:G:N2	34:YA:633:A:OP2	2.36	0.50
34:YA:1329:U:H5''	34:YA:1330:C:H5	1.76	0.50
34:YA:1598:C:O3'	52:YX:35:THR:OG1	2.28	0.50
34:YA:1791:A:H3'	34:YA:1792:G:H8	1.76	0.50
45:YQ:27:VAL:C	45:YQ:105:GLU:OE2	2.55	0.50
1:QA:1058:G:OP1	3:QC:199:LYS:NZ	2.42	0.50
1:QA:1071:C:H2'	1:QA:1072:G:H8	1.77	0.50
5:QE:35:GLY:HA3	5:QE:112:LEU:HB3	1.92	0.50
32:R8:25:MET:HE2	44:RP:64:LYS:CB	2.41	0.50
34:RA:181:A:H1'	34:RA:435:C:H5'	1.93	0.50
34:RA:560:C:H4'	49:RU:52:ARG:HH12	1.76	0.50
34:RA:1652:A:N6	46:RR:11:ASN:OD1	2.42	0.50
45:RQ:135:ASP:OD2	54:RZ:81:ARG:NH2	2.45	0.50
1:XA:578:C:O2'	1:XA:728:A:N3	2.38	0.50
1:XA:1469:G:H2'	1:XA:1470:G:H8	1.76	0.50
1:XA:1503:A:C5	1:XA:1531:A:C2	3.00	0.50
34:YA:605:C:O2	34:YA:657:U:O2'	2.29	0.50
37:YE:7:VAL:HG11	48:YT:1:MET:HE1	1.94	0.50
47:YS:39:ILE:HD12	47:YS:85:VAL:HG11	1.94	0.50
3:QC:9:GLY:HA2	3:QC:12:LEU:HG	1.94	0.50
13:QM:24:GLY:CA	13:QM:66:LEU:HD21	2.39	0.50
13:QM:36:LYS:HD2	13:QM:59:TYR:HE1	1.77	0.50
14:QN:37:PHE:HD2	14:QN:44:LEU:HD22	1.77	0.50
34:RA:302:C:OP2	53:RY:73:ARG:NH1	2.39	0.50
34:RA:1341:U:OP2	34:RA:1394:U:O2'	2.28	0.50
1:XA:376:G:H5''	16:XP:5:ARG:HB2	1.94	0.50
1:XA:401:C:O2'	1:XA:621:A:N3	2.41	0.50
2:XB:212:GLN:OE1	2:XB:235:SER:HB2	2.09	0.50
24:Y0:23:VAL:HG21	34:YA:857:C:H4'	1.94	0.50
34:YA:577:G:O2'	34:YA:1254:A:OP1	2.29	0.50
34:YA:665:C:H2'	34:YA:666:G:H8	1.77	0.50
38:YF:110:LEU:HD11	38:YF:181:LEU:HD13	1.94	0.50
48:YT:119:LYS:O	48:YT:123:GLN:HG2	2.10	0.50
1:QA:1066:C:N4	1:QA:1191:A:H62	2.10	0.49
1:QA:1250:A:OP1	9:QI:67:GLY:N	2.41	0.49
9:QI:26:VAL:HG22	9:QI:61:ALA:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:QI:63:ILE:HG21	9:QI:77:ILE:HG12	1.93	0.49
34:RA:581:C:H2'	34:RA:582:G:C8	2.47	0.49
34:RA:1882:C:H3'	34:RA:1883:G:H8	1.77	0.49
34:RA:2841:C:H2'	34:RA:2842:G:H8	1.77	0.49
1:XA:1101:A:N6	2:XB:176:GLU:OE2	2.45	0.49
1:XA:1233:G:O2'	1:XA:1365:G:OP1	2.30	0.49
29:Y5:19:ARG:NH2	34:YA:1264:G:OP1	2.34	0.49
45:YQ:77:LYS:NZ	45:YQ:83:MET:O	2.44	0.49
1:QA:713:G:H2'	1:QA:714:G:C8	2.47	0.49
41:RI:88:ILE:HD12	41:RI:121:LYS:HA	1.94	0.49
1:XA:107:G:H3'	1:XA:108:G:H21	1.77	0.49
1:XA:581:G:OP1	15:XO:65:ARG:NH1	2.44	0.49
27:Y3:37:LEU:HB2	27:Y3:43:ILE:HG21	1.94	0.49
34:YA:2508:G:H1	34:YA:2580:U:H3	1.58	0.49
34:YA:2571:C:O2'	37:YE:146:THR:O	2.30	0.49
46:YR:28:LEU:HD23	46:YR:48:VAL:HG11	1.93	0.49
1:QA:938:A:N3	1:QA:1376:U:O2'	2.39	0.49
34:RA:30:G:O2'	34:RA:1214:A:N3	2.39	0.49
4:XD:105:VAL:HG11	4:XD:126:ILE:HD13	1.94	0.49
4:XD:187:ARG:NH1	4:XD:193:ASP:OD2	2.45	0.49
30:Y6:5:VAL:HA	30:Y6:27:LYS:HE2	1.94	0.49
34:YA:270(R):G:H2'	34:YA:270(S):G:H8	1.77	0.49
34:YA:1538:G:H2'	34:YA:1539:G:H8	1.77	0.49
38:YF:157:VAL:HG21	38:YF:181:LEU:HD23	1.93	0.49
1:QA:440:A:N6	1:QA:493:G:H21	2.06	0.49
1:QA:742:G:OP2	15:QO:35:ARG:NH2	2.44	0.49
3:QC:85:ARG:HG3	3:QC:88:ARG:HH21	1.78	0.49
13:QM:34:LEU:HD13	13:QM:41:PRO:HG3	1.93	0.49
34:RA:2392:A:H1'	44:RP:60:MET:HE3	1.94	0.49
39:RG:16:ARG:HH21	39:RG:28:VAL:HG22	1.78	0.49
42:RN:112:LEU:HG	42:RN:116:LEU:HD11	1.93	0.49
34:YA:546:C:OP1	34:YA:547:A:N6	2.45	0.49
34:YA:1983:C:H4'	34:YA:2606:C:H4'	1.93	0.49
40:YH:7:LEU:HD12	40:YH:8:PRO:HD2	1.93	0.49
44:YP:86:LYS:HB3	44:YP:118:GLY:HA3	1.93	0.49
1:QA:1406:U:O2	1:QA:1517:G:N2	2.41	0.49
5:QE:50:GLU:HB2	5:QE:53:LEU:HD13	1.94	0.49
8:QH:91:ARG:HB2	12:QL:7:ILE:HG13	1.94	0.49
33:R9:2:LYS:NZ	33:R9:31:LYS:O	2.41	0.49
34:RA:299:A:H5'	53:RY:86:ARG:HH21	1.78	0.49
34:RA:1045:A:H5''	34:RA:1046:A:H5'	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:1510:A:O2'	34:RA:1512:G:N7	2.44	0.49
34:RA:2047:U:H2'	34:RA:2048:G:H8	1.77	0.49
41:RI:124:GLY:H	41:RI:142:VAL:HG13	1.78	0.49
45:RQ:52:VAL:HG13	54:RZ:183:LEU:HD13	1.95	0.49
1:XA:256:U:OP1	17:XQ:17:LYS:NZ	2.43	0.49
1:XA:266:G:H5'	1:XA:268:C:H41	1.77	0.49
1:XA:1255:G:O2'	1:XA:1258:G:N3	2.39	0.49
10:XJ:9:ARG:HB2	10:XJ:95:GLU:HB3	1.93	0.49
34:YA:28:A:N6	34:YA:512:G:O2'	2.45	0.49
34:YA:2211:G:H21	34:YA:2212:A:H2	1.59	0.49
53:YY:29:GLU:HB3	53:YY:38:ILE:HD12	1.94	0.49
1:QA:1322:C:O2	1:QA:1322:C:H2'	2.11	0.49
1:QA:1355:G:H2'	1:QA:1356:G:H8	1.77	0.49
34:RA:1678:G:H22	34:RA:1989:G:N2	2.10	0.49
42:RN:114:ARG:NH1	42:RN:114:ARG:HG2	2.27	0.49
43:RO:104:ARG:NH1	43:RO:121:VAL:O	2.45	0.49
1:XA:1296:C:OP1	13:XM:44:ARG:NH2	2.42	0.49
3:XC:11:ARG:NH2	3:XC:177:THR:O	2.34	0.49
10:XJ:44:VAL:HG11	10:XJ:46:ARG:HH21	1.77	0.49
34:YA:270(M):U:OP2	41:YI:50:ARG:NH1	2.46	0.49
34:YA:1491:G:H2'	34:YA:1492:G:H8	1.77	0.49
34:YA:2081:C:H2'	34:YA:2082:A:H8	1.76	0.49
34:YA:2468:G:O2'	34:YA:2481:G:N2	2.46	0.49
1:QA:522:C:H41	12:QL:53:ARG:HH22	1.60	0.49
13:QM:22:ILE:HB	13:QM:25:ILE:HB	1.95	0.49
49:RU:109:LEU:HD23	50:RV:47:VAL:HG21	1.93	0.49
1:XA:28:G:O2'	1:XA:296:U:OP1	2.29	0.49
25:Y1:6:GLU:HB3	25:Y1:91:LYS:HD2	1.94	0.49
27:Y3:3:ARG:CG	27:Y3:59:VAL:HB	2.43	0.49
34:YA:2311:A:H1'	39:YG:82:LEU:HD11	1.94	0.49
1:QA:745:C:OP1	1:QA:851:G:O2'	2.30	0.49
30:R6:37:ARG:HA	30:R6:48:VAL:HA	1.93	0.49
51:RW:92:ARG:NH1	51:RW:94:ASP:OD1	2.46	0.49
1:XA:347:G:H1'	1:XA:348:G:H5'	1.94	0.49
1:XA:1068:G:OP1	1:XA:1387:G:O2'	2.31	0.49
13:XM:7:VAL:HG23	39:YG:115:ARG:HH22	1.77	0.49
31:Y7:7:PRO:HB2	34:YA:1309:G:H4'	1.94	0.49
34:YA:458:G:O2'	34:YA:469:G:O6	2.30	0.49
34:YA:2125:G:O2'	34:YA:2173:A:N6	2.46	0.49
34:YA:2154:G:H2'	34:YA:2155:G:H8	1.78	0.49
34:YA:2185:C:H2'	34:YA:2186:G:H8	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:2438:U:O2'	34:YA:2440:C:OP1	2.28	0.49
44:YP:80:TYR:HE1	44:YP:111:ARG:HD2	1.78	0.49
1:QA:562:C:H1'	12:QL:15:ARG:HD2	1.94	0.49
1:QA:867:G:O2'	1:QA:873:A:N1	2.44	0.49
2:QB:137:ARG:HG3	2:QB:138:LEU:HD12	1.95	0.49
12:QL:49:ASN:ND2	12:QL:92:ASP:OD2	2.43	0.49
34:RA:589:C:H2'	34:RA:590:A:C8	2.48	0.49
36:RD:5:LYS:HG2	36:RD:17:THR:HG22	1.95	0.49
37:RE:57:LYS:HA	37:RE:57:LYS:HE3	1.95	0.49
39:RG:23:PHE:HE2	39:RG:168:GLU:HA	1.78	0.49
41:RI:1:MET:N	41:RI:21:VAL:O	2.38	0.49
1:XA:8:A:N6	4:XD:208:SER:O	2.45	0.49
34:YA:1826:G:O2'	36:YD:242:ARG:NH2	2.44	0.49
34:YA:1952:A:N3	34:YA:2560:C:O2'	2.41	0.49
34:YA:2495:G:H5''	45:YQ:81:VAL:HG12	1.95	0.49
34:YA:2707:G:H2'	34:YA:2708:G:H8	1.78	0.49
1:QA:397:A:N7	1:QA:547:A:O2'	2.46	0.49
1:QA:1322:C:OP2	19:QS:78:ARG:CZ	2.61	0.49
1:QA:1386:G:H2'	1:QA:1387:G:H8	1.78	0.49
34:RA:1066:U:O2'	34:RA:1068:G:OP2	2.23	0.49
34:RA:1769:G:O2'	34:RA:1958:C:OP1	2.30	0.49
37:RE:10:GLY:HA3	48:RT:8:LYS:HD3	1.95	0.49
40:RH:103:LEU:HD22	40:RH:105:LEU:HD23	1.95	0.49
11:XK:86:GLY:O	11:XK:91:ARG:NH1	2.43	0.49
33:Y9:22:ARG:HH12	34:YA:2741:A:H5''	1.78	0.49
34:YA:181:A:H1'	34:YA:435:C:H5'	1.95	0.49
34:YA:839:U:H1'	34:YA:1191:G:H1'	1.93	0.49
1:QA:1005:A:OP2	1:QA:1006:C:N4	2.46	0.48
1:QA:1342:C:H2'	1:QA:1343:G:C8	2.47	0.48
4:QD:64:LEU:HB2	4:QD:198:VAL:HG11	1.95	0.48
9:QI:28:VAL:HG22	9:QI:63:ILE:HB	1.94	0.48
9:QI:117:HIS:HE1	9:QI:123:PRO:HB3	1.77	0.48
34:RA:2646:C:OP2	34:RA:2732:G:O2'	2.27	0.48
36:RD:142:VAL:HG23	36:RD:193:VAL:HA	1.94	0.48
37:RE:38:THR:OG1	37:RE:40:GLU:OE1	2.30	0.48
39:RG:120:LEU:HB2	39:RG:180:PHE:HA	1.95	0.48
1:XA:923:A:O2'	1:XA:1399:C:OP2	2.27	0.48
12:XL:84:LEU:HD22	12:XL:104:VAL:HG21	1.95	0.48
34:YA:27:G:N2	34:YA:513:A:OP2	2.46	0.48
34:YA:265:A:N1	34:YA:427:U:O2'	2.40	0.48
34:YA:1882:C:H3'	34:YA:1883:G:H8	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:YT:77:PRO:HB2	48:YT:80:SER:HB2	1.95	0.48
1:QA:991:U:O4	1:QA:1212:U:O2'	2.28	0.48
34:RA:1288:U:O3'	34:RA:1647:G:N2	2.46	0.48
34:RA:2844:G:H3'	34:RA:2845:G:H8	1.78	0.48
36:RD:108:PRO:HD2	36:RD:111:LEU:HD22	1.94	0.48
1:XA:1123:A:H4'	10:XJ:36:GLY:HA3	1.95	0.48
1:XA:1500:A:H5''	1:XA:1508:G:H5''	1.95	0.48
3:XC:81:GLY:O	3:XC:85:ARG:CG	2.61	0.48
13:XM:93:ARG:HH21	34:YA:887:A:H5'	1.78	0.48
34:YA:918:A:N3	35:YB:80:U:O2'	2.44	0.48
1:QA:662:G:O2'	1:QA:836:G:OP1	2.28	0.48
15:QO:8:LYS:HG3	15:QO:31:LEU:HD11	1.95	0.48
48:RT:112:ARG:CG	48:RT:112:ARG:NH1	2.73	0.48
50:RV:51:VAL:C	50:RV:53:GLU:N	2.70	0.48
17:XQ:15:MET:HE1	17:XQ:43:LEU:HD22	1.94	0.48
34:YA:837:C:N3	34:YA:941:A:N6	2.61	0.48
36:YD:125:ILE:N	36:YD:125:ILE:CD1	2.76	0.48
38:YF:101:LEU:HD23	38:YF:106:ARG:HG2	1.94	0.48
45:YQ:28:ALA:HB3	45:YQ:67:ARG:HH12	1.78	0.48
3:QC:58:GLU:HB3	3:QC:65:ALA:HB3	1.95	0.48
4:QD:133:VAL:HG12	4:QD:135:LEU:H	1.77	0.48
34:RA:24:G:O2'	51:RW:78:GLU:O	2.30	0.48
34:RA:265:A:N6	34:RA:427:U:O2'	2.47	0.48
34:RA:630:G:N2	34:RA:633:A:OP2	2.39	0.48
34:RA:1800:C:N4	34:RA:1817:G:H22	2.11	0.48
36:RD:182:LEU:H	36:RD:272:ALA:HB3	1.78	0.48
40:RH:109:PHE:CZ	40:RH:152:ARG:HD2	2.49	0.48
1:XA:277:C:H5''	17:XQ:68:ARG:HH21	1.78	0.48
1:XA:452:A:N6	1:XA:480:U:H3	2.06	0.48
3:XC:130:VAL:HG21	3:XC:157:ILE:HG23	1.96	0.48
36:YD:77:ALA:HB3	36:YD:117:VAL:HG13	1.95	0.48
1:QA:279:A:OP2	17:QQ:95:TYR:OH	2.29	0.48
1:QA:1127:G:N2	1:QA:1145:C:O2	2.40	0.48
9:QI:8:GLY:O	9:QI:15:ALA:N	2.45	0.48
10:QJ:8:LEU:HB3	10:QJ:16:LEU:HD11	1.96	0.48
34:RA:71:A:H62	34:RA:114:U:H1'	1.79	0.48
34:RA:918:A:N3	35:RB:80:U:O2'	2.42	0.48
39:RG:29:TRP:O	39:RG:33:ARG:NH1	2.45	0.48
39:RG:83:ARG:NH1	39:RG:83:ARG:CG	2.77	0.48
43:RO:12:ASP:HB3	43:RO:98:VAL:HG12	1.96	0.48
49:RU:92:ARG:CG	49:RU:95:LEU:HD23	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:RU:94:ASN:C	49:RU:96:ALA:H	2.21	0.48
1:XA:356:A:N3	1:XA:368:U:O2'	2.40	0.48
34:YA:1113:U:H2'	34:YA:1114:G:C8	2.49	0.48
34:YA:2047:U:H2'	34:YA:2048:G:H8	1.77	0.48
34:YA:2315:G:OP1	39:YG:36:LYS:NZ	2.39	0.48
34:YA:2647:U:O2	34:YA:2673:G:O6	2.32	0.48
41:YL:30:LEU:HB3	41:YL:36:ALA:HB3	1.96	0.48
1:QA:521:G:HO2'	1:QA:536:C:HO2'	1.58	0.48
20:QT:100:ILE:HG13	20:QT:102:GLY:H	1.78	0.48
34:RA:9:U:OP1	42:RN:115:ARG:NH2	2.46	0.48
34:RA:2495:G:H5''	45:RQ:81:VAL:HG12	1.95	0.48
54:RZ:69:THR:HG22	54:RZ:90:VAL:HG22	1.95	0.48
1:XA:1243:C:OP2	21:XU:10:ARG:NH2	2.47	0.48
4:XD:88:VAL:HG12	5:XE:97:GLY:HA3	1.94	0.48
3:QC:150:LYS:HB3	3:QC:201:TYR:HB2	1.95	0.48
34:RA:1485:G:H1	34:RA:1504:C:H42	1.60	0.48
35:RB:102:G:N3	54:RZ:73:GLN:NE2	2.54	0.48
37:RE:21:VAL:HG23	37:RE:185:LYS:HE3	1.94	0.48
1:XA:559:A:H4'	1:XA:560:U:H3'	1.95	0.48
1:XA:1187:G:H4'	9:XI:111:ARG:HH21	1.79	0.48
12:XL:114:LYS:O	12:XL:117:ARG:NH1	2.46	0.48
22:XV:37:T6A:HN1	22:XV:38:A:H1'	1.79	0.48
39:YG:5:VAL:HG11	39:YG:100:TRP:HB3	1.96	0.48
48:YT:50:ILE:HD11	48:YT:100:TYR:HA	1.95	0.48
1:QA:619:U:N3	4:QD:134:ASP:OD1	2.39	0.48
1:QA:963:G:H21	10:QJ:55:LYS:HE3	1.78	0.48
1:QA:1323:G:N2	1:QA:1361:G:O2'	2.47	0.48
1:QA:1492:A:OP1	12:QL:47:LYS:HG3	2.13	0.48
11:QK:34:ASP:OD1	11:QK:38:ASN:N	2.47	0.48
34:RA:514:A:N3	34:RA:581:C:O2'	2.41	0.48
34:RA:2441:C:OP2	34:RA:2586:C:O2'	2.30	0.48
45:RQ:24:GLY:H	45:RQ:101:ARG:HD2	1.79	0.48
45:RQ:103:MET:HE1	45:RQ:127:ILE:HD11	1.96	0.48
1:XA:165:C:H2'	1:XA:166:G:H8	1.79	0.48
1:XA:1141:C:H2'	1:XA:1142:G:H8	1.78	0.48
45:YQ:75:THR:HG21	45:YQ:85:LYS:HE3	1.96	0.48
1:QA:1250:A:H2	1:QA:1370:G:H1'	1.79	0.48
2:QB:8:LYS:HG3	2:QB:10:LEU:H	1.79	0.48
12:QL:113:ARG:HH21	12:QL:116:SER:HB2	1.78	0.48
32:R8:27:THR:HB	34:RA:2361:A:P	2.54	0.48
34:RA:679:C:H2'	34:RA:680:G:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:1316:U:H2'	34:RA:1317:A:H8	1.79	0.48
39:RG:106:LEU:HA	39:RG:110:ALA:HB3	1.95	0.48
44:RP:18:ARG:HE	44:RP:21:ARG:HG3	1.78	0.48
45:RQ:8:LYS:HA	54:RZ:197:ILE:HB	1.96	0.48
50:RV:52:VAL:C	50:RV:54:GLY:H	2.22	0.48
30:Y6:21:TYR:OH	30:Y6:39:TYR:O	2.32	0.48
34:YA:589:C:H2'	34:YA:590:A:C8	2.48	0.48
34:YA:617:G:OP1	38:YF:40:GLN:NE2	2.47	0.48
2:QB:6:THR:O	2:QB:217:ARG:NH1	2.47	0.48
34:RA:83:G:O2'	34:RA:102:G:N2	2.46	0.48
36:RD:247:ALA:HA	36:RD:253:GLN:HA	1.96	0.48
48:RT:102:ILE:HB	48:RT:110:ILE:CD1	2.42	0.48
34:YA:679:C:H2'	34:YA:680:G:H8	1.78	0.48
36:YD:108:PRO:HD2	36:YD:111:LEU:HD22	1.95	0.48
38:YF:198:ALA:HA	38:YF:201:VAL:HG12	1.95	0.48
39:YG:83:ARG:C	39:YG:85:GLY:N	2.70	0.48
40:YH:3:ARG:HH21	40:YH:5:GLY:H	1.59	0.48
1:QA:618:C:H5'	1:QA:619:U:H5''	1.96	0.47
3:QC:84:ILE:HG23	3:QC:85:ARG:HD2	1.95	0.47
6:QF:9:VAL:HB	6:QF:87:ARG:HB2	1.95	0.47
11:QK:62:GLN:HG3	11:QK:97:ALA:HB2	1.96	0.47
17:QQ:15:MET:HE1	17:QQ:43:LEU:HD22	1.96	0.47
28:R4:26:SER:OG	28:R4:27:THR:N	2.47	0.47
34:RA:550:G:H2'	34:RA:551:G:H8	1.80	0.47
34:RA:1449:A:O2'	34:RA:1530:G:N2	2.45	0.47
34:RA:1972:A:H2'	34:RA:1973:G:H8	1.79	0.47
34:RA:2791:C:H4'	34:RA:2792:G:H5'	1.96	0.47
41:RI:125:GLU:OE1	41:RI:141:LYS:HG2	2.14	0.47
3:XC:190:ARG:HA	3:XC:195:VAL:HG22	1.95	0.47
34:YA:81:G:HO2'	34:YA:295:G:HO2'	1.60	0.47
34:YA:574:C:N3	37:YE:145:LYS:NZ	2.62	0.47
42:YN:14:VAL:HG21	42:YN:33:LEU:HD23	1.96	0.47
49:YU:91:ASP:OD1	49:YU:96:ALA:HA	2.13	0.47
1:QA:28:G:O2'	1:QA:296:U:OP1	2.32	0.47
1:QA:1343:G:H4'	9:QI:122:ALA:HB3	1.95	0.47
9:QI:85:LEU:HD11	9:QI:96:LEU:HD11	1.95	0.47
34:RA:672:C:OP2	44:RP:42:SER:OG	2.31	0.47
34:RA:1278:A:H2'	34:RA:1279:G:C8	2.49	0.47
40:RH:12:PRO:HG3	40:RH:48:GLY:O	2.13	0.47
40:RH:24:VAL:HG13	40:RH:37:VAL:HG21	1.96	0.47
41:RI:9:LEU:HD13	41:RI:9:LEU:HA	1.70	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:XY:28:G:H2'	55:XY:29:G:H8	1.79	0.47
34:YA:59:U:H3	34:YA:68:G:H1	1.63	0.47
34:YA:151:C:H2'	34:YA:152:G:H8	1.79	0.47
34:YA:764:A:N3	36:YD:213:ARG:NH1	2.61	0.47
43:YO:87:ILE:HD12	43:YO:91:LEU:HA	1.96	0.47
1:QA:1189:C:C5'	3:QC:5:ILE:HD13	2.33	0.47
1:QA:1368:G:O2'	10:QJ:46:ARG:NH2	2.47	0.47
2:QB:87:ARG:NH1	2:QB:220:ASP:OD1	2.47	0.47
3:QC:172:ARG:HG2	3:QC:174:PRO:HD3	1.96	0.47
5:QE:79:GLU:HG2	8:QH:104:ARG:HH11	1.78	0.47
5:QE:107:ARG:O	5:QE:111:GLU:HB2	2.13	0.47
34:RA:219:G:N3	34:RA:234:C:O2'	2.47	0.47
34:RA:837:C:N3	34:RA:941:A:N6	2.61	0.47
34:RA:2118:U:O2	34:RA:2148:G:O2'	2.31	0.47
36:RD:146:GLU:HB2	36:RD:189:CYS:HB3	1.97	0.47
38:RF:113:ALA:HB2	38:RF:183:VAL:HG23	1.96	0.47
1:XA:1510:U:H2'	1:XA:1511:G:C8	2.48	0.47
34:YA:303:U:H2'	34:YA:304:G:H8	1.78	0.47
34:YA:443:A:H2'	38:YF:45:ARG:HH12	1.79	0.47
34:YA:704:G:O2'	34:YA:726:G:N2	2.47	0.47
34:YA:1791:A:N6	34:YA:1828:G:O2'	2.39	0.47
34:YA:2521:C:O2'	34:YA:2564:A:N3	2.44	0.47
1:QA:34:C:H2'	1:QA:35:G:H8	1.78	0.47
1:QA:346:G:H1'	1:QA:347:G:H5'	1.96	0.47
1:QA:501:C:H2'	1:QA:502:G:C8	2.49	0.47
1:QA:1510:U:H2'	1:QA:1511:G:H8	1.79	0.47
2:QB:77:ALA:HB2	2:QB:211:ILE:HD13	1.96	0.47
34:RA:807:U:OP2	44:RP:41:ARG:NH1	2.48	0.47
34:RA:2627:G:N2	34:RA:2777:G:OP2	2.44	0.47
37:RE:201:THR:HG22	37:RE:203:LYS:H	1.78	0.47
45:RQ:31:ASP:OD1	54:RZ:122:ARG:NH2	2.46	0.47
5:XE:12:LEU:HB3	5:XE:31:LEU:HB3	1.96	0.47
34:YA:1678:G:N2	34:YA:1989:G:H22	2.13	0.47
54:YZ:47:VAL:O	54:YZ:51:ALA:N	2.47	0.47
25:R1:78:LYS:HD3	34:RA:270(S):G:H1'	1.97	0.47
29:R5:4:HIS:O	34:RA:2056:G:N2	2.47	0.47
32:R8:25:MET:HE2	44:RP:64:LYS:CG	2.44	0.47
34:RA:1478:G:H2'	34:RA:1479:G:H8	1.80	0.47
39:RG:38:VAL:HB	39:RG:158:ALA:HB3	1.97	0.47
43:RO:25:LEU:HB2	43:RO:38:VAL:HG13	1.95	0.47
43:RO:87:ILE:HD12	43:RO:91:LEU:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:419:C:OP1	1:XA:513:C:O2'	2.32	0.47
34:YA:956:G:OP2	45:YQ:14:ARG:NH2	2.48	0.47
34:YA:2140:C:H2'	34:YA:2141:G:H8	1.79	0.47
34:YA:2308:G:C2	39:YG:80:PHE:HZ	2.32	0.47
39:YG:82:LEU:HD23	39:YG:82:LEU:N	2.28	0.47
1:QA:861:G:HO2'	1:QA:874:G:HO2'	1.60	0.47
9:QI:116:LYS:HE3	9:QI:120:ARG:HA	1.95	0.47
44:RP:107:LYS:NZ	44:RP:107:LYS:CB	2.73	0.47
4:XD:98:GLU:HG2	4:XD:189:PRO:HG3	1.95	0.47
34:YA:822:U:H2'	34:YA:823:G:H8	1.80	0.47
34:YA:867:C:N3	34:YA:912:C:O2'	2.43	0.47
34:YA:2692:C:H2'	34:YA:2693:A:H8	1.79	0.47
36:YD:121:PRO:HB3	36:YD:135:PHE:HE2	1.76	0.47
39:YG:71:THR:N	39:YG:89:GLY:O	2.46	0.47
43:YO:25:LEU:HB2	43:YO:38:VAL:HG13	1.96	0.47
1:QA:401:C:OP2	4:QD:73:ARG:NH1	2.48	0.47
1:QA:714:G:H2'	1:QA:715:A:C8	2.49	0.47
1:QA:979:C:OP1	1:QA:1223:C:N4	2.48	0.47
1:QA:1356:G:H2'	1:QA:1357:A:C8	2.49	0.47
19:QS:53:ASN:ND2	19:QS:76:PRO:O	2.45	0.47
34:RA:180:G:N1	34:RA:214:G:N7	2.54	0.47
34:RA:728:G:H5''	36:RD:13:ARG:HH21	1.79	0.47
36:RD:26:LYS:NZ	36:RD:28:GLU:O	2.41	0.47
48:RT:120:ARG:HA	48:RT:123:GLN:HB2	1.95	0.47
51:RW:111:HIS:CD2	51:RW:113:LYS:H	2.32	0.47
53:RY:14:LEU:HB2	53:RY:75:ILE:HD11	1.97	0.47
1:XA:21:G:H2'	1:XA:22:G:C8	2.50	0.47
1:XA:359:U:H2'	1:XA:360:A:C8	2.49	0.47
1:XA:715:A:H2'	1:XA:716:A:C8	2.49	0.47
3:XC:150:LYS:HG3	3:XC:169:ALA:HB2	1.97	0.47
11:XK:21:ILE:HB	11:XK:84:VAL:HG12	1.96	0.47
27:Y3:5:LYS:HG2	27:Y3:57:GLU:HB3	1.97	0.47
34:YA:83:G:O2'	34:YA:102:G:N2	2.47	0.47
34:YA:1571:A:H2'	34:YA:1572:A:H8	1.80	0.47
36:YD:143:HIS:ND1	36:YD:194:GLY:O	2.43	0.47
39:YG:19:LEU:HD13	39:YG:32:PRO:HD2	1.96	0.47
48:YT:26:ASP:HB2	48:YT:91:ARG:HA	1.96	0.47
49:YU:90:VAL:HG11	50:YV:40:LEU:HG	1.97	0.47
52:YX:54:VAL:HG22	52:YX:81:VAL:HG23	1.95	0.47
1:QA:323:U:OP1	20:QT:26:ASN:ND2	2.45	0.47
3:QC:47:LEU:HD22	3:QC:76:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:R1:97:LEU:HD22	34:RA:270(T):G:H5''	1.96	0.47
27:R3:40:THR:HG22	27:R3:42:ALA:H	1.80	0.47
34:RA:679:C:H2'	34:RA:680:G:H8	1.79	0.47
36:RD:121:PRO:CB	36:RD:135:PHE:CE2	2.75	0.47
36:RD:199:ALA:C	36:RD:201:HIS:N	2.73	0.47
10:XJ:57:LYS:HE2	10:XJ:60:ARG:HH22	1.80	0.47
34:YA:1972:A:H2'	34:YA:1973:G:H8	1.80	0.47
34:YA:2069:G:N1	34:YA:2443:C:N3	2.63	0.47
34:YA:2500:U:O2'	34:YA:2504:U:OP1	2.29	0.47
43:YO:120:GLU:OE1	48:YT:67:SER:OG	2.32	0.47
34:RA:1278:A:H2'	34:RA:1279:G:H8	1.79	0.47
34:RA:1830:C:H2'	34:RA:1831:G:H8	1.80	0.47
38:RF:40:GLN:HE22	38:RF:182:ASN:HB2	1.79	0.47
1:XA:939:G:H21	1:XA:1374:A:H61	1.62	0.47
1:XA:1209:C:O2'	1:XA:1214:C:N4	2.44	0.47
13:XM:75:ALA:HA	13:XM:78:ILE:HG12	1.96	0.47
16:XP:5:ARG:NH2	16:XP:27:LYS:O	2.48	0.47
34:YA:1278:A:H2'	34:YA:1279:G:H8	1.80	0.47
34:YA:1954:G:O2'	34:YA:1956:U:O4	2.31	0.47
34:YA:2646:C:OP2	34:YA:2732:G:O2'	2.27	0.47
39:YG:37:VAL:HG22	39:YG:159:VAL:HG12	1.96	0.47
48:YT:19:LEU:HD22	48:YT:86:ILE:HG22	1.96	0.47
1:QA:269:C:H2'	1:QA:270:A:H8	1.80	0.47
1:QA:362:G:N2	1:QA:365:U:OP2	2.46	0.47
1:QA:521:G:O2'	1:QA:536:C:O2'	2.31	0.47
7:QG:88:PRO:HG2	7:QG:152:ALA:HB2	1.97	0.47
34:RA:2052:G:H4'	37:RE:143:ASN:H	1.78	0.47
41:RI:80:PRO:HB2	41:RI:146:ALA:HB2	1.97	0.47
41:RI:120:ILE:CD1	41:RI:126:TYR:CD2	2.98	0.47
41:RI:123:LEU:HD12	41:RI:123:LEU:N	2.02	0.47
1:XA:636:U:H5'	17:XQ:2:PRO:HG3	1.96	0.47
1:XA:1366:C:O2'	10:XJ:60:ARG:NH1	2.48	0.47
12:XL:77:LEU:HD21	12:XL:107:ALA:HB2	1.97	0.47
34:YA:270(N):G:O4'	41:YI:50:ARG:NH2	2.48	0.47
34:YA:743:G:O2'	34:YA:1659:U:OP1	2.29	0.47
34:YA:900:A:H3'	34:YA:901:A:H8	1.80	0.47
34:YA:1231:G:H2'	34:YA:1232:G:H8	1.79	0.47
34:YA:1441:G:H2'	34:YA:1442:G:H8	1.79	0.47
34:YA:1664:A:H61	34:YA:1996:C:H42	1.63	0.47
44:YP:71:VAL:HG13	44:YP:72:PRO:HA	1.97	0.47
48:YT:35:LYS:HE3	48:YT:38:ASN:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:YZ:5:LEU:HD11	54:YZ:44:PHE:HA	1.97	0.47
54:YZ:53:ILE:C	54:YZ:55:HIS:N	2.72	0.47
1:QA:578:C:O2'	1:QA:728:A:N3	2.42	0.46
2:QB:198:ASP:OD1	8:QH:68:ARG:NH1	2.43	0.46
31:R7:8:ASN:HB3	31:R7:11:LYS:HB3	1.97	0.46
34:RA:839:U:H1'	34:RA:1191:G:H1'	1.97	0.46
34:RA:1508:A:O2'	34:RA:1509:C:O4'	2.33	0.46
34:RA:2696:U:H2'	34:RA:2697:G:C8	2.50	0.46
39:RG:135:LEU:HD13	39:RG:140:ILE:HD11	1.95	0.46
48:RT:111:ARG:C	48:RT:113:LYS:N	2.70	0.46
50:RV:47:VAL:O	50:RV:47:VAL:HG13	2.13	0.46
14:YN:27:CYS:SG	14:YN:28:GLY:N	2.88	0.46
34:YA:554:U:H2'	34:YA:556:G:C8	2.50	0.46
34:YA:952:G:OP1	45:YQ:16:ARG:NH1	2.48	0.46
34:YA:1228:G:OP2	49:YU:16:LYS:NZ	2.39	0.46
34:YA:1769:G:O2'	34:YA:1958:C:OP1	2.32	0.46
42:YN:6:PRO:HG3	42:YN:41:ASP:HB2	1.96	0.46
45:YQ:111:GLU:OE1	45:YQ:133:ARG:NH2	2.48	0.46
48:YT:120:ARG:HA	48:YT:123:GLN:CD	2.39	0.46
34:RA:2375:G:N2	34:RA:2378:A:OP2	2.41	0.46
40:RH:146:ALA:O	40:RH:150:ALA:HB3	2.15	0.46
41:RI:30:LEU:HB3	41:RI:36:ALA:HB3	1.97	0.46
4:XD:166:LYS:HB2	4:XD:178:VAL:HG11	1.98	0.46
8:XH:34:GLU:OE1	8:XH:37:ARG:NH2	2.48	0.46
31:Y7:13:ALA:HB2	31:Y7:46:VAL:HG11	1.97	0.46
33:Y9:16:VAL:HG22	33:Y9:25:VAL:HG22	1.97	0.46
34:YA:987:G:O2'	34:YA:1000:A:N3	2.37	0.46
34:YA:1103:A:H5'	34:YA:1104:C:H5	1.79	0.46
1:QA:56:U:H2'	1:QA:57:G:C8	2.51	0.46
34:RA:347:A:H2'	34:RA:348:G:H8	1.80	0.46
34:RA:402:A:N3	34:RA:406:G:O2'	2.46	0.46
34:RA:1636:C:H2'	34:RA:1637:A:C8	2.51	0.46
35:RB:28:C:H5''	47:RS:29:PHE:HE2	1.78	0.46
36:RD:148:GLU:HB2	36:RD:151:LYS:HD2	1.97	0.46
37:RE:74:PRO:HG2	37:RE:77:ILE:HG22	1.96	0.46
1:XA:125:U:O3'	1:XA:633:G:N2	2.49	0.46
1:XA:452:A:H2'	1:XA:453:A:H8	1.81	0.46
10:XJ:23:ILE:HD12	10:XJ:85:LEU:HD11	1.96	0.46
34:YA:1818:U:H2'	36:YD:157:ARG:HG2	1.96	0.46
34:YA:1824:G:N3	36:YD:254:THR:OG1	2.48	0.46
36:YD:26:LYS:NZ	36:YD:28:GLU:O	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:YW:111:HIS:HD2	51:YW:113:LYS:H	1.63	0.46
1:QA:1510:U:H2'	1:QA:1511:G:C8	2.50	0.46
4:QD:19:LEU:HD22	4:QD:67:ILE:HD11	1.98	0.46
34:RA:2416:C:O3'	44:RP:64:LYS:NZ	2.48	0.46
34:RA:2561:A:H4'	43:RO:40:VAL:HG11	1.98	0.46
2:XB:98:LEU:H	2:XB:101:MET:HE3	1.80	0.46
34:YA:1266:G:O5'	51:YW:15:ARG:NH2	2.48	0.46
34:YA:2630:G:H2'	34:YA:2631:G:H8	1.79	0.46
1:QA:673:G:H2'	1:QA:674:G:C8	2.50	0.46
1:QA:967:C:O2'	9:QI:125:TYR:OH	2.30	0.46
1:QA:985:C:H2'	1:QA:986:A:H8	1.79	0.46
1:QA:1309:G:N7	13:QM:99:ARG:NH2	2.63	0.46
13:QM:13:LYS:HD3	13:QM:44:ARG:HD3	1.98	0.46
33:R9:22:ARG:HH12	34:RA:2741:A:H5''	1.80	0.46
1:XA:675:A:H1'	11:XK:116:HIS:CD2	2.51	0.46
7:XG:35:LYS:HD3	7:XG:38:LEU:HD12	1.97	0.46
34:YA:270(R):G:H2'	34:YA:270(S):G:C8	2.50	0.46
34:YA:1819:A:H5''	36:YD:161:THR:HG21	1.98	0.46
41:YI:12:LEU:HD23	41:YI:12:LEU:HA	1.75	0.46
1:QA:824:C:H2'	1:QA:825:G:H8	1.80	0.46
34:RA:458:G:O2'	34:RA:469:G:O6	2.32	0.46
43:RO:120:GLU:OE1	48:RT:67:SER:OG	2.34	0.46
1:XA:335:C:O2'	1:XA:1433:A:N3	2.43	0.46
1:XA:405:U:O4	4:XD:2:GLY:N	2.49	0.46
1:XA:946:A:O2'	1:XA:1333:A:N3	2.43	0.46
13:XM:7:VAL:HG11	39:YG:139:LEU:HD13	1.98	0.46
34:YA:534:U:H5'	49:YU:42:ALA:HB1	1.98	0.46
34:YA:648:G:H2'	34:YA:649:G:H8	1.81	0.46
34:YA:2849:U:O4	48:YT:23:ARG:NH1	2.42	0.46
41:YI:92:VAL:CB	41:YI:120:ILE:CG2	2.77	0.46
41:YI:109:ILE:HB	41:YI:130:TYR:CZ	2.51	0.46
1:QA:159:G:O2'	1:QA:161:A:N7	2.45	0.46
1:QA:376:G:H5''	16:QP:5:ARG:HB2	1.97	0.46
1:QA:407:G:H2'	1:QA:408:A:C8	2.51	0.46
1:QA:946:A:H2'	1:QA:947:G:C8	2.51	0.46
1:QA:1033:G:H2'	1:QA:1034:G:H4'	1.98	0.46
1:QA:1105:A:H2'	1:QA:1106:G:H8	1.81	0.46
11:QK:58:PRO:HB2	11:QK:93:GLN:HG3	1.96	0.46
13:QM:3:ARG:HE	13:QM:9:ILE:HG21	1.80	0.46
34:RA:941:A:N3	34:RA:1190:G:O2'	2.48	0.46
38:RF:31:HIS:NE2	38:RF:35:GLU:OE2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:RH:84:SER:HB2	40:RH:133:VAL:O	2.16	0.46
40:RH:159:GLU:HG3	40:RH:171:LEU:HD11	1.97	0.46
1:XA:243:A:H4'	1:XA:244:U:H3'	1.97	0.46
1:XA:448:A:OP2	1:XA:485:G:N2	2.43	0.46
1:XA:1342:C:H2'	1:XA:1343:G:H8	1.79	0.46
1:XA:1491:G:H5'	12:XL:47:LYS:HE3	1.98	0.46
2:XB:105:PHE:HA	2:XB:108:ILE:HG22	1.98	0.46
34:YA:414:C:H2'	34:YA:415:A:C8	2.51	0.46
34:YA:2133:G:O2'	34:YA:2158:A:N1	2.48	0.46
34:YA:2405:G:O2'	34:YA:2411:A:N6	2.48	0.46
38:YF:167:ALA:HB1	38:YF:173:VAL:HG11	1.98	0.46
46:YR:24:GLN:HG3	46:YR:44:LEU:HD13	1.97	0.46
49:YU:62:ILE:HD11	49:YU:93:LYS:HD2	1.97	0.46
54:YZ:100:VAL:HG21	54:YZ:134:PRO:HG2	1.96	0.46
6:QF:1:MET:HE3	6:QF:66:GLU:HG2	1.97	0.46
24:R0:35:ASN:HD22	34:RA:2354:G:H4'	1.81	0.46
37:RE:63:LEU:O	37:RE:73:GLU:CD	2.59	0.46
40:RH:89:ILE:O	40:RH:129:THR:OG1	2.34	0.46
40:RH:101:ARG:HE	40:RH:117:PRO:HG2	1.81	0.46
1:XA:54:C:N4	1:XA:353:A:OP2	2.43	0.46
3:XC:9:GLY:HA2	3:XC:12:LEU:HG	1.97	0.46
5:XE:34:VAL:HG11	5:XE:63:ARG:HE	1.81	0.46
19:XS:63:THR:OG1	19:XS:65:ASN:OD1	2.34	0.46
1:QA:21:G:H2'	1:QA:22:G:C8	2.50	0.46
1:QA:922:G:H4'	5:QE:20:GLN:HA	1.98	0.46
34:RA:579:G:O2'	34:RA:2019:A:OP1	2.32	0.46
35:RB:8:U:O2	35:RB:112:G:N2	2.38	0.46
53:RY:102:CYS:SG	53:RY:103:GLY:N	2.89	0.46
1:XA:714:G:H2'	1:XA:715:A:C8	2.50	0.46
4:XD:62:GLN:HE22	4:XD:65:ARG:HH21	1.63	0.46
5:XE:91:LEU:HD13	5:XE:120:THR:HG22	1.98	0.46
17:XQ:18:THR:OG1	17:XQ:69:LYS:NZ	2.45	0.46
34:YA:1800:C:H42	34:YA:1817:G:N2	2.14	0.46
34:YA:2115:G:N2	34:YA:2164:C:OP2	2.48	0.46
52:YX:12:VAL:HB	52:YX:27:THR:HG23	1.98	0.46
54:YZ:70:LEU:HG	54:YZ:91:LEU:HD21	1.98	0.46
1:QA:1034:G:H2'	1:QA:1035:A:C8	2.51	0.46
18:QR:58:LEU:HD23	18:QR:62:GLU:HB3	1.98	0.46
19:QS:41:VAL:HG12	19:QS:43:GLU:H	1.81	0.46
36:RD:199:ALA:C	36:RD:201:HIS:H	2.24	0.46
39:RG:82:LEU:HD23	39:RG:82:LEU:HA	1.81	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	2.49	0.46
34:YA:75:G:H22	34:YA:111:A:H2	1.64	0.46
52:YX:55:ASN:HB2	52:YX:80:ILE:HG23	1.98	0.46
54:YZ:74:VAL:HG23	54:YZ:86:VAL:HG22	1.97	0.46
3:QC:131:ARG:NH2	3:QC:166:GLU:OE2	2.49	0.45
24:R0:21:LEU:HD21	24:R0:41:ARG:HH11	1.80	0.45
30:R6:21:TYR:OH	30:R6:39:TYR:O	2.34	0.45
32:R8:30:ARG:CZ	44:RP:62:LEU:HD12	2.45	0.45
34:RA:414:C:H2'	34:RA:415:A:H8	1.82	0.45
34:RA:1086:A:OP1	34:RA:1104:C:O2'	2.27	0.45
34:RA:1791:A:H3'	34:RA:1792:G:H8	1.80	0.45
1:XA:186:C:H5'	20:XT:78:ALA:HB1	1.97	0.45
1:XA:377:G:H2'	1:XA:378:G:H8	1.80	0.45
1:XA:452:A:H4'	16:XP:72:ARG:HH12	1.81	0.45
1:XA:957:U:H3	1:XA:960:U:H5''	1.81	0.45
1:XA:1342:C:H2'	1:XA:1343:G:C8	2.51	0.45
8:XH:97:VAL:HG21	8:XH:128:GLY:HA2	1.98	0.45
13:XM:40:ASN:HB2	13:XM:43:THR:HG23	1.97	0.45
19:XS:16:LEU:O	19:XS:20:LEU:HB2	2.16	0.45
27:Y3:2:PRO:HA	27:Y3:39:ASP:CB	2.45	0.45
34:YA:767:U:H2'	34:YA:768:G:H8	1.82	0.45
34:YA:1278:A:H2'	34:YA:1279:G:C8	2.52	0.45
34:YA:1571:A:H2'	34:YA:1572:A:C8	2.51	0.45
34:YA:2100:G:O6	34:YA:2189:U:O2	2.34	0.45
1:QA:677:U:O2	1:QA:777:A:O2'	2.33	0.45
7:QG:16:LEU:HD12	9:QI:44:VAL:HG23	1.98	0.45
34:RA:2010:G:H5''	51:RW:42:ARG:HB2	1.98	0.45
41:RI:9:LEU:CD2	41:RI:35:LEU:HD13	2.46	0.45
41:RI:80:PRO:HA	41:RI:143:SER:HB2	1.98	0.45
1:XA:398:C:H2'	1:XA:399:G:H8	1.81	0.45
1:XA:1129:C:O2	1:XA:1132:C:N4	2.50	0.45
1:XA:1137:C:O2'	1:XA:1138:G:N2	2.49	0.45
1:XA:1323:G:H2'	1:XA:1324:A:C8	2.51	0.45
1:XA:1423:G:H5'	43:YO:49:ARG:HH12	1.79	0.45
3:XC:39:ILE:HD12	3:XC:91:LEU:HD22	1.97	0.45
12:XL:49:ASN:ND2	12:XL:92:ASP:OD2	2.48	0.45
23:XX:-14:G:H2'	23:XX:-13:G:C8	2.52	0.45
1:QA:390:C:H2'	1:QA:391:G:C8	2.51	0.45
34:RA:390:A:H4'	34:RA:391:G:H5'	1.98	0.45
34:RA:1105:U:H2'	34:RA:1106:G:H8	1.81	0.45
34:RA:1815:A:OP2	36:RD:54:ARG:NH2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:RG:73:ALA:HB1	39:RG:82:LEU:HD13	1.99	0.45
40:RH:9:ILE:CG2	40:RH:50:VAL:O	2.64	0.45
45:RQ:75:THR:HG21	45:RQ:85:LYS:HE3	1.97	0.45
47:RS:66:ALA:HA	47:RS:69:VAL:HG12	1.98	0.45
1:XA:309:G:H2'	1:XA:310:G:H8	1.81	0.45
5:XE:35:GLY:HA3	5:XE:112:LEU:HB3	1.97	0.45
9:XI:28:VAL:HA	9:XI:63:ILE:HB	1.97	0.45
16:XP:67:THR:O	16:XP:71:ARG:N	2.44	0.45
26:Y2:65:ASN:ND2	34:YA:72:U:O4	2.48	0.45
34:YA:483:A:O2'	53:YY:49:VAL:O	2.33	0.45
34:YA:704:G:H1'	34:YA:727:A:H61	1.80	0.45
34:YA:776:G:N7	34:YA:793:A:O2'	2.49	0.45
34:RA:985:C:H2'	34:RA:986:C:H6	1.80	0.45
34:RA:1824:G:N3	36:RD:254:THR:OG1	2.49	0.45
1:XA:45:U:H2'	1:XA:46:G:H8	1.80	0.45
20:XT:62:LEU:HA	20:XT:65:LYS:HB2	1.98	0.45
40:YH:21:PRO:O	40:YH:23:ARG:NH1	2.49	0.45
43:YO:97:ARG:H	43:YO:117:LEU:HD13	1.81	0.45
51:YW:86:LEU:HD22	51:YW:96:ILE:HD11	1.97	0.45
1:QA:272:C:H2'	1:QA:273:A:H8	1.82	0.45
1:QA:546:G:H4'	1:QA:548:G:H4'	1.99	0.45
1:QA:715:A:H2'	1:QA:716:A:C8	2.51	0.45
1:QA:1376:U:OP1	7:QG:94:ARG:NH1	2.48	0.45
34:RA:17:G:HO2'	49:RU:25:TRP:CD1	2.35	0.45
34:RA:605:C:O2	34:RA:657:U:O2'	2.34	0.45
34:RA:2229:C:H2'	34:RA:2230:G:H8	1.81	0.45
34:RA:2328:A:H2'	34:RA:2329:G:H8	1.79	0.45
43:RO:104:ARG:HH11	43:RO:121:VAL:HG12	1.81	0.45
49:RU:108:GLU:OE1	50:RV:47:VAL:HG11	2.17	0.45
1:XA:748:C:H1'	1:XA:749:C:H5	1.80	0.45
1:XA:1060:C:H2'	1:XA:1061:G:H8	1.82	0.45
9:XI:50:LEU:HD22	9:XI:81:ILE:HG21	1.98	0.45
18:XR:70:ILE:O	18:XR:74:ARG:HB2	2.16	0.45
34:YA:971:C:O2'	34:YA:983:A:N3	2.39	0.45
35:YB:23:G:H2'	35:YB:24:G:C5	2.51	0.45
22:QV:22:G:H2'	22:QV:23:A:H8	1.82	0.45
24:R0:39:ARG:HH21	34:RA:2355:C:H1'	1.82	0.45
34:RA:576:U:H2'	34:RA:577:G:C8	2.51	0.45
35:RB:24:G:H1'	35:RB:27:C:H41	1.82	0.45
36:RD:145:VAL:HB	36:RD:155:LEU:HB2	1.98	0.45
41:RI:9:LEU:HD21	41:RI:35:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:RP:52:GLU:OE2	44:RP:58:THR:OG1	2.33	0.45
1:XA:34:C:H2'	1:XA:35:G:C8	2.51	0.45
1:XA:707:C:OP1	11:XK:85:ARG:NH1	2.48	0.45
1:XA:718:G:O6	18:XR:74:ARG:NH1	2.50	0.45
1:XA:1240:U:OP1	7:XG:119:ARG:NH2	2.49	0.45
31:Y7:47:ARG:HH12	52:YX:60:ARG:HH22	1.62	0.45
34:YA:576:U:H2'	34:YA:577:G:C8	2.52	0.45
34:YA:2074:U:H2'	34:YA:2075:U:C6	2.51	0.45
50:YV:24:LYS:HA	50:YV:92:THR:HG23	1.98	0.45
1:QA:1113:C:H4'	3:QC:14:ILE:HG13	1.99	0.45
2:QB:93:VAL:HG11	2:QB:97:TRP:HD1	1.81	0.45
3:QC:77:ILE:HD12	3:QC:84:ILE:HG21	1.98	0.45
34:RA:1153:C:H5'	49:RU:76:TYR:HE2	1.81	0.45
34:RA:1470:G:O2'	34:RA:1522:G:O6	2.33	0.45
34:RA:1952:A:N3	34:RA:2560:C:O2'	2.40	0.45
34:RA:2008:C:H2'	34:RA:2009:G:H8	1.82	0.45
34:RA:2659:G:N2	34:RA:2662:A:OP2	2.50	0.45
45:RQ:137:TYR:HD1	54:RZ:74:VAL:HG11	1.81	0.45
46:RR:33:ARG:HD3	46:RR:113:LEU:HD11	1.99	0.45
1:XA:662:G:O2'	1:XA:836:G:OP1	2.35	0.45
1:XA:769:G:H4'	1:XA:1513:A:H4'	1.99	0.45
34:YA:1826:G:OP1	36:YD:224:ALA:N	2.50	0.45
49:YU:74:LEU:HD21	49:YU:110:VAL:HG13	1.98	0.45
1:QA:143:A:H2	1:QA:220:G:H1	1.64	0.45
1:QA:1030:C:O2'	1:QA:1031:G:O4'	2.34	0.45
2:QB:51:LEU:HD23	2:QB:201:ILE:HD12	1.98	0.45
16:QP:34:GLU:OE2	16:QP:55:ARG:NH2	2.47	0.45
24:R0:67:VAL:HG22	24:R0:81:VAL:HG22	1.97	0.45
34:RA:1732:A:H3'	34:RA:1733:G:H8	1.81	0.45
34:RA:2123:G:H2'	34:RA:2124:G:H8	1.81	0.45
34:RA:2579:C:H2'	34:RA:2580:U:H6	1.82	0.45
49:RU:92:ARG:HG2	49:RU:95:LEU:HD22	1.88	0.45
1:XA:269:C:H2'	1:XA:270:A:H8	1.82	0.45
1:XA:642:A:N3	8:XH:113:SER:OG	2.42	0.45
30:Y6:11:LEU:HB2	30:Y6:21:TYR:HB2	1.97	0.45
34:YA:1491:G:H2'	34:YA:1492:G:C8	2.52	0.45
34:YA:1782:C:H1'	34:YA:2609:U:H5''	1.98	0.45
42:YN:23:LEU:HB2	42:YN:62:VAL:HG12	1.99	0.45
47:YS:71:ARG:O	47:YS:107:GLU:OE1	2.34	0.45
1:QA:593:G:H1	1:QA:646:U:H3	1.65	0.45
1:QA:736:C:H2'	1:QA:737:A:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1023:G:H3'	1:QA:1024:G:H5''	1.98	0.45
1:QA:1060:C:H2'	1:QA:1061:G:H8	1.81	0.45
1:QA:1151:A:H2'	1:QA:1152:A:C8	2.51	0.45
5:QE:102:ALA:O	5:QE:107:ARG:NH2	2.50	0.45
22:QV:37:T6A:HN1	22:QV:38:A:H1'	1.82	0.45
34:RA:958:U:OP2	45:RQ:14:ARG:NH1	2.49	0.45
36:RD:108:PRO:CA	36:RD:196:VAL:O	2.65	0.45
1:XA:272:C:H2'	1:XA:273:A:H8	1.82	0.45
1:XA:546:G:H4'	1:XA:548:G:H4'	1.98	0.45
28:Y4:40:HIS:CD2	39:YG:112:PRO:HB3	2.52	0.45
34:YA:414:C:O2	34:YA:1864:U:O2'	2.33	0.45
34:YA:890:A:H2'	34:YA:892:G:H8	1.82	0.45
34:YA:919:G:N2	34:YA:2269:A:OP2	2.50	0.45
34:YA:1449:A:C4	34:YA:1529:A:H2	2.35	0.45
51:YW:111:HIS:CD2	51:YW:113:LYS:H	2.34	0.45
1:QA:970:C:N4	9:QI:128:ARG:O	2.42	0.45
1:QA:985:C:H2'	1:QA:986:A:C8	2.52	0.45
34:RA:414:C:H2'	34:RA:415:A:C8	2.52	0.45
34:RA:740:U:H2'	34:RA:741:G:C8	2.51	0.45
34:RA:1316:U:H2'	34:RA:1317:A:C8	2.52	0.45
34:RA:1667:G:O2'	34:RA:1991:U:O4	2.31	0.45
34:RA:1819:A:H5''	36:RD:161:THR:HG21	1.99	0.45
34:RA:2404:C:O3'	44:RP:77:ARG:NH2	2.50	0.45
34:RA:2544:G:H1'	34:RA:2646:C:H4'	1.99	0.45
34:RA:2623:G:OP1	34:RA:2826:A:O2'	2.27	0.45
39:RG:73:ALA:HB1	39:RG:82:LEU:CD1	2.47	0.45
1:XA:407:G:H2'	1:XA:408:A:C8	2.51	0.45
27:Y3:3:ARG:CG	27:Y3:60:GLU:OXT	2.64	0.45
34:YA:297:C:OP1	53:YY:87:LYS:NZ	2.42	0.45
34:YA:679:C:H2'	34:YA:680:G:C8	2.51	0.45
34:YA:784:A:N6	34:YA:2072:G:O2'	2.49	0.45
34:YA:2071:A:H2'	34:YA:2072:G:C8	2.52	0.45
34:YA:2291:U:O2'	34:YA:2374:C:O2	2.35	0.45
34:YA:2590:A:H2'	34:YA:2591:C:H6	1.82	0.45
37:YE:2:LYS:HG2	37:YE:200:GLU:HB2	1.99	0.45
39:YG:106:LEU:HA	39:YG:110:ALA:HB3	1.98	0.45
45:YQ:103:MET:HE1	45:YQ:125:LEU:HD13	1.99	0.45
47:YS:26:LEU:HB3	47:YS:87:PHE:HA	1.99	0.45
1:QA:131:C:O2'	1:QA:262:A:N3	2.46	0.44
22:QV:65:C:H2'	22:QV:66:A:C8	2.52	0.44
34:RA:281:G:H21	34:RA:359:A:H62	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:2318:G:H1	47:RS:2:ALA:HA	1.82	0.44
34:RA:2377:A:O2'	47:RS:111:GLU:O	2.29	0.44
35:RB:8:U:O4	35:RB:112:G:O6	2.35	0.44
38:RF:40:GLN:HA	38:RF:43:LYS:HG2	1.99	0.44
11:XK:52:GLY:H	11:XK:55:LYS:HE2	1.82	0.44
34:YA:17:G:H4'	49:YU:25:TRP:HE1	1.82	0.44
34:YA:818:G:N1	34:YA:1188:U:OP2	2.35	0.44
34:YA:975:G:N2	34:YA:1156:A:O2'	2.50	0.44
34:YA:2737:G:H2'	34:YA:2738:A:C8	2.52	0.44
53:YY:20:TYR:HB3	53:YY:23:ARG:HG3	1.99	0.44
1:QA:407:G:H2'	1:QA:408:A:H8	1.81	0.44
1:QA:806:C:H2'	1:QA:807:A:H8	1.82	0.44
1:QA:890:G:O2'	1:QA:906:G:O6	2.31	0.44
2:QB:70:PHE:O	2:QB:93:VAL:N	2.46	0.44
24:R0:55:ARG:NH1	34:RA:2364:C:OP1	2.48	0.44
29:R5:12:SER:HB3	34:RA:2020:A:H5'	1.99	0.44
34:RA:604:G:OP1	44:RP:90:ARG:NH1	2.50	0.44
34:RA:2123:G:H2'	34:RA:2124:G:C8	2.52	0.44
39:RG:68:PRO:HB3	39:RG:92:VAL:HB	1.98	0.44
39:RG:81:LYS:HA	39:RG:81:LYS:HD2	1.57	0.44
50:RV:55:ALA:HA	50:RV:101:GLY:HA2	2.00	0.44
52:RX:12:VAL:HB	52:RX:27:THR:HG23	1.99	0.44
1:XA:707:C:H2'	1:XA:708:C:H6	1.82	0.44
1:XA:1541:U:H3	23:XX:-14:G:H1	1.66	0.44
3:XC:19:GLU:O	3:XC:40:ARG:NH2	2.50	0.44
10:XJ:23:ILE:HG23	10:XJ:85:LEU:HD11	1.99	0.44
29:Y5:4:HIS:O	34:YA:2056:G:N2	2.50	0.44
36:YD:108:PRO:HB3	36:YD:143:HIS:CE1	2.52	0.44
54:YZ:6:LYS:HD3	54:YZ:8:TYR:CZ	2.52	0.44
1:QA:407:G:OP1	4:QD:115:ARG:NH1	2.50	0.44
1:QA:687:A:N6	1:QA:701:C:O4'	2.51	0.44
25:R1:19:GLN:HG3	34:RA:2080:G:H5'	1.98	0.44
34:RA:851:U:H2'	34:RA:852:G:H8	1.82	0.44
37:RE:144:ARG:HB3	37:RE:145:LYS:H	1.70	0.44
49:RU:109:LEU:CD2	50:RV:47:VAL:HG21	2.47	0.44
1:XA:22:G:H4'	1:XA:885:G:C8	2.52	0.44
1:XA:67:C:H2'	1:XA:68:G:C8	2.52	0.44
1:XA:438:G:N2	1:XA:496:A:H62	2.13	0.44
1:XA:501:C:H2'	1:XA:502:G:H8	1.82	0.44
1:XA:579:G:H5'	1:XA:728:A:H1'	1.99	0.44
17:XQ:53:LEU:HD23	17:XQ:85:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:XV:22:G:H2'	22:XV:23:A:H8	1.82	0.44
25:Y1:17:SER:HB2	25:Y1:40:ARG:HD2	2.00	0.44
27:Y3:37:LEU:N	27:Y3:37:LEU:CD1	2.73	0.44
34:YA:729:G:C6	34:YA:1775:U:N3	2.85	0.44
34:YA:1399:C:H2'	34:YA:1400:G:H8	1.81	0.44
34:YA:2151:G:H2'	34:YA:2152:G:H8	1.81	0.44
45:YQ:65:PHE:HD2	45:YQ:105:GLU:O	2.00	0.44
1:QA:448:A:OP2	1:QA:485:G:N2	2.39	0.44
1:QA:782:A:H62	1:QA:800:G:H21	1.66	0.44
3:QC:124:ILE:HG21	3:QC:196:LEU:HG	1.99	0.44
19:QS:15:LEU:HD11	19:QS:35:SER:HB3	1.98	0.44
34:RA:1598:C:O3'	52:RX:35:THR:OG1	2.36	0.44
34:RA:1995:U:O2	43:RO:3:GLN:NE2	2.36	0.44
34:RA:2037:G:H2'	34:RA:2038:G:C8	2.53	0.44
34:RA:2378:A:H4'	47:RS:23:ARG:NH1	2.33	0.44
54:RZ:48:PHE:HE1	54:RZ:53:ILE:HG22	1.82	0.44
1:XA:1386:G:H2'	1:XA:1387:G:H8	1.81	0.44
6:XF:48:LEU:HD22	18:XR:77:GLY:HA3	1.98	0.44
22:XV:50:C:H2'	22:XV:51:A:C8	2.53	0.44
26:Y2:17:SER:HB3	26:Y2:20:GLU:HG2	1.99	0.44
34:YA:373:U:H2'	34:YA:374:A:H8	1.81	0.44
34:YA:807:U:H2'	34:YA:808:G:H8	1.82	0.44
41:YI:118:LYS:CB	41:YI:119:PRO:HD2	2.42	0.44
4:QD:195:ALA:HB1	6:XF:16:GLN:HG3	1.98	0.44
34:RA:1380:G:O2'	34:RA:1569:A:N6	2.50	0.44
34:RA:2250:G:C4	45:RQ:82:ARG:HG3	2.53	0.44
36:RD:245:PRO:HA	36:RD:246:PRO:HD3	1.83	0.44
41:RI:118:LYS:HB3	41:RI:118:LYS:HE3	1.50	0.44
42:RN:47:ALA:HB2	42:RN:112:LEU:HD11	1.98	0.44
1:XA:166:G:H2'	1:XA:167:G:H8	1.83	0.44
1:XA:486:U:H2'	1:XA:487:A:H8	1.82	0.44
1:XA:674:G:H2'	1:XA:675:A:C8	2.49	0.44
1:XA:738:C:H5''	6:XF:69:GLU:HB2	2.00	0.44
1:XA:1492:A:OP2	12:XL:47:LYS:HG2	2.17	0.44
7:XG:111:ARG:NH2	7:XG:126:ASP:OD2	2.41	0.44
11:XK:108:ILE:O	18:XR:87:ARG:N	2.45	0.44
33:Y9:19:ARG:NE	34:YA:2756:U:OP2	2.39	0.44
34:YA:219:G:N3	34:YA:234:C:O2'	2.49	0.44
34:YA:569:U:O2'	34:YA:983:A:N1	2.46	0.44
34:YA:1651:G:N7	46:YR:11:ASN:ND2	2.65	0.44
39:YG:59:GLU:OE1	39:YG:153:ARG:NH2	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:537:G:H5''	12:QL:113:ARG:HH12	1.83	0.44
10:QJ:34:VAL:HG23	10:QJ:74:ILE:HA	2.00	0.44
25:R1:45:ASN:HB2	34:RA:397:G:H5''	1.99	0.44
26:R2:6:VAL:HG13	26:R2:59:ARG:HE	1.82	0.44
28:R4:5:ILE:O	39:RG:67:LYS:NZ	2.51	0.44
34:RA:39:C:O2	38:RF:46:ARG:NH2	2.50	0.44
34:RA:288:C:H2'	34:RA:289:A:H8	1.83	0.44
34:RA:468:G:H5''	38:RF:60:SER:HB2	2.00	0.44
34:RA:746:A:O2'	34:RA:2611:U:O2'	2.29	0.44
34:RA:1026:U:H1'	34:RA:1027:A:H5''	1.99	0.44
34:RA:1600:C:OP1	52:RX:58:HIS:NE2	2.32	0.44
34:RA:2291:U:O2'	34:RA:2374:C:O2	2.34	0.44
34:RA:2304:G:H22	34:RA:2312:U:H3	1.65	0.44
38:RF:167:ALA:HB1	38:RF:173:VAL:HG11	1.98	0.44
1:XA:235:C:H2'	1:XA:236:G:H8	1.81	0.44
1:XA:1354:C:H2'	1:XA:1355:G:H8	1.83	0.44
14:XN:23:ARG:NH1	14:XN:28:GLY:O	2.51	0.44
34:YA:1416:G:H2'	34:YA:1417:C:C6	2.53	0.44
36:YD:121:PRO:HB3	36:YD:135:PHE:HD2	1.77	0.44
1:QA:1249:C:N4	1:QA:1288:A:OP2	2.51	0.44
12:QL:47:LYS:N	12:QL:48:PRO:HD2	2.33	0.44
33:R9:16:VAL:HG11	34:RA:1032:A:H4'	2.00	0.44
34:RA:323:G:H2'	38:RF:169:ASN:ND2	2.33	0.44
34:RA:2246:G:H2'	34:RA:2247:A:C8	2.53	0.44
36:RD:155:LEU:HD23	36:RD:177:LEU:HD11	1.99	0.44
41:RI:14:ASP:OD1	41:RI:17:GLN:OE1	2.35	0.44
2:XB:179:LYS:HA	8:XH:72:PRO:HD3	1.99	0.44
5:XE:110:LEU:HD13	5:XE:118:ILE:HD13	1.98	0.44
34:YA:814:C:H1'	34:YA:1226:G:H21	1.82	0.44
34:YA:2352:A:N6	34:YA:2365:G:O2'	2.51	0.44
40:YH:121:ILE:HD11	40:YH:140:LYS:HG2	2.00	0.44
42:YN:128:HIS:NE2	42:YN:134:ARG:HD3	2.32	0.44
2:QB:80:ILE:HD11	2:QB:208:ILE:HG23	1.99	0.44
5:QE:16:THR:OG1	5:QE:27:ARG:O	2.34	0.44
32:R8:55:ALA:HB1	44:RP:49:ARG:O	2.17	0.44
34:RA:1042:G:O6	34:RA:1113:U:O2	2.36	0.44
34:RA:1231:G:H2'	34:RA:1232:G:H8	1.83	0.44
34:RA:1569:A:H4'	36:RD:61:LEU:HD11	1.99	0.44
48:RT:125:ARG:O	48:RT:128:GLU:HB3	2.18	0.44
1:XA:18:C:H4'	1:XA:1078:U:H3	1.81	0.44
1:XA:877:C:H2'	1:XA:878:G:H8	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:XC:76:VAL:HG23	3:XC:77:ILE:HG13	2.00	0.44
4:XD:17:VAL:N	4:XD:33:MET:HE1	2.33	0.44
13:XM:65:LYS:NZ	13:XM:73:GLU:OE1	2.49	0.44
15:XO:67:LEU:HB3	15:XO:78:TYR:HE1	1.82	0.44
34:YA:389:G:N1	44:YP:71:VAL:O	2.43	0.44
34:YA:1316:U:H2'	34:YA:1317:A:C8	2.52	0.44
34:YA:2099:U:O4	34:YA:2190:G:O6	2.36	0.44
34:YA:2453:A:H2'	34:YA:2454:G:H8	1.83	0.44
37:YE:52:LEU:CD2	37:YE:77:ILE:HD12	2.48	0.44
39:YG:16:ARG:HH21	39:YG:28:VAL:HG22	1.81	0.44
39:YG:41:GLN:NE2	39:YG:56:ALA:HB1	2.33	0.44
53:YY:28:LYS:N	53:YY:38:ILE:O	2.44	0.44
1:QA:634:C:H2'	1:QA:635:G:H8	1.83	0.44
1:QA:838:G:H1	1:QA:848:C:H42	1.66	0.44
7:QG:111:ARG:NH2	7:QG:126:ASP:OD2	2.44	0.44
25:R1:53:VAL:HG13	25:R1:74:VAL:HG13	2.00	0.44
37:RE:36:ARG:HH12	37:RE:86:PRO:HD2	1.83	0.44
45:RQ:77:LYS:NZ	45:RQ:83:MET:O	2.38	0.44
1:XA:320:C:H2'	1:XA:321:A:C8	2.53	0.44
1:XA:1491:G:C5'	12:XL:47:LYS:HE3	2.48	0.44
3:XC:42:LEU:HA	3:XC:45:LYS:HG2	2.00	0.44
34:YA:307:G:H21	34:YA:330:A:H62	1.66	0.44
34:YA:1353:A:H2'	34:YA:1354:A:C8	2.53	0.44
34:YA:2561:A:H4'	43:YO:40:VAL:HG11	2.00	0.44
41:YI:130:TYR:O	41:YI:136:VAL:O	2.36	0.44
52:YX:25:LYS:HB3	52:YX:80:ILE:HD11	2.00	0.44
54:YZ:4:ARG:HG2	54:YZ:58:VAL:HB	2.00	0.44
1:QA:452:A:H62	1:QA:480:U:H3	1.64	0.43
1:QA:946:A:H2'	1:QA:947:G:H8	1.82	0.43
13:QM:65:LYS:C	13:QM:66:LEU:HG	2.43	0.43
26:R2:18:PRO:HA	26:R2:21:LEU:HD12	2.00	0.43
32:R8:36:LYS:HB3	32:R8:40:GLU:HG2	1.99	0.43
34:RA:1354:A:H3'	34:RA:1355:G:H8	1.83	0.43
34:RA:2329:G:H2'	34:RA:2330:G:C8	2.53	0.43
34:RA:2859:G:H2'	34:RA:2860:A:C8	2.53	0.43
46:RR:104:ARG:HG3	46:RR:107:ASP:HB3	2.00	0.43
24:Y0:46:LYS:HD2	24:Y0:78:TYR:HE1	1.82	0.43
34:YA:177:G:H3'	34:YA:178:G:H8	1.83	0.43
34:YA:787:U:H5''	34:YA:788:A:H5'	2.00	0.43
34:YA:847:U:H3	34:YA:934:G:N2	2.16	0.43
34:YA:949:C:H2'	34:YA:950:G:H8	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:2391:G:O2'	34:YA:2422:A:N7	2.51	0.43
34:YA:2845:G:H2'	34:YA:2846:G:C8	2.53	0.43
47:YS:18:ILE:HG13	47:YS:88:ASP:HA	1.99	0.43
48:YT:20:PRO:HD2	48:YT:86:ILE:HG23	2.00	0.43
1:QA:1022:G:H2'	1:QA:1023:G:H8	1.84	0.43
4:QD:109:GLY:HA3	4:QD:165:MET:HG2	1.99	0.43
22:QV:50:C:H2'	22:QV:51:A:C8	2.52	0.43
30:R6:10:LEU:HD21	34:RA:2419:U:H4'	2.00	0.43
34:RA:520:G:H2'	34:RA:521:G:H8	1.83	0.43
34:RA:704:G:O2'	34:RA:726:G:N2	2.48	0.43
34:RA:2578:G:OP1	34:RA:2614:A:N6	2.51	0.43
35:RB:116:G:H4'	47:RS:54:LEU:HD22	2.00	0.43
50:RV:1:MET:HE2	50:RV:43:GLU:HB2	1.98	0.43
1:XA:262:A:H5''	20:XT:76:ALA:HB2	2.01	0.43
1:XA:802:A:H3'	1:XA:803:G:H8	1.81	0.43
6:XF:97:PHE:HB2	18:XR:32:ARG:HE	1.84	0.43
24:Y0:49:LYS:HE2	47:YS:43:GLU:HG3	2.00	0.43
34:YA:37:C:H2'	34:YA:38:A:H8	1.83	0.43
34:YA:414:C:H2'	34:YA:415:A:H8	1.83	0.43
34:YA:996:A:H4'	49:YU:92:ARG:HE	1.79	0.43
34:YA:2791:C:H5	34:YA:2893:G:H3'	1.83	0.43
34:YA:2841:C:H2'	34:YA:2842:G:H8	1.81	0.43
40:YH:17:VAL:HG22	40:YH:26:VAL:HG12	2.01	0.43
40:YH:122:THR:HB	40:YH:134:SER:HB2	1.99	0.43
49:YU:83:LEU:HD12	49:YU:113:ALA:HB2	2.00	0.43
1:QA:45:U:H2'	1:QA:46:G:C8	2.53	0.43
1:QA:692:U:OP1	11:QK:124:LYS:NZ	2.42	0.43
1:QA:1298:C:H4'	1:QA:1299:A:C8	2.53	0.43
8:QH:9:MET:HG3	8:QH:26:VAL:HG11	1.99	0.43
34:RA:1203:G:O6	34:RA:1204:A:N6	2.52	0.43
34:RA:1435:G:N2	34:RA:1477:A:O2'	2.50	0.43
1:XA:946:A:H2'	1:XA:947:G:C8	2.53	0.43
13:XM:23:TYR:HD2	13:XM:67:GLU:HA	1.84	0.43
34:YA:520:G:H2'	34:YA:521:G:H8	1.83	0.43
34:YA:907:U:O2'	45:YQ:101:ARG:NH2	2.48	0.43
34:YA:1173:G:N2	34:YA:1175:U:O4	2.44	0.43
34:YA:2630:G:H2'	34:YA:2631:G:C8	2.53	0.43
34:YA:2853:C:H2'	34:YA:2854:G:H8	1.83	0.43
41:YI:131:LYS:CB	41:YI:135:GLU:HA	2.43	0.43
45:YQ:34:LEU:HB2	45:YQ:118:LEU:HD22	2.00	0.43
1:QA:1172:C:H2'	1:QA:1173:G:H8	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1221:G:OP1	1:QA:1321:C:N4	2.51	0.43
34:RA:13:A:O2'	34:RA:15:G:N7	2.46	0.43
34:RA:2749:A:H4'	40:RH:62:LYS:HB3	1.99	0.43
37:RE:176:ILE:HB	37:RE:181:LEU:HB2	1.99	0.43
3:XC:20:SER:HG	3:XC:22:TRP:NE1	2.16	0.43
3:XC:88:ARG:HE	3:XC:101:LEU:HB2	1.84	0.43
12:XL:104:VAL:HG13	12:XL:105:TYR:CD2	2.52	0.43
29:Y5:52:TYR:OH	34:YA:2883:A:OP1	2.34	0.43
34:YA:1139:G:O2'	34:YA:1143:A:N1	2.38	0.43
34:YA:1339:G:H5''	52:YX:16:LYS:HD3	2.00	0.43
34:YA:1853:A:N3	34:YA:2233:U:O2'	2.41	0.43
36:YD:108:PRO:HG2	36:YD:111:LEU:HB2	2.01	0.43
45:YQ:58:PHE:HD2	45:YQ:61:GLY:HA3	1.82	0.43
52:YX:53:LYS:NZ	52:YX:55:ASN:OD1	2.51	0.43
1:QA:636:U:H2'	1:QA:637:G:H8	1.82	0.43
1:QA:1492:A:OP2	12:QL:47:LYS:HE3	2.16	0.43
2:QB:19:HIS:ND1	2:QB:20:GLU:OE2	2.51	0.43
3:QC:8:ILE:HG23	3:QC:16:ARG:HG2	1.98	0.43
13:QM:5:ALA:C	13:QM:67:GLU:OE2	2.62	0.43
25:R1:80:LEU:HD12	25:R1:81:LYS:HG3	2.01	0.43
31:R7:20:ALA:HA	31:R7:23:ARG:HD3	2.01	0.43
34:RA:2845:G:H2'	34:RA:2846:G:C8	2.54	0.43
48:RT:107:ASP:O	48:RT:110:ILE:CG2	2.47	0.43
52:RX:55:ASN:HB2	52:RX:80:ILE:HG23	2.01	0.43
1:XA:296:U:O2'	1:XA:556:C:O2	2.34	0.43
11:XK:33:THR:HA	11:XK:39:PRO:HA	2.00	0.43
18:XR:50:ILE:HG13	18:XR:74:ARG:HH22	1.83	0.43
27:Y3:40:THR:HG22	27:Y3:42:ALA:H	1.84	0.43
44:YP:88:LEU:HD11	44:YP:114:ILE:HD12	2.00	0.43
48:YT:3:ARG:HG3	48:YT:7:ILE:HG12	2.00	0.43
1:QA:1432:G:OP1	48:RT:108:ARG:N	2.48	0.43
13:QM:90:LEU:HD23	13:QM:93:ARG:HE	1.84	0.43
34:RA:749:C:H5'	34:RA:1271:G:H1'	2.00	0.43
34:RA:1155:A:H5''	49:RU:55:ARG:CZ	2.49	0.43
40:RH:9:ILE:CG2	40:RH:50:VAL:H	2.26	0.43
52:RX:57:LEU:HG	52:RX:78:LYS:HB2	2.00	0.43
1:XA:969:A:OP1	10:XJ:55:LYS:NZ	2.51	0.43
19:XS:10:PHE:HB2	19:XS:39:THR:HG22	2.01	0.43
34:YA:807:U:OP2	44:YP:41:ARG:NH2	2.51	0.43
34:YA:1779:U:OP2	34:YA:1784:A:N6	2.39	0.43
36:YD:142:VAL:HG23	36:YD:193:VAL:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:375:U:OP1	16:QP:69:THR:OG1	2.28	0.43
1:QA:1048:G:H1'	1:QA:1215:G:H5''	2.01	0.43
1:QA:1355:G:H2'	1:QA:1356:G:C8	2.54	0.43
1:QA:1414:U:H2'	1:QA:1415:G:C8	2.53	0.43
19:QS:10:PHE:HE2	19:QS:16:LEU:HB2	1.84	0.43
34:RA:78:A:H2'	34:RA:79:G:H8	1.83	0.43
34:RA:848:G:H2'	34:RA:849:A:C8	2.53	0.43
34:RA:1844:C:H2'	34:RA:1845:G:H8	1.84	0.43
34:RA:2103:C:N4	34:RA:2187:G:O6	2.52	0.43
54:RZ:97:GLU:HA	54:RZ:127:LYS:HA	2.00	0.43
54:RZ:102:LEU:HD11	54:RZ:124:ILE:HB	1.99	0.43
1:XA:563:A:H2'	1:XA:567:G:C8	2.53	0.43
1:XA:652:U:O4	1:XA:752:G:O2'	2.25	0.43
1:XA:1151:A:O2'	10:XJ:70:ARG:NH2	2.52	0.43
55:XY:34:G:H2'	55:XY:35:A:C8	2.54	0.43
34:YA:784:A:C5	36:YD:229:VAL:HG21	2.54	0.43
34:YA:1021:A:H61	34:YA:1142(A):A:H61	1.66	0.43
34:YA:1800:C:H42	34:YA:1817:G:H22	1.65	0.43
1:QA:1010:G:H2'	1:QA:1011:G:C8	2.53	0.43
1:QA:1469:G:H2'	1:QA:1470:G:H8	1.84	0.43
5:QE:78:HIS:HB3	8:QH:107:LEU:HD12	2.01	0.43
9:QI:20:ARG:O	9:QI:60:ASP:N	2.52	0.43
34:RA:2458:G:O2'	34:RA:2460:U:O4	2.33	0.43
1:XA:359:U:H2'	1:XA:360:A:H8	1.84	0.43
1:XA:1492:A:P	12:XL:47:LYS:HG2	2.58	0.43
2:XB:223:ILE:HA	2:XB:226:ARG:HB3	2.00	0.43
4:XD:20:TYR:CD1	4:XD:106:TYR:OH	2.70	0.43
34:YA:2241:A:H2'	34:YA:2242:G:C8	2.54	0.43
34:YA:2626:C:H2'	34:YA:2627:G:C8	2.54	0.43
34:YA:2689:U:OP2	34:YA:2872:G:N2	2.50	0.43
42:YN:47:ALA:HB2	42:YN:112:LEU:HD11	2.00	0.43
46:YR:51:LEU:HD22	46:YR:66:VAL:HG13	2.01	0.43
54:YZ:59:LEU:HA	54:YZ:59:LEU:HD13	1.72	0.43
1:QA:309:G:H2'	1:QA:310:G:H8	1.83	0.43
2:QB:115:LEU:HD13	2:QB:145:LEU:HB3	2.01	0.43
3:QC:4:LYS:HA	3:QC:4:LYS:HD3	1.65	0.43
7:QG:24:THR:HA	7:QG:27:ILE:HG22	2.00	0.43
9:QI:19:LEU:HD23	9:QI:59:PHE:HD2	1.84	0.43
9:QI:125:TYR:HE2	9:QI:127:LYS:HD3	1.83	0.43
25:R1:17:SER:HB2	25:R1:40:ARG:HD2	2.01	0.43
34:RA:442:G:H1'	38:RF:48:THR:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:1771:C:H2'	34:RA:1772:G:C8	2.54	0.43
34:RA:1827:C:OP2	36:RD:222:ARG:NH1	2.51	0.43
34:RA:2487:G:H2'	34:RA:2488:A:H8	1.83	0.43
40:RH:99:VAL:HG23	40:RH:102:ALA:HB3	2.00	0.43
41:RI:131:LYS:CG	41:RI:135:GLU:OE1	2.66	0.43
46:RR:77:ARG:O	46:RR:81:ASP:HB2	2.19	0.43
48:RT:120:ARG:HA	48:RT:123:GLN:OE1	2.18	0.43
2:XB:98:LEU:HB2	2:XB:101:MET:HE3	2.01	0.43
6:XF:10:LEU:HD13	6:XF:61:LEU:HD13	2.00	0.43
7:XG:136:LYS:HA	7:XG:139:GLU:HG2	2.01	0.43
34:YA:557:U:H2'	34:YA:558:G:H8	1.83	0.43
34:YA:870:A:OP1	45:YQ:6:ARG:NH2	2.50	0.43
34:YA:1057:A:N6	34:YA:1087:G:OP2	2.52	0.43
34:YA:1266:G:O2'	34:YA:2012:G:O6	2.33	0.43
49:YU:93:LYS:HB2	49:YU:93:LYS:HE2	1.36	0.43
3:QC:191:THR:OG1	3:QC:194:GLY:O	2.35	0.43
5:QE:143:ARG:NE	8:QH:77:GLU:OE2	2.51	0.43
7:QG:71:PRO:O	7:QG:96:GLN:NE2	2.52	0.43
9:QI:42:ARG:NH2	9:QI:71:SER:O	2.52	0.43
17:QQ:18:THR:OG1	17:QQ:69:LYS:NZ	2.40	0.43
31:R7:42:LEU:HD12	34:RA:126:A:H61	1.83	0.43
34:RA:993:G:OP1	49:RU:50:ARG:NH2	2.46	0.43
34:RA:1416:G:H2'	34:RA:1417:C:C6	2.54	0.43
39:RG:82:LEU:HD23	39:RG:86:MET:HB3	2.00	0.43
45:RQ:43:THR:HG22	45:RQ:94:VAL:HG12	2.01	0.43
1:XA:269:C:H2'	1:XA:270:A:C8	2.53	0.43
1:XA:452:A:N7	1:XA:480:U:O4	2.52	0.43
1:XA:946:A:H2'	1:XA:947:G:H8	1.83	0.43
1:XA:1469:G:H2'	1:XA:1470:G:C8	2.54	0.43
5:XE:78:HIS:HE1	5:XE:80:ILE:HD13	1.84	0.43
26:Y2:28:LYS:HD2	26:Y2:53:LEU:HD11	2.00	0.43
34:YA:775:G:H4'	34:YA:776:G:H5'	1.99	0.43
34:YA:1028:A:H2'	34:YA:1029:A:C8	2.54	0.43
34:YA:2531:A:H61	34:YA:2662:A:H61	1.65	0.43
34:YA:2692:C:H2'	34:YA:2693:A:C8	2.54	0.43
45:YQ:27:VAL:HG13	45:YQ:105:GLU:CG	2.49	0.43
1:QA:923:A:O2'	1:QA:1399:C:OP2	2.34	0.42
26:R2:17:SER:HB3	26:R2:20:GLU:HG2	2.00	0.42
32:R8:63:PRO:HB2	32:R8:65:GLU:CD	2.43	0.42
34:RA:586:A:N1	34:RA:809:G:O2'	2.48	0.42
34:RA:2304:G:N2	34:RA:2312:U:H3	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:RV:75:PHE:HA	50:RV:81:TYR:HD2	1.83	0.42
1:XA:427:U:O2'	1:XA:541:G:OP1	2.28	0.42
1:XA:1316:G:N2	1:XA:1319:A:OP2	2.43	0.42
23:XX:-12:C:H2'	23:XX:-11:A:C8	2.52	0.42
34:YA:58:G:O2'	34:YA:73:A:N1	2.49	0.42
34:YA:468:G:H5''	38:YF:60:SER:HB2	2.00	0.42
34:YA:521:G:H2'	34:YA:522:G:H8	1.84	0.42
34:YA:1434:A:H61	34:YA:1558:A:N6	2.17	0.42
34:YA:1507:A:O2'	34:YA:1509:C:O2	2.34	0.42
34:YA:2315:G:H21	39:YG:128:ARG:HH22	1.67	0.42
40:YH:46:GLU:HB2	40:YH:49:VAL:HB	2.01	0.42
49:YU:96:ALA:O	49:YU:99:ALA:CB	2.66	0.42
1:QA:912:C:H2'	1:QA:913:A:C8	2.53	0.42
1:QA:1064:G:H1'	1:QA:1066:C:C6	2.54	0.42
1:QA:1238:A:OP1	1:QA:1335:C:O2'	2.27	0.42
10:QJ:30:SER:O	10:QJ:78:ASN:ND2	2.51	0.42
34:RA:121:G:H4'	34:RA:149:A:H5'	2.01	0.42
34:RA:191:A:H2'	34:RA:192:C:H6	1.84	0.42
39:RG:73:ALA:HB2	39:RG:82:LEU:CD2	2.49	0.42
47:RS:85:VAL:HG23	47:RS:112:PHE:HE1	1.84	0.42
1:XA:562:C:O2'	12:XL:16:GLU:O	2.37	0.42
1:XA:736:C:H2'	1:XA:737:A:H8	1.84	0.42
1:XA:891:U:H2'	1:XA:892:A:H8	1.85	0.42
22:XV:50:C:H2'	22:XV:51:A:H8	1.85	0.42
34:YA:39:C:O2	38:YF:46:ARG:NH2	2.48	0.42
34:YA:2233:U:H2'	34:YA:2234:G:C8	2.54	0.42
34:YA:2591:C:H2'	34:YA:2592:G:C8	2.54	0.42
36:YD:164:GLN:OE1	36:YD:176:ARG:NH2	2.47	0.42
47:YS:66:ALA:HA	47:YS:69:VAL:HG12	2.00	0.42
1:QA:269:C:H2'	1:QA:270:A:C8	2.54	0.42
1:QA:908:A:H2'	1:QA:909:A:H8	1.83	0.42
1:QA:1221:G:H4'	19:QS:77:THR:HG21	2.01	0.42
4:QD:96:LEU:HD22	4:QD:139:ARG:HE	1.84	0.42
5:QE:11:ILE:HG23	5:QE:12:LEU:HD23	2.00	0.42
24:R0:51:VAL:O	47:RS:20:ARG:NH2	2.49	0.42
43:RO:76:ALA:HB3	48:RT:75:ILE:HD12	2.01	0.42
48:RT:66:VAL:HA	48:RT:71:GLY:HA2	2.01	0.42
54:RZ:70:LEU:HB2	54:RZ:91:LEU:HD21	2.01	0.42
1:XA:936:C:O2	1:XA:1382:C:N4	2.49	0.42
1:XA:1503:A:C6	1:XA:1531:A:H2	2.37	0.42
7:XG:30:ILE:HG23	7:XG:39:ALA:HB1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:XG:140:ASP:O	7:XG:143:ARG:HG2	2.19	0.42
34:YA:142:G:H2'	34:YA:143:C:H6	1.85	0.42
34:YA:197:A:H2	34:YA:2434:A:H62	1.68	0.42
34:YA:210:C:H2'	34:YA:211:A:C8	2.54	0.42
34:YA:579:G:O2'	34:YA:2019:A:OP1	2.34	0.42
34:YA:675:A:N3	34:YA:2443:C:O2'	2.47	0.42
34:YA:863:A:H2'	34:YA:864:G:C8	2.54	0.42
34:YA:2030:A:H4'	34:YA:2031:A:C8	2.53	0.42
34:YA:2618:G:H21	37:YE:150:VAL:HG21	1.84	0.42
48:YT:92:GLY:O	48:YT:120:ARG:NH2	2.52	0.42
1:QA:300:A:O2'	1:QA:564:C:N3	2.41	0.42
34:RA:529:A:H8	34:RA:530:G:C6	2.38	0.42
34:RA:1005:C:H2'	34:RA:1006:C:C6	2.55	0.42
34:RA:2693:A:H2'	34:RA:2694:G:H8	1.84	0.42
38:RF:118:ALA:HB2	38:RF:123:LEU:HD23	2.01	0.42
51:RW:111:HIS:HD2	51:RW:113:LYS:H	1.67	0.42
54:RZ:13:GLU:HB3	54:RZ:18:LEU:HD11	2.01	0.42
1:XA:1211:U:H5'	1:XA:1212:U:H5'	2.01	0.42
1:XA:1492:A:OP1	12:XL:47:LYS:HG3	2.19	0.42
2:XB:88:ALA:HB2	2:XB:219:VAL:HG13	2.00	0.42
3:XC:179:ARG:HB2	3:XC:206:GLU:HG3	2.02	0.42
20:XT:43:LEU:HD23	20:XT:51:GLU:HG3	2.01	0.42
34:YA:142:G:H2'	34:YA:143:C:C6	2.55	0.42
34:YA:2181:G:H2'	34:YA:2182:G:C8	2.54	0.42
38:YF:12:LEU:HB3	38:YF:126:VAL:HA	2.02	0.42
40:YH:54:ARG:HD2	40:YH:65:HIS:CG	2.54	0.42
54:YZ:166:SER:HB3	54:YZ:168:GLU:N	2.32	0.42
1:QA:390:C:H2'	1:QA:391:G:H8	1.85	0.42
1:QA:1022:G:H2'	1:QA:1023:G:C8	2.55	0.42
1:QA:1287:A:H2	1:QA:1353:G:H1'	1.84	0.42
12:QL:84:LEU:HB2	12:QL:104:VAL:HG21	2.01	0.42
34:RA:1689:A:OP2	34:RA:1698:A:N6	2.50	0.42
34:RA:2836:U:H2'	34:RA:2837:G:C8	2.55	0.42
38:RF:198:ALA:HA	38:RF:201:VAL:HG12	2.01	0.42
1:XA:490:G:OP2	4:XD:132:ARG:NH2	2.52	0.42
1:XA:812:C:H4'	1:XA:813:U:H5'	2.00	0.42
4:XD:18:LYS:N	4:XD:33:MET:HE1	2.33	0.42
4:XD:116:GLN:HE21	4:XD:157:LEU:HD21	1.83	0.42
6:XF:35:ALA:HB1	6:XF:65:VAL:HG11	2.01	0.42
7:XG:76:ARG:O	7:XG:87:VAL:N	2.45	0.42
34:YA:729:G:C5	36:YD:208:LYS:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:848:G:H2'	34:YA:849:A:C8	2.54	0.42
34:YA:948:G:H1	34:YA:969:U:H3	1.67	0.42
34:YA:2313:C:H5''	39:YG:91:ARG:HD3	2.01	0.42
47:YS:106:ARG:C	47:YS:106:ARG:HD2	2.43	0.42
6:QF:94:GLN:OE1	18:QR:32:ARG:NH1	2.50	0.42
8:QH:12:ARG:HD2	8:QH:26:VAL:HG12	2.02	0.42
13:QM:57:ARG:NH2	28:R4:34:GLU:O	2.53	0.42
18:QR:86:VAL:HG12	18:QR:87:ARG:HG2	2.01	0.42
34:RA:840:C:H2'	34:RA:841:A:H8	1.82	0.42
34:RA:2036:C:H2'	34:RA:2037:G:H8	1.84	0.42
40:RH:18:GLU:HB2	40:RH:25:LYS:HB2	2.02	0.42
46:RR:104:ARG:HE	46:RR:111:LEU:HD21	1.85	0.42
50:RV:59:ALA:HB1	50:RV:94:LEU:HB3	2.02	0.42
1:XA:681:C:H2'	1:XA:682:G:H8	1.85	0.42
1:XA:782:A:H62	1:XA:800:G:H21	1.67	0.42
1:XA:851:G:H2'	1:XA:852:G:H8	1.85	0.42
1:XA:1054:C:OP2	1:XA:1054:C:H4'	2.20	0.42
1:XA:1054:C:C5	55:XY:34:G:H1'	2.55	0.42
1:XA:1118:C:H1'	1:XA:1179:A:C5	2.55	0.42
1:XA:1157:A:N6	1:XA:1178:G:N3	2.68	0.42
1:XA:1427:U:H2'	1:XA:1428:A:C8	2.55	0.42
4:XD:20:TYR:HE1	4:XD:106:TYR:HH	1.56	0.42
32:Y8:58:ILE:HA	32:Y8:61:LEU:HD12	2.02	0.42
34:YA:36:G:N3	34:YA:450:G:O2'	2.50	0.42
34:YA:1062:G:C8	34:YA:1088:A:H2'	2.55	0.42
34:YA:1138:G:H21	42:YN:106:MET:HE3	1.85	0.42
34:YA:1636:C:H2'	34:YA:1637:A:C8	2.55	0.42
34:YA:2546:U:H5''	34:YA:2547:U:H5'	2.01	0.42
34:YA:2707:G:H2'	34:YA:2708:G:C8	2.55	0.42
28:R4:28:LYS:HA	28:R4:29:PRO:HD3	1.92	0.42
32:R8:26:LYS:HG2	32:R8:47:LYS:HD2	2.01	0.42
34:RA:946:G:O6	34:RA:972:G:N2	2.53	0.42
34:RA:1138:G:H21	42:RN:106:MET:HE3	1.84	0.42
34:RA:1638:C:O2	34:RA:2698:U:O2'	2.33	0.42
35:RB:8:U:P	47:RS:15:ARG:HH22	2.43	0.42
40:RH:9:ILE:HG22	40:RH:10:PRO:N	2.29	0.42
40:RH:106:THR:HG22	40:RH:112:PRO:HB3	2.01	0.42
45:RQ:20:ALA:HB3	54:RZ:79:ARG:HE	1.85	0.42
50:RV:14:VAL:HB	50:RV:96:ILE:HG13	2.02	0.42
54:RZ:48:PHE:CZ	54:RZ:53:ILE:HG23	2.55	0.42
1:XA:554:C:H2'	1:XA:555:C:H6	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:XT:33:ILE:HD12	20:XT:63:ILE:HG13	2.01	0.42
34:YA:439:G:H2'	34:YA:440:G:C8	2.55	0.42
34:YA:1309:G:O2'	34:YA:1611:C:O2'	2.32	0.42
34:YA:1626:G:H5''	34:YA:1627:G:H5'	2.02	0.42
34:YA:2311:A:H1'	39:YG:82:LEU:CD1	2.48	0.42
34:YA:2455:G:H2'	34:YA:2456:C:C6	2.54	0.42
40:YH:26:VAL:HG21	40:YH:75:ALA:HB1	2.01	0.42
48:YT:122:ASP:HA	48:YT:125:ARG:HD2	2.00	0.42
49:YU:28:ARG:NH1	49:YU:38:THR:OG1	2.47	0.42
1:QA:224:C:H2'	1:QA:225:C:H6	1.85	0.42
26:R2:53:LEU:HA	26:R2:56:GLN:HG2	2.02	0.42
34:RA:627:A:H4'	34:RA:628:G:H5'	2.02	0.42
45:RQ:11:LYS:HZ1	45:RQ:87:LYS:HD3	1.85	0.42
1:XA:45:U:H2'	1:XA:46:G:C8	2.55	0.42
1:XA:628:G:H2'	1:XA:629:G:C8	2.54	0.42
3:XC:8:ILE:HG23	3:XC:16:ARG:HE	1.85	0.42
8:XH:14:ARG:NH2	8:XH:83:ILE:O	2.43	0.42
34:YA:380:U:H2'	34:YA:381:G:H8	1.84	0.42
34:YA:573:G:N1	34:YA:2031:A:OP2	2.38	0.42
34:YA:2441:C:OP2	34:YA:2586:C:O2'	2.37	0.42
41:YI:110:ASP:N	41:YI:130:TYR:OH	2.42	0.42
1:QA:165:C:H2'	1:QA:166:G:C8	2.55	0.42
1:QA:769:G:H4'	1:QA:1513:A:H4'	2.02	0.42
1:QA:1368:G:H5''	9:QI:112:LYS:HB3	2.02	0.42
2:QB:97:TRP:HZ2	2:QB:102:LEU:HD13	1.84	0.42
3:QC:181:ASN:ND2	3:QC:205:GLY:O	2.53	0.42
12:QL:32:PHE:HB3	12:QL:84:LEU:HD11	2.02	0.42
20:QT:71:THR:HG22	20:QT:72:LEU:HD12	2.01	0.42
34:RA:698:C:O2'	34:RA:734:A:N6	2.43	0.42
34:RA:1423:G:H2'	34:RA:1424:G:H8	1.85	0.42
38:RF:186:ILE:HD12	38:RF:192:LEU:HD11	2.01	0.42
42:RN:115:ARG:O	42:RN:115:ARG:HG3	2.20	0.42
47:RS:4:LEU:N	47:RS:4:LEU:CD1	2.82	0.42
49:RU:95:LEU:HD22	49:RU:95:LEU:H	1.82	0.42
1:XA:1252:A:H61	1:XA:1285:A:H61	1.66	0.42
2:XB:168:THR:HA	2:XB:171:ALA:HB2	2.02	0.42
3:XC:119:ARG:HG2	3:XC:140:ARG:HH12	1.85	0.42
4:XD:15:GLU:OE2	4:XD:59:ARG:NH1	2.53	0.42
34:YA:210:C:H2'	34:YA:211:A:H8	1.85	0.42
34:YA:1113:U:H2'	34:YA:1114:G:H8	1.85	0.42
34:YA:2696:U:H2'	34:YA:2697:G:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:YG:62:LEU:HG	39:YG:143:GLU:HB3	2.00	0.42
53:YY:14:LEU:HD22	53:YY:82:PRO:HG3	2.01	0.42
1:QA:324:G:OP1	20:QT:70:SER:OG	2.38	0.42
13:QM:67:GLU:HB3	13:QM:68:GLY:H	1.62	0.42
34:RA:2690:C:OP1	46:RR:17:ARG:NH2	2.53	0.42
36:RD:153:ALA:O	36:RD:157:ARG:NH1	2.53	0.42
39:RG:73:ALA:CB	39:RG:82:LEU:CD1	2.97	0.42
39:RG:79:ASN:HB2	39:RG:80:PHE:CD1	2.55	0.42
44:RP:89:ALA:O	44:RP:121:LYS:NZ	2.46	0.42
45:RQ:7:MET:HE1	45:RQ:73:PRO:HG3	2.01	0.42
1:XA:603:U:H2'	1:XA:604:G:C8	2.55	0.42
34:YA:2787:C:H1'	37:YE:62:PRO:HG3	2.00	0.42
44:YP:8:PRO:HB2	44:YP:12:ALA:HB3	2.02	0.42
1:QA:137:C:H2'	1:QA:138:G:H8	1.85	0.41
1:QA:1060:C:H2'	1:QA:1061:G:C8	2.54	0.41
3:QC:70:VAL:HG12	3:QC:72:LYS:H	1.85	0.41
11:QK:86:GLY:O	11:QK:91:ARG:NH1	2.53	0.41
14:QN:48:ALA:HB2	14:QN:53:LEU:HD12	2.02	0.41
34:RA:532:A:H4'	34:RA:533:G:C8	2.55	0.41
34:RA:1105:U:H2'	34:RA:1106:G:C8	2.55	0.41
34:RA:2074:U:H2'	34:RA:2075:U:C6	2.55	0.41
40:RH:83:TYR:O	40:RH:83:TYR:CD2	2.70	0.41
41:RI:9:LEU:HB2	41:RI:12:LEU:HB2	2.02	0.41
42:RN:6:PRO:HG3	42:RN:41:ASP:HB2	2.01	0.41
47:RS:28:VAL:HG11	47:RS:98:VAL:HG12	2.02	0.41
54:RZ:5:LEU:HB2	54:RZ:59:LEU:HD23	2.02	0.41
1:XA:337:C:H2'	1:XA:338:A:H8	1.85	0.41
1:XA:1128:C:H5'	9:XI:16:ARG:HH22	1.85	0.41
34:YA:459:U:H2'	34:YA:460:A:H8	1.85	0.41
34:YA:550:G:H2'	34:YA:551:G:H8	1.85	0.41
34:YA:1159:U:H2'	34:YA:1160:G:H8	1.85	0.41
34:YA:1296:G:OP1	34:YA:2709:G:O2'	2.27	0.41
34:YA:2502:G:H5''	34:YA:2503:A:H5''	2.01	0.41
43:YO:68:GLU:HG3	43:YO:78:ARG:HD3	2.01	0.41
47:YS:15:ARG:NE	47:YS:88:ASP:OD1	2.53	0.41
49:YU:92:ARG:NH1	49:YU:92:ARG:CG	2.79	0.41
1:QA:45:U:H2'	1:QA:46:G:H8	1.85	0.41
1:QA:359:U:H2'	1:QA:360:A:H8	1.85	0.41
1:QA:790:A:OP1	22:QV:38:A:O2'	2.33	0.41
1:QA:1066:C:N4	1:QA:1191:A:C6	2.82	0.41
1:QA:1351:U:H3	1:QA:1371:G:H1	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:QI:10:ARG:HG3	9:QI:75:ASP:HB3	2.01	0.41
34:RA:270(V):G:H2'	34:RA:270(W):G:H8	1.86	0.41
34:RA:557:U:H2'	34:RA:558:G:C8	2.54	0.41
34:RA:582:G:H2'	34:RA:583:G:H8	1.84	0.41
34:RA:811:U:H2'	44:RP:21:ARG:HA	2.03	0.41
34:RA:1980:G:O2'	34:RA:1982:C:OP2	2.36	0.41
34:RA:2567:G:H2'	34:RA:2568:C:C6	2.55	0.41
36:RD:260:ARG:HH22	36:RD:270:ILE:HD12	1.84	0.41
40:RH:88:LEU:HD22	40:RH:165:ALA:HB2	2.02	0.41
54:RZ:203:GLU:H	54:RZ:203:GLU:HG2	1.68	0.41
18:XR:58:LEU:HD23	18:XR:62:GLU:HB3	2.02	0.41
34:YA:331:A:H62	34:YA:1210:A:H8	1.66	0.41
34:YA:685:A:OP1	34:YA:686:G:N2	2.50	0.41
34:YA:910:A:H2'	34:YA:911:A:C8	2.55	0.41
34:YA:2086:U:H2'	34:YA:2087:G:C8	2.55	0.41
41:YI:12:LEU:HB3	41:YI:13:GLY:H	1.57	0.41
46:YR:38:VAL:HG22	46:YR:112:ALA:HB2	2.01	0.41
49:YU:96:ALA:O	49:YU:99:ALA:N	2.39	0.41
53:YY:14:LEU:HB2	53:YY:75:ILE:HD11	2.02	0.41
2:QB:236:TYR:HB2	2:QB:237:ALA:H	1.57	0.41
22:QV:12:U:OP1	34:RA:1908:C:O2'	2.38	0.41
34:RA:1853:A:N3	34:RA:2233:U:O2'	2.43	0.41
34:RA:2086:U:H2'	34:RA:2087:G:C8	2.55	0.41
34:RA:2692:C:H2'	34:RA:2693:A:H8	1.85	0.41
35:RB:43:C:O2	39:RG:93:THR:OG1	2.34	0.41
39:RG:37:VAL:O	39:RG:94:LEU:N	2.47	0.41
39:RG:138:GLN:HG2	39:RG:144:ILE:HG21	2.01	0.41
42:RN:16:ILE:HG21	42:RN:26:LEU:HD11	2.01	0.41
2:XB:51:LEU:HA	2:XB:54:THR:HG22	2.01	0.41
34:YA:1299:G:H22	34:YA:1640:C:H5'	1.85	0.41
34:YA:2392:A:H8	44:YP:61:ARG:HG2	1.85	0.41
34:YA:2641:G:H2'	34:YA:2642:G:H8	1.85	0.41
47:YS:34:HIS:O	47:YS:97:ARG:NH2	2.54	0.41
54:YZ:59:LEU:HB3	54:YZ:61:LEU:HD12	2.03	0.41
2:QB:16:HIS:HA	2:QB:210:SER:HB2	2.02	0.41
2:QB:32:ILE:HD11	2:QB:190:THR:HG22	2.01	0.41
11:QK:38:ASN:HA	11:QK:39:PRO:HD3	1.90	0.41
22:QV:60:U:H5''	22:QV:61:C:C5	2.56	0.41
34:RA:1826:G:H4'	36:RD:242:ARG:HH21	1.84	0.41
34:RA:2233:U:H2'	34:RA:2234:G:C8	2.56	0.41
39:RG:73:ALA:CB	39:RG:82:LEU:HD11	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:RH:31:GLY:HA3	40:RH:136:ILE:HD13	2.02	0.41
45:RQ:4:PRO:HG3	45:RQ:69:PHE:HE2	1.86	0.41
1:XA:112:G:H4'	1:XA:389:A:H4'	2.02	0.41
1:XA:264:U:O2'	17:XQ:64:PRO:O	2.34	0.41
4:XD:19:LEU:HD21	4:XD:197:PRO:HG2	1.93	0.41
4:XD:19:LEU:CD1	4:XD:63:LYS:CG	2.94	0.41
4:XD:119:GLN:HG2	4:XD:123:HIS:CD2	2.56	0.41
15:XO:88:ARG:NH1	34:YA:713:G:OP2	2.41	0.41
32:Y8:34:TRP:CE2	32:Y8:35:GLN:HG3	2.55	0.41
34:YA:642:G:H21	34:YA:646:A:H2	1.67	0.41
34:YA:949:C:H2'	34:YA:950:G:C8	2.55	0.41
34:YA:1408:C:H2'	34:YA:1409:C:C6	2.55	0.41
34:YA:1423:G:H2'	34:YA:1424:G:H8	1.84	0.41
36:YD:182:LEU:HB2	36:YD:271:ILE:HB	2.01	0.41
1:QA:130:A:H5'	17:QQ:63:ARG:HH11	1.85	0.41
1:QA:636:U:H5'	17:QQ:2:PRO:HG3	2.02	0.41
1:QA:1123:A:H4'	10:QJ:36:GLY:HA3	2.03	0.41
1:QA:1427:U:H2'	1:QA:1428:A:C8	2.56	0.41
3:QC:24:ALA:HB2	3:QC:32:LEU:HD22	2.01	0.41
40:RH:12:PRO:HG3	40:RH:48:GLY:C	2.46	0.41
41:RI:72:LEU:HG	41:RI:138:ILE:HD13	2.02	0.41
44:RP:29:LYS:HD2	44:RP:30:THR:HG23	2.01	0.41
1:XA:323:U:OP1	20:XT:26:ASN:ND2	2.45	0.41
1:XA:337:C:H2'	1:XA:338:A:C8	2.56	0.41
1:XA:1071:C:H5''	5:XE:49:PRO:HG2	2.02	0.41
26:Y2:41:ILE:HD11	26:Y2:44:LEU:HD12	2.01	0.41
34:YA:1800:C:O2	34:YA:1817:G:O6	2.38	0.41
34:YA:2853:C:H2'	34:YA:2854:G:C8	2.55	0.41
37:YE:52:LEU:HB3	37:YE:76:ARG:HD3	2.02	0.41
1:QA:628:G:H2'	1:QA:629:G:C8	2.55	0.41
1:QA:636:U:H2'	1:QA:637:G:C8	2.55	0.41
12:QL:24:VAL:HG13	12:QL:98:TYR:HE1	1.85	0.41
20:QT:26:ASN:HA	20:QT:29:LYS:HG2	2.01	0.41
34:RA:380:U:H2'	34:RA:381:G:H8	1.86	0.41
34:RA:828:U:H4'	34:RA:831:G:N1	2.36	0.41
34:RA:1525:G:H2'	34:RA:1526:G:C8	2.56	0.41
34:RA:2445:G:P	38:RF:74:ARG:HH22	2.43	0.41
34:RA:2639:A:O2'	42:RN:97:ARG:NH2	2.53	0.41
50:RV:52:VAL:HG23	50:RV:54:GLY:H	1.84	0.41
54:RZ:128:VAL:HG11	54:RZ:133:ILE:HA	2.02	0.41
1:XA:624:C:H2'	1:XA:625:G:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:1297:C:H42	7:XG:115:ARG:HH21	1.68	0.41
1:XA:1347:G:H22	1:XA:1373:G:H3'	1.85	0.41
1:XA:1409:C:H2'	1:XA:1410:G:H8	1.86	0.41
1:XA:1412:C:H2'	1:XA:1413:A:C8	2.55	0.41
11:XK:31:THR:HA	11:XK:42:TRP:HA	2.01	0.41
25:Y1:60:PHE:HB3	25:Y1:62:VAL:HG13	2.02	0.41
34:YA:941:A:O2'	34:YA:1190:G:O3'	2.36	0.41
34:YA:1205:U:C4	38:YF:171:PRO:HA	2.56	0.41
34:YA:2312:U:O2	39:YG:40:ASN:ND2	2.53	0.41
34:YA:2836:U:H2'	34:YA:2837:G:C8	2.55	0.41
1:QA:522:C:H41	12:QL:53:ARG:NH2	2.18	0.41
34:RA:270:A:OP2	34:RA:270(Y):G:N1	2.53	0.41
34:RA:504:U:H5''	34:RA:505:A:H5'	2.01	0.41
34:RA:2627:G:O2'	34:RA:2781:A:N1	2.41	0.41
39:RG:73:ALA:HB2	39:RG:82:LEU:HD11	2.03	0.41
40:RH:153:LYS:HD3	40:RH:162:ILE:HG13	2.02	0.41
1:XA:736:C:H2'	1:XA:737:A:C8	2.55	0.41
1:XA:985:C:H2'	1:XA:986:A:C8	2.56	0.41
1:XA:1392:G:N2	1:XA:1502:A:H8	2.19	0.41
1:XA:1513:A:H2'	1:XA:1514:C:C6	2.55	0.41
12:XL:45:PRO:HG3	12:XL:53:ARG:HD3	2.02	0.41
29:Y5:19:ARG:HH21	34:YA:1265:A:H3'	1.86	0.41
42:YN:47:ALA:O	42:YN:119:ARG:NH1	2.51	0.41
43:YO:1:MET:HB2	43:YO:32:TYR:HB3	2.01	0.41
45:YQ:62:GLY:HA2	54:YZ:116:VAL:HG21	2.02	0.41
45:YQ:66:ILE:C	45:YQ:68:ILE:H	2.29	0.41
1:QA:196:A:OP1	20:QT:68:LYS:NZ	2.40	0.41
1:QA:627:G:H2'	1:QA:628:G:H8	1.85	0.41
1:QA:950:U:H2'	1:QA:951:G:C8	2.56	0.41
34:RA:1063:G:OP1	34:RA:1065:U:O2'	2.34	0.41
34:RA:2683:C:H5'	48:RT:58:ASN:HD22	1.84	0.41
34:RA:2853:C:H2'	34:RA:2854:G:C8	2.56	0.41
36:RD:108:PRO:HB3	36:RD:143:HIS:CE1	2.56	0.41
39:RG:22:ARG:HH12	39:RG:175:LEU:HD11	1.85	0.41
39:RG:135:LEU:HB2	39:RG:155:MET:HB3	2.01	0.41
1:XA:409:G:H5''	4:XD:25:ARG:HG3	2.02	0.41
4:XD:61:LYS:HE3	4:XD:61:LYS:HB3	1.91	0.41
5:XE:72:GLN:HE22	5:XE:144:THR:HG22	1.86	0.41
13:XM:66:LEU:HB3	13:XM:67:GLU:H	1.66	0.41
18:XR:37:VAL:O	18:XR:41:LYS:N	2.53	0.41
22:XV:65:C:H2'	22:XV:66:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Y6:38:LYS:NZ	34:YA:2347:C:OP1	2.38	0.41
33:Y9:25:VAL:HB	33:Y9:34:GLN:HB2	2.02	0.41
34:YA:545:G:N2	34:YA:548:A:OP2	2.45	0.41
34:YA:1535:U:H5'	34:YA:1537:C:N3	2.36	0.41
34:YA:2743:C:HO2'	40:YH:153:LYS:NZ	2.19	0.41
50:YV:6:LYS:HB2	50:YV:39:LEU:HD21	2.03	0.41
1:QA:134:A:H61	16:QP:25:ARG:NH1	2.18	0.41
1:QA:348:G:H2'	1:QA:349:A:H8	1.85	0.41
1:QA:514:C:H2'	1:QA:515:G:C8	2.54	0.41
1:QA:539:A:H2'	1:QA:540:G:C8	2.56	0.41
1:QA:639:G:H2'	1:QA:640:A:H8	1.86	0.41
5:QE:78:HIS:HE1	5:QE:80:ILE:HD13	1.85	0.41
6:QF:95:GLU:HA	6:QF:96:PRO:HD3	1.95	0.41
7:QG:27:ILE:HD12	7:QG:27:ILE:HA	1.89	0.41
24:R0:38:VAL:HB	24:R0:59:LEU:HD12	2.02	0.41
32:R8:46:ARG:NH1	34:RA:630:G:OP1	2.53	0.41
34:RA:629:G:N3	34:RA:639:U:O2'	2.53	0.41
34:RA:689:A:H2'	34:RA:690:G:C8	2.56	0.41
34:RA:1258:C:H2'	34:RA:1259:G:C8	2.56	0.41
34:RA:1791:A:H5'	36:RD:206:LEU:HD12	2.02	0.41
34:RA:2081:C:H2'	34:RA:2082:A:H8	1.85	0.41
34:RA:2696:U:H2'	34:RA:2697:G:H8	1.84	0.41
34:RA:2718:G:O2'	34:RA:2847:U:OP1	2.34	0.41
37:RE:29:GLY:HA2	37:RE:180:ASN:HB3	2.02	0.41
42:RN:21:LYS:HE2	42:RN:21:LYS:HB2	1.82	0.41
1:XA:590:C:OP1	8:XH:30:ARG:N	2.50	0.41
1:XA:1119:C:H2'	1:XA:1120:G:C8	2.54	0.41
1:XA:1287:A:H2'	1:XA:1288:A:C8	2.56	0.41
1:XA:1288:A:H2'	1:XA:1289:A:C8	2.56	0.41
1:XA:1308:U:H2'	1:XA:1309:G:H8	1.85	0.41
1:XA:1507:A:H2'	1:XA:1508:G:C8	2.56	0.41
3:XC:9:GLY:HA3	14:XN:49:HIS:HA	2.03	0.41
4:XD:104:VAL:HG21	4:XD:140:VAL:HG21	2.02	0.41
5:XE:48:ALA:HB2	5:XE:57:LYS:HE3	2.03	0.41
10:XJ:51:ARG:CZ	10:XJ:61:GLU:HB3	2.51	0.41
27:Y3:26:LEU:O	27:Y3:35:ARG:HG2	2.21	0.41
34:YA:271(D):G:H2'	34:YA:272:G:C8	2.56	0.41
34:YA:288:C:H2'	34:YA:289:A:C8	2.55	0.41
34:YA:813:U:H2'	34:YA:814:C:C6	2.56	0.41
34:YA:996:A:O2'	49:YU:92:ARG:NE	2.54	0.41
34:YA:1441:G:H2'	34:YA:1442:G:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:1800:C:N3	34:YA:1817:G:N1	2.68	0.41
34:YA:1812:A:H2'	34:YA:1813:G:H8	1.86	0.41
34:YA:1817:G:OP2	36:YD:157:ARG:NH2	2.54	0.41
34:YA:1918:A:O2'	34:YA:1920:C:N4	2.54	0.41
34:YA:2051:A:H4'	37:YE:141:ILE:HG12	2.03	0.41
34:YA:2096:U:O4	34:YA:2193:G:O6	2.39	0.41
34:YA:2708:G:H2'	34:YA:2709:G:H8	1.86	0.41
40:YH:164:TYR:HB2	40:YH:167:GLU:HB2	2.02	0.41
41:YI:13:GLY:HA2	41:YI:17:GLN:HG3	2.02	0.41
43:YO:8:LEU:HB2	43:YO:19:ILE:HG13	2.03	0.41
45:YQ:13:GLN:O	45:YQ:72:LYS:NZ	2.43	0.41
51:YW:22:ASP:OD1	51:YW:25:ARG:NH1	2.49	0.41
1:QA:34:C:H2'	1:QA:35:G:C8	2.55	0.41
1:QA:662:G:H2'	1:QA:663:A:C8	2.55	0.41
1:QA:1228:C:H4'	13:QM:116:THR:HA	2.03	0.41
3:QC:150:LYS:HE3	3:QC:167:TRP:HE1	1.85	0.41
12:QL:60:LEU:HD12	12:QL:62:SER:H	1.86	0.41
24:R0:23:VAL:HG21	34:RA:857:C:H4'	2.03	0.41
34:RA:1662:C:O2'	34:RA:2687:U:OP1	2.37	0.41
34:RA:2314:C:H2'	34:RA:2315:G:C8	2.55	0.41
34:RA:2329:G:H2'	34:RA:2330:G:H8	1.86	0.41
34:RA:2406:U:C2	44:RP:72:PRO:HB2	2.56	0.41
34:RA:2710:C:H2'	34:RA:2711:A:C8	2.56	0.41
35:RB:42:C:H5''	39:RG:69:ALA:HB2	2.02	0.41
41:RI:46:ALA:O	41:RI:50:ARG:HG2	2.21	0.41
44:RP:58:THR:C	44:RP:60:MET:H	2.29	0.41
47:RS:10:ARG:HG2	47:RS:13:ARG:HH22	1.86	0.41
49:RU:90:VAL:HG11	50:RV:40:LEU:HG	2.02	0.41
1:XA:76:G:H1	1:XA:93:U:H3	1.68	0.41
6:XF:99:ALA:HB1	18:XR:23:LYS:HE3	2.03	0.41
7:XG:13:GLN:HA	7:XG:14:PRO:HD3	1.95	0.41
15:XO:17:ARG:HH12	15:XO:77:ARG:NH1	2.19	0.41
24:Y0:35:ASN:HD22	34:YA:2354:G:H4'	1.87	0.41
25:Y1:28:GLY:HA2	34:YA:2397:G:H5''	2.03	0.41
30:Y6:10:LEU:HD13	30:Y6:19:ARG:HD3	2.02	0.41
34:YA:24:G:O2'	51:YW:78:GLU:O	2.35	0.41
34:YA:299:A:N1	34:YA:322:A:O2'	2.50	0.41
34:YA:303:U:H2'	34:YA:304:G:C8	2.56	0.41
34:YA:700:G:O2'	34:YA:1632:A:N3	2.47	0.41
34:YA:2123:G:H2'	34:YA:2124:G:H8	1.86	0.41
36:YD:13:ARG:NH1	36:YD:16:MET:SD	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:YO:78:ARG:HH21	48:YT:103:ARG:NH2	2.19	0.41
51:YW:1:MET:C	51:YW:64:MET:HE2	2.30	0.41
1:QA:486:U:H2'	1:QA:487:A:H8	1.86	0.40
1:QA:552:U:H2'	1:QA:553:A:H8	1.85	0.40
1:QA:851:G:H2'	1:QA:852:G:H8	1.85	0.40
1:QA:1492:A:OP1	12:QL:47:LYS:CG	2.69	0.40
4:QD:101:LEU:HB2	4:QD:138:TYR:HB3	2.03	0.40
5:QE:93:PRO:HG2	8:QH:105:ARG:HE	1.86	0.40
20:QT:29:LYS:O	20:QT:33:ILE:HG12	2.21	0.40
34:RA:626:U:O4	44:RP:81:GLN:NE2	2.52	0.40
34:RA:949:C:H2'	34:RA:950:G:C8	2.56	0.40
34:RA:1782:C:H1'	34:RA:2609:U:H5''	2.03	0.40
1:XA:881:G:P	12:XL:12:ARG:HH22	2.45	0.40
1:XA:1151:A:H2'	1:XA:1152:A:C8	2.56	0.40
1:XA:1286:A:N3	21:XU:22:ARG:NH2	2.69	0.40
1:XA:1492:A:H2'	1:XA:1493:A:C4	2.55	0.40
4:XD:85:LYS:HD2	4:XD:92:VAL:HG11	2.03	0.40
11:XK:21:ILE:HG12	11:XK:30:VAL:HG12	2.03	0.40
21:XU:10:ARG:HG2	21:XU:13:ILE:HD12	2.03	0.40
24:Y0:19:LYS:NZ	34:YA:2387:U:O2'	2.54	0.40
34:YA:513:A:O2'	34:YA:1217:C:OP1	2.34	0.40
34:YA:840:C:H2'	34:YA:841:A:H8	1.86	0.40
34:YA:2036:C:H2'	34:YA:2037:G:H8	1.85	0.40
34:YA:2698:U:H2'	34:YA:2699:C:C6	2.56	0.40
40:YH:116:GLU:HA	40:YH:117:PRO:HD3	1.95	0.40
42:YN:39:ARG:HB2	42:YN:48:MET:HE1	2.02	0.40
47:YS:78:LEU:HD11	47:YS:108:GLY:O	2.21	0.40
48:YT:27:THR:HB	48:YT:90:GLN:HB3	2.03	0.40
1:QA:690:G:H22	11:QK:55:LYS:NZ	2.19	0.40
1:QA:1356:G:H2'	1:QA:1357:A:H8	1.85	0.40
25:R1:87:PRO:HA	25:R1:90:ILE:HG22	2.02	0.40
27:R3:16:PRO:HA	34:RA:969:U:H5'	2.04	0.40
32:R8:52:LYS:NZ	34:RA:834:C:H4'	2.31	0.40
34:RA:1681:G:O2'	34:RA:1762:A:O2'	2.25	0.40
34:RA:2014:A:H4'	51:RW:92:ARG:HH12	1.86	0.40
37:RE:57:LYS:HA	37:RE:57:LYS:CE	2.49	0.40
42:RN:35:ARG:HH21	42:RN:42:TRP:HZ2	1.69	0.40
45:RQ:115:MET:HG2	45:RQ:131:ILE:HG21	2.04	0.40
1:XA:165:C:H2'	1:XA:166:G:C8	2.56	0.40
1:XA:677:U:H3	1:XA:713:G:H22	1.69	0.40
1:XA:779:C:H5''	11:XK:122:LYS:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:1446:A:H4'	48:YT:125:ARG:HH12	1.86	0.40
32:Y8:12:LYS:NZ	34:YA:249:C:O2	2.43	0.40
34:YA:191:A:H2'	34:YA:192:C:H6	1.87	0.40
34:YA:1780:A:O2'	34:YA:1781:C:O2	2.36	0.40
34:YA:1791:A:H4'	36:YD:206:LEU:HB2	2.03	0.40
34:YA:2590:A:H2'	34:YA:2591:C:C6	2.56	0.40
36:YD:245:PRO:HA	36:YD:246:PRO:HD3	1.79	0.40
46:YR:3:HIS:O	46:YR:5:LYS:N	2.53	0.40
1:QA:539:A:H2'	1:QA:540:G:H8	1.86	0.40
1:QA:1220:G:H2'	1:QA:1221:G:H8	1.85	0.40
1:QA:1408:A:HO2'	34:RA:1916:A:H61	1.68	0.40
32:R8:61:LEU:HD22	32:R8:61:LEU:HA	1.91	0.40
34:RA:570:G:H2'	34:RA:2030:A:C5	2.57	0.40
34:RA:588:U:H1'	38:RF:90:PHE:HB3	2.02	0.40
34:RA:648:G:H2'	34:RA:649:G:H8	1.85	0.40
34:RA:815:C:OP2	50:RV:83:ARG:NH1	2.54	0.40
34:RA:2443:C:H2'	34:RA:2444:G:C8	2.57	0.40
34:RA:2630:G:H2'	34:RA:2631:G:C8	2.55	0.40
37:RE:119:ARG:HG3	37:RE:160:TYR:HB2	2.02	0.40
39:RG:41:GLN:HE22	39:RG:43:LEU:HD21	1.87	0.40
39:RG:97:ASP:HA	39:RG:100:TRP:HD1	1.86	0.40
1:XA:1095:U:OP2	1:XA:1108:G:N1	2.49	0.40
1:XA:1435:G:H2'	1:XA:1436:U:C6	2.56	0.40
1:XA:1492:A:OP1	12:XL:47:LYS:CG	2.69	0.40
8:XH:100:ILE:HA	8:XH:101:PRO:HD3	1.93	0.40
11:XK:11:LYS:HD2	11:XK:12:ARG:HB2	2.04	0.40
22:XV:60:U:H5''	22:XV:61:C:C5	2.56	0.40
34:YA:271(D):G:H2'	34:YA:272:G:H8	1.86	0.40
34:YA:673:C:H5''	38:YF:81:PRO:HD2	2.03	0.40
34:YA:1434:A:H61	34:YA:1558:A:H62	1.69	0.40
34:YA:2020:A:H4'	49:YU:25:TRP:HZ3	1.85	0.40
34:YA:2037:G:H2'	34:YA:2038:G:C8	2.57	0.40
37:YE:24:THR:HG21	37:YE:188:VAL:HB	2.03	0.40
39:YG:150:ASP:OD1	39:YG:153:ARG:NH1	2.55	0.40
1:QA:380:G:N2	1:QA:383:A:OP2	2.40	0.40
1:QA:779:C:H5''	11:QK:122:LYS:HG2	2.04	0.40
1:QA:855:G:OP2	1:QA:871:U:N3	2.42	0.40
1:QA:1145:C:H4'	1:QA:1146:A:H8	1.86	0.40
1:QA:1244:C:H2'	1:QA:1245:A:C8	2.57	0.40
17:QQ:11:VAL:HG12	17:QQ:85:VAL:HG22	2.04	0.40
26:R2:14:ARG:NH1	26:R2:66:GLU:OE1	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:R8:31:HIS:ND1	32:R8:32:LEU:HG	2.36	0.40
34:RA:439:G:H2'	34:RA:440:G:C8	2.57	0.40
34:RA:1113:U:H2'	34:RA:1114:G:C8	2.56	0.40
34:RA:1265:A:H61	34:RA:2013:A:H5''	1.86	0.40
34:RA:2291:U:OP1	34:RA:2380:C:O2'	2.38	0.40
34:RA:2487:G:H2'	34:RA:2488:A:C8	2.56	0.40
34:RA:2841:C:H2'	34:RA:2842:G:C8	2.57	0.40
39:RG:106:LEU:HD12	39:RG:110:ALA:HB3	2.04	0.40
51:RW:24:ILE:HD13	51:RW:36:LEU:HD11	2.03	0.40
1:XA:582:U:OP2	1:XA:758:G:N1	2.42	0.40
1:XA:753:A:OP1	15:XO:69:TYR:OH	2.33	0.40
10:XJ:52:GLY:HA2	10:XJ:53:PRO:HD3	1.91	0.40
28:Y4:5:ILE:HD12	39:YG:67:LYS:HE2	2.04	0.40
34:YA:551:G:H5'	34:YA:1220:A:H1'	2.03	0.40
34:YA:828:U:H4'	34:YA:831:G:N1	2.36	0.40
34:YA:1062:G:H1'	34:YA:1088:A:C5	2.57	0.40
34:YA:1927:A:H2'	34:YA:1928:A:C8	2.56	0.40
34:YA:2212:A:H1'	34:YA:2215:G:C5	2.56	0.40
34:YA:2506:U:O2	56:Z8:76:PPU:O2'	2.38	0.40
34:YA:2730:C:H2'	34:YA:2731:G:H8	1.86	0.40
37:YE:32:PRO:HA	37:YE:90:THR:HA	2.02	0.40
45:YQ:27:VAL:HG13	45:YQ:105:GLU:CD	2.42	0.40
46:YR:104:ARG:HG3	46:YR:107:ASP:HB3	2.04	0.40
1:QA:745:C:H2'	1:QA:746:A:C8	2.57	0.40
1:QA:1025:U:O2'	1:QA:1026:G:O4'	2.37	0.40
4:QD:152:SER:HA	4:QD:155:LEU:HD13	2.03	0.40
4:QD:173:TRP:CD1	4:QD:174:LEU:HG	2.56	0.40
32:R8:22:VAL:HB	32:R8:53:PRO:HB3	2.03	0.40
34:RA:271(D):G:H2'	34:RA:272:G:H8	1.87	0.40
34:RA:411:G:OP2	34:RA:2406:U:O2'	2.32	0.40
34:RA:1791:A:N6	34:RA:1828:G:O2'	2.50	0.40
36:RD:231:HIS:CD2	36:RD:249:PRO:HG3	2.56	0.40
45:RQ:17:LEU:HA	45:RQ:98:LYS:HE2	2.04	0.40
54:RZ:24:LEU:HD13	54:RZ:41:LEU:HD12	2.04	0.40
1:XA:789:U:H1'	1:XA:792:A:H2	1.87	0.40
6:XF:80:ARG:NE	6:XF:88:VAL:HB	2.37	0.40
34:YA:18:C:O2'	34:YA:553:U:OP1	2.40	0.40
34:YA:1888:G:OP2	34:YA:1888:G:N2	2.51	0.40
34:YA:1992:G:N2	34:YA:1996:C:O2'	2.55	0.40
34:YA:2131:G:H4'	34:YA:2132:U:H4'	2.03	0.40
34:YA:2154:G:H2'	34:YA:2155:G:C8	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:2291:U:H2'	34:YA:2292:C:C6	2.56	0.40
34:YA:2314:C:H2'	34:YA:2315:G:H8	1.87	0.40
34:YA:2497:A:H1'	34:YA:2498:C:H5	1.85	0.40
37:YE:54:GLN:NE2	37:YE:76:ARG:HG2	2.37	0.40
43:YO:111:PHE:HB3	43:YO:114:ILE:HD12	2.04	0.40
46:YR:79:LEU:HD12	46:YR:83:ILE:HB	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	233/256 (91%)	210 (90%)	22 (9%)	1 (0%)	30	59
2	XB	234/256 (91%)	211 (90%)	22 (9%)	1 (0%)	30	59
3	QC	203/239 (85%)	195 (96%)	8 (4%)	0	100	100
3	XC	203/239 (85%)	191 (94%)	10 (5%)	2 (1%)	12	41
4	QD	206/209 (99%)	202 (98%)	4 (2%)	0	100	100
4	XD	206/209 (99%)	195 (95%)	9 (4%)	2 (1%)	12	41
5	QE	149/162 (92%)	145 (97%)	4 (3%)	0	100	100
5	XE	149/162 (92%)	140 (94%)	9 (6%)	0	100	100
6	QF	99/101 (98%)	97 (98%)	2 (2%)	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%)	151 (99%)	2 (1%)	0	100	100
8	QH	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
8	XH	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
9	QI	125/128 (98%)	116 (93%)	9 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	XI	124/128 (97%)	114 (92%)	10 (8%)	0	100	100
10	QJ	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
10	XJ	94/105 (90%)	85 (90%)	9 (10%)	0	100	100
11	QK	117/129 (91%)	111 (95%)	6 (5%)	0	100	100
11	XK	114/129 (88%)	106 (93%)	8 (7%)	0	100	100
12	QL	123/131 (94%)	115 (94%)	7 (6%)	1 (1%)	16	45
12	XL	120/131 (92%)	109 (91%)	11 (9%)	0	100	100
13	QM	118/126 (94%)	103 (87%)	13 (11%)	2 (2%)	7	31
13	XM	117/126 (93%)	102 (87%)	14 (12%)	1 (1%)	14	43
14	QN	58/61 (95%)	52 (90%)	5 (9%)	1 (2%)	7	31
14	XN	58/61 (95%)	52 (90%)	5 (9%)	1 (2%)	7	31
15	QO	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
15	XO	85/89 (96%)	82 (96%)	3 (4%)	0	100	100
16	QP	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
16	XP	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
17	QQ	98/105 (93%)	96 (98%)	2 (2%)	0	100	100
17	XQ	98/105 (93%)	96 (98%)	2 (2%)	0	100	100
18	QR	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
18	XR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
19	QS	81/93 (87%)	75 (93%)	6 (7%)	0	100	100
19	XS	82/93 (88%)	72 (88%)	10 (12%)	0	100	100
20	QT	97/106 (92%)	90 (93%)	7 (7%)	0	100	100
20	XT	97/106 (92%)	86 (89%)	10 (10%)	1 (1%)	12	41
21	QU	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
21	XU	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
24	R0	74/85 (87%)	71 (96%)	3 (4%)	0	100	100
24	Y0	73/85 (86%)	71 (97%)	2 (3%)	0	100	100
25	R1	95/98 (97%)	84 (88%)	11 (12%)	0	100	100
25	Y1	91/98 (93%)	81 (89%)	10 (11%)	0	100	100
26	R2	67/72 (93%)	63 (94%)	4 (6%)	0	100	100
26	Y2	66/72 (92%)	64 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	R3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	Y3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	R4	67/71 (94%)	56 (84%)	11 (16%)	0	100	100
28	Y4	67/71 (94%)	53 (79%)	13 (19%)	1 (2%)	8	33
29	R5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
29	Y5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
30	R6	51/54 (94%)	51 (100%)	0	0	100	100
30	Y6	51/54 (94%)	51 (100%)	0	0	100	100
31	R7	45/49 (92%)	44 (98%)	1 (2%)	0	100	100
31	Y7	46/49 (94%)	46 (100%)	0	0	100	100
32	R8	62/65 (95%)	50 (81%)	8 (13%)	4 (6%)	1	10
32	Y8	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
33	R9	35/37 (95%)	35 (100%)	0	0	100	100
33	Y9	35/37 (95%)	35 (100%)	0	0	100	100
36	RD	270/276 (98%)	254 (94%)	15 (6%)	1 (0%)	30	59
36	YD	270/276 (98%)	257 (95%)	13 (5%)	0	100	100
37	RE	203/206 (98%)	170 (84%)	33 (16%)	0	100	100
37	YE	202/206 (98%)	189 (94%)	11 (5%)	2 (1%)	12	41
38	RF	200/210 (95%)	185 (92%)	15 (8%)	0	100	100
38	YF	200/210 (95%)	183 (92%)	17 (8%)	0	100	100
39	RG	179/182 (98%)	159 (89%)	17 (10%)	3 (2%)	7	31
39	YG	179/182 (98%)	160 (89%)	18 (10%)	1 (1%)	21	51
40	RH	172/180 (96%)	152 (88%)	17 (10%)	3 (2%)	7	31
40	YH	171/180 (95%)	164 (96%)	7 (4%)	0	100	100
41	RI	144/148 (97%)	127 (88%)	14 (10%)	3 (2%)	5	27
41	YI	144/148 (97%)	127 (88%)	12 (8%)	5 (4%)	3	20
42	RN	136/140 (97%)	122 (90%)	13 (10%)	1 (1%)	18	48
42	YN	136/140 (97%)	120 (88%)	15 (11%)	1 (1%)	18	48
43	RO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
43	YO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
44	RP	148/150 (99%)	126 (85%)	20 (14%)	2 (1%)	9	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	YP	145/150 (97%)	137 (94%)	7 (5%)	1 (1%)	18	48
45	RQ	139/141 (99%)	122 (88%)	16 (12%)	1 (1%)	18	48
45	YQ	139/141 (99%)	122 (88%)	15 (11%)	2 (1%)	9	34
46	RR	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
46	YR	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	14	43
47	RS	109/112 (97%)	90 (83%)	17 (16%)	2 (2%)	6	30
47	YS	109/112 (97%)	94 (86%)	15 (14%)	0	100	100
48	RT	135/146 (92%)	122 (90%)	13 (10%)	0	100	100
48	YT	135/146 (92%)	124 (92%)	11 (8%)	0	100	100
49	RU	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	14	43
49	YU	115/118 (98%)	105 (91%)	8 (7%)	2 (2%)	7	31
50	RV	99/101 (98%)	86 (87%)	11 (11%)	2 (2%)	6	28
50	YV	99/101 (98%)	87 (88%)	11 (11%)	1 (1%)	12	41
51	RW	111/113 (98%)	106 (96%)	5 (4%)	0	100	100
51	YW	111/113 (98%)	105 (95%)	5 (4%)	1 (1%)	14	43
52	RX	90/96 (94%)	87 (97%)	3 (3%)	0	100	100
52	YX	90/96 (94%)	87 (97%)	3 (3%)	0	100	100
53	RY	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
53	YY	105/110 (96%)	103 (98%)	2 (2%)	0	100	100
54	RZ	201/206 (98%)	186 (92%)	14 (7%)	1 (0%)	24	55
54	YZ	201/206 (98%)	186 (92%)	12 (6%)	3 (2%)	8	33
All	All	11484/12126 (95%)	10639 (93%)	787 (7%)	58 (0%)	24	55

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	R8	62	LEU
40	RH	12	PRO
41	RI	132	PRO
44	RP	108	LYS
50	RV	46	VAL
50	RV	50	PRO
41	YI	118	LYS
41	YI	132	PRO
50	YV	50	PRO

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Mol	Chain	Res	Type
14	QN	17	LYS
32	R8	27	THR
39	RG	82	LEU
39	RG	84	LYS
41	RI	119	PRO
47	RS	4	LEU
4	XD	20	TYR
4	XD	32	ALA
37	YE	147	PRO
44	YP	63	PRO
49	YU	95	LEU
54	YZ	13	GLU
54	YZ	166	SER
2	QB	234	PRO
13	QM	66	LEU
40	RH	129	THR
49	RU	97	ASP
2	XB	234	PRO
49	YU	93	LYS
12	QL	105	TYR
39	RG	81	LYS
40	RH	126	PRO
14	XN	17	LYS
41	YI	12	LEU
45	YQ	67	ARG
13	QM	69	GLU
32	R8	52	LYS
36	RD	200	ASP
42	RN	23	LEU
3	XC	12	LEU
28	Y4	48	ARG
37	YE	52	LEU
46	YR	4	LEU
51	YW	65	LEU
41	RI	133	HIS
47	RS	88	ASP
13	XM	106	ASN
39	YG	82	LEU
41	YI	10	GLU
42	YN	22	THR
32	R8	38	GLY
44	RP	109	GLY

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Mol	Chain	Res	Type
54	RZ	53	ILE
20	XT	96	GLY
45	RQ	78	PRO
3	XC	81	GLY
41	YI	119	PRO
45	YQ	78	PRO
54	YZ	167	PRO

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%)	200 (98%)	3 (2%)	57	66
2	XB	204/220 (93%)	204 (100%)	0	100	100
3	QC	159/188 (85%)	158 (99%)	1 (1%)	78	77
3	XC	159/188 (85%)	158 (99%)	1 (1%)	78	77
4	QD	180/181 (99%)	179 (99%)	1 (1%)	78	77
4	XD	180/181 (99%)	179 (99%)	1 (1%)	78	77
5	QE	116/123 (94%)	116 (100%)	0	100	100
5	XE	116/123 (94%)	116 (100%)	0	100	100
6	QF	90/90 (100%)	90 (100%)	0	100	100
6	XF	90/90 (100%)	90 (100%)	0	100	100
7	QG	126/127 (99%)	126 (100%)	0	100	100
7	XG	126/127 (99%)	125 (99%)	1 (1%)	73	74
8	QH	118/119 (99%)	118 (100%)	0	100	100
8	XH	118/119 (99%)	117 (99%)	1 (1%)	73	74
9	QI	98/99 (99%)	94 (96%)	4 (4%)	27	50
9	XI	97/99 (98%)	96 (99%)	1 (1%)	68	72
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	86/92 (94%)	85 (99%)	1 (1%)	63	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	QK	90/99 (91%)	90 (100%)	0	100	100
11	XK	88/99 (89%)	88 (100%)	0	100	100
12	QL	104/108 (96%)	103 (99%)	1 (1%)	68	72
12	XL	103/108 (95%)	102 (99%)	1 (1%)	68	72
13	QM	96/101 (95%)	95 (99%)	1 (1%)	68	72
13	XM	95/101 (94%)	95 (100%)	0	100	100
14	QN	49/50 (98%)	48 (98%)	1 (2%)	48	63
14	XN	49/50 (98%)	49 (100%)	0	100	100
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%)	72 (100%)	0	100	100
16	XP	72/74 (97%)	72 (100%)	0	100	100
17	QQ	95/97 (98%)	95 (100%)	0	100	100
17	XQ	95/97 (98%)	95 (100%)	0	100	100
18	QR	61/77 (79%)	61 (100%)	0	100	100
18	XR	61/77 (79%)	61 (100%)	0	100	100
19	QS	72/80 (90%)	72 (100%)	0	100	100
19	XS	73/80 (91%)	73 (100%)	0	100	100
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
24	R0	61/67 (91%)	61 (100%)	0	100	100
24	Y0	61/67 (91%)	61 (100%)	0	100	100
25	R1	82/83 (99%)	82 (100%)	0	100	100
25	Y1	78/83 (94%)	78 (100%)	0	100	100
26	R2	64/67 (96%)	64 (100%)	0	100	100
26	Y2	64/67 (96%)	63 (98%)	1 (2%)	55	65
27	R3	51/52 (98%)	51 (100%)	0	100	100
27	Y3	51/52 (98%)	43 (84%)	8 (16%)	2	13
28	R4	62/63 (98%)	62 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	Y4	62/63 (98%)	61 (98%)	1 (2%)	55	65
29	R5	51/52 (98%)	51 (100%)	0	100	100
29	Y5	51/52 (98%)	51 (100%)	0	100	100
30	R6	51/52 (98%)	51 (100%)	0	100	100
30	Y6	51/52 (98%)	51 (100%)	0	100	100
31	R7	40/42 (95%)	40 (100%)	0	100	100
31	Y7	41/42 (98%)	41 (100%)	0	100	100
32	R8	54/55 (98%)	45 (83%)	9 (17%)	2	12
32	Y8	54/55 (98%)	54 (100%)	0	100	100
33	R9	34/34 (100%)	34 (100%)	0	100	100
33	Y9	34/34 (100%)	34 (100%)	0	100	100
36	RD	214/218 (98%)	214 (100%)	0	100	100
36	YD	214/218 (98%)	213 (100%)	1 (0%)	81	78
37	RE	165/166 (99%)	162 (98%)	3 (2%)	51	64
37	YE	165/166 (99%)	163 (99%)	2 (1%)	63	70
38	RF	161/166 (97%)	160 (99%)	1 (1%)	78	77
38	YF	161/166 (97%)	161 (100%)	0	100	100
39	RG	155/156 (99%)	149 (96%)	6 (4%)	28	51
39	YG	155/156 (99%)	151 (97%)	4 (3%)	40	58
40	RH	145/148 (98%)	137 (94%)	8 (6%)	19	44
40	YH	144/148 (97%)	144 (100%)	0	100	100
41	RI	122/124 (98%)	114 (93%)	8 (7%)	15	40
41	YI	122/124 (98%)	116 (95%)	6 (5%)	22	46
42	RN	117/119 (98%)	114 (97%)	3 (3%)	40	58
42	YN	117/119 (98%)	117 (100%)	0	100	100
43	RO	100/100 (100%)	100 (100%)	0	100	100
43	YO	100/100 (100%)	100 (100%)	0	100	100
44	RP	116/116 (100%)	114 (98%)	2 (2%)	53	65
44	YP	114/116 (98%)	112 (98%)	2 (2%)	51	64
45	RQ	111/111 (100%)	110 (99%)	1 (1%)	70	73
45	YQ	111/111 (100%)	108 (97%)	3 (3%)	39	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	RR	100/101 (99%)	100 (100%)	0	100	100
46	YR	100/101 (99%)	100 (100%)	0	100	100
47	RS	87/88 (99%)	87 (100%)	0	100	100
47	YS	87/88 (99%)	86 (99%)	1 (1%)	65	71
48	RT	120/127 (94%)	117 (98%)	3 (2%)	42	59
48	YT	120/127 (94%)	119 (99%)	1 (1%)	73	74
49	RU	93/94 (99%)	92 (99%)	1 (1%)	65	71
49	YU	93/94 (99%)	91 (98%)	2 (2%)	45	61
50	RV	82/82 (100%)	80 (98%)	2 (2%)	43	60
50	YV	82/82 (100%)	79 (96%)	3 (4%)	30	52
51	RW	92/92 (100%)	92 (100%)	0	100	100
51	YW	92/92 (100%)	90 (98%)	2 (2%)	45	61
52	RX	74/78 (95%)	74 (100%)	0	100	100
52	YX	74/78 (95%)	74 (100%)	0	100	100
53	RY	88/91 (97%)	88 (100%)	0	100	100
53	YY	88/91 (97%)	88 (100%)	0	100	100
54	RZ	174/179 (97%)	170 (98%)	4 (2%)	44	61
54	YZ	174/179 (97%)	169 (97%)	5 (3%)	37	56
All	All	9706/10064 (96%)	9594 (99%)	112 (1%)	63	70

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	QB	155	LEU
2	QB	231	GLU
2	QB	236	TYR
3	QC	4	LYS
4	QD	162	LEU
9	QI	2	GLU
9	QI	10	ARG
9	QI	37	PHE
9	QI	74	ILE
12	QL	104	VAL
13	QM	67	GLU
14	QN	27	CYS
32	R8	26	LYS

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Mol	Chain	Res	Type
32	R8	29	LYS
32	R8	30	ARG
32	R8	35	GLN
32	R8	44	LYS
32	R8	47	LYS
32	R8	61	LEU
32	R8	64	TYR
32	R8	65	GLU
37	RE	16	ARG
37	RE	59	VAL
37	RE	145	LYS
38	RF	169	ASN
39	RG	79	ASN
39	RG	80	PHE
39	RG	81	LYS
39	RG	82	LEU
39	RG	83	ARG
39	RG	84	LYS
40	RH	11	VAL
40	RH	50	VAL
40	RH	81	GLU
40	RH	83	TYR
40	RH	125	VAL
40	RH	126	PRO
40	RH	127	GLU
40	RH	152	ARG
41	RI	9	LEU
41	RI	10	GLU
41	RI	78	THR
41	RI	81	VAL
41	RI	118	LYS
41	RI	120	ILE
41	RI	123	LEU
41	RI	142	VAL
42	RN	21	LYS
42	RN	22	THR
42	RN	114	ARG
44	RP	107	LYS
44	RP	108	LYS
45	RQ	18	LYS
48	RT	99	LEU
48	RT	112	ARG

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Mol	Chain	Res	Type
48	RT	125	ARG
49	RU	92	ARG
50	RV	50	PRO
50	RV	75	PHE
54	RZ	53	ILE
54	RZ	71	VAL
54	RZ	161	VAL
54	RZ	165	VAL
3	XC	79	ARG
4	XD	31	CYS
7	XG	50	ILE
8	XH	103	VAL
9	XI	81	ILE
10	XJ	47	PHE
12	XL	104	VAL
26	Y2	47	ASN
27	Y3	2	PRO
27	Y3	4	LEU
27	Y3	5	LYS
27	Y3	36	VAL
27	Y3	37	LEU
27	Y3	58	VAL
27	Y3	59	VAL
27	Y3	60	GLU
28	Y4	56	VAL
36	YD	125	ILE
37	YE	52	LEU
37	YE	75	VAL
39	YG	41	GLN
39	YG	82	LEU
39	YG	83	ARG
39	YG	84	LYS
41	YI	9	LEU
41	YI	12	LEU
41	YI	14	ASP
41	YI	120	ILE
41	YI	131	LYS
41	YI	133	HIS
44	YP	70	GLN
44	YP	71	VAL
45	YQ	64	ILE
45	YQ	66	ILE

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Mol	Chain	Res	Type
45	YQ	103	MET
47	YS	106	ARG
48	YT	125	ARG
49	YU	40	PHE
49	YU	93	LYS
50	YV	24	LYS
50	YV	50	PRO
50	YV	51	VAL
51	YW	63	ASP
51	YW	64	MET
54	YZ	53	ILE
54	YZ	54	HIS
54	YZ	58	VAL
54	YZ	59	LEU
54	YZ	165	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
2	QB	224	GLN
3	QC	118	GLN
3	QC	170	GLN
4	QD	74	GLN
4	QD	77	ASN
4	QD	129	ASN
4	QD	161	ASN
5	QE	141	GLN
7	QG	64	GLN
7	QG	68	ASN
9	QI	3	GLN
9	QI	117	HIS
9	QI	124	GLN
11	QK	116	HIS
12	QL	80	HIS
15	QO	62	GLN
16	QP	13	HIS
16	QP	65	GLN
19	QS	47	HIS
26	R2	65	ASN
30	R6	26	ASN
30	R6	29	ASN
36	RD	227	ASN

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Mol	Chain	Res	Type
37	RE	35	GLN
37	RE	143	ASN
38	RF	203	GLN
39	RG	41	GLN
39	RG	66	GLN
39	RG	79	ASN
39	RG	121	ASN
40	RH	139	GLN
41	RI	17	GLN
42	RN	101	HIS
44	RP	27	HIS
45	RQ	141	GLN
46	RR	31	HIS
48	RT	58	ASN
48	RT	90	GLN
49	RU	72	HIS
49	RU	117	GLN
54	RZ	32	HIS
54	RZ	121	HIS
3	XC	3	ASN
4	XD	103	ASN
4	XD	161	ASN
4	XD	201	GLN
5	XE	72	GLN
7	XG	11	GLN
7	XG	28	ASN
7	XG	148	ASN
8	XH	82	HIS
9	XI	38	GLN
10	XJ	78	ASN
12	XL	80	HIS
13	XM	40	ASN
15	XO	50	HIS
18	XR	63	GLN
20	XT	75	ASN
28	Y4	40	HIS
28	Y4	46	GLN
30	Y6	26	ASN
30	Y6	29	ASN
37	YE	137	HIS
38	YF	40	GLN
39	YG	41	GLN

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Mol	Chain	Res	Type
40	YH	65	HIS
43	YO	3	GLN
44	YP	68	GLN
45	YQ	57	HIS
46	YR	31	HIS
46	YR	71	GLN
48	YT	90	GLN
51	YW	60	ASN
54	YZ	55	HIS
54	YZ	73	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1522 (98%)	266 (17%)	30 (2%)
1	XA	1509/1522 (99%)	295 (19%)	25 (1%)
22	QV	72/76 (94%)	17 (23%)	0
22	XV	72/76 (94%)	17 (23%)	0
23	QX	2/23 (8%)	0	0
23	XX	22/23 (95%)	4 (18%)	2 (9%)
34	RA	2877/2915 (98%)	550 (19%)	37 (1%)
34	YA	2880/2915 (98%)	513 (17%)	37 (1%)
35	RB	119/122 (97%)	16 (13%)	1 (0%)
35	YB	119/122 (97%)	18 (15%)	1 (0%)
55	XY	16/17 (94%)	3 (18%)	0
56	Z6	1/3 (33%)	0	0
56	Z8	1/3 (33%)	0	0
All	All	9188/9339 (98%)	1699 (18%)	133 (1%)

All (1699) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	9	G
1	QA	31	G
1	QA	32	A
1	QA	39	G
1	QA	48	C
1	QA	50	A
1	QA	51	A
1	QA	64	G

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Mol	Chain	Res	Type
1	QA	65	U
1	QA	91	C
1	QA	95	G
1	QA	101	A
1	QA	116	A
1	QA	120	A
1	QA	121	C
1	QA	122	G
1	QA	129(A)	G
1	QA	144	G
1	QA	146	G
1	QA	151	A
1	QA	157	G
1	QA	158	G
1	QA	160	A
1	QA	163	C
1	QA	169	C
1	QA	173	U
1	QA	174	C
1	QA	189	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	216	G
1	QA	220	G
1	QA	244	U
1	QA	245	C
1	QA	247	G
1	QA	250	A
1	QA	251	G
1	QA	267	C
1	QA	270	A
1	QA	281	G
1	QA	289	G
1	QA	298	A
1	QA	314	C
1	QA	321	A
1	QA	328	C
1	QA	329	A

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Mol	Chain	Res	Type
1	QA	332	G
1	QA	343	U
1	QA	344	A
1	QA	346	G
1	QA	347	G
1	QA	351	G
1	QA	352	C
1	QA	353	A
1	QA	354	G
1	QA	356	A
1	QA	367	U
1	QA	372	C
1	QA	373	A
1	QA	389	A
1	QA	397	A
1	QA	398	C
1	QA	406	G
1	QA	411	A
1	QA	412	A
1	QA	413	G
1	QA	414	A
1	QA	421	U
1	QA	422	C
1	QA	423	G
1	QA	428	G
1	QA	429	U
1	QA	435	C
1	QA	455	C
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	508	C
1	QA	509	A
1	QA	510	A
1	QA	511	C
1	QA	518	C
1	QA	521	G
1	QA	527	G

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Mol	Chain	Res	Type
1	QA	532	A
1	QA	533	A
1	QA	545	C
1	QA	547	A
1	QA	559	A
1	QA	564	C
1	QA	568	G
1	QA	572	A
1	QA	573	A
1	QA	574	A
1	QA	576	G
1	QA	577	G
1	QA	618	C
1	QA	630	G
1	QA	631	G
1	QA	653	A
1	QA	665	A
1	QA	666	G
1	QA	686	U
1	QA	688	G
1	QA	701	C
1	QA	702	A
1	QA	703	G
1	QA	704	A
1	QA	722	A
1	QA	731	G
1	QA	748	C
1	QA	754	C
1	QA	755	G
1	QA	760	G
1	QA	777	A
1	QA	785	G
1	QA	792	A
1	QA	793	U
1	QA	794	A
1	QA	813	U
1	QA	817	C
1	QA	819	A
1	QA	821	G
1	QA	828	A
1	QA	841	U
1	QA	842	C

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Mol	Chain	Res	Type
1	QA	843	U
1	QA	848	C
1	QA	859	A
1	QA	871	U
1	QA	872	A
1	QA	902	G
1	QA	914	A
1	QA	926	G
1	QA	927	G
1	QA	934	C
1	QA	960	U
1	QA	961	U
1	QA	968	A
1	QA	969	A
1	QA	971	G
1	QA	974	A
1	QA	976	G
1	QA	977	A
1	QA	991	U
1	QA	992	U
1	QA	993	G
1	QA	994	A
1	QA	1001	G
1	QA	1002	G
1	QA	1004	A
1	QA	1006	C
1	QA	1008	C
1	QA	1020	U
1	QA	1024	G
1	QA	1025	U
1	QA	1027	C
1	QA	1028	C
1	QA	1029	G
1	QA	1030	C
1	QA	1031	G
1	QA	1032(A)	G
1	QA	1033	G
1	QA	1034	G
1	QA	1054	C
1	QA	1064	G
1	QA	1065	U
1	QA	1066	C

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Mol	Chain	Res	Type
1	QA	1080	A
1	QA	1081	G
1	QA	1094	G
1	QA	1095	U
1	QA	1101	A
1	QA	1108	G
1	QA	1124	G
1	QA	1125	U
1	QA	1126	U
1	QA	1130	A
1	QA	1131	G
1	QA	1136	U
1	QA	1137	C
1	QA	1138	G
1	QA	1139	G
1	QA	1140	C
1	QA	1146	A
1	QA	1157	A
1	QA	1158	C
1	QA	1159	U
1	QA	1160	G
1	QA	1171	G
1	QA	1178	G
1	QA	1181	G
1	QA	1182	G
1	QA	1183	A
1	QA	1184	G
1	QA	1187	G
1	QA	1196	U
1	QA	1201	A
1	QA	1202	G
1	QA	1212	U
1	QA	1213	A
1	QA	1215	G
1	QA	1224	G
1	QA	1225	A
1	QA	1238	A
1	QA	1240	U
1	QA	1241	G
1	QA	1256	A
1	QA	1257	U
1	QA	1258	G

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Mol	Chain	Res	Type
1	QA	1270	C
1	QA	1280	A
1	QA	1281	U
1	QA	1286	A
1	QA	1287	A
1	QA	1297	C
1	QA	1298	C
1	QA	1299	A
1	QA	1300	G
1	QA	1302	U
1	QA	1303	C
1	QA	1305	G
1	QA	1319	A
1	QA	1320	C
1	QA	1321	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	1364	U
1	QA	1378	C
1	QA	1397	C
1	QA	1398	A
1	QA	1419	G
1	QA	1442	G
1	QA	1446	A
1	QA	1447	G
1	QA	1452	C
1	QA	1453	G
1	QA	1492	A
1	QA	1494	G
1	QA	1499	A
1	QA	1502	A
1	QA	1504	G

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Mol	Chain	Res	Type
1	QA	1506	U
1	QA	1517	G
1	QA	1520	G
1	QA	1529	G
1	QA	1530	G
22	QV	2	G
22	QV	8	U
22	QV	19	G
22	QV	21	A
22	QV	30	G
22	QV	33	U
22	QV	37	T6A
22	QV	48	C
22	QV	49	G
22	QV	53	G
22	QV	54	U
22	QV	55	U
22	QV	57	G
22	QV	59	A
22	QV	61	C
22	QV	74	C
22	QV	76	A
34	RA	14	A
34	RA	15	G
34	RA	27	G
34	RA	34	C
34	RA	35	G
34	RA	46	C
34	RA	51	G
34	RA	55	G
34	RA	72	U
34	RA	74	A
34	RA	75	G
34	RA	83	G
34	RA	101	G
34	RA	103	A
34	RA	118	A
34	RA	119	A
34	RA	120	U
34	RA	131	G
34	RA	139	G
34	RA	140	A

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Mol	Chain	Res	Type
34	RA	177	G
34	RA	181	A
34	RA	196	A
34	RA	199	A
34	RA	215	G
34	RA	216	A
34	RA	221	A
34	RA	222	A
34	RA	223	A
34	RA	226	G
34	RA	229	A
34	RA	230	U
34	RA	233	A
34	RA	248	G
34	RA	249	C
34	RA	252	G
34	RA	265	A
34	RA	266	G
34	RA	270(L)	U
34	RA	270(M)	U
34	RA	270(N)	G
34	RA	270(P)	C
34	RA	271(C)	U
34	RA	273(F)	C
34	RA	275	G
34	RA	276	A
34	RA	277	C
34	RA	278	A
34	RA	299	A
34	RA	311	A
34	RA	323	G
34	RA	324	A
34	RA	329	G
34	RA	330	A
34	RA	338	G
34	RA	346	A
34	RA	352	G
34	RA	363(F)	A
34	RA	364	C
34	RA	371	A
34	RA	372	G
34	RA	373	U

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Mol	Chain	Res	Type
34	RA	386	G
34	RA	395	U
34	RA	405	U
34	RA	406	G
34	RA	411	G
34	RA	412	A
34	RA	428	A
34	RA	444	C
34	RA	448	U
34	RA	454	A
34	RA	455	C
34	RA	456	C
34	RA	457	A
34	RA	470	A
34	RA	481	G
34	RA	501	A
34	RA	504	U
34	RA	505	A
34	RA	509	C
34	RA	513	A
34	RA	527	C
34	RA	529	A
34	RA	531	C
34	RA	532	A
34	RA	533	G
34	RA	537	C
34	RA	539	G
34	RA	540	G
34	RA	546	C
34	RA	547	A
34	RA	549	G
34	RA	556	G
34	RA	563	G
34	RA	571	A
34	RA	573	G
34	RA	574	C
34	RA	575	A
34	RA	588	U
34	RA	603	A
34	RA	607	U
34	RA	614	U
34	RA	615	G

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Mol	Chain	Res	Type
34	RA	616	A
34	RA	617	G
34	RA	627	A
34	RA	634	C
34	RA	637	A
34	RA	638	G
34	RA	645	C
34	RA	646	A
34	RA	647	G
34	RA	651	G
34	RA	652	C
34	RA	654	A
34	RA	654(A)	G
34	RA	669	G
34	RA	686	G
34	RA	722	A
34	RA	726	G
34	RA	730	C
34	RA	753	C
34	RA	765	G
34	RA	776	G
34	RA	782	A
34	RA	784	A
34	RA	785	G
34	RA	789	A
34	RA	790	C
34	RA	791	C
34	RA	792	G
34	RA	800	A
34	RA	805	G
34	RA	812	C
34	RA	819	A
34	RA	827	U
34	RA	828	U
34	RA	831	G
34	RA	847	U
34	RA	856	C
34	RA	857	C
34	RA	859	G
34	RA	866	A
34	RA	869	G
34	RA	882	G

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Mol	Chain	Res	Type
34	RA	884	C
34	RA	885	C
34	RA	886	C
34	RA	888	C
34	RA	889	C
34	RA	896	A
34	RA	898	C
34	RA	900	A
34	RA	907	U
34	RA	910	A
34	RA	914	C
34	RA	915	C
34	RA	917	A
34	RA	932	G
34	RA	941	A
34	RA	945	A
34	RA	946	G
34	RA	953	A
34	RA	959	A
34	RA	961	C
34	RA	973	A
34	RA	974	G
34	RA	974(A)	C
34	RA	980	A
34	RA	983	A
34	RA	996	A
34	RA	1003	G
34	RA	1012	U
34	RA	1013	C
34	RA	1022	G
34	RA	1023	U
34	RA	1025	G
34	RA	1026	U
34	RA	1027	A
34	RA	1033	U
34	RA	1036	G
34	RA	1038	C
34	RA	1042	G
34	RA	1045	A
34	RA	1046	A
34	RA	1047	G
34	RA	1054	A

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Mol	Chain	Res	Type
34	RA	1058	G
34	RA	1060	U
34	RA	1063	G
34	RA	1064	C
34	RA	1065	U
34	RA	1066	U
34	RA	1067	A
34	RA	1068	G
34	RA	1070	A
34	RA	1071	G
34	RA	1073	A
34	RA	1074	G
34	RA	1076	C
34	RA	1078	U
34	RA	1079	C
34	RA	1080	C
34	RA	1082	U
34	RA	1083	U
34	RA	1084	A
34	RA	1085	A
34	RA	1086	A
34	RA	1088	A
34	RA	1090	U
34	RA	1092	C
34	RA	1093	G
34	RA	1094	U
34	RA	1096	A
34	RA	1097	U
34	RA	1098	A
34	RA	1109	C
34	RA	1112	G
34	RA	1122	G
34	RA	1130	U
34	RA	1131	G
34	RA	1135	C
34	RA	1136	G
34	RA	1140	C
34	RA	1142(A)	A
34	RA	1173	G
34	RA	1174	A
34	RA	1175	U
34	RA	1176	G

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Mol	Chain	Res	Type
34	RA	1187	G
34	RA	1195	G
34	RA	1204	A
34	RA	1205	U
34	RA	1206	G
34	RA	1210	A
34	RA	1211	U
34	RA	1220	A
34	RA	1236	G
34	RA	1238	G
34	RA	1253	A
34	RA	1256	G
34	RA	1265	A
34	RA	1271	G
34	RA	1272	A
34	RA	1273	U
34	RA	1300	U
34	RA	1301	A
34	RA	1312	U
34	RA	1313	U
34	RA	1314	C
34	RA	1329	U
34	RA	1332	G
34	RA	1349	A
34	RA	1352	U
34	RA	1365	A
34	RA	1370	C
34	RA	1378	A
34	RA	1379	A
34	RA	1384	A
34	RA	1385	G
34	RA	1395	A
34	RA	1403	C
34	RA	1404	C
34	RA	1407	C
34	RA	1411	C
34	RA	1416	G
34	RA	1419	A
34	RA	1420	U
34	RA	1421	G
34	RA	1428	C
34	RA	1434	A

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Mol	Chain	Res	Type
34	RA	1444(A)	A
34	RA	1445	C
34	RA	1449	A
34	RA	1449(A)	G
34	RA	1455	G
34	RA	1459	G
34	RA	1460	A
34	RA	1461	G
34	RA	1471	A
34	RA	1480	G
34	RA	1482	U
34	RA	1483	G
34	RA	1487	G
34	RA	1493	C
34	RA	1497	U
34	RA	1504	C
34	RA	1506	C
34	RA	1507	A
34	RA	1508	A
34	RA	1510	A
34	RA	1511	A
34	RA	1514	U
34	RA	1522	G
34	RA	1523	U
34	RA	1528	A
34	RA	1535	U
34	RA	1536	A
34	RA	1537	C
34	RA	1538	G
34	RA	1543	A
34	RA	1545	A
34	RA	1547	C
34	RA	1558	A
34	RA	1559	G
34	RA	1566	A
34	RA	1569	A
34	RA	1578	U
34	RA	1580	A
34	RA	1581	G
34	RA	1583	A
34	RA	1586	A
34	RA	1587	A

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Mol	Chain	Res	Type
34	RA	1598	C
34	RA	1608	A
34	RA	1609	A
34	RA	1616	A
34	RA	1617	C
34	RA	1640	C
34	RA	1648	C
34	RA	1654	A
34	RA	1667	G
34	RA	1668	A
34	RA	1674	G
34	RA	1725	G
34	RA	1728	G
34	RA	1729	A
34	RA	1730	U
34	RA	1731	G
34	RA	1733	G
34	RA	1743	G
34	RA	1756	G
34	RA	1762	A
34	RA	1763	G
34	RA	1764	G
34	RA	1769	G
34	RA	1773	A
34	RA	1776	G
34	RA	1779	U
34	RA	1780	A
34	RA	1782	C
34	RA	1787	A
34	RA	1791	A
34	RA	1799	G
34	RA	1800	C
34	RA	1801	G
34	RA	1816	G
34	RA	1820	U
34	RA	1828	G
34	RA	1835	G
34	RA	1847	A
34	RA	1848	A
34	RA	1858	G
34	RA	1869	G
34	RA	1870	C

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Mol	Chain	Res	Type
34	RA	1872	A
34	RA	1878	G
34	RA	1882	C
34	RA	1888	G
34	RA	1889	A
34	RA	1903	G
34	RA	1906	G
34	RA	1913	A
34	RA	1914	C
34	RA	1929	G
34	RA	1930	G
34	RA	1936	A
34	RA	1939	U
34	RA	1940	U
34	RA	1955	U
34	RA	1963	U
34	RA	1965	C
34	RA	1967	C
34	RA	1969	A
34	RA	1970	A
34	RA	1971	A
34	RA	1972	A
34	RA	1982	C
34	RA	1992	G
34	RA	1993	U
34	RA	2004	G
34	RA	2020	A
34	RA	2021	C
34	RA	2023	G
34	RA	2031	A
34	RA	2032	G
34	RA	2033	A
34	RA	2043	C
34	RA	2052	G
34	RA	2055	C
34	RA	2056	G
34	RA	2059	A
34	RA	2060	A
34	RA	2061	G
34	RA	2062	A
34	RA	2069	G
34	RA	2093	G

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Mol	Chain	Res	Type
34	RA	2111	C
34	RA	2113	U
34	RA	2114	A
34	RA	2115	G
34	RA	2116	G
34	RA	2117	A
34	RA	2118	U
34	RA	2126	A
34	RA	2127	G
34	RA	2128	C
34	RA	2132	U
34	RA	2133	G
34	RA	2136	C
34	RA	2147	G
34	RA	2148	G
34	RA	2158	A
34	RA	2164	C
34	RA	2166	G
34	RA	2167	U
34	RA	2168	G
34	RA	2169	A
34	RA	2173	A
34	RA	2182	G
34	RA	2189	U
34	RA	2190	G
34	RA	2194	G
34	RA	2198	A
34	RA	2199	A
34	RA	2210	G
34	RA	2211	G
34	RA	2212	A
34	RA	2215	G
34	RA	2225	A
34	RA	2238	G
34	RA	2239	G
34	RA	2243	U
34	RA	2266	A
34	RA	2275	C
34	RA	2278	A
34	RA	2280	G
34	RA	2283	C
34	RA	2287	A

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Mol	Chain	Res	Type
34	RA	2288	A
34	RA	2305	A
34	RA	2307	G
34	RA	2308	G
34	RA	2309	A
34	RA	2310	A
34	RA	2311	A
34	RA	2313	C
34	RA	2319	G
34	RA	2320	A
34	RA	2325	G
34	RA	2334	G
34	RA	2336	A
34	RA	2342	C
34	RA	2346	A
34	RA	2347	C
34	RA	2350	C
34	RA	2361	A
34	RA	2362	G
34	RA	2372	G
34	RA	2383	G
34	RA	2385	C
34	RA	2391	G
34	RA	2392	A
34	RA	2394	C
34	RA	2402	C
34	RA	2403	C
34	RA	2424	C
34	RA	2425	A
34	RA	2429	G
34	RA	2430	A
34	RA	2435	A
34	RA	2439	A
34	RA	2440	C
34	RA	2441	C
34	RA	2447	G
34	RA	2448	A
34	RA	2469	A
34	RA	2478	A
34	RA	2481	G
34	RA	2494	G
34	RA	2498	C

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Mol	Chain	Res	Type
34	RA	2502	G
34	RA	2505	G
34	RA	2518	A
34	RA	2519	U
34	RA	2529	G
34	RA	2542	A
34	RA	2543	G
34	RA	2554	U
34	RA	2564	A
34	RA	2567	G
34	RA	2569	G
34	RA	2572	A
34	RA	2573	C
34	RA	2585	U
34	RA	2602	A
34	RA	2609	U
34	RA	2611	U
34	RA	2612	C
34	RA	2615	U
34	RA	2623	G
34	RA	2629	A
34	RA	2646	C
34	RA	2655	G
34	RA	2665	A
34	RA	2673	G
34	RA	2689	U
34	RA	2690	C
34	RA	2702	U
34	RA	2707	G
34	RA	2712(A)	A
34	RA	2713	A
34	RA	2714	G
34	RA	2726	U
34	RA	2732	G
34	RA	2733	A
34	RA	2744	G
34	RA	2748	A
34	RA	2751	G
34	RA	2761	G
34	RA	2764	A
34	RA	2765	A
34	RA	2766	G

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Mol	Chain	Res	Type
34	RA	2778	A
34	RA	2779	U
34	RA	2780	G
34	RA	2789	C
34	RA	2790	A
34	RA	2791	C
34	RA	2792	G
34	RA	2797	U
34	RA	2798	C
34	RA	2818	G
34	RA	2820	A
34	RA	2821	A
34	RA	2833	G
34	RA	2834	G
34	RA	2835	A
34	RA	2847	U
34	RA	2867	G
34	RA	2872	G
34	RA	2873	A
34	RA	2879	C
34	RA	2880	C
34	RA	2886	G
34	RA	2892	A
34	RA	2894	G
34	RA	2895	U
34	RA	2897	U
35	RB	8	U
35	RB	13	A
35	RB	15	A
35	RB	16	G
35	RB	19	G
35	RB	21	G
35	RB	25	A
35	RB	41	U
35	RB	42	C
35	RB	45	A
35	RB	52	A
35	RB	56	G
35	RB	67	G
35	RB	73	A
35	RB	108	C
35	RB	109	G

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Mol	Chain	Res	Type
1	XA	6	G
1	XA	7	G
1	XA	31	G
1	XA	32	A
1	XA	39	G
1	XA	47	C
1	XA	48	C
1	XA	51	A
1	XA	56	U
1	XA	61	G
1	XA	65	U
1	XA	66	G
1	XA	79	G
1	XA	89	U
1	XA	92	G
1	XA	95	G
1	XA	101	A
1	XA	115	G
1	XA	116	A
1	XA	121	C
1	XA	130	A
1	XA	144	G
1	XA	147	G
1	XA	151	A
1	XA	156	G
1	XA	161	A
1	XA	163	C
1	XA	169	C
1	XA	172	A
1	XA	174	C
1	XA	190	G
1	XA	191(A)	G
1	XA	195	A
1	XA	196	A
1	XA	197	A
1	XA	208	U
1	XA	209	U
1	XA	210	U
1	XA	244	U
1	XA	245	C
1	XA	247	G
1	XA	251	G

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Mol	Chain	Res	Type
1	XA	267	C
1	XA	281	G
1	XA	289	G
1	XA	306	G
1	XA	314	C
1	XA	321	A
1	XA	328	C
1	XA	329	A
1	XA	332	G
1	XA	343	U
1	XA	345	C
1	XA	346	G
1	XA	347	G
1	XA	348	G
1	XA	351	G
1	XA	352	C
1	XA	353	A
1	XA	354	G
1	XA	356	A
1	XA	359	U
1	XA	363	A
1	XA	367	U
1	XA	372	C
1	XA	373	A
1	XA	384	G
1	XA	389	A
1	XA	397	A
1	XA	398	C
1	XA	406	G
1	XA	411	A
1	XA	412	A
1	XA	413	G
1	XA	421	U
1	XA	422	C
1	XA	423	G
1	XA	428	G
1	XA	429	U
1	XA	440	A
1	XA	442	C
1	XA	452	A
1	XA	465	A
1	XA	466	C

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Mol	Chain	Res	Type
1	XA	467	G
1	XA	482	A
1	XA	484	G
1	XA	485	G
1	XA	486	U
1	XA	492	G
1	XA	496	A
1	XA	497	U
1	XA	509	A
1	XA	510	A
1	XA	511	C
1	XA	518	C
1	XA	519	C
1	XA	521	G
1	XA	524	G
1	XA	527	G
1	XA	529	G
1	XA	530	G
1	XA	531	U
1	XA	532	A
1	XA	533	A
1	XA	547	A
1	XA	548	G
1	XA	559	A
1	XA	561	U
1	XA	564	C
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	657	G
1	XA	665	A
1	XA	666	G
1	XA	686	U
1	XA	688	G
1	XA	690	G
1	XA	702	A

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Mol	Chain	Res	Type
1	XA	703	G
1	XA	704	A
1	XA	723	U
1	XA	731	G
1	XA	734	G
1	XA	749	C
1	XA	754	C
1	XA	755	G
1	XA	777	A
1	XA	792	A
1	XA	793	U
1	XA	794	A
1	XA	799	G
1	XA	812	C
1	XA	813	U
1	XA	816	A
1	XA	817	C
1	XA	821	G
1	XA	828	A
1	XA	836	G
1	XA	841	U
1	XA	842	C
1	XA	843	U
1	XA	848	C
1	XA	859	A
1	XA	871	U
1	XA	872	A
1	XA	902	G
1	XA	914	A
1	XA	916	G
1	XA	926	G
1	XA	927	G
1	XA	934	C
1	XA	935	A
1	XA	958	A
1	XA	960	U
1	XA	968	A
1	XA	969	A
1	XA	972	C
1	XA	974	A
1	XA	975	A
1	XA	976	G

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Mol	Chain	Res	Type
1	XA	977	A
1	XA	982	U
1	XA	991	U
1	XA	992	U
1	XA	993	G
1	XA	994	A
1	XA	1003	G
1	XA	1004	A
1	XA	1005	A
1	XA	1006	C
1	XA	1009	G
1	XA	1024	G
1	XA	1025	U
1	XA	1028	C
1	XA	1029	G
1	XA	1031	G
1	XA	1032(A)	G
1	XA	1032(B)	G
1	XA	1038	C
1	XA	1039	C
1	XA	1040	U
1	XA	1041	A
1	XA	1042	G
1	XA	1046	A
1	XA	1053	G
1	XA	1054	C
1	XA	1055	A
1	XA	1064	G
1	XA	1066	C
1	XA	1081	G
1	XA	1085	U
1	XA	1094	G
1	XA	1101	A
1	XA	1108	G
1	XA	1115	C
1	XA	1124	G
1	XA	1125	U
1	XA	1126	U
1	XA	1127	G
1	XA	1129	C
1	XA	1130	A
1	XA	1131	G

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Mol	Chain	Res	Type
1	XA	1136	U
1	XA	1137	C
1	XA	1138	G
1	XA	1139	G
1	XA	1146	A
1	XA	1157	A
1	XA	1158	C
1	XA	1159	U
1	XA	1160	G
1	XA	1162	C
1	XA	1169	A
1	XA	1176	A
1	XA	1177	G
1	XA	1181	G
1	XA	1182	G
1	XA	1183	A
1	XA	1187	G
1	XA	1196	U
1	XA	1200	C
1	XA	1201	A
1	XA	1212	U
1	XA	1225	A
1	XA	1236	A
1	XA	1238	A
1	XA	1240	U
1	XA	1241	G
1	XA	1256	A
1	XA	1257	U
1	XA	1258	G
1	XA	1260	C
1	XA	1270	C
1	XA	1273	G
1	XA	1280	A
1	XA	1281	U
1	XA	1282	C
1	XA	1286	A
1	XA	1287	A
1	XA	1290	G
1	XA	1291	G
1	XA	1298	C
1	XA	1299	A
1	XA	1300	G

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Mol	Chain	Res	Type
1	XA	1301	U
1	XA	1302	U
1	XA	1303	C
1	XA	1305	G
1	XA	1310	G
1	XA	1311	G
1	XA	1318	A
1	XA	1319	A
1	XA	1320	C
1	XA	1323	G
1	XA	1331	G
1	XA	1335	C
1	XA	1336	C
1	XA	1340	A
1	XA	1347	G
1	XA	1348	U
1	XA	1362(A)	C
1	XA	1394	A
1	XA	1397	C
1	XA	1400	C
1	XA	1419	G
1	XA	1442	G
1	XA	1446	A
1	XA	1452	C
1	XA	1453	G
1	XA	1454	G
1	XA	1487	G
1	XA	1492	A
1	XA	1493	A
1	XA	1494	G
1	XA	1497	G
1	XA	1498	U
1	XA	1499	A
1	XA	1502	A
1	XA	1504	G
1	XA	1506	U
1	XA	1517	G
1	XA	1520	G
1	XA	1529	G
1	XA	1530	G
1	XA	1533	C
1	XA	1538	C

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Mol	Chain	Res	Type
1	XA	1541	U
22	XV	2	G
22	XV	8	U
22	XV	19	G
22	XV	21	A
22	XV	30	G
22	XV	33	U
22	XV	37	T6A
22	XV	48	C
22	XV	49	G
22	XV	53	G
22	XV	54	U
22	XV	55	U
22	XV	57	G
22	XV	59	A
22	XV	61	C
22	XV	74	C
22	XV	76	A
23	XX	-4	U
23	XX	-3	A
23	XX	-2	A
23	XX	4	U
55	XY	28	G
55	XY	30	G
55	XY	43	C
34	YA	9	U
34	YA	11	G
34	YA	15	G
34	YA	34	C
34	YA	35	G
34	YA	46	C
34	YA	51	G
34	YA	61	G
34	YA	74	A
34	YA	75	G
34	YA	101	G
34	YA	102	G
34	YA	118	A
34	YA	120	U
34	YA	125	G
34	YA	131	G
34	YA	140	A

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Mol	Chain	Res	Type
34	YA	155	C
34	YA	162	U
34	YA	196	A
34	YA	199	A
34	YA	214	G
34	YA	215	G
34	YA	216	A
34	YA	221	A
34	YA	222	A
34	YA	223	A
34	YA	226	G
34	YA	228	A
34	YA	229	A
34	YA	230	U
34	YA	232	G
34	YA	242	G
34	YA	243	U
34	YA	248	G
34	YA	252	G
34	YA	270(L)	U
34	YA	270(M)	U
34	YA	270(N)	G
34	YA	270(P)	C
34	YA	270(Y)	G
34	YA	271(B)	G
34	YA	271(C)	U
34	YA	271(D)	G
34	YA	274	G
34	YA	275	G
34	YA	276	A
34	YA	278	A
34	YA	279	C
34	YA	299	A
34	YA	311	A
34	YA	323	G
34	YA	324	A
34	YA	329	G
34	YA	330	A
34	YA	332	A
34	YA	352	G
34	YA	363	G
34	YA	363(E)	U

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Mol	Chain	Res	Type
34	YA	364	C
34	YA	371	A
34	YA	372	G
34	YA	386	G
34	YA	387	U
34	YA	396	G
34	YA	404	C
34	YA	405	U
34	YA	406	G
34	YA	411	G
34	YA	412	A
34	YA	428	A
34	YA	443	A
34	YA	444	C
34	YA	448	U
34	YA	457	A
34	YA	470	A
34	YA	481	G
34	YA	504	U
34	YA	505	A
34	YA	509	C
34	YA	512	G
34	YA	518	G
34	YA	531	C
34	YA	532	A
34	YA	533	G
34	YA	537	C
34	YA	539	G
34	YA	540	G
34	YA	541	C
34	YA	546	C
34	YA	547	A
34	YA	563	G
34	YA	568	U
34	YA	573	G
34	YA	575	A
34	YA	603	A
34	YA	607	U
34	YA	614	U
34	YA	617	G
34	YA	622	G
34	YA	627	A

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Mol	Chain	Res	Type
34	YA	634	C
34	YA	637	A
34	YA	638	G
34	YA	645	C
34	YA	646	A
34	YA	651	G
34	YA	654	A
34	YA	654(A)	G
34	YA	669	G
34	YA	686	G
34	YA	717	G
34	YA	722	A
34	YA	726	G
34	YA	730	C
34	YA	753	C
34	YA	764	A
34	YA	765	G
34	YA	782	A
34	YA	784	A
34	YA	785	G
34	YA	788	A
34	YA	789	A
34	YA	790	C
34	YA	791	C
34	YA	805	G
34	YA	812	C
34	YA	819	A
34	YA	827	U
34	YA	831	G
34	YA	847	U
34	YA	856	C
34	YA	857	C
34	YA	860	U
34	YA	866	A
34	YA	881	G
34	YA	882	G
34	YA	884	C
34	YA	886	C
34	YA	888	C
34	YA	889	C
34	YA	896	A
34	YA	897	C

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Mol	Chain	Res	Type
34	YA	900	A
34	YA	907	U
34	YA	910	A
34	YA	915	C
34	YA	917	A
34	YA	932	G
34	YA	941	A
34	YA	945	A
34	YA	946	G
34	YA	953	A
34	YA	959	A
34	YA	961	C
34	YA	974	G
34	YA	974(A)	C
34	YA	980	A
34	YA	983	A
34	YA	996	A
34	YA	1011	G
34	YA	1012	U
34	YA	1013	C
34	YA	1015	G
34	YA	1022	G
34	YA	1023	U
34	YA	1026	U
34	YA	1027	A
34	YA	1033	U
34	YA	1046	A
34	YA	1047	G
34	YA	1050	A
34	YA	1053	C
34	YA	1057	A
34	YA	1059	G
34	YA	1060	U
34	YA	1061	U
34	YA	1062	G
34	YA	1067	A
34	YA	1068	G
34	YA	1070	A
34	YA	1071	G
34	YA	1073	A
34	YA	1077	A
34	YA	1078	U

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Mol	Chain	Res	Type
34	YA	1082	U
34	YA	1083	U
34	YA	1084	A
34	YA	1085	A
34	YA	1086	A
34	YA	1088	A
34	YA	1089	G
34	YA	1093	G
34	YA	1095	A
34	YA	1096	A
34	YA	1097	U
34	YA	1103	A
34	YA	1104	C
34	YA	1109	C
34	YA	1110	G
34	YA	1130	U
34	YA	1135	C
34	YA	1136	G
34	YA	1139	G
34	YA	1141	U
34	YA	1142	U
34	YA	1142(A)	A
34	YA	1155	A
34	YA	1173	G
34	YA	1174	A
34	YA	1175	U
34	YA	1176	G
34	YA	1179	C
34	YA	1204	A
34	YA	1205	U
34	YA	1210	A
34	YA	1211	U
34	YA	1220	A
34	YA	1236	G
34	YA	1238	G
34	YA	1252	G
34	YA	1253	A
34	YA	1256	G
34	YA	1265	A
34	YA	1271	G
34	YA	1272	A
34	YA	1275	A

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Mol	Chain	Res	Type
34	YA	1300	U
34	YA	1301	A
34	YA	1314	C
34	YA	1329	U
34	YA	1349	A
34	YA	1365	A
34	YA	1368	G
34	YA	1370	C
34	YA	1378	A
34	YA	1379	A
34	YA	1384	A
34	YA	1385	G
34	YA	1392	A
34	YA	1395	A
34	YA	1406	U
34	YA	1407	C
34	YA	1411	C
34	YA	1416	G
34	YA	1419	A
34	YA	1420	U
34	YA	1421	G
34	YA	1428	C
34	YA	1444(A)	A
34	YA	1445	C
34	YA	1449	A
34	YA	1449(A)	G
34	YA	1455	G
34	YA	1460	A
34	YA	1461	G
34	YA	1467	C
34	YA	1471	A
34	YA	1478	G
34	YA	1482	U
34	YA	1483	G
34	YA	1487	G
34	YA	1493	C
34	YA	1496	A
34	YA	1497	U
34	YA	1507	A
34	YA	1510	A
34	YA	1511	A
34	YA	1522	G

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Mol	Chain	Res	Type
34	YA	1528	A
34	YA	1533	C
34	YA	1535	U
34	YA	1536	A
34	YA	1537	C
34	YA	1540	G
34	YA	1543	A
34	YA	1544	C
34	YA	1545	A
34	YA	1558	A
34	YA	1559	G
34	YA	1566	A
34	YA	1569	A
34	YA	1578	U
34	YA	1585	C
34	YA	1586	A
34	YA	1591	G
34	YA	1598	C
34	YA	1608	A
34	YA	1609	A
34	YA	1616	A
34	YA	1617	C
34	YA	1640	C
34	YA	1648	C
34	YA	1654	A
34	YA	1674	G
34	YA	1695	G
34	YA	1725	G
34	YA	1728	G
34	YA	1729	A
34	YA	1731	G
34	YA	1732	A
34	YA	1733	G
34	YA	1743	G
34	YA	1749	A
34	YA	1753	G
34	YA	1754	C
34	YA	1756	G
34	YA	1763	G
34	YA	1764	G
34	YA	1769	G
34	YA	1773	A

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Mol	Chain	Res	Type
34	YA	1779	U
34	YA	1780	A
34	YA	1781	C
34	YA	1787	A
34	YA	1791	A
34	YA	1799	G
34	YA	1800	C
34	YA	1801	G
34	YA	1816	G
34	YA	1829	A
34	YA	1835	G
34	YA	1847	A
34	YA	1858	G
34	YA	1869	G
34	YA	1870	C
34	YA	1872	A
34	YA	1878	G
34	YA	1882	C
34	YA	1884	A
34	YA	1889	A
34	YA	1903	G
34	YA	1906	G
34	YA	1913	A
34	YA	1914	C
34	YA	1919	A
34	YA	1929	G
34	YA	1930	G
34	YA	1936	A
34	YA	1939	U
34	YA	1940	U
34	YA	1955	U
34	YA	1956	U
34	YA	1963	U
34	YA	1964	G
34	YA	1967	C
34	YA	1969	A
34	YA	1970	A
34	YA	1971	A
34	YA	1972	A
34	YA	1982	C
34	YA	1992	G
34	YA	1993	U

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Mol	Chain	Res	Type
34	YA	2020	A
34	YA	2021	C
34	YA	2023	G
34	YA	2031	A
34	YA	2033	A
34	YA	2043	C
34	YA	2052	G
34	YA	2055	C
34	YA	2056	G
34	YA	2059	A
34	YA	2060	A
34	YA	2061	G
34	YA	2062	A
34	YA	2069	G
34	YA	2093	G
34	YA	2100	G
34	YA	2111	C
34	YA	2114	A
34	YA	2115	G
34	YA	2116	G
34	YA	2118	U
34	YA	2120	G
34	YA	2126	A
34	YA	2127	G
34	YA	2131	G
34	YA	2132	U
34	YA	2133	G
34	YA	2134	A
34	YA	2136	C
34	YA	2147	G
34	YA	2148	G
34	YA	2152	G
34	YA	2156	G
34	YA	2157	G
34	YA	2158	A
34	YA	2159	G
34	YA	2166	G
34	YA	2168	G
34	YA	2169	A
34	YA	2173	A
34	YA	2180	U
34	YA	2189	U

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Mol	Chain	Res	Type
34	YA	2190	G
34	YA	2192	G
34	YA	2198	A
34	YA	2210	G
34	YA	2211	G
34	YA	2212	A
34	YA	2213	U
34	YA	2215	G
34	YA	2225	A
34	YA	2238	G
34	YA	2239	G
34	YA	2243	U
34	YA	2266	A
34	YA	2275	C
34	YA	2278	A
34	YA	2279	G
34	YA	2283	C
34	YA	2287	A
34	YA	2288	A
34	YA	2305	A
34	YA	2307	G
34	YA	2308	G
34	YA	2309	A
34	YA	2311	A
34	YA	2320	A
34	YA	2325	G
34	YA	2334	G
34	YA	2335	A
34	YA	2345	G
34	YA	2346	A
34	YA	2347	C
34	YA	2350	C
34	YA	2383	G
34	YA	2385	C
34	YA	2403	C
34	YA	2406	U
34	YA	2407	G
34	YA	2410	G
34	YA	2423	U
34	YA	2425	A
34	YA	2427	C
34	YA	2428	G

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Mol	Chain	Res	Type
34	YA	2429	G
34	YA	2430	A
34	YA	2435	A
34	YA	2439	A
34	YA	2441	C
34	YA	2447	G
34	YA	2448	A
34	YA	2450	A
34	YA	2469	A
34	YA	2470	G
34	YA	2494	G
34	YA	2498	C
34	YA	2502	G
34	YA	2505	G
34	YA	2518	A
34	YA	2529	G
34	YA	2554	U
34	YA	2558	C
34	YA	2564	A
34	YA	2566	A
34	YA	2567	G
34	YA	2572	A
34	YA	2576	G
34	YA	2578	G
34	YA	2585	U
34	YA	2602	A
34	YA	2609	U
34	YA	2611	U
34	YA	2612	C
34	YA	2615	U
34	YA	2629	A
34	YA	2646	C
34	YA	2655	G
34	YA	2665	A
34	YA	2673	G
34	YA	2682	U
34	YA	2689	U
34	YA	2702	U
34	YA	2712	U
34	YA	2712(A)	A
34	YA	2713	A
34	YA	2714	G

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Mol	Chain	Res	Type
34	YA	2726	U
34	YA	2732	G
34	YA	2733	A
34	YA	2744	G
34	YA	2748	A
34	YA	2751	G
34	YA	2761	G
34	YA	2764	A
34	YA	2765	A
34	YA	2766	G
34	YA	2769	C
34	YA	2777	G
34	YA	2778	A
34	YA	2779	U
34	YA	2780	G
34	YA	2790	A
34	YA	2791	C
34	YA	2797	U
34	YA	2818	G
34	YA	2820	A
34	YA	2821	A
34	YA	2823	A
34	YA	2833	G
34	YA	2834	G
34	YA	2835	A
34	YA	2847	U
34	YA	2867	G
34	YA	2868	A
34	YA	2872	G
34	YA	2873	A
34	YA	2880	C
34	YA	2891	G
34	YA	2892	A
34	YA	2893	G
35	YB	8	U
35	YB	9	G
35	YB	13	A
35	YB	15	A
35	YB	16	G
35	YB	19	G
35	YB	21	G
35	YB	22	U

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Mol	Chain	Res	Type
35	YB	25	A
35	YB	32	C
35	YB	41	U
35	YB	42	C
35	YB	44	G
35	YB	45	A
35	YB	56	G
35	YB	67	G
35	YB	73	A
35	YB	109	G

All (133) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	QA	64	G
1	QA	115	G
1	QA	119	A
1	QA	243	A
1	QA	244	U
1	QA	250	A
1	QA	266	G
1	QA	328	C
1	QA	410	G
1	QA	412	A
1	QA	481	G
1	QA	484	G
1	QA	485	G
1	QA	509	A
1	QA	687	A
1	QA	703	G
1	QA	753	A
1	QA	792	A
1	QA	812	C
1	QA	913	A
1	QA	992	U
1	QA	1065	U
1	QA	1200	C
1	QA	1285	A
1	QA	1297	C
1	QA	1336	C
1	QA	1346	A
1	QA	1347	G

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Mol	Chain	Res	Type
1	QA	1498	U
1	QA	1528	U
34	RA	221	A
34	RA	222	A
34	RA	229	A
34	RA	271(B)	G
34	RA	345	A
34	RA	372	G
34	RA	404	C
34	RA	503	A
34	RA	512	G
34	RA	587	C
34	RA	637	A
34	RA	752	A
34	RA	846	C
34	RA	856	C
34	RA	1022	G
34	RA	1026	U
34	RA	1053	C
34	RA	1057	A
34	RA	1065	U
34	RA	1067	A
34	RA	1073	A
34	RA	1204	A
34	RA	1210	A
34	RA	1312	U
34	RA	1427	A
34	RA	1558	A
34	RA	1653	G
34	RA	1819	A
34	RA	1992	G
34	RA	2060	A
34	RA	2126	A
34	RA	2361	A
34	RA	2439	A
34	RA	2566	A
34	RA	2610	C
34	RA	2689	U
34	RA	2832	U
35	RB	66	A
1	XA	60	A
1	XA	78	G

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Mol	Chain	Res	Type
1	XA	115	G
1	XA	243	A
1	XA	244	U
1	XA	250	A
1	XA	266	G
1	XA	328	C
1	XA	410	G
1	XA	412	A
1	XA	481	G
1	XA	484	G
1	XA	485	G
1	XA	509	A
1	XA	687	A
1	XA	703	G
1	XA	753	A
1	XA	812	C
1	XA	913	A
1	XA	992	U
1	XA	1027	C
1	XA	1285	A
1	XA	1297	C
1	XA	1310	G
1	XA	1498	U
23	XX	-5	G
23	XX	-3	A
34	YA	195	A
34	YA	221	A
34	YA	229	A
34	YA	241	A
34	YA	242	G
34	YA	271(B)	G
34	YA	278	A
34	YA	404	C
34	YA	503	A
34	YA	637	A
34	YA	752	A
34	YA	846	C
34	YA	856	C
34	YA	859	G
34	YA	974	G
34	YA	1022	G
34	YA	1026	U

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Mol	Chain	Res	Type
34	YA	1085	A
34	YA	1109	C
34	YA	1178	C
34	YA	1204	A
34	YA	1210	A
34	YA	1427	A
34	YA	1460	A
34	YA	1558	A
34	YA	1653	G
34	YA	1694	C
34	YA	1799	G
34	YA	1992	G
34	YA	2406	U
34	YA	2566	A
34	YA	2610	C
34	YA	2681	C
34	YA	2712	U
34	YA	2776	A
34	YA	2832	U
34	YA	2867	G
35	YB	66	A

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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
22	MNU	XV	34	23,22	21,24,25	1.28	3 (14%)	27,34,37	1.82	8 (29%)
22	T6A	QV	37	22	31,34,35	1.40	4 (12%)	43,49,52	2.06	11 (25%)
22	T6A	XV	37	22	31,34,35	1.38	3 (9%)	43,49,52	2.03	10 (23%)
56	PPU	Z8	76	34,56	37,40,41	1.28	4 (10%)	47,57,60	2.10	14 (29%)
56	PPU	Z6	76	34,56	37,40,41	1.27	5 (13%)	47,57,60	2.06	15 (31%)
22	MNU	QV	34	23,22	21,24,25	1.26	3 (14%)	27,34,37	1.63	7 (25%)

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
22	MNU	XV	34	23,22	-	0/10/28/29	0/2/2/2
22	T6A	QV	37	22	-	16/23/41/42	0/3/3/3
22	T6A	XV	37	22	-	17/23/41/42	0/3/3/3
56	PPU	Z8	76	34,56	-	4/25/43/44	0/4/4/4
56	PPU	Z6	76	34,56	-	4/25/43/44	0/4/4/4
22	MNU	QV	34	23,22	-	1/10/28/29	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z8	76	PPU	C5-C4	5.00	1.48	1.39
56	Z6	76	PPU	C5-C4	4.91	1.47	1.39
22	QV	37	T6A	C5-C4	4.78	1.47	1.39
22	XV	37	T6A	C5-C4	4.64	1.47	1.39
22	XV	34	MNU	C2-N1	3.19	1.43	1.38
56	Z8	76	PPU	C5-C6	3.02	1.49	1.41
56	Z6	76	PPU	C5-C6	3.00	1.49	1.41
22	QV	34	MNU	C2-N1	2.98	1.43	1.38
22	QV	34	MNU	C4-N3	-2.83	1.33	1.38
22	XV	34	MNU	C4-N3	-2.82	1.33	1.38
22	QV	37	T6A	C5-C6	2.75	1.48	1.41
22	XV	37	T6A	C5-N7	-2.64	1.34	1.39
22	XV	37	T6A	C5-C6	2.58	1.48	1.41
22	QV	37	T6A	C5-N7	-2.43	1.34	1.39
56	Z6	76	PPU	C8-N7	2.35	1.36	1.31
56	Z8	76	PPU	C8-N7	2.23	1.36	1.31
22	QV	34	MNU	C2-N3	-2.23	1.34	1.38
56	Z6	76	PPU	C5-N7	-2.14	1.35	1.39
22	XV	34	MNU	C2-N3	-2.09	1.34	1.38
56	Z8	76	PPU	C5-N7	-2.09	1.35	1.39
22	QV	37	T6A	C8-N7	2.07	1.35	1.31
56	Z6	76	PPU	C4-N9	-2.00	1.33	1.37

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	XV	37	T6A	C5-C4-N3	-6.75	117.42	126.72
22	QV	37	T6A	C5-C4-N3	-6.63	117.59	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	XV	37	T6A	N3-C4-N9	5.76	136.96	127.17
22	QV	37	T6A	N3-C4-N9	5.62	136.72	127.17
56	Z8	76	PPU	C5-C4-N3	-5.58	119.03	126.72
56	Z6	76	PPU	C5-C4-N3	-5.56	119.06	126.72
22	XV	34	MNU	N3-C2-N1	4.53	120.79	114.89
22	QV	34	MNU	N3-C2-N1	4.35	120.55	114.89
56	Z8	76	PPU	C2-N1-C6	4.32	122.39	111.83
56	Z8	76	PPU	N3-C4-N9	4.19	134.29	127.17
56	Z6	76	PPU	N3-C4-N9	4.19	134.28	127.17
22	XV	34	MNU	C1'-N1-C2	4.14	125.03	117.59
56	Z6	76	PPU	C2-N1-C6	4.13	121.93	111.83
56	Z6	76	PPU	C9-N6-C6	-4.00	110.33	120.52
22	QV	37	T6A	C2-N3-C4	3.99	121.58	111.83
22	QV	37	T6A	N6-C10-N11	3.98	119.25	113.77
22	XV	37	T6A	C2-N3-C4	3.92	121.41	111.83
56	Z6	76	PPU	N1-C6-N6	3.88	121.58	116.86
56	Z8	76	PPU	C10-N6-C6	-3.86	110.71	120.52
56	Z8	76	PPU	C4-C5-N7	-3.85	106.18	110.58
56	Z6	76	PPU	C10-N6-C6	-3.82	110.80	120.52
56	Z6	76	PPU	C4-C5-N7	-3.80	106.23	110.58
56	Z8	76	PPU	N1-C6-N6	3.79	121.48	116.86
22	XV	34	MNU	C4-N3-C2	-3.68	122.52	127.34
56	Z8	76	PPU	C9-N6-C6	-3.66	111.22	120.52
56	Z8	76	PPU	C2-N3-C4	3.53	120.46	111.83
56	Z6	76	PPU	C2-N3-C4	3.31	119.92	111.83
22	QV	37	T6A	N3-C2-N1	-3.26	123.65	128.58
22	QV	34	MNU	C1'-N1-C2	3.25	123.42	117.59
22	QV	34	MNU	C4-N3-C2	-3.24	123.09	127.34
22	XV	37	T6A	C4-C5-N7	-3.19	106.93	110.58
22	XV	37	T6A	N6-C10-N11	3.17	118.13	113.77
22	QV	37	T6A	C4-C5-N7	-3.16	106.97	110.58
56	Z8	76	PPU	C10-N6-C9	-3.08	106.29	116.18
56	Z8	76	PPU	N3-C2-N1	-3.06	123.94	128.58
22	XV	34	MNU	O2-C2-N3	-3.06	115.84	121.49
22	XV	37	T6A	N3-C2-N1	-3.05	123.96	128.58
22	XV	34	MNU	C1'-N1-C6	-2.94	116.32	121.15
22	QV	34	MNU	O2-C2-N3	-2.92	116.11	121.49
56	Z6	76	PPU	C10-N6-C9	-2.77	107.28	116.18
22	XV	34	MNU	C6-N1-C2	-2.73	118.58	121.30
22	XV	37	T6A	C5-N7-C8	2.71	107.71	103.45
22	XV	37	T6A	C4-N9-C8	2.65	108.53	105.74
56	Z8	76	PPU	C5-N7-C8	2.61	107.56	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	Z8	76	PPU	C3'-N3'-C	-2.61	119.23	123.20
56	Z6	76	PPU	C5-N7-C8	2.60	107.53	103.45
22	QV	37	T6A	C4-N9-C8	2.56	108.43	105.74
22	QV	37	T6A	C5-N7-C8	2.56	107.47	103.45
56	Z6	76	PPU	N3-C2-N1	-2.54	124.73	128.58
22	QV	34	MNU	C6-N1-C2	-2.51	118.80	121.30
56	Z6	76	PPU	C4-N9-C8	2.50	108.37	105.74
22	QV	37	T6A	C6-C5-N7	2.49	135.14	132.43
22	XV	37	T6A	C1'-N9-C8	-2.39	121.78	127.09
56	Z6	76	PPU	C5-C6-N6	-2.33	121.64	125.33
22	QV	37	T6A	O10-C10-N6	-2.32	119.51	123.64
22	XV	34	MNU	O4-C4-C5	-2.29	120.86	124.71
56	Z8	76	PPU	C4-N9-C8	2.24	108.09	105.74
56	Z8	76	PPU	C5-C6-N6	-2.22	121.82	125.33
56	Z6	76	PPU	C2'-C1'-N9	-2.17	107.92	113.30
22	QV	34	MNU	O4-C4-C5	-2.16	121.07	124.71
22	QV	37	T6A	C1'-N9-C8	-2.15	122.33	127.09
22	XV	34	MNU	C5-C4-N3	2.13	118.47	115.21
22	XV	37	T6A	C6-C5-N7	2.11	134.73	132.43
22	QV	34	MNU	C1'-N1-C6	-2.09	117.71	121.15
56	Z6	76	PPU	C3'-N3'-C	-2.09	120.02	123.20

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	QV	34	MNU	C5-C7-N8-C9
22	QV	37	T6A	O4'-C1'-N9-C8
22	QV	37	T6A	O4'-C1'-N9-C4
22	QV	37	T6A	C5-C6-N6-C10
22	QV	37	T6A	O10-C10-N6-C6
22	QV	37	T6A	N11-C10-N6-C6
22	QV	37	T6A	N6-C10-N11-C12
22	QV	37	T6A	O10-C10-N11-C12
22	QV	37	T6A	N11-C12-C13-ODA
22	QV	37	T6A	N11-C12-C13-ODB
22	XV	37	T6A	O4'-C1'-N9-C8
22	XV	37	T6A	O4'-C1'-N9-C4
22	XV	37	T6A	C5-C6-N6-C10
22	XV	37	T6A	O10-C10-N6-C6
22	XV	37	T6A	N11-C10-N6-C6
22	XV	37	T6A	N6-C10-N11-C12

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Mol	Chain	Res	Type	Atoms
22	XV	37	T6A	O10-C10-N11-C12
22	XV	37	T6A	N11-C12-C13-ODA
22	XV	37	T6A	N11-C12-C13-ODB
56	Z6	76	PPU	C5-C6-N6-C9
22	QV	37	T6A	C3'-C4'-C5'-O5'
22	XV	37	T6A	C3'-C4'-C5'-O5'
56	Z6	76	PPU	CE1-CZ-OC-CM
56	Z8	76	PPU	CE1-CZ-OC-CM
22	XV	37	T6A	C4'-C5'-O5'-P
56	Z6	76	PPU	CE2-CZ-OC-CM
56	Z8	76	PPU	CE2-CZ-OC-CM
22	QV	37	T6A	O4'-C4'-C5'-O5'
22	XV	37	T6A	O4'-C4'-C5'-O5'
22	QV	37	T6A	C4'-C5'-O5'-P
56	Z6	76	PPU	N1-C6-N6-C9
56	Z8	76	PPU	C5-C6-N6-C9
22	QV	37	T6A	C13-C12-N11-C10
22	QV	37	T6A	C13-C12-C14-O14
22	XV	37	T6A	C13-C12-C14-O14
22	XV	37	T6A	C13-C12-C14-C15
56	Z8	76	PPU	N1-C6-N6-C9
22	XV	37	T6A	N1-C6-N6-C10
22	XV	37	T6A	C13-C12-N11-C10
22	QV	37	T6A	N1-C6-N6-C10
22	QV	37	T6A	C14-C12-N11-C10
22	XV	37	T6A	C14-C12-N11-C10

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	QV	37	T6A	1	0
22	XV	37	T6A	1	0
56	Z8	76	PPU	2	0
22	QV	34	MNU	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1253 ligands modelled in this entry, 1251 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	$\# Z > 2$
58	SF4	QD	301	4	0,12,12	-	-	-		
58	SF4	XD	301	-	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
58	SF4	QD	301	4	-	-	0/6/5/5
58	SF4	XD	301	-	-	-	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	1500/1522 (98%)	0.33	51 (3%) 48 28	78, 129, 224, 338	0
1	XA	1511/1522 (99%)	0.38	57 (3%) 44 26	74, 126, 218, 321	0
2	QB	235/256 (91%)	0.16	3 (1%) 75 49	133, 173, 225, 251	0
2	XB	236/256 (92%)	0.37	5 (2%) 63 38	107, 157, 207, 237	0
3	QC	205/239 (85%)	0.12	3 (1%) 72 45	113, 165, 211, 257	0
3	XC	205/239 (85%)	0.39	7 (3%) 48 28	104, 144, 192, 229	0
4	QD	208/209 (99%)	0.36	7 (3%) 48 28	97, 130, 176, 204	0
4	XD	208/209 (99%)	0.48	11 (5%) 32 20	81, 121, 169, 223	0
5	QE	151/162 (93%)	-0.10	0 100 100	85, 128, 164, 214	0
5	XE	151/162 (93%)	0.20	1 (0%) 84 62	74, 114, 151, 196	0
6	QF	101/101 (100%)	0.28	3 (2%) 52 31	100, 129, 164, 175	0
6	XF	101/101 (100%)	0.14	0 100 100	108, 136, 171, 205	0
7	QG	155/156 (99%)	0.68	14 (9%) 15 11	121, 159, 205, 242	0
7	XG	155/156 (99%)	0.68	15 (9%) 13 11	111, 153, 200, 226	0
8	QH	137/138 (99%)	0.43	5 (3%) 46 27	100, 135, 176, 221	0
8	XH	137/138 (99%)	0.40	4 (2%) 53 31	98, 128, 163, 171	0
9	QI	127/128 (99%)	1.40	26 (20%) 2 3	128, 168, 217, 239	0
9	XI	126/128 (98%)	0.88	20 (15%) 5 5	117, 160, 211, 241	0
10	QJ	99/105 (94%)	0.48	6 (6%) 27 17	136, 177, 221, 261	0
10	XJ	96/105 (91%)	0.64	8 (8%) 17 12	128, 163, 208, 231	0
11	QK	119/129 (92%)	0.80	11 (9%) 14 11	105, 136, 187, 207	0
11	XK	116/129 (89%)	0.55	4 (3%) 48 28	84, 125, 171, 211	0
12	QL	125/131 (95%)	0.64	7 (5%) 30 19	84, 112, 156, 230	0
12	XL	122/131 (93%)	0.67	12 (9%) 13 11	75, 103, 136, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	120/126 (95%)	1.00	19 (15%) 5 5	121, 178, 222, 280	0
13	XM	119/126 (94%)	0.80	13 (10%) 10 10	104, 155, 213, 233	0
14	QN	60/61 (98%)	0.42	2 (3%) 49 29	133, 170, 205, 236	0
14	XN	60/61 (98%)	1.08	6 (10%) 12 11	108, 140, 186, 197	0
15	QO	88/89 (98%)	0.27	3 (3%) 48 28	95, 129, 172, 202	0
15	XO	87/89 (97%)	-0.03	0 100 100	78, 111, 152, 167	0
16	QP	84/88 (95%)	0.44	1 (1%) 76 50	80, 111, 155, 183	0
16	XP	84/88 (95%)	0.42	2 (2%) 59 35	100, 136, 184, 221	0
17	QQ	100/105 (95%)	0.43	4 (4%) 42 25	86, 115, 152, 165	0
17	XQ	100/105 (95%)	0.55	8 (8%) 18 13	85, 126, 161, 185	0
18	QR	70/88 (79%)	0.38	1 (1%) 73 47	101, 134, 187, 244	0
18	XR	70/88 (79%)	0.18	0 100 100	100, 129, 178, 194	0
19	QS	83/93 (89%)	0.45	2 (2%) 59 35	131, 177, 220, 247	0
19	XS	84/93 (90%)	0.30	1 (1%) 76 50	124, 160, 210, 218	0
20	QT	99/106 (93%)	0.49	5 (5%) 33 21	84, 111, 178, 222	0
20	XT	99/106 (93%)	0.75	9 (9%) 15 11	112, 146, 194, 225	0
21	QU	25/27 (92%)	1.19	4 (16%) 5 5	129, 172, 201, 214	0
21	XU	25/27 (92%)	0.77	3 (12%) 9 8	125, 158, 197, 211	0
22	QV	72/76 (94%)	1.02	7 (9%) 13 11	130, 238, 297, 362	0
22	XV	72/76 (94%)	0.85	7 (9%) 13 11	109, 220, 253, 332	0
23	QX	3/23 (13%)	0.64	0 100 100	104, 104, 106, 132	0
23	XX	23/23 (100%)	1.34	6 (26%) 1 2	107, 195, 248, 277	0
24	R0	76/85 (89%)	0.27	1 (1%) 75 49	83, 111, 144, 173	0
24	Y0	75/85 (88%)	0.57	1 (1%) 75 49	75, 102, 139, 175	0
25	R1	97/98 (98%)	0.95	8 (8%) 17 12	66, 104, 162, 225	0
25	Y1	93/98 (94%)	0.86	6 (6%) 25 16	63, 90, 146, 181	0
26	R2	69/72 (95%)	0.50	2 (2%) 53 31	97, 128, 171, 236	0
26	Y2	68/72 (94%)	0.40	2 (2%) 53 31	71, 93, 136, 184	0
27	R3	59/60 (98%)	0.30	0 100 100	85, 117, 153, 229	0
27	Y3	59/60 (98%)	0.71	3 (5%) 33 21	82, 107, 145, 180	0
28	R4	69/71 (97%)	0.25	1 (1%) 73 47	139, 181, 227, 245	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
28	Y4	69/71 (97%)	0.51	3 (4%)	40	23	126, 183, 242, 277	0
29	R5	59/60 (98%)	0.47	4 (6%)	23	16	59, 88, 161, 188	0
29	Y5	59/60 (98%)	0.15	1 (1%)	69	42	58, 106, 195, 205	0
30	R6	53/54 (98%)	0.98	8 (15%)	5	6	154, 213, 254, 262	0
30	Y6	53/54 (98%)	0.73	5 (9%)	14	11	177, 210, 240, 259	0
31	R7	47/49 (95%)	0.55	2 (4%)	40	23	54, 75, 104, 138	0
31	Y7	48/49 (97%)	0.19	2 (4%)	40	24	54, 66, 100, 130	0
32	R8	64/65 (98%)	0.76	3 (4%)	36	22	76, 98, 145, 196	0
32	Y8	64/65 (98%)	0.87	4 (6%)	26	17	72, 89, 128, 153	0
33	R9	37/37 (100%)	1.51	9 (24%)	2	2	176, 195, 233, 256	0
33	Y9	37/37 (100%)	1.13	2 (5%)	31	19	145, 193, 249, 254	0
34	RA	2881/2915 (98%)	0.56	157 (5%)	31	19	59, 98, 232, 354	0
34	YA	2883/2915 (98%)	0.53	156 (5%)	31	19	55, 92, 228, 366	0
35	RB	120/122 (98%)	0.21	1 (0%)	82	60	109, 165, 211, 244	0
35	YB	120/122 (98%)	0.74	9 (7%)	20	14	110, 148, 185, 223	0
36	RD	272/276 (98%)	0.55	12 (4%)	39	23	56, 83, 116, 157	0
36	YD	272/276 (98%)	0.22	5 (1%)	67	41	45, 76, 110, 138	0
37	RE	205/206 (99%)	0.71	24 (11%)	9	9	56, 93, 153, 199	0
37	YE	204/206 (99%)	0.86	28 (13%)	6	7	54, 97, 150, 205	0
38	RF	202/210 (96%)	0.71	22 (10%)	10	10	62, 108, 161, 212	0
38	YF	202/210 (96%)	0.61	17 (8%)	17	12	51, 93, 146, 179	0
39	RG	181/182 (99%)	0.59	8 (4%)	39	23	124, 173, 220, 288	0
39	YG	181/182 (99%)	0.65	10 (5%)	30	19	116, 151, 197, 223	0
40	RH	174/180 (96%)	1.00	25 (14%)	6	6	100, 167, 226, 292	0
40	YH	173/180 (96%)	0.56	11 (6%)	25	17	82, 114, 156, 185	0
41	RI	146/148 (98%)	0.79	19 (13%)	7	7	93, 138, 193, 228	0
41	YI	146/148 (98%)	0.39	3 (2%)	63	38	82, 134, 178, 225	0
42	RN	138/140 (98%)	0.88	13 (9%)	14	11	69, 110, 164, 196	0
42	YN	138/140 (98%)	0.72	11 (7%)	18	13	66, 112, 167, 208	0
43	RO	122/122 (100%)	0.12	5 (4%)	41	24	52, 86, 117, 138	0
43	YO	122/122 (100%)	0.37	2 (1%)	70	44	55, 89, 118, 155	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RP	150/150 (100%)	0.60	7 (4%) 36 22	62, 114, 164, 237	0
44	YP	147/150 (98%)	0.40	5 (3%) 48 28	53, 97, 141, 166	0
45	RQ	141/141 (100%)	0.46	6 (4%) 40 23	72, 112, 158, 208	0
45	YQ	141/141 (100%)	0.66	13 (9%) 14 11	68, 102, 148, 216	0
46	RR	117/118 (99%)	0.19	2 (1%) 69 42	56, 86, 120, 208	0
46	YR	117/118 (99%)	0.41	4 (3%) 48 28	61, 92, 125, 170	0
47	RS	111/112 (99%)	0.54	6 (5%) 31 19	119, 154, 214, 254	0
47	YS	111/112 (99%)	0.75	7 (6%) 26 17	107, 144, 196, 226	0
48	RT	137/146 (93%)	0.31	6 (4%) 39 23	64, 95, 158, 188	0
48	YT	137/146 (93%)	0.56	6 (4%) 39 23	54, 104, 172, 232	0
49	RU	117/118 (99%)	0.80	12 (10%) 12 11	66, 101, 160, 193	0
49	YU	117/118 (99%)	0.57	5 (4%) 40 23	56, 110, 164, 242	0
50	RV	101/101 (100%)	0.44	7 (6%) 23 15	83, 122, 167, 271	0
50	YV	101/101 (100%)	0.52	6 (5%) 28 18	71, 120, 174, 217	0
51	RW	113/113 (100%)	0.57	10 (8%) 15 12	60, 84, 134, 233	0
51	YW	113/113 (100%)	0.31	3 (2%) 56 33	58, 85, 138, 204	0
52	RX	92/96 (95%)	0.57	6 (6%) 25 16	69, 102, 145, 159	0
52	YX	92/96 (95%)	0.43	5 (5%) 31 19	58, 80, 111, 181	0
53	RY	107/110 (97%)	1.10	14 (13%) 7 7	91, 125, 168, 188	0
53	YY	107/110 (97%)	0.86	8 (7%) 20 14	75, 107, 152, 174	0
54	RZ	203/206 (98%)	0.20	0 100 100	114, 153, 202, 282	0
54	YZ	203/206 (98%)	0.47	11 (5%) 31 19	108, 142, 192, 226	0
55	XY	17/17 (100%)	0.45	0 100 100	141, 155, 229, 295	0
56	Z6	2/3 (66%)	0.07	0 100 100	136, 136, 136, 146	0
56	Z8	2/3 (66%)	0.78	0 100 100	129, 129, 129, 136	0
All	All	20886/21465 (97%)	0.51	1137 (5%) 31 19	45, 118, 209, 366	0

All (1137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	QI	116	LYS	8.7
37	RE	130	GLY	8.4
53	RY	62	GLU	8.2

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Mol	Chain	Res	Type	RSRZ
37	YE	153	GLY	7.5
22	XV	1	G	7.0
34	YA	2602	A	6.9
9	QI	111	ARG	6.8
7	QG	81	GLY	6.4
34	YA	669	G	6.3
9	QI	106	ALA	6.2
9	QI	117	HIS	6.2
12	XL	28	LYS	6.2
9	QI	115	GLY	6.2
9	QI	127	LYS	6.1
38	YF	66	PRO	6.0
9	QI	110	GLU	6.0
47	YS	22	GLY	5.8
22	XV	76	A	5.6
34	YA	745	G	5.6
7	QG	153	HIS	5.5
34	YA	2062	A	5.5
22	XV	74	C	5.4
51	RW	93	ALA	5.4
9	XI	115	GLY	5.4
37	YE	152	LYS	5.3
48	YT	104	ASN	5.2
34	RA	1087	G	5.2
25	Y1	91	LYS	5.1
25	Y1	11	ARG	5.1
54	YZ	17	ALA	5.1
9	XI	118	LYS	5.1
34	YA	2618	G	5.1
13	QM	102	ARG	5.0
25	Y1	92	LYS	5.0
34	RA	1103	A	5.0
40	YH	58	GLU	5.0
34	YA	744	G	4.9
9	QI	120	ARG	4.9
51	RW	92	ARG	4.9
44	RP	61	ARG	4.8
9	QI	125	TYR	4.8
9	XI	116	LYS	4.8
37	RE	155	LYS	4.7
37	YE	141	ILE	4.7
37	YE	159	HIS	4.7

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Mol	Chain	Res	Type	RSRZ
38	YF	70	THR	4.7
34	YA	2619	C	4.6
38	RF	72	ARG	4.6
1	QA	1451	A	4.6
45	YQ	80	GLU	4.6
34	YA	1272	A	4.5
51	RW	94	ASP	4.5
38	RF	62	ARG	4.5
13	QM	78	ILE	4.5
9	XI	127	LYS	4.4
42	YN	77	GLY	4.4
42	YN	75	TYR	4.4
34	RA	967	C	4.4
34	RA	2402	C	4.4
53	YY	64	GLU	4.4
14	XN	2	ALA	4.4
53	YY	1	MET	4.4
48	YT	106	SER	4.4
34	YA	1379	A	4.4
19	XS	76	PRO	4.4
33	R9	14	CYS	4.4
38	YF	85	GLY	4.4
1	QA	1202	G	4.4
34	RA	2400	G	4.4
11	XK	120	ARG	4.4
34	RA	2609	U	4.3
45	YQ	135	ASP	4.3
34	RA	747	U	4.3
34	YA	789	A	4.3
11	QK	125	PHE	4.3
33	R9	26	ILE	4.3
45	YQ	92	GLY	4.3
7	XG	4	ARG	4.3
34	RA	389	G	4.2
34	YA	2003	G	4.2
13	XM	102	ARG	4.2
34	RA	6	A	4.2
34	YA	1816	G	4.2
40	RH	83	TYR	4.2
34	YA	2578	G	4.1
35	YB	84	C	4.1
34	YA	1130	U	4.1

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Mol	Chain	Res	Type	RSRZ
13	QM	87	TYR	4.1
49	RU	28	ARG	4.1
41	YI	118	LYS	4.0
10	QJ	59	SER	4.0
34	YA	755	C	4.0
39	RG	155	MET	4.0
34	YA	791	C	4.0
34	YA	2571	C	4.0
38	YF	72	ARG	4.0
38	RF	65	TRP	4.0
13	QM	94	ARG	4.0
35	YB	88	C	3.9
1	XA	1529	G	3.9
10	XJ	98	ILE	3.9
34	RA	2581	G	3.9
7	QG	8	GLU	3.9
22	QV	1	G	3.9
9	QI	123	PRO	3.9
51	RW	85	VAL	3.9
10	QJ	61	GLU	3.9
1	XA	81	G	3.8
22	XV	75	C	3.8
34	RA	2357	U	3.8
47	YS	77	ALA	3.8
12	XL	8	ASN	3.8
25	R1	65	SER	3.8
34	YA	2439	A	3.8
34	YA	2506	U	3.8
37	RE	127	ASP	3.8
1	XA	1094	G	3.8
2	QB	214	ILE	3.8
34	RA	1083	U	3.8
11	XK	20	TYR	3.8
9	QI	114	TYR	3.7
40	YH	64	LEU	3.7
1	XA	1527	C	3.7
34	YA	34	C	3.7
45	YQ	83	MET	3.7
35	YB	1	U	3.7
34	YA	461	C	3.7
53	RY	42	VAL	3.7
9	QI	119	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
35	YB	85	G	3.7
7	XG	5	ARG	3.7
10	XJ	49	VAL	3.7
4	XD	50	ARG	3.6
28	R4	3	GLU	3.6
34	YA	753	C	3.6
1	QA	1438	G	3.6
13	QM	95	GLY	3.6
2	XB	167	PRO	3.6
10	XJ	6	ILE	3.6
37	YE	138	PRO	3.6
52	YX	69	TYR	3.6
36	RD	240	ALA	3.6
37	YE	162	ALA	3.6
34	RA	744	G	3.6
7	QG	152	ALA	3.6
24	Y0	30	VAL	3.6
42	YN	76	SER	3.6
12	QL	28	LYS	3.5
52	YX	68	ARG	3.5
30	Y6	22	ALA	3.5
34	YA	2758	A	3.5
23	XX	0	G	3.5
37	RE	144	ARG	3.5
48	RT	94	ALA	3.5
12	XL	13	LYS	3.5
39	YG	36	LYS	3.5
34	RA	2062	A	3.5
1	XA	79	G	3.5
37	YE	154	LYS	3.5
42	RN	84	LYS	3.5
49	RU	90	VAL	3.5
1	QA	1531	A	3.4
53	RY	22	GLY	3.4
50	RV	82	ARG	3.4
36	YD	107	ALA	3.4
41	RI	18	VAL	3.4
1	XA	1346	A	3.4
52	RX	68	ARG	3.4
34	RA	186	G	3.4
35	YB	83	G	3.4
34	RA	1104	C	3.4

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Mol	Chain	Res	Type	RSRZ
10	QJ	58	ASP	3.4
15	QO	88	ARG	3.4
7	XG	3	ARG	3.4
8	XH	136	GLU	3.4
34	YA	469	G	3.4
34	RA	34	C	3.4
34	YA	756	C	3.4
7	QG	4	ARG	3.4
13	XM	99	ARG	3.4
13	QM	85	GLY	3.3
38	YF	56	GLU	3.3
40	RH	151	ILE	3.3
49	RU	97	ASP	3.3
34	YA	363	G	3.3
10	QJ	62	HIS	3.3
38	RF	79	GLY	3.3
38	RF	131	GLY	3.3
1	XA	897	C	3.3
54	YZ	193	GLU	3.3
34	YA	722	A	3.3
49	RU	25	TRP	3.3
37	YE	113	PHE	3.3
51	RW	91	GLY	3.3
49	YU	97	ASP	3.3
34	RA	1992	G	3.3
53	RY	24	VAL	3.3
51	RW	86	LEU	3.3
41	RI	85	GLU	3.3
12	XL	7	ILE	3.3
47	RS	108	GLY	3.3
34	YA	859	G	3.3
25	R1	90	ILE	3.3
37	YE	149	ARG	3.2
37	YE	147	PRO	3.2
34	YA	982	C	3.2
41	RI	16	GLY	3.2
1	QA	1188	A	3.2
34	RA	265	A	3.2
34	YA	460	A	3.2
34	RA	1661	G	3.2
34	RA	2505	G	3.2
33	R9	11	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
40	RH	168	PRO	3.2
43	RO	1	MET	3.2
53	YY	50	ARG	3.2
34	YA	1536	A	3.2
34	YA	1618	A	3.2
40	YH	68	THR	3.2
41	RI	20	ASP	3.2
48	YT	69	GLY	3.2
33	Y9	26	ILE	3.2
53	RY	29	GLU	3.2
30	R6	11	LEU	3.2
34	RA	1078	U	3.2
40	RH	166	GLY	3.2
9	XI	125	TYR	3.2
51	RW	90	ARG	3.2
45	RQ	91	GLU	3.2
1	QA	1466	C	3.2
42	RN	1	MET	3.2
51	RW	81	ALA	3.2
1	XA	1511	G	3.2
34	RA	739	G	3.2
34	YA	2505	G	3.2
38	YF	62	ARG	3.2
49	RU	36	ARG	3.2
17	QQ	24	GLU	3.2
30	Y6	24	GLU	3.2
34	YA	181	A	3.1
12	XL	19	ARG	3.1
32	R8	59	LYS	3.1
40	RH	35	VAL	3.1
32	Y8	2	PRO	3.1
34	RA	799	G	3.1
34	RA	2401	U	3.1
34	YA	1273	U	3.1
52	YX	66	LEU	3.1
53	RY	107	ASP	3.1
34	RA	1755	A	3.1
1	XA	822	C	3.1
34	YA	2063	C	3.1
12	QL	19	ARG	3.1
38	RF	75	HIS	3.1
34	RA	214	G	3.1

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Mol	Chain	Res	Type	RSRZ
34	RA	2270	G	3.1
35	YB	87	G	3.1
1	XA	5	U	3.1
7	QG	82	GLY	3.1
38	YF	131	GLY	3.1
2	XB	138	LEU	3.1
36	RD	46	GLN	3.1
3	XC	167	TRP	3.1
48	RT	106	SER	3.1
53	RY	10	GLY	3.1
34	RA	2398	U	3.1
34	YA	741	G	3.1
37	RE	128	SER	3.1
38	RF	89	VAL	3.1
40	RH	33	LEU	3.1
34	RA	2403	C	3.1
50	RV	48	GLY	3.1
37	YE	155	LYS	3.0
34	RA	101	G	3.0
34	YA	728	G	3.0
34	YA	2642	G	3.0
4	XD	91	SER	3.0
53	YY	3	VAL	3.0
34	RA	1086	A	3.0
41	RI	2	LYS	3.0
37	RE	79	ARG	3.0
13	QM	67	GLU	3.0
42	RN	68	GLU	3.0
34	YA	1781	C	3.0
12	XL	21	LYS	3.0
34	RA	2611	U	3.0
34	YA	694	U	3.0
34	YA	2609	U	3.0
41	RI	27	ARG	3.0
34	YA	2709	G	3.0
34	RA	2015	A	3.0
34	YA	751	A	3.0
40	RH	82	GLY	3.0
27	Y3	56	VAL	3.0
41	RI	19	VAL	3.0
34	RA	1663	C	3.0
49	RU	14	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
29	R5	9	LYS	3.0
38	YF	71	GLY	3.0
50	RV	80	GLN	3.0
7	XG	99	LEU	3.0
1	QA	570	G	3.0
1	XA	1394	A	3.0
34	YA	746	A	3.0
34	YA	2346	A	3.0
35	YB	86	G	3.0
42	YN	78	TYR	3.0
45	YQ	91	GLU	3.0
9	QI	112	LYS	3.0
49	YU	90	VAL	3.0
40	RH	138	LYS	2.9
54	YZ	25	PRO	2.9
9	QI	108	VAL	2.9
30	Y6	23	THR	2.9
36	RD	217	ARG	2.9
37	YE	146	THR	2.9
44	RP	65	ARG	2.9
40	RH	150	ALA	2.9
1	XA	80	G	2.9
22	QV	52	G	2.9
53	YY	107	ASP	2.9
43	RO	68	GLU	2.9
4	XD	120	LEU	2.9
21	QU	2	GLY	2.9
37	RE	150	VAL	2.9
11	XK	123	LYS	2.9
9	QI	40	LEU	2.9
53	RY	64	GLU	2.9
21	XU	2	GLY	2.9
40	RH	5	GLY	2.9
29	R5	8	LYS	2.9
34	RA	673	C	2.9
34	YA	698	C	2.9
34	YA	737	C	2.9
53	RY	61	ILE	2.9
10	XJ	59	SER	2.9
13	QM	15	VAL	2.9
37	RE	148	GLY	2.9
54	YZ	191	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
9	XI	119	ALA	2.9
34	YA	980	A	2.9
42	RN	138	LEU	2.9
9	QI	37	PHE	2.9
11	QK	20	TYR	2.9
10	XJ	60	ARG	2.9
11	XK	126	ARG	2.9
40	RH	152	ARG	2.9
1	QA	20	U	2.9
1	QA	1062	U	2.9
34	RA	383	U	2.9
34	RA	2055	C	2.9
1	XA	769	G	2.9
1	XA	971	G	2.9
1	XA	1526	G	2.9
34	YA	674	G	2.9
34	YA	1659	U	2.9
27	Y3	9	VAL	2.9
13	XM	33	ALA	2.9
33	R9	27	CYS	2.9
12	XL	15	ARG	2.9
38	RF	81	PRO	2.9
50	RV	36	PRO	2.9
9	XI	117	HIS	2.8
34	RA	227	A	2.8
34	RA	1177	A	2.8
34	YA	2042	A	2.8
37	YE	158	GLY	2.8
50	YV	52	VAL	2.8
39	RG	34	LEU	2.8
50	YV	45	THR	2.8
1	XA	345	C	2.8
34	RA	889	C	2.8
35	YB	12	C	2.8
12	XL	47	LYS	2.8
34	RA	748	G	2.8
38	RF	59	TYR	2.8
9	XI	110	GLU	2.8
3	QC	124	ILE	2.8
13	QM	75	ALA	2.8
1	QA	915	A	2.8
1	XA	975	A	2.8

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Mol	Chain	Res	Type	RSRZ
47	YS	7	TYR	2.8
17	QQ	35	VAL	2.8
37	YE	143	ASN	2.8
39	RG	137	GLU	2.8
42	RN	46	VAL	2.8
25	R1	77	ALA	2.8
34	RA	1140	C	2.8
34	YA	435	C	2.8
34	YA	790	C	2.8
34	YA	2620	C	2.8
13	QM	114	ARG	2.8
17	XQ	37	LYS	2.8
34	RA	2018	G	2.8
17	XQ	35	VAL	2.8
38	RF	88	VAL	2.8
52	RX	69	TYR	2.8
4	XD	130	GLY	2.8
1	QA	968	A	2.8
34	YA	2712(A)	A	2.8
30	Y6	38	LYS	2.8
40	YH	4	ILE	2.8
34	YA	2039	C	2.8
38	YF	132	VAL	2.8
3	QC	10	PHE	2.8
7	XG	47	CYS	2.8
34	RA	738	G	2.8
34	RA	1139	G	2.8
34	RA	2717	G	2.8
34	YA	275	G	2.8
44	RP	79	ARG	2.8
37	RE	117	MET	2.8
47	RS	109	GLY	2.8
1	QA	1450	U	2.8
8	QH	3	THR	2.8
46	RR	9	LYS	2.8
20	XT	83	ARG	2.7
32	R8	50	LEU	2.7
34	RA	1258	C	2.7
40	RH	125	VAL	2.7
40	RH	141	VAL	2.7
11	QK	124	LYS	2.7
42	YN	80	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
22	XV	2	G	2.7
34	YA	707	G	2.7
34	YA	1131	G	2.7
34	YA	1807	G	2.7
34	YA	2100	G	2.7
36	RD	27	THR	2.7
8	XH	91	ARG	2.7
9	QI	107	ARG	2.7
22	XV	73	A	2.7
34	RA	752	A	2.7
34	RA	1097	U	2.7
4	QD	198	VAL	2.7
37	YE	150	VAL	2.7
42	YN	62	VAL	2.7
4	XD	30	LYS	2.7
42	RN	111	PRO	2.7
37	YE	130	GLY	2.7
1	XA	1344	C	2.7
4	QD	77	ASN	2.7
34	RA	461	C	2.7
34	RA	1064	C	2.7
34	YA	693	C	2.7
34	YA	1836	C	2.7
20	QT	73	HIS	2.7
1	QA	411	A	2.7
1	XA	799	G	2.7
6	QF	45	LEU	2.7
34	RA	743	G	2.7
17	XQ	68	ARG	2.7
25	R1	11	ARG	2.7
45	RQ	80	GLU	2.7
1	XA	1528	U	2.7
23	XX	4	U	2.7
24	R0	53	MET	2.7
34	RA	580	C	2.7
41	RI	140	LEU	2.7
3	XC	50	ALA	2.7
7	XG	2	ALA	2.7
7	XG	8	GLU	2.7
20	QT	29	LYS	2.7
1	XA	1188	A	2.7
9	XI	109	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
40	YH	19	VAL	2.7
1	XA	630	G	2.7
34	RA	83	G	2.7
34	YA	1678	G	2.7
33	R9	12	ASP	2.7
40	YH	39	PRO	2.7
42	RN	132	ALA	2.7
3	XC	166	GLU	2.7
37	RE	145	LYS	2.7
42	RN	59	LYS	2.7
1	XA	810	C	2.7
1	XA	1538	C	2.7
34	YA	2690	C	2.7
38	RF	74	ARG	2.6
48	YT	11	GLU	2.6
1	XA	809	G	2.6
34	RA	2399	G	2.6
51	YW	92	ARG	2.6
7	QG	103	TRP	2.6
12	QL	129	ALA	2.6
9	QI	70	LYS	2.6
14	XN	58	LYS	2.6
37	YE	142	GLY	2.6
42	RN	127	ASP	2.6
34	RA	246	C	2.6
47	YS	28	VAL	2.6
22	QV	31	A	2.6
34	RA	1614	A	2.6
34	RA	2602	A	2.6
34	YA	984	A	2.6
13	QM	113	PRO	2.6
17	XQ	26	GLN	2.6
34	YA	2585	U	2.6
36	RD	216	GLY	2.6
49	YU	35	ALA	2.6
50	RV	8	GLY	2.6
1	XA	1224	G	2.6
26	Y2	11	GLU	2.6
34	RA	1089	G	2.6
34	RA	1416	G	2.6
34	RA	1667	G	2.6
34	YA	270(Y)	G	2.6

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Mol	Chain	Res	Type	RSRZ
34	YA	2004	G	2.6
44	RP	25	SER	2.6
53	RY	63	LYS	2.6
1	QA	1063	C	2.6
34	RA	1754	C	2.6
34	YA	2021	C	2.6
33	R9	20	HIS	2.6
12	XL	92	ASP	2.6
34	RA	229	A	2.6
34	YA	1508	A	2.6
34	YA	1762	A	2.6
1	XA	1235	U	2.6
45	YQ	81	VAL	2.6
13	XM	2	ALA	2.6
33	Y9	5	ALA	2.6
36	YD	111	LEU	2.6
54	YZ	164	ALA	2.6
13	QM	92	HIS	2.6
38	RF	76	GLY	2.6
1	XA	579	G	2.6
10	QJ	54	PHE	2.6
34	YA	530	G	2.6
34	YA	668	G	2.6
7	QG	90	GLU	2.6
14	QN	29	ARG	2.6
33	R9	13	LYS	2.6
29	Y5	7	PRO	2.6
34	YA	270(B)	A	2.6
34	YA	470	A	2.6
1	XA	359	U	2.6
34	RA	2506	U	2.6
43	RO	110	GLY	2.6
5	XE	81	GLU	2.5
38	YF	74	ARG	2.5
41	RI	10	GLU	2.5
53	YY	63	LYS	2.5
15	QO	45	VAL	2.5
10	XJ	58	ASP	2.5
1	QA	1331	G	2.5
9	XI	106	ALA	2.5
34	YA	252	G	2.5
34	YA	2190	G	2.5

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Mol	Chain	Res	Type	RSRZ
39	YG	102	PHE	2.5
42	YN	36	GLY	2.5
2	XB	214	ILE	2.5
14	XN	13	THR	2.5
8	QH	91	ARG	2.5
9	QI	121	ARG	2.5
12	QL	18	VAL	2.5
13	QM	60	VAL	2.5
47	YS	43	GLU	2.5
1	QA	975	A	2.5
1	QA	1357	A	2.5
12	XL	27	LEU	2.5
34	YA	1302	A	2.5
39	RG	86	MET	2.5
40	RH	29	PRO	2.5
42	YN	79	PRO	2.5
45	YQ	45	GLN	2.5
46	YR	46	GLY	2.5
38	RF	70	THR	2.5
50	YV	7	THR	2.5
9	XI	121	ARG	2.5
25	R1	98	LEU	2.5
40	RH	86	GLU	2.5
41	RI	37	VAL	2.5
1	QA	1190	G	2.5
1	XA	898	G	2.5
34	RA	968	G	2.5
34	RA	2694	G	2.5
1	XA	811	C	2.5
34	RA	756	C	2.5
34	YA	574	C	2.5
38	RF	77	ASP	2.5
41	RI	39	ALA	2.5
13	XM	10	PRO	2.5
22	QV	76	A	2.5
34	RA	2016	U	2.5
9	XI	111	ARG	2.5
53	YY	62	GLU	2.5
54	YZ	28	MET	2.5
38	RF	83	PHE	2.5
49	RU	40	PHE	2.5
25	Y1	77	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
13	XM	97	PRO	2.5
14	XN	7	ILE	2.5
37	YE	148	GLY	2.5
4	QD	64	LEU	2.5
9	QI	128	ARG	2.5
52	YX	65	ARG	2.5
11	QK	87	THR	2.5
9	XI	114	TYR	2.5
20	XT	73	HIS	2.5
31	R7	1	MET	2.5
45	RQ	83	MET	2.5
1	XA	422	C	2.5
34	YA	1830	C	2.5
34	YA	2710	C	2.5
34	RA	1862	G	2.5
34	YA	1219	G	2.5
34	YA	2182	G	2.5
14	QN	37	PHE	2.5
1	XA	1196	U	2.5
1	XA	968	A	2.5
23	XX	-2	A	2.5
34	RA	2693	A	2.5
34	YA	750	A	2.5
34	YA	1434	A	2.5
49	RU	35	ALA	2.5
37	YE	74	PRO	2.5
38	YF	95	ARG	2.5
39	YG	34	LEU	2.5
47	YS	41	ASP	2.5
40	RH	144	VAL	2.5
32	Y8	54	GLU	2.4
36	RD	59	LYS	2.4
38	RF	82	ILE	2.4
38	YF	22	ALA	2.4
54	YZ	192	ALA	2.4
37	RE	63	LEU	2.4
11	QK	126	ARG	2.4
7	XG	34	GLY	2.4
50	YV	48	GLY	2.4
34	RA	1053	C	2.4
34	YA	754	C	2.4
34	YA	961	C	2.4

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Mol	Chain	Res	Type	RSRZ
34	YA	2579	C	2.4
1	XA	1380	U	2.4
2	QB	168	THR	2.4
19	QS	79	THR	2.4
1	QA	886	G	2.4
1	XA	572	A	2.4
1	XA	1508	G	2.4
34	YA	270(X)	G	2.4
34	YA	723	G	2.4
34	YA	743	G	2.4
34	YA	2358	G	2.4
34	YA	2581	G	2.4
37	RE	116	VAL	2.4
21	QU	18	TYR	2.4
33	R9	15	LYS	2.4
37	YE	151	TYR	2.4
49	RU	32	PHE	2.4
54	YZ	88	PHE	2.4
4	QD	67	ILE	2.4
26	Y2	66	GLU	2.4
37	YE	63	LEU	2.4
46	YR	41	ALA	2.4
48	RT	114	LEU	2.4
50	YV	77	ALA	2.4
39	RG	72	ARG	2.4
16	XP	35	LYS	2.4
40	YH	136	ILE	2.4
38	YF	75	HIS	2.4
39	YG	164	GLU	2.4
41	YI	41	GLU	2.4
43	YO	45	GLU	2.4
1	QA	1397	C	2.4
29	R5	2	ALA	2.4
34	RA	335	C	2.4
34	YA	708	C	2.4
1	XA	1531	A	2.4
4	XD	29	PRO	2.4
34	RA	586	A	2.4
34	RA	1084	A	2.4
34	RA	2054	A	2.4
34	RA	2577	A	2.4
34	YA	727	A	2.4

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Mol	Chain	Res	Type	RSRZ
34	YA	752	A	2.4
40	RH	41	MET	2.4
43	YO	110	GLY	2.4
1	XA	631	G	2.4
34	RA	776	G	2.4
34	YA	11	G	2.4
34	YA	272	G	2.4
34	YA	738	G	2.4
34	YA	832	G	2.4
35	YB	76	G	2.4
40	YH	43	VAL	2.4
20	QT	36	LEU	2.4
54	YZ	195	GLU	2.4
20	XT	76	ALA	2.4
41	RI	36	ALA	2.4
46	RR	2	ARG	2.4
4	XD	18	LYS	2.4
30	R6	8	LYS	2.4
52	YX	67	GLY	2.4
3	XC	64	VAL	2.4
34	YA	1808	U	2.4
40	RH	136	ILE	2.4
44	RP	62	LEU	2.4
1	QA	1189	C	2.4
34	RA	1660	C	2.4
1	QA	1101	A	2.4
23	XX	-3	A	2.4
34	RA	2060	A	2.4
34	YA	670	A	2.4
34	YA	1677	A	2.4
45	RQ	16	ARG	2.4
53	RY	40	GLU	2.4
9	XI	46	ALA	2.4
1	QA	929	G	2.4
1	XA	1187	G	2.4
34	RA	2413	G	2.4
34	YA	180	G	2.4
7	QG	156	TRP	2.4
39	RG	87	PRO	2.4
39	YG	32	PRO	2.4
40	RH	28	GLY	2.4
9	QI	126	SER	2.4

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Mol	Chain	Res	Type	RSRZ
41	RI	86	THR	2.4
48	RT	102	ILE	2.4
48	YT	6	LEU	2.4
7	XG	20	ASP	2.4
15	QO	68	ARG	2.4
47	RS	88	ASP	2.4
37	YE	145	LYS	2.4
1	XA	1532	U	2.3
34	YA	456	C	2.3
37	YE	128	SER	2.3
48	RT	104	ASN	2.3
1	QA	412	A	2.3
1	QA	908	A	2.3
6	QF	8	ILE	2.3
17	XQ	36	ILE	2.3
34	RA	222	A	2.3
34	RA	472	A	2.3
34	RA	634	C	2.3
34	RA	1098	A	2.3
34	RA	1102	C	2.3
38	RF	78	ILE	2.3
41	RI	12	LEU	2.3
20	XT	23	ARG	2.3
50	YV	81	TYR	2.3
1	QA	1053	G	2.3
34	RA	680	G	2.3
34	RA	745	G	2.3
36	RD	4	LYS	2.3
37	RE	154	LYS	2.3
40	RH	119	GLU	2.3
9	XI	126	SER	2.3
20	QT	55	ILE	2.3
3	XC	198	VAL	2.3
9	QI	41	VAL	2.3
47	YS	98	VAL	2.3
7	QG	5	ARG	2.3
13	QM	88	ARG	2.3
37	RE	151	TYR	2.3
1	QA	1459	C	2.3
1	XA	896	C	2.3
2	XB	120	ALA	2.3
13	XM	30	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
53	RY	105	ALA	2.3
8	QH	4	ASP	2.3
38	RF	56	GLU	2.3
30	Y6	36	LEU	2.3
46	YR	10	LEU	2.3
51	YW	86	LEU	2.3
37	RE	159	HIS	2.3
40	YH	21	PRO	2.3
45	YQ	90	VAL	2.3
26	R2	8	LYS	2.3
29	R5	19	ARG	2.3
34	YA	179	G	2.3
34	YA	1426	G	2.3
17	QQ	95	TYR	2.3
37	YE	163	GLU	2.3
40	RH	124	GLU	2.3
8	QH	23	SER	2.3
40	RH	38	SER	2.3
37	RE	137	HIS	2.3
1	QA	1111	A	2.3
1	XA	87	A	2.3
11	QK	71	LYS	2.3
34	RA	8	A	2.3
34	RA	1654	A	2.3
1	QA	1128	C	2.3
34	RA	2356	C	2.3
4	XD	26	CYS	2.3
39	RG	135	LEU	2.3
49	RU	95	LEU	2.3
4	QD	167	GLY	2.3
21	QU	4	GLY	2.3
45	YQ	21	THR	2.3
34	RA	798	G	2.3
34	RA	944	G	2.3
34	RA	1264	G	2.3
34	YA	2548	G	2.3
34	RA	1066	U	2.3
34	YA	1639	U	2.3
34	YA	2514	U	2.3
2	QB	68	ILE	2.3
14	XN	27	CYS	2.3
16	XP	32	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
34	YA	2451	A	2.3
1	XA	1342	C	2.3
31	Y7	48	LYS	2.3
34	RA	273(B)	C	2.3
34	YA	949	C	2.3
36	RD	5	LYS	2.3
37	RE	142	GLY	2.3
44	YP	53	GLY	2.3
52	RX	33	LYS	2.3
48	RT	96	ARG	2.3
13	QM	103	THR	2.2
25	Y1	16	ASN	2.2
30	R6	30	THR	2.2
7	XG	120	ILE	2.2
39	YG	163	ALA	2.2
7	XG	11	GLN	2.2
9	QI	124	GLN	2.2
25	Y1	42	GLN	2.2
26	R2	46	GLN	2.2
13	QM	121	LYS	2.2
27	Y3	17	LYS	2.2
36	RD	266	SER	2.2
17	XQ	96	GLU	2.2
1	QA	685	G	2.2
1	QA	1061	G	2.2
1	QA	1233	G	2.2
1	QA	1368	G	2.2
1	XA	800	G	2.2
23	XX	-1	U	2.2
34	RA	577	G	2.2
34	RA	801	G	2.2
34	RA	859	G	2.2
34	RA	1026	U	2.2
34	RA	2067	G	2.2
34	YA	1026	U	2.2
34	YA	2029	G	2.2
34	YA	2574	G	2.2
35	RB	16	G	2.2
38	RF	66	PRO	2.2
45	YQ	86	GLY	2.2
49	YU	36	ARG	2.2
8	XH	133	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
23	XX	8	A	2.2
34	RA	578	A	2.2
34	RA	2587	A	2.2
34	YA	529	A	2.2
36	YD	93	ALA	2.2
36	YD	240	ALA	2.2
9	QI	118	LYS	2.2
34	RA	654(B)	C	2.2
34	YA	2699	C	2.2
47	RS	7	TYR	2.2
20	QT	17	ARG	2.2
28	Y4	54	GLY	2.2
31	Y7	46	VAL	2.2
39	YG	160	VAL	2.2
46	YR	48	VAL	2.2
10	QJ	48	THR	2.2
6	QF	55	ASP	2.2
16	QP	29	ASP	2.2
20	XT	9	ASN	2.2
36	RD	220	HIS	2.2
44	RP	27	HIS	2.2
1	QA	1341	U	2.2
34	YA	1431	U	2.2
1	QA	769	G	2.2
1	QA	887	G	2.2
21	QU	15	ARG	2.2
34	RA	307	G	2.2
34	RA	742	G	2.2
34	RA	2318	G	2.2
34	YA	406	G	2.2
34	YA	739	G	2.2
34	YA	801	G	2.2
4	XD	80	GLU	2.2
34	RA	653	A	2.2
34	RA	1269	A	2.2
34	RA	1762	A	2.2
34	YA	1562	A	2.2
34	YA	2577	A	2.2
7	XG	43	PHE	2.2
1	XA	312	C	2.2
7	QG	37	ASN	2.2
34	RA	456	C	2.2

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Mol	Chain	Res	Type	RSRZ
34	RA	2610	C	2.2
34	YA	1258	C	2.2
37	RE	143	ASN	2.2
25	R1	32	LYS	2.2
4	QD	120	LEU	2.2
21	XU	15	ARG	2.2
39	YG	136	ARG	2.2
47	RS	32	LEU	2.2
51	YW	90	ARG	2.2
9	XI	26	VAL	2.2
41	RI	92	VAL	2.2
36	YD	108	PRO	2.2
37	YE	139	GLY	2.2
38	RF	61	GLY	2.2
40	RH	93	GLY	2.2
49	RU	108	GLU	2.2
38	YF	78	ILE	2.2
40	RH	92	ILE	2.2
34	RA	2897	U	2.2
34	YA	757	U	2.2
53	YY	71	LYS	2.2
37	RE	156	MET	2.2
1	XA	771	G	2.2
13	XM	56	LEU	2.2
25	R1	94	LEU	2.2
34	RA	205	G	2.2
34	RA	583	G	2.2
34	RA	676	A	2.2
34	RA	1256	G	2.2
34	RA	1325	G	2.2
34	YA	681	G	2.2
34	YA	1062	G	2.2
34	YA	1252	G	2.2
34	YA	1274	A	2.2
34	YA	2513	G	2.2
41	YI	128	LEU	2.2
51	RW	13	SER	2.2
28	Y4	35	VAL	2.2
12	QL	29	GLY	2.2
34	RA	2692	C	2.2
34	RA	2870	C	2.2
34	YA	970	C	2.2

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Mol	Chain	Res	Type	RSRZ
34	YA	2183	C	2.2
42	YN	81	GLY	2.2
3	QC	91	LEU	2.2
8	XH	25	ASP	2.1
34	RA	1778	U	2.1
40	YH	60	ARG	2.1
45	YQ	141	GLN	2.1
53	RY	50	ARG	2.1
7	XG	21	VAL	2.1
13	XM	15	VAL	2.1
17	XQ	23	VAL	2.1
41	RI	97	ILE	2.1
44	RP	126	VAL	2.1
39	YG	23	PHE	2.1
4	XD	46	LYS	2.1
13	XM	120	LYS	2.1
42	RN	37	LYS	2.1
34	RA	1085	A	2.1
34	RA	2725	A	2.1
1	QA	1187	G	2.1
34	RA	1678	G	2.1
34	RA	1816	G	2.1
34	RA	2141	G	2.1
34	RA	2444	G	2.1
34	YA	1232	G	2.1
9	XI	15	ALA	2.1
7	XG	10	ARG	2.1
1	QA	1113	C	2.1
11	QK	129	SER	2.1
34	RA	393	C	2.1
34	RA	857	C	2.1
34	RA	884	C	2.1
34	RA	1417	C	2.1
34	RA	1782	C	2.1
34	YA	721	C	2.1
34	YA	1660	C	2.1
51	RW	63	ASP	2.1
9	QI	44	VAL	2.1
20	XT	34	LYS	2.1
30	R6	17	LYS	2.1
44	YP	36	LYS	2.1
45	RQ	104	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
13	QM	68	GLY	2.1
18	QR	80	PRO	2.1
42	RN	79	PRO	2.1
48	YT	109	GLU	2.1
1	QA	1358	U	2.1
1	XA	820	U	2.1
1	XA	1472	U	2.1
12	QL	27	LEU	2.1
34	RA	373	U	2.1
30	R6	2	ALA	2.1
31	R7	13	ALA	2.1
38	RF	206	ILE	2.1
10	XJ	24	VAL	2.1
37	YE	133	LYS	2.1
52	RX	51	VAL	2.1
22	QV	69	A	2.1
34	RA	567	A	2.1
13	XM	90	LEU	2.1
1	QA	168	G	2.1
1	XA	78	G	2.1
1	XA	570	G	2.1
34	RA	382	G	2.1
34	YA	742	G	2.1
1	XA	719	C	2.1
34	RA	749	C	2.1
34	RA	837	C	2.1
34	YA	1656	C	2.1
34	YA	2026	C	2.1
20	XT	77	ALA	2.1
25	R1	91	LYS	2.1
1	QA	82	U	2.1
12	XL	101	VAL	2.1
22	QV	43	U	2.1
34	RA	273(E)	U	2.1
34	YA	1188	U	2.1
38	RF	132	VAL	2.1
38	YF	193	VAL	2.1
53	RY	39	VAL	2.1
20	XT	20	LEU	2.1
21	XU	11	GLY	2.1
30	R6	21	TYR	2.1
37	RE	65	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
7	QG	146	GLU	2.1
52	RX	45	THR	2.1
37	RE	76	ARG	2.1
1	QA	1179	A	2.1
7	QG	2	ALA	2.1
34	YA	471	A	2.1
34	YA	777	A	2.1
11	QK	122	LYS	2.1
32	Y8	5	LYS	2.1
37	RE	205	ALA	2.1
4	XD	77	ASN	2.1
13	QM	74	VAL	2.1
13	XM	7	VAL	2.1
28	Y4	50	VAL	2.1
47	RS	98	VAL	2.1
9	XI	47	LEU	2.1
39	YG	106	LEU	2.1
41	RI	30	LEU	2.1
42	RN	91	LEU	2.1
1	QA	88	C	2.1
34	RA	201	C	2.1
34	RA	1076	C	2.1
34	RA	2140	C	2.1
34	YA	1607	C	2.1
34	YA	2040	C	2.1
1	QA	306	G	2.1
1	QA	1347	G	2.1
1	XA	760	G	2.1
1	XA	1523	G	2.1
22	XV	10	G	2.1
30	R6	42	TRP	2.1
34	RA	252	G	2.1
34	RA	585	G	2.1
34	RA	1764	G	2.1
34	YA	2121	G	2.1
37	RE	124	GLY	2.1
38	YF	65	TRP	2.1
54	YZ	190	GLU	2.1
36	RD	54	ARG	2.1
1	QA	1348	U	2.1
1	XA	1240	U	2.1
34	YA	810	U	2.1

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Mol	Chain	Res	Type	RSRZ
39	RG	36	LYS	2.1
50	RV	78	LYS	2.1
2	XB	188	ALA	2.1
9	XI	37	PHE	2.1
3	XC	153	VAL	2.1
7	QG	99	LEU	2.1
52	RX	66	LEU	2.1
1	QA	415	A	2.0
1	QA	1110	A	2.0
19	QS	83	HIS	2.0
33	R9	32	HIS	2.0
17	XQ	30	PRO	2.0
34	RA	213	A	2.0
34	YA	1095	A	2.0
7	XG	103	TRP	2.0
37	YE	111	ARG	2.0
43	RO	81	ASP	2.0
44	YP	29	LYS	2.0
49	RU	37	GLU	2.0
50	RV	74	LYS	2.0
1	XA	1054	C	2.0
1	XA	1066	C	2.0
9	QI	109	VAL	2.0
30	R6	48	VAL	2.0
34	RA	462	C	2.0
34	RA	574	C	2.0
34	RA	737	C	2.0
34	RA	1662	C	2.0
34	RA	2363	C	2.0
34	RA	2789	C	2.0
34	YA	766	C	2.0
34	YA	1804	C	2.0
34	YA	2175	C	2.0
41	RI	77	LEU	2.0
42	YN	82	LEU	2.0
42	YN	138	LEU	2.0
49	YU	117	GLN	2.0
1	QA	251	G	2.0
22	QV	53	G	2.0
34	YA	2455	G	2.0
34	RA	387	U	2.0
34	RA	2017	U	2.0

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Mol	Chain	Res	Type	RSRZ
34	YA	2041	U	2.0
45	YQ	100	GLY	2.0
4	QD	30	LYS	2.0
11	QK	12	ARG	2.0
37	YE	135	HIS	2.0
38	YF	93	LYS	2.0
45	YQ	77	LYS	2.0
10	XJ	48	THR	2.0
13	QM	64	TRP	2.0
8	QH	73	ASP	2.0
40	YH	34	GLU	2.0
54	YZ	178	GLU	2.0
12	QL	128	ALA	2.0
20	XT	95	ALA	2.0
36	RD	215	LEU	2.0
44	YP	40	SER	2.0
9	XI	124	GLN	2.0
13	XM	101	GLN	2.0
34	RA	1254	A	2.0
34	RA	1510	A	2.0
45	RQ	27	VAL	2.0
11	QK	88	GLY	2.0
11	QK	123	LYS	2.0
12	XL	89	ARG	2.0
32	Y8	38	GLY	2.0
37	RE	136	ARG	2.0
43	RO	32	TYR	2.0
1	QA	328	C	2.0
1	QA	1112	C	2.0
3	XC	10	PHE	2.0
17	QQ	49	GLU	2.0
32	R8	54	GLU	2.0
34	RA	2784	C	2.0
34	YA	965	C	2.0
34	YA	1233	C	2.0
42	RN	96	GLU	2.0
41	RI	96	ASP	2.0
44	YP	45	LEU	2.0
34	RA	1012	U	2.0
34	YA	767	U	2.0
14	XN	56	VAL	2.0
40	RH	169	VAL	2.0

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

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(Å ²)	Q<0.9
22	T6A	QV	37	32/33	0.73	0.15	155,169,201,204	0
22	T6A	XV	37	32/33	0.88	0.18	105,112,148,175	0
22	MNU	QV	34	23/24	0.89	0.10	128,129,139,148	0
56	PPU	Z8	76	37/38	0.90	0.16	88,94,130,143	0
22	MNU	XV	34	23/24	0.92	0.13	103,106,117,124	0
56	PPU	Z6	76	37/38	0.93	0.14	88,101,129,133	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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(Å ²)	Q<0.9
57	MG	YA	3398	1/1	0.05	0.16	82,82,82,82	0
57	MG	RB	201	1/1	0.32	0.15	87,87,87,87	0
57	MG	YB	210	1/1	0.45	0.10	82,82,82,82	0
57	MG	RA	3267	1/1	0.46	0.32	76,76,76,76	0
57	MG	RA	3446	1/1	0.51	0.08	65,65,65,65	0
57	MG	YA	3448	1/1	0.51	0.17	91,91,91,91	0
57	MG	RA	3259	1/1	0.51	0.13	73,73,73,73	0
57	MG	YA	3287	1/1	0.53	0.26	92,92,92,92	0
57	MG	YA	3496	1/1	0.55	0.16	72,72,72,72	0
57	MG	RY	201	1/1	0.56	0.12	104,104,104,104	0
57	MG	RA	3428	1/1	0.56	0.37	46,46,46,46	0
57	MG	YB	213	1/1	0.57	0.26	57,57,57,57	0
57	MG	RA	3355	1/1	0.59	0.20	75,75,75,75	0
57	MG	RA	3208	1/1	0.60	0.20	78,78,78,78	0
57	MG	RA	3295	1/1	0.61	0.10	64,64,64,64	0
57	MG	RA	3451	1/1	0.61	0.12	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3310	1/1	0.62	0.16	62,62,62,62	0
57	MG	RA	3362	1/1	0.63	0.15	68,68,68,68	0
57	MG	YB	207	1/1	0.63	0.14	107,107,107,107	0
57	MG	QA	1655	1/1	0.63	0.28	98,98,98,98	0
57	MG	YA	3466	1/1	0.63	0.22	73,73,73,73	0
57	MG	RA	3139	1/1	0.64	0.15	38,38,38,38	0
57	MG	RA	3186	1/1	0.65	0.14	90,90,90,90	0
57	MG	QA	1672	1/1	0.65	0.30	76,76,76,76	0
57	MG	RA	3321	1/1	0.65	0.13	53,53,53,53	0
57	MG	RA	3449	1/1	0.65	0.26	100,100,100,100	0
57	MG	YA	3336	1/1	0.65	0.23	79,79,79,79	0
57	MG	QA	1661	1/1	0.65	0.20	113,113,113,113	0
57	MG	RA	3405	1/1	0.66	0.25	82,82,82,82	0
57	MG	RA	3414	1/1	0.66	0.08	39,39,39,39	0
57	MG	YA	3525	1/1	0.66	0.32	46,46,46,46	0
57	MG	YA	3225	1/1	0.66	0.12	64,64,64,64	0
57	MG	YA	3409	1/1	0.66	0.18	74,74,74,74	0
57	MG	RA	3171	1/1	0.66	0.12	70,70,70,70	0
57	MG	YA	3410	1/1	0.67	0.08	60,60,60,60	0
57	MG	RA	3400	1/1	0.67	0.25	69,69,69,69	0
57	MG	YA	3453	1/1	0.67	0.10	51,51,51,51	0
57	MG	YB	206	1/1	0.68	0.27	75,75,75,75	0
57	MG	RA	3369	1/1	0.68	0.30	91,91,91,91	0
57	MG	YA	3499	1/1	0.68	0.10	77,77,77,77	0
57	MG	RA	3404	1/1	0.68	0.25	85,85,85,85	0
57	MG	RA	3195	1/1	0.69	0.30	95,95,95,95	0
57	MG	RA	3277	1/1	0.69	0.21	81,81,81,81	0
57	MG	YB	208	1/1	0.69	0.11	76,76,76,76	0
57	MG	RA	3444	1/1	0.69	0.20	57,57,57,57	0
57	MG	YA	3528	1/1	0.69	0.10	51,51,51,51	0
57	MG	RA	3353	1/1	0.70	0.10	67,67,67,67	0
57	MG	RA	3395	1/1	0.70	0.18	77,77,77,77	0
57	MG	YA	3426	1/1	0.70	0.19	62,62,62,62	0
57	MG	YA	3375	1/1	0.70	0.21	67,67,67,67	0
57	MG	RA	3422	1/1	0.70	0.09	57,57,57,57	0
57	MG	YA	3298	1/1	0.71	0.32	78,78,78,78	0
57	MG	RQ	203	1/1	0.71	0.19	83,83,83,83	0
57	MG	YA	3405	1/1	0.72	0.13	61,61,61,61	0
57	MG	RA	3383	1/1	0.72	0.33	71,71,71,71	0
57	MG	YA	3349	1/1	0.72	0.21	86,86,86,86	0
57	MG	RA	3418	1/1	0.72	0.10	59,59,59,59	0
57	MG	YA	3508	1/1	0.72	0.14	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3270	1/1	0.72	0.29	75,75,75,75	0
57	MG	YO	201	1/1	0.72	0.18	70,70,70,70	0
57	MG	RA	3322	1/1	0.73	0.09	59,59,59,59	0
57	MG	YA	3436	1/1	0.73	0.15	75,75,75,75	0
57	MG	RA	3084	1/1	0.73	0.21	38,38,38,38	0
57	MG	YA	3400	1/1	0.73	0.07	68,68,68,68	0
57	MG	RA	3425	1/1	0.74	0.10	73,73,73,73	0
57	MG	XA	1612	1/1	0.74	0.14	73,73,73,73	0
57	MG	YA	3345	1/1	0.74	0.12	38,38,38,38	0
57	MG	YA	3195	1/1	0.74	0.15	46,46,46,46	0
57	MG	RA	3427	1/1	0.74	0.23	81,81,81,81	0
57	MG	YA	3382	1/1	0.74	0.07	97,97,97,97	0
57	MG	RA	3310	1/1	0.74	0.09	71,71,71,71	0
57	MG	RA	3437	1/1	0.74	0.19	69,69,69,69	0
57	MG	YD	302	1/1	0.74	0.39	102,102,102,102	0
57	MG	RA	3360	1/1	0.74	0.10	38,38,38,38	0
57	MG	YA	3160	1/1	0.75	0.25	80,80,80,80	0
57	MG	YA	3290	1/1	0.75	0.15	97,97,97,97	0
57	MG	RA	3430	1/1	0.75	0.21	67,67,67,67	0
57	MG	YE	304	1/1	0.75	0.12	114,114,114,114	0
57	MG	YA	3305	1/1	0.75	0.39	81,81,81,81	0
57	MG	RA	3190	1/1	0.76	0.21	55,55,55,55	0
57	MG	RA	3317	1/1	0.76	0.23	48,48,48,48	0
57	MG	XM	201	1/1	0.76	0.11	97,97,97,97	0
57	MG	RA	3124	1/1	0.76	0.23	68,68,68,68	0
57	MG	YA	3424	1/1	0.76	0.23	65,65,65,65	0
57	MG	RA	3111	1/1	0.76	0.11	54,54,54,54	0
57	MG	YA	3203	1/1	0.76	0.26	38,38,38,38	0
57	MG	RA	3228	1/1	0.76	0.13	38,38,38,38	0
57	MG	RA	3298	1/1	0.76	0.07	62,62,62,62	0
57	MG	YA	3463	1/1	0.76	0.07	72,72,72,72	0
57	MG	YA	3273	1/1	0.76	0.10	45,45,45,45	0
57	MG	RA	3306	1/1	0.76	0.10	58,58,58,58	0
57	MG	YB	204	1/1	0.77	0.27	38,38,38,38	0
57	MG	XA	1669	1/1	0.77	0.14	83,83,83,83	0
57	MG	YA	3362	1/1	0.77	0.07	73,73,73,73	0
57	MG	YA	3209	1/1	0.77	0.07	38,38,38,38	0
57	MG	RA	3385	1/1	0.77	0.07	67,67,67,67	0
57	MG	YA	3046	1/1	0.77	0.38	61,61,61,61	0
57	MG	YA	3509	1/1	0.77	0.26	63,63,63,63	0
57	MG	RA	3193	1/1	0.77	0.15	59,59,59,59	0
57	MG	YN	201	1/1	0.77	0.09	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3368	1/1	0.77	0.16	56,56,56,56	0
57	MG	RA	3246	1/1	0.78	0.15	38,38,38,38	0
57	MG	YA	3311	1/1	0.78	0.07	38,38,38,38	0
57	MG	YA	3322	1/1	0.78	0.10	42,42,42,42	0
57	MG	RA	3343	1/1	0.78	0.09	51,51,51,51	0
57	MG	RA	3392	1/1	0.78	0.14	51,51,51,51	0
57	MG	YA	3456	1/1	0.78	0.16	66,66,66,66	0
57	MG	YA	3188	1/1	0.78	0.12	45,45,45,45	0
57	MG	YA	3190	1/1	0.78	0.10	73,73,73,73	0
57	MG	RA	3256	1/1	0.79	0.09	38,38,38,38	0
57	MG	RB	203	1/1	0.79	0.12	77,77,77,77	0
57	MG	RA	3307	1/1	0.79	0.18	76,76,76,76	0
57	MG	RA	3292	1/1	0.79	0.28	69,69,69,69	0
57	MG	QA	1645	1/1	0.79	0.10	82,82,82,82	0
57	MG	RA	3001	1/1	0.79	0.20	66,66,66,66	0
57	MG	RA	3412	1/1	0.79	0.14	82,82,82,82	0
57	MG	YA	3380	1/1	0.79	0.11	38,38,38,38	0
57	MG	YA	3443	1/1	0.79	0.11	58,58,58,58	0
57	MG	YA	3222	1/1	0.79	0.24	121,121,121,121	0
57	MG	YX	102	1/1	0.79	0.26	95,95,95,95	0
57	MG	RA	3204	1/1	0.80	0.23	77,77,77,77	0
57	MG	RN	201	1/1	0.80	0.39	57,57,57,57	0
57	MG	YA	3216	1/1	0.80	0.09	70,70,70,70	0
57	MG	YA	3367	1/1	0.80	0.11	52,52,52,52	0
57	MG	RA	3152	1/1	0.80	0.17	38,38,38,38	0
57	MG	RA	3406	1/1	0.80	0.09	44,44,44,44	0
57	MG	YA	3242	1/1	0.80	0.09	63,63,63,63	0
57	MG	YA	3512	1/1	0.80	0.10	77,77,77,77	0
57	MG	YA	3396	1/1	0.80	0.12	69,69,69,69	0
57	MG	RA	3302	1/1	0.80	0.14	66,66,66,66	0
57	MG	RA	3227	1/1	0.80	0.14	65,65,65,65	0
57	MG	XA	1673	1/1	0.80	0.10	48,48,48,48	0
57	MG	YA	3408	1/1	0.80	0.11	56,56,56,56	0
57	MG	RA	3268	1/1	0.80	0.10	59,59,59,59	0
57	MG	YA	3012	1/1	0.80	0.16	69,69,69,69	0
57	MG	QF	201	1/1	0.80	0.12	91,91,91,91	0
57	MG	RA	3450	1/1	0.80	0.07	54,54,54,54	0
57	MG	RA	3424	1/1	0.80	0.10	65,65,65,65	0
57	MG	RA	3455	1/1	0.80	0.10	57,57,57,57	0
57	MG	RA	3149	1/1	0.80	0.18	75,75,75,75	0
57	MG	YA	3342	1/1	0.80	0.07	52,52,52,52	0
57	MG	RA	3314	1/1	0.81	0.17	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3460	1/1	0.81	0.14	58,58,58,58	0
57	MG	RA	3242	1/1	0.81	0.26	83,83,83,83	0
57	MG	QA	1649	1/1	0.81	0.11	64,64,64,64	0
57	MG	YA	3479	1/1	0.81	0.20	57,57,57,57	0
57	MG	YA	3483	1/1	0.81	0.09	49,49,49,49	0
57	MG	YA	3501	1/1	0.82	0.28	38,38,38,38	0
57	MG	RA	3286	1/1	0.82	0.21	41,41,41,41	0
57	MG	YA	3355	1/1	0.82	0.15	98,98,98,98	0
57	MG	YA	3433	1/1	0.82	0.21	78,78,78,78	0
57	MG	YA	3201	1/1	0.82	0.56	92,92,92,92	0
57	MG	YA	3441	1/1	0.82	0.08	38,38,38,38	0
57	MG	RA	3461	1/1	0.82	0.37	38,38,38,38	0
57	MG	YA	3301	1/1	0.82	0.23	42,42,42,42	0
57	MG	YA	3304	1/1	0.82	0.17	44,44,44,44	0
57	MG	RA	3162	1/1	0.82	0.12	38,38,38,38	0
57	MG	RA	3083	1/1	0.82	0.29	62,62,62,62	0
57	MG	YB	212	1/1	0.82	0.06	65,65,65,65	0
57	MG	RA	3173	1/1	0.82	0.11	44,44,44,44	0
57	MG	YA	3140	1/1	0.82	0.10	38,38,38,38	0
57	MG	YA	3328	1/1	0.82	0.15	53,53,53,53	0
57	MG	RA	3201	1/1	0.82	0.09	70,70,70,70	0
57	MG	RA	3117	1/1	0.82	0.19	38,38,38,38	0
57	MG	RA	3452	1/1	0.82	0.27	69,69,69,69	0
57	MG	YA	3250	1/1	0.83	0.18	54,54,54,54	0
57	MG	YA	3261	1/1	0.83	0.11	62,62,62,62	0
57	MG	Y0	101	1/1	0.83	0.21	65,65,65,65	0
57	MG	RA	3038	1/1	0.83	0.23	38,38,38,38	0
57	MG	YA	3493	1/1	0.83	0.17	96,96,96,96	0
57	MG	RA	3089	1/1	0.83	0.35	38,38,38,38	0
57	MG	RA	3053	1/1	0.83	0.21	38,38,38,38	0
57	MG	RA	3155	1/1	0.83	0.07	52,52,52,52	0
57	MG	YA	3165	1/1	0.83	0.11	38,38,38,38	0
57	MG	YA	3404	1/1	0.83	0.07	60,60,60,60	0
57	MG	YA	3171	1/1	0.83	0.26	54,54,54,54	0
57	MG	YA	3406	1/1	0.83	0.16	62,62,62,62	0
57	MG	RA	3372	1/1	0.83	0.07	49,49,49,49	0
57	MG	YA	3535	1/1	0.83	0.15	38,38,38,38	0
57	MG	RA	3156	1/1	0.83	0.15	59,59,59,59	0
57	MG	RA	3061	1/1	0.83	0.23	38,38,38,38	0
57	MG	RA	3122	1/1	0.83	0.18	73,73,73,73	0
57	MG	RA	3211	1/1	0.83	0.18	63,63,63,63	0
57	MG	RA	3431	1/1	0.83	0.15	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1656	1/1	0.83	0.16	55,55,55,55	0
57	MG	RA	3351	1/1	0.83	0.24	59,59,59,59	0
57	MG	YA	3346	1/1	0.83	0.32	81,81,81,81	0
57	MG	RA	3179	1/1	0.83	0.08	74,74,74,74	0
57	MG	YA	3354	1/1	0.83	0.06	40,40,40,40	0
57	MG	RA	3239	1/1	0.83	0.15	54,54,54,54	0
57	MG	YA	3356	1/1	0.83	0.11	38,38,38,38	0
59	ZN	R5	101	1/1	0.83	0.29	88,88,88,88	0
57	MG	RA	3396	1/1	0.84	0.14	38,38,38,38	0
57	MG	YA	3248	1/1	0.84	0.07	54,54,54,54	0
57	MG	YA	3170	1/1	0.84	0.11	64,64,64,64	0
57	MG	RA	3079	1/1	0.84	0.10	50,50,50,50	0
57	MG	RA	3384	1/1	0.84	0.06	40,40,40,40	0
57	MG	YA	3007	1/1	0.84	0.15	71,71,71,71	0
57	MG	YA	3514	1/1	0.84	0.40	85,85,85,85	0
57	MG	YA	3353	1/1	0.84	0.06	50,50,50,50	0
57	MG	YA	3284	1/1	0.84	0.10	38,38,38,38	0
57	MG	RA	3254	1/1	0.84	0.11	38,38,38,38	0
57	MG	YA	3020	1/1	0.84	0.13	53,53,53,53	0
57	MG	RA	3081	1/1	0.84	0.26	63,63,63,63	0
57	MG	YA	3444	1/1	0.84	0.26	55,55,55,55	0
57	MG	YA	3053	1/1	0.84	0.24	38,38,38,38	0
57	MG	YA	3211	1/1	0.84	0.07	65,65,65,65	0
57	MG	YA	3069	1/1	0.84	0.14	44,44,44,44	0
57	MG	RA	3070	1/1	0.84	0.13	38,38,38,38	0
57	MG	RA	3483	1/1	0.84	0.16	65,65,65,65	0
57	MG	YA	3397	1/1	0.84	0.20	52,52,52,52	0
57	MG	YA	3314	1/1	0.84	0.21	66,66,66,66	0
57	MG	YA	3320	1/1	0.84	0.14	54,54,54,54	0
57	MG	YQ	201	1/1	0.84	0.20	77,77,77,77	0
57	MG	YA	3486	1/1	0.84	0.08	87,87,87,87	0
57	MG	YA	3239	1/1	0.84	0.19	38,38,38,38	0
59	ZN	Y6	101	1/1	0.84	0.37	106,106,106,106	0
57	MG	YA	3299	1/1	0.85	0.07	43,43,43,43	0
57	MG	YA	3423	1/1	0.85	0.15	73,73,73,73	0
57	MG	YA	3087	1/1	0.85	0.31	38,38,38,38	0
57	MG	RA	3453	1/1	0.85	0.23	71,71,71,71	0
57	MG	RA	3199	1/1	0.85	0.09	56,56,56,56	0
57	MG	RA	3244	1/1	0.85	0.11	38,38,38,38	0
57	MG	YA	3364	1/1	0.85	0.16	56,56,56,56	0
57	MG	RA	3442	1/1	0.85	0.18	58,58,58,58	0
57	MG	QA	1647	1/1	0.85	0.06	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3377	1/1	0.85	0.08	38,38,38,38	0
57	MG	YA	3319	1/1	0.85	0.13	38,38,38,38	0
57	MG	RA	3073	1/1	0.85	0.10	38,38,38,38	0
57	MG	YB	209	1/1	0.85	0.09	51,51,51,51	0
57	MG	YA	3014	1/1	0.85	0.09	69,69,69,69	0
57	MG	RA	3426	1/1	0.85	0.16	91,91,91,91	0
57	MG	YA	3334	1/1	0.85	0.12	64,64,64,64	0
57	MG	YA	3471	1/1	0.85	0.15	47,47,47,47	0
57	MG	YA	3197	1/1	0.85	0.12	38,38,38,38	0
57	MG	RA	3141	1/1	0.85	0.13	57,57,57,57	0
57	MG	RA	3413	1/1	0.85	0.07	45,45,45,45	0
57	MG	YA	3492	1/1	0.85	0.10	52,52,52,52	0
57	MG	RA	3378	1/1	0.85	0.10	73,73,73,73	0
57	MG	YA	3082	1/1	0.85	0.25	38,38,38,38	0
57	MG	YA	3350	1/1	0.85	0.06	54,54,54,54	0
59	ZN	YY	202	1/1	0.85	0.23	93,93,93,93	0
57	MG	RA	3467	1/1	0.86	0.15	51,51,51,51	0
57	MG	RA	3471	1/1	0.86	0.23	38,38,38,38	0
57	MG	YA	3323	1/1	0.86	0.26	38,38,38,38	0
57	MG	RA	3008	1/1	0.86	0.06	38,38,38,38	0
57	MG	YA	3329	1/1	0.86	0.09	38,38,38,38	0
57	MG	RA	3016	1/1	0.86	0.19	38,38,38,38	0
57	MG	RA	3352	1/1	0.86	0.16	55,55,55,55	0
57	MG	RA	3128	1/1	0.86	0.19	38,38,38,38	0
57	MG	RO	201	1/1	0.86	0.22	63,63,63,63	0
57	MG	YA	3202	1/1	0.86	0.12	38,38,38,38	0
57	MG	RP	203	1/1	0.86	0.30	79,79,79,79	0
57	MG	YA	3204	1/1	0.86	0.08	67,67,67,67	0
57	MG	RA	3207	1/1	0.86	0.13	75,75,75,75	0
57	MG	RA	3129	1/1	0.86	0.06	52,52,52,52	0
57	MG	RA	3281	1/1	0.86	0.10	49,49,49,49	0
57	MG	XA	1615	1/1	0.86	0.06	47,47,47,47	0
57	MG	RA	3176	1/1	0.86	0.12	40,40,40,40	0
57	MG	RA	3291	1/1	0.86	0.06	46,46,46,46	0
57	MG	XL	201	1/1	0.86	0.09	42,42,42,42	0
57	MG	RA	3177	1/1	0.86	0.18	38,38,38,38	0
57	MG	YA	3376	1/1	0.86	0.17	77,77,77,77	0
57	MG	RA	3020	1/1	0.86	0.35	38,38,38,38	0
57	MG	RA	3380	1/1	0.86	0.08	38,38,38,38	0
57	MG	YA	3267	1/1	0.86	0.27	61,61,61,61	0
57	MG	YA	3008	1/1	0.86	0.09	56,56,56,56	0
57	MG	RA	3231	1/1	0.86	0.15	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3299	1/1	0.86	0.10	71,71,71,71	0
57	MG	YA	3399	1/1	0.86	0.14	38,38,38,38	0
57	MG	YA	3016	1/1	0.86	0.20	38,38,38,38	0
57	MG	RA	3234	1/1	0.86	0.17	75,75,75,75	0
57	MG	YA	3291	1/1	0.86	0.09	61,61,61,61	0
57	MG	RA	3238	1/1	0.86	0.16	53,53,53,53	0
57	MG	RA	3101	1/1	0.86	0.13	57,57,57,57	0
57	MG	QA	1617	1/1	0.86	0.17	60,60,60,60	0
57	MG	YA	3070	1/1	0.86	0.18	38,38,38,38	0
57	MG	RA	3005	1/1	0.86	0.20	38,38,38,38	0
57	MG	YP	201	1/1	0.86	0.34	72,72,72,72	0
57	MG	RA	3121	1/1	0.86	0.27	38,38,38,38	0
57	MG	RA	3247	1/1	0.86	0.07	38,38,38,38	0
57	MG	RA	3197	1/1	0.86	0.11	51,51,51,51	0
57	MG	YA	3315	1/1	0.86	0.10	38,38,38,38	0
57	MG	RA	3411	1/1	0.86	0.19	71,71,71,71	0
57	MG	YA	3474	1/1	0.87	0.26	38,38,38,38	0
57	MG	YA	3308	1/1	0.87	0.26	66,66,66,66	0
57	MG	RA	3357	1/1	0.87	0.08	57,57,57,57	0
57	MG	YA	3381	1/1	0.87	0.17	39,39,39,39	0
57	MG	RA	3358	1/1	0.87	0.10	74,74,74,74	0
57	MG	RA	3133	1/1	0.87	0.20	38,38,38,38	0
57	MG	RA	3134	1/1	0.87	0.19	38,38,38,38	0
57	MG	YA	3498	1/1	0.87	0.10	45,45,45,45	0
57	MG	RB	205	1/1	0.87	0.21	68,68,68,68	0
57	MG	RE	304	1/1	0.87	0.14	38,38,38,38	0
57	MG	YA	3032	1/1	0.87	0.24	38,38,38,38	0
57	MG	RA	3062	1/1	0.87	0.14	61,61,61,61	0
57	MG	YA	3326	1/1	0.87	0.08	73,73,73,73	0
57	MG	YA	3235	1/1	0.87	0.15	38,38,38,38	0
57	MG	RA	3409	1/1	0.87	0.18	43,43,43,43	0
57	MG	RA	3185	1/1	0.87	0.14	93,93,93,93	0
57	MG	QA	1633	1/1	0.87	0.14	73,73,73,73	0
57	MG	YB	203	1/1	0.87	0.08	107,107,107,107	0
57	MG	YA	3413	1/1	0.87	0.12	56,56,56,56	0
57	MG	RA	3188	1/1	0.87	0.08	67,67,67,67	0
57	MG	XA	1605	1/1	0.87	0.10	61,61,61,61	0
57	MG	YA	3127	1/1	0.87	0.18	70,70,70,70	0
57	MG	YA	3132	1/1	0.87	0.07	38,38,38,38	0
57	MG	XA	1611	1/1	0.87	0.12	39,39,39,39	0
57	MG	YA	3351	1/1	0.87	0.24	38,38,38,38	0
57	MG	RA	3144	1/1	0.87	0.12	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3221	1/1	0.87	0.09	38,38,38,38	0
57	MG	RA	3421	1/1	0.87	0.07	38,38,38,38	0
57	MG	YA	3449	1/1	0.87	0.09	56,56,56,56	0
57	MG	YA	3451	1/1	0.87	0.06	63,63,63,63	0
57	MG	RA	3131	1/1	0.87	0.14	48,48,48,48	0
57	MG	RA	3194	1/1	0.87	0.14	48,48,48,48	0
57	MG	YQ	202	1/1	0.87	0.11	82,82,82,82	0
57	MG	YR	202	1/1	0.87	0.12	38,38,38,38	0
57	MG	RA	3175	1/1	0.87	0.16	70,70,70,70	0
57	MG	RA	3356	1/1	0.87	0.07	49,49,49,49	0
59	ZN	R9	101	1/1	0.87	0.44	88,88,88,88	0
59	ZN	RY	202	1/1	0.87	0.28	88,88,88,88	0
57	MG	YA	3003	1/1	0.87	0.10	67,67,67,67	0
57	MG	YA	3006	1/1	0.87	0.14	38,38,38,38	0
57	MG	XA	1617	1/1	0.88	0.15	38,38,38,38	0
57	MG	YA	3194	1/1	0.88	0.15	64,64,64,64	0
57	MG	XA	1620	1/1	0.88	0.12	38,38,38,38	0
57	MG	XA	1645	1/1	0.88	0.20	43,43,43,43	0
57	MG	R1	101	1/1	0.88	0.17	38,38,38,38	0
57	MG	RA	3398	1/1	0.88	0.11	38,38,38,38	0
57	MG	RA	3025	1/1	0.88	0.16	38,38,38,38	0
57	MG	RA	3192	1/1	0.88	0.26	38,38,38,38	0
57	MG	XS	101	1/1	0.88	0.05	51,51,51,51	0
57	MG	RA	3078	1/1	0.88	0.19	40,40,40,40	0
57	MG	YA	3214	1/1	0.88	0.06	38,38,38,38	0
57	MG	YA	3352	1/1	0.88	0.17	48,48,48,48	0
57	MG	RA	3035	1/1	0.88	0.22	38,38,38,38	0
57	MG	YA	3485	1/1	0.88	0.15	76,76,76,76	0
57	MG	YA	3219	1/1	0.88	0.07	38,38,38,38	0
57	MG	YA	3488	1/1	0.88	0.15	63,63,63,63	0
57	MG	QA	1670	1/1	0.88	0.16	38,38,38,38	0
57	MG	RA	3044	1/1	0.88	0.13	38,38,38,38	0
57	MG	YA	3357	1/1	0.88	0.10	91,91,91,91	0
57	MG	RA	3454	1/1	0.88	0.20	60,60,60,60	0
57	MG	RA	3046	1/1	0.88	0.25	38,38,38,38	0
57	MG	QA	1671	1/1	0.88	0.07	38,38,38,38	0
57	MG	YA	3244	1/1	0.88	0.07	38,38,38,38	0
57	MG	RA	3138	1/1	0.88	0.06	38,38,38,38	0
57	MG	RA	3415	1/1	0.88	0.05	63,63,63,63	0
57	MG	RA	3417	1/1	0.88	0.17	38,38,38,38	0
57	MG	YA	3522	1/1	0.88	0.27	38,38,38,38	0
57	MG	YA	3044	1/1	0.88	0.19	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3057	1/1	0.88	0.41	38,38,38,38	0
57	MG	YA	3390	1/1	0.88	0.12	74,74,74,74	0
57	MG	YB	202	1/1	0.88	0.18	38,38,38,38	0
57	MG	YA	3395	1/1	0.88	0.13	86,86,86,86	0
57	MG	RA	3255	1/1	0.88	0.24	38,38,38,38	0
57	MG	YA	3060	1/1	0.88	0.24	38,38,38,38	0
57	MG	RA	3376	1/1	0.88	0.17	76,76,76,76	0
57	MG	QA	1601	1/1	0.88	0.11	38,38,38,38	0
57	MG	QA	1668	1/1	0.88	0.10	55,55,55,55	0
57	MG	YA	3083	1/1	0.88	0.10	38,38,38,38	0
57	MG	RA	3260	1/1	0.88	0.11	60,60,60,60	0
57	MG	YA	3102	1/1	0.88	0.18	38,38,38,38	0
57	MG	YD	301	1/1	0.88	0.33	38,38,38,38	0
57	MG	YA	3106	1/1	0.88	0.23	38,38,38,38	0
57	MG	RA	3220	1/1	0.88	0.23	53,53,53,53	0
57	MG	RA	3328	1/1	0.88	0.22	94,94,94,94	0
57	MG	RA	3387	1/1	0.88	0.08	64,64,64,64	0
57	MG	YA	3416	1/1	0.88	0.13	53,53,53,53	0
57	MG	YA	3142	1/1	0.88	0.09	38,38,38,38	0
57	MG	XA	1604	1/1	0.88	0.07	76,76,76,76	0
57	MG	RA	3332	1/1	0.88	0.06	38,38,38,38	0
57	MG	YX	101	1/1	0.88	0.11	81,81,81,81	0
57	MG	YA	3432	1/1	0.88	0.20	56,56,56,56	0
57	MG	YA	3168	1/1	0.88	0.17	44,44,44,44	0
57	MG	RA	3148	1/1	0.88	0.08	45,45,45,45	0
57	MG	YA	3437	1/1	0.88	0.07	68,68,68,68	0
57	MG	RA	3439	1/1	0.88	0.17	52,52,52,52	0
57	MG	RA	3441	1/1	0.88	0.10	64,64,64,64	0
57	MG	YA	3143	1/1	0.89	0.06	42,42,42,42	0
57	MG	RA	3463	1/1	0.89	0.30	87,87,87,87	0
57	MG	RA	3382	1/1	0.89	0.10	38,38,38,38	0
57	MG	YA	3166	1/1	0.89	0.08	38,38,38,38	0
57	MG	YA	3297	1/1	0.89	0.10	50,50,50,50	0
57	MG	YA	3490	1/1	0.89	0.04	39,39,39,39	0
57	MG	RA	3280	1/1	0.89	0.11	42,42,42,42	0
57	MG	RA	3477	1/1	0.89	0.28	38,38,38,38	0
57	MG	YA	3386	1/1	0.89	0.07	38,38,38,38	0
57	MG	RA	3329	1/1	0.89	0.27	38,38,38,38	0
57	MG	QA	1657	1/1	0.89	0.19	63,63,63,63	0
57	MG	RA	3341	1/1	0.89	0.05	38,38,38,38	0
57	MG	RA	3285	1/1	0.89	0.11	38,38,38,38	0
57	MG	YA	3309	1/1	0.89	0.10	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3349	1/1	0.89	0.10	41,41,41,41	0
57	MG	RA	3009	1/1	0.89	0.10	65,65,65,65	0
57	MG	YA	3017	1/1	0.89	0.08	38,38,38,38	0
57	MG	YA	3019	1/1	0.89	0.23	49,49,49,49	0
57	MG	RA	3436	1/1	0.89	0.13	77,77,77,77	0
57	MG	RA	3287	1/1	0.89	0.16	70,70,70,70	0
57	MG	RA	3245	1/1	0.89	0.10	38,38,38,38	0
57	MG	RA	3214	1/1	0.89	0.08	73,73,73,73	0
57	MG	YA	3212	1/1	0.89	0.13	53,53,53,53	0
57	MG	YA	3049	1/1	0.89	0.34	38,38,38,38	0
57	MG	QA	1605	1/1	0.89	0.21	47,47,47,47	0
57	MG	QA	1652	1/1	0.89	0.12	68,68,68,68	0
57	MG	RA	3196	1/1	0.89	0.07	50,50,50,50	0
57	MG	YA	3339	1/1	0.89	0.11	38,38,38,38	0
57	MG	RA	3119	1/1	0.89	0.10	38,38,38,38	0
57	MG	YA	3343	1/1	0.89	0.09	38,38,38,38	0
57	MG	YA	3230	1/1	0.89	0.09	38,38,38,38	0
57	MG	RA	3229	1/1	0.89	0.11	38,38,38,38	0
57	MG	RA	3024	1/1	0.89	0.26	38,38,38,38	0
57	MG	RA	3266	1/1	0.89	0.19	61,61,61,61	0
57	MG	XA	1626	1/1	0.89	0.17	38,38,38,38	0
57	MG	XA	1633	1/1	0.89	0.14	38,38,38,38	0
57	MG	RA	3158	1/1	0.89	0.10	86,86,86,86	0
57	MG	YA	3260	1/1	0.89	0.21	38,38,38,38	0
57	MG	QA	1608	1/1	0.89	0.09	54,54,54,54	0
57	MG	YA	3457	1/1	0.89	0.09	72,72,72,72	0
57	MG	YA	3136	1/1	0.89	0.12	53,53,53,53	0
57	MG	QA	1604	1/1	0.89	0.10	38,38,38,38	0
57	MG	RA	3279	1/1	0.89	0.14	51,51,51,51	0
57	MG	YA	3363	1/1	0.89	0.06	49,49,49,49	0
57	MG	YA	3274	1/1	0.89	0.23	38,38,38,38	0
57	MG	YA	3475	1/1	0.89	0.13	38,38,38,38	0
57	MG	YA	3445	1/1	0.90	0.12	69,69,69,69	0
57	MG	YA	3447	1/1	0.90	0.16	38,38,38,38	0
57	MG	RA	3004	1/1	0.90	0.23	38,38,38,38	0
57	MG	RA	3037	1/1	0.90	0.23	38,38,38,38	0
57	MG	YA	3450	1/1	0.90	0.23	70,70,70,70	0
57	MG	YA	3196	1/1	0.90	0.12	38,38,38,38	0
57	MG	YA	3330	1/1	0.90	0.10	42,42,42,42	0
57	MG	YA	3454	1/1	0.90	0.07	53,53,53,53	0
57	MG	YA	3455	1/1	0.90	0.06	38,38,38,38	0
57	MG	RA	3174	1/1	0.90	0.13	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3249	1/1	0.90	0.10	38,38,38,38	0
57	MG	YA	3338	1/1	0.90	0.14	38,38,38,38	0
57	MG	RA	3468	1/1	0.90	0.13	55,55,55,55	0
57	MG	RA	3305	1/1	0.90	0.12	44,44,44,44	0
57	MG	YA	3013	1/1	0.90	0.10	52,52,52,52	0
57	MG	RA	3363	1/1	0.90	0.09	38,38,38,38	0
57	MG	RA	3419	1/1	0.90	0.15	41,41,41,41	0
57	MG	YA	3476	1/1	0.90	0.11	47,47,47,47	0
57	MG	RA	3367	1/1	0.90	0.27	56,56,56,56	0
57	MG	RB	202	1/1	0.90	0.06	57,57,57,57	0
57	MG	RA	3206	1/1	0.90	0.28	71,71,71,71	0
57	MG	YA	3218	1/1	0.90	0.20	99,99,99,99	0
57	MG	QA	1628	1/1	0.90	0.06	52,52,52,52	0
57	MG	YA	3221	1/1	0.90	0.11	59,59,59,59	0
57	MG	YA	3043	1/1	0.90	0.34	38,38,38,38	0
57	MG	RA	3309	1/1	0.90	0.14	59,59,59,59	0
57	MG	RA	3042	1/1	0.90	0.15	38,38,38,38	0
57	MG	QA	1611	1/1	0.90	0.21	38,38,38,38	0
57	MG	YA	3236	1/1	0.90	0.15	38,38,38,38	0
57	MG	YA	3238	1/1	0.90	0.07	38,38,38,38	0
57	MG	YA	3502	1/1	0.90	0.07	45,45,45,45	0
57	MG	RA	3085	1/1	0.90	0.30	38,38,38,38	0
57	MG	YA	3374	1/1	0.90	0.07	38,38,38,38	0
57	MG	YA	3511	1/1	0.90	0.06	41,41,41,41	0
57	MG	RA	3429	1/1	0.90	0.05	38,38,38,38	0
57	MG	RA	3218	1/1	0.90	0.15	57,57,57,57	0
57	MG	YA	3517	1/1	0.90	0.24	38,38,38,38	0
57	MG	RA	3180	1/1	0.90	0.11	77,77,77,77	0
57	MG	YA	3074	1/1	0.90	0.22	38,38,38,38	0
57	MG	RA	3325	1/1	0.90	0.08	54,54,54,54	0
57	MG	XA	1608	1/1	0.90	0.11	38,38,38,38	0
57	MG	QA	1663	1/1	0.90	0.20	65,65,65,65	0
57	MG	YA	3269	1/1	0.90	0.09	57,57,57,57	0
57	MG	RA	3090	1/1	0.90	0.27	38,38,38,38	0
57	MG	RA	3440	1/1	0.90	0.11	51,51,51,51	0
57	MG	YA	3114	1/1	0.90	0.21	38,38,38,38	0
57	MG	RA	3096	1/1	0.90	0.15	38,38,38,38	0
57	MG	YA	3129	1/1	0.90	0.31	38,38,38,38	0
57	MG	XA	1619	1/1	0.90	0.17	38,38,38,38	0
57	MG	RA	3049	1/1	0.90	0.23	38,38,38,38	0
57	MG	RA	3010	1/1	0.90	0.15	38,38,38,38	0
57	MG	RA	3346	1/1	0.90	0.18	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1641	1/1	0.90	0.15	38,38,38,38	0
57	MG	XA	1643	1/1	0.90	0.09	38,38,38,38	0
57	MG	QH	201	1/1	0.90	0.11	60,60,60,60	0
57	MG	XA	1662	1/1	0.90	0.20	64,64,64,64	0
57	MG	YA	3307	1/1	0.90	0.07	38,38,38,38	0
57	MG	RA	3019	1/1	0.90	0.20	38,38,38,38	0
57	MG	QM	201	1/1	0.90	0.15	54,54,54,54	0
57	MG	QA	1619	1/1	0.90	0.07	61,61,61,61	0
57	MG	YA	3176	1/1	0.90	0.10	76,76,76,76	0
57	MG	YA	3182	1/1	0.90	0.21	38,38,38,38	0
57	MG	YA	3184	1/1	0.90	0.15	38,38,38,38	0
57	MG	RA	3354	1/1	0.90	0.08	38,38,38,38	0
57	MG	YA	3189	1/1	0.90	0.11	41,41,41,41	0
57	MG	QA	1624	1/1	0.90	0.06	50,50,50,50	0
57	MG	YA	3193	1/1	0.90	0.16	38,38,38,38	0
57	MG	RA	3300	1/1	0.91	0.14	38,38,38,38	0
57	MG	RA	3065	1/1	0.91	0.09	38,38,38,38	0
57	MG	RA	3165	1/1	0.91	0.12	38,38,38,38	0
57	MG	Y1	101	1/1	0.91	0.07	38,38,38,38	0
57	MG	YA	3180	1/1	0.91	0.09	38,38,38,38	0
57	MG	YA	3313	1/1	0.91	0.28	67,67,67,67	0
57	MG	RA	3222	1/1	0.91	0.09	38,38,38,38	0
57	MG	YA	3004	1/1	0.91	0.24	38,38,38,38	0
57	MG	YA	3316	1/1	0.91	0.06	38,38,38,38	0
57	MG	QA	1621	1/1	0.91	0.17	38,38,38,38	0
57	MG	RA	3088	1/1	0.91	0.17	38,38,38,38	0
57	MG	YA	3321	1/1	0.91	0.12	68,68,68,68	0
57	MG	RA	3420	1/1	0.91	0.12	45,45,45,45	0
57	MG	YA	3192	1/1	0.91	0.11	72,72,72,72	0
57	MG	RA	3261	1/1	0.91	0.23	49,49,49,49	0
57	MG	RA	3313	1/1	0.91	0.11	59,59,59,59	0
57	MG	RA	3142	1/1	0.91	0.14	45,45,45,45	0
57	MG	RA	3371	1/1	0.91	0.17	56,56,56,56	0
57	MG	RA	3316	1/1	0.91	0.19	70,70,70,70	0
57	MG	RA	3373	1/1	0.91	0.09	47,47,47,47	0
57	MG	YA	3467	1/1	0.91	0.09	38,38,38,38	0
57	MG	RP	202	1/1	0.91	0.22	51,51,51,51	0
57	MG	YA	3031	1/1	0.91	0.20	38,38,38,38	0
57	MG	YA	3340	1/1	0.91	0.23	41,41,41,41	0
57	MG	RA	3230	1/1	0.91	0.14	45,45,45,45	0
57	MG	YA	3034	1/1	0.91	0.26	38,38,38,38	0
57	MG	QA	1622	1/1	0.91	0.06	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RT	201	1/1	0.91	0.18	56,56,56,56	0
57	MG	RA	3275	1/1	0.91	0.13	65,65,65,65	0
57	MG	XA	1601	1/1	0.91	0.08	38,38,38,38	0
57	MG	YA	3217	1/1	0.91	0.12	58,58,58,58	0
57	MG	YA	3051	1/1	0.91	0.20	38,38,38,38	0
57	MG	YA	3052	1/1	0.91	0.26	38,38,38,38	0
57	MG	RA	3323	1/1	0.91	0.16	38,38,38,38	0
57	MG	YA	3497	1/1	0.91	0.09	40,40,40,40	0
57	MG	RA	3146	1/1	0.91	0.22	38,38,38,38	0
57	MG	YA	3061	1/1	0.91	0.23	38,38,38,38	0
57	MG	YA	3226	1/1	0.91	0.05	38,38,38,38	0
57	MG	XA	1607	1/1	0.91	0.21	38,38,38,38	0
57	MG	YA	3503	1/1	0.91	0.26	69,69,69,69	0
57	MG	RA	3236	1/1	0.91	0.04	38,38,38,38	0
57	MG	QA	1613	1/1	0.91	0.09	38,38,38,38	0
57	MG	YA	3080	1/1	0.91	0.17	38,38,38,38	0
57	MG	YA	3371	1/1	0.91	0.21	77,77,77,77	0
57	MG	RA	3093	1/1	0.91	0.16	38,38,38,38	0
57	MG	YA	3241	1/1	0.91	0.20	64,64,64,64	0
57	MG	RA	3338	1/1	0.91	0.07	50,50,50,50	0
57	MG	YA	3524	1/1	0.91	0.40	54,54,54,54	0
57	MG	YA	3086	1/1	0.91	0.26	38,38,38,38	0
57	MG	YA	3378	1/1	0.91	0.07	44,44,44,44	0
57	MG	RA	3151	1/1	0.91	0.07	38,38,38,38	0
57	MG	RA	3443	1/1	0.91	0.10	38,38,38,38	0
57	MG	YA	3251	1/1	0.91	0.05	38,38,38,38	0
57	MG	YA	3257	1/1	0.91	0.12	38,38,38,38	0
57	MG	RA	3094	1/1	0.91	0.14	38,38,38,38	0
57	MG	YA	3113	1/1	0.91	0.21	38,38,38,38	0
57	MG	RA	3040	1/1	0.91	0.24	38,38,38,38	0
57	MG	YA	3116	1/1	0.91	0.13	38,38,38,38	0
57	MG	YA	3120	1/1	0.91	0.27	38,38,38,38	0
57	MG	YA	3125	1/1	0.91	0.24	38,38,38,38	0
57	MG	RA	3347	1/1	0.91	0.11	61,61,61,61	0
57	MG	YA	3403	1/1	0.91	0.10	43,43,43,43	0
57	MG	YA	3277	1/1	0.91	0.27	46,46,46,46	0
57	MG	QA	1660	1/1	0.91	0.13	44,44,44,44	0
57	MG	QA	1654	1/1	0.91	0.06	83,83,83,83	0
57	MG	RA	3191	1/1	0.91	0.42	38,38,38,38	0
57	MG	XA	1655	1/1	0.91	0.07	53,53,53,53	0
57	MG	RA	3407	1/1	0.91	0.09	60,60,60,60	0
57	MG	XA	1664	1/1	0.91	0.05	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3145	1/1	0.91	0.14	60,60,60,60	0
57	MG	YA	3419	1/1	0.91	0.06	38,38,38,38	0
57	MG	YA	3420	1/1	0.91	0.08	38,38,38,38	0
57	MG	YY	201	1/1	0.91	0.14	77,77,77,77	0
57	MG	YA	3421	1/1	0.91	0.18	38,38,38,38	0
59	ZN	R6	101	1/1	0.91	0.41	88,88,88,88	0
57	MG	RA	3296	1/1	0.91	0.11	38,38,38,38	0
57	MG	RA	3250	1/1	0.91	0.04	44,44,44,44	0
57	MG	RA	3253	1/1	0.91	0.21	38,38,38,38	0
57	MG	YA	3306	1/1	0.91	0.13	54,54,54,54	0
57	MG	RA	3147	1/1	0.92	0.18	67,67,67,67	0
57	MG	RA	3445	1/1	0.92	0.10	38,38,38,38	0
57	MG	YA	3018	1/1	0.92	0.15	38,38,38,38	0
57	MG	RA	3318	1/1	0.92	0.14	38,38,38,38	0
57	MG	XA	1606	1/1	0.92	0.13	38,38,38,38	0
57	MG	YA	3022	1/1	0.92	0.22	38,38,38,38	0
57	MG	YA	3025	1/1	0.92	0.09	38,38,38,38	0
57	MG	RA	3109	1/1	0.92	0.12	95,95,95,95	0
57	MG	RA	3205	1/1	0.92	0.10	84,84,84,84	0
57	MG	YA	3033	1/1	0.92	0.34	38,38,38,38	0
57	MG	XA	1610	1/1	0.92	0.09	73,73,73,73	0
57	MG	YA	3040	1/1	0.92	0.09	45,45,45,45	0
57	MG	YA	3042	1/1	0.92	0.20	38,38,38,38	0
57	MG	RA	3087	1/1	0.92	0.18	38,38,38,38	0
57	MG	RA	3150	1/1	0.92	0.07	42,42,42,42	0
57	MG	QA	1603	1/1	0.92	0.17	38,38,38,38	0
57	MG	RA	3210	1/1	0.92	0.07	56,56,56,56	0
57	MG	YA	3464	1/1	0.92	0.07	63,63,63,63	0
57	MG	RA	3331	1/1	0.92	0.23	66,66,66,66	0
57	MG	RA	3460	1/1	0.92	0.24	38,38,38,38	0
57	MG	YA	3215	1/1	0.92	0.36	62,62,62,62	0
57	MG	YA	3473	1/1	0.92	0.05	38,38,38,38	0
57	MG	XA	1621	1/1	0.92	0.23	38,38,38,38	0
57	MG	RA	3135	1/1	0.92	0.27	46,46,46,46	0
57	MG	XA	1629	1/1	0.92	0.23	38,38,38,38	0
57	MG	YA	3478	1/1	0.92	0.07	40,40,40,40	0
57	MG	YA	3062	1/1	0.92	0.14	38,38,38,38	0
57	MG	RA	3377	1/1	0.92	0.33	38,38,38,38	0
57	MG	RA	3464	1/1	0.92	0.08	38,38,38,38	0
57	MG	YA	3223	1/1	0.92	0.12	38,38,38,38	0
57	MG	YA	3487	1/1	0.92	0.06	47,47,47,47	0
57	MG	RA	3336	1/1	0.92	0.07	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1644	1/1	0.92	0.14	38,38,38,38	0
57	MG	YA	3227	1/1	0.92	0.09	38,38,38,38	0
57	MG	RA	3153	1/1	0.92	0.12	53,53,53,53	0
57	MG	RA	3340	1/1	0.92	0.06	64,64,64,64	0
57	MG	XA	1656	1/1	0.92	0.10	53,53,53,53	0
57	MG	YA	3366	1/1	0.92	0.13	68,68,68,68	0
57	MG	XA	1660	1/1	0.92	0.08	61,61,61,61	0
57	MG	YA	3370	1/1	0.92	0.21	48,48,48,48	0
57	MG	YA	3095	1/1	0.92	0.15	38,38,38,38	0
57	MG	YA	3372	1/1	0.92	0.09	51,51,51,51	0
57	MG	YA	3098	1/1	0.92	0.15	38,38,38,38	0
57	MG	YA	3099	1/1	0.92	0.24	38,38,38,38	0
57	MG	YA	3100	1/1	0.92	0.20	38,38,38,38	0
57	MG	YA	3246	1/1	0.92	0.29	66,66,66,66	0
57	MG	RA	3187	1/1	0.92	0.19	38,38,38,38	0
57	MG	YA	3379	1/1	0.92	0.15	57,57,57,57	0
57	MG	YA	3521	1/1	0.92	0.10	38,38,38,38	0
57	MG	XA	1663	1/1	0.92	0.04	38,38,38,38	0
57	MG	RA	3479	1/1	0.92	0.09	69,69,69,69	0
57	MG	RA	3136	1/1	0.92	0.14	38,38,38,38	0
57	MG	XA	1671	1/1	0.92	0.06	71,71,71,71	0
57	MG	YA	3529	1/1	0.92	0.12	38,38,38,38	0
57	MG	YA	3530	1/1	0.92	0.20	50,50,50,50	0
57	MG	YA	3389	1/1	0.92	0.13	53,53,53,53	0
57	MG	RA	3047	1/1	0.92	0.10	38,38,38,38	0
57	MG	YA	3393	1/1	0.92	0.23	77,77,77,77	0
57	MG	XE	201	1/1	0.92	0.07	55,55,55,55	0
57	MG	RA	3157	1/1	0.92	0.05	38,38,38,38	0
57	MG	RA	3223	1/1	0.92	0.16	38,38,38,38	0
57	MG	R0	101	1/1	0.92	0.10	38,38,38,38	0
57	MG	RE	302	1/1	0.92	0.17	48,48,48,48	0
57	MG	YA	3138	1/1	0.92	0.18	38,38,38,38	0
57	MG	YA	3402	1/1	0.92	0.08	59,59,59,59	0
57	MG	RA	3433	1/1	0.92	0.10	64,64,64,64	0
57	MG	Y7	101	1/1	0.92	0.10	56,56,56,56	0
57	MG	Y8	101	1/1	0.92	0.18	48,48,48,48	0
57	MG	YA	3002	1/1	0.92	0.09	38,38,38,38	0
57	MG	YA	3296	1/1	0.92	0.11	38,38,38,38	0
57	MG	YA	3146	1/1	0.92	0.14	38,38,38,38	0
57	MG	YA	3149	1/1	0.92	0.07	38,38,38,38	0
57	MG	YA	3158	1/1	0.92	0.06	38,38,38,38	0
57	MG	YA	3415	1/1	0.92	0.18	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3082	1/1	0.92	0.14	38,38,38,38	0
57	MG	RA	3007	1/1	0.92	0.08	38,38,38,38	0
57	MG	RA	3168	1/1	0.92	0.11	38,38,38,38	0
57	MG	RA	3143	1/1	0.92	0.15	51,51,51,51	0
57	MG	RQ	201	1/1	0.92	0.12	38,38,38,38	0
57	MG	RA	3270	1/1	0.92	0.05	84,84,84,84	0
57	MG	RA	3022	1/1	0.92	0.19	38,38,38,38	0
57	MG	YA	3177	1/1	0.92	0.11	38,38,38,38	0
57	MG	YA	3179	1/1	0.92	0.09	38,38,38,38	0
57	MG	RA	3075	1/1	0.92	0.26	38,38,38,38	0
57	MG	RA	3482	1/1	0.93	0.13	38,38,38,38	0
57	MG	YA	3055	1/1	0.93	0.19	38,38,38,38	0
57	MG	YA	3446	1/1	0.93	0.11	38,38,38,38	0
57	MG	RA	3333	1/1	0.93	0.12	47,47,47,47	0
57	MG	YA	3325	1/1	0.93	0.12	38,38,38,38	0
57	MG	XA	1658	1/1	0.93	0.07	50,50,50,50	0
57	MG	YA	3327	1/1	0.93	0.06	38,38,38,38	0
57	MG	RA	3335	1/1	0.93	0.14	38,38,38,38	0
57	MG	XA	1661	1/1	0.93	0.05	63,63,63,63	0
57	MG	QA	1606	1/1	0.93	0.09	77,77,77,77	0
57	MG	YA	3207	1/1	0.93	0.11	49,49,49,49	0
57	MG	RA	3337	1/1	0.93	0.19	91,91,91,91	0
57	MG	YA	3076	1/1	0.93	0.09	38,38,38,38	0
57	MG	QA	1612	1/1	0.93	0.09	52,52,52,52	0
57	MG	XA	1665	1/1	0.93	0.21	38,38,38,38	0
57	MG	RA	3432	1/1	0.93	0.05	66,66,66,66	0
57	MG	QA	1659	1/1	0.93	0.07	38,38,38,38	0
57	MG	RA	3048	1/1	0.93	0.15	38,38,38,38	0
57	MG	YA	3090	1/1	0.93	0.17	38,38,38,38	0
57	MG	YA	3347	1/1	0.93	0.12	38,38,38,38	0
57	MG	RA	3100	1/1	0.93	0.42	96,96,96,96	0
57	MG	RA	3345	1/1	0.93	0.05	38,38,38,38	0
57	MG	QA	1635	1/1	0.93	0.15	63,63,63,63	0
57	MG	RA	3235	1/1	0.93	0.11	38,38,38,38	0
57	MG	YA	3101	1/1	0.93	0.12	38,38,38,38	0
57	MG	YA	3482	1/1	0.93	0.14	67,67,67,67	0
57	MG	RA	3348	1/1	0.93	0.12	39,39,39,39	0
57	MG	YA	3103	1/1	0.93	0.13	38,38,38,38	0
57	MG	YA	3228	1/1	0.93	0.15	38,38,38,38	0
57	MG	RR	201	1/1	0.93	0.08	38,38,38,38	0
57	MG	YA	3109	1/1	0.93	0.09	38,38,38,38	0
57	MG	YA	3112	1/1	0.93	0.14	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3237	1/1	0.93	0.12	38,38,38,38	0
57	MG	RA	3183	1/1	0.93	0.09	65,65,65,65	0
57	MG	YA	3495	1/1	0.93	0.08	40,40,40,40	0
57	MG	RA	3237	1/1	0.93	0.18	52,52,52,52	0
57	MG	RA	3103	1/1	0.93	0.17	38,38,38,38	0
57	MG	XA	1602	1/1	0.93	0.16	47,47,47,47	0
57	MG	XA	1603	1/1	0.93	0.22	38,38,38,38	0
57	MG	YA	3500	1/1	0.93	0.17	38,38,38,38	0
57	MG	YA	3245	1/1	0.93	0.08	39,39,39,39	0
57	MG	RA	3312	1/1	0.93	0.09	53,53,53,53	0
57	MG	YA	3247	1/1	0.93	0.23	38,38,38,38	0
57	MG	YA	3506	1/1	0.93	0.11	101,101,101,101	0
57	MG	RA	3107	1/1	0.93	0.14	38,38,38,38	0
57	MG	YA	3130	1/1	0.93	0.23	38,38,38,38	0
57	MG	YA	3131	1/1	0.93	0.18	38,38,38,38	0
57	MG	RA	3278	1/1	0.93	0.05	43,43,43,43	0
57	MG	YA	3011	1/1	0.93	0.11	81,81,81,81	0
57	MG	RA	3209	1/1	0.93	0.08	39,39,39,39	0
57	MG	RA	3030	1/1	0.93	0.41	38,38,38,38	0
57	MG	YA	3388	1/1	0.93	0.07	61,61,61,61	0
57	MG	XA	1609	1/1	0.93	0.10	38,38,38,38	0
57	MG	RA	3012	1/1	0.93	0.27	38,38,38,38	0
57	MG	YA	3271	1/1	0.93	0.21	38,38,38,38	0
57	MG	RA	3319	1/1	0.93	0.13	38,38,38,38	0
57	MG	RA	3282	1/1	0.93	0.07	38,38,38,38	0
57	MG	YA	3275	1/1	0.93	0.16	38,38,38,38	0
57	MG	XA	1613	1/1	0.93	0.08	38,38,38,38	0
57	MG	YA	3154	1/1	0.93	0.10	49,49,49,49	0
57	MG	YA	3155	1/1	0.93	0.07	38,38,38,38	0
57	MG	YB	205	1/1	0.93	0.06	38,38,38,38	0
57	MG	RA	3284	1/1	0.93	0.15	38,38,38,38	0
57	MG	YA	3021	1/1	0.93	0.18	43,43,43,43	0
57	MG	RA	3161	1/1	0.93	0.06	38,38,38,38	0
57	MG	RA	3058	1/1	0.93	0.20	38,38,38,38	0
57	MG	YA	3030	1/1	0.93	0.26	38,38,38,38	0
57	MG	QA	1639	1/1	0.93	0.14	43,43,43,43	0
57	MG	RA	3465	1/1	0.93	0.06	38,38,38,38	0
57	MG	YA	3302	1/1	0.93	0.11	38,38,38,38	0
57	MG	YA	3412	1/1	0.93	0.07	38,38,38,38	0
57	MG	RA	3017	1/1	0.93	0.18	38,38,38,38	0
57	MG	YA	3414	1/1	0.93	0.09	38,38,38,38	0
57	MG	RA	3330	1/1	0.93	0.10	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3037	1/1	0.93	0.20	38,38,38,38	0
57	MG	RA	3018	1/1	0.93	0.18	38,38,38,38	0
57	MG	XA	1635	1/1	0.93	0.14	38,38,38,38	0
57	MG	YA	3183	1/1	0.93	0.14	86,86,86,86	0
57	MG	RA	3474	1/1	0.93	0.10	38,38,38,38	0
57	MG	YA	3186	1/1	0.93	0.17	58,58,58,58	0
57	MG	YA	3312	1/1	0.93	0.20	38,38,38,38	0
57	MG	RA	3475	1/1	0.93	0.07	65,65,65,65	0
57	MG	RA	3375	1/1	0.93	0.09	47,47,47,47	0
57	MG	QA	1625	1/1	0.93	0.10	58,58,58,58	0
57	MG	YA	3050	1/1	0.93	0.26	38,38,38,38	0
57	MG	XA	1646	1/1	0.93	0.24	38,38,38,38	0
57	MG	XA	1653	1/1	0.93	0.09	58,58,58,58	0
57	MG	QA	1607	1/1	0.94	0.09	38,38,38,38	0
57	MG	YA	3205	1/1	0.94	0.05	81,81,81,81	0
57	MG	YA	3206	1/1	0.94	0.09	38,38,38,38	0
57	MG	RA	3072	1/1	0.94	0.25	38,38,38,38	0
57	MG	RA	3200	1/1	0.94	0.11	38,38,38,38	0
57	MG	RA	3043	1/1	0.94	0.22	38,38,38,38	0
57	MG	XQ	201	1/1	0.94	0.07	65,65,65,65	0
57	MG	YA	3093	1/1	0.94	0.22	38,38,38,38	0
57	MG	RA	3102	1/1	0.94	0.16	38,38,38,38	0
57	MG	RA	3438	1/1	0.94	0.09	45,45,45,45	0
57	MG	RA	3003	1/1	0.94	0.07	38,38,38,38	0
57	MG	RA	3045	1/1	0.94	0.13	38,38,38,38	0
57	MG	RA	3290	1/1	0.94	0.09	38,38,38,38	0
57	MG	QA	1638	1/1	0.94	0.10	38,38,38,38	0
57	MG	YA	3459	1/1	0.94	0.23	38,38,38,38	0
57	MG	RA	3145	1/1	0.94	0.05	38,38,38,38	0
57	MG	RA	3388	1/1	0.94	0.07	46,46,46,46	0
57	MG	YA	3224	1/1	0.94	0.13	51,51,51,51	0
57	MG	YA	3107	1/1	0.94	0.10	38,38,38,38	0
57	MG	YA	3005	1/1	0.94	0.07	58,58,58,58	0
57	MG	YA	3470	1/1	0.94	0.12	42,42,42,42	0
57	MG	RA	3293	1/1	0.94	0.16	42,42,42,42	0
57	MG	RA	3394	1/1	0.94	0.05	61,61,61,61	0
57	MG	YA	3229	1/1	0.94	0.06	38,38,38,38	0
57	MG	RA	3248	1/1	0.94	0.07	38,38,38,38	0
57	MG	YA	3009	1/1	0.94	0.06	38,38,38,38	0
57	MG	YA	3118	1/1	0.94	0.13	38,38,38,38	0
57	MG	YA	3119	1/1	0.94	0.19	38,38,38,38	0
57	MG	RA	3178	1/1	0.94	0.05	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1626	1/1	0.94	0.15	59,59,59,59	0
57	MG	YA	3484	1/1	0.94	0.06	47,47,47,47	0
57	MG	YA	3358	1/1	0.94	0.10	38,38,38,38	0
57	MG	YA	3126	1/1	0.94	0.11	38,38,38,38	0
57	MG	RA	3251	1/1	0.94	0.05	62,62,62,62	0
57	MG	RA	3401	1/1	0.94	0.15	57,57,57,57	0
57	MG	YA	3015	1/1	0.94	0.08	38,38,38,38	0
57	MG	XA	1614	1/1	0.94	0.08	38,38,38,38	0
57	MG	YA	3368	1/1	0.94	0.11	43,43,43,43	0
57	MG	YA	3369	1/1	0.94	0.14	53,53,53,53	0
57	MG	RA	3402	1/1	0.94	0.09	38,38,38,38	0
57	MG	XA	1616	1/1	0.94	0.05	51,51,51,51	0
57	MG	RA	3115	1/1	0.94	0.09	40,40,40,40	0
57	MG	RA	3181	1/1	0.94	0.09	38,38,38,38	0
57	MG	RA	3116	1/1	0.94	0.22	38,38,38,38	0
57	MG	QA	1640	1/1	0.94	0.05	77,77,77,77	0
57	MG	QA	1623	1/1	0.94	0.10	62,62,62,62	0
57	MG	YA	3027	1/1	0.94	0.19	38,38,38,38	0
57	MG	YA	3505	1/1	0.94	0.05	47,47,47,47	0
57	MG	RA	3410	1/1	0.94	0.15	57,57,57,57	0
57	MG	YA	3507	1/1	0.94	0.07	40,40,40,40	0
57	MG	RA	3308	1/1	0.94	0.09	38,38,38,38	0
57	MG	QA	1630	1/1	0.94	0.22	38,38,38,38	0
57	MG	XA	1638	1/1	0.94	0.05	48,48,48,48	0
57	MG	YA	3384	1/1	0.94	0.05	60,60,60,60	0
57	MG	RA	3470	1/1	0.94	0.11	38,38,38,38	0
57	MG	YA	3515	1/1	0.94	0.18	38,38,38,38	0
57	MG	YA	3163	1/1	0.94	0.09	41,41,41,41	0
57	MG	YA	3520	1/1	0.94	0.18	38,38,38,38	0
57	MG	RA	3031	1/1	0.94	0.20	38,38,38,38	0
57	MG	YA	3278	1/1	0.94	0.11	38,38,38,38	0
57	MG	YA	3523	1/1	0.94	0.10	38,38,38,38	0
57	MG	YA	3391	1/1	0.94	0.17	38,38,38,38	0
57	MG	YA	3279	1/1	0.94	0.10	38,38,38,38	0
57	MG	YA	3038	1/1	0.94	0.16	38,38,38,38	0
57	MG	YA	3285	1/1	0.94	0.07	42,42,42,42	0
57	MG	RA	3262	1/1	0.94	0.12	40,40,40,40	0
57	MG	YA	3288	1/1	0.94	0.04	38,38,38,38	0
57	MG	YA	3537	1/1	0.94	0.13	38,38,38,38	0
57	MG	YB	201	1/1	0.94	0.10	88,88,88,88	0
57	MG	YA	3041	1/1	0.94	0.16	38,38,38,38	0
57	MG	RA	3263	1/1	0.94	0.16	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3293	1/1	0.94	0.13	38,38,38,38	0
57	MG	YA	3294	1/1	0.94	0.11	38,38,38,38	0
57	MG	RA	3086	1/1	0.94	0.09	38,38,38,38	0
57	MG	XA	1650	1/1	0.94	0.04	43,43,43,43	0
57	MG	QA	1631	1/1	0.94	0.04	68,68,68,68	0
57	MG	YA	3048	1/1	0.94	0.12	38,38,38,38	0
57	MG	YA	3181	1/1	0.94	0.17	38,38,38,38	0
57	MG	YB	211	1/1	0.94	0.04	72,72,72,72	0
57	MG	XA	1654	1/1	0.94	0.05	45,45,45,45	0
57	MG	RA	3361	1/1	0.94	0.07	56,56,56,56	0
57	MG	RA	3060	1/1	0.94	0.14	38,38,38,38	0
57	MG	QV	101	1/1	0.94	0.07	38,38,38,38	0
57	MG	YE	303	1/1	0.94	0.21	40,40,40,40	0
57	MG	RA	3273	1/1	0.94	0.06	38,38,38,38	0
57	MG	QA	1610	1/1	0.94	0.10	38,38,38,38	0
57	MG	RA	3232	1/1	0.94	0.09	38,38,38,38	0
57	MG	RA	3370	1/1	0.94	0.09	38,38,38,38	0
57	MG	QA	1664	1/1	0.94	0.25	38,38,38,38	0
57	MG	YA	3066	1/1	0.94	0.17	38,38,38,38	0
57	MG	YQ	203	1/1	0.94	0.09	38,38,38,38	0
57	MG	RA	3068	1/1	0.94	0.18	38,38,38,38	0
57	MG	YA	3425	1/1	0.94	0.09	75,75,75,75	0
57	MG	XA	1667	1/1	0.94	0.09	66,66,66,66	0
57	MG	YA	3431	1/1	0.94	0.13	58,58,58,58	0
57	MG	XA	1668	1/1	0.94	0.26	38,38,38,38	0
57	MG	RA	3326	1/1	0.94	0.05	94,94,94,94	0
57	MG	YA	3318	1/1	0.94	0.07	38,38,38,38	0
57	MG	YA	3077	1/1	0.94	0.17	38,38,38,38	0
57	MG	YA	3439	1/1	0.94	0.18	38,38,38,38	0
57	MG	RA	3374	1/1	0.94	0.05	77,77,77,77	0
57	MG	RA	3013	1/1	0.95	0.19	38,38,38,38	0
57	MG	YA	3442	1/1	0.95	0.06	38,38,38,38	0
57	MG	RA	3416	1/1	0.95	0.06	38,38,38,38	0
57	MG	RA	3164	1/1	0.95	0.04	38,38,38,38	0
57	MG	YA	3067	1/1	0.95	0.15	38,38,38,38	0
57	MG	RA	3080	1/1	0.95	0.23	38,38,38,38	0
57	MG	RA	3365	1/1	0.95	0.09	77,77,77,77	0
57	MG	YA	3073	1/1	0.95	0.09	48,48,48,48	0
57	MG	YA	3198	1/1	0.95	0.04	39,39,39,39	0
57	MG	XA	1666	1/1	0.95	0.04	38,38,38,38	0
57	MG	YA	3075	1/1	0.95	0.05	38,38,38,38	0
57	MG	YA	3324	1/1	0.95	0.08	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3320	1/1	0.95	0.11	56,56,56,56	0
57	MG	RA	3167	1/1	0.95	0.04	38,38,38,38	0
57	MG	YA	3078	1/1	0.95	0.15	38,38,38,38	0
57	MG	RB	206	1/1	0.95	0.04	79,79,79,79	0
57	MG	RB	207	1/1	0.95	0.06	47,47,47,47	0
57	MG	YA	3208	1/1	0.95	0.06	55,55,55,55	0
57	MG	YA	3461	1/1	0.95	0.05	47,47,47,47	0
57	MG	YA	3462	1/1	0.95	0.12	73,73,73,73	0
57	MG	YA	3333	1/1	0.95	0.11	38,38,38,38	0
57	MG	RE	301	1/1	0.95	0.13	38,38,38,38	0
57	MG	YA	3465	1/1	0.95	0.10	54,54,54,54	0
57	MG	YA	3084	1/1	0.95	0.07	38,38,38,38	0
57	MG	RA	3034	1/1	0.95	0.15	38,38,38,38	0
57	MG	YA	3468	1/1	0.95	0.11	38,38,38,38	0
57	MG	XK	201	1/1	0.95	0.05	55,55,55,55	0
57	MG	RA	3140	1/1	0.95	0.07	38,38,38,38	0
57	MG	YA	3092	1/1	0.95	0.11	38,38,38,38	0
57	MG	RA	3324	1/1	0.95	0.10	38,38,38,38	0
57	MG	RA	3172	1/1	0.95	0.07	43,43,43,43	0
57	MG	YA	3096	1/1	0.95	0.09	38,38,38,38	0
57	MG	YA	3220	1/1	0.95	0.10	38,38,38,38	0
57	MG	RA	3283	1/1	0.95	0.15	38,38,38,38	0
57	MG	YA	3481	1/1	0.95	0.05	65,65,65,65	0
57	MG	RA	3327	1/1	0.95	0.12	38,38,38,38	0
57	MG	RA	3054	1/1	0.95	0.11	38,38,38,38	0
57	MG	RA	3002	1/1	0.95	0.05	38,38,38,38	0
57	MG	RA	3114	1/1	0.95	0.20	58,58,58,58	0
57	MG	YA	3001	1/1	0.95	0.08	38,38,38,38	0
57	MG	RA	3036	1/1	0.95	0.12	38,38,38,38	0
57	MG	RA	3288	1/1	0.95	0.16	38,38,38,38	0
57	MG	YA	3489	1/1	0.95	0.12	47,47,47,47	0
57	MG	RA	3435	1/1	0.95	0.09	46,46,46,46	0
57	MG	QA	1673	1/1	0.95	0.05	54,54,54,54	0
57	MG	YA	3361	1/1	0.95	0.36	85,85,85,85	0
57	MG	YA	3494	1/1	0.95	0.14	38,38,38,38	0
57	MG	YA	3231	1/1	0.95	0.06	38,38,38,38	0
57	MG	YA	3232	1/1	0.95	0.07	38,38,38,38	0
57	MG	RA	3334	1/1	0.95	0.21	54,54,54,54	0
57	MG	QA	1642	1/1	0.95	0.08	38,38,38,38	0
57	MG	RA	3118	1/1	0.95	0.11	38,38,38,38	0
57	MG	RA	3386	1/1	0.95	0.06	38,38,38,38	0
57	MG	RA	3213	1/1	0.95	0.09	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3252	1/1	0.95	0.11	38,38,38,38	0
57	MG	RA	3389	1/1	0.95	0.06	38,38,38,38	0
57	MG	RA	3390	1/1	0.95	0.06	38,38,38,38	0
57	MG	QA	1636	1/1	0.95	0.05	38,38,38,38	0
57	MG	RA	3393	1/1	0.95	0.07	41,41,41,41	0
57	MG	RA	3448	1/1	0.95	0.06	84,84,84,84	0
57	MG	RA	3216	1/1	0.95	0.18	38,38,38,38	0
57	MG	RA	3064	1/1	0.95	0.13	38,38,38,38	0
57	MG	YA	3133	1/1	0.95	0.07	38,38,38,38	0
57	MG	YA	3255	1/1	0.95	0.10	38,38,38,38	0
57	MG	RA	3219	1/1	0.95	0.11	38,38,38,38	0
57	MG	YA	3259	1/1	0.95	0.17	38,38,38,38	0
57	MG	RA	3301	1/1	0.95	0.09	38,38,38,38	0
57	MG	YA	3385	1/1	0.95	0.07	38,38,38,38	0
57	MG	YA	3139	1/1	0.95	0.18	65,65,65,65	0
57	MG	YA	3263	1/1	0.95	0.04	38,38,38,38	0
57	MG	YA	3264	1/1	0.95	0.24	38,38,38,38	0
57	MG	QA	1665	1/1	0.95	0.04	47,47,47,47	0
57	MG	YA	3527	1/1	0.95	0.11	53,53,53,53	0
57	MG	YA	3023	1/1	0.95	0.22	38,38,38,38	0
57	MG	YA	3392	1/1	0.95	0.05	38,38,38,38	0
57	MG	RA	3021	1/1	0.95	0.14	38,38,38,38	0
57	MG	YA	3144	1/1	0.95	0.06	38,38,38,38	0
57	MG	YA	3536	1/1	0.95	0.06	38,38,38,38	0
57	MG	YA	3272	1/1	0.95	0.17	38,38,38,38	0
57	MG	RA	3127	1/1	0.95	0.15	38,38,38,38	0
57	MG	RA	3458	1/1	0.95	0.22	38,38,38,38	0
57	MG	YA	3147	1/1	0.95	0.10	51,51,51,51	0
57	MG	RA	3403	1/1	0.95	0.17	38,38,38,38	0
57	MG	YA	3401	1/1	0.95	0.22	38,38,38,38	0
57	MG	QA	1632	1/1	0.95	0.11	59,59,59,59	0
57	MG	RA	3462	1/1	0.95	0.08	38,38,38,38	0
57	MG	XA	1636	1/1	0.95	0.09	38,38,38,38	0
57	MG	QA	1616	1/1	0.95	0.12	38,38,38,38	0
57	MG	YA	3161	1/1	0.95	0.08	38,38,38,38	0
57	MG	RA	3264	1/1	0.95	0.06	38,38,38,38	0
57	MG	QA	1609	1/1	0.95	0.21	38,38,38,38	0
57	MG	RA	3408	1/1	0.95	0.13	38,38,38,38	0
57	MG	RA	3098	1/1	0.95	0.09	38,38,38,38	0
57	MG	YA	3169	1/1	0.95	0.17	38,38,38,38	0
57	MG	YD	303	1/1	0.95	0.05	38,38,38,38	0
57	MG	RA	3469	1/1	0.95	0.10	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1647	1/1	0.95	0.12	42,42,42,42	0
57	MG	YA	3172	1/1	0.95	0.20	86,86,86,86	0
57	MG	YA	3417	1/1	0.95	0.09	44,44,44,44	0
57	MG	RA	3028	1/1	0.95	0.06	38,38,38,38	0
57	MG	YA	3300	1/1	0.95	0.11	38,38,38,38	0
57	MG	XA	1651	1/1	0.95	0.12	38,38,38,38	0
57	MG	XA	1652	1/1	0.95	0.05	99,99,99,99	0
57	MG	RA	3159	1/1	0.95	0.22	38,38,38,38	0
57	MG	RA	3473	1/1	0.95	0.08	38,38,38,38	0
57	MG	RA	3315	1/1	0.95	0.07	38,38,38,38	0
57	MG	YA	3428	1/1	0.95	0.06	64,64,64,64	0
57	MG	RA	3359	1/1	0.95	0.09	38,38,38,38	0
57	MG	YA	3054	1/1	0.95	0.19	38,38,38,38	0
57	MG	RA	3476	1/1	0.95	0.07	38,38,38,38	0
57	MG	YA	3187	1/1	0.95	0.07	38,38,38,38	0
59	ZN	Y5	101	1/1	0.95	0.22	94,94,94,94	0
57	MG	YA	3056	1/1	0.95	0.11	38,38,38,38	0
57	MG	QA	1641	1/1	0.95	0.07	62,62,62,62	0
57	MG	QA	1634	1/1	0.96	0.10	38,38,38,38	0
57	MG	YA	3373	1/1	0.96	0.07	38,38,38,38	0
57	MG	YA	3472	1/1	0.96	0.07	70,70,70,70	0
57	MG	RA	3233	1/1	0.96	0.15	64,64,64,64	0
57	MG	RQ	202	1/1	0.96	0.10	49,49,49,49	0
57	MG	YA	3108	1/1	0.96	0.13	38,38,38,38	0
57	MG	RA	3271	1/1	0.96	0.10	38,38,38,38	0
57	MG	YA	3477	1/1	0.96	0.15	65,65,65,65	0
57	MG	YA	3199	1/1	0.96	0.23	38,38,38,38	0
57	MG	RA	3272	1/1	0.96	0.09	38,38,38,38	0
57	MG	RA	3163	1/1	0.96	0.06	42,42,42,42	0
57	MG	RA	3108	1/1	0.96	0.10	79,79,79,79	0
57	MG	YA	3115	1/1	0.96	0.07	38,38,38,38	0
57	MG	YA	3039	1/1	0.96	0.27	38,38,38,38	0
57	MG	YA	3117	1/1	0.96	0.14	38,38,38,38	0
57	MG	RA	3023	1/1	0.96	0.06	38,38,38,38	0
57	MG	YA	3387	1/1	0.96	0.04	38,38,38,38	0
57	MG	QA	1620	1/1	0.96	0.06	48,48,48,48	0
57	MG	RA	3112	1/1	0.96	0.11	38,38,38,38	0
57	MG	YA	3121	1/1	0.96	0.04	38,38,38,38	0
57	MG	YA	3303	1/1	0.96	0.07	38,38,38,38	0
57	MG	YA	3122	1/1	0.96	0.08	38,38,38,38	0
57	MG	RA	3113	1/1	0.96	0.17	38,38,38,38	0
57	MG	RA	3241	1/1	0.96	0.25	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3045	1/1	0.96	0.34	38,38,38,38	0
57	MG	YA	3128	1/1	0.96	0.10	44,44,44,44	0
57	MG	R3	101	1/1	0.96	0.06	43,43,43,43	0
57	MG	YA	3047	1/1	0.96	0.05	38,38,38,38	0
57	MG	RA	3027	1/1	0.96	0.16	38,38,38,38	0
57	MG	QA	1618	1/1	0.96	0.07	38,38,38,38	0
57	MG	RA	3029	1/1	0.96	0.15	38,38,38,38	0
57	MG	QA	1650	1/1	0.96	0.07	55,55,55,55	0
57	MG	RA	3466	1/1	0.96	0.14	38,38,38,38	0
57	MG	QA	1651	1/1	0.96	0.04	41,41,41,41	0
57	MG	RA	3120	1/1	0.96	0.08	45,45,45,45	0
57	MG	YA	3407	1/1	0.96	0.17	54,54,54,54	0
57	MG	RA	3032	1/1	0.96	0.12	38,38,38,38	0
57	MG	YA	3510	1/1	0.96	0.04	46,46,46,46	0
57	MG	RA	3077	1/1	0.96	0.17	38,38,38,38	0
57	MG	YA	3059	1/1	0.96	0.09	38,38,38,38	0
57	MG	Y0	102	1/1	0.96	0.23	38,38,38,38	0
57	MG	QA	1602	1/1	0.96	0.16	38,38,38,38	0
57	MG	YA	3516	1/1	0.96	0.30	38,38,38,38	0
57	MG	RA	3125	1/1	0.96	0.20	38,38,38,38	0
57	MG	YA	3518	1/1	0.96	0.23	38,38,38,38	0
57	MG	YA	3519	1/1	0.96	0.32	38,38,38,38	0
57	MG	YA	3233	1/1	0.96	0.05	38,38,38,38	0
57	MG	YA	3234	1/1	0.96	0.06	38,38,38,38	0
57	MG	YA	3063	1/1	0.96	0.08	38,38,38,38	0
57	MG	YA	3418	1/1	0.96	0.13	38,38,38,38	0
57	MG	YA	3064	1/1	0.96	0.18	38,38,38,38	0
57	MG	YA	3065	1/1	0.96	0.19	38,38,38,38	0
57	MG	YA	3526	1/1	0.96	0.15	41,41,41,41	0
57	MG	RA	3294	1/1	0.96	0.10	38,38,38,38	0
57	MG	YA	3331	1/1	0.96	0.06	91,91,91,91	0
57	MG	YA	3332	1/1	0.96	0.06	54,54,54,54	0
57	MG	RA	3184	1/1	0.96	0.09	38,38,38,38	0
57	MG	YA	3531	1/1	0.96	0.07	56,56,56,56	0
57	MG	YA	3240	1/1	0.96	0.07	38,38,38,38	0
57	MG	RA	3126	1/1	0.96	0.10	38,38,38,38	0
57	MG	YA	3429	1/1	0.96	0.06	45,45,45,45	0
57	MG	YA	3430	1/1	0.96	0.04	41,41,41,41	0
57	MG	RA	3297	1/1	0.96	0.08	38,38,38,38	0
57	MG	RA	3339	1/1	0.96	0.14	38,38,38,38	0
57	MG	XA	1630	1/1	0.96	0.12	38,38,38,38	0
57	MG	YA	3341	1/1	0.96	0.16	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3167	1/1	0.96	0.04	38,38,38,38	0
57	MG	QA	1643	1/1	0.96	0.24	38,38,38,38	0
57	MG	YA	3440	1/1	0.96	0.06	38,38,38,38	0
57	MG	YA	3344	1/1	0.96	0.09	38,38,38,38	0
57	MG	RA	3257	1/1	0.96	0.09	38,38,38,38	0
57	MG	RA	3258	1/1	0.96	0.11	38,38,38,38	0
57	MG	RA	3154	1/1	0.96	0.11	38,38,38,38	0
57	MG	YA	3252	1/1	0.96	0.08	38,38,38,38	0
57	MG	YA	3254	1/1	0.96	0.09	38,38,38,38	0
57	MG	YA	3010	1/1	0.96	0.06	90,90,90,90	0
57	MG	YA	3175	1/1	0.96	0.11	38,38,38,38	0
57	MG	YE	301	1/1	0.96	0.15	38,38,38,38	0
57	MG	XA	1639	1/1	0.96	0.12	38,38,38,38	0
57	MG	XA	1640	1/1	0.96	0.04	38,38,38,38	0
57	MG	RA	3055	1/1	0.96	0.11	38,38,38,38	0
57	MG	XA	1642	1/1	0.96	0.06	43,43,43,43	0
57	MG	RA	3226	1/1	0.96	0.14	38,38,38,38	0
57	MG	YA	3266	1/1	0.96	0.14	38,38,38,38	0
57	MG	YA	3359	1/1	0.96	0.06	38,38,38,38	0
57	MG	QA	1644	1/1	0.96	0.06	59,59,59,59	0
57	MG	YR	201	1/1	0.96	0.16	38,38,38,38	0
57	MG	YA	3458	1/1	0.96	0.04	38,38,38,38	0
57	MG	RA	3130	1/1	0.96	0.05	48,48,48,48	0
57	MG	QA	1666	1/1	0.96	0.07	43,43,43,43	0
57	MG	RA	3265	1/1	0.96	0.16	38,38,38,38	0
58	SF4	XD	301	8/8	0.96	0.09	88,97,160,164	0
59	ZN	QN	101	1/1	0.96	0.09	94,94,94,94	0
57	MG	YA	3365	1/1	0.96	0.11	49,49,49,49	0
57	MG	XA	1649	1/1	0.96	0.05	60,60,60,60	0
57	MG	RE	303	1/1	0.96	0.08	38,38,38,38	0
57	MG	RA	3399	1/1	0.96	0.12	38,38,38,38	0
59	ZN	XN	101	1/1	0.96	0.06	134,134,134,134	0
59	ZN	Y4	101	1/1	0.96	0.30	88,88,88,88	0
57	MG	RA	3132	1/1	0.96	0.19	38,38,38,38	0
57	MG	RA	3311	1/1	0.96	0.05	50,50,50,50	0
57	MG	RA	3106	1/1	0.96	0.08	77,77,77,77	0
57	MG	YA	3026	1/1	0.97	0.14	38,38,38,38	0
57	MG	QA	1627	1/1	0.97	0.09	53,53,53,53	0
57	MG	YA	3281	1/1	0.97	0.18	49,49,49,49	0
57	MG	YA	3029	1/1	0.97	0.06	38,38,38,38	0
57	MG	YA	3480	1/1	0.97	0.07	44,44,44,44	0
57	MG	RA	3095	1/1	0.97	0.06	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3286	1/1	0.97	0.10	38,38,38,38	0
57	MG	YA	3191	1/1	0.97	0.13	38,38,38,38	0
57	MG	YA	3383	1/1	0.97	0.10	52,52,52,52	0
57	MG	RA	3447	1/1	0.97	0.05	38,38,38,38	0
57	MG	YA	3289	1/1	0.97	0.26	38,38,38,38	0
57	MG	YA	3104	1/1	0.97	0.06	42,42,42,42	0
57	MG	RA	3051	1/1	0.97	0.16	38,38,38,38	0
57	MG	XA	1657	1/1	0.97	0.05	38,38,38,38	0
57	MG	RA	3097	1/1	0.97	0.04	38,38,38,38	0
57	MG	YA	3491	1/1	0.97	0.19	38,38,38,38	0
57	MG	YA	3036	1/1	0.97	0.09	38,38,38,38	0
57	MG	YA	3111	1/1	0.97	0.14	38,38,38,38	0
57	MG	RA	3074	1/1	0.97	0.12	38,38,38,38	0
57	MG	YA	3200	1/1	0.97	0.04	38,38,38,38	0
57	MG	YA	3394	1/1	0.97	0.05	38,38,38,38	0
57	MG	RA	3212	1/1	0.97	0.04	54,54,54,54	0
57	MG	RA	3099	1/1	0.97	0.06	38,38,38,38	0
57	MG	RA	3052	1/1	0.97	0.05	38,38,38,38	0
57	MG	RA	3182	1/1	0.97	0.14	47,47,47,47	0
57	MG	RA	3289	1/1	0.97	0.18	38,38,38,38	0
57	MG	RA	3457	1/1	0.97	0.16	38,38,38,38	0
57	MG	RA	3026	1/1	0.97	0.15	38,38,38,38	0
57	MG	YA	3504	1/1	0.97	0.08	66,66,66,66	0
57	MG	QA	1615	1/1	0.97	0.04	38,38,38,38	0
57	MG	RA	3039	1/1	0.97	0.12	38,38,38,38	0
57	MG	XA	1670	1/1	0.97	0.10	38,38,38,38	0
57	MG	YA	3123	1/1	0.97	0.05	38,38,38,38	0
57	MG	YA	3213	1/1	0.97	0.04	38,38,38,38	0
57	MG	RA	3104	1/1	0.97	0.04	38,38,38,38	0
57	MG	QA	1648	1/1	0.97	0.04	44,44,44,44	0
57	MG	RA	3041	1/1	0.97	0.15	38,38,38,38	0
57	MG	YA	3513	1/1	0.97	0.09	38,38,38,38	0
57	MG	RA	3225	1/1	0.97	0.28	38,38,38,38	0
57	MG	QA	1637	1/1	0.97	0.06	38,38,38,38	0
57	MG	QA	1629	1/1	0.97	0.05	38,38,38,38	0
57	MG	QA	1614	1/1	0.97	0.05	38,38,38,38	0
57	MG	RA	3137	1/1	0.97	0.08	38,38,38,38	0
57	MG	RA	3379	1/1	0.97	0.03	38,38,38,38	0
57	MG	YA	3058	1/1	0.97	0.11	38,38,38,38	0
57	MG	YA	3137	1/1	0.97	0.27	38,38,38,38	0
57	MG	RA	3063	1/1	0.97	0.15	38,38,38,38	0
57	MG	XA	1618	1/1	0.97	0.04	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3381	1/1	0.97	0.10	38,38,38,38	0
57	MG	YA	3422	1/1	0.97	0.04	55,55,55,55	0
57	MG	YA	3141	1/1	0.97	0.13	50,50,50,50	0
57	MG	RA	3011	1/1	0.97	0.06	38,38,38,38	0
57	MG	RA	3303	1/1	0.97	0.07	38,38,38,38	0
57	MG	RA	3033	1/1	0.97	0.11	38,38,38,38	0
57	MG	XA	1627	1/1	0.97	0.09	38,38,38,38	0
57	MG	XA	1628	1/1	0.97	0.06	38,38,38,38	0
57	MG	YA	3533	1/1	0.97	0.09	38,38,38,38	0
57	MG	YA	3534	1/1	0.97	0.12	38,38,38,38	0
57	MG	RA	3342	1/1	0.97	0.18	51,51,51,51	0
57	MG	YA	3148	1/1	0.97	0.06	38,38,38,38	0
57	MG	YA	3068	1/1	0.97	0.22	38,38,38,38	0
57	MG	YA	3538	1/1	0.97	0.09	38,38,38,38	0
57	MG	YA	3150	1/1	0.97	0.06	38,38,38,38	0
57	MG	YA	3434	1/1	0.97	0.27	62,62,62,62	0
57	MG	YA	3153	1/1	0.97	0.05	38,38,38,38	0
57	MG	QA	1667	1/1	0.97	0.04	38,38,38,38	0
57	MG	YA	3438	1/1	0.97	0.13	75,75,75,75	0
57	MG	XA	1632	1/1	0.97	0.08	38,38,38,38	0
57	MG	YA	3157	1/1	0.97	0.07	38,38,38,38	0
57	MG	YA	3071	1/1	0.97	0.22	38,38,38,38	0
57	MG	YA	3072	1/1	0.97	0.08	38,38,38,38	0
57	MG	RA	3481	1/1	0.97	0.09	38,38,38,38	0
57	MG	YA	3162	1/1	0.97	0.16	38,38,38,38	0
57	MG	RA	3344	1/1	0.97	0.10	38,38,38,38	0
57	MG	YA	3348	1/1	0.97	0.09	38,38,38,38	0
57	MG	YA	3164	1/1	0.97	0.19	38,38,38,38	0
57	MG	YA	3249	1/1	0.97	0.23	38,38,38,38	0
57	MG	RA	3169	1/1	0.97	0.04	63,63,63,63	0
57	MG	RA	3170	1/1	0.97	0.04	38,38,38,38	0
57	MG	YE	302	1/1	0.97	0.07	38,38,38,38	0
57	MG	RA	3434	1/1	0.97	0.09	38,38,38,38	0
57	MG	YA	3452	1/1	0.97	0.04	38,38,38,38	0
57	MG	YA	3253	1/1	0.97	0.21	38,38,38,38	0
57	MG	RA	3069	1/1	0.97	0.09	38,38,38,38	0
57	MG	YA	3079	1/1	0.97	0.09	56,56,56,56	0
57	MG	RB	204	1/1	0.97	0.14	40,40,40,40	0
57	MG	RA	3202	1/1	0.97	0.06	38,38,38,38	0
57	MG	RA	3203	1/1	0.97	0.09	55,55,55,55	0
57	MG	YA	3360	1/1	0.97	0.05	38,38,38,38	0
57	MG	YA	3173	1/1	0.97	0.04	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3262	1/1	0.97	0.14	38,38,38,38	0
57	MG	YA	3174	1/1	0.97	0.08	38,38,38,38	0
57	MG	RA	3350	1/1	0.97	0.04	38,38,38,38	0
58	SF4	QD	301	8/8	0.97	0.06	88,107,133,212	0
57	MG	RA	3274	1/1	0.97	0.24	55,55,55,55	0
57	MG	QJ	201	1/1	0.97	0.19	60,60,60,60	0
57	MG	YA	3268	1/1	0.97	0.11	38,38,38,38	0
57	MG	YA	3178	1/1	0.97	0.04	48,48,48,48	0
57	MG	RA	3397	1/1	0.97	0.07	45,45,45,45	0
57	MG	RA	3091	1/1	0.97	0.08	40,40,40,40	0
57	MG	RA	3071	1/1	0.97	0.09	38,38,38,38	0
57	MG	YA	3094	1/1	0.97	0.10	38,38,38,38	0
57	MG	RA	3243	1/1	0.97	0.24	38,38,38,38	0
57	MG	YA	3024	1/1	0.97	0.09	38,38,38,38	0
59	ZN	Y9	101	1/1	0.97	0.29	90,90,90,90	0
57	MG	RP	201	1/1	0.97	0.11	41,41,41,41	0
57	MG	XA	1672	1/1	0.98	0.07	38,38,38,38	0
57	MG	RA	3015	1/1	0.98	0.11	38,38,38,38	0
57	MG	XA	1637	1/1	0.98	0.04	38,38,38,38	0
57	MG	YA	3028	1/1	0.98	0.11	38,38,38,38	0
57	MG	RA	3166	1/1	0.98	0.07	39,39,39,39	0
57	MG	RA	3006	1/1	0.98	0.17	38,38,38,38	0
57	MG	RA	3456	1/1	0.98	0.04	48,48,48,48	0
57	MG	RA	3364	1/1	0.98	0.07	38,38,38,38	0
57	MG	YA	3335	1/1	0.98	0.05	38,38,38,38	0
57	MG	RA	3304	1/1	0.98	0.04	38,38,38,38	0
57	MG	YA	3337	1/1	0.98	0.04	38,38,38,38	0
57	MG	YA	3276	1/1	0.98	0.14	38,38,38,38	0
57	MG	RA	3459	1/1	0.98	0.13	38,38,38,38	0
57	MG	YA	3035	1/1	0.98	0.07	38,38,38,38	0
57	MG	RA	3366	1/1	0.98	0.10	38,38,38,38	0
57	MG	YA	3532	1/1	0.98	0.05	38,38,38,38	0
57	MG	YA	3280	1/1	0.98	0.10	38,38,38,38	0
57	MG	RA	3092	1/1	0.98	0.12	40,40,40,40	0
57	MG	YA	3469	1/1	0.98	0.06	38,38,38,38	0
57	MG	YA	3282	1/1	0.98	0.18	38,38,38,38	0
57	MG	YA	3283	1/1	0.98	0.04	38,38,38,38	0
57	MG	RA	3066	1/1	0.98	0.07	38,38,38,38	0
57	MG	RA	3391	1/1	0.98	0.20	38,38,38,38	0
57	MG	XA	1648	1/1	0.98	0.08	38,38,38,38	0
57	MG	RA	3067	1/1	0.98	0.03	38,38,38,38	0
57	MG	YA	3411	1/1	0.98	0.04	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3215	1/1	0.98	0.12	38,38,38,38	0
57	MG	RA	3269	1/1	0.98	0.16	38,38,38,38	0
57	MG	YA	3085	1/1	0.98	0.10	38,38,38,38	0
57	MG	RA	3105	1/1	0.98	0.05	38,38,38,38	0
57	MG	YA	3292	1/1	0.98	0.19	38,38,38,38	0
57	MG	YA	3134	1/1	0.98	0.24	38,38,38,38	0
57	MG	YA	3185	1/1	0.98	0.04	38,38,38,38	0
57	MG	RA	3217	1/1	0.98	0.23	38,38,38,38	0
57	MG	YA	3088	1/1	0.98	0.09	42,42,42,42	0
57	MG	YA	3089	1/1	0.98	0.21	38,38,38,38	0
57	MG	RA	3076	1/1	0.98	0.04	38,38,38,38	0
57	MG	QA	1669	1/1	0.98	0.12	38,38,38,38	0
57	MG	QA	1658	1/1	0.98	0.04	38,38,38,38	0
57	MG	XA	1622	1/1	0.98	0.06	38,38,38,38	0
57	MG	XA	1623	1/1	0.98	0.10	91,91,91,91	0
57	MG	YA	3427	1/1	0.98	0.07	38,38,38,38	0
57	MG	XA	1659	1/1	0.98	0.04	38,38,38,38	0
57	MG	XA	1624	1/1	0.98	0.26	38,38,38,38	0
57	MG	XA	1625	1/1	0.98	0.05	38,38,38,38	0
57	MG	QA	1662	1/1	0.98	0.06	54,54,54,54	0
57	MG	RA	3110	1/1	0.98	0.03	38,38,38,38	0
57	MG	RA	3240	1/1	0.98	0.11	38,38,38,38	0
57	MG	RA	3123	1/1	0.98	0.09	38,38,38,38	0
57	MG	YA	3435	1/1	0.98	0.03	39,39,39,39	0
57	MG	YA	3151	1/1	0.98	0.13	81,81,81,81	0
57	MG	YA	3152	1/1	0.98	0.04	55,55,55,55	0
57	MG	RA	3224	1/1	0.98	0.21	38,38,38,38	0
57	MG	YA	3105	1/1	0.98	0.05	38,38,38,38	0
57	MG	YA	3256	1/1	0.98	0.25	38,38,38,38	0
57	MG	XA	1631	1/1	0.98	0.04	38,38,38,38	0
59	ZN	R4	101	1/1	0.98	0.22	88,88,88,88	0
57	MG	YA	3317	1/1	0.98	0.11	38,38,38,38	0
57	MG	YA	3258	1/1	0.98	0.23	38,38,38,38	0
57	MG	RA	3478	1/1	0.98	0.11	38,38,38,38	0
57	MG	RA	3056	1/1	0.98	0.03	43,43,43,43	0
57	MG	YA	3159	1/1	0.98	0.07	38,38,38,38	0
57	MG	XA	1634	1/1	0.98	0.05	43,43,43,43	0
57	MG	YA	3210	1/1	0.98	0.13	38,38,38,38	0
57	MG	YA	3110	1/1	0.98	0.04	38,38,38,38	0
57	MG	YA	3265	1/1	0.98	0.12	38,38,38,38	0
57	MG	RA	3480	1/1	0.98	0.04	38,38,38,38	0
57	MG	YA	3091	1/1	0.99	0.03	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3156	1/1	0.99	0.03	38,38,38,38	0
57	MG	QA	1653	1/1	0.99	0.03	58,58,58,58	0
57	MG	QA	1646	1/1	0.99	0.03	58,58,58,58	0
57	MG	YA	3124	1/1	0.99	0.04	38,38,38,38	0
57	MG	RA	3050	1/1	0.99	0.11	38,38,38,38	0
57	MG	YA	3081	1/1	0.99	0.10	38,38,38,38	0
57	MG	YA	3057	1/1	0.99	0.03	38,38,38,38	0
57	MG	YA	3097	1/1	0.99	0.06	38,38,38,38	0
57	MG	RA	3276	1/1	0.99	0.07	54,54,54,54	0
57	MG	RA	3189	1/1	0.99	0.10	38,38,38,38	0
57	MG	YA	3295	1/1	0.99	0.12	38,38,38,38	0
57	MG	RA	3472	1/1	0.99	0.19	38,38,38,38	0
57	MG	RA	3059	1/1	0.99	0.07	38,38,38,38	0
57	MG	RA	3423	1/1	0.99	0.04	38,38,38,38	0
57	MG	RA	3198	1/1	0.99	0.03	46,46,46,46	0
57	MG	YA	3135	1/1	0.99	0.06	38,38,38,38	0
57	MG	YA	3243	1/1	0.99	0.03	38,38,38,38	0
57	MG	RA	3160	1/1	0.99	0.03	38,38,38,38	0
57	MG	RA	3014	1/1	0.99	0.04	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.