



Full wwPDB EM Validation Report ⓘ

May 11, 2026 – 06:06 PM EDT

PDB ID : 9DOV / pdb_00009dov
EMDB ID : EMD-47093
Title : Hypopseudouridylated yeast 80S bound with Taura syndrome virus (TSV) internal ribosome entry site (IRES) and hygromycin B
Authors : Zhao, Y.; Li, H.
Deposited on : 2024-09-19
Resolution : 2.49 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

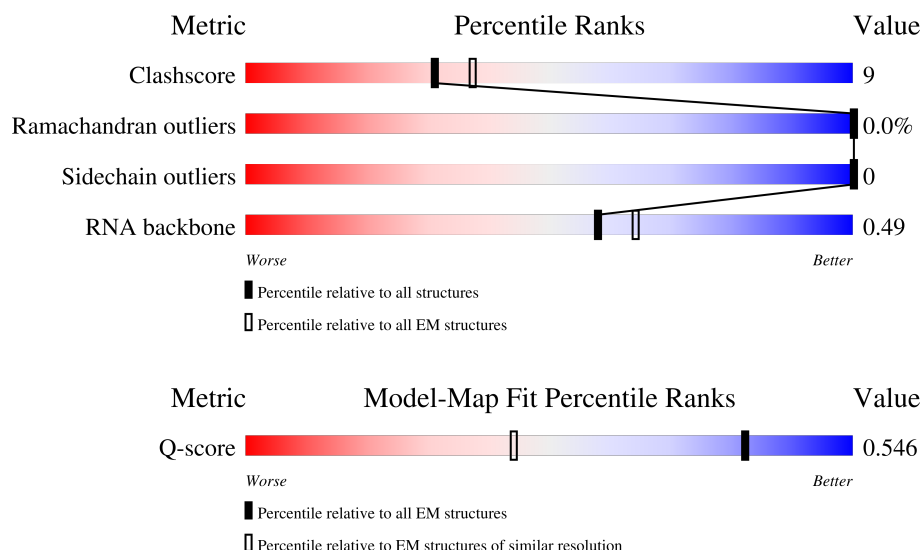
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.49 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	6237 (2.00 - 2.99)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	BA	252	
2	BB	255	
3	BC	254	

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Mol	Chain	Length	Quality of chain
4	BE	261	
5	BG	236	
6	BH	190	
7	BI	200	
8	BJ	197	
9	BL	156	
10	BN	151	
11	BO	137	
12	BV	87	
13	BW	130	
14	BX	145	
15	BY	135	
16	Ba	119	
17	Bb	82	
18	Be	63	
19	BD	240	
20	BF	225	
21	BK	105	
22	BP	142	
23	BQ	143	
24	BR	136	
25	BS	146	
26	BT	144	
27	BU	121	
28	BZ	108	

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Mol	Chain	Length	Quality of chain
29	Bc	67	
30	Bd	56	
31	Bg	319	
32	Bf	152	
33	BM	143	
34	B5	1798	
35	AA	254	
36	AB	387	
37	AC	362	
38	A1	3360	
39	A3	121	
40	A4	158	
41	AD	297	
42	AE	176	
43	AF	244	
44	AG	256	
45	AH	191	
46	AI	221	
47	AJ	174	
48	AL	199	
49	AM	138	
50	AN	204	
51	AO	199	
52	AP	184	
53	AQ	186	

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Mol	Chain	Length	Quality of chain
54	AR	189	
55	AS	178	
56	AT	160	
57	AU	121	
58	AV	137	
59	AW	155	
60	AX	142	
61	AY	127	
62	AZ	136	
63	Aa	149	
64	Ab	59	
65	Ac	105	
66	Ad	113	
67	Ae	130	
68	Af	107	
69	Ag	121	
70	Ah	120	
71	Ai	100	
72	Aj	88	
73	Ak	78	
74	Al	51	
75	Am	128	
76	An	25	
77	Ao	106	
78	Ap	92	

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Mol	Chain	Length	Quality of chain
79	E	217	<p>100% 67% 32%</p>
80	EC	202	<p>94% 21% 47% 28%</p>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	G7M	B5	1575	X	-	-	-

2 Entry composition

There are 83 unique types of molecules in this entry. The entry contains 205978 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	BA	206	Total	C	N	O	S	0	0
			1612	1034	285	291	2		

- Molecule 2 is a protein called Small ribosomal subunit protein eS1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BB	214	Total	C	N	O	S	0	0
			1709	1084	310	311	4		

- Molecule 3 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	BC	217	Total	C	N	O	S	0	0
			1635	1047	289	297	2		

- Molecule 4 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	BE	260	Total	C	N	O	S	0	0
			2068	1316	389	360	3		

- Molecule 5 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BG	226	Total	C	N	O	S	0	0
			1820	1142	350	325	3		

- Molecule 6 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	BH	184	Total	C	N	O	0	0
			1481	951	265	265		

- Molecule 7 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BI	188	Total	C	N	O	S	0	0
			1489	925	298	264	2		

- Molecule 8 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BJ	185	Total	C	N	O	S	0	0
			1494	943	289	261	1		

- Molecule 9 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BL	155	Total	C	N	O	S	0	0
			1244	798	235	208	3		

- Molecule 10 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	BN	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 11 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BO	127	Total	C	N	O	S	0	0
			941	578	186	174	3		

- Molecule 12 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BV	87	Total	C	N	O	S	0	0
			684	420	125	137	2		

- Molecule 13 is a protein called Small ribosomal subunit protein uS8A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BW	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 14 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BX	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 15 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BY	134	Total	C	N	O	S	0	0
			1073	676	208	189			

- Molecule 16 is a protein called Small ribosomal subunit protein eS26B.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Ba	97	Total	C	N	O	S	0	0
			769	475	160	129	5		

- Molecule 17 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Bb	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 18 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Be	60	Total	C	N	O	S	0	0
			475	299	98	77	1		

- Molecule 19 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	BD	223	Total	C	N	O	S	0	0
			1734	1101	313	314	6		

- Molecule 20 is a protein called Rps5p.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	BF	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		

- Molecule 21 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BK	96	Total	C	N	O	S	0	0
			817	529	133	153	2		

- Molecule 22 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BP	124	Total	C	N	O	S	0	0
			991	631	187	166	7		

- Molecule 23 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BQ	141	Total	C	N	O	S	0	0
			1105	708	203	194			

- Molecule 24 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BR	121	Total	C	N	O	S	0	0
			975	611	183	179	2		

- Molecule 25 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BS	145	Total	C	N	O	S	0	0
			1192	743	237	210	2		

- Molecule 26 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BT	141	Total	C	N	O	S	0	0
			1095	685	206	202	2		

- Molecule 27 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BU	107	Total	C	N	O	S	0	0
			855	539	156	159	1		

- Molecule 28 is a protein called Small ribosomal subunit protein eS25A.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	BZ	69	Total	C	N	O	0	0
			558	357	103	98		

- Molecule 29 is a protein called Small ribosomal subunit protein eS28A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Bc	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 30 is a protein called Small ribosomal subunit protein uS14A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Bd	53	Total	C	N	O	S	0	0
			443	275	92	72	4		

- Molecule 31 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Bg	312	Total	C	N	O	S	0	0
			2401	1522	410	461	8		

- Molecule 32 is a protein called RPS31 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Bf	57	Total	C	N	O	S	0	0
			454	288	86	77	3		

- Molecule 33 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BM	121	Total	C	N	O	S	0	0
			913	574	162	175	2		

- Molecule 34 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	B5	1782	Total	C	N	O	P	1	0
			38004	17005	6718	12499	1782		

- Molecule 35 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	AA	247	Total	C	N	O	S	0	0
			1878	1170	381	326	1		

- Molecule 36 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	AB	386	Total	C	N	O	S	0	0
			3080	1955	584	533	8		

- Molecule 37 is a protein called Large ribosomal subunit protein uL4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	AC	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 38 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	A1	3198	Total	C	N	O	P	0	0
			68445	30596	12331	22320	3198		

- Molecule 39 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	A3	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 40 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	A4	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 41 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AD	292	Total	C	N	O	S	0	0
			2341	1478	408	453	2		

- Molecule 42 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	AE	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 43 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	AF	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 44 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	AG	230	Total	C	N	O	S	0	0
			1798	1149	323	323	3		

- Molecule 45 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	AH	190	Total	C	N	O	S	0	0
			1510	957	273	276	4		

- Molecule 46 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	AI	205	Total	C	N	O	S	0	0
			1672	1063	316	288	5		

- Molecule 47 is a protein called Large ribosomal subunit protein uL5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	AJ	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 48 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AL	193	Total	C	N	O		0	0
			1543	962	315	266			

- Molecule 49 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AM	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 50 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	AN	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 51 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AO	197	Total	C	N	O	S	197	0
			1555	1003	289	262	1		

- Molecule 52 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	AP	175	Total	C	N	O	S	0	0
			1388	862	277	249			

- Molecule 53 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	AQ	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 54 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AR	188	Total	C	N	O	S	0	0
			1521	935	326	260			

- Molecule 55 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	AS	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 56 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AT	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 57 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	AU	100	Total	C	N	O	S	0	0
			796	516	131	149			

- Molecule 58 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AV	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 59 is a protein called Large ribosomal subunit protein eL24A.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AW	63	Total	C	N	O	S	0	0
			521	336	102	82	1		

- Molecule 60 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AX	121	Total	C	N	O	S	0	0
			968	623	170	173	2		

- Molecule 61 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AY	126	Total	C	N	O	S	0	0
			993	625	192	176			

- Molecule 62 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AZ	135	Total	C	N	O	S	0	0
			1092	710	202	180			

- Molecule 63 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Aa	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 64 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Ab	58	Total	C	N	O		0	0
			462	289	100	73			

- Molecule 65 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Ac	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 66 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Ad	109	Total	C	N	O	S	0	0
			890	565	168	156	1		

- Molecule 67 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Ae	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 68 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Af	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 69 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Ag	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 70 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Ah	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 71 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Ai	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 72 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Aj	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 73 is a protein called Large ribosomal subunit protein eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Ak	77	Total	C	N	O		0	0
			612	391	115	106			

- Molecule 74 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Al	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 75 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Am	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 76 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	An	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 77 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Ao	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 78 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Ap	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 79 is a protein called Large ribosomal subunit protein uL1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	E	217	Total	C	N	O	S	0	0
			1718	1097	299	312	10		

- Molecule 80 is a RNA chain called TSV IRES RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	EC	193	Total	C	N	O	P	0	0
			4112	1838	734	1347	193		

- Molecule 81 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

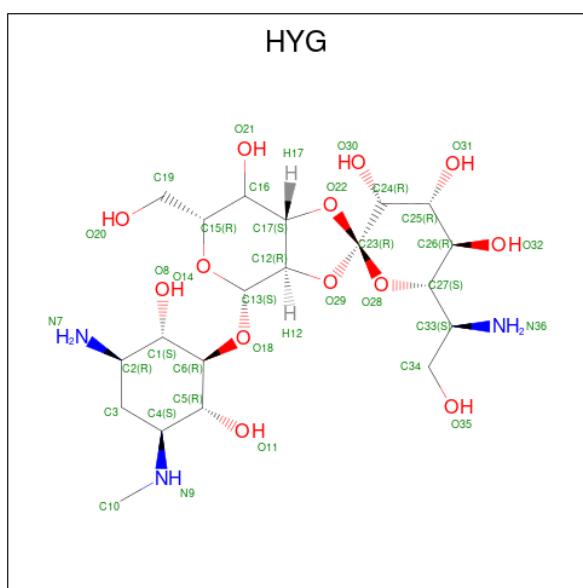
Mol	Chain	Residues	Atoms		AltConf
81	BE	1	Total	Mg	0
			1	1	
81	BN	1	Total	Mg	0
			1	1	
81	Ba	1	Total	Mg	0
			1	1	
81	B5	61	Total	Mg	0
			61	61	
81	AA	1	Total	Mg	0
			1	1	
81	AB	2	Total	Mg	0
			2	2	
81	A1	177	Total	Mg	0
			177	177	
81	A3	2	Total	Mg	0
			2	2	
81	A4	6	Total	Mg	0
			6	6	

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Mol	Chain	Residues	Atoms		AltConf
81	AI	1	Total	Mg	0
			1	1	
81	AN	1	Total	Mg	0
			1	1	
81	AP	1	Total	Mg	0
			1	1	
81	Ae	1	Total	Mg	0
			1	1	
81	Af	1	Total	Mg	0
			1	1	

- Molecule 82 is HYGROMYCIN B (CCD ID: HYG) (formula: $C_{20}H_{37}N_3O_{13}$).



Mol	Chain	Residues	Atoms				AltConf
82	B5	1	Total	C	N	O	0
			36	20	3	13	

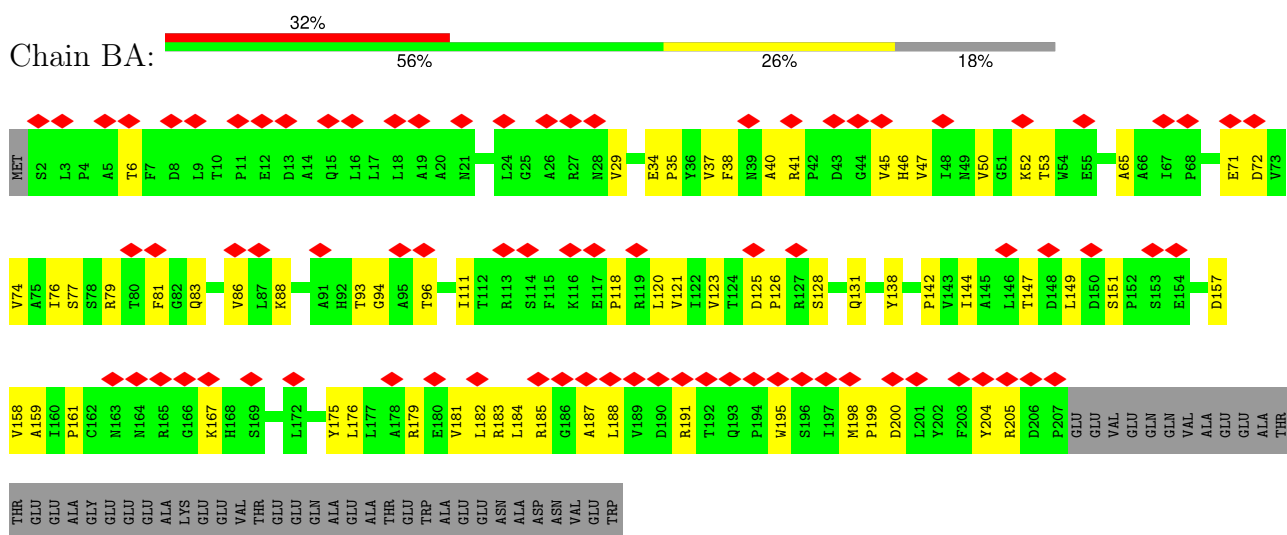
- Molecule 83 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
83	Ao	1	Total	Zn	0
			1	1	

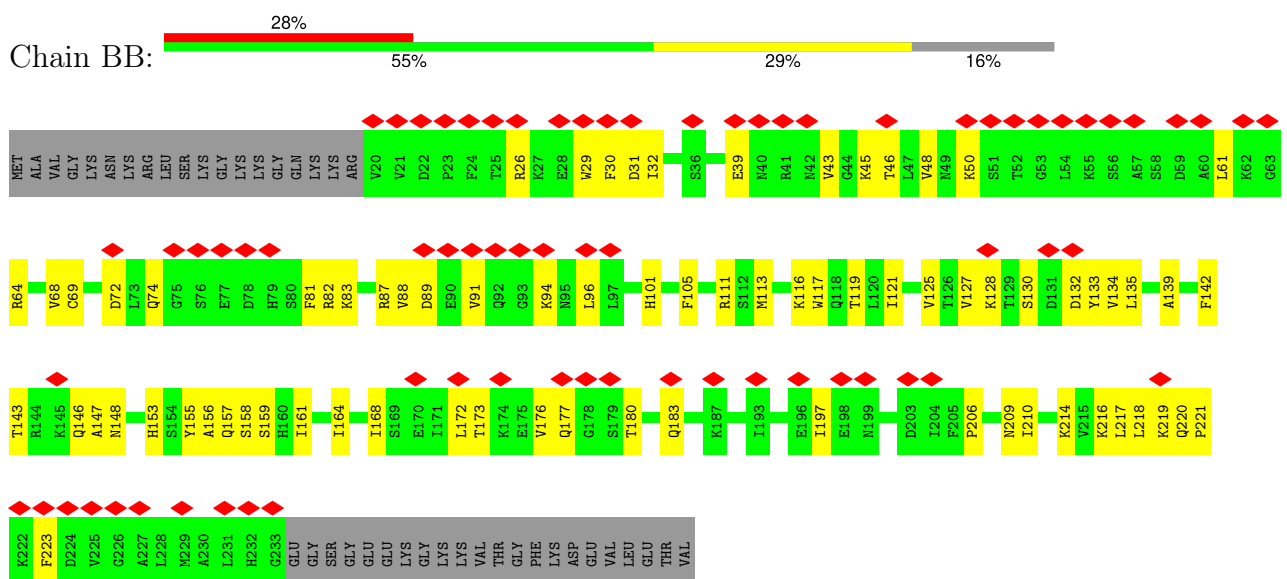
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

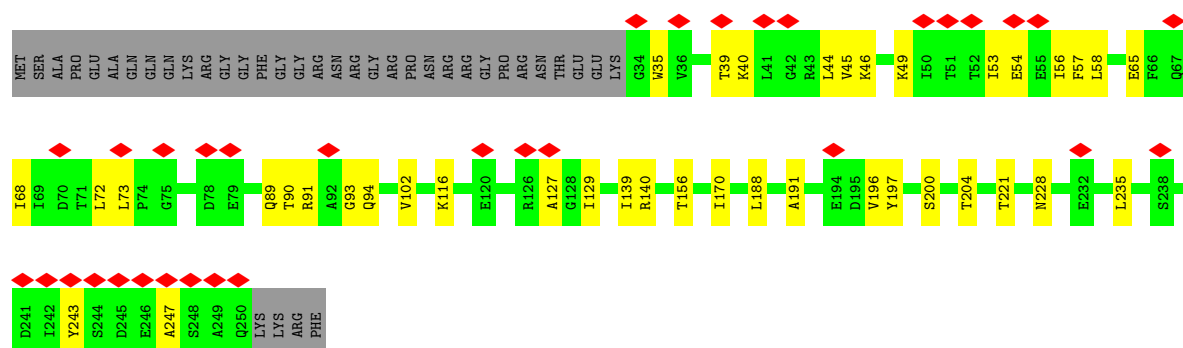
• Molecule 1: 40S ribosomal protein S0-A



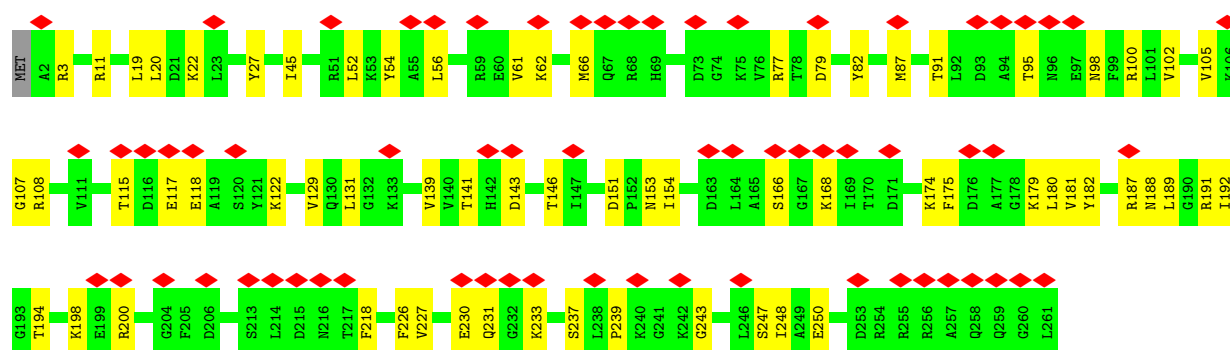
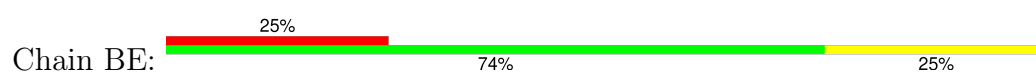
• Molecule 2: Small ribosomal subunit protein eS1A



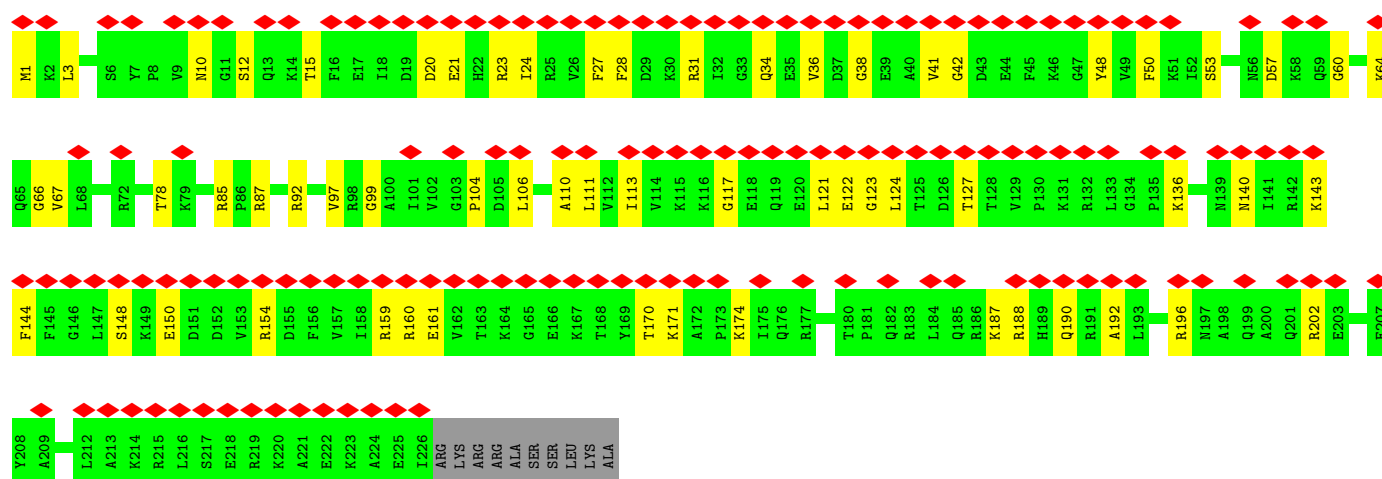
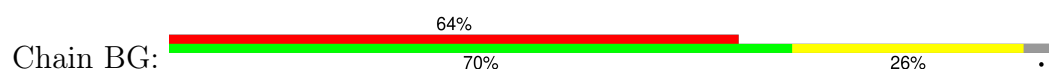
• Molecule 3: Small ribosomal subunit protein uS5



• Molecule 4: 40S ribosomal protein S4-A

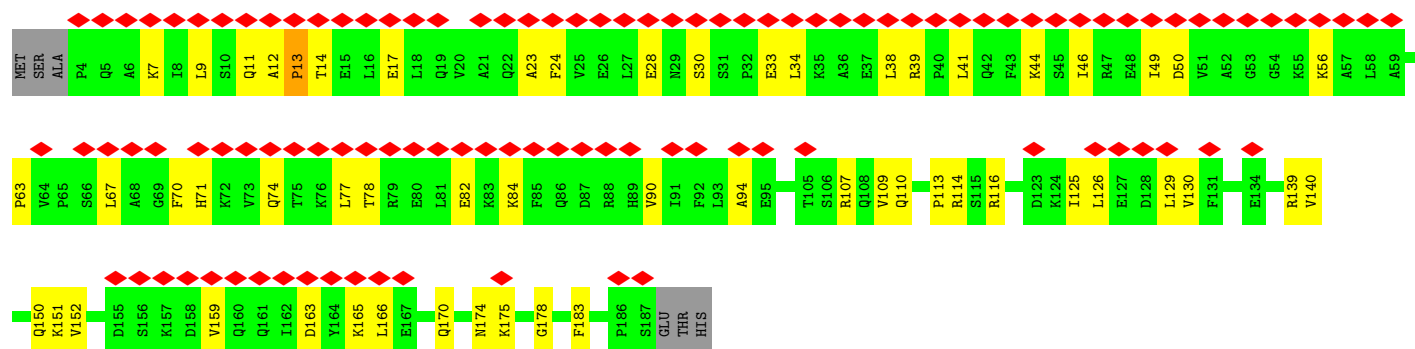


• Molecule 5: 40S ribosomal protein S6-A

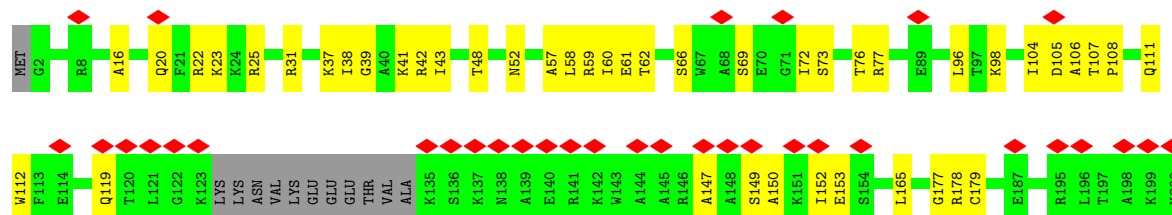


• Molecule 6: 40S ribosomal protein S7-A

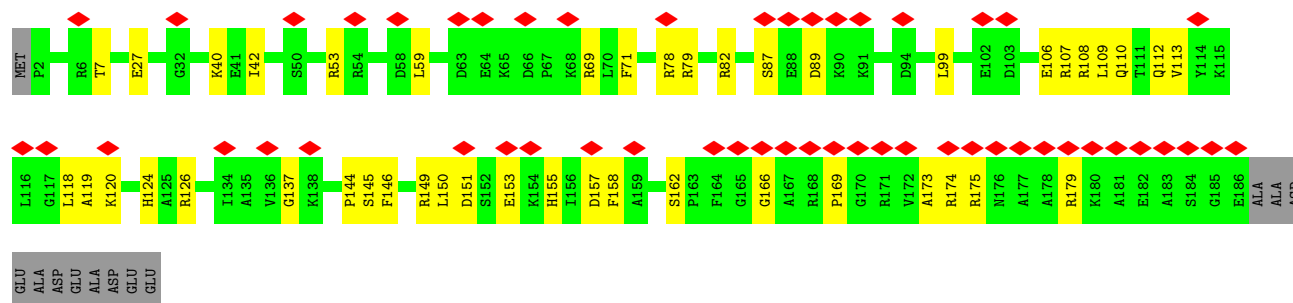
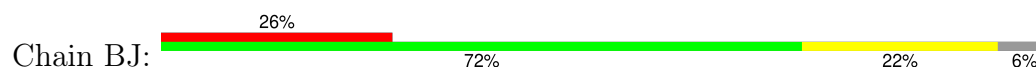




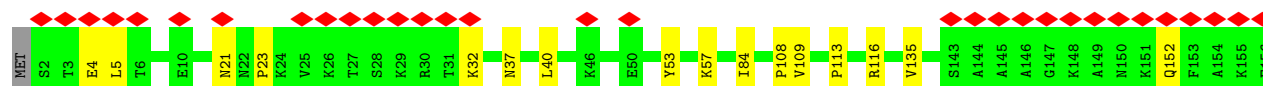
• Molecule 7: 40S ribosomal protein S8-A



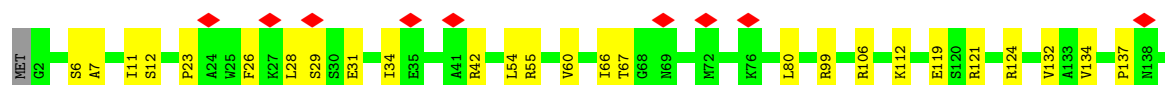
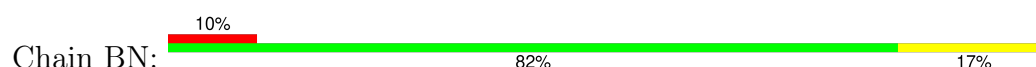
• Molecule 8: 40S ribosomal protein S9-A

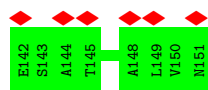


• Molecule 9: 40S ribosomal protein S11-A

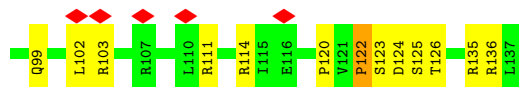
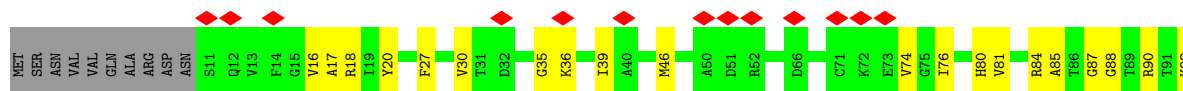


• Molecule 10: 40S ribosomal protein S13

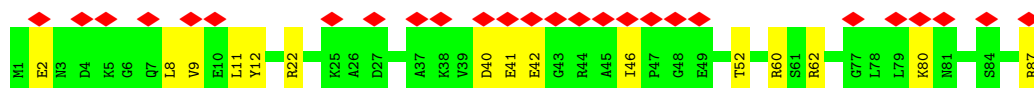
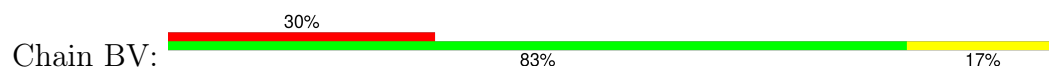




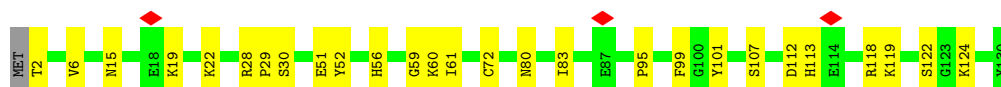
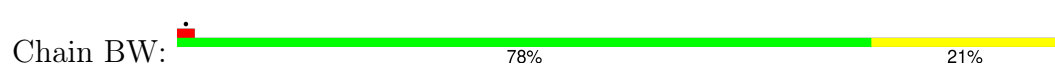
- Molecule 11: 40S ribosomal protein S14-A



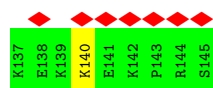
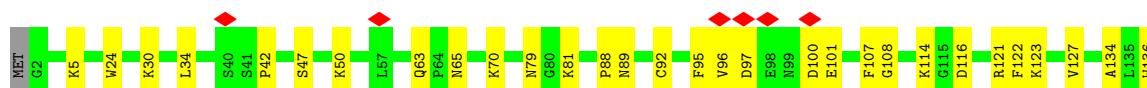
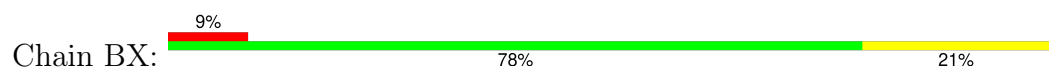
- Molecule 12: 40S ribosomal protein S21-A



- Molecule 13: Small ribosomal subunit protein uS8A

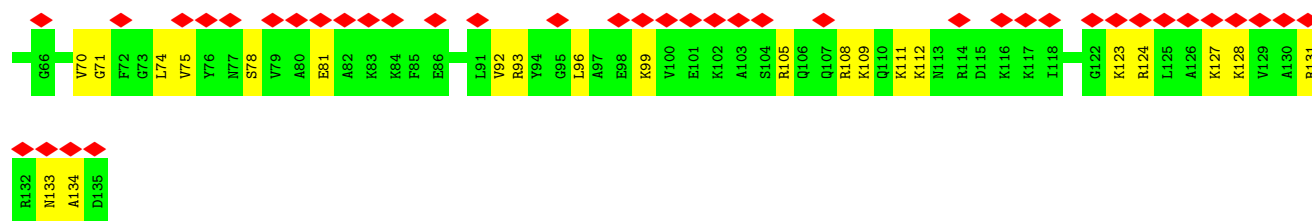


- Molecule 14: 40S ribosomal protein S23-A

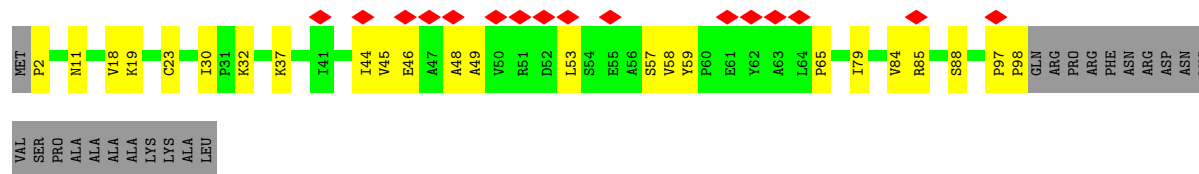


- Molecule 15: 40S ribosomal protein S24-A

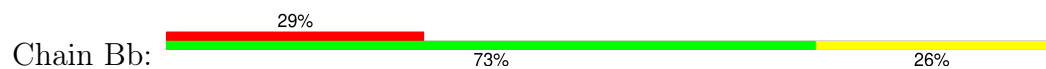




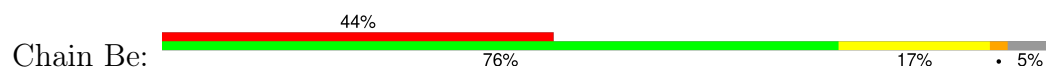
- Molecule 16: Small ribosomal subunit protein eS26B



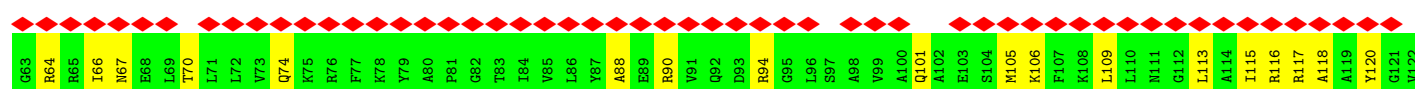
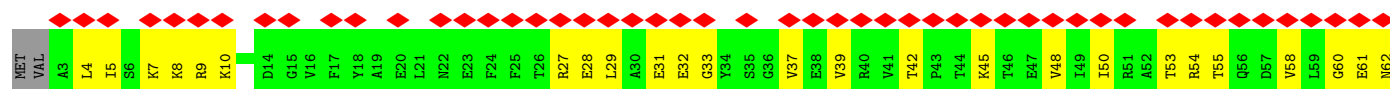
- Molecule 17: 40S ribosomal protein S27-A



- Molecule 18: 40S ribosomal protein S30-A

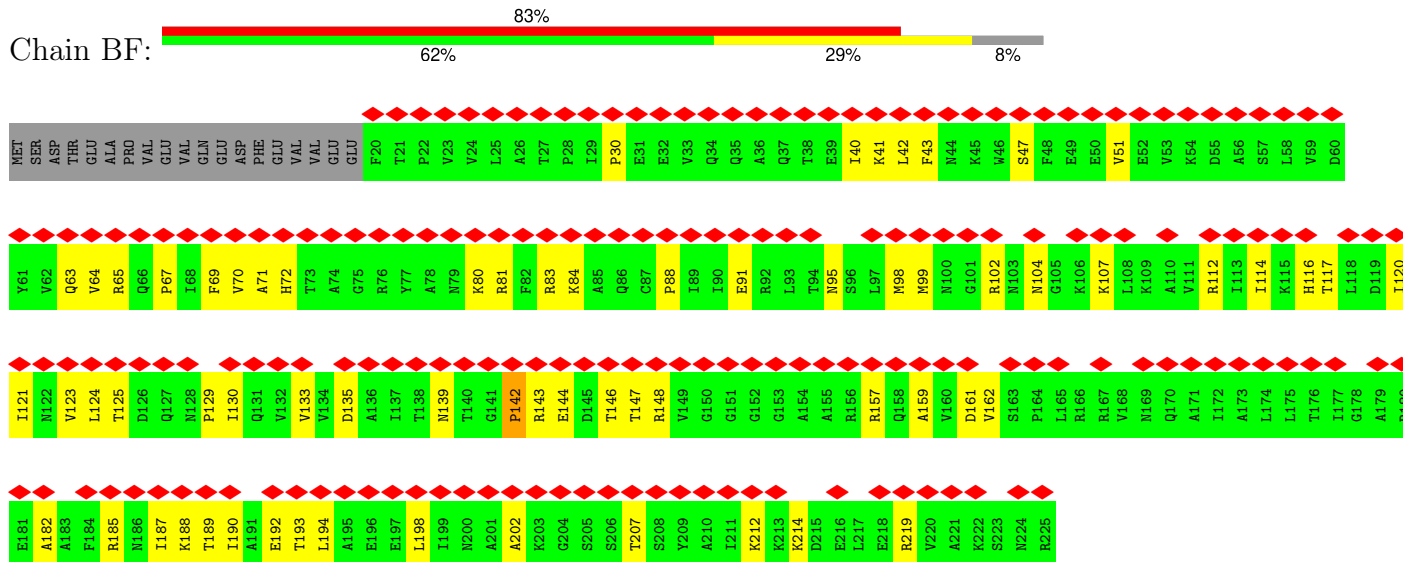


- Molecule 19: Small ribosomal subunit protein uS3



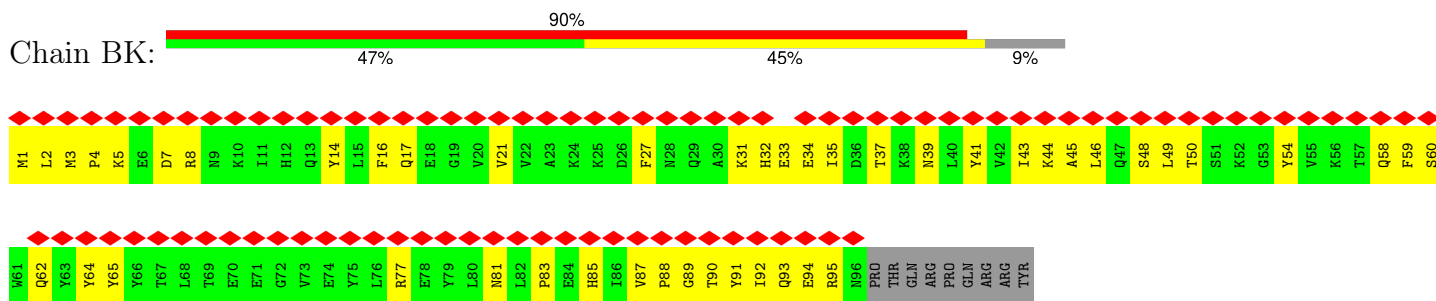
- Molecule 20: Rps5p

Chain BF:



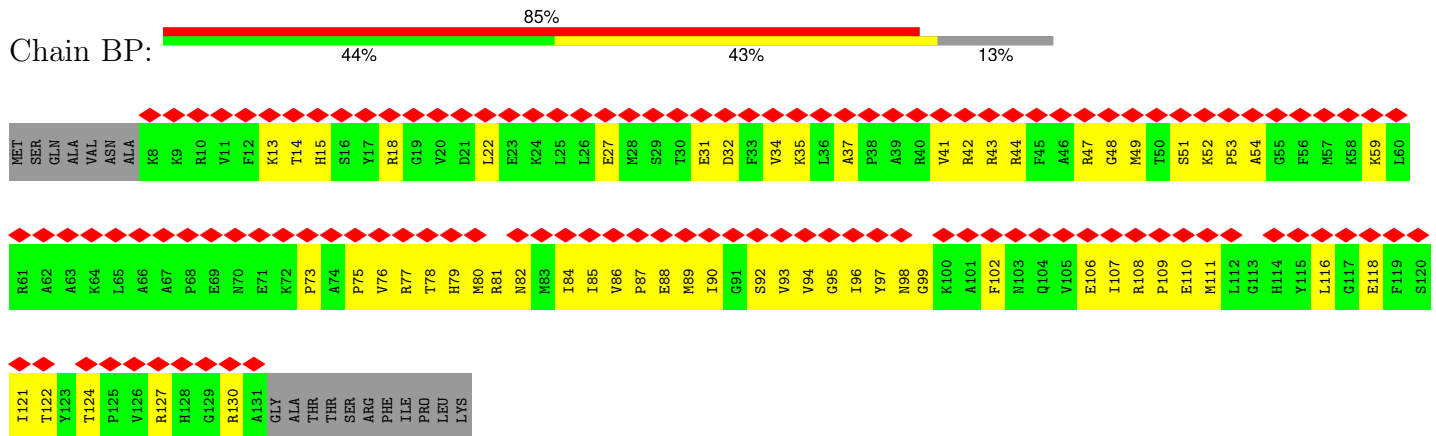
- Molecule 21: 40S ribosomal protein S10-A

Chain BK:



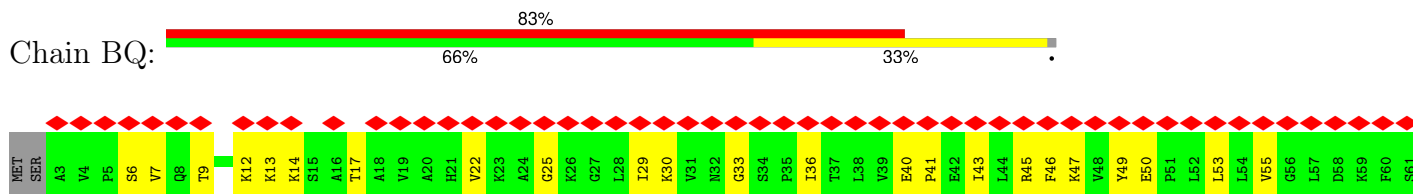
- Molecule 22: Small ribosomal subunit protein uS19

Chain BP:



- Molecule 23: 40S ribosomal protein S16-A

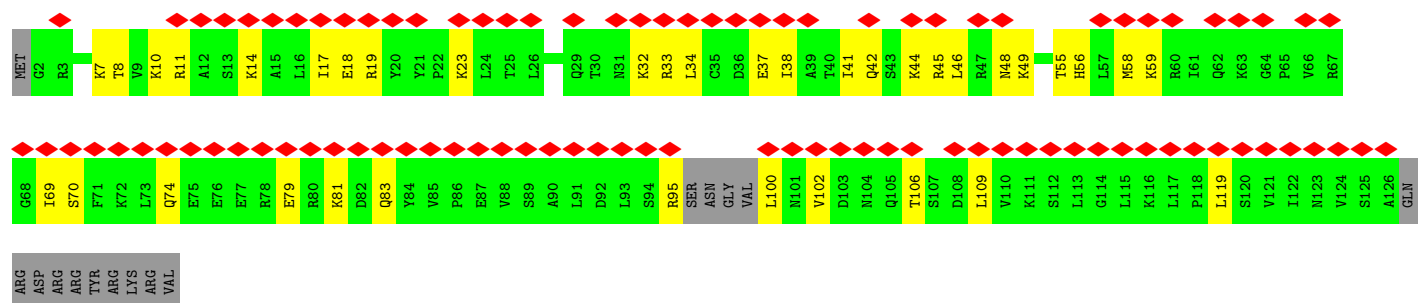
Chain BQ:





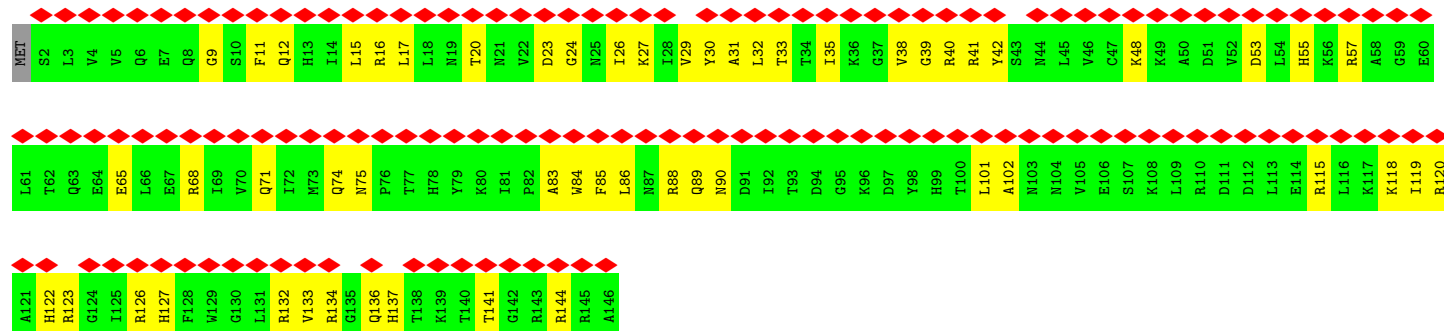
• Molecule 24: 40S ribosomal protein S17-A

Chain BR:



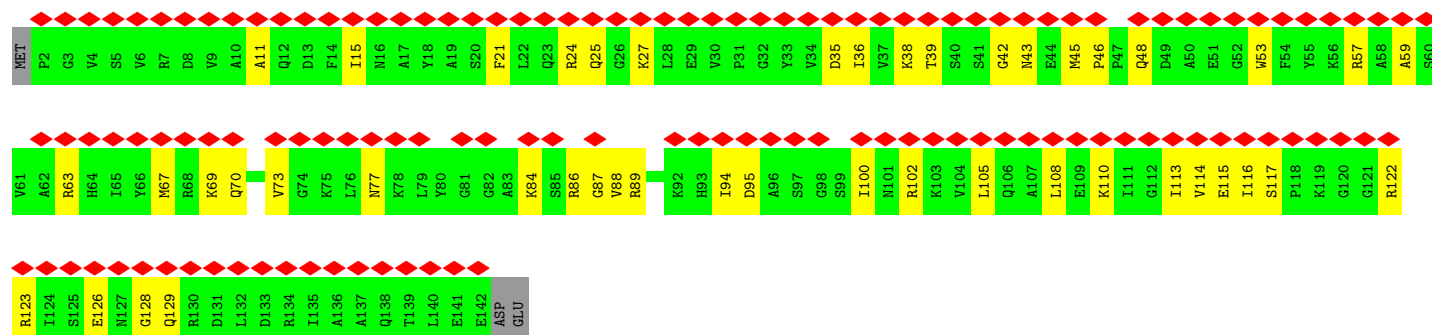
• Molecule 25: 40S ribosomal protein S18-A

Chain BS:



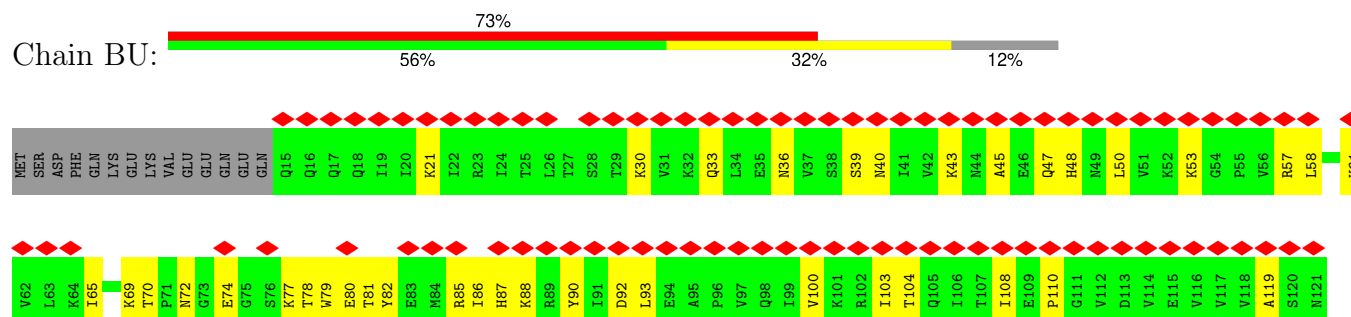
• Molecule 26: 40S ribosomal protein S19-A

Chain BT:



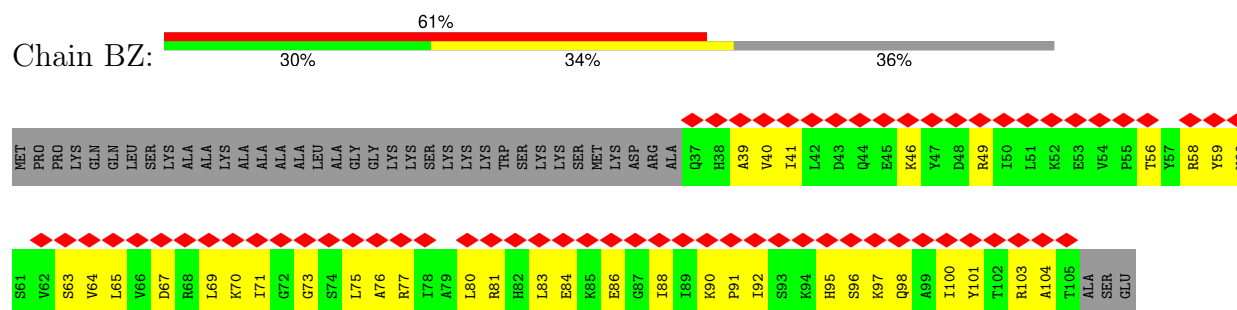
- Molecule 27: Small ribosomal subunit protein uS10

Chain BU:



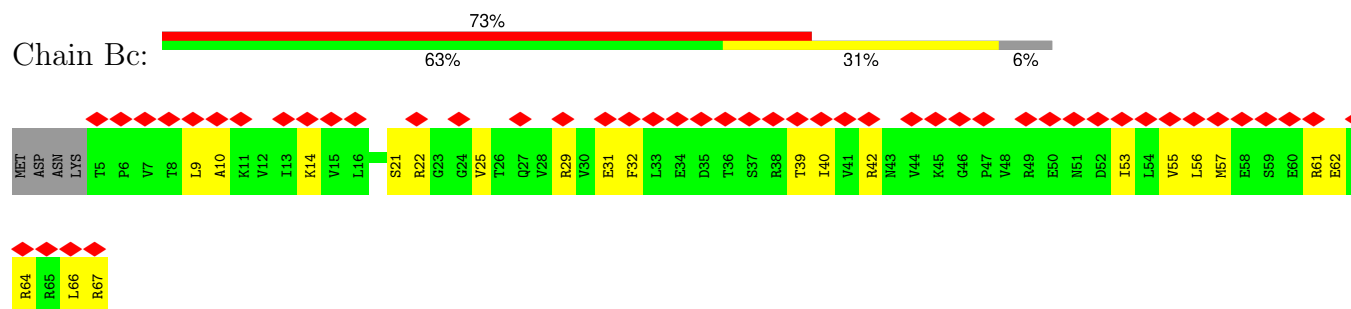
- Molecule 28: Small ribosomal subunit protein eS25A

Chain BZ:



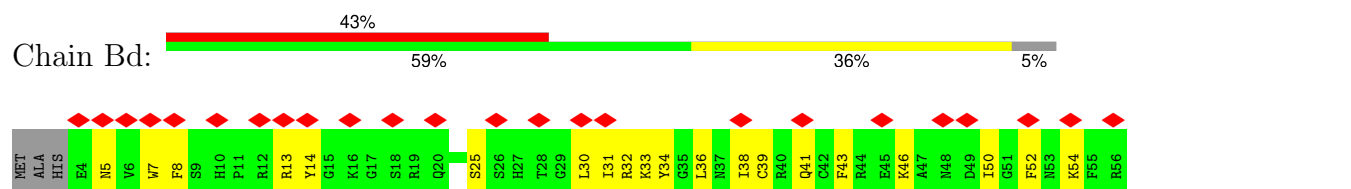
- Molecule 29: Small ribosomal subunit protein eS28A

Chain Bc:



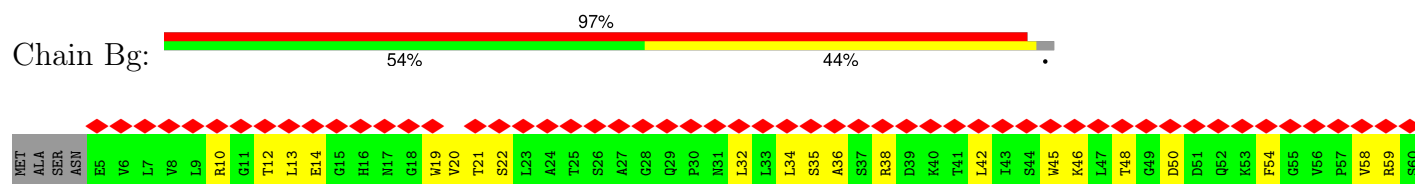
- Molecule 30: Small ribosomal subunit protein uS14A

Chain Bd:



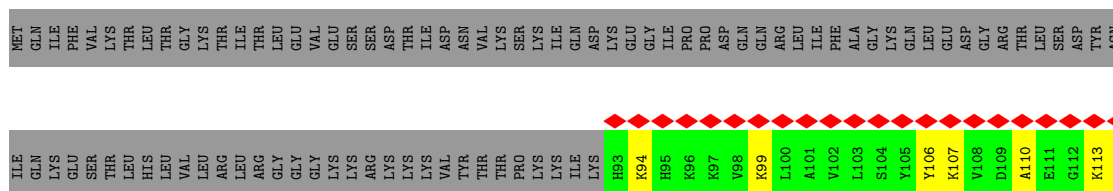
- Molecule 31: Guanine nucleotide-binding protein subunit beta-like protein

Chain Bg:

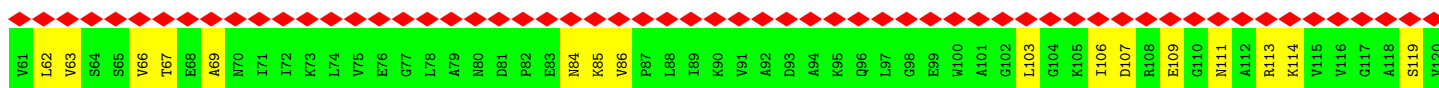
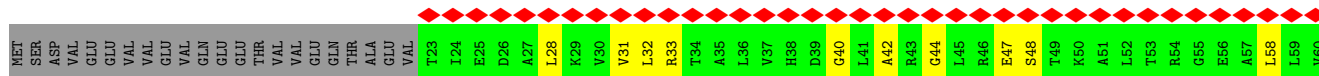




• Molecule 32: RPS31 isoform 1

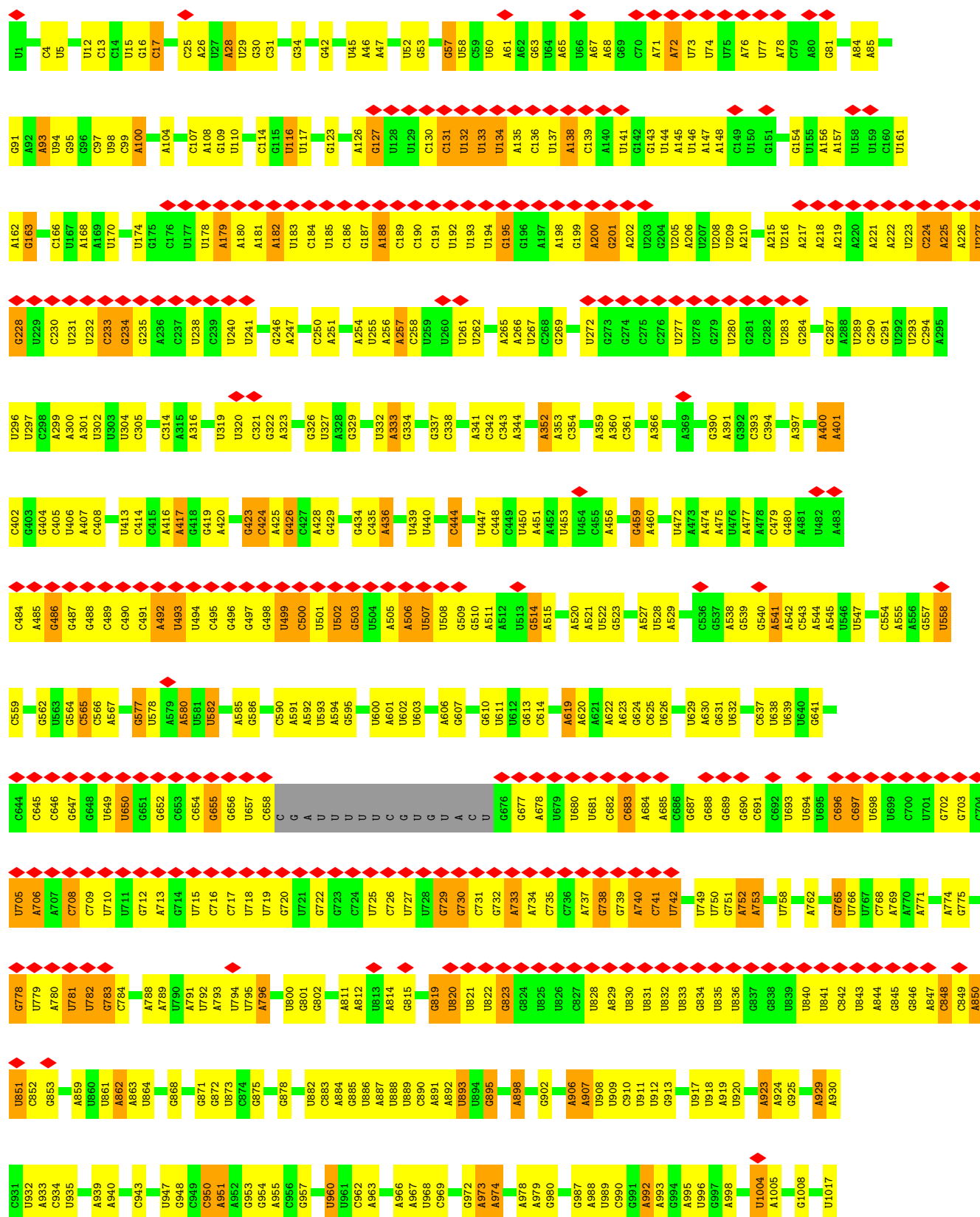


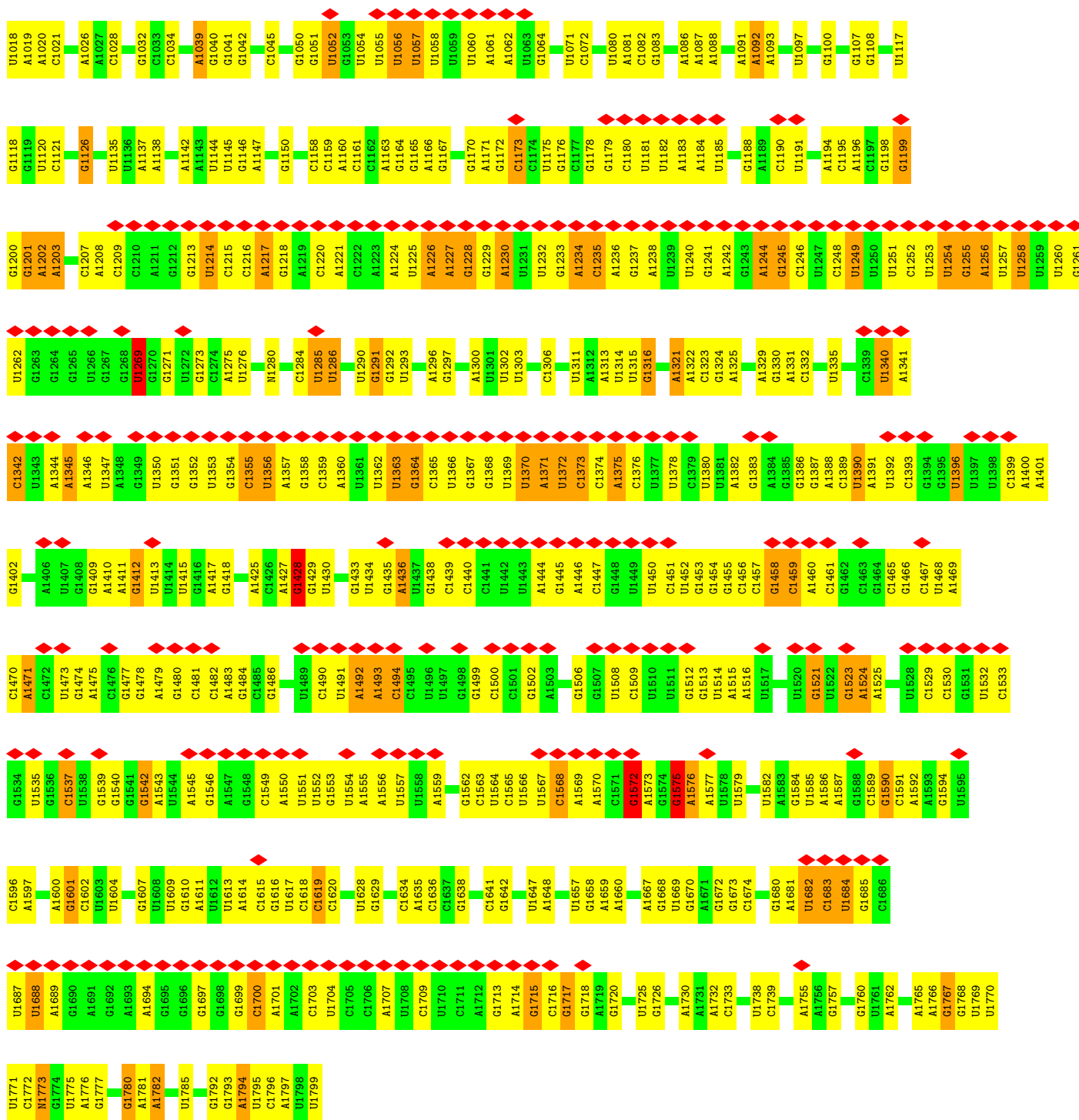
• Molecule 33: Small ribosomal subunit protein eS12



• Molecule 34: 18S rRNA

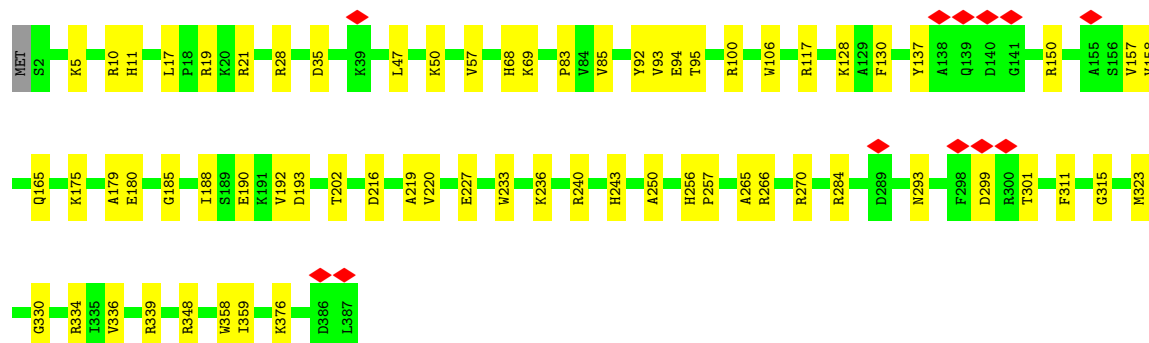
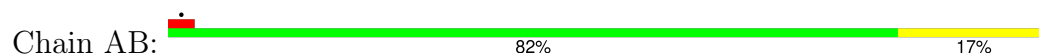




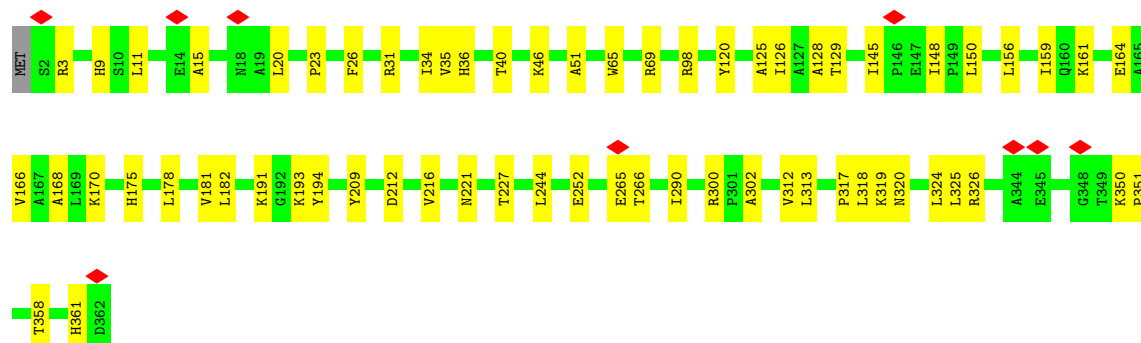
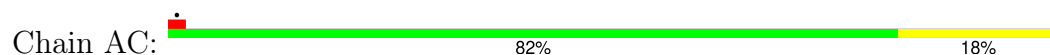




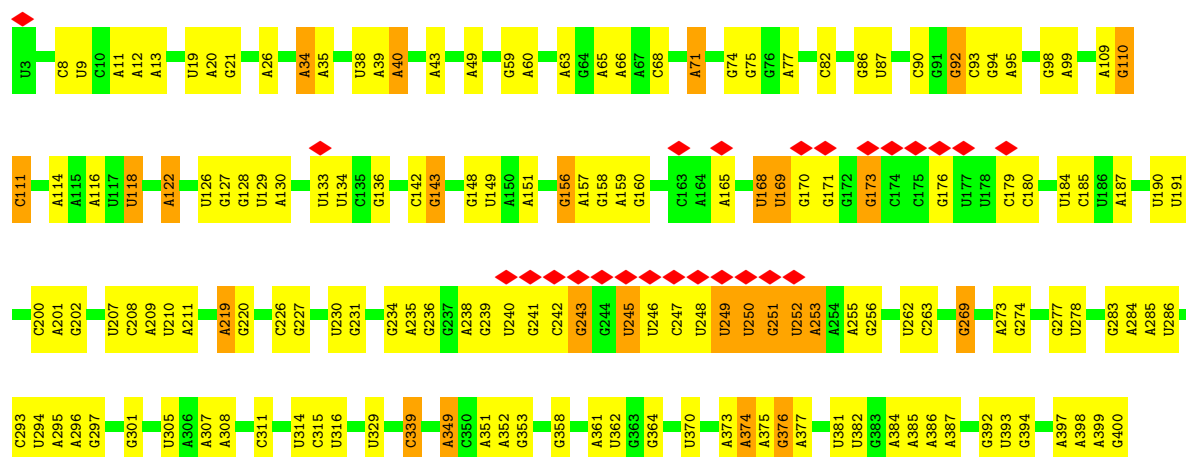
- Molecule 36: 60S ribosomal protein L3

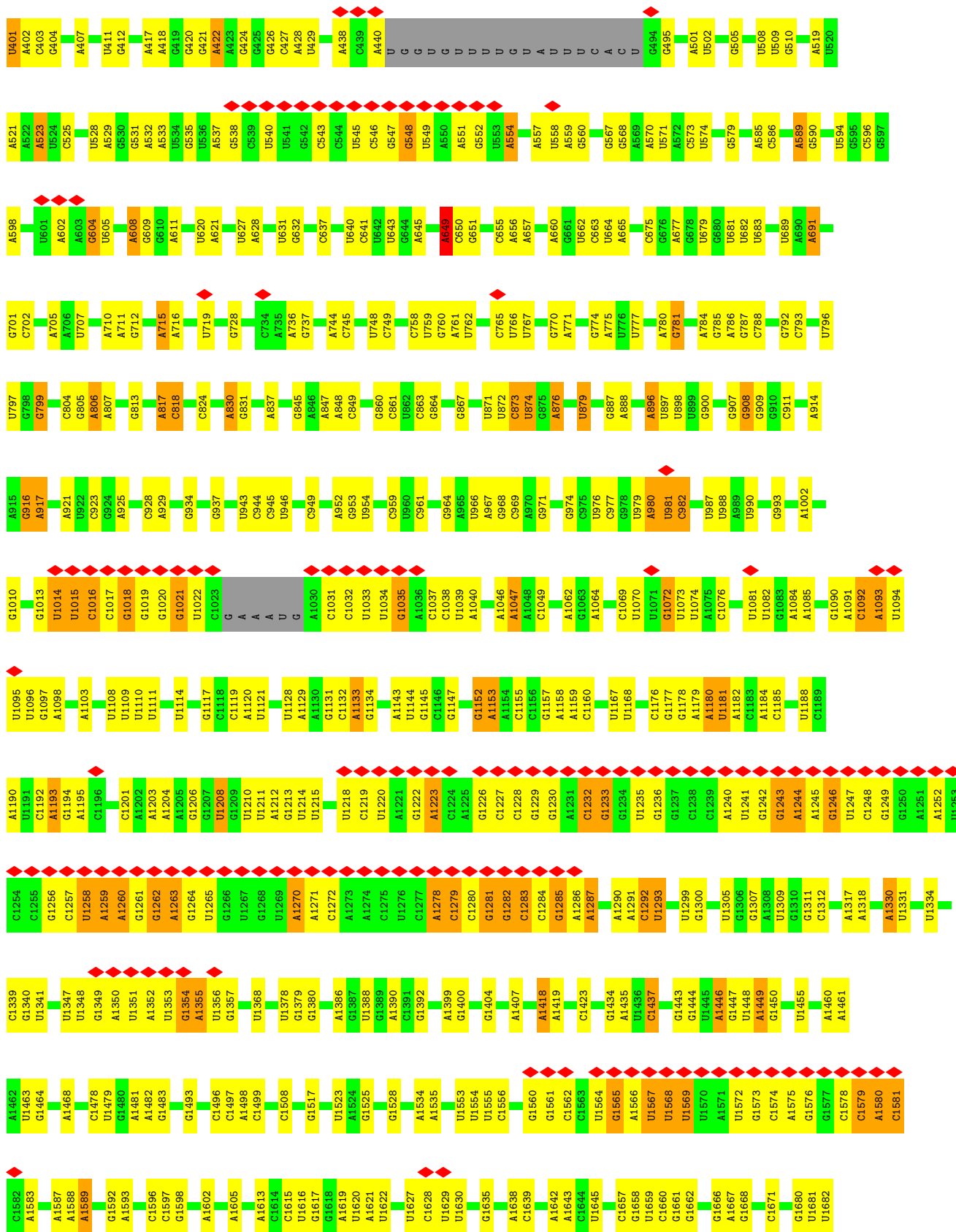


- Molecule 37: Large ribosomal subunit protein uL4A

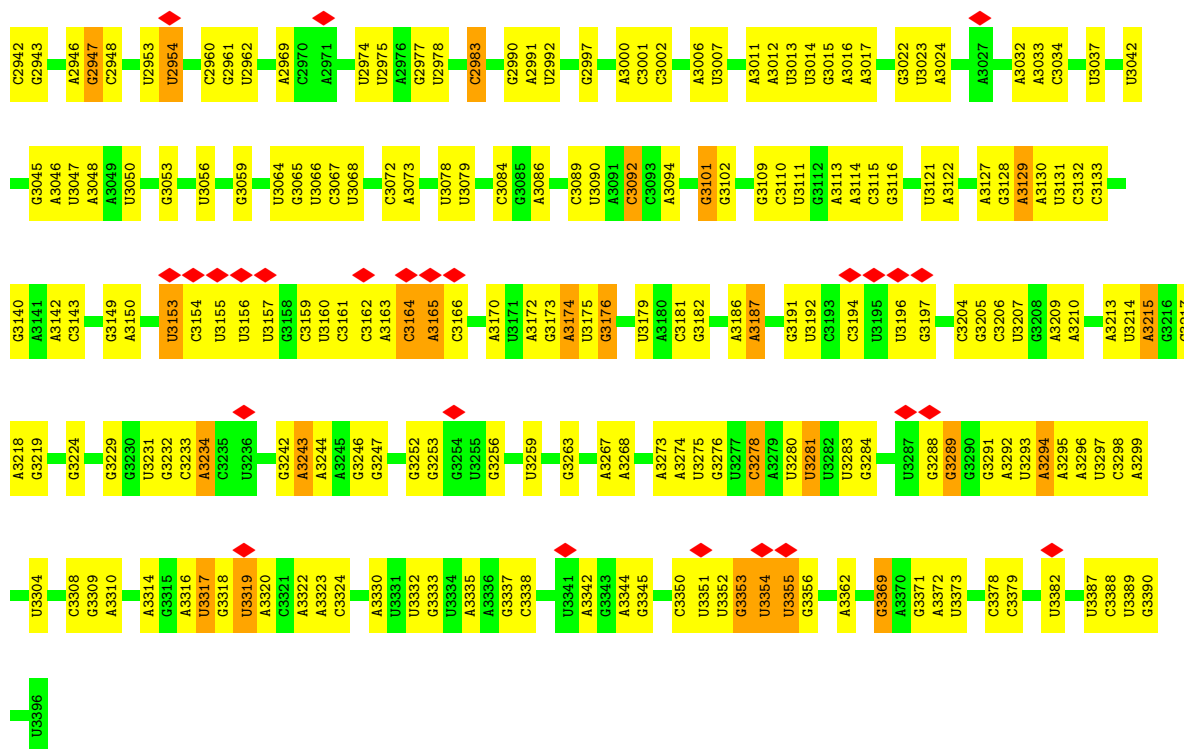


- Molecule 38: 25S rRNA

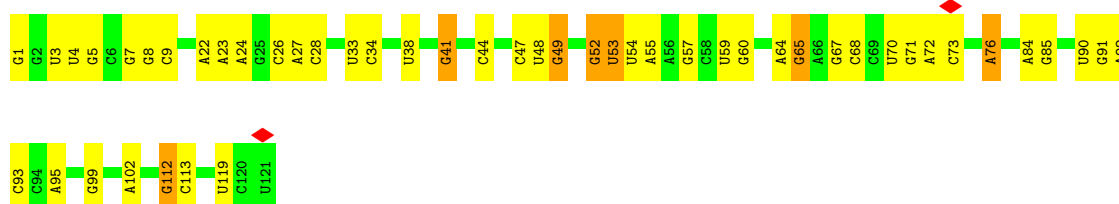




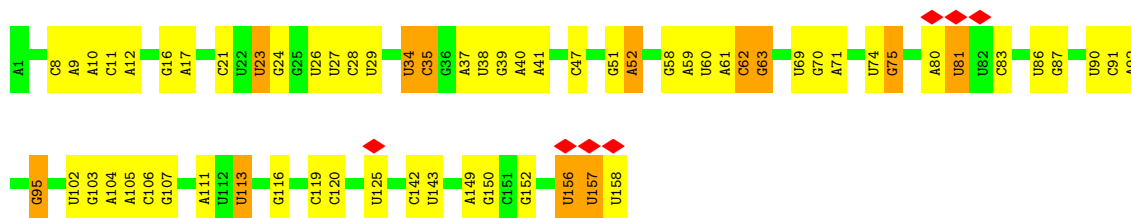
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A2748	G2749	U2750	G2751	U2752	G2753	U2757	U2763	A2762	A2763	U2767	U2768	A2769	C2772	C2773	G2777	G2778	A2779	A2780	U2781	U2782	G2791	A2792	G2793	G2796	C2797	C2798	A2799	G2800	A2801	A2802	A2803	C2810	A2811	C2812	G2813	G2814	G2815	G2816	A2817	U2818	A2819	G2824	U2829	G2830	U2835	C2836	U2842	U2843								
C2545	C2546	A2547	C2548	G2549	C2552	U2553	A2554	A2557	C2560	A2561	A2562	C2566	C2567	C2568	A2569	U2570	U2571	C2572	G2573	G2585	U2588	U2592	A2593	A2594	A2595	G2606	G2607	G2608	U2611	U2612	U2613	G2614	G2615	G2616	G2619	A2626	U2629	C2630	U2631	G2632	U2633	U2634	A2637	A2640	U2641											
A2642	G2651	U2652	U2655	A2656	A2657	G2660	G2672	A2673	A2674	C2675	A2676	G2677	A2678	A2679	A2680	U2681	C2682	U2683	C2684	C2685	U2688	A2689	A2690	A2691	A2696	U2697	G2698	A2703	A2704	C2709	C2710	C2711	G2714	U2719	C2720	U2723	U2724	U2728	U2729	A2736	C2737	U2744	A2745	A2746	A2747											
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A2402	G2403	A2404	C2405	C2406	C2407	U2408	U2411	C2415	U2416	U2417	G2418	A2419	C2420	U2421	U2426	U2427	U2428	A2438	A2439	G2440	A2441	G2442	A2443	C2444	A2445	U2446	A2447	G2448	A2449	G2450	G2451	G2452	U2453	G2454	U2455	A2456	G2457	A2458	A2459	U2460	A2461	A2462	G2463	U2464	G2465	G2466	G2467	A2468	G2469	C2470	U2471	U2472	C2473	G2474		
G2475	C2476	G2477	C2478	C2479	A2480	G2481	U2482	G2483	A2484	A2485	A2486	U2487	C2488	C2489	C2490	A2491	C2492	U2493	A2494	C2495	C2496	U2497	U2498	U2499	A2500	U2501	A2502	G2503	U2504	U2505	U2506	C2507	U2508	U2509	C2512	U2513	U2514	A2515	A2520	U2521	G2522	A2523	G2524	G2525	C2526	G2527	A2535	A2536	U2537	U2538	C2539	A2540	U2541	U2542	U2543	U2544
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G2206	A2207	C2208	A2209	G2210	A2213	A2214	A2215	G2216	A2217	G2218	A2219	A2220	A2223	A2224	U2225	A2228	A2229	C2230	C2231	A2232	A2233	U2241	A2242	G2249	U2253	A2256	C2257	U2258	A2259	U2260	A2262	U2266	C2267	U2268	U2269	A2270	A2271	G2272	G2273	C2278	A2279	A2280	A2281	U2282	G2288	A2291	U2292									
A2106	A2107	C2108	U2112	A2113	C2114	G2115	A2116	A2117	G2122	A2131	U2140	A2142	A2143	A2144	A2145	U2148	A2149	G2150	C2151	A2152	U2153	C2156	G2157	A2158	U2159	G2160	A2161	U2162	C2163	G2169	U2176	C2177	G2180	C2181	G2185	A2188	U2189	C2192	C2197	G2201	C2202	U2203	C2204	U2205												
C	C	U	U	G	U	U	U	U	C	A	G	G	C	U	C	G	A	G	G	U	U	U	G	U	U	A	G	A	C	U	C	U	U	U	U	U	U	U	A	A2093	C2094	G2095	A2096	C												
A	G	C	G	G	G	C	G	C	G	U	U	G	A	C	U	G	C	U	U	G	U	C	C	C	U	U	U	U	C	C	U	G	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C					
U1886	U1887	C1791	C1792	U1899	A1797	A1798	A1799	A1800	A1801	C1802	C1805	C1806	U1807	G1808	A1809	A1810	G1811	A1812	A1813	A1814	U1815	A1816	U1817	U1818	U1819	U1820	U1821	G1830	U1831	C1832	G1833	U1834	A1842	C1846	C1849	A1850	G1851	C1856	C1857	G1863	A1864	A1865	C1866	G1875	G1876	A1879	U1880	U1888	U1890							



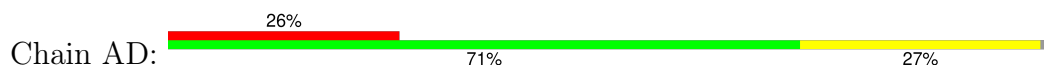
• Molecule 39: 5S rRNA

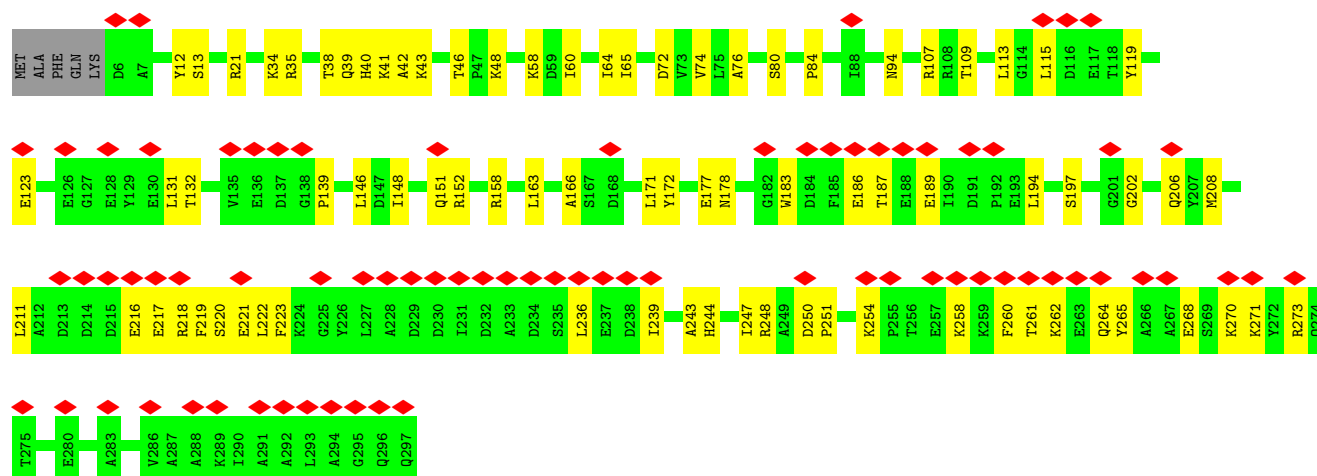


• Molecule 40: 5.8S rRNA

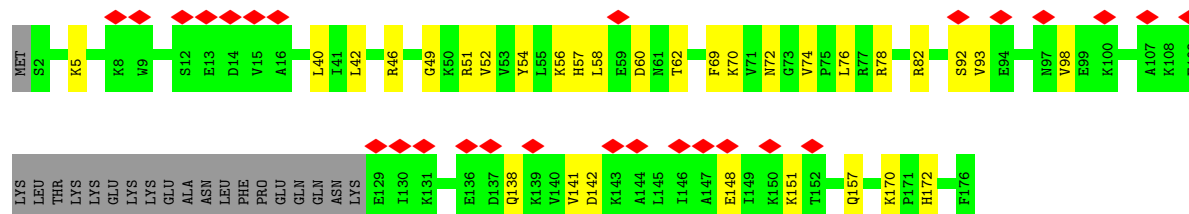
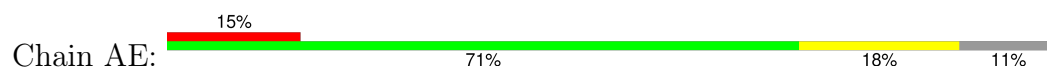


• Molecule 41: Large ribosomal subunit protein uL18

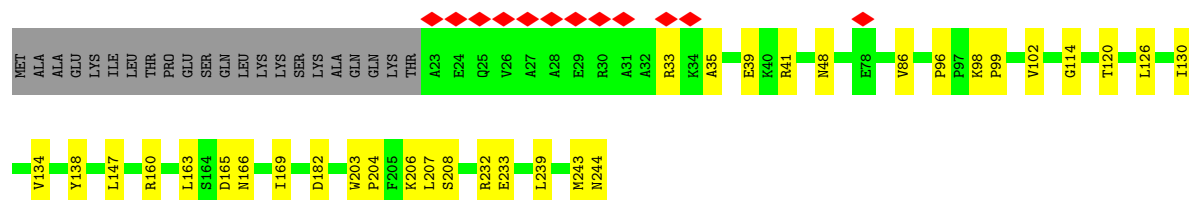
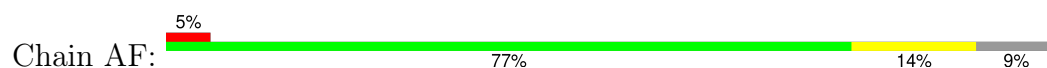




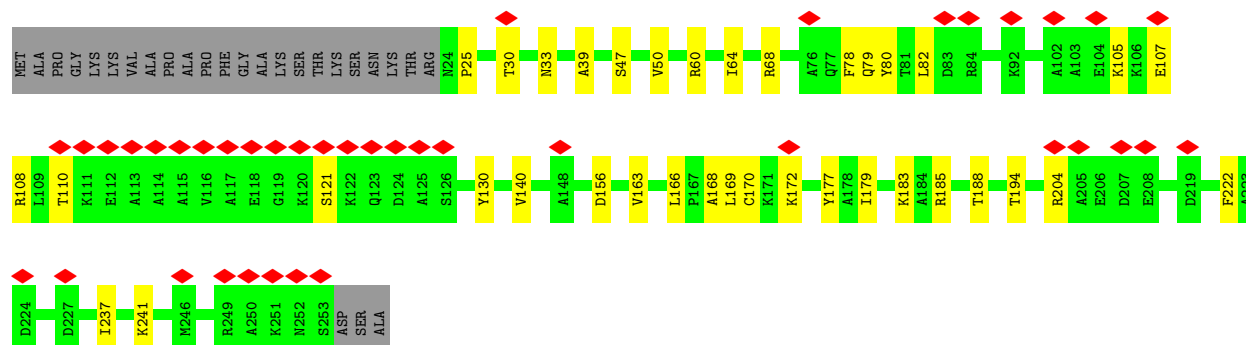
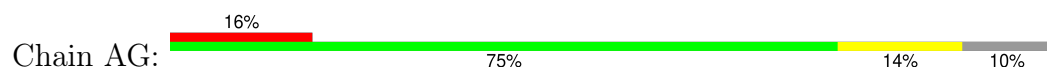
- Molecule 42: 60S ribosomal protein L6-A



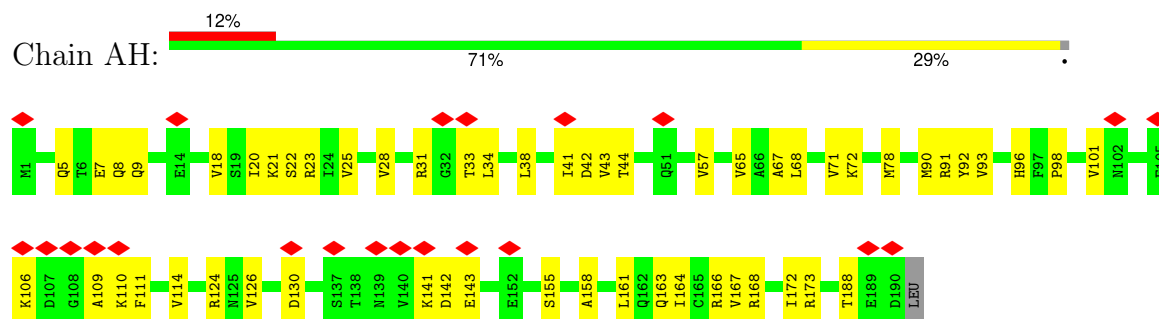
- Molecule 43: 60S ribosomal protein L7-A



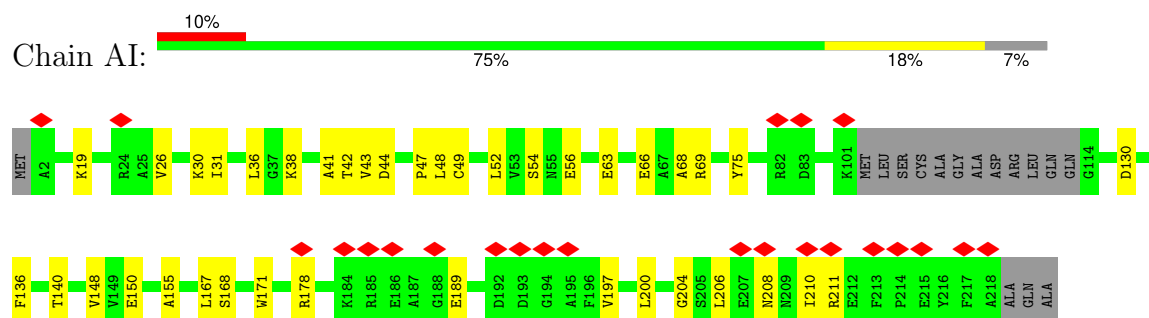
- Molecule 44: 60S ribosomal protein L8-A



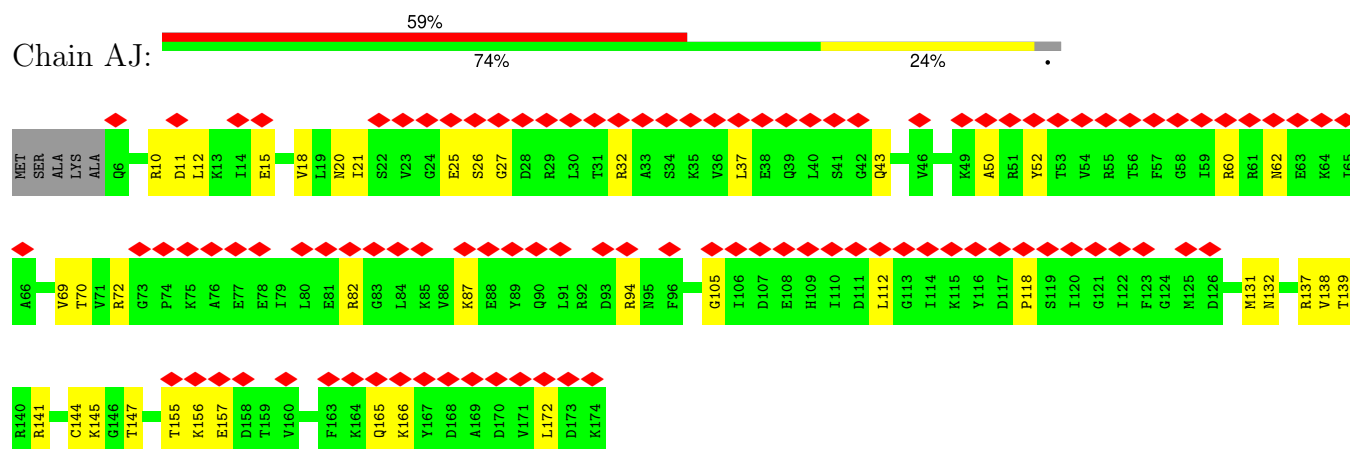
- Molecule 45: 60S ribosomal protein L9-A



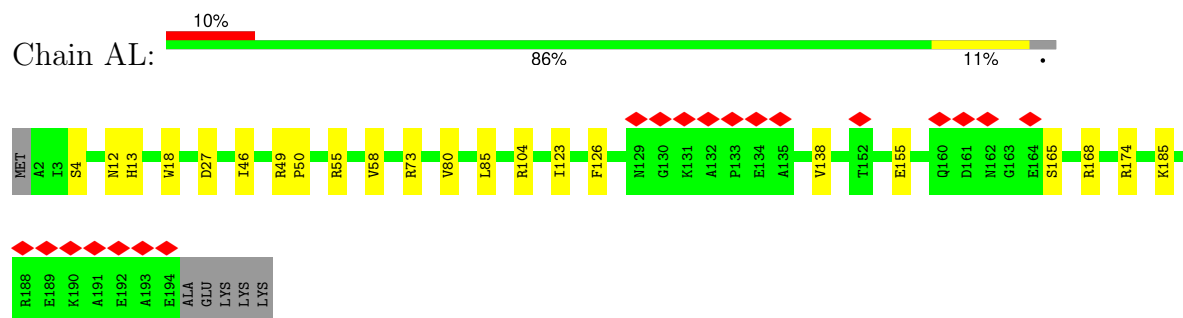
- Molecule 46: Large ribosomal subunit protein uL16



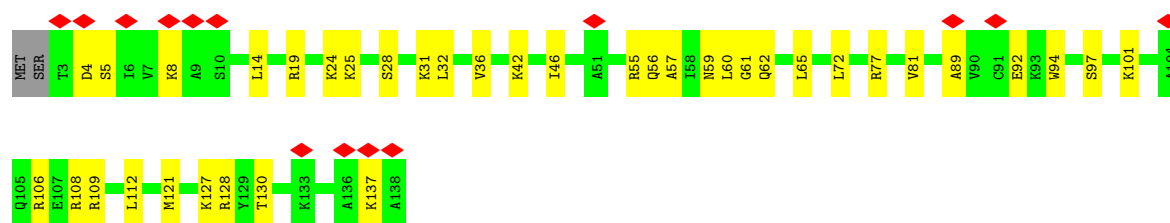
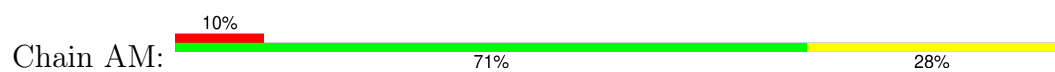
- Molecule 47: Large ribosomal subunit protein uL5A



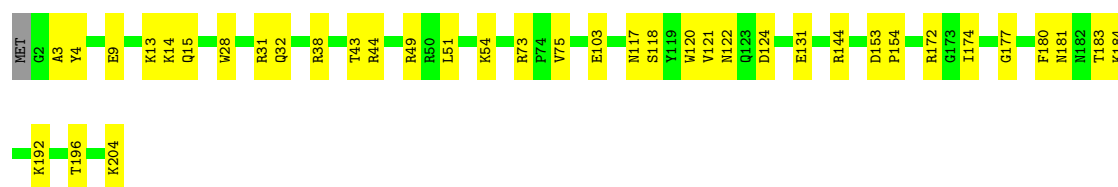
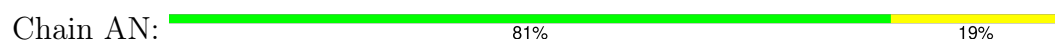
- Molecule 48: 60S ribosomal protein L13-A



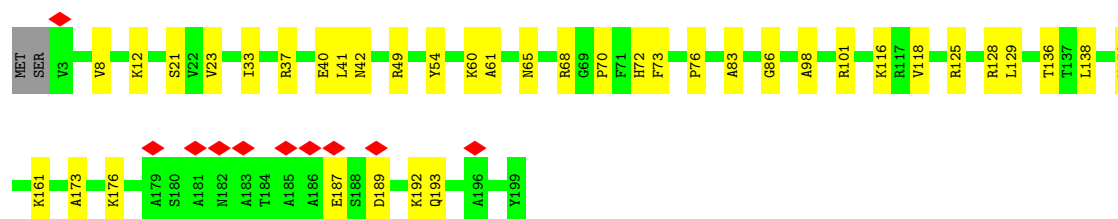
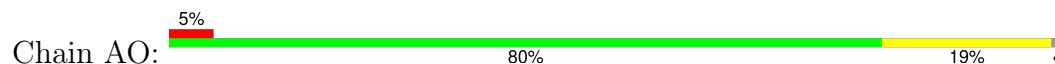
- Molecule 49: 60S ribosomal protein L14-A



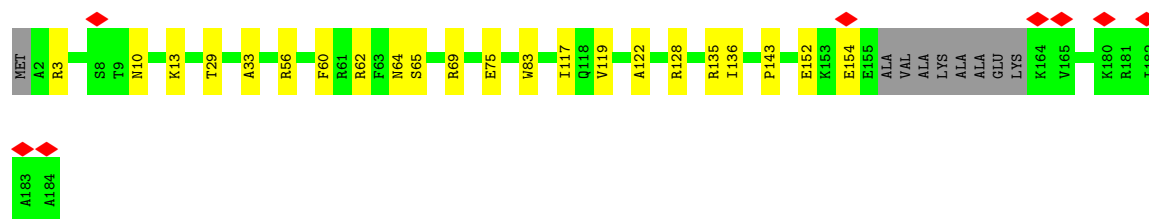
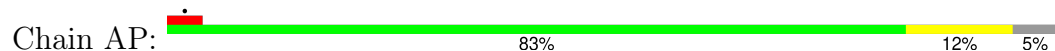
- Molecule 50: 60S ribosomal protein L15-A



- Molecule 51: 60S ribosomal protein L16-A



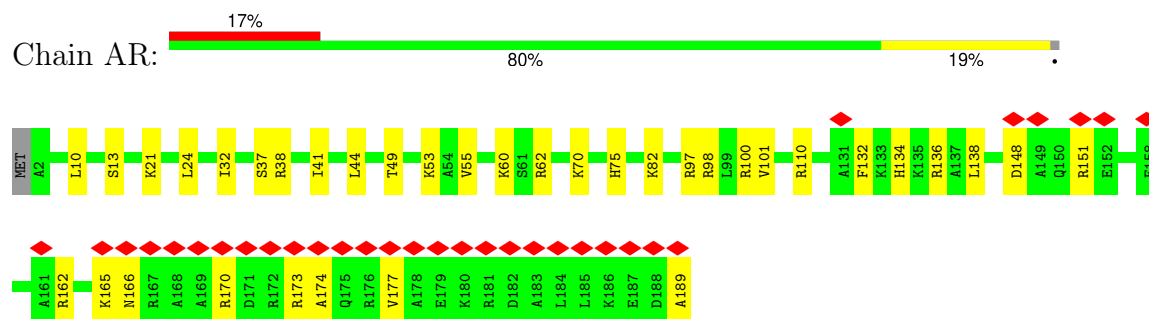
- Molecule 52: 60S ribosomal protein L17-A



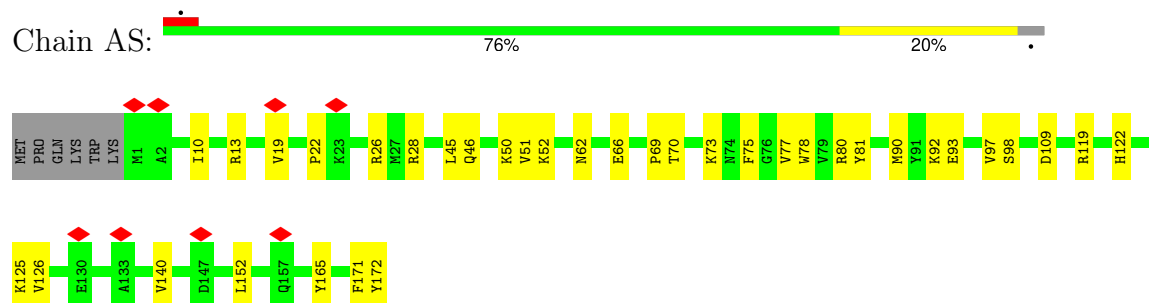
- Molecule 53: 60S ribosomal protein L18-A



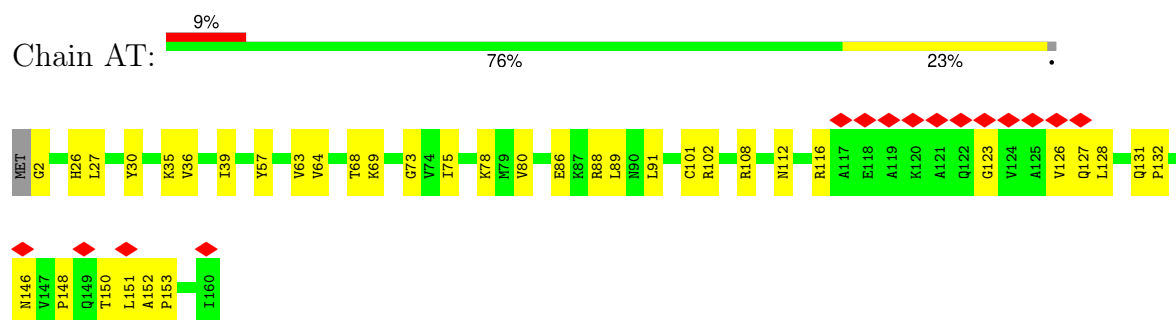
- Molecule 54: 60S ribosomal protein L19-A



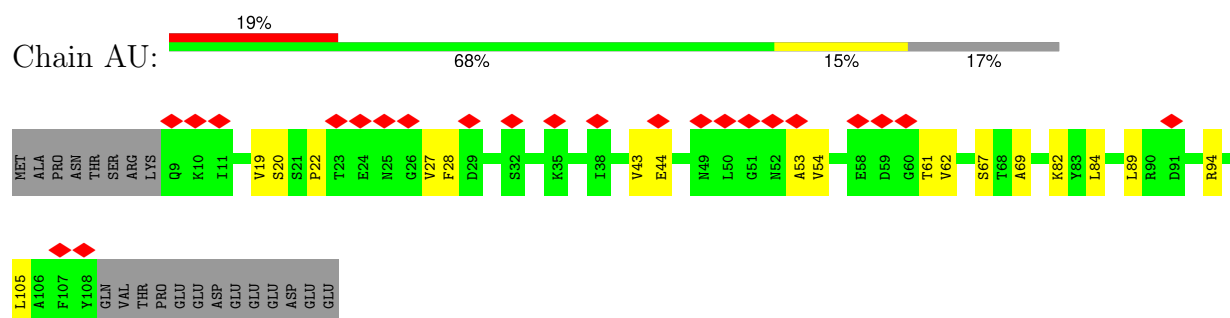
- Molecule 55: 60S ribosomal protein L20



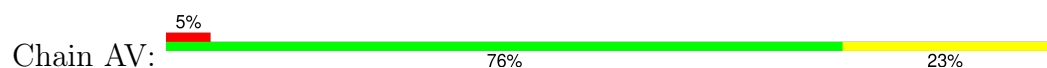
- Molecule 56: 60S ribosomal protein L21-A

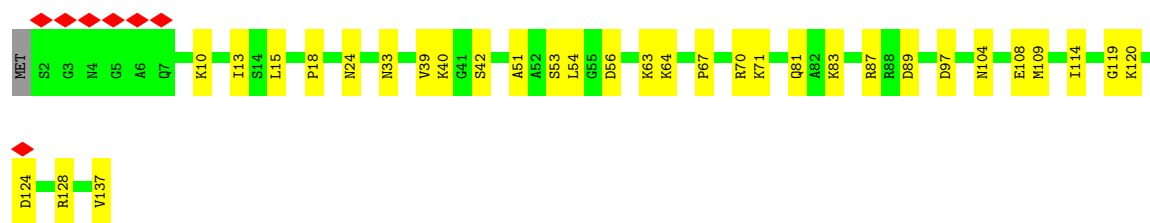


- Molecule 57: 60S ribosomal protein L22-A



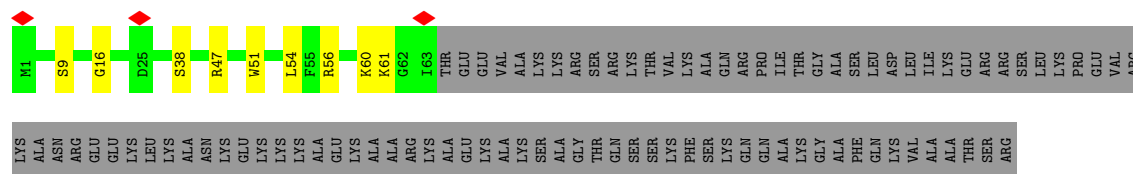
- Molecule 58: 60S ribosomal protein L23-A





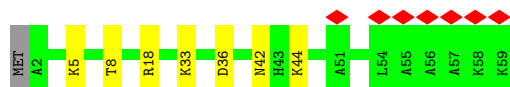
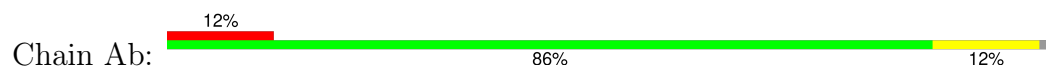
- Molecule 59: Large ribosomal subunit protein eL24A

Chain AW: 35% 6% 59%

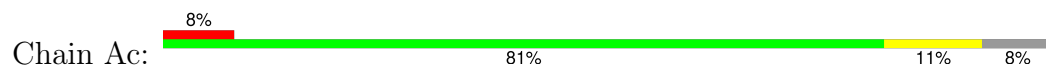




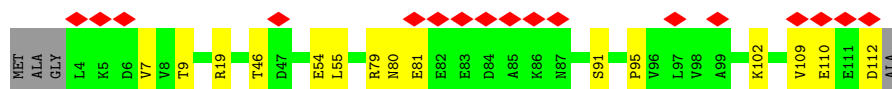
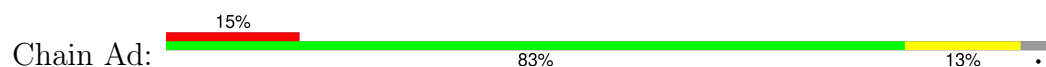
- Molecule 64: Large ribosomal subunit protein eL29



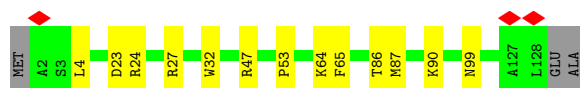
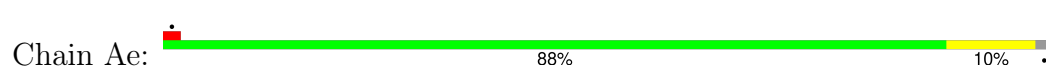
- Molecule 65: 60S ribosomal protein L30



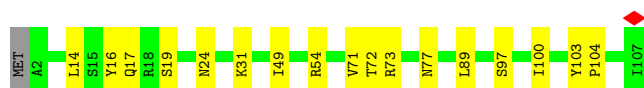
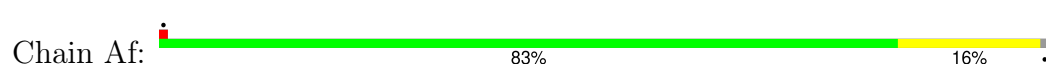
- Molecule 66: 60S ribosomal protein L31-A



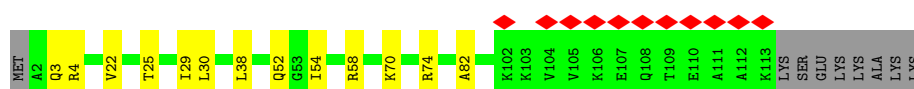
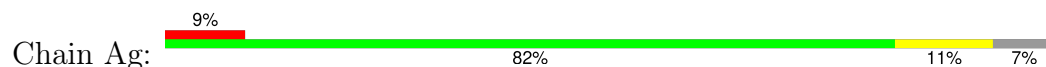
- Molecule 67: Large ribosomal subunit protein eL32



- Molecule 68: 60S ribosomal protein L33-A



- Molecule 69: 60S ribosomal protein L34-A



- Molecule 70: 60S ribosomal protein L35-A

Figure 1: The number of genes in each cluster. The chart shows the distribution of genes across 21 clusters. The clusters are labeled on the x-axis, and the number of genes is indicated by the height of the bars. The bars are color-coded: green for clusters with a red diamond above them, and yellow for others. The y-axis ranges from 0 to 100.

Cluster	Number of Genes (approx.)
MET	10
A2	45
L9	25
K12	20
L36	55
S37	50
R38	50
K45	25
K49	20
V66	20
G72	55
Y75	20
K83	20
R86	20
R90	20
E102	20
I109	20
K115	20
I118	20
K119	55
A120	55

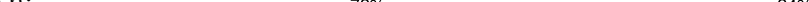
-
- Number of genes
- 100
90
80
70
60
50
40
30
20
10
0
- MET T2 T19 G10 L11 N12 K13 K25 K30 L43 I47 S51 E54 N63 E66 K67 R68 A69 R70 K75 N92 A95 A96 S97 R98 R99 H100

-
- | Amino Acid | Relative Abundance (%) |
|------------|------------------------|
| MET | 100 |
| G2 | ~90 |
| S7 | ~85 |
| K14 | ~80 |
| R24 | ~75 |
| F27 | ~70 |
| C34 | ~65 |
| K43 | ~60 |
| K52 | ~55 |
| R55 | ~50 |
| G81 | ~45 |
| S84 | ~40 |
| K85 | ~35 |
| A86 | ~30 |
| S87 | ~25 |
| A88 | ~20 |

- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | A2 | I5 | T6 | D7 | I8 | K9 | Q10 | F11 | L12 | F13 | L14 | D19 | V20 | K26 | I27 | N28 | K29 | K30 | L31 | N32 | K33 | A34 | G35 | K36 | P37 | F38 | R39 | Q40 | T41 | K42 | F43 | K44 | D58 | A59 | G60 | X61 | L66 | O67 | S68 | L69 | P70 | P71 | R77 | L78 |
|-----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

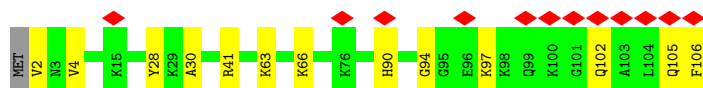
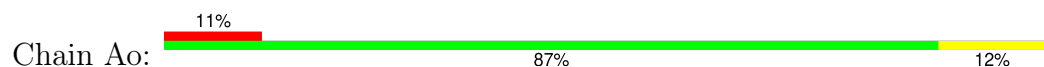
-

- | TILE | GLN | PHE | VAL | LYS | THR | HIS | LEU | VAL | LEU | ARG | GLY | I77 | I78 | E79 | P80 | S81 | L82 | S87 | K88 | D92 | Y100 | P104 | F106 | R106 | A107 | R113 | K125 | R126 | L127 | R128 | | | | | | | | | | | | | | | | | | | | | |
|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | GLN | PHE | VAL | LYS | THR | LEU | LEU | GLY | LYS | THR | LEU | VAL | GLU | SER | ASP | THR | TLE | ASP | ASN | VAL | LYS | LYS | TLE | GLN | ASP | LYS | GLY | TLE | PRO | PRO | ASP | GLN | GLN | ARG | LEU | PHE | ALA | GLY | LYS | GLN | LEU | GLU | ASP | GLY | ARG | THR | LEU | SER | ASP | TVR | ASN |

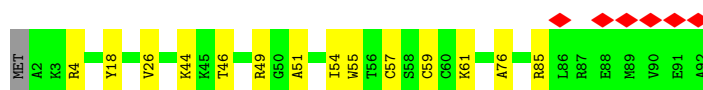
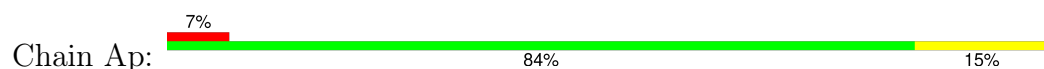
- Chain An: 



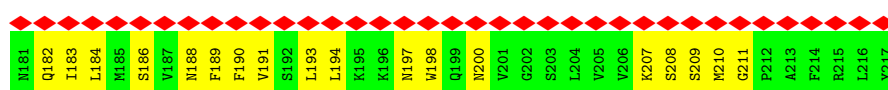
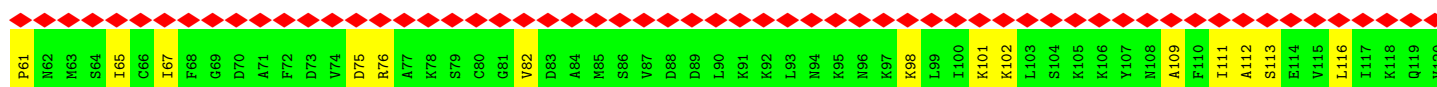
- Molecule 77: 60S ribosomal protein L42-A



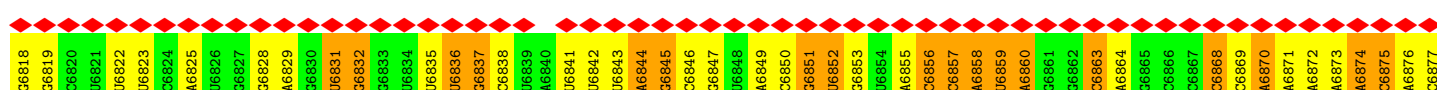
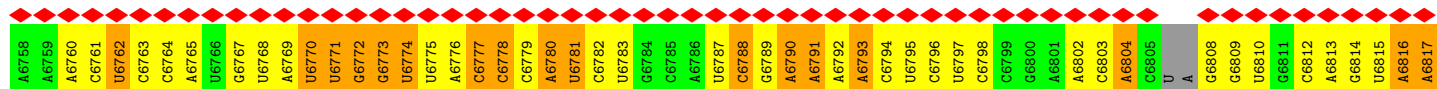
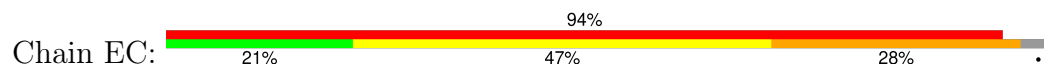
- Molecule 78: 60S ribosomal protein L43-A



- Molecule 79: Large ribosomal subunit protein uL1A



- Molecule 80: TSV IRES RNA



G6878	U6879	G6880	U	G	A6883	G6884	G6885	A6886	G6887	A6888	A6889	A6890	G6891	U6892	G6893	G6894	G6895	A6896	G6897	U6898	G6899	A6900	G6901	U6902	U6903	U6904	G6905	G6906	G6907	G6908	A6909	A6910	A6911	G6912	U6913	A6914	G6915	A6916	G6917	A6918	G6919	G6920	G6921	G6922	G6923	G6924	G6925	U6926	U6927	G6928	G6929	G6930	U6931	G6932	G6933	U6934	G6935	G6936	G6937
A6938	G6939	U6940	U6941	A6942	A6943	U6944	U6945	A6946	A6947	U6948	G6949	G6950	G6951	U6952	G6953	C	U	A6954	A	C	C																																						

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	112542	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	5.134	Depositor
Minimum map value	-2.613	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.181	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	423.19998, 423.19998, 423.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, OMU, A2M, HIC, 1MA, XSX, OMC, UR3, MG, OMG, 4AC, HYG, MA6, ZN, G7M

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	BA	0.17	0/1653	0.42	0/2261
2	BB	0.20	0/1735	0.48	0/2335
3	BC	0.17	0/1665	0.33	0/2263
4	BE	0.17	0/2109	0.39	0/2839
5	BG	0.14	0/1844	0.34	0/2464
6	BH	0.16	0/1506	0.45	2/2028 (0.1%)
7	BI	0.16	0/1514	0.38	0/2021
8	BJ	0.15	0/1519	0.39	0/2035
9	BL	0.16	0/1272	0.36	0/1712
10	BN	0.17	0/1215	0.37	0/1638
11	BO	0.19	0/952	0.48	1/1279 (0.1%)
12	BV	0.15	0/693	0.37	0/935
13	BW	0.18	0/1038	0.34	0/1395
14	BX	0.18	0/1139	0.44	0/1518
15	BY	0.15	0/1087	0.39	0/1449
16	Ba	0.20	0/782	0.48	0/1047
17	Bb	0.17	0/620	0.40	0/838
18	Be	0.16	0/483	0.43	0/643
19	BD	0.22	0/1759	0.42	0/2368
20	BF	0.22	1/1629 (0.1%)	0.57	6/2202 (0.3%)
21	BK	0.16	0/837	0.44	0/1131
22	BP	0.15	0/1012	0.39	0/1356
23	BQ	0.14	0/1125	0.39	0/1510
24	BR	0.12	0/984	0.35	0/1318
25	BS	0.16	0/1211	0.39	0/1628
26	BT	0.18	0/1113	0.46	1/1494 (0.1%)
27	BU	0.14	0/865	0.37	0/1169
28	BZ	0.15	0/566	0.37	0/761
29	Bc	0.15	0/499	0.38	0/670
30	Bd	0.17	0/453	0.44	0/602
31	Bg	0.16	0/2454	0.45	0/3340
32	Bf	0.15	0/462	0.46	0/617

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BM	0.14	0/921	0.43	0/1245
34	B5	0.18	4/41880 (0.0%)	0.29	0/65248
35	AA	0.21	0/1912	0.38	0/2569
36	AB	0.19	0/3138	0.37	0/4217
37	AC	0.20	0/2800	0.40	0/3790
38	A1	0.23	1/75561 (0.0%)	0.32	0/117806
39	A3	0.18	0/2883	0.28	0/4491
40	A4	0.21	0/3746	0.32	0/5832
41	AD	0.23	1/2390 (0.0%)	0.44	1/3225 (0.0%)
42	AE	0.17	0/1260	0.39	0/1694
43	AF	0.20	0/1821	0.38	0/2451
44	AG	0.18	0/1830	0.41	0/2469
45	AH	0.22	0/1531	0.41	0/2062
46	AI	0.17	0/1708	0.34	0/2290
47	AJ	0.17	0/1374	0.46	0/1842
48	AL	0.18	0/1568	0.38	0/2106
49	AM	0.18	0/1068	0.35	0/1438
50	AN	0.20	0/1757	0.34	0/2354
51	AO	0.20	0/1585	0.36	0/2128
52	AP	0.19	0/1410	0.35	0/1893
53	AQ	0.18	0/1465	0.33	0/1965
54	AR	0.18	0/1538	0.34	0/2050
55	AS	0.20	0/1481	0.43	0/1990
56	AT	0.19	0/1300	0.40	0/1743
57	AU	0.16	0/812	0.38	0/1099
58	AV	0.20	0/1018	0.37	0/1369
59	AW	0.20	0/533	0.36	0/707
60	AX	0.19	0/983	0.34	0/1325
61	AY	0.20	0/1004	0.41	0/1341
62	AZ	0.18	0/1118	0.35	0/1497
63	Aa	0.24	0/1204	0.43	0/1612
64	Ab	0.18	0/473	0.31	0/629
65	Ac	0.16	0/751	0.29	0/1008
66	Ad	0.18	0/904	0.35	0/1213
67	Ae	0.20	0/1041	0.37	0/1394
68	Af	0.21	0/868	0.39	0/1168
69	Ag	0.21	0/890	0.38	0/1189
70	Ah	0.17	0/978	0.34	0/1301
71	Ai	0.18	0/778	0.36	0/1034
72	Aj	0.21	0/696	0.35	0/923
73	Ak	0.18	0/618	0.39	0/826
74	Al	0.21	0/443	0.36	0/588
75	Am	0.16	0/423	0.35	0/562

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	An	0.32	0/234	0.67	0/300
77	Ao	0.18	0/860	0.36	0/1136
78	Ap	0.18	0/701	0.34	0/934
79	E	0.13	0/1745	0.37	1/2342 (0.0%)
80	EC	0.12	0/4595	0.29	0/7149
All	All	0.20	7/219392 (0.0%)	0.34	12/322410 (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
11	BO	0	1
14	BX	0	2
34	B5	3	0
41	AD	0	1
43	AF	0	1
44	AG	0	2
76	An	0	2
All	All	3	9

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	AD	84	PRO	N-CD	-6.92	1.38	1.47
34	B5	1575	G7M	O3'-P	5.61	1.61	1.56
20	BF	30	PRO	CG-CD	-5.54	1.31	1.50
38	A1	2281	A2M	O3'-P	5.12	1.61	1.56
34	B5	541	A2M	O3'-P	5.11	1.61	1.56
34	B5	619	A2M	O3'-P	5.08	1.61	1.56
34	B5	436	A2M	O3'-P	5.03	1.61	1.56

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	AD	84	PRO	CA-N-CD	-12.46	94.56	112.00
20	BF	30	PRO	N-CD-CG	-10.26	87.81	103.20
11	BO	74	VAL	N-CA-C	-7.94	106.16	113.71
6	BH	13	PRO	CA-C-N	7.62	135.42	121.70
6	BH	13	PRO	C-N-CA	7.62	135.42	121.70
20	BF	142	PRO	N-CD-CG	-6.87	92.90	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	BF	30	PRO	CA-N-CD	-6.70	102.62	112.00
26	BT	36	ILE	N-CA-C	-6.11	107.34	113.20
20	BF	142	PRO	CA-CB-CG	-6.09	92.93	104.50
20	BF	30	PRO	CA-CB-CG	-6.00	93.10	104.50
20	BF	142	PRO	CA-N-CD	-5.54	104.25	112.00
79	E	172	VAL	N-CA-C	-5.31	108.32	113.53

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
34	B5	1575	G7M	C3',C4',C2'

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
41	AD	43	LYS	Peptide
43	AF	232	ARG	Peptide
44	AG	121	SER	Peptide
44	AG	30	THR	Peptide
76	An	15	ARG	Sidechain
76	An	23	ARG	Sidechain
11	BO	122	PRO	Peptide
14	BX	63	GLN	Peptide
14	BX	88	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BA	1612	0	1623	41	0
2	BB	1709	0	1784	58	0
3	BC	1635	0	1723	27	0
4	BE	2068	0	2154	45	0
5	BG	1820	0	1918	45	0
6	BH	1481	0	1572	41	0
7	BI	1489	0	1525	36	0
8	BJ	1494	0	1573	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	BL	1244	0	1314	12	0
10	BN	1192	0	1255	21	0
11	BO	941	0	979	27	0
12	BV	684	0	672	13	0
13	BW	1021	0	1060	20	0
14	BX	1121	0	1196	24	0
15	BY	1073	0	1132	35	0
16	Ba	769	0	818	22	0
17	Bb	610	0	633	20	0
18	Be	475	0	525	13	0
19	BD	1734	0	1817	50	0
20	BF	1609	0	1675	66	0
21	BK	817	0	804	37	0
22	BP	991	0	1035	52	0
23	BQ	1105	0	1166	42	0
24	BR	975	0	1039	34	0
25	BS	1192	0	1222	43	0
26	BT	1095	0	1114	47	0
27	BU	855	0	917	33	0
28	BZ	558	0	598	33	0
29	Bc	497	0	535	17	0
30	Bd	443	0	436	23	0
31	Bg	2401	0	2356	116	0
32	Bf	454	0	465	12	0
33	BM	913	0	955	26	0
34	B5	38004	0	19143	680	0
35	AA	1878	0	1946	37	0
36	AB	3080	0	3158	48	0
37	AC	2748	0	2859	46	0
38	A1	68445	0	34455	743	0
39	A3	2579	0	1304	40	0
40	A4	3353	0	1695	42	0
41	AD	2341	0	2290	57	0
42	AE	1239	0	1326	20	0
43	AF	1784	0	1862	23	0
44	AG	1798	0	1894	22	0
45	AH	1510	0	1576	42	0
46	AI	1672	0	1711	23	0
47	AJ	1353	0	1383	36	0
48	AL	1543	0	1608	21	0
49	AM	1053	0	1149	29	0
50	AN	1720	0	1779	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	AO	1555	0	1659	25	0
52	AP	1388	0	1423	16	0
53	AQ	1441	0	1543	21	0
54	AR	1521	0	1617	33	0
55	AS	1445	0	1487	33	0
56	AT	1276	0	1323	32	0
57	AU	796	0	812	11	0
58	AV	1003	0	1048	21	0
59	AW	521	0	551	6	0
60	AX	968	0	1036	9	0
61	AY	993	0	1081	23	0
62	AZ	1092	0	1155	22	0
63	Aa	1173	0	1215	36	0
64	Ab	462	0	491	6	0
65	Ac	743	0	797	7	0
66	Ad	890	0	938	9	0
67	Ae	1020	0	1090	9	0
68	Af	850	0	880	12	0
69	Ag	880	0	945	10	0
70	Ah	969	0	1078	17	0
71	Ai	771	0	849	12	0
72	Aj	681	0	687	9	0
73	Ak	612	0	682	16	0
74	Al	436	0	475	8	0
75	Am	417	0	459	7	0
76	An	233	0	279	5	0
77	Ao	847	0	914	10	0
78	Ap	694	0	738	10	0
79	E	1718	0	1811	55	0
80	EC	4112	0	2080	87	0
81	A1	177	0	0	0	0
81	A3	2	0	0	0	0
81	A4	6	0	0	0	0
81	AA	1	0	0	0	0
81	AB	2	0	0	0	0
81	AI	1	0	0	0	0
81	AN	1	0	0	0	0
81	AP	1	0	0	0	0
81	Ae	1	0	0	0	0
81	Af	1	0	0	0	0
81	B5	61	0	0	0	0
81	BE	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
81	BN	1	0	0	0	0
81	Ba	1	0	0	0	0
82	B5	36	0	36	3	0
83	Ao	1	0	0	0	0
All	All	205978	0	151907	3098	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 9.

All (3098) 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)
82:B5:1801:HYG:O14	82:B5:1801:HYG:C15	1.63	1.42
34:B5:1499:G:H1	34:B5:1508:U:H3	1.10	0.94
26:BT:113:ILE:HD12	26:BT:128:GLY:HA2	1.51	0.91
38:A1:2445:A:N6	38:A1:2503:G:C6	2.40	0.89
34:B5:1214:U:H5''	34:B5:1244:A:H8	1.37	0.89
31:Bg:122:ILE:HB	31:Bg:134:TRP:HB2	1.56	0.88
2:BB:132:ASP:HB2	2:BB:221:PRO:HB3	1.59	0.85
49:AM:55:ARG:NH1	55:AS:70:THR:O	2.10	0.84
13:BW:2:THR:N	34:B5:1034:C:HO2'	1.76	0.84
38:A1:3234:A:H61	38:A1:3253:G:H1	1.22	0.83
18:Be:43:ARG:O	18:Be:54:ARG:NH2	2.10	0.83
38:A1:1785:U:H5''	69:Ag:38:LEU:HD11	1.60	0.83
31:Bg:89:LEU:HB2	31:Bg:103:PHE:HB2	1.62	0.82
27:BU:85:ARG:HH22	34:B5:1335:U:H5'	1.45	0.81
45:AH:20:ILE:HG22	45:AH:25:VAL:HA	1.63	0.81
34:B5:65:A:H2	34:B5:84:A:H62	1.29	0.81
40:A4:63:G:O2'	70:Ah:49:LYS:NZ	2.14	0.80
14:BX:121:ARG:NH2	34:B5:1135:U:OP2	2.14	0.80
23:BQ:30:LYS:HE2	23:BQ:33:GLY:HA2	1.63	0.80
63:Aa:60:TYR:HE2	63:Aa:63:LYS:HA	1.46	0.80
47:AJ:165:GLN:HG3	47:AJ:166:LYS:H	1.45	0.80
20:BF:148:ARG:HH21	29:Bc:22:ARG:HH12	1.30	0.79
24:BR:37:GLU:HG3	31:Bg:150:TRP:HZ3	1.46	0.79
26:BT:113:ILE:HG23	26:BT:114:VAL:HG13	1.64	0.79
75:Am:104:PRO:HG2	75:Am:107:ALA:HB2	1.65	0.79
50:AN:177:GLY:O	50:AN:184:LYS:NZ	2.16	0.79
14:BX:42:PRO:HA	14:BX:81:LYS:HD2	1.65	0.79
19:BD:164:VAL:HA	19:BD:168:ILE:HD13	1.65	0.79
38:A1:1016:C:N4	38:A1:1035:G:O6	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BS:38:VAL:HG23	25:BS:42:TYR:HB3	1.64	0.78
31:Bg:12:THR:HG22	31:Bg:311:ARG:HG2	1.65	0.78
38:A1:952:A:OP1	64:Ab:18:ARG:NH2	2.15	0.78
45:AH:34:LEU:HD11	45:AH:78:MET:HB2	1.65	0.78
41:AD:64:ILE:HD12	41:AD:109:THR:HG21	1.65	0.78
32:Bf:124:PRO:HD2	32:Bf:143:LYS:HG2	1.66	0.78
63:Aa:56:VAL:HG12	63:Aa:57:GLY:H	1.49	0.78
30:Bd:7:TRP:NE1	34:B5:1451:C:O2'	2.12	0.77
27:BU:74:GLU:OE2	34:B5:1428:OMG:N2	2.17	0.77
58:AV:109:MET:HE1	58:AV:114:ILE:HD11	1.66	0.77
46:AI:30:LYS:HG3	46:AI:63:GLU:HG3	1.64	0.77
25:BS:74:GLN:HG2	25:BS:101:LEU:HD11	1.66	0.77
80:EC:6853:G:H22	80:EC:6875:C:H42	1.33	0.77
18:Be:43:ARG:NH2	34:B5:590:C:OP1	2.18	0.76
26:BT:102:ARG:NH2	34:B5:1502:G:N7	2.32	0.76
34:B5:1697:G:H1	34:B5:1704:U:H3	1.32	0.76
28:BZ:46:LYS:HZ3	28:BZ:49:ARG:HG2	1.50	0.76
34:B5:992:A:O2'	34:B5:1785:U:O2	2.02	0.76
6:BH:67:LEU:HD22	6:BH:94:ALA:HB2	1.68	0.75
34:B5:1699:G:H21	34:B5:1700:C:H4'	1.49	0.75
26:BT:25:GLN:HB3	26:BT:27:LYS:HG2	1.67	0.75
38:A1:1232:C:H42	38:A1:1257:C:H42	1.33	0.75
41:AD:40:HIS:HD2	41:AD:42:ALA:H	1.34	0.75
34:B5:1180:C:H42	34:B5:1458:G:H1	1.34	0.75
79:E:30:GLU:O	79:E:171:ASN:ND2	2.20	0.75
20:BF:102:ARG:NH1	34:B5:1473:U:O2'	2.19	0.75
56:AT:88:ARG:NH1	64:Ab:33:LYS:O	2.19	0.75
38:A1:3278:C:OP1	68:Af:54:ARG:NH2	2.19	0.75
38:A1:126:U:OP1	50:AN:144:ARG:NH1	2.19	0.75
20:BF:41:LYS:HG2	20:BF:47:SER:HB2	1.69	0.74
37:AC:145:ILE:HD11	37:AC:150:LEU:HD22	1.69	0.74
22:BP:32:ASP:HA	22:BP:35:LYS:HE3	1.69	0.74
31:Bg:307:ASP:OD2	31:Bg:311:ARG:NH2	2.19	0.74
28:BZ:39:ALA:HB3	28:BZ:71:ILE:HA	1.70	0.74
8:BJ:110:GLN:HE22	8:BJ:126:ARG:HB2	1.53	0.74
24:BR:95:ARG:NH2	24:BR:100:LEU:O	2.20	0.74
6:BH:49:ILE:HD12	6:BH:175:LYS:HG2	1.70	0.74
23:BQ:95:LYS:HA	31:Bg:59:ARG:HH12	1.53	0.73
34:B5:1672:G:H2'	34:B5:1673:G:C8	2.22	0.73
38:A1:2457:G:N3	38:A1:2486:A:N6	2.37	0.73
73:Ak:5:ILE:HG21	73:Ak:11:PHE:HB2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:EC:6851:G:O2'	80:EC:6852:U:O5'	2.05	0.73
19:BD:42:THR:OG1	19:BD:45:LYS:O	2.06	0.73
29:Bc:61:ARG:NH1	29:Bc:62:GLU:O	2.21	0.73
37:AC:170:LYS:HG3	37:AC:175:HIS:HB2	1.71	0.73
57:AU:19:VAL:HG23	57:AU:105:LEU:HD22	1.69	0.73
8:BJ:107:ARG:NH2	8:BJ:153:GLU:OE2	2.21	0.73
38:A1:2465:G:N1	79:E:33:GLU:OE2	2.22	0.73
39:A3:119:U:OP2	41:AD:258:LYS:NZ	2.21	0.73
38:A1:1846:C:OP1	38:A1:1849:C:N4	2.21	0.73
38:A1:2674:A:H5''	47:AJ:105:GLY:HA3	1.69	0.73
39:A3:8:G:O6	41:AD:21:ARG:NH2	2.22	0.72
23:BQ:14:LYS:NZ	34:B5:1610:G:N7	2.37	0.72
4:BE:19:LEU:HD11	4:BE:108:ARG:HD2	1.71	0.72
15:BY:57:VAL:HB	15:BY:60:PHE:HE2	1.54	0.72
20:BF:114:ILE:HA	20:BF:117:THR:HG22	1.71	0.72
24:BR:102:VAL:HG21	24:BR:119:LEU:HD12	1.71	0.72
25:BS:41:ARG:HG2	34:B5:1565:C:H5''	1.72	0.72
38:A1:845:G:H21	38:A1:848:A:H2	1.38	0.72
4:BE:153:ASN:O	4:BE:174:LYS:NZ	2.22	0.72
11:BO:99:GLN:NE2	16:Ba:45:VAL:O	2.22	0.72
36:AB:240:ARG:NH2	38:A1:1907:C:O2	2.22	0.72
38:A1:2457:G:H2'	38:A1:2458:A:H2'	1.71	0.72
26:BT:105:LEU:HD12	26:BT:122:ARG:HD2	1.72	0.72
4:BE:107:GLY:HA2	4:BE:189:LEU:HD22	1.71	0.71
34:B5:1055:U:O2	34:B5:1064:G:O6	2.07	0.71
38:A1:2501:U:H3'	38:A1:2502:A:H8	1.53	0.71
34:B5:1396:U:H3	34:B5:1402:G:H1	1.37	0.71
80:EC:6944:U:H2'	80:EC:6945:U:H4'	1.71	0.71
3:BC:40:LYS:HG3	3:BC:247:ALA:HB1	1.72	0.71
31:Bg:197:SER:HB2	31:Bg:216:LYS:HB2	1.72	0.71
37:AC:318:LEU:H	37:AC:324:LEU:HD12	1.56	0.71
63:Aa:60:TYR:CE2	63:Aa:63:LYS:HA	2.25	0.71
23:BQ:139:GLN:NE2	34:B5:1465:C:OP1	2.24	0.71
38:A1:3268:A:OP1	42:AE:46:ARG:NH2	2.23	0.71
35:AA:21:ARG:HD3	38:A1:824:C:H5''	1.70	0.71
38:A1:1243:G:N3	38:A1:1270:A:O2'	2.24	0.71
38:A1:3092:C:O2'	38:A1:3094:A:OP2	2.08	0.71
38:A1:3319:U:H5'	38:A1:3320:A:H5'	1.72	0.71
79:E:45:ARG:NH2	80:EC:6817:A:OP1	2.24	0.71
52:AP:122:ALA:HB3	52:AP:143:PRO:HB2	1.73	0.70
19:BD:7:LYS:HA	19:BD:10:LYS:HG2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:AT:127:GLN:OE1	56:AT:131:GLN:NE2	2.24	0.70
23:BQ:30:LYS:HE3	34:B5:1365:C:H5''	1.73	0.70
34:B5:924:A:H2'	34:B5:925:G:C8	2.25	0.70
20:BF:189:THR:OG1	20:BF:192:GLU:OE1	2.08	0.70
54:AR:44:LEU:HB3	54:AR:49:THR:HB	1.74	0.70
3:BC:91:ARG:HH11	34:B5:1147:A:H5''	1.55	0.70
37:AC:265:GLU:HG3	37:AC:266:THR:HG23	1.74	0.70
38:A1:2444:C:O2'	71:AI:63:ASN:OD1	2.09	0.70
40:A4:75:G:OP2	61:AY:74:TYR:OH	2.07	0.70
38:A1:118:U:N3	38:A1:122:A:OP2	2.20	0.70
80:EC:6904:U:O2'	80:EC:6906:G:N7	2.23	0.70
34:B5:1354:G:H3'	34:B5:1355:C:H5''	1.72	0.69
1:BA:53:THR:HG22	1:BA:161:PRO:HG2	1.72	0.69
12:BV:40:ASP:HB2	12:BV:46:ILE:HD11	1.75	0.69
25:BS:12:GLN:HE22	25:BS:15:LEU:HB3	1.56	0.69
37:AC:98:ARG:NH2	38:A1:804:C:OP1	2.25	0.69
38:A1:2836:C:H5	38:A1:2852:C:H42	1.39	0.69
54:AR:148:ASP:OD1	54:AR:151:ARG:NH2	2.25	0.69
80:EC:6815:U:H3'	80:EC:6816:A:H5''	1.72	0.69
57:AU:61:THR:HG23	57:AU:62:VAL:HG23	1.72	0.69
21:BK:5:LYS:HE3	34:B5:1255:G:H4'	1.73	0.69
34:B5:1356:U:O2	34:B5:1367:G:O6	2.10	0.69
34:B5:174:U:H3	34:B5:266:A:H62	1.41	0.69
34:B5:851:U:OP1	54:AR:173:ARG:NH2	2.25	0.69
8:BJ:144:PRO:HD2	34:B5:474:A:H5''	1.74	0.69
15:BY:105:ARG:NH2	34:B5:459:G:OP2	2.26	0.69
38:A1:2798:C:H5''	38:A1:2800:G:H5'	1.73	0.69
6:BH:82:GLU:OE2	6:BH:165:LYS:NZ	2.25	0.69
24:BR:45:ARG:NH2	34:B5:1331:A:OP1	2.24	0.69
25:BS:71:GLN:O	25:BS:75:ASN:ND2	2.26	0.69
31:Bg:223:TRP:HD1	31:Bg:230:ALA:HB2	1.57	0.69
34:B5:852:C:H2'	34:B5:853:G:C8	2.28	0.69
26:BT:117:SER:HB2	26:BT:123:ARG:HG2	1.74	0.69
31:Bg:32:LEU:HD22	31:Bg:94:VAL:HG21	1.75	0.69
11:BO:20:TYR:HB3	11:BO:27:PHE:HB2	1.74	0.69
28:BZ:77:ARG:NH2	34:B5:1532:U:OP2	2.25	0.69
37:AC:300:ARG:O	53:AQ:39:ARG:NH2	2.25	0.69
34:B5:71:A:N6	34:B5:72:A:N3	2.39	0.68
34:B5:647:G:H21	34:B5:687:G:H1	1.39	0.68
38:A1:417:A:H2'	38:A1:418:A:C8	2.27	0.68
22:BP:86:VAL:HG12	22:BP:88:GLU:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Bg:178:VAL:HG23	31:Bg:192:PHE:HB2	1.75	0.68
38:A1:2500:A:N7	38:A1:2502:A:N6	2.40	0.68
38:A1:2796:G:N7	77:Ao:63:LYS:NZ	2.39	0.68
62:AZ:70:PRO:HG3	62:AZ:115:LYS:HB2	1.75	0.68
6:BH:11:GLN:HG3	6:BH:13:PRO:HD2	1.75	0.68
34:B5:1369:U:H1'	34:B5:1372:U:H2'	1.75	0.68
58:AV:63:LYS:O	58:AV:70:ARG:NH1	2.27	0.68
5:BG:12:SER:OG	5:BG:124:LEU:O	2.12	0.68
38:A1:3016:A:H2'	38:A1:3017:A:H8	1.58	0.68
48:AL:155:GLU:OE2	63:Aa:86:LYS:NZ	2.19	0.68
5:BG:140:ASN:ND2	34:B5:168:A:OP1	2.27	0.68
34:B5:1456:C:OP1	34:B5:1457:C:O2'	2.10	0.68
56:AT:68:THR:HG22	56:AT:69:LYS:H	1.58	0.68
35:AA:241:ARG:NH2	38:A1:2156:C:OP1	2.26	0.68
34:B5:852:C:OP2	54:AR:173:ARG:NH1	2.26	0.68
38:A1:799:G:O2'	48:AL:18:TRP:NE1	2.24	0.68
38:A1:3016:A:H2'	38:A1:3017:A:C8	2.29	0.68
27:BU:87:HIS:ND1	34:B5:1383:G:OP1	2.27	0.68
35:AA:215:ASN:ND2	38:A1:2969:A:N7	2.41	0.68
38:A1:2213:A:H2'	38:A1:2214:A:C8	2.29	0.68
38:A1:3234:A:N6	38:A1:3253:G:H1	1.92	0.68
36:AB:95:THR:HG23	38:A1:3243:A:H4'	1.74	0.67
38:A1:1388:U:O2'	67:Ae:99:ASN:O	2.11	0.67
38:A1:2453:U:H4'	38:A1:2461:A:H5''	1.75	0.67
2:BB:72:ASP:OD1	16:Ba:59:TYR:OH	2.09	0.67
36:AB:128:LYS:NZ	38:A1:3294:A:OP1	2.27	0.67
38:A1:1015:U:O2'	38:A1:1016:C:O5'	2.12	0.67
53:AQ:95:GLU:OE1	53:AQ:95:GLU:N	2.26	0.67
73:Ak:9:LYS:HA	73:Ak:9:LYS:HE3	1.75	0.67
19:BD:106:LYS:HG3	19:BD:175:VAL:HG22	1.76	0.67
34:B5:739:G:OP2	34:B5:739:G:N2	2.25	0.67
73:Ak:32:ASN:HD21	73:Ak:36:LYS:H	1.43	0.67
31:Bg:303:ALA:HB3	31:Bg:313:TRP:HZ3	1.59	0.67
65:Ac:17:VAL:HG11	65:Ac:92:ILE:HD12	1.76	0.67
13:BW:15:ASN:ND2	13:BW:72:CYS:O	2.28	0.67
29:Bc:66:LEU:HD23	29:Bc:67:ARG:HG2	1.77	0.67
80:EC:6770:U:H3	80:EC:6772:G:H21	1.42	0.67
19:BD:27:ARG:NH2	34:B5:1436:A:OP2	2.28	0.67
41:AD:202:GLY:O	41:AD:206:GLN:NE2	2.27	0.67
25:BS:133:VAL:HG12	34:B5:1545:A:H5''	1.77	0.67
34:B5:1687:U:H3	34:B5:1715:G:H1	1.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:AC:361:HIS:O	55:AS:28:ARG:NH1	2.27	0.67
38:A1:38:U:H4'	63:Aa:32:ARG:HD2	1.77	0.67
48:AL:4:SER:O	63:Aa:44:ASN:ND2	2.28	0.67
16:Ba:44:ILE:HG23	16:Ba:45:VAL:HG23	1.77	0.67
65:Ac:24:THR:HG23	65:Ac:93:LEU:HD11	1.78	0.67
32:Bf:121:CYS:SG	32:Bf:122:SER:N	2.68	0.66
7:BI:107:THR:O	7:BI:111:GLN:NE2	2.28	0.66
34:B5:1041:G:H2'	34:B5:1042:G:C8	2.30	0.66
31:Bg:182:ASN:ND2	31:Bg:185:GLN:OE1	2.26	0.66
36:AB:219:ALA:HB2	36:AB:336:VAL:HG23	1.78	0.66
36:AB:266:ARG:NH2	38:A1:2392:C:O2'	2.26	0.66
38:A1:2960:C:H2'	38:A1:2961:G:C8	2.31	0.66
20:BF:63:GLN:HB3	20:BF:88:PRO:HA	1.76	0.66
34:B5:1284:C:H4'	34:B5:1285:U:H5'	1.78	0.66
38:A1:3215:A:H5'	49:AM:121:MET:HE1	1.77	0.66
39:A3:91:G:N2	46:AI:56:GLU:OE2	2.27	0.66
45:AH:41:ILE:HD11	45:AH:67:ALA:HB1	1.78	0.66
4:BE:100:ARG:HH21	4:BE:118:GLU:HG2	1.60	0.66
10:BN:11:ILE:HG13	10:BN:12:SER:H	1.59	0.66
79:E:12:HIS:HA	79:E:15:GLU:HG2	1.77	0.66
79:E:131:ALA:O	79:E:133:LYS:NZ	2.27	0.66
19:BD:109:LEU:HD12	19:BD:184:ILE:HD11	1.78	0.66
26:BT:42:GLY:HA2	26:BT:84:LYS:HE3	1.76	0.66
33:BM:106:ILE:HB	33:BM:109:GLU:HG2	1.76	0.66
1:BA:111:ILE:HD11	34:B5:1292:G:H21	1.60	0.66
10:BN:23:PRO:HD2	10:BN:26:PHE:HB2	1.78	0.66
28:BZ:56:THR:H	28:BZ:103:ARG:HE	1.41	0.66
34:B5:1051:G:H3'	34:B5:1052:U:H4'	1.76	0.66
34:B5:1220:C:H2'	34:B5:1221:A:H8	1.60	0.66
38:A1:664:U:H2'	38:A1:665:A:C8	2.31	0.66
52:AP:10:ASN:HD22	52:AP:13:LYS:HE2	1.60	0.66
29:Bc:9:LEU:HD12	29:Bc:53:ILE:HG22	1.78	0.66
24:BR:8:THR:HG21	34:B5:1330:G:H21	1.59	0.66
25:BS:83:ALA:HA	25:BS:86:LEU:HD13	1.75	0.66
27:BU:65:ILE:HG22	30:Bd:33:LYS:HD3	1.78	0.66
38:A1:251:G:H1'	38:A1:253:A:C5	2.31	0.66
31:Bg:179:LYS:HZ2	31:Bg:190:ALA:N	1.92	0.66
34:B5:1237:G:H2'	34:B5:1238:A:H8	1.61	0.66
38:A1:1627:U:O2	38:A1:1817:G:O6	2.14	0.66
38:A1:2895:G:O2'	75:Am:100:TYR:O	2.14	0.66
45:AH:5:GLN:HE21	45:AH:7:GLU:HG2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:Am:88:LYS:HA	75:Am:92:ASP:HB3	1.78	0.66
61:AY:51:ARG:HG2	61:AY:52:ARG:H	1.59	0.65
82:B5:1801:HYG:C15	82:B5:1801:HYG:C13	2.73	0.65
39:A3:44:C:OP2	47:AJ:137:ARG:NH2	2.29	0.65
53:AQ:40:THR:HG22	53:AQ:42:ALA:H	1.60	0.65
26:BT:69:LYS:HD3	34:B5:1367:G:H5''	1.77	0.65
33:BM:114:LYS:HE3	34:B5:1225:U:OP2	1.96	0.65
34:B5:486:G:O2'	34:B5:488:G:OP2	2.14	0.65
38:A1:1261:G:N2	38:A1:1261:G:OP2	2.29	0.65
38:A1:1635:G:N2	38:A1:1638:A:OP2	2.26	0.65
4:BE:129:VAL:HG22	4:BE:139:VAL:HG12	1.78	0.65
4:BE:151:ASP:HB3	4:BE:154:ILE:HG13	1.77	0.65
7:BI:152:ILE:HG13	7:BI:153:GLU:H	1.61	0.65
14:BX:65:ASN:ND2	14:BX:116:ASP:OD2	2.28	0.65
19:BD:132:LYS:HB3	19:BD:189:MET:HG2	1.78	0.65
37:AC:161:LYS:HB2	37:AC:164:GLU:HG2	1.77	0.65
38:A1:424:G:O2'	67:Ae:23:ASP:OD1	2.15	0.65
22:BP:110:GLU:HB2	25:BS:119:ILE:HD11	1.79	0.65
24:BR:79:GLU:O	24:BR:83:GLN:NE2	2.29	0.65
26:BT:70:GLN:HG3	26:BT:123:ARG:HB3	1.78	0.65
34:B5:1683:C:O2'	34:B5:1684:U:O5'	2.14	0.65
38:A1:1014:U:O2'	38:A1:1015:U:O5'	2.13	0.65
5:BG:159:ARG:HH21	5:BG:170:THR:HG23	1.60	0.65
26:BT:108:LEU:HB3	26:BT:113:ILE:CG2	2.26	0.65
36:AB:85:VAL:HG22	36:AB:202:THR:HG22	1.78	0.65
38:A1:2445:A:C5	38:A1:2503:G:N1	2.65	0.65
34:B5:590:C:H2'	34:B5:591:A:H8	1.61	0.65
41:AD:166:ALA:HB1	41:AD:171:LEU:HD21	1.79	0.65
58:AV:108:GLU:HA	58:AV:128:ARG:HG3	1.78	0.65
34:B5:782:U:H4'	34:B5:783:G:H5''	1.78	0.65
38:A1:760:G:O2'	38:A1:770:G:N2	2.29	0.65
38:A1:2767:U:O2'	77:Ao:30:ALA:O	2.13	0.65
54:AR:98:ARG:NH1	54:AR:132:PHE:O	2.30	0.65
38:A1:3291:G:H2'	38:A1:3292:A:H8	1.61	0.65
56:AT:89:LEU:HD23	56:AT:91:LEU:HD21	1.78	0.65
25:BS:144:ARG:NE	34:B5:1172:G:OP1	2.30	0.65
34:B5:227:U:O2'	34:B5:834:G:N2	2.30	0.65
38:A1:1757:A:OP1	57:AU:94:ARG:NH2	2.27	0.65
38:A1:3252:G:H2'	38:A1:3253:G:C8	2.32	0.65
33:BM:42:ALA:HB3	33:BM:122:VAL:HB	1.79	0.64
38:A1:1799:A:H2'	38:A1:1800:A:C8	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:1805:C:H2'	38:A1:1806:A:H8	1.62	0.64
61:AY:83:ASP:O	61:AY:84:LYS:HG3	1.97	0.64
34:B5:1220:C:H2'	34:B5:1221:A:C8	2.32	0.64
38:A1:2588:U:OP1	44:AG:241:LYS:NZ	2.30	0.64
42:AE:52:VAL:HG12	42:AE:74:VAL:HG11	1.78	0.64
19:BD:8:LYS:HD3	27:BU:61:LYS:HE2	1.79	0.64
68:Af:72:THR:HG22	68:Af:73:ARG:HG3	1.78	0.64
17:Bb:81:ARG:HG3	17:Bb:82:LYS:HG2	1.79	0.64
19:BD:205:ALA:O	24:BR:42:GLN:NE2	2.29	0.64
34:B5:590:C:H2'	34:B5:591:A:C8	2.31	0.64
34:B5:1354:G:N2	34:B5:1372:U:O3'	2.31	0.64
38:A1:412:G:OP1	52:AP:62:ARG:NH1	2.30	0.64
38:A1:1667:A:H2'	38:A1:1668:G:C8	2.31	0.64
6:BH:17:GLU:HB3	6:BH:46:ILE:HG13	1.80	0.64
38:A1:284:A:OP2	77:Ao:41:ARG:NH1	2.27	0.64
21:BK:77:ARG:NH1	21:BK:83:PRO:O	2.31	0.64
62:AZ:72:ILE:HD11	62:AZ:107:ARG:HB2	1.79	0.64
66:Ad:110:GLU:HG2	66:Ad:112:ASP:H	1.61	0.64
31:Bg:135:THR:HG23	31:Bg:141:LEU:HD11	1.78	0.64
38:A1:3050:U:O2'	59:AW:16:GLY:O	2.14	0.64
67:Ae:4:LEU:HD12	67:Ae:90:LYS:HB3	1.79	0.64
30:Bd:7:TRP:O	30:Bd:7:TRP:HD1	1.80	0.64
34:B5:1235:C:N4	34:B5:1245:G:O6	2.30	0.64
38:A1:874:U:N3	38:A1:2978:U:OP1	2.25	0.64
7:BI:48:THR:OG1	7:BI:52:ASN:O	2.16	0.64
34:B5:1525:A:N3	34:B5:1589:C:O2'	2.29	0.64
38:A1:1233:G:N2	38:A1:1256:G:OP1	2.31	0.64
10:BN:29:SER:OG	10:BN:31:GLU:OE1	2.16	0.63
20:BF:192:GLU:OE2	28:BZ:98:GLN:NE2	2.31	0.63
21:BK:87:VAL:HG12	21:BK:89:GLY:H	1.63	0.63
32:Bf:107:LYS:HB3	32:Bf:110:ALA:HB2	1.78	0.63
38:A1:1661:G:H2'	38:A1:1662:G:C8	2.32	0.63
34:B5:705:U:O2'	34:B5:732:G:O2'	2.15	0.63
34:B5:871:G:H2'	34:B5:872:G:C8	2.33	0.63
38:A1:831:G:O2'	38:A1:1864:A:N3	2.31	0.63
6:BH:74:GLN:OE1	6:BH:78:THR:OG1	2.16	0.63
33:BM:44:GLY:O	33:BM:48:SER:OG	2.14	0.63
34:B5:1248:C:H2'	34:B5:1249:U:H5	1.62	0.63
38:A1:1747:G:H21	73:Ak:2:ALA:HB3	1.63	0.63
45:AH:126:VAL:HG23	45:AH:164:ILE:HD13	1.80	0.63
49:AM:14:LEU:O	49:AM:19:ARG:NH1	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:AS:66:GLU:OE1	55:AS:73:LYS:NZ	2.25	0.63
2:BB:101:HIS:HA	2:BB:217:LEU:HD22	1.81	0.63
4:BE:188:ASN:HD21	4:BE:218:PHE:HD2	1.46	0.63
34:B5:514:G:H1	34:B5:543:C:H5	1.46	0.63
38:A1:3042:U:OP2	38:A1:3092:C:N4	2.24	0.63
66:Ad:7:VAL:HG21	66:Ad:79:ARG:HH21	1.63	0.63
27:BU:82:TYR:HB3	30:Bd:52:PHE:HB3	1.78	0.63
34:B5:1458:G:O2'	34:B5:1459:C:OP1	2.15	0.63
36:AB:68:HIS:CE1	36:AB:69:LYS:HE3	2.34	0.63
38:A1:1062:A:O2'	56:AT:108:ARG:NH2	2.30	0.63
38:A1:1786:G:H2'	38:A1:1787:A:C8	2.34	0.63
50:AN:51:LEU:O	50:AN:117:ASN:ND2	2.30	0.63
34:B5:1370:U:H3	34:B5:1374:C:H41	1.46	0.63
34:B5:1533:C:H4'	34:B5:1539:G:C6	2.33	0.63
38:A1:1750:A:OP2	73:Ak:42:LYS:NZ	2.26	0.63
38:A1:3354:U:H4'	38:A1:3355:U:H4'	1.81	0.63
39:A3:1:G:O3'	41:AD:273:ARG:NH2	2.31	0.63
50:AN:121:VAL:HG21	50:AN:131:GLU:HG3	1.81	0.63
34:B5:835:U:H2'	34:B5:836:U:H5	1.62	0.63
79:E:30:GLU:HB2	79:E:209:SER:HB3	1.80	0.63
19:BD:33:GLY:HA3	19:BD:53:THR:HG22	1.81	0.62
20:BF:64:VAL:HG12	20:BF:65:ARG:H	1.63	0.62
33:BM:32:LEU:HB3	33:BM:33:ARG:HH21	1.63	0.62
34:B5:126:A:H62	34:B5:291:G:H21	1.46	0.62
34:B5:1477:G:H2'	34:B5:1478:G:C8	2.34	0.62
38:A1:1244:A:H1'	38:A1:1271:A:H4'	1.81	0.62
38:A1:1597:C:H5'	38:A1:1696:A:H1'	1.80	0.62
34:B5:110:U:OP1	34:B5:753:A:O2'	2.17	0.62
38:A1:173:G:O6	38:A1:245:U:O2	2.17	0.62
2:BB:39:GLU:HB2	2:BB:74:GLN:HA	1.80	0.62
34:B5:1434:U:O2'	34:B5:1436:A:OP1	2.17	0.62
38:A1:596:C:OP1	43:AF:33:ARG:NH1	2.33	0.62
38:A1:792:G:H5''	63:Aa:2:PRO:HD3	1.79	0.62
38:A1:1596:C:H2'	38:A1:1597:C:C6	2.34	0.62
48:AL:46:ILE:HG22	48:AL:49:ARG:HB2	1.80	0.62
55:AS:92:LYS:NZ	55:AS:109:ASP:OD2	2.32	0.62
32:Bf:133:ALA:HB3	32:Bf:140:TYR:HB2	1.81	0.62
33:BM:44:GLY:HA3	33:BM:47:GLU:HB2	1.81	0.62
5:BG:161:GLU:HA	5:BG:170:THR:HA	1.81	0.62
38:A1:537:A:H61	38:A1:554:A:H1'	1.62	0.62
15:BY:108:ARG:NH2	34:B5:444:C:OP2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:BD:120:TYR:HA	19:BD:123:VAL:HG12	1.81	0.62
21:BK:27:PHE:HE1	21:BK:43:ILE:HD11	1.65	0.62
28:BZ:60:VAL:HB	28:BZ:101:TYR:HB2	1.80	0.62
38:A1:3214:U:OP2	49:AM:128:ARG:NH2	2.32	0.62
41:AD:208:MET:HB2	41:AD:219:PHE:HE1	1.63	0.62
2:BB:32:ILE:HA	2:BB:96:LEU:HB2	1.81	0.62
41:AD:38:THR:HG23	56:AT:30:TYR:HB3	1.82	0.62
80:EC:6929:C:H2'	80:EC:6930:G:C8	2.35	0.62
7:BI:62:THR:HG22	7:BI:77:ARG:HG2	1.82	0.62
34:B5:12:U:H2'	34:B5:13:C:C6	2.35	0.62
34:B5:1297:G:N2	34:B5:1300:A:OP2	2.25	0.62
59:AW:47:ARG:HG2	59:AW:54:LEU:HG	1.81	0.62
59:AW:60:LYS:O	59:AW:60:LYS:HD2	2.00	0.62
15:BY:29:HIS:ND1	15:BY:29:HIS:O	2.32	0.62
38:A1:655:C:H2'	38:A1:656:A:H8	1.65	0.62
34:B5:564:G:N2	34:B5:577:G:OP1	2.29	0.62
34:B5:1171:A:H2'	34:B5:1172:G:C8	2.34	0.62
80:EC:6857:C:O2'	80:EC:6858:A:OP1	2.16	0.62
80:EC:6903:U:H3	80:EC:6909:A:N6	1.97	0.62
2:BB:30:PHE:CE1	2:BB:94:LYS:HA	2.35	0.61
7:BI:57:ALA:HB2	7:BI:177:GLY:HA2	1.81	0.61
7:BI:104:ILE:HG13	7:BI:105:ASP:H	1.66	0.61
11:BO:39:ILE:HD13	11:BO:76:ILE:HD11	1.82	0.61
36:AB:92:TYR:HB2	36:AB:157:VAL:HB	1.82	0.61
38:A1:1493:G:O6	74:A1:2:ALA:N	2.33	0.61
5:BG:188:ARG:NH2	34:B5:284:G:O6	2.33	0.61
7:BI:16:ALA:HB2	34:B5:354:C:H5''	1.82	0.61
20:BF:117:THR:HA	20:BF:120:ILE:HD13	1.82	0.61
34:B5:234:G:N1	34:B5:235:G:N3	2.49	0.61
34:B5:690:G:H2'	34:B5:691:C:C6	2.35	0.61
34:B5:1232:U:H2'	34:B5:1233:G:C8	2.35	0.61
38:A1:252:U:H5'	38:A1:253:A:H5'	1.82	0.61
38:A1:1863:G:N1	38:A1:1866:C:OP2	2.26	0.61
2:BB:88:VAL:HG21	2:BB:96:LEU:HD23	1.81	0.61
22:BP:41:VAL:HG13	22:BP:84:ILE:HD13	1.82	0.61
34:B5:63:G:O2'	34:B5:170:U:OP1	2.17	0.61
34:B5:1477:G:H2'	34:B5:1478:G:H8	1.64	0.61
38:A1:2491:A:H5'	79:E:207:LYS:HG3	1.82	0.61
43:AF:163:LEU:HD13	43:AF:169:ILE:HD11	1.81	0.61
65:Ac:24:THR:OG1	65:Ac:91:SER:OG	2.17	0.61
80:EC:6922:G:H1	80:EC:6931:U:H3	1.45	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BT:88:VAL:HG13	34:B5:1172:G:H21	1.65	0.61
34:B5:895:G:H1	34:B5:917:U:H3	1.47	0.61
19:BD:4:LEU:HB2	34:B5:1490:C:H5	1.64	0.61
25:BS:35:ILE:HD11	25:BS:102:ALA:HB2	1.83	0.61
26:BT:126:GLU:OE1	34:B5:1358:G:O2'	2.18	0.61
38:A1:1256:G:H2'	38:A1:1257:C:O4'	2.00	0.61
49:AM:24:LYS:NZ	49:AM:61:GLY:O	2.28	0.61
3:BC:139:ILE:HD13	3:BC:191:ALA:HB1	1.82	0.61
10:BN:124:ARG:NH2	34:B5:967:A:OP2	2.32	0.61
26:BT:77:ASN:HB3	26:BT:95:ASP:HB3	1.82	0.61
31:Bg:174:ASN:O	31:Bg:198:ASN:ND2	2.33	0.61
1:BA:147:THR:OG1	1:BA:151:SER:OG	2.17	0.61
9:BL:152:GLN:HB3	10:BN:137:PRO:HD3	1.83	0.61
38:A1:316:U:O2'	71:Ai:30:LYS:NZ	2.23	0.61
45:AH:90:MET:CE	45:AH:158:ALA:HA	2.31	0.61
15:BY:55:VAL:HG22	15:BY:75:VAL:HG22	1.82	0.61
26:BT:24:ARG:HH22	26:BT:25:GLN:HG2	1.65	0.61
31:Bg:42:LEU:HD11	31:Bg:68:VAL:HG11	1.82	0.61
47:AJ:139:THR:HG22	47:AJ:147:THR:HA	1.81	0.61
18:Be:55:ARG:NH1	34:B5:558:U:OP1	2.33	0.61
22:BP:98:ASN:O	34:B5:1183:A:N6	2.34	0.61
34:B5:1171:A:O2'	34:B5:1570:A:N3	2.31	0.61
38:A1:2445:A:N6	38:A1:2503:G:C5	2.68	0.61
5:BG:10:ASN:ND2	5:BG:127:THR:O	2.34	0.61
47:AJ:141:ARG:NH2	47:AJ:144:CYS:O	2.33	0.61
7:BI:61:GLU:HG2	7:BI:62:THR:HG23	1.83	0.60
34:B5:848:C:H2'	34:B5:849:C:H6	1.65	0.60
41:AD:60:ILE:HB	41:AD:80:SER:HB2	1.83	0.60
49:AM:36:VAL:HG12	49:AM:72:LEU:HD21	1.83	0.60
49:AM:72:LEU:HD11	49:AM:81:VAL:HG12	1.82	0.60
18:Be:25:GLU:O	34:B5:506:A:N6	2.29	0.60
26:BT:88:VAL:HG21	34:B5:1543:A:H5'	1.82	0.60
34:B5:1542:G:N1	34:B5:1568:C:O2'	2.29	0.60
38:A1:353:G:O6	72:Aj:55:ARG:NH2	2.32	0.60
15:BY:56:SER:HB3	15:BY:74:LEU:HB2	1.81	0.60
35:AA:67:TYR:OH	38:A1:2525:G:N7	2.33	0.60
39:A3:84:A:H2'	39:A3:85:G:C8	2.36	0.60
44:AG:163:VAL:HA	44:AG:166:LEU:HD13	1.82	0.60
49:AM:109:ARG:HA	49:AM:112:LEU:HD13	1.84	0.60
8:BJ:162:SER:O	8:BJ:166:GLY:N	2.34	0.60
24:BR:7:LYS:HD2	24:BR:11:ARG:HH21	1.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:BR:44:LYS:NZ	34:B5:1386:G:OP2	2.34	0.60
34:B5:133:U:O2	34:B5:134:U:O2'	2.18	0.60
38:A1:784:A:OP2	53:AQ:69:ARG:NH1	2.32	0.60
38:A1:1566:A:H5''	38:A1:1567:U:H5	1.66	0.60
38:A1:3295:A:H2'	38:A1:3296:A:C8	2.36	0.60
68:Af:49:ILE:HG12	68:Af:100:ILE:HG12	1.82	0.60
2:BB:29:TRP:CD1	2:BB:45:LYS:HZ1	2.20	0.60
26:BT:108:LEU:HB3	26:BT:113:ILE:HG21	1.83	0.60
35:AA:118:GLU:OE1	38:A1:2177:G:N1	2.34	0.60
38:A1:375:A:OP2	61:AY:89:LYS:NZ	2.33	0.60
38:A1:2960:C:H2'	38:A1:2961:G:H8	1.65	0.60
38:A1:3110:C:O3'	45:AH:155:SER:OG	2.18	0.60
5:BG:140:ASN:HA	5:BG:143:LYS:HG2	1.82	0.60
20:BF:143:ARG:NH1	29:Bc:57:MET:HE1	2.16	0.60
22:BP:43:ARG:NH1	34:B5:1551:U:OP2	2.35	0.60
34:B5:939:A:H2'	34:B5:940:A:C8	2.37	0.60
34:B5:1226:A:O2'	34:B5:1256:A:N6	2.34	0.60
38:A1:1228:C:H2'	38:A1:1229:G:C8	2.37	0.60
38:A1:2747:A:H2'	38:A1:2748:A:C8	2.36	0.60
38:A1:2843:U:OP2	38:A1:2844:C:N4	2.29	0.60
45:AH:163:GLN:O	45:AH:166:ARG:NE	2.34	0.60
50:AN:181:ASN:HA	50:AN:184:LYS:HE2	1.82	0.60
79:E:208:SER:O	79:E:211:GLY:N	2.34	0.60
5:BG:57:ASP:HA	5:BG:106:LEU:HA	1.82	0.60
20:BF:133:VAL:HG22	20:BF:198:LEU:HD11	1.82	0.60
23:BQ:12:LYS:NZ	23:BQ:17:THR:OG1	2.34	0.60
36:AB:299:ASP:HB3	36:AB:301:THR:HG22	1.84	0.60
37:AC:20:LEU:HD11	37:AC:252:GLU:HG3	1.84	0.60
38:A1:2800:G:O6	63:Aa:42:ARG:NH2	2.34	0.60
80:EC:6813:A:H2'	80:EC:6814:G:C8	2.37	0.60
80:EC:6891:G:O6	80:EC:6940:U:O2	2.20	0.60
12:BV:22:ARG:NH2	13:BW:19:LYS:O	2.35	0.60
37:AC:31:ARG:HG3	37:AC:120:TYR:OH	2.02	0.60
8:BJ:119:ALA:O	8:BJ:124:HIS:ND1	2.24	0.60
17:Bb:67:THR:OG1	17:Bb:70:LYS:O	2.19	0.60
38:A1:2220:A2M:H2	38:A1:2225:U:C5	2.37	0.60
31:Bg:172:ALA:HB3	31:Bg:202:LEU:HD22	1.83	0.60
38:A1:2901:G:O2'	38:A1:3024:A:N1	2.35	0.60
79:E:58:CYS:HB3	79:E:152:ARG:HB3	1.83	0.60
3:BC:228:ASN:HD22	3:BC:228:ASN:C	2.09	0.59
4:BE:3:ARG:HH21	34:B5:93:A:H4'	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:BK:3:MET:SD	21:BK:8:ARG:NH2	2.75	0.59
34:B5:223:U:H2'	34:B5:224:C:H6	1.67	0.59
36:AB:250:ALA:HB3	38:A1:2880:U:H1'	1.84	0.59
38:A1:1084:A:OP1	56:AT:35:LYS:NZ	2.32	0.59
38:A1:2220:A2M:H2	38:A1:2225:U:H5	1.66	0.59
39:A3:67:G:O2'	41:AD:13:SER:O	2.20	0.59
62:AZ:11:ALA:HB3	62:AZ:80:LEU:HD12	1.83	0.59
77:Ao:105:GLN:HG3	77:Ao:106:PHE:HD1	1.67	0.59
80:EC:6764:C:H2'	80:EC:6765:A:C8	2.36	0.59
12:BV:62:ARG:HH22	34:B5:1039:A:H4'	1.66	0.59
41:AD:34:LYS:HA	56:AT:27:LEU:HD11	1.84	0.59
45:AH:124:ARG:NH1	45:AH:164:ILE:O	2.36	0.59
58:AV:24:ASN:ND2	58:AV:97:ASP:OD2	2.33	0.59
19:BD:135:GLU:HG3	19:BD:153:ALA:HB2	1.83	0.59
38:A1:3322:A:H2'	38:A1:3323:A:C8	2.37	0.59
42:AE:92:SER:N	42:AE:148:GLU:OE2	2.31	0.59
1:BA:120:LEU:HD12	1:BA:142:PRO:HB2	1.85	0.59
9:BL:108:PRO:HB2	9:BL:135:VAL:HG22	1.85	0.59
31:Bg:244:ALA:HB3	31:Bg:253:ALA:HB3	1.85	0.59
34:B5:698:U:N3	34:B5:741:C:C4	2.70	0.59
40:A4:142:C:OP1	50:AN:38:ARG:NH1	2.35	0.59
80:EC:6812:C:H2'	80:EC:6813:A:C8	2.37	0.59
29:Bc:61:ARG:HH12	29:Bc:64:ARG:HG2	1.68	0.59
31:Bg:65:SER:OG	31:Bg:86:ASP:OD1	2.20	0.59
31:Bg:223:TRP:CD1	31:Bg:230:ALA:HB2	2.37	0.59
38:A1:651:G:O2'	38:A1:1435:A:OP1	2.20	0.59
38:A1:1717:U:H2'	38:A1:1718:G:C8	2.37	0.59
80:EC:6855:A:H3'	80:EC:6856:C:H5''	1.85	0.59
20:BF:188:LYS:HD2	28:BZ:63:SER:HB3	1.83	0.59
27:BU:21:LYS:HG3	27:BU:119:ALA:HB3	1.84	0.59
33:BM:40:GLY:HA2	33:BM:124:LYS:HB2	1.83	0.59
34:B5:1179:G:H2'	34:B5:1180:C:C6	2.37	0.59
38:A1:358:G:N2	38:A1:361:A:OP2	2.33	0.59
38:A1:1176:C:H2'	38:A1:1177:G:N2	2.18	0.59
2:BB:113:MET:HE2	2:BB:142:PHE:HE2	1.66	0.59
8:BJ:173:ALA:HB2	34:B5:511:A:H5'	1.85	0.59
10:BN:99:ARG:HG2	10:BN:99:ARG:HH11	1.68	0.59
27:BU:100:VAL:O	27:BU:104:THR:OG1	2.20	0.59
38:A1:170:G:H2'	38:A1:171:G:C8	2.37	0.59
38:A1:655:C:H2'	38:A1:656:A:C8	2.38	0.59
43:AF:120:THR:HG22	56:AT:132:PRO:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:AM:14:LEU:N	49:AM:19:ARG:HH12	2.01	0.59
80:EC:6813:A:H2'	80:EC:6814:G:H8	1.67	0.59
34:B5:1291:G:H22	34:B5:1324:G:N2	2.00	0.59
36:AB:315:GLY:HA2	38:A1:3379:C:H4'	1.85	0.59
38:A1:2953:U:H2'	38:A1:2954:U:H2'	1.85	0.59
40:A4:37:A:H5''	40:A4:39:G:O4'	2.03	0.59
42:AE:170:LYS:HB3	42:AE:172:HIS:CE1	2.37	0.59
55:AS:77:VAL:HG22	55:AS:126:VAL:HG23	1.83	0.59
1:BA:126:PRO:HG2	1:BA:151:SER:HB2	1.85	0.59
3:BC:39:THR:OG1	3:BC:65:GLU:OE1	2.21	0.59
3:BC:53:ILE:HA	3:BC:56:ILE:HD12	1.85	0.59
8:BJ:27:GLU:HG2	8:BJ:42:ILE:HG21	1.84	0.59
8:BJ:53:ARG:NH2	8:BJ:99:LEU:O	2.35	0.59
38:A1:1748:G:OP1	73:AK:44:LYS:HE3	2.03	0.59
38:A1:2538:U:O2'	38:A1:2539:C:O4'	2.17	0.59
50:AN:31:ARG:NH1	50:AN:124:ASP:OD2	2.36	0.59
52:AP:13:LYS:NZ	52:AP:154:GLU:OE1	2.34	0.59
21:BK:14:TYR:OH	21:BK:34:GLU:OE2	2.18	0.58
36:AB:117:ARG:HA	36:AB:175:LYS:HD2	1.84	0.58
38:A1:1798:A:H2'	38:A1:1799:A:C8	2.38	0.58
38:A1:2445:A:C6	38:A1:2503:G:C6	2.91	0.58
38:A1:2629:U:O4	56:AT:2:GLY:N	2.35	0.58
39:A3:53:U:O2'	39:A3:55:A:N7	2.35	0.58
39:A3:112:G:H2'	39:A3:113:C:C6	2.38	0.58
71:AI:51:SER:HB2	71:AI:54:GLU:HG3	1.85	0.58
34:B5:479:C:O2	34:B5:510:G:N2	2.36	0.58
36:AB:5:LYS:HE2	38:A1:2878:G:H5''	1.85	0.58
38:A1:1696:A:H2'	38:A1:1697:A:C8	2.39	0.58
7:BI:60:ILE:HD11	7:BI:179:CYS:SG	2.44	0.58
14:BX:92:CYS:HA	14:BX:95:PHE:HD2	1.68	0.58
22:BP:110:GLU:O	25:BS:115:ARG:NH2	2.36	0.58
25:BS:123:ARG:O	25:BS:127:HIS:ND1	2.36	0.58
34:B5:1697:G:O6	34:B5:1704:U:O4	2.21	0.58
38:A1:428:A:H2'	38:A1:429:U:C6	2.39	0.58
38:A1:2253:G:O2'	80:EC:6894:C:O2'	2.21	0.58
39:A3:48:U:H1'	41:AD:222:LEU:HD22	1.85	0.58
11:BO:17:ALA:HB3	11:BO:81:VAL:HA	1.85	0.58
20:BF:219:ARG:HH22	80:EC:6845:G:P	2.25	0.58
22:BP:43:ARG:NH2	34:B5:1552:U:OP2	2.36	0.58
34:B5:58:U:OP1	34:B5:456:A:O2'	2.21	0.58
34:B5:1474:G:H2'	34:B5:1475:A:H8	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:1474:G:H2'	34:B5:1475:A:C8	2.38	0.58
35:AA:54:ARG:NH2	38:A1:2176:U:OP1	2.37	0.58
40:A4:9:A:H2'	40:A4:10:A:C8	2.39	0.58
48:AL:55:ARG:NH1	48:AL:73:ARG:O	2.33	0.58
34:B5:1429:G:H2'	34:B5:1430:U:C6	2.39	0.58
35:AA:118:GLU:HG3	35:AA:125:ALA:HB3	1.86	0.58
66:Ad:9:THR:HG23	66:Ad:109:VAL:HG13	1.84	0.58
79:E:32:VAL:HG23	79:E:169:VAL:HB	1.85	0.58
2:BB:88:VAL:CG2	2:BB:96:LEU:HD23	2.34	0.58
21:BK:32:HIS:CD2	21:BK:33:GLU:H	2.22	0.58
21:BK:64:TYR:OH	34:B5:1435:G:O6	2.18	0.58
29:Bc:31:GLU:HB3	29:Bc:39:THR:HG22	1.85	0.58
38:A1:1021:G:H21	38:A1:1031:C:H2'	1.67	0.58
38:A1:1147:G:OP1	67:Ae:47:ARG:NH1	2.35	0.58
55:AS:80:ARG:HG2	55:AS:122:HIS:HB2	1.85	0.58
5:BG:188:ARG:NH1	34:B5:284:G:N7	2.47	0.58
10:BN:121:ARG:NH1	34:B5:868:G:OP1	2.36	0.58
11:BO:88:GLY:O	11:BO:92:LYS:NZ	2.31	0.58
38:A1:2369:G:H2'	38:A1:2370:G:C8	2.39	0.58
61:AY:74:TYR:CD2	61:AY:77:LYS:HG2	2.38	0.58
80:EC:6884:G:H2'	80:EC:6885:G:H8	1.68	0.58
16:Ba:84:VAL:O	34:B5:1797:A:N6	2.35	0.58
22:BP:93:VAL:HG12	22:BP:106:GLU:HB3	1.86	0.58
27:BU:65:ILE:HD11	30:Bd:43:PHE:CZ	2.39	0.58
61:AY:74:TYR:CE2	61:AY:77:LYS:HG2	2.38	0.58
14:BX:24:TRP:HE3	14:BX:30:LYS:HD2	1.69	0.58
19:BD:113:LEU:HD22	19:BD:118:ALA:HB2	1.86	0.58
22:BP:44:ARG:HH21	22:BP:52:LYS:HZ1	1.51	0.58
23:BQ:46:PHE:HA	23:BQ:49:TYR:HD1	1.68	0.58
25:BS:27:LYS:HA	25:BS:57:ARG:HA	1.85	0.58
34:B5:108:A:H2'	34:B5:109:G:C8	2.39	0.58
34:B5:186:C:H2'	34:B5:187:G:O4'	2.03	0.58
38:A1:519:A:OP1	55:AS:62:ASN:ND2	2.27	0.58
42:AE:42:LEU:O	42:AE:49:GLY:N	2.32	0.58
68:Af:14:LEU:HD11	68:Af:31:LYS:HB2	1.85	0.58
20:BF:70:VAL:HG11	23:BQ:47:LYS:HD3	1.86	0.58
22:BP:13:LYS:NZ	22:BP:14:THR:O	2.37	0.58
34:B5:185:U:H2'	34:B5:186:C:C6	2.38	0.58
38:A1:1069:C:H2'	38:A1:1070:U:C6	2.39	0.58
51:AO:98[A]:ALA:HA	51:AO:101[A]:ARG:HE	1.69	0.58
61:AY:51:ARG:HG2	61:AY:52:ARG:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BI:41:LYS:HB2	7:BI:60:ILE:HG22	1.85	0.57
20:BF:185:ARG:HH22	34:B5:1572:OMG:H4'	1.69	0.57
31:Bg:42:LEU:HB2	31:Bg:61:PHE:HB2	1.86	0.57
34:B5:1291:G:H22	34:B5:1324:G:H22	1.53	0.57
34:B5:1359:C:H2'	34:B5:1360:A:C8	2.38	0.57
36:AB:83:PRO:O	36:AB:165:GLN:NE2	2.32	0.57
38:A1:168:U:O2'	38:A1:169:U:OP1	2.20	0.57
38:A1:1621:A:H2'	38:A1:1622:U:C6	2.39	0.57
38:A1:2561:A:HO2'	38:A1:2562:A:H8	1.52	0.57
4:BE:62:LYS:HD2	4:BE:66:MET:HE3	1.86	0.57
14:BX:121:ARG:HH22	34:B5:1135:U:P	2.26	0.57
30:Bd:32:ARG:NH2	34:B5:1596:C:O2	2.37	0.57
38:A1:1330:A:OP1	68:Af:19:SER:OG	2.22	0.57
38:A1:2782:U:OP1	48:AL:185:LYS:NZ	2.32	0.57
2:BB:30:PHE:CD2	2:BB:96:LEU:HD12	2.39	0.57
29:Bc:42:ARG:NH1	29:Bc:61:ARG:O	2.38	0.57
31:Bg:270:LEU:HD21	31:Bg:273:ASP:HB2	1.86	0.57
4:BE:105:VAL:HG22	4:BE:243:GLY:HA2	1.86	0.57
7:BI:43:ILE:HG12	7:BI:57:ALA:HA	1.86	0.57
34:B5:182:A:H2'	34:B5:183:U:C6	2.39	0.57
79:E:98:LYS:HE3	79:E:102:LYS:HE2	1.87	0.57
27:BU:103:ILE:HG23	27:BU:104:THR:HG23	1.86	0.57
34:B5:815:G:H21	54:AR:162:ARG:HH22	1.51	0.57
34:B5:1370:U:H3	34:B5:1374:C:N4	2.02	0.57
38:A1:1261:G:O2'	38:A1:1262:G:N7	2.37	0.57
38:A1:2219:A:H2'	38:A1:2220:A2M:H8	1.85	0.57
49:AM:42:LYS:HA	49:AM:60:LEU:HD12	1.86	0.57
80:EC:6919:G:H3'	80:EC:6920:C:H6	1.69	0.57
6:BH:166:LEU:HD12	6:BH:183:PHE:CG	2.39	0.57
34:B5:844:A:H2'	34:B5:845:G:H8	1.69	0.57
34:B5:1214:U:H2'	34:B5:1215:C:C6	2.39	0.57
37:AC:36:HIS:O	37:AC:40:THR:HG23	2.04	0.57
38:A1:2185:G:O2'	38:A1:2314:U:OP2	2.21	0.57
40:A4:40:A:H2'	40:A4:41:A:C8	2.39	0.57
44:AG:183:LYS:HB2	44:AG:194:THR:HG23	1.87	0.57
63:Aa:36:GLY:HA3	63:Aa:40:HIS:CE1	2.40	0.57
80:EC:6831:U:H1'	80:EC:6832:G:N7	2.20	0.57
1:BA:35:PRO:O	1:BA:52:LYS:NZ	2.33	0.57
8:BJ:137:GLY:HA2	8:BJ:155:HIS:HB3	1.86	0.57
20:BF:98:MET:O	20:BF:104:ASN:ND2	2.38	0.57
31:Bg:156:VAL:HG22	31:Bg:169:ILE:HG22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BG:202:ARG:NH2	34:B5:127:G:O6	2.38	0.57
21:BK:14:TYR:HD2	21:BK:17:GLN:HE21	1.53	0.57
25:BS:29:VAL:HG23	25:BS:30:TYR:HD1	1.70	0.57
35:AA:117:GLU:HB2	35:AA:162:ALA:HB1	1.87	0.57
36:AB:19:ARG:NH2	38:A1:3045:G:OP1	2.37	0.57
36:AB:220:VAL:O	36:AB:334:ARG:NH1	2.37	0.57
38:A1:2526:C:H2'	38:A1:2527:G:C8	2.40	0.57
62:AZ:47:GLU:HB3	62:AZ:69:LYS:HB3	1.87	0.57
2:BB:113:MET:HE3	2:BB:209:ASN:HB3	1.86	0.57
15:BY:6:THR:HG23	15:BY:28:LEU:HB3	1.86	0.57
24:BR:102:VAL:HB	24:BR:106:THR:HG23	1.87	0.57
34:B5:1290:U:H2'	34:B5:1291:G:C8	2.39	0.57
34:B5:1291:G:H1	34:B5:1324:G:H22	1.51	0.57
34:B5:1409:G:N2	34:B5:1412:G:OP2	2.35	0.57
38:A1:1560:G:N2	38:A1:1579:C:H42	2.03	0.57
38:A1:1694:U:H5	38:A1:1752:A:N1	2.02	0.57
38:A1:1940:G:H21	38:A1:3362:A:H8	1.52	0.57
56:AT:68:THR:HG22	56:AT:69:LYS:N	2.20	0.57
15:BY:124:ARG:HA	15:BY:127:LYS:HB3	1.87	0.57
20:BF:95:ASN:O	34:B5:1611:A:O2'	2.22	0.57
20:BF:139:ASN:ND2	20:BF:202:ALA:O	2.38	0.57
30:Bd:13:ARG:NH1	34:B5:1554:U:OP1	2.38	0.57
34:B5:882:U:H5''	78:Ap:85:ARG:HH11	1.69	0.57
34:B5:1352:G:H2'	34:B5:1353:U:O4'	2.05	0.57
38:A1:1613:A:OP1	73:Ak:2:ALA:N	2.38	0.57
45:AH:28:VAL:HG13	45:AH:33:THR:HG22	1.87	0.57
1:BA:93:THR:HG22	1:BA:94:GLY:H	1.70	0.56
31:Bg:111:MET:HG3	31:Bg:152:SER:HA	1.87	0.56
34:B5:912:U:OP1	34:B5:913:G:O2'	2.18	0.56
34:B5:1180:C:N4	34:B5:1458:G:H1	2.01	0.56
38:A1:129:U:H2'	38:A1:130:A:C8	2.39	0.56
40:A4:80:A:H5'	40:A4:81:U:H5'	1.87	0.56
41:AD:76:ALA:HB3	41:AD:109:THR:HG22	1.87	0.56
3:BC:188:LEU:HD13	3:BC:196:VAL:HG11	1.87	0.56
7:BI:178:ARG:NH1	34:B5:258:C:O2	2.37	0.56
15:BY:41:ARG:NH1	15:BY:55:VAL:O	2.39	0.56
19:BD:61:GLU:OE1	19:BD:62:ASN:ND2	2.37	0.56
34:B5:591:A:H2'	34:B5:592:A:C8	2.40	0.56
38:A1:1120:A:H2'	38:A1:1121:U:C6	2.40	0.56
38:A1:1390:A:N6	38:A1:1418:A:O2'	2.37	0.56
72:Aj:85:LYS:HG3	72:Aj:86:ALA:H	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BW:107:SER:HB3	34:B5:802:G:H21	1.70	0.56
17:Bb:50:ALA:O	17:Bb:51:GLN:HG2	2.05	0.56
20:BF:70:VAL:HG13	20:BF:72:HIS:H	1.70	0.56
22:BP:99:GLY:HA2	34:B5:1453:G:H21	1.70	0.56
26:BT:15:ILE:HG23	26:BT:59:ALA:HB3	1.86	0.56
30:Bd:7:TRP:O	30:Bd:7:TRP:CD1	2.58	0.56
31:Bg:155:ARG:O	31:Bg:170:ILE:HG12	2.05	0.56
32:Bf:94:LYS:NZ	34:B5:1232:U:O4	2.35	0.56
34:B5:407:A:H2'	34:B5:408:C:C6	2.40	0.56
34:B5:751:G:H2'	34:B5:752:A:H8	1.69	0.56
34:B5:822:U:H2'	34:B5:823:G:O4'	2.05	0.56
34:B5:1248:C:H2'	34:B5:1249:U:C5	2.40	0.56
38:A1:364:G:OP2	72:Aj:52:LYS:NZ	2.24	0.56
38:A1:662:U:H2'	38:A1:663:OMC:C6	2.40	0.56
52:AP:13:LYS:HB3	52:AP:152:GLU:HB2	1.87	0.56
61:AY:86:THR:HG22	61:AY:96:PRO:HA	1.87	0.56
80:EC:6783:U:H3	80:EC:6813:A:H61	1.54	0.56
80:EC:6788:C:O4'	80:EC:6809:G:N2	2.38	0.56
24:BR:32:LYS:NZ	34:B5:1388:A:OP2	2.37	0.56
38:A1:1751:G:H5'	73:Ak:26:LYS:HE2	1.88	0.56
38:A1:2697:A:H2'	38:A1:2698:G:C8	2.40	0.56
5:BG:48:TYR:HE2	5:BG:117:GLY:H	1.54	0.56
5:BG:67:VAL:HG13	5:BG:99:GLY:HA2	1.86	0.56
11:BO:102:LEU:HG	16:Ba:53:LEU:HD21	1.87	0.56
17:Bb:51:GLN:OE1	34:B5:957:G:N2	2.38	0.56
20:BF:190:ILE:HG12	34:B5:1473:U:C5	2.40	0.56
34:B5:1160:A:H2'	34:B5:1161:C:C6	2.40	0.56
34:B5:1466:G:O2'	34:B5:1602:C:OP1	2.23	0.56
38:A1:1791:C:H2'	38:A1:1792:C:C6	2.40	0.56
38:A1:2203:U:H2'	38:A1:2204:C:C6	2.40	0.56
44:AG:25:PRO:HB3	62:AZ:125:GLY:H	1.68	0.56
45:AH:8:GLN:HB3	45:AH:72:LYS:HD2	1.86	0.56
20:BF:120:ILE:HA	20:BF:123:VAL:HG22	1.88	0.56
20:BF:219:ARG:NE	80:EC:6841:U:O2	2.38	0.56
34:B5:1316:G:HO2'	34:B5:1401:A:HO2'	1.53	0.56
61:AY:48:LEU:HD13	61:AY:115:ARG:HH21	1.71	0.56
62:AZ:26:VAL:HG12	62:AZ:27:LYS:HG3	1.86	0.56
4:BE:27:TYR:O	34:B5:447:U:O2'	2.24	0.56
4:BE:230:GLU:OE1	4:BE:233:LYS:NZ	2.39	0.56
26:BT:86:ARG:NH2	34:B5:1601:G:OP1	2.33	0.56
35:AA:127:ALA:HB2	35:AA:134:VAL:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:AC:181:VAL:O	37:AC:182:LEU:HG	2.04	0.56
38:A1:596:C:P	43:AF:33:ARG:HH12	2.29	0.56
38:A1:2673:A:OP1	47:AJ:94:ARG:NE	2.39	0.56
62:AZ:15:ARG:HD2	62:AZ:79:HIS:CD2	2.40	0.56
14:BX:42:PRO:HG2	14:BX:122:PHE:HZ	1.71	0.56
15:BY:123:LYS:O	15:BY:127:LYS:N	2.35	0.56
23:BQ:29:ILE:HG21	23:BQ:36:ILE:HD12	1.86	0.56
38:A1:993:G:N3	38:A1:2637:A:H2'	2.21	0.56
38:A1:3174:A:OP1	68:Af:97:SER:OG	2.17	0.56
36:AB:57:VAL:HG12	36:AB:358:TRP:HB3	1.87	0.56
37:AC:326:ARG:O	43:AF:41:ARG:NH1	2.39	0.56
38:A1:2294:U:OP2	58:AV:71:LYS:NZ	2.34	0.56
18:Be:53:LYS:O	18:Be:54:ARG:HB2	2.05	0.56
26:BT:48:GLN:HG3	34:B5:1477:G:H1'	1.88	0.56
28:BZ:90:LYS:HG3	28:BZ:104:ALA:HA	1.87	0.56
31:Bg:21:THR:OG1	31:Bg:69:GLN:O	2.22	0.56
31:Bg:68:VAL:HA	31:Bg:84:SER:HA	1.88	0.56
34:B5:1738:U:H2'	34:B5:1739:C:C6	2.41	0.56
38:A1:129:U:H2'	38:A1:130:A:H8	1.71	0.56
38:A1:631:U:H2'	38:A1:632:G:C8	2.41	0.56
38:A1:1084:A:H2'	38:A1:1085:A:C8	2.41	0.56
46:AI:140:THR:HG21	46:AI:148:VAL:HG11	1.87	0.56
51:AO:187[A]:GLU:HA	51:AO:192[A]:LYS:NZ	2.21	0.56
58:AV:120:LYS:NZ	58:AV:124:ASP:OD1	2.34	0.56
79:E:189:PHE:HE1	79:E:193:LEU:HD22	1.70	0.56
19:BD:166:ASP:O	19:BD:190:ARG:NH2	2.31	0.55
25:BS:20:THR:HG21	25:BS:35:ILE:HG13	1.88	0.55
31:Bg:102:ARG:HH12	34:B5:1342:C:C5'	2.18	0.55
34:B5:1687:U:O4	34:B5:1715:G:O6	2.24	0.55
38:A1:40:A:H5''	63:Aa:35:ALA:HB1	1.89	0.55
38:A1:307:A:H2'	38:A1:308:A:C8	2.41	0.55
38:A1:966:U:H2'	38:A1:967:A:C8	2.41	0.55
20:BF:81:ARG:NH2	34:B5:1615:C:OP1	2.33	0.55
24:BR:7:LYS:N	34:B5:1316:G:OP1	2.38	0.55
24:BR:41:ILE:HG23	24:BR:46:LEU:HD23	1.88	0.55
25:BS:84:TRP:HA	25:BS:89:GLN:NE2	2.21	0.55
37:AC:11:LEU:HD21	37:AC:156:LEU:HB2	1.88	0.55
38:A1:269:G:H5''	50:AN:14:LYS:HE2	1.87	0.55
38:A1:627:U:H2'	38:A1:628:A:C8	2.41	0.55
38:A1:799:G:OP2	63:Aa:32:ARG:NH1	2.39	0.55
38:A1:1284:C:H3'	38:A1:1285:G:C8	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:2197:OMC:N4	38:A1:2241:U:H2'	2.21	0.55
38:A1:2631:U:OP1	38:A1:2757:U:O2'	2.18	0.55
38:A1:3116:G:OP1	38:A1:3116:G:N2	2.37	0.55
63:Aa:24:LYS:O	63:Aa:26:ARG:HG2	2.05	0.55
65:Ac:32:LYS:O	65:Ac:36:GLN:HG3	2.06	0.55
4:BE:146:THR:HG21	34:B5:123:G:H21	1.70	0.55
6:BH:30:SER:OG	6:BH:33:GLU:OE2	2.24	0.55
31:Bg:38:ARG:HD3	31:Bg:67:ILE:HD13	1.87	0.55
38:A1:1230:G:N2	38:A1:1260:A:N3	2.54	0.55
38:A1:3017:A:N1	38:A1:3037:U:H5	2.04	0.55
45:AH:101:VAL:HG22	45:AH:114:VAL:HG22	1.88	0.55
49:AM:89:ALA:HB1	49:AM:92:GLU:OE2	2.07	0.55
28:BZ:92:ILE:HD13	28:BZ:100:ILE:HG13	1.88	0.55
34:B5:654:C:H41	34:B5:655:G:H21	1.53	0.55
44:AG:78:PHE:O	44:AG:79:GLN:HG3	2.07	0.55
9:BL:57:LYS:NZ	34:B5:326:G:OP1	2.39	0.55
20:BF:219:ARG:HH12	80:EC:6844:A:H4'	1.72	0.55
35:AA:245:LEU:HD23	35:AA:247:ARG:HE	1.72	0.55
38:A1:528:U:H2'	38:A1:529:A:C8	2.41	0.55
38:A1:916:G:H5'	38:A1:917:A:OP1	2.06	0.55
38:A1:2745:G:N2	38:A1:2748:A:OP2	2.35	0.55
15:BY:112:LYS:NZ	34:B5:57:G:OP1	2.35	0.55
31:Bg:179:LYS:NZ	31:Bg:188:ILE:HG13	2.21	0.55
31:Bg:303:ALA:HB3	31:Bg:313:TRP:CZ3	2.41	0.55
34:B5:1081:A:H2	34:B5:1082:C:H42	1.54	0.55
38:A1:1724:U:H1'	38:A1:1725:C:C6	2.41	0.55
38:A1:3280:U:O2'	38:A1:3281:U:O5'	2.24	0.55
41:AD:40:HIS:CD2	56:AT:69:LYS:HA	2.41	0.55
42:AE:138:GLN:NE2	42:AE:142:ASP:OD2	2.38	0.55
51:AO:76[A]:PRO:HB3	51:AO:138[A]:LEU:HB3	1.88	0.55
11:BO:99:GLN:HE21	16:Ba:46:GLU:HG3	1.72	0.55
17:Bb:36:LYS:O	17:Bb:77:THR:OG1	2.22	0.55
26:BT:11:ALA:O	26:BT:15:ILE:HD12	2.07	0.55
34:B5:407:A:H2'	34:B5:408:C:H6	1.72	0.55
34:B5:950:C:H2'	34:B5:951:A:C8	2.41	0.55
47:AJ:43:GLN:NE2	47:AJ:70:THR:O	2.39	0.55
61:AY:63:LYS:HE3	61:AY:97:ILE:HD13	1.89	0.55
31:Bg:10:ARG:NH1	31:Bg:50:ASP:O	2.29	0.55
34:B5:520:A:H2'	34:B5:521:A:C8	2.42	0.55
38:A1:1596:C:H2'	38:A1:1597:C:H6	1.72	0.55
38:A1:3160:U:H2'	38:A1:3161:C:H6	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:A3:55:A:H1'	47:AJ:10:ARG:HB2	1.88	0.55
45:AH:90:MET:SD	45:AH:161:LEU:HD11	2.47	0.55
79:E:65:ILE:HA	79:E:109:ALA:HB3	1.89	0.55
17:Bb:64:CYS:HB3	17:Bb:73:LEU:HD23	1.89	0.55
19:BD:94:ARG:NH2	19:BD:125:TYR:OH	2.39	0.55
34:B5:436:A2M:H8	34:B5:436:A2M:O5'	2.07	0.55
34:B5:968:U:H2'	34:B5:969:C:O4'	2.07	0.55
34:B5:1439:C:H2'	34:B5:1440:C:C6	2.42	0.55
38:A1:3101:G:H2'	38:A1:3102:G:C8	2.42	0.55
51:AO:12[A]:LYS:HD2	51:AO:37[A]:ARG:NH2	2.21	0.55
1:BA:41:ARG:HG2	1:BA:45:VAL:O	2.06	0.55
3:BC:35:TRP:CZ3	3:BC:46:LYS:HD3	2.42	0.55
4:BE:52:LEU:HB3	4:BE:54:TYR:CD1	2.42	0.55
34:B5:52:U:H2'	34:B5:53:G:H8	1.72	0.55
34:B5:499:U:H3'	34:B5:500:C:H5''	1.89	0.55
34:B5:580:A:O2'	34:B5:582:U:OP1	2.25	0.55
34:B5:891:A:H2'	34:B5:892:A:H8	1.71	0.55
34:B5:1772:C:H2'	34:B5:1773:4AC:H6	1.89	0.55
37:AC:317:PRO:C	37:AC:319:LYS:H	2.15	0.55
45:AH:41:ILE:HG23	45:AH:43:VAL:HG13	1.89	0.55
4:BE:115:THR:HG23	4:BE:117:GLU:H	1.72	0.54
22:BP:48:GLY:C	22:BP:49:MET:HE2	2.32	0.54
26:BT:89:ARG:NH1	34:B5:1562:G:OP1	2.39	0.54
31:Bg:73:LEU:HD23	31:Bg:74:THR:N	2.22	0.54
34:B5:791:A:H2'	34:B5:792:U:C6	2.43	0.54
34:B5:1285:U:H4'	34:B5:1286:U:O5'	2.07	0.54
35:AA:30:ARG:HG2	35:AA:74:GLU:HG3	1.88	0.54
37:AC:156:LEU:HD12	37:AC:159:ILE:HD12	1.89	0.54
38:A1:2445:A:H61	38:A1:2502:A:H2	1.53	0.54
44:AG:130:TYR:HB2	44:AG:204:ARG:NH1	2.22	0.54
79:E:112:ALA:N	79:E:135:PRO:HB3	2.22	0.54
80:EC:6791:A:C5	80:EC:6793:A:H1'	2.42	0.54
15:BY:35:VAL:HG23	15:BY:36:SER:H	1.70	0.54
38:A1:1092:C:O2'	38:A1:1093:A:OP1	2.24	0.54
38:A1:2273:G:O2'	38:A1:2311:G:O6	2.23	0.54
40:A4:69:U:H2'	40:A4:70:G:O4'	2.07	0.54
48:AL:126:PHE:HD2	70:Ah:115:LYS:HE2	1.72	0.54
62:AZ:116:LYS:O	62:AZ:120:GLU:HG2	2.07	0.54
80:EC:6853:G:N2	80:EC:6875:C:H42	2.04	0.54
20:BF:124:LEU:HD23	28:BZ:58:ARG:HD2	1.89	0.54
25:BS:42:TYR:HA	25:BS:85:PHE:HE2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Bg:48:THR:OG1	31:Bg:50:ASP:OD1	2.23	0.54
31:Bg:305:TYR:HD2	31:Bg:311:ARG:NH1	2.05	0.54
34:B5:183:U:H2'	34:B5:184:C:C6	2.43	0.54
38:A1:12:A:H2'	38:A1:13:A:C8	2.42	0.54
38:A1:2352:A:H5''	52:AP:83:TRP:O	2.08	0.54
41:AD:260:PHE:HB3	41:AD:264:GLN:NE2	2.22	0.54
69:Ag:74:ARG:NH2	69:Ag:82:ALA:HB2	2.22	0.54
79:E:113:SER:HB3	79:E:116:LEU:HD13	1.88	0.54
20:BF:120:ILE:HG12	28:BZ:59:TYR:HE1	1.72	0.54
34:B5:629:U:H2'	34:B5:630:A:H8	1.72	0.54
34:B5:1591:C:H2'	34:B5:1592:A:H8	1.73	0.54
37:AC:209:TYR:OH	38:A1:689:U:O4	2.24	0.54
38:A1:1528:G:O2'	38:A1:1588:A:N3	2.39	0.54
40:A4:52:A:H5'	74:Al:21:ARG:HD3	1.90	0.54
41:AD:250:ASP:OD2	41:AD:254:LYS:NZ	2.40	0.54
42:AE:56:LYS:HD2	42:AE:98:VAL:HG22	1.89	0.54
53:AQ:157:PRO:HD3	63:Aa:47:LYS:HD2	1.89	0.54
23:BQ:82:ARG:NH2	23:BQ:113:ASP:OD2	2.41	0.54
24:BR:49:LYS:NZ	34:B5:1390:U:OP2	2.41	0.54
25:BS:26:ILE:HG13	25:BS:31:ALA:HB2	1.89	0.54
31:Bg:289:ALA:HB2	31:Bg:305:TYR:HE1	1.73	0.54
34:B5:228:G:C4	34:B5:835:U:H1'	2.43	0.54
34:B5:1201:G:N2	34:B5:1600:A:O5'	2.41	0.54
38:A1:2344:U:H2'	38:A1:2345:A:C8	2.43	0.54
39:A3:70:U:H2'	39:A3:71:G:C8	2.42	0.54
40:A4:103:G:OP2	40:A4:105:A:O2'	2.24	0.54
79:E:18:LYS:HD3	79:E:21:ASN:HD21	1.71	0.54
2:BB:48:VAL:HG21	2:BB:61:LEU:HD21	1.90	0.54
31:Bg:289:ALA:HB2	31:Bg:305:TYR:CE1	2.42	0.54
34:B5:233:C:O2'	34:B5:234:G:N2	2.40	0.54
34:B5:428:A:H2'	34:B5:429:G:O4'	2.08	0.54
34:B5:472:U:O2'	34:B5:769:A:N3	2.37	0.54
34:B5:1198:G:OP1	34:B5:1199:G:O2'	2.21	0.54
38:A1:1448:U:H2'	38:A1:1449:A2M:H8	1.90	0.54
38:A1:2728:G:C6	56:AT:80:VAL:HG11	2.43	0.54
39:A3:4:U:H2'	39:A3:5:G:H8	1.73	0.54
2:BB:30:PHE:CE2	2:BB:96:LEU:HD12	2.42	0.54
2:BB:180:THR:O	2:BB:183:GLN:N	2.40	0.54
5:BG:48:TYR:HE1	5:BG:121:LEU:HD21	1.72	0.54
38:A1:19:U:H2'	38:A1:20:A:C8	2.42	0.54
38:A1:1447:G:OP1	52:AP:65:SER:OG	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:1808:G:OP1	62:AZ:135:ARG:NH2	2.40	0.54
45:AH:31:ARG:NH2	45:AH:188:THR:OG1	2.41	0.54
46:AI:19:LYS:HE2	46:AI:26:VAL:HB	1.88	0.54
13:BW:80:ASN:OD1	13:BW:124:LYS:NZ	2.40	0.54
34:B5:1091:A:H4'	34:B5:1092:A:O4'	2.08	0.54
34:B5:1345:A:N1	34:B5:1380:U:H5	2.04	0.54
40:A4:74:U:C4	61:AY:74:TYR:HD1	2.25	0.54
46:AI:206:LEU:O	46:AI:210:ILE:HG12	2.08	0.54
47:AJ:25:GLU:HG3	47:AJ:26:SER:H	1.73	0.54
79:E:134:PHE:HZ	80:EC:6773:G:H21	1.56	0.54
2:BB:82:ARG:HG2	2:BB:105:PHE:CE1	2.43	0.54
7:BI:76:THR:HG21	7:BI:104:ILE:HD12	1.88	0.54
22:BP:81:ARG:NH1	22:BP:97:TYR:O	2.41	0.54
32:Bf:99:LYS:H	32:Bf:99:LYS:HD2	1.73	0.54
38:A1:307:A:H2'	38:A1:308:A:H8	1.72	0.54
38:A1:2449:A:H3'	38:A1:2450:G:H8	1.73	0.54
38:A1:3113:A:H2'	38:A1:3114:A:O4'	2.08	0.54
79:E:188:ASN:HA	79:E:191:VAL:HB	1.90	0.54
80:EC:6860:A:H61	80:EC:6870:A:H1'	1.73	0.54
3:BC:102:VAL:HG11	3:BC:129:ILE:HG12	1.90	0.54
26:BT:24:ARG:NH2	26:BT:25:GLN:HG2	2.23	0.54
31:Bg:122:ILE:O	31:Bg:134:TRP:N	2.32	0.54
34:B5:1146:G:H2'	34:B5:1147:A:C8	2.43	0.54
34:B5:1628:U:H2'	34:B5:1629:G:C8	2.43	0.54
38:A1:1203:A:H2'	38:A1:1204:A:C8	2.43	0.54
38:A1:2416:U:H2'	38:A1:2417:OMU:H6	1.90	0.54
50:AN:103:GLU:OE2	50:AN:118:SER:OG	2.24	0.54
21:BK:31:LYS:O	21:BK:39:ASN:ND2	2.40	0.53
33:BM:133:LEU:HG	33:BM:136:ILE:HD13	1.89	0.53
34:B5:31:C:O2'	34:B5:547:U:OP1	2.25	0.53
34:B5:143:G:H2'	34:B5:144:U:C6	2.43	0.53
38:A1:2218:G:OP1	71:Ai:68:ARG:NH2	2.41	0.53
38:A1:2897:A:H5''	75:Am:125:LYS:HD2	1.89	0.53
38:A1:3294:A:H2'	38:A1:3295:A:O4'	2.08	0.53
45:AH:9:GLN:O	45:AH:72:LYS:HE2	2.08	0.53
47:AJ:60:ARG:HH12	80:EC:6798:C:H4'	1.72	0.53
6:BH:12:ALA:HB3	6:BH:13:PRO:HD3	1.89	0.53
6:BH:78:THR:HG23	6:BH:90:VAL:HG23	1.90	0.53
7:BI:106:ALA:HB2	7:BI:165:LEU:HG	1.89	0.53
27:BU:47:GLN:HG3	27:BU:48:HIS:ND1	2.24	0.53
36:AB:94:GLU:HG3	51:AO:152[A]:VAL:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:1262:G:O2'	38:A1:1264:G:O4'	2.25	0.53
38:A1:1777:U:H2'	38:A1:1778:G:C8	2.43	0.53
38:A1:1899:G:O2'	38:A1:2334:U:O4	2.20	0.53
40:A4:71:A:OP2	61:AY:51:ARG:NH1	2.41	0.53
58:AV:18:PRO:HA	58:AV:51:ALA:HA	1.90	0.53
34:B5:738:G:H2'	34:B5:739:G:N3	2.24	0.53
34:B5:1482:C:P	34:B5:1521:G:H22	2.31	0.53
37:AC:11:LEU:HD22	37:AC:168:ALA:HB1	1.89	0.53
38:A1:531:G:H2'	38:A1:532:A:C8	2.43	0.53
38:A1:759:U:H2'	38:A1:760:G:O4'	2.08	0.53
79:E:17:LEU:HD22	79:E:172:VAL:HG22	1.89	0.53
8:BJ:120:LYS:HE3	34:B5:479:C:H4'	1.90	0.53
22:BP:37:ALA:HB1	22:BP:41:VAL:HB	1.90	0.53
31:Bg:22:SER:HB2	31:Bg:70:ASP:HA	1.91	0.53
36:AB:17:LEU:HD21	36:AB:233:TRP:HH2	1.74	0.53
38:A1:351:A:N6	74:Al:37:TYR:O	2.41	0.53
38:A1:2445:A:C6	38:A1:2503:G:N1	2.77	0.53
40:A4:26:U:H2'	40:A4:27:U:C6	2.44	0.53
50:AN:9:GLU:OE2	50:AN:13:LYS:NZ	2.36	0.53
58:AV:39:VAL:HG13	58:AV:42:SER:OG	2.08	0.53
1:BA:74:VAL:HB	1:BA:121:VAL:HG12	1.90	0.53
2:BB:89:ASP:HB3	2:BB:223:PHE:CE1	2.44	0.53
6:BH:9:LEU:HD11	6:BH:17:GLU:HG3	1.91	0.53
10:BN:99:ARG:HG2	10:BN:99:ARG:NH1	2.23	0.53
19:BD:55:THR:HB	19:BD:90:ARG:HD3	1.90	0.53
22:BP:124:THR:HG21	34:B5:1182:U:H4'	1.91	0.53
24:BR:23:LYS:NZ	31:Bg:149:ASP:OD2	2.42	0.53
29:Bc:9:LEU:HD11	29:Bc:55:VAL:HG22	1.90	0.53
34:B5:1163:A:N3	34:B5:1613:U:O2'	2.32	0.53
38:A1:1667:A:H2'	38:A1:1668:G:H8	1.73	0.53
51:AO:189[A]:ASP:O	51:AO:193[A]:GLN:HG3	2.08	0.53
8:BJ:59:LEU:HD22	8:BJ:69:ARG:HA	1.89	0.53
8:BJ:113:VAL:HG13	8:BJ:118:LEU:HD23	1.89	0.53
10:BN:99:ARG:NH2	10:BN:119:GLU:OE2	2.38	0.53
14:BX:134:ALA:HB1	14:BX:140:LYS:HD3	1.90	0.53
26:BT:39:THR:HA	26:BT:100:ILE:HD12	1.89	0.53
33:BM:136:ILE:HA	33:BM:139:HIS:CE1	2.44	0.53
34:B5:850:A:OP1	54:AR:166:ASN:HB2	2.08	0.53
38:A1:114:A:OP1	50:AN:54:LYS:NZ	2.40	0.53
45:AH:38:LEU:HD21	45:AH:71:VAL:HG13	1.89	0.53
79:E:6:SER:HA	79:E:9:VAL:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:EC:6899:C:H2'	80:EC:6900:A:H8	1.73	0.53
1:BA:147:THR:HG21	1:BA:159:ALA:HB1	1.90	0.53
3:BC:170:ILE:HB	3:BC:197:TYR:HB2	1.91	0.53
5:BG:136:LYS:NZ	5:BG:174:LYS:O	2.31	0.53
18:Be:56:MET:HE2	34:B5:590:C:H5'	1.89	0.53
25:BS:30:TYR:O	25:BS:33:THR:OG1	2.25	0.53
28:BZ:90:LYS:NZ	28:BZ:103:ARG:O	2.36	0.53
57:AU:20:SER:HG	57:AU:61:THR:HG1	1.56	0.53
1:BA:198:MET:HG2	1:BA:200:ASP:H	1.72	0.53
18:Be:29:LYS:HD2	18:Be:35:TYR:HE1	1.73	0.53
38:A1:1620:U:H2'	38:A1:1621:A:C8	2.44	0.53
38:A1:3160:U:H2'	38:A1:3161:C:C6	2.44	0.53
49:AM:32:LEU:HD11	49:AM:94:TRP:CD2	2.44	0.53
50:AN:121:VAL:HG12	50:AN:122:ASN:HD22	1.74	0.53
1:BA:6:THR:HG22	1:BA:191:ARG:HH11	1.74	0.53
16:Ba:97:PRO:HG2	16:Ba:98:PRO:HD3	1.88	0.53
20:BF:84:LYS:NZ	34:B5:1614:A:OP2	2.40	0.53
34:B5:868:G:H1	34:B5:960:U:H3	1.57	0.53
37:AC:350:LYS:HG2	37:AC:351:PRO:HD2	1.91	0.53
38:A1:1799:A:H2'	38:A1:1800:A:H8	1.74	0.53
38:A1:2816:G:N2	38:A1:2819:A:OP2	2.41	0.53
38:A1:2909:U:H2'	38:A1:2910:A:O4'	2.09	0.53
1:BA:79:ARG:HH21	1:BA:81:PHE:HD2	1.56	0.53
22:BP:111:MET:HG2	25:BS:119:ILE:HG23	1.89	0.53
38:A1:2724:OMU:OP1	56:AT:78:LYS:NZ	2.40	0.53
38:A1:3231:U:H2'	38:A1:3232:G:H8	1.73	0.53
41:AD:178:ASN:HA	41:AD:183:TRP:CD2	2.44	0.53
63:Aa:60:TYR:CD2	63:Aa:63:LYS:HB2	2.44	0.53
78:Ap:46:THR:OG1	78:Ap:57:CYS:SG	2.65	0.53
4:BE:22:LYS:NZ	34:B5:758:U:OP1	2.42	0.52
15:BY:32:ARG:CZ	15:BY:35:VAL:HG12	2.39	0.52
27:BU:53:LYS:HE2	34:B5:1345:A:H5'	1.90	0.52
34:B5:17:C:O2'	34:B5:1137:A:N1	2.40	0.52
38:A1:760:G:H1'	38:A1:771:A:N6	2.24	0.52
38:A1:1460:A:H2'	38:A1:1461:A:C8	2.45	0.52
56:AT:152:ALA:HB1	56:AT:153:PRO:HD2	1.91	0.52
2:BB:214:LYS:NZ	34:B5:886:U:OP1	2.29	0.52
5:BG:187:LYS:NZ	34:B5:139:C:O2'	2.41	0.52
24:BR:56:HIS:NE2	34:B5:1401:A:OP1	2.38	0.52
26:BT:84:LYS:HD2	26:BT:94:ILE:HD12	1.91	0.52
31:Bg:74:THR:HA	31:Bg:115:ILE:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:706:A:H3'	34:B5:708:C:H5''	1.91	0.52
38:A1:1259:A:O2'	38:A1:1260:A:O5'	2.21	0.52
80:EC:6804:A:O2'	80:EC:6808:G:N2	2.33	0.52
5:BG:122:GLU:OE1	5:BG:122:GLU:N	2.42	0.52
6:BH:34:LEU:HD12	6:BH:38:LEU:HB3	1.91	0.52
11:BO:46:MET:HE3	34:B5:898:A:H4'	1.91	0.52
23:BQ:40:GLU:CD	23:BQ:41:PRO:HA	2.35	0.52
26:BT:39:THR:OG1	34:B5:1478:G:OP1	2.24	0.52
31:Bg:35:SER:HB3	31:Bg:45:TRP:HZ3	1.74	0.52
34:B5:406:U:H2'	34:B5:407:A:H8	1.75	0.52
38:A1:1157:G:H2'	38:A1:1158:A:O4'	2.08	0.52
38:A1:1553:U:H4'	38:A1:1554:U:H5'	1.91	0.52
38:A1:2180:G:H2'	38:A1:2181:C:C6	2.44	0.52
38:A1:2458:A:C6	38:A1:2477:G:H5''	2.44	0.52
39:A3:70:U:H2'	39:A3:71:G:H8	1.74	0.52
79:E:39:LYS:N	79:E:200:ASN:O	2.43	0.52
4:BE:95:THR:HG22	15:BY:16:PRO:HG2	1.89	0.52
19:BD:67:ASN:ND2	21:BK:91:TYR:O	2.43	0.52
21:BK:45:ALA:O	21:BK:48:SER:OG	2.26	0.52
24:BR:33:ARG:NH2	34:B5:1387:G:OP1	2.43	0.52
34:B5:1564:U:H2'	34:B5:1565:C:C6	2.45	0.52
34:B5:1619:C:H2'	34:B5:1620:C:H6	1.72	0.52
35:AA:180:LEU:HD22	78:Ap:18:TYR:HB3	1.91	0.52
38:A1:1076:C:C6	64:Ab:42:ASN:ND2	2.77	0.52
41:AD:107:ARG:HD2	41:AD:248:ARG:HD3	1.92	0.52
45:AH:22:SER:OG	45:AH:23:ARG:N	2.43	0.52
80:EC:6869:C:O2'	80:EC:6870:A:O4'	2.28	0.52
80:EC:6890:A:H2'	80:EC:6891:G:C8	2.45	0.52
80:EC:6919:G:C2	80:EC:6920:C:H1'	2.45	0.52
2:BB:69:CYS:HA	2:BB:83:LYS:HA	1.92	0.52
4:BE:188:ASN:OD1	4:BE:191:ARG:HD3	2.09	0.52
8:BJ:175:ARG:HE	8:BJ:179:ARG:HH12	1.56	0.52
20:BF:143:ARG:HH21	20:BF:214:LYS:HZ3	1.58	0.52
26:BT:27:LYS:O	26:BT:110:LYS:NZ	2.43	0.52
33:BM:111:ASN:HB3	33:BM:113:ARG:HB3	1.92	0.52
34:B5:185:U:H2'	34:B5:186:C:H6	1.75	0.52
38:A1:1223:A:N1	38:A1:1287:A:O2'	2.32	0.52
38:A1:1257:C:H2'	38:A1:1258:U:C6	2.45	0.52
38:A1:1834:U:OP2	74:Al:10:LYS:NZ	2.42	0.52
62:AZ:88:ASP:H	62:AZ:121:ARG:HH22	1.57	0.52
79:E:75:ASP:OD1	79:E:76:ARG:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:58:LEU:HD13	12:BV:12:TYR:HD2	1.73	0.52
31:Bg:172:ALA:HB2	31:Bg:178:VAL:HG12	1.92	0.52
31:Bg:305:TYR:CD2	31:Bg:311:ARG:NH1	2.78	0.52
36:AB:190:GLU:HA	36:AB:193:ASP:HB2	1.90	0.52
80:EC:6837:G:H2'	80:EC:6838:C:C6	2.44	0.52
5:BG:92:ARG:O	34:B5:405:C:O2'	2.24	0.52
15:BY:15:ASN:HD21	15:BY:18:LEU:HD12	1.75	0.52
31:Bg:214:ALA:HB1	31:Bg:240:VAL:HG23	1.91	0.52
34:B5:223:U:H2'	34:B5:224:C:C6	2.44	0.52
34:B5:850:A:H4'	54:AR:165:LYS:HD3	1.91	0.52
34:B5:1450:U:H2'	34:B5:1451:C:H6	1.75	0.52
38:A1:3013:U:H2'	38:A1:3014:U:C6	2.45	0.52
45:AH:167:VAL:HG23	45:AH:172:ILE:HG22	1.92	0.52
80:EC:6926:U:OP2	80:EC:6928:G:N1	2.39	0.52
4:BE:118:GLU:OE2	4:BE:237:SER:N	2.41	0.52
27:BU:70:THR:OG1	27:BU:72:ASN:OD1	2.28	0.52
34:B5:156:A:H2'	34:B5:157:A:O4'	2.10	0.52
37:AC:51:ALA:O	40:A4:26:U:O2'	2.28	0.52
37:AC:166:VAL:HG13	37:AC:170:LYS:NZ	2.25	0.52
38:A1:314:U:H2'	38:A1:315:C:C6	2.44	0.52
38:A1:1193:A:OP1	51:AO:49[A]:ARG:NH2	2.42	0.52
38:A1:2228:A:H2'	38:A1:2229:A:C8	2.44	0.52
1:BA:188:LEU:HD22	1:BA:195:TRP:HE1	1.75	0.52
31:Bg:38:ARG:HA	31:Bg:67:ILE:HG23	1.91	0.52
34:B5:1166:A:H2'	34:B5:1167:G:O4'	2.10	0.52
35:AA:69:TYR:OH	38:A1:2557:A:OP1	2.21	0.52
38:A1:656:A:H2'	38:A1:657:A:C8	2.45	0.52
38:A1:1278:A:H5''	38:A1:1279:C:H5	1.74	0.52
38:A1:1498:A:H2'	38:A1:1499:C:C6	2.44	0.52
38:A1:2364:G:H22	38:A1:2396:G:H1'	1.74	0.52
38:A1:2535:A:C2	38:A1:2536:A:H1'	2.45	0.52
38:A1:3324:C:OP1	66:Ad:19:ARG:NH1	2.37	0.52
46:AI:189:GLU:HG3	46:AI:200:LEU:HB3	1.92	0.52
47:AJ:15:GLU:HG2	47:AJ:132:ASN:HD21	1.74	0.52
68:Af:17:GLN:O	68:Af:24:ASN:N	2.42	0.52
20:BF:98:MET:HE1	20:BF:107:LYS:HA	1.91	0.52
24:BR:33:ARG:HG3	31:Bg:127:ARG:NH1	2.25	0.52
26:BT:45:MET:SD	26:BT:46:PRO:HD2	2.50	0.52
31:Bg:150:TRP:HE1	31:Bg:174:ASN:HD22	1.58	0.52
34:B5:146:U:H2'	34:B5:147:A:H8	1.75	0.52
34:B5:179:A:H3'	34:B5:180:A:C8	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:1208:A:H8	34:B5:1269:OMU:H6	1.74	0.52
34:B5:1241:G:H2'	34:B5:1242:A:O4'	2.10	0.52
34:B5:1469:A:H2'	34:B5:1470:C:C6	2.45	0.52
36:AB:216:ASP:HB2	36:AB:339:ARG:HB3	1.92	0.52
38:A1:1718:G:H2'	38:A1:1719:G:H8	1.74	0.52
38:A1:3084:C:O2'	38:A1:3332:U:OP1	2.23	0.52
38:A1:3233:C:H2'	38:A1:3234:A:C8	2.44	0.52
80:EC:6902:U:H4'	80:EC:6903:U:H5'	1.92	0.52
13:BW:30:SER:HB2	13:BW:61:ILE:HG13	1.93	0.51
22:BP:122:THR:HG21	34:B5:1454:G:H4'	1.92	0.51
34:B5:690:G:H2'	34:B5:691:C:H6	1.75	0.51
34:B5:1171:A:H2'	34:B5:1172:G:H8	1.73	0.51
38:A1:400:G:H4'	38:A1:401:U:H5''	1.92	0.51
38:A1:2357:A:H2'	38:A1:2358:A:C8	2.45	0.51
38:A1:2585:G:H2'	38:A1:2585:G:N3	2.25	0.51
38:A1:2592:G:H4'	38:A1:2594:C:C2	2.45	0.51
38:A1:2801:A:O2'	38:A1:2802:A:H2'	2.10	0.51
41:AD:146:LEU:HD22	41:AD:163:LEU:HD13	1.91	0.51
41:AD:268:GLU:O	41:AD:271:LYS:HG2	2.10	0.51
47:AJ:60:ARG:HH22	80:EC:6798:C:H4'	1.75	0.51
58:AV:15:LEU:HD13	58:AV:51:ALA:HB3	1.92	0.51
62:AZ:104:PRO:HA	62:AZ:107:ARG:HG2	1.92	0.51
80:EC:6771:U:O2'	80:EC:6777:C:N3	2.43	0.51
2:BB:218:LEU:O	2:BB:219:LYS:HE2	2.11	0.51
5:BG:50:PHE:HE1	5:BG:113:ILE:HG13	1.75	0.51
6:BH:114:ARG:NH1	34:B5:637:C:O2	2.37	0.51
11:BO:35:GLY:O	34:B5:918:U:O2'	2.25	0.51
20:BF:142:PRO:O	20:BF:142:PRO:HG2	2.10	0.51
23:BQ:55:VAL:HG21	23:BQ:105:LEU:HD23	1.92	0.51
34:B5:646:C:H2'	34:B5:647:G:O4'	2.10	0.51
34:B5:1575:G7M:H4'	34:B5:1576:A:OP2	2.10	0.51
38:A1:1718:G:H2'	38:A1:1719:G:C8	2.45	0.51
38:A1:2367:A:H2'	38:A1:2368:A:C8	2.45	0.51
38:A1:2544:U:H2'	38:A1:2545:C:C6	2.45	0.51
45:AH:92:TYR:CD2	45:AH:142:ASP:HB2	2.45	0.51
49:AM:4:ASP:OD1	49:AM:5:SER:N	2.41	0.51
80:EC:6828:G:H2'	80:EC:6829:A:H8	1.75	0.51
2:BB:216:LYS:NZ	34:B5:885:G:OP1	2.40	0.51
20:BF:185:ARG:NH2	34:B5:1572:OMG:H4'	2.25	0.51
31:Bg:110:VAL:HA	31:Bg:126:SER:HA	1.92	0.51
34:B5:1087:A:H2'	34:B5:1088:A:C8	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:1254:U:O2'	34:B5:1255:G:O4'	2.27	0.51
34:B5:1594:G:OP2	34:B5:1596:C:N4	2.44	0.51
37:AC:325:LEU:HD23	38:A1:598:A:H4'	1.91	0.51
38:A1:2160:G:H2'	38:A1:2161:G:H8	1.76	0.51
40:A4:47:C:H1'	40:A4:61:A:H2'	1.91	0.51
50:AN:192:LYS:O	50:AN:196:THR:OG1	2.25	0.51
7:BI:66:SER:HA	7:BI:73:SER:HA	1.92	0.51
9:BL:84:ILE:HG13	9:BL:109:VAL:HB	1.92	0.51
13:BW:119:LYS:HG2	34:B5:687:G:H5''	1.92	0.51
17:Bb:56:CYS:SG	17:Bb:57:GLU:N	2.83	0.51
37:AC:46:LYS:NZ	38:A1:691:A:OP1	2.42	0.51
38:A1:219:A:HO2'	38:A1:220:G:H21	1.58	0.51
38:A1:792:G:H2'	38:A1:793:C:C6	2.45	0.51
38:A1:1615:C:H2'	38:A1:1616:U:C6	2.45	0.51
51:AO:116[A]:LYS:NZ	55:AS:165:TYR:O	2.42	0.51
52:AP:33:ALA:HB1	52:AP:117:ILE:HG12	1.92	0.51
80:EC:6934:U:O2'	80:EC:6935:G:O5'	2.18	0.51
4:BE:79:ASP:HB3	4:BE:82:TYR:HB2	1.93	0.51
4:BE:187:ARG:NH1	34:B5:752:A:OP1	2.43	0.51
10:BN:42:ARG:HB3	65:Ac:97:ASP:OD1	2.11	0.51
15:BY:92:VAL:HG11	15:BY:99:LYS:HB2	1.92	0.51
16:Ba:32:LYS:O	16:Ba:37:LYS:NZ	2.38	0.51
23:BQ:13:LYS:HG3	23:BQ:14:LYS:H	1.75	0.51
31:Bg:216:LYS:HA	31:Bg:239:GLU:OE1	2.11	0.51
34:B5:1371:A:H4'	34:B5:1373:C:H5'	1.91	0.51
34:B5:1776:A:H2'	34:B5:1777:G:C8	2.46	0.51
38:A1:2697:A:H2'	38:A1:2698:G:H8	1.76	0.51
38:A1:2767:U:H2'	38:A1:2768:U:C6	2.46	0.51
38:A1:3332:U:H2'	38:A1:3333:G:O4'	2.11	0.51
44:AG:169:LEU:HA	71:AI:43:LEU:HD11	1.93	0.51
1:BA:176:LEU:O	1:BA:179:ARG:N	2.43	0.51
26:BT:57:ARG:NE	34:B5:1479:A:OP1	2.33	0.51
34:B5:1214:U:H5''	34:B5:1244:A:C8	2.30	0.51
38:A1:269:G:O6	50:AN:15:GLN:NE2	2.40	0.51
38:A1:792:G:H2'	38:A1:793:C:H6	1.75	0.51
38:A1:3006:A:H2'	38:A1:3007:U:O4'	2.11	0.51
46:AI:49:CYS:HB3	46:AI:168:SER:HB3	1.92	0.51
51:AO:61[A]:ALA:HA	51:AO:70[A]:PRO:HD2	1.90	0.51
78:Ap:49:ARG:HB2	78:Ap:55:TRP:CZ3	2.46	0.51
79:E:189:PHE:O	79:E:193:LEU:N	2.33	0.51
2:BB:197:ILE:HG22	2:BB:210:ILE:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BI:42:ARG:HG3	7:BI:58:LEU:HB2	1.93	0.51
8:BJ:106:GLU:O	8:BJ:112:GLN:NE2	2.43	0.51
34:B5:116:U:H2'	34:B5:117:U:C6	2.46	0.51
34:B5:625:C:H2'	34:B5:626:U:C6	2.45	0.51
35:AA:183:GLY:HA2	38:A1:896:A:H5''	1.92	0.51
38:A1:2526:C:H2'	38:A1:2527:G:H8	1.76	0.51
38:A1:3000:A:H2'	38:A1:3001:C:C6	2.45	0.51
73:AK:32:ASN:ND2	73:AK:36:LYS:H	2.08	0.51
80:EC:6808:G:O2'	80:EC:6809:G:O4'	2.28	0.51
1:BA:29:VAL:HG22	1:BA:149:LEU:HB3	1.92	0.51
1:BA:198:MET:SD	1:BA:198:MET:N	2.75	0.51
13:BW:118:ARG:NH1	34:B5:687:G:OP1	2.44	0.51
27:BU:53:LYS:HB2	27:BU:92:ASP:HB3	1.93	0.51
31:Bg:131:ILE:HB	31:Bg:144:LEU:HB2	1.93	0.51
34:B5:1120:U:H2'	34:B5:1121:C:C6	2.45	0.51
36:AB:376:LYS:NZ	38:A1:3330:A:OP2	2.43	0.51
37:AC:193:LYS:NZ	40:A4:21:C:OP1	2.32	0.51
38:A1:407:A:C2	40:A4:17:A:H1'	2.46	0.51
38:A1:585:A:H4'	68:Af:72:THR:HG23	1.93	0.51
38:A1:1132:C:H2'	38:A1:1133:A2M:H8	1.91	0.51
38:A1:2768:U:H2'	38:A1:2769:A:H8	1.76	0.51
43:AF:138:TYR:CE2	43:AF:233:GLU:HB2	2.46	0.51
80:EC:6885:G:H2'	80:EC:6886:A:C8	2.46	0.51
1:BA:138:TYR:OH	34:B5:1296:A:OP1	2.25	0.51
26:BT:73:VAL:O	26:BT:77:ASN:ND2	2.44	0.51
34:B5:341:A:H2'	34:B5:342:C:C6	2.46	0.51
34:B5:891:A:H2'	34:B5:892:A:C8	2.46	0.51
34:B5:1374:C:H2'	34:B5:1375:A:O4'	2.10	0.51
38:A1:90:C:OP1	63:Aa:59:ARG:NH1	2.42	0.51
38:A1:219:A:O2'	38:A1:220:G:N2	2.36	0.51
41:AD:186:GLU:HG2	41:AD:187:THR:HG23	1.93	0.51
2:BB:146:GLN:OE1	2:BB:206:PRO:HG3	2.09	0.51
20:BF:43:PHE:HE1	20:BF:71:ALA:H	1.58	0.51
22:BP:127:ARG:HB3	22:BP:130:ARG:HG2	1.93	0.51
31:Bg:179:LYS:HZ1	31:Bg:188:ILE:HG13	1.76	0.51
31:Bg:254:ALA:HB3	31:Bg:261:LYS:HE3	1.93	0.51
34:B5:1542:G:H22	34:B5:1568:C:H1'	1.75	0.51
38:A1:523:A:O2'	55:AS:69:PRO:HD2	2.11	0.51
38:A1:1090:G:H2'	38:A1:1091:A:H8	1.75	0.51
38:A1:1181:U:O4	51:AO:21[A]:SER:OG	2.20	0.51
39:A3:22:A:H2'	39:A3:23:A:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AL:27:ASP:OD2	48:AL:27:ASP:N	2.40	0.51
13:BW:22:LYS:HA	17:Bb:3:LEU:HB2	1.94	0.50
15:BY:26:ASP:HB3	15:BY:70:VAL:HG23	1.93	0.50
30:Bd:7:TRP:CZ3	34:B5:1242:A:H1'	2.45	0.50
34:B5:654:C:H41	34:B5:655:G:N2	2.09	0.50
38:A1:1108:U:H2'	38:A1:1109:U:C6	2.46	0.50
38:A1:1283:C:H3'	38:A1:1283:C:OP2	2.11	0.50
38:A1:1657:C:O2'	38:A1:1797:A:OP2	2.21	0.50
38:A1:2223:A:H2'	38:A1:2224:A:C8	2.46	0.50
38:A1:3084:C:OP1	59:AW:38:SER:OG	2.26	0.50
43:AF:98:LYS:HB3	43:AF:99:PRO:HD3	1.93	0.50
47:AJ:18:VAL:HG22	47:AJ:70:THR:HG22	1.93	0.50
2:BB:87:ARG:HG2	2:BB:101:HIS:HB2	1.93	0.50
3:BC:53:ILE:HD13	3:BC:73:LEU:HD11	1.94	0.50
7:BI:152:ILE:HG13	7:BI:153:GLU:N	2.26	0.50
15:BY:26:ASP:HA	15:BY:70:VAL:HA	1.93	0.50
22:BP:27:GLU:HG3	22:BP:88:GLU:HA	1.93	0.50
22:BP:44:ARG:NH1	22:BP:82:ASN:O	2.42	0.50
22:BP:48:GLY:O	22:BP:49:MET:HE2	2.12	0.50
22:BP:89:MET:HE2	22:BP:94:VAL:HG22	1.93	0.50
26:BT:88:VAL:HG12	34:B5:1601:G:N2	2.26	0.50
26:BT:122:ARG:HH22	34:B5:1500:C:P	2.34	0.50
29:Bc:14:LYS:HB3	29:Bc:29:ARG:HB3	1.93	0.50
31:Bg:169:ILE:HG13	31:Bg:181:TRP:HB2	1.92	0.50
31:Bg:252:LEU:HD23	31:Bg:265:LEU:HB3	1.94	0.50
34:B5:1224:A:H2'	34:B5:1225:U:C6	2.46	0.50
34:B5:1566:U:N3	34:B5:1567:U:O4	2.44	0.50
37:AC:126:ILE:O	37:AC:129:THR:OG1	2.22	0.50
38:A1:2213:A:H2'	38:A1:2214:A:H8	1.76	0.50
40:A4:12:A:OP1	52:AP:3:ARG:NH2	2.41	0.50
50:AN:43:THR:HG23	50:AN:44:ARG:HG3	1.93	0.50
57:AU:43:VAL:HG12	57:AU:44:GLU:OE1	2.12	0.50
63:Aa:96:LYS:C	63:Aa:98:THR:H	2.19	0.50
80:EC:6910:A:H2'	80:EC:6911:A:O4'	2.11	0.50
5:BG:66:GLY:HA2	34:B5:1681:A:H1'	1.91	0.50
14:BX:5:LYS:NZ	34:B5:614:C:OP2	2.39	0.50
26:BT:84:LYS:NZ	34:B5:1563:C:OP1	2.38	0.50
34:B5:688:G:H2'	34:B5:689:G:H8	1.76	0.50
34:B5:1346:A:H62	34:B5:1370:U:H6	1.58	0.50
34:B5:1450:U:H2'	34:B5:1451:C:C6	2.46	0.50
34:B5:1480:G:H2'	34:B5:1481:C:O4'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:1110:U:H2'	38:A1:1111:U:C6	2.45	0.50
38:A1:2144:A:H1'	38:A1:2281:A2M:N6	2.27	0.50
38:A1:3308:C:O2'	52:AP:69:ARG:O	2.23	0.50
41:AD:216:GLU:O	41:AD:220:SER:N	2.44	0.50
45:AH:18:VAL:O	49:AM:5:SER:HB2	2.11	0.50
80:EC:6780:A:H2'	80:EC:6781:U:C4	2.46	0.50
80:EC:6891:G:H2'	80:EC:6892:U:H6	1.76	0.50
2:BB:32:ILE:HG12	2:BB:96:LEU:HD22	1.92	0.50
16:Ba:88:SER:HA	34:B5:1628:U:H5'	1.94	0.50
34:B5:680:U:H2'	34:B5:682:C:H41	1.76	0.50
34:B5:841:U:H2'	34:B5:842:C:C6	2.46	0.50
34:B5:1738:U:H2'	34:B5:1739:C:H6	1.75	0.50
35:AA:5:ILE:HG22	35:AA:208:ASP:O	2.10	0.50
36:AB:250:ALA:HB1	38:A1:2947:G:C2	2.47	0.50
38:A1:787:G:H2'	38:A1:788:C:C6	2.47	0.50
38:A1:1659:U:H2'	38:A1:1660:C:C6	2.47	0.50
38:A1:3187:A:C2	55:AS:171:PHE:HB3	2.46	0.50
5:BG:154:ARG:HD3	34:B5:78:A:N7	2.26	0.50
19:BD:120:TYR:HE1	19:BD:152:PHE:HD2	1.59	0.50
19:BD:137:VAL:HG22	19:BD:185:LYS:HB2	1.92	0.50
31:Bg:112:SER:HB2	31:Bg:154:VAL:H	1.76	0.50
31:Bg:255:ALA:HB1	31:Bg:289:ALA:HB3	1.93	0.50
32:Bf:138:ARG:NH1	34:B5:1236:A:N3	2.59	0.50
34:B5:52:U:H2'	34:B5:53:G:C8	2.47	0.50
34:B5:138:A:N6	34:B5:266:A:H61	2.10	0.50
34:B5:751:G:H2'	34:B5:752:A:C8	2.46	0.50
34:B5:1172:G:H2'	34:B5:1173:C:C6	2.46	0.50
37:AC:166:VAL:HG13	37:AC:170:LYS:HZ2	1.77	0.50
38:A1:249:U:H1'	38:A1:251:G:O5'	2.11	0.50
38:A1:374:A:N3	38:A1:376:G:H5''	2.26	0.50
38:A1:2344:U:H2'	38:A1:2345:A:H8	1.76	0.50
38:A1:3373:U:OP2	66:Ad:102:LYS:NZ	2.28	0.50
8:BJ:150:LEU:HA	8:BJ:153:GLU:HG2	1.94	0.50
14:BX:89:ASN:HB2	14:BX:92:CYS:SG	2.52	0.50
19:BD:162:GLN:HB3	34:B5:1332:C:O2'	2.12	0.50
31:Bg:114:ASP:OD2	31:Bg:156:VAL:N	2.37	0.50
34:B5:100:A2M:H8	34:B5:100:A2M:O5'	2.12	0.50
34:B5:795:U:H2'	34:B5:796:A2M:H8	1.93	0.50
34:B5:1483:A:H2'	34:B5:1484:G:C8	2.46	0.50
38:A1:710:A:H2'	38:A1:711:A:C8	2.47	0.50
38:A1:1805:C:H2'	38:A1:1806:A:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:2438:A:H2'	38:A1:2439:A:H8	1.76	0.50
38:A1:2683:U:H2'	38:A1:2684:C:C6	2.47	0.50
76:An:1:MET:HG2	76:An:6:ARG:HB2	1.94	0.50
80:EC:6891:G:H2'	80:EC:6892:U:C6	2.47	0.50
3:BC:53:ILE:HG23	3:BC:72:LEU:HB3	1.93	0.50
15:BY:57:VAL:HB	15:BY:60:PHE:CE2	2.42	0.50
21:BK:49:LEU:HD21	21:BK:54:TYR:HB2	1.92	0.50
22:BP:78:THR:OG1	22:BP:80:MET:SD	2.65	0.50
34:B5:683:C:H2'	34:B5:684:A:C8	2.47	0.50
34:B5:1471:A:H2	34:B5:1474:G:N3	2.10	0.50
38:A1:1013:G:H2'	38:A1:1014:U:O4'	2.12	0.50
38:A1:1069:C:H2'	38:A1:1070:U:H6	1.76	0.50
38:A1:1246:G:H2'	38:A1:1247:U:C6	2.46	0.50
38:A1:1312:C:O2'	51:AO:83[A]:ALA:O	2.29	0.50
40:A4:142:C:H2'	40:A4:143:U:C6	2.46	0.50
45:AH:161:LEU:HA	45:AH:164:ILE:HG12	1.94	0.50
50:AN:73:ARG:HG2	50:AN:75:VAL:HG13	1.94	0.50
55:AS:22:PRO:O	56:AT:146:ASN:ND2	2.32	0.50
62:AZ:101:PHE:O	62:AZ:107:ARG:NH2	2.44	0.50
80:EC:6760:A:H2'	80:EC:6761:C:O4'	2.11	0.50
80:EC:6929:C:H2'	80:EC:6930:G:H8	1.76	0.50
4:BE:200:ARG:NH1	34:B5:737:A:OP1	2.44	0.50
5:BG:123:GLY:O	5:BG:127:THR:OG1	2.29	0.50
38:A1:2427:U:H2'	38:A1:2428:U:C6	2.47	0.50
41:AD:34:LYS:HE3	56:AT:30:TYR:CZ	2.46	0.50
41:AD:244:HIS:O	41:AD:248:ARG:HG2	2.11	0.50
51:AO:173[A]:ALA:HA	51:AO:176[A]:LYS:HE2	1.93	0.50
6:BH:109:VAL:HG12	6:BH:110:GLN:H	1.77	0.50
20:BF:112:ARG:HD3	23:BQ:43:ILE:HD12	1.93	0.50
21:BK:14:TYR:CD1	21:BK:35:ILE:HD11	2.47	0.50
26:BT:21:PHE:O	26:BT:24:ARG:NH2	2.45	0.50
30:Bd:31:ILE:HG22	34:B5:1199:G:N1	2.27	0.50
34:B5:15:U:H2'	34:B5:16:G:O4'	2.12	0.50
34:B5:205:U:C2	34:B5:206:A:C8	3.00	0.50
34:B5:1056:U:OP2	34:B5:1057:U:H5'	2.12	0.50
34:B5:1180:C:N3	34:B5:1458:G:N2	2.53	0.50
34:B5:1452:U:C2	34:B5:1453:G:C8	3.00	0.50
35:AA:136:ILE:HA	35:AA:148:VAL:HG12	1.93	0.50
38:A1:169:U:H5	38:A1:253:A:N1	2.09	0.50
38:A1:876:A2M:H5''	38:A1:1890:U:H5''	1.94	0.50
38:A1:879:U:O2'	52:AP:135:ARG:NH2	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:1560:G:O2'	38:A1:1561:G:O4'	2.29	0.50
38:A1:2160:G:H2'	38:A1:2161:G:C8	2.47	0.50
38:A1:3165:A:H2'	38:A1:3166:C:C6	2.46	0.50
48:AL:50:PRO:HG3	70:Ah:118:ILE:HD11	1.93	0.50
63:Aa:85:ASP:N	63:Aa:85:ASP:OD1	2.43	0.50
1:BA:38:PHE:O	1:BA:47:VAL:HB	2.12	0.49
2:BB:81:PHE:CD2	2:BB:82:ARG:HG3	2.47	0.49
3:BC:156:THR:HG22	13:BW:99:PHE:HZ	1.76	0.49
5:BG:140:ASN:O	5:BG:144:PHE:HB2	2.12	0.49
21:BK:41:TYR:HD1	21:BK:44:LYS:HD3	1.77	0.49
25:BS:40:ARG:NH1	34:B5:1539:G:H4'	2.26	0.49
30:Bd:31:ILE:HG22	34:B5:1199:G:H1	1.77	0.49
34:B5:319:U:H4'	34:B5:323:A:C8	2.46	0.49
34:B5:1641:C:H2'	34:B5:1642:G:C8	2.47	0.49
37:AC:34:ILE:HD12	37:AC:120:TYR:CE2	2.47	0.49
38:A1:82:C:H4'	50:AN:204:LYS:HE3	1.94	0.49
38:A1:92:G:H5'	38:A1:94:G:N7	2.27	0.49
38:A1:1262:G:H3'	38:A1:1263:A:H4'	1.93	0.49
38:A1:2961:G:H2'	38:A1:2962:U:C6	2.47	0.49
38:A1:3387:U:H2'	38:A1:3388:C:C6	2.47	0.49
47:AJ:62:ASN:ND2	77:Ao:102:GLN:O	2.45	0.49
55:AS:46:GLN:NE2	55:AS:51:VAL:O	2.39	0.49
7:BI:23:LYS:NZ	34:B5:391:A:OP2	2.38	0.49
19:BD:211:PRO:HG2	24:BR:19:ARG:HB2	1.94	0.49
34:B5:209:U:H2'	34:B5:210:A:H8	1.77	0.49
34:B5:424:C:O2'	34:B5:426:G:OP1	2.23	0.49
34:B5:1160:A:H2'	34:B5:1161:C:H6	1.76	0.49
34:B5:1360:A:N1	34:B5:1364:G:C6	2.80	0.49
38:A1:650:OMC:H2'	38:A1:651:G:C8	2.47	0.49
38:A1:2219:A:H2'	38:A1:2220:A2M:C8	2.42	0.49
45:AH:7:GLU:O	45:AH:8:GLN:NE2	2.44	0.49
69:Ag:3:GLN:HE22	69:Ag:29:ILE:HB	1.77	0.49
71:Ai:99:ARG:HD2	71:Ai:100:HIS:ND1	2.28	0.49
80:EC:6809:G:H2'	80:EC:6810:U:C6	2.47	0.49
5:BG:148:SER:OG	5:BG:150:GLU:O	2.28	0.49
22:BP:42:ARG:NH2	34:B5:1549:C:OP1	2.39	0.49
25:BS:137:HIS:NE2	34:B5:1457:C:O4'	2.45	0.49
34:B5:1482:C:N4	34:B5:1524:A:OP2	2.44	0.49
38:A1:532:A:H2'	38:A1:533:A:C8	2.47	0.49
38:A1:1120:A:H2'	38:A1:1121:U:H6	1.76	0.49
38:A1:3204:C:H2'	38:A1:3205:G:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:3322:A:H2'	38:A1:3323:A:H8	1.76	0.49
41:AD:34:LYS:O	41:AD:38:THR:OG1	2.21	0.49
60:AX:50:ALA:O	70:Ah:66:VAL:HG21	2.12	0.49
2:BB:128:LYS:HB3	2:BB:134:VAL:HG22	1.94	0.49
21:BK:1:MET:H3	21:BK:41:TYR:HE1	1.58	0.49
34:B5:505:A:H2'	34:B5:507:U:C2	2.47	0.49
34:B5:729:G:OP2	34:B5:730:G:H8	1.96	0.49
34:B5:947:U:H2'	34:B5:948:G:C8	2.47	0.49
34:B5:1647:U:H2'	34:B5:1648:A:C8	2.47	0.49
37:AC:221:ASN:ND2	38:A1:209:A:N3	2.57	0.49
38:A1:1688:U:H2'	38:A1:1689:U:C6	2.47	0.49
38:A1:2748:A:C2	41:AD:35:ARG:HG3	2.47	0.49
41:AD:41:LYS:HB2	56:AT:68:THR:O	2.12	0.49
41:AD:65:ILE:HG12	41:AD:74:VAL:HG22	1.94	0.49
45:AH:90:MET:O	45:AH:143:GLU:HG3	2.13	0.49
63:Aa:86:LYS:NZ	63:Aa:90:TYR:HE2	2.10	0.49
1:BA:167:LYS:NZ	1:BA:204:TYR:O	2.37	0.49
2:BB:164:ILE:O	2:BB:168:ILE:HG12	2.13	0.49
21:BK:88:PRO:HG3	21:BK:92:ILE:O	2.13	0.49
34:B5:393:C:H2'	34:B5:394:C:C6	2.48	0.49
34:B5:800:U:H2'	34:B5:801:G:H8	1.77	0.49
34:B5:1569:A:H2'	34:B5:1570:A:C8	2.48	0.49
36:AB:250:ALA:HB1	38:A1:2947:G:N3	2.27	0.49
38:A1:1311:G:N2	51:AO:86[A]:GLY:O	2.26	0.49
38:A1:3267:A:H2'	42:AE:69:PHE:CZ	2.47	0.49
39:A3:57:G:H4'	47:AJ:138:VAL:HG11	1.94	0.49
68:Af:16:TYR:OH	68:Af:89:LEU:O	2.30	0.49
14:BX:30:LYS:HE3	14:BX:34:LEU:HD11	1.95	0.49
14:BX:92:CYS:HA	14:BX:95:PHE:CD2	2.47	0.49
23:BQ:49:TYR:HB3	23:BQ:53:LEU:HD12	1.95	0.49
34:B5:849:C:C2	34:B5:850:A:C8	3.00	0.49
34:B5:1553:G:N2	34:B5:1555:A:H3'	2.26	0.49
34:B5:1713:G:H2'	34:B5:1714:A:C8	2.48	0.49
36:AB:180:GLU:OE2	38:A1:3002:C:O2'	2.27	0.49
38:A1:1592:G:OP1	69:Ag:58:ARG:NH2	2.37	0.49
39:A3:90:U:H2'	39:A3:91:G:O4'	2.13	0.49
71:Ai:9:ILE:HA	71:Ai:13:LYS:HD3	1.94	0.49
1:BA:157:ASP:OD1	12:BV:60:ARG:NE	2.37	0.49
8:BJ:109:LEU:HB2	8:BJ:146:PHE:HB3	1.94	0.49
25:BS:48:LYS:HD2	26:BT:35:ASP:OD1	2.13	0.49
33:BM:66:VAL:HG13	33:BM:67:THR:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BM:129:GLU:HB2	33:BM:133:LEU:HD13	1.94	0.49
34:B5:688:G:H2'	34:B5:689:G:C8	2.48	0.49
34:B5:1237:G:N2	34:B5:1249:U:O4	2.45	0.49
34:B5:1240:U:O2'	34:B5:1242:A:N7	2.40	0.49
34:B5:1253:U:N3	34:B5:1254:U:O4	2.45	0.49
34:B5:1396:U:O4	34:B5:1402:G:O6	2.31	0.49
38:A1:74:G:H5''	48:AL:104:ARG:HH21	1.77	0.49
38:A1:775:A:OP1	64:Ab:44:LYS:NZ	2.45	0.49
38:A1:1666:G:H2'	38:A1:1667:A:C8	2.47	0.49
38:A1:2683:U:H2'	38:A1:2684:C:H6	1.77	0.49
2:BB:64:ARG:NE	11:BO:36:LYS:HD3	2.28	0.49
4:BE:87:MET:HG3	4:BE:122:LYS:HB2	1.95	0.49
6:BH:24:PHE:HE1	6:BH:77:LEU:HD21	1.78	0.49
6:BH:170:GLN:O	6:BH:174:ASN:ND2	2.42	0.49
8:BJ:119:ALA:O	8:BJ:120:LYS:HG2	2.11	0.49
23:BQ:45:ARG:HG3	23:BQ:49:TYR:CE1	2.48	0.49
24:BR:17:ILE:HD11	24:BR:58:MET:SD	2.53	0.49
31:Bg:182:ASN:HD22	31:Bg:185:GLN:CD	2.20	0.49
33:BM:106:ILE:HG13	33:BM:107:ASP:H	1.77	0.49
34:B5:161:U:H2'	34:B5:162:A:C8	2.47	0.49
34:B5:416:A:H3'	34:B5:417:A:H8	1.78	0.49
38:A1:370:U:H4'	38:A1:404:G:H5'	1.95	0.49
38:A1:945:C:H2'	38:A1:946:U:C6	2.47	0.49
38:A1:2444:C:H2'	38:A1:2445:A:O4'	2.13	0.49
38:A1:2458:A:N6	38:A1:2478:C:OP2	2.33	0.49
50:AN:180:PHE:O	50:AN:184:LYS:HG3	2.13	0.49
52:AP:29:THR:HG22	52:AP:119:VAL:HG21	1.95	0.49
6:BH:28:GLU:HB2	6:BH:34:LEU:HD13	1.95	0.49
23:BQ:142:TYR:HE2	34:B5:1579:U:H5''	1.76	0.49
34:B5:366:A:OP1	34:B5:758:U:O2'	2.24	0.49
35:AA:44:ILE:HD13	35:AA:87:PHE:CE1	2.47	0.49
37:AC:170:LYS:NZ	37:AC:178:LEU:HD13	2.28	0.49
38:A1:230:U:H2'	38:A1:231:G:O4'	2.12	0.49
38:A1:818:C:O2'	72:Aj:7:SER:OG	2.26	0.49
38:A1:1785:U:H2'	38:A1:1786:G:C8	2.48	0.49
38:A1:1911:A:H2	38:A1:2122:G:C8	2.31	0.49
38:A1:2445:A:C5	38:A1:2503:G:C2	3.01	0.49
39:A3:4:U:H2'	39:A3:5:G:C8	2.47	0.49
41:AD:218:ARG:HA	41:AD:221:GLU:HG2	1.94	0.49
4:BE:175:PHE:CE1	4:BE:198:LYS:HD3	2.48	0.49
6:BH:9:LEU:HD21	6:BH:17:GLU:OE2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BH:44:LYS:HE3	6:BH:63:PRO:HG3	1.94	0.49
10:BN:60:VAL:HG13	10:BN:66:ILE:HD12	1.95	0.49
22:BP:31:GLU:HA	22:BP:34:VAL:HG22	1.94	0.49
26:BT:11:ALA:HB1	34:B5:1480:G:H4'	1.94	0.49
30:Bd:7:TRP:CH2	34:B5:1242:A:H1'	2.48	0.49
38:A1:631:U:H2'	38:A1:632:G:H8	1.77	0.49
38:A1:2232:A:H2'	38:A1:2233:A:C8	2.48	0.49
38:A1:2406:C:H2'	38:A1:2407:C:C6	2.48	0.49
38:A1:2679:A:H2	38:A1:2680:A:H62	1.60	0.49
38:A1:2688:U:OP1	41:AD:12:TYR:OH	2.16	0.49
38:A1:3047:U:O2'	38:A1:3048:A:H5'	2.13	0.49
38:A1:3067:C:H3'	54:AR:62:ARG:HH22	1.78	0.49
44:AG:107:GLU:O	44:AG:110:THR:OG1	2.25	0.49
45:AH:23:ARG:HH12	45:AH:42:ASP:H	1.60	0.49
7:BI:98:LYS:HB3	34:B5:329:G:H5''	1.95	0.48
16:Ba:23:CYS:HB2	16:Ba:30:ILE:HD11	1.95	0.48
34:B5:479:C:H2'	34:B5:480:G:H8	1.78	0.48
34:B5:906:A:H2'	34:B5:907:A:C8	2.48	0.48
38:A1:3162:C:H2'	38:A1:3163:A:H8	1.78	0.48
67:Ae:86:THR:HG23	67:Ae:87:MET:HG2	1.93	0.48
73:Ak:32:ASN:HD21	73:Ak:36:LYS:N	2.09	0.48
7:BI:73:SER:OG	34:B5:257:A:H1'	2.13	0.48
19:BD:161:GLY:HA3	34:B5:1331:A:H61	1.76	0.48
20:BF:40:ILE:HB	20:BF:67:PRO:HB2	1.96	0.48
25:BS:29:VAL:HG23	25:BS:30:TYR:CD1	2.46	0.48
34:B5:12:U:H2'	34:B5:13:C:H6	1.78	0.48
34:B5:183:U:H2'	34:B5:184:C:H6	1.78	0.48
34:B5:1482:C:O5'	34:B5:1521:G:N2	2.37	0.48
1:BA:34:GLU:O	1:BA:37:VAL:HG22	2.13	0.48
8:BJ:108:ARG:NH1	8:BJ:145:SER:HB3	2.28	0.48
23:BQ:30:LYS:HD2	23:BQ:66:ARG:HG2	1.95	0.48
27:BU:61:LYS:HB2	27:BU:86:ILE:HB	1.95	0.48
34:B5:848:C:H2'	34:B5:849:C:C6	2.46	0.48
34:B5:1682:U:O2'	34:B5:1683:C:O5'	2.31	0.48
34:B5:1770:U:H2'	34:B5:1771:U:C6	2.48	0.48
35:AA:181:LYS:HB2	38:A1:860:G:C5	2.49	0.48
36:AB:150:ARG:NH2	38:A1:3242:G:O6	2.46	0.48
38:A1:1292:C:O2'	38:A1:1293:U:OP1	2.28	0.48
40:A4:8:C:H2'	40:A4:9:A:C8	2.48	0.48
53:AQ:176:ARG:HA	53:AQ:182:LYS:O	2.13	0.48
79:E:149:THR:HA	79:E:152:ARG:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:77:SER:HB2	1:BA:86:VAL:HG21	1.95	0.48
7:BI:20:GLN:NE2	7:BI:22:ARG:O	2.47	0.48
7:BI:72:ILE:HD13	7:BI:112:TRP:CD2	2.48	0.48
22:BP:22:LEU:HD21	22:BP:109:PRO:HG3	1.94	0.48
27:BU:79:TRP:CE2	34:B5:1604:U:H5'	2.48	0.48
31:Bg:123:ILE:HG13	31:Bg:133:VAL:HG23	1.94	0.48
32:Bf:106:TYR:CZ	32:Bf:117:LEU:HD12	2.48	0.48
33:BM:130:THR:HG22	33:BM:132:GLU:H	1.79	0.48
34:B5:1311:U:O2'	34:B5:1313:A:N7	2.36	0.48
38:A1:806:A:N3	38:A1:2812:C:O2'	2.43	0.48
38:A1:1446:A:H5''	52:AP:65:SER:OG	2.13	0.48
38:A1:2520:A:H2'	38:A1:2521:U:C6	2.48	0.48
39:A3:27:A:H2'	39:A3:28:C:C6	2.48	0.48
41:AD:132:THR:HB	41:AD:172:TYR:HB2	1.95	0.48
49:AM:19:ARG:HH11	49:AM:65:LEU:HD23	1.78	0.48
80:EC:6886:A:H2'	80:EC:6887:G:C8	2.49	0.48
2:BB:176:VAL:HG12	2:BB:177:GLN:H	1.78	0.48
6:BH:13:PRO:HB2	6:BH:14:THR:HG22	1.95	0.48
19:BD:178:ARG:HD2	19:BD:179:GLN:HG3	1.94	0.48
25:BS:41:ARG:HG3	25:BS:85:PHE:CZ	2.48	0.48
26:BT:88:VAL:HG12	34:B5:1601:G:H22	1.78	0.48
29:Bc:40:ILE:HD12	29:Bc:42:ARG:HH11	1.77	0.48
31:Bg:14:GLU:HG2	31:Bg:14:GLU:O	2.13	0.48
31:Bg:74:THR:HA	31:Bg:115:ILE:CD1	2.44	0.48
34:B5:85:A:N3	34:B5:148:A:O2'	2.43	0.48
36:AB:21:ARG:HG2	38:A1:2991:A:OP1	2.14	0.48
37:AC:23:PRO:HD2	37:AC:26:PHE:CD2	2.49	0.48
38:A1:682:U:H5''	38:A1:683:U:H5	1.79	0.48
38:A1:1232:C:H42	38:A1:1257:C:N4	2.05	0.48
41:AD:270:LYS:HA	41:AD:273:ARG:HD2	1.95	0.48
63:Aa:86:LYS:HZ3	63:Aa:90:TYR:HE2	1.60	0.48
79:E:57:ASN:OD1	79:E:182:GLN:NE2	2.47	0.48
2:BB:116:LYS:HG2	2:BB:117:TRP:H	1.77	0.48
6:BH:7:LYS:HG2	54:AR:189:ALA:HA	1.95	0.48
19:BD:220:PRO:O	31:Bg:193:ILE:HG23	2.13	0.48
25:BS:134:ARG:HB2	25:BS:136:GLN:HE22	1.79	0.48
29:Bc:10:ALA:HA	29:Bc:32:PHE:HA	1.94	0.48
34:B5:1466:G:H2'	34:B5:1467:C:C6	2.49	0.48
34:B5:1591:C:H2'	34:B5:1592:A:C8	2.49	0.48
38:A1:20:A:H2'	38:A1:21:G:C8	2.49	0.48
38:A1:761:A:H2'	38:A1:762:U:C6	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:1184:A:H2'	38:A1:1185:C:C6	2.49	0.48
47:AJ:43:GLN:HE21	47:AJ:69:VAL:HG22	1.77	0.48
56:AT:57:TYR:CG	56:AT:89:LEU:HD21	2.49	0.48
78:Ap:44:LYS:HD2	78:Ap:59:CYS:SG	2.53	0.48
2:BB:31:ASP:OD1	2:BB:32:ILE:N	2.45	0.48
6:BH:41:LEU:HD12	6:BH:70:PHE:CD1	2.49	0.48
12:BV:41:GLU:O	12:BV:42:GLU:HG3	2.14	0.48
12:BV:87:ARG:HD2	17:Bb:2:VAL:HG21	1.95	0.48
15:BY:109:LYS:NZ	34:B5:459:G:OP1	2.46	0.48
17:Bb:70:LYS:NZ	34:B5:1050:G:OP1	2.43	0.48
22:BP:59:LYS:HE3	34:B5:1240:U:O4	2.14	0.48
23:BQ:7:VAL:HG22	23:BQ:92:TYR:HD2	1.79	0.48
23:BQ:77:GLN:O	23:BQ:81:ILE:HD12	2.14	0.48
34:B5:1521:G:O2'	34:B5:1523:G:OP2	2.24	0.48
38:A1:110:G:C2	38:A1:111:C:H1'	2.49	0.48
38:A1:900:G:H1'	38:A1:1589:A:N6	2.29	0.48
38:A1:1340:G:H2'	38:A1:1341:U:C6	2.49	0.48
38:A1:2356:A:H61	38:A1:2983:C:H5	1.62	0.48
38:A1:2465:G:H22	79:E:33:GLU:HG3	1.79	0.48
3:BC:44:LEU:HD11	3:BC:243:TYR:HB3	1.95	0.48
6:BH:139:ARG:O	6:BH:151:LYS:N	2.41	0.48
19:BD:67:ASN:HD21	21:BK:95:ARG:NH1	2.11	0.48
24:BR:69:ILE:O	24:BR:74:GLN:NE2	2.47	0.48
34:B5:231:U:C2	34:B5:233:C:H1'	2.49	0.48
34:B5:304:U:H2'	34:B5:305:C:C6	2.48	0.48
34:B5:1202:A:H1'	34:B5:1207:C:H42	1.79	0.48
38:A1:87:U:OP1	53:AQ:167:SER:OG	2.30	0.48
38:A1:525:C:OP2	49:AM:77:ARG:NH2	2.47	0.48
38:A1:2506:U:HO2'	38:A1:2507:C:P	2.37	0.48
44:AG:78:PHE:C	44:AG:80:TYR:H	2.22	0.48
62:AZ:121:ARG:HD2	62:AZ:126:LYS:HD2	1.96	0.48
2:BB:89:ASP:HB3	2:BB:223:PHE:HE1	1.77	0.48
2:BB:130:SER:HB2	2:BB:180:THR:HG22	1.96	0.48
22:BP:98:ASN:HB2	22:BP:122:THR:HA	1.96	0.48
31:Bg:150:TRP:HE1	31:Bg:174:ASN:ND2	2.12	0.48
34:B5:861:U:H3'	34:B5:862:A:C8	2.49	0.48
34:B5:1226:A:H5''	34:B5:1229:G:H4'	1.95	0.48
34:B5:1755:A:N3	80:EC:6951:C:O2'	2.47	0.48
38:A1:1214:U:H2'	38:A1:1215:U:C6	2.48	0.48
38:A1:1619:A:H2'	38:A1:1620:U:O4'	2.14	0.48
38:A1:1922:A:H2'	38:A1:1923:C:O4'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:AI:36:LEU:HD21	46:AI:69:ARG:HD3	1.96	0.48
55:AS:46:GLN:HE22	55:AS:52:LYS:HA	1.78	0.48
79:E:112:ALA:H	79:E:135:PRO:HB3	1.78	0.48
8:BJ:157:ASP:OD2	8:BJ:158:PHE:N	2.38	0.48
21:BK:16:PHE:CE1	21:BK:89:GLY:HA3	2.49	0.48
31:Bg:46:LYS:HE2	31:Bg:58:VAL:HG11	1.96	0.48
35:AA:14:SER:OG	38:A1:911:C:OP1	2.32	0.48
38:A1:2506:U:O2'	38:A1:2507:C:OP1	2.25	0.48
38:A1:2861:U:H2'	38:A1:2862:U:O4'	2.14	0.48
51:AO:40[A]:GLU:HG3	51:AO:40[A]:GLU:O	2.14	0.48
77:Ao:2:VAL:N	77:Ao:90:HIS:O	2.46	0.48
19:BD:116:ARG:HH11	19:BD:117:ARG:NH2	2.12	0.47
20:BF:51:VAL:HG21	20:BF:130:ILE:HD11	1.96	0.47
23:BQ:127:LYS:HE2	23:BQ:131:GLY:O	2.14	0.47
34:B5:71:A:H2'	34:B5:72:A:H4'	1.96	0.47
34:B5:1780:G:N3	38:A1:2262:A:O2'	2.45	0.47
38:A1:68:C:OP2	38:A1:301:G:N2	2.44	0.47
38:A1:1037:C:H2'	38:A1:1038:C:H6	1.79	0.47
38:A1:1738:C:H1'	69:Ag:52:GLN:HE21	1.78	0.47
57:AU:53:ALA:HB1	57:AU:69:ALA:HB2	1.96	0.47
80:EC:6885:G:H2'	80:EC:6886:A:H8	1.79	0.47
2:BB:121:ILE:HG12	2:BB:161:ILE:HD12	1.96	0.47
10:BN:106:ARG:HH21	34:B5:1019:A:H5''	1.79	0.47
15:BY:46:GLU:O	15:BY:49:LYS:HE3	2.13	0.47
21:BK:60:SER:HB2	21:BK:65:TYR:CE1	2.50	0.47
25:BS:53:ASP:OD1	25:BS:55:HIS:ND1	2.47	0.47
31:Bg:300:THR:HG23	31:Bg:314:GLN:HB3	1.96	0.47
34:B5:492:A:H4'	34:B5:493:U:C5	2.49	0.47
34:B5:1524:A:H2'	34:B5:1525:A:C8	2.49	0.47
38:A1:887:G:H2'	38:A1:888:A:C8	2.49	0.47
38:A1:1565:G:C2	38:A1:1566:A:C8	3.02	0.47
38:A1:2974:U:H2'	38:A1:2975:U:C6	2.49	0.47
41:AD:217:GLU:HA	41:AD:220:SER:HB2	1.96	0.47
51:AO:65[A]:ASN:HB3	51:AO:68[A]:ARG:HG2	1.95	0.47
1:BA:72:ASP:HB2	1:BA:118:PRO:HA	1.97	0.47
22:BP:15:HIS:CE1	22:BP:110:GLU:HG2	2.49	0.47
29:Bc:42:ARG:HE	29:Bc:56:LEU:HD22	1.79	0.47
34:B5:844:A:H2'	34:B5:845:G:C8	2.48	0.47
34:B5:884:A:H2'	34:B5:885:G:C8	2.48	0.47
38:A1:422:A:C2	38:A1:2363:A:H4'	2.48	0.47
38:A1:1525:G:H5'	38:A1:1830:G:OP2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:1627:U:C2	38:A1:1817:G:O6	2.67	0.47
38:A1:1807:G:H5''	62:AZ:135:ARG:NH1	2.29	0.47
38:A1:2216:G:H22	38:A1:2229:A:H2	1.60	0.47
44:AG:168:ALA:HB3	71:AI:47:ILE:HD11	1.96	0.47
44:AG:172:LYS:HD3	71:AI:43:LEU:HD12	1.96	0.47
57:AU:22:PRO:HB2	57:AU:28:PHE:HB2	1.96	0.47
79:E:113:SER:HA	79:E:138:VAL:HG12	1.95	0.47
80:EC:6763:C:H2'	80:EC:6764:C:C6	2.49	0.47
16:Ba:11:ASN:OD1	34:B5:934:C:H1'	2.14	0.47
20:BF:120:ILE:CG1	28:BZ:59:TYR:HE1	2.28	0.47
22:BP:77:ARG:HH22	34:B5:1240:U:H5''	1.79	0.47
31:Bg:35:SER:O	31:Bg:42:LEU:HG	2.14	0.47
34:B5:250:C:H2'	34:B5:251:A:H8	1.80	0.47
34:B5:815:G:N3	54:AR:162:ARG:NH2	2.62	0.47
34:B5:1144:U:H2'	34:B5:1145:U:C6	2.48	0.47
34:B5:1178:G:H5'	34:B5:1190:C:H42	1.79	0.47
34:B5:1226:A:H2	34:B5:1229:G:N3	2.11	0.47
34:B5:1451:C:C2	34:B5:1452:U:C5	3.02	0.47
35:AA:140:ASN:O	35:AA:144:ASN:HA	2.14	0.47
38:A1:585:A:H2'	38:A1:586:C:C6	2.49	0.47
38:A1:1119:C:H2'	38:A1:1120:A:H8	1.79	0.47
38:A1:1517:G:OP1	74:AI:22:PRO:HG3	2.14	0.47
39:A3:23:A:H2'	39:A3:24:A:C8	2.50	0.47
39:A3:92:A:C5	39:A3:93:C:H1'	2.50	0.47
40:A4:113:U:H5''	74:AI:7:PHE:HB2	1.95	0.47
72:Aj:14:LYS:HD3	74:AI:51:ILE:HD11	1.96	0.47
11:BO:123:SER:HA	34:B5:929:A:C8	2.49	0.47
24:BR:45:ARG:NH1	34:B5:1332:C:OP2	2.47	0.47
34:B5:1179:G:H2'	34:B5:1180:C:H6	1.78	0.47
37:AC:358:THR:HG21	56:AT:148:PRO:HG2	1.97	0.47
38:A1:837:A:OP2	78:Ap:4:ARG:NE	2.38	0.47
38:A1:990:U:H1'	56:AT:101:CYS:HB3	1.97	0.47
38:A1:1047:A:N3	38:A1:2633:U:O2'	2.46	0.47
38:A1:2835:U:H2'	38:A1:2836:C:O2	2.15	0.47
46:AI:42:THR:HG22	46:AI:44:ASP:H	1.79	0.47
47:AJ:155:THR:HG22	47:AJ:156:LYS:N	2.29	0.47
49:AM:97:SER:O	49:AM:101:LYS:HG2	2.14	0.47
76:An:23:ARG:HG2	76:An:23:ARG:O	2.14	0.47
4:BE:175:PHE:HE1	4:BE:198:LYS:HD3	1.80	0.47
5:BG:60:GLY:O	34:B5:154:G:N2	2.32	0.47
14:BX:50:LYS:HD3	14:BX:101:GLU:OE2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BS:11:PHE:HB2	28:BZ:41:ILE:HG13	1.96	0.47
30:Bd:30:LEU:HA	30:Bd:39:CYS:HA	1.97	0.47
31:Bg:22:SER:HB3	31:Bg:36:ALA:HB3	1.95	0.47
36:AB:47:LEU:HD11	36:AB:179:ALA:HB3	1.97	0.47
37:AC:65:TRP:HB3	37:AC:69:ARG:HD3	1.97	0.47
38:A1:11:A:H2'	38:A1:12:A:C8	2.49	0.47
38:A1:1143:A:H5'	38:A1:1368:U:H1'	1.95	0.47
38:A1:1534:A:H2'	38:A1:1535:A:C8	2.49	0.47
38:A1:3182:G:H4'	51:AO:161[A]:LYS:HD3	1.97	0.47
41:AD:261:THR:O	41:AD:264:GLN:HG3	2.15	0.47
45:AH:126:VAL:HG21	45:AH:161:LEU:HB3	1.95	0.47
47:AJ:21:ILE:HG13	47:AJ:37:LEU:HD11	1.96	0.47
52:AP:60:PHE:HB3	52:AP:64:ASN:HB3	1.96	0.47
80:EC:6891:G:O2'	80:EC:6892:U:H5'	2.15	0.47
2:BB:134:VAL:HG12	2:BB:218:LEU:HD12	1.95	0.47
16:Ba:44:ILE:HG21	16:Ba:65:PRO:HG2	1.97	0.47
16:Ba:45:VAL:O	16:Ba:46:GLU:HG3	2.14	0.47
18:Be:31:LYS:HD3	34:B5:545:A:H2'	1.95	0.47
19:BD:39:VAL:HG22	19:BD:48:VAL:HG12	1.96	0.47
20:BF:147:THR:HG21	29:Bc:25:VAL:HG22	1.96	0.47
22:BP:18:ARG:HE	25:BS:90:ASN:CG	2.22	0.47
22:BP:79:HIS:CD2	34:B5:1241:G:C4	3.03	0.47
28:BZ:58:ARG:N	80:EC:6863:C:O2	2.42	0.47
31:Bg:182:ASN:HD21	31:Bg:184:ASN:HB2	1.78	0.47
31:Bg:253:ALA:HB1	31:Bg:292:LEU:HD11	1.97	0.47
34:B5:1552:U:H2'	34:B5:1553:G:O4'	2.15	0.47
35:AA:101:VAL:HG22	35:AA:165:VAL:HG22	1.97	0.47
35:AA:142:ASP:O	35:AA:143:GLU:HG3	2.15	0.47
38:A1:316:U:HO2'	71:Ai:30:LYS:HZ1	1.54	0.47
38:A1:707:U:OP1	38:A1:780:A:O2'	2.20	0.47
38:A1:874:U:OP2	38:A1:1907:C:O2'	2.27	0.47
38:A1:1671:C:OP1	54:AR:60:LYS:HE3	2.15	0.47
38:A1:2150:G:O2'	38:A1:2189:U:OP1	2.33	0.47
38:A1:2506:U:H2'	38:A1:2507:C:C6	2.49	0.47
38:A1:2882:U:H2'	38:A1:2883:U:C6	2.49	0.47
39:A3:47:C:OP2	41:AD:158:ARG:HD3	2.15	0.47
40:A4:91:C:H2'	40:A4:92:A:C8	2.50	0.47
58:AV:81:GLN:HG2	58:AV:83:LYS:H	1.79	0.47
73:Ak:7:ASP:HB3	73:Ak:10:GLN:HG2	1.97	0.47
10:BN:6:SER:OG	10:BN:7:ALA:N	2.47	0.47
20:BF:64:VAL:HG12	20:BF:65:ARG:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:BQ:46:PHE:HA	23:BQ:49:TYR:CD1	2.47	0.47
23:BQ:129:PHE:CE2	27:BU:78:THR:HA	2.50	0.47
31:Bg:214:ALA:HB1	31:Bg:240:VAL:CG2	2.45	0.47
34:B5:1493:A:H1'	34:B5:1494:C:H5	1.79	0.47
37:AC:35:VAL:HG11	37:AC:244:LEU:HD13	1.96	0.47
38:A1:201:A:H2'	38:A1:202:G:H8	1.80	0.47
38:A1:349:A:C4	40:A4:24:G:H1'	2.50	0.47
38:A1:1478:C:H2'	38:A1:1479:U:C6	2.50	0.47
38:A1:3333:G:N2	38:A1:3369:G:O2'	2.48	0.47
41:AD:197:SER:O	41:AD:202:GLY:N	2.37	0.47
46:AI:38:LYS:HB3	46:AI:41:ALA:HB2	1.97	0.47
60:AX:57:LEU:HD12	60:AX:61:LYS:HG3	1.97	0.47
80:EC:6851:G:O2'	80:EC:6852:U:H6	1.98	0.47
18:Be:29:LYS:HD2	18:Be:35:TYR:CE1	2.50	0.47
21:BK:2:LEU:HD11	34:B5:1258:U:H4'	1.97	0.47
25:BS:23:ASP:OD1	25:BS:24:GLY:N	2.48	0.47
34:B5:209:U:H2'	34:B5:210:A:C8	2.50	0.47
34:B5:1291:G:N2	34:B5:1324:G:H22	2.12	0.47
38:A1:159:A:H2'	38:A1:160:G:H8	1.78	0.47
38:A1:954:U:H5	38:A1:967:A:N1	2.12	0.47
38:A1:1190:A:H4'	75:Am:113:ARG:HH22	1.78	0.47
39:A3:71:G:H2'	39:A3:72:A:C8	2.50	0.47
46:AI:48:LEU:HD11	46:AI:167:LEU:HD11	1.95	0.47
47:AJ:137:ARG:HG2	47:AJ:141:ARG:HG3	1.96	0.47
48:AL:138:VAL:HG21	70:Ah:118:ILE:HB	1.97	0.47
55:AS:81:TYR:CE2	55:AS:90:MET:HE3	2.49	0.47
79:E:53:LEU:HG	79:E:54:LYS:H	1.79	0.47
79:E:191:VAL:HG13	79:E:197:ASN:OD1	2.15	0.47
1:BA:131:GLN:NE2	34:B5:1321:A:N7	2.58	0.47
14:BX:92:CYS:HG	14:BX:136:TRP:CD1	2.33	0.47
19:BD:7:LYS:HG2	34:B5:1515:A:OP2	2.15	0.47
19:BD:37:VAL:HG12	19:BD:50:ILE:HG22	1.97	0.47
22:BP:43:ARG:HE	22:BP:47:ARG:HD2	1.80	0.47
22:BP:87:PRO:HA	22:BP:90:ILE:HG13	1.97	0.47
27:BU:33:GLN:NE2	27:BU:110:PRO:O	2.48	0.47
31:Bg:74:THR:OG1	31:Bg:76:ASP:OD1	2.20	0.47
34:B5:413:U:H2'	34:B5:414:OMC:H6	1.80	0.47
34:B5:509:G:H2'	34:B5:510:G:C8	2.50	0.47
34:B5:950:C:O2'	34:B5:951:A:OP1	2.22	0.47
38:A1:283:G:OP2	38:A1:285:A:O2'	2.24	0.47
38:A1:1014:U:H2'	38:A1:1015:U:C2	2.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:1621:A:H2'	38:A1:1622:U:H6	1.78	0.47
38:A1:2675:C:H5''	38:A1:2676:A:H2'	1.95	0.47
40:A4:40:A:H2'	40:A4:41:A:H8	1.78	0.47
63:Aa:56:VAL:HG12	63:Aa:57:GLY:N	2.25	0.47
79:E:65:ILE:HD11	79:E:82:VAL:HG11	1.97	0.47
14:BX:107:PHE:HE1	14:BX:123:LYS:HB3	1.79	0.46
31:Bg:161:LYS:HB3	31:Bg:164:ASP:OD1	2.15	0.46
32:Bf:135:HIS:O	32:Bf:136:LYS:HD3	2.15	0.46
33:BM:28:LEU:HA	33:BM:31:VAL:HG12	1.96	0.46
34:B5:828:U:H2'	34:B5:829:A:O4'	2.15	0.46
38:A1:246:U:H2'	38:A1:247:C:C6	2.50	0.46
38:A1:262:U:H2'	38:A1:263:C:O4'	2.16	0.46
38:A1:1134:G:O2'	38:A1:2642:A:N3	2.40	0.46
38:A1:1616:U:H2'	38:A1:1617:G:C8	2.50	0.46
38:A1:2373:A:N3	38:A1:2824:G:O2'	2.30	0.46
39:A3:52:G:O2'	39:A3:53:U:OP1	2.32	0.46
56:AT:39:ILE:HD12	56:AT:63:VAL:HG22	1.97	0.46
73:Ak:27:ILE:HD13	73:Ak:39:ARG:NH2	2.30	0.46
80:EC:6790:A:N6	80:EC:6797:U:OP2	2.42	0.46
22:BP:85:ILE:HD12	22:BP:107:ILE:HD12	1.97	0.46
33:BM:58:LEU:HD23	33:BM:58:LEU:H	1.79	0.46
34:B5:1227:A:N6	34:B5:1256:A:H5''	2.31	0.46
34:B5:1617:U:H2'	34:B5:1618:C:C6	2.50	0.46
38:A1:339:C:OP1	38:A1:1380:G:O2'	2.31	0.46
38:A1:1211:U:H2'	38:A1:1212:A:C8	2.50	0.46
44:AG:47:SER:HA	44:AG:50:VAL:HG23	1.97	0.46
45:AH:130:ASP:OD1	45:AH:130:ASP:N	2.47	0.46
1:BA:79:ARG:O	1:BA:83:GLN:HG3	2.14	0.46
5:BG:20:ASP:OD2	5:BG:23:ARG:HG3	2.16	0.46
11:BO:103:ARG:HH21	16:Ba:49:ALA:HB2	1.79	0.46
17:Bb:64:CYS:HA	17:Bb:73:LEU:HA	1.97	0.46
17:Bb:77:THR:OG1	17:Bb:78:SER:N	2.48	0.46
19:BD:161:GLY:O	19:BD:164:VAL:HG12	2.15	0.46
27:BU:69:LYS:HG2	27:BU:80:GLU:HB2	1.98	0.46
34:B5:98:U:H2'	34:B5:99:C:C6	2.51	0.46
34:B5:781:U:H4'	34:B5:782:U:C6	2.50	0.46
34:B5:819:G:C4	34:B5:853:G:N2	2.83	0.46
34:B5:823:G:O6	34:B5:850:A:N6	2.47	0.46
36:AB:233:TRP:CD1	36:AB:265:ALA:HB1	2.50	0.46
38:A1:604:G:H2'	38:A1:605:U:C6	2.49	0.46
38:A1:2207:A:N6	38:A1:2233:A:OP2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Ad:55:LEU:HB2	66:Ad:95:PRO:HD3	1.97	0.46
5:BG:187:LYS:O	5:BG:190:GLN:HG2	2.16	0.46
14:BX:47:SER:HB2	34:B5:600:U:H1'	1.96	0.46
22:BP:96:ILE:HD11	22:BP:116:LEU:HD22	1.97	0.46
23:BQ:95:LYS:CA	31:Bg:59:ARG:HH12	2.22	0.46
34:B5:953:G:H2'	34:B5:954:G:C8	2.50	0.46
34:B5:1170:G:C2	34:B5:1171:A:C8	3.04	0.46
34:B5:1292:G:H2'	34:B5:1293:U:C6	2.51	0.46
34:B5:1694:A:N6	34:B5:1707:A:H62	2.14	0.46
36:AB:35:ASP:OD1	36:AB:185:GLY:N	2.40	0.46
38:A1:158:G:H2'	38:A1:159:A:H8	1.80	0.46
38:A1:643:U:O2'	38:A1:1153:A:N1	2.40	0.46
38:A1:675:C:O2'	38:A1:679:U:OP1	2.29	0.46
38:A1:1580:A:H4'	38:A1:1581:C:C2	2.50	0.46
38:A1:1744:G:H2'	38:A1:1745:C:C6	2.51	0.46
38:A1:2681:U:OP1	47:AJ:50:ALA:HA	2.16	0.46
60:AX:46:TYR:CD1	70:Ah:75:TYR:HB3	2.50	0.46
79:E:29:LEU:HD11	79:E:61:PRO:HD2	1.98	0.46
13:BW:56:HIS:O	34:B5:861:U:O2'	2.31	0.46
14:BX:96:VAL:HA	14:BX:127:VAL:HG21	1.96	0.46
25:BS:39:GLY:N	34:B5:1566:U:H5''	2.31	0.46
26:BT:53:TRP:HH2	26:BT:100:ILE:HD13	1.81	0.46
26:BT:129:GLN:NE2	34:B5:1358:G:O2'	2.48	0.46
31:Bg:87:LYS:HD2	31:Bg:107:LYS:O	2.16	0.46
35:AA:138:GLY:HA3	35:AA:147:ARG:CZ	2.45	0.46
38:A1:567:G:H2'	38:A1:568:G:C8	2.51	0.46
38:A1:987:U:H2'	38:A1:988:U:C6	2.50	0.46
38:A1:3291:G:H2'	38:A1:3292:A:C8	2.47	0.46
40:A4:10:A:H2'	40:A4:11:C:C6	2.51	0.46
43:AF:208:SER:O	43:AF:243:MET:HB2	2.16	0.46
68:Af:49:ILE:HD11	68:Af:71:VAL:HG22	1.96	0.46
80:EC:6846:C:N4	80:EC:6847:G:O6	2.48	0.46
2:BB:156:ALA:HB3	2:BB:161:ILE:HD11	1.98	0.46
4:BE:180:LEU:HB2	4:BE:230:GLU:O	2.16	0.46
9:BL:37:ASN:OD1	34:B5:247:A:H4'	2.16	0.46
11:BO:80:HIS:HD1	11:BO:114:ARG:HB2	1.79	0.46
16:Ba:58:VAL:HG23	16:Ba:59:TYR:CD2	2.51	0.46
19:BD:105:MET:HE3	19:BD:105:MET:HB2	1.85	0.46
31:Bg:22:SER:CB	31:Bg:70:ASP:HA	2.46	0.46
34:B5:585:A:H2'	34:B5:586:G:C8	2.51	0.46
34:B5:878:G:OP1	34:B5:943:C:O2'	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:1278:A:N3	38:A1:1278:A:H2'	2.30	0.46
38:A1:1597:C:H2'	38:A1:1598:G:C8	2.50	0.46
38:A1:1627:U:O2	38:A1:1817:G:C6	2.69	0.46
38:A1:2438:A:H2'	38:A1:2439:A:C8	2.50	0.46
38:A1:3353:G:H5'	38:A1:3354:U:C5	2.50	0.46
48:AL:165:SER:HA	63:Aa:135:GLU:OE2	2.16	0.46
80:EC:6937:G:H2'	80:EC:6939:C:H41	1.81	0.46
3:BC:44:LEU:HG	3:BC:49:LYS:HB2	1.96	0.46
19:BD:42:THR:HA	27:BU:108:ILE:HD11	1.98	0.46
21:BK:58:GLN:OE1	21:BK:58:GLN:N	2.49	0.46
23:BQ:9:THR:HA	34:B5:1340:U:O4	2.15	0.46
25:BS:65:GLU:HA	25:BS:68:ARG:HE	1.80	0.46
34:B5:447:U:H2'	34:B5:448:C:O4'	2.16	0.46
34:B5:565:C:H4'	34:B5:566:C:H6	1.80	0.46
34:B5:947:U:H2'	34:B5:948:G:H8	1.80	0.46
34:B5:1188:G:O2'	34:B5:1430:U:OP1	2.31	0.46
34:B5:1585:U:N3	34:B5:1611:A:H2	2.14	0.46
38:A1:142:C:H2'	38:A1:143:G:O4'	2.16	0.46
38:A1:2203:U:H2'	38:A1:2204:C:H6	1.80	0.46
49:AM:59:ASN:HB3	49:AM:62:GLN:OE1	2.15	0.46
63:Aa:60:TYR:HD2	63:Aa:63:LYS:HB2	1.80	0.46
79:E:157:PHE:HA	79:E:165:LEU:HD11	1.98	0.46
12:BV:2:GLU:HA	12:BV:8:LEU:HA	1.98	0.46
27:BU:39:SER:O	27:BU:43:LYS:HG3	2.16	0.46
32:Bf:113:LYS:HG3	32:Bf:114:VAL:H	1.80	0.46
33:BM:135:MET:HA	33:BM:138:GLU:HB3	1.97	0.46
34:B5:886:U:H2'	34:B5:887:A:H8	1.80	0.46
34:B5:1356:U:H2'	34:B5:1357:A:C8	2.50	0.46
34:B5:1685:G:H8	34:B5:1685:G:O5'	1.99	0.46
34:B5:1773:4AC:OP2	76:An:4:LYS:HB2	2.16	0.46
38:A1:1248:C:H2'	38:A1:1249:G:C8	2.51	0.46
38:A1:1290:A:H2'	38:A1:1291:A:C8	2.51	0.46
57:AU:27:VAL:HG12	57:AU:89:LEU:HD11	1.97	0.46
80:EC:6858:A:H4'	80:EC:6859:U:O5'	2.16	0.46
17:Bb:55:THR:OG1	17:Bb:60:SER:HA	2.15	0.46
20:BF:91:GLU:OE2	20:BF:107:LYS:NZ	2.39	0.46
20:BF:117:THR:O	20:BF:121:ILE:HD12	2.15	0.46
21:BK:16:PHE:O	21:BK:90:THR:OG1	2.34	0.46
31:Bg:178:VAL:HG21	31:Bg:223:TRP:CH2	2.50	0.46
38:A1:38:U:H2'	38:A1:39:A:O4'	2.16	0.46
39:A3:3:U:H2'	39:A3:4:U:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:AE:76:LEU:HD11	42:AE:141:VAL:HG21	1.98	0.46
46:AI:43:VAL:HG21	46:AI:197:VAL:HG13	1.97	0.46
47:AJ:15:GLU:OE2	47:AJ:72:ARG:NH1	2.48	0.46
50:AN:44:ARG:NH1	50:AN:120:TRP:O	2.48	0.46
60:AX:108:LEU:HD23	60:AX:125:ARG:HD3	1.97	0.46
6:BH:130:VAL:HG13	6:BH:130:VAL:O	2.16	0.46
18:Be:20:LYS:HE2	18:Be:20:LYS:HB2	1.67	0.46
21:BK:93:GLN:HG2	21:BK:94:GLU:N	2.31	0.46
27:BU:81:THR:O	30:Bd:54:LYS:HG2	2.16	0.46
34:B5:413:U:H2'	34:B5:414:OMC:C6	2.50	0.46
34:B5:1175:U:H2'	34:B5:1176:G:H8	1.80	0.46
34:B5:1252:C:H2'	34:B5:1253:U:O4'	2.16	0.46
38:A1:71:A:P	63:Aa:67:HIS:HE2	2.39	0.46
38:A1:238:A:H2'	38:A1:239:G:O4'	2.16	0.46
38:A1:362:U:O4	72:Aj:24:ARG:NH2	2.49	0.46
38:A1:748:U:H2'	38:A1:749:C:C6	2.51	0.46
38:A1:2894:C:H5'	45:AH:168:ARG:HH21	1.81	0.46
38:A1:3296:A:H2'	38:A1:3297:U:C6	2.51	0.46
49:AM:28:SER:HA	49:AM:31:LYS:HE2	1.98	0.46
62:AZ:95:VAL:HG13	62:AZ:96:VAL:HG13	1.98	0.46
5:BG:92:ARG:NH1	34:B5:1674:C:OP1	2.43	0.45
8:BJ:78:ARG:O	8:BJ:82:ARG:HB2	2.16	0.45
8:BJ:82:ARG:O	8:BJ:150:LEU:HB3	2.16	0.45
25:BS:127:HIS:CE1	25:BS:133:VAL:HG11	2.51	0.45
27:BU:45:ALA:HA	27:BU:50:LEU:HD13	1.98	0.45
28:BZ:91:PRO:HB3	28:BZ:101:TYR:CE2	2.51	0.45
31:Bg:63:GLY:HA2	34:B5:1341:A:OP1	2.17	0.45
31:Bg:113:VAL:HG23	31:Bg:124:SER:HB3	1.98	0.45
31:Bg:127:ARG:HA	31:Bg:150:TRP:HB2	1.97	0.45
33:BM:42:ALA:HB2	33:BM:124:LYS:HE3	1.97	0.45
34:B5:256:A:H2'	34:B5:257:A:O4'	2.16	0.45
34:B5:800:U:H2'	34:B5:801:G:C8	2.51	0.45
38:A1:1039:U:H2'	38:A1:1040:A:C8	2.51	0.45
38:A1:1242:G:H3'	38:A1:1243:G:C8	2.51	0.45
38:A1:1378:U:H2'	38:A1:1379:G:C8	2.51	0.45
38:A1:1498:A:H2'	38:A1:1499:C:H6	1.81	0.45
38:A1:2501:U:H3'	38:A1:2502:A:C8	2.44	0.45
38:A1:2594:C:H2'	38:A1:2595:A:O4'	2.16	0.45
39:A3:33:U:H2'	39:A3:34:C:C6	2.51	0.45
44:AG:82:LEU:HD13	44:AG:222:PHE:HE2	1.82	0.45
45:AH:109:ALA:C	45:AH:110:LYS:HG2	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AJ:50:ALA:HB3	47:AJ:62:ASN:N	2.31	0.45
49:AM:25:LYS:HE2	49:AM:62:GLN:HG3	1.98	0.45
60:AX:46:TYR:HD1	70:Ah:75:TYR:HB3	1.80	0.45
2:BB:111:ARG:HH22	34:B5:930:A:HO2'	1.64	0.45
15:BY:53:ASP:CG	15:BY:96:LEU:HD21	2.42	0.45
20:BF:112:ARG:HD3	23:BQ:43:ILE:HG23	1.98	0.45
34:B5:107:C:H2'	34:B5:108:A:C8	2.51	0.45
34:B5:406:U:H2'	34:B5:407:A:C8	2.51	0.45
34:B5:923:A:H2'	34:B5:924:A:C8	2.50	0.45
38:A1:226:C:H2'	38:A1:227:G:O4'	2.16	0.45
38:A1:1801:U:H2'	38:A1:1802:C:C6	2.51	0.45
38:A1:1810:A:H2'	38:A1:1811:G:C8	2.51	0.45
38:A1:1831:U:H2'	38:A1:1832:C:C6	2.51	0.45
38:A1:3209:A:C4	49:AM:106:ARG:HD3	2.50	0.45
38:A1:3273:A:H2'	38:A1:3274:A:C8	2.51	0.45
38:A1:3283:U:H2'	38:A1:3284:G:H8	1.81	0.45
1:BA:65:ALA:HB2	1:BA:181:VAL:HG23	1.98	0.45
2:BB:147:ALA:O	2:BB:148:ASN:OD1	2.34	0.45
4:BE:194:THR:HG21	4:BE:231:GLN:OE1	2.16	0.45
7:BI:98:LYS:NZ	34:B5:329:G:OP1	2.46	0.45
7:BI:119:GLN:HG2	7:BI:150:ALA:HB1	1.98	0.45
18:Be:3:LYS:HD3	18:Be:3:LYS:HA	1.71	0.45
20:BF:112:ARG:HA	20:BF:112:ARG:HD2	1.77	0.45
22:BP:118:GLU:O	25:BS:122:HIS:N	2.49	0.45
27:BU:88:LYS:NZ	34:B5:1347:U:O4	2.49	0.45
35:AA:142:ASP:OD1	35:AA:142:ASP:N	2.50	0.45
38:A1:394:G:N1	38:A1:397:A:OP2	2.49	0.45
38:A1:1566:A:N3	38:A1:1566:A:H2'	2.32	0.45
38:A1:2720:G:OP1	53:AQ:180:ARG:NH2	2.44	0.45
38:A1:2762:A:H2'	38:A1:2763:U:H6	1.81	0.45
43:AF:147:LEU:HA	43:AF:244:ASN:HD21	1.79	0.45
45:AH:106:LYS:HE3	45:AH:111:PHE:HE2	1.81	0.45
4:BE:45:ILE:HG13	4:BE:61:VAL:HG21	1.99	0.45
8:BJ:149:ARG:C	8:BJ:151:ASP:H	2.25	0.45
14:BX:70:LYS:NZ	34:B5:567:A:OP1	2.50	0.45
22:BP:76:VAL:O	22:BP:95:GLY:N	2.50	0.45
31:Bg:19:TRP:CE2	31:Bg:306:THR:HB	2.52	0.45
31:Bg:66:HIS:CG	31:Bg:67:ILE:H	2.34	0.45
34:B5:1669:U:H2'	34:B5:1670:G:O4'	2.17	0.45
36:AB:284:ARG:NH1	36:AB:293:ASN:O	2.49	0.45
37:AC:9:HIS:HA	37:AC:15:ALA:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:501:A:H2'	38:A1:502:U:C6	2.51	0.45
38:A1:2108:C:H1'	38:A1:3344:A:C8	2.51	0.45
38:A1:2696:A:H2'	38:A1:2697:A:C8	2.52	0.45
41:AD:40:HIS:CD2	41:AD:42:ALA:H	2.23	0.45
53:AQ:148:GLU:OE2	53:AQ:151:ARG:NH1	2.48	0.45
60:AX:131:ASP:OD1	60:AX:131:ASP:N	2.49	0.45
1:BA:40:ALA:HB2	1:BA:46:HIS:CD2	2.51	0.45
1:BA:179:ARG:O	1:BA:183:ARG:HG2	2.16	0.45
21:BK:14:TYR:HE1	21:BK:21:VAL:HG23	1.82	0.45
28:BZ:95:HIS:ND1	28:BZ:96:SER:O	2.32	0.45
34:B5:91:G:OP1	34:B5:397:A:N6	2.48	0.45
34:B5:885:G:H2'	34:B5:886:U:C6	2.52	0.45
34:B5:1080:U:H2'	34:B5:1081:A:C8	2.52	0.45
34:B5:1181:U:H2'	34:B5:1182:U:O4'	2.17	0.45
34:B5:1321:A:H4'	34:B5:1322:A:O5'	2.16	0.45
34:B5:1529:C:H2'	34:B5:1530:C:C6	2.50	0.45
34:B5:1609:U:H2'	34:B5:1610:G:O4'	2.16	0.45
36:AB:348:ARG:NH1	38:A1:3037:U:H5''	2.32	0.45
38:A1:148:G:OP2	50:AN:4:TYR:OH	2.17	0.45
38:A1:928:C:H2'	38:A1:929:A:C8	2.52	0.45
38:A1:1194:G:H2'	38:A1:1195:A:C8	2.51	0.45
38:A1:1281:G:N2	38:A1:1282:G:O6	2.49	0.45
38:A1:1482:A:H4'	38:A1:1483:G:OP2	2.16	0.45
38:A1:2768:U:H2'	38:A1:2769:A:C8	2.52	0.45
42:AE:148:GLU:HA	42:AE:151:LYS:HE2	1.99	0.45
54:AR:13:SER:OG	54:AR:38:ARG:NH2	2.44	0.45
58:AV:10:LYS:HE2	58:AV:56:ASP:OD2	2.17	0.45
79:E:60:ARG:O	79:E:152:ARG:NH2	2.45	0.45
7:BI:147:ALA:C	7:BI:149:SER:H	2.25	0.45
28:BZ:92:ILE:HB	28:BZ:100:ILE:HG23	1.98	0.45
31:Bg:169:ILE:O	31:Bg:181:TRP:N	2.50	0.45
31:Bg:179:LYS:HZ1	31:Bg:189:GLU:N	2.15	0.45
33:BM:67:THR:C	33:BM:69:ALA:H	2.24	0.45
34:B5:740:A:H1'	34:B5:847:A:OP1	2.16	0.45
34:B5:1215:C:H2'	34:B5:1216:C:C6	2.52	0.45
37:AC:125:ALA:HA	37:AC:244:LEU:HD11	1.99	0.45
38:A1:691:A:N1	40:A4:28:C:O2'	2.42	0.45
38:A1:1616:U:H2'	38:A1:1617:G:H8	1.82	0.45
38:A1:1671:C:H5''	54:AR:60:LYS:NZ	2.32	0.45
38:A1:2204:C:H2'	38:A1:2205:U:O4'	2.16	0.45
38:A1:3164:C:O2'	38:A1:3165:A:H8	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:AR:24:LEU:HD13	54:AR:32:ILE:HG21	1.98	0.45
80:EC:6918:A:H3'	80:EC:6919:G:H8	1.82	0.45
4:BE:102:VAL:HG23	4:BE:239:PRO:HG3	1.99	0.45
5:BG:27:PHE:CE1	5:BG:36:VAL:HG11	2.52	0.45
15:BY:108:ARG:HA	15:BY:111:LYS:HE3	1.99	0.45
16:Ba:85:ARG:O	16:Ba:85:ARG:HD3	2.17	0.45
26:BT:122:ARG:NH1	34:B5:1499:G:OP1	2.50	0.45
35:AA:2:GLY:HA3	38:A1:2415:C:OP1	2.16	0.45
38:A1:573:C:H2'	38:A1:574:U:C6	2.51	0.45
38:A1:952:A:H4'	38:A1:968:G:N2	2.32	0.45
38:A1:1719:G:OP1	54:AR:110:ARG:NH1	2.49	0.45
38:A1:3023:U:H2'	38:A1:3024:A:H8	1.82	0.45
38:A1:3159:C:H2'	38:A1:3160:U:H6	1.81	0.45
38:A1:3298:C:C2	38:A1:3299:A:C8	3.04	0.45
41:AD:148:ILE:HB	41:AD:151:GLN:HB3	1.98	0.45
43:AF:130:ILE:HD12	43:AF:134:VAL:HG11	1.99	0.45
44:AG:68:ARG:HD3	44:AG:237:ILE:O	2.16	0.45
45:AH:167:VAL:C	45:AH:168:ARG:HD2	2.42	0.45
2:BB:29:TRP:HD1	2:BB:45:LYS:HZ1	1.61	0.45
2:BB:119:THR:HB	2:BB:143:THR:HG23	1.99	0.45
7:BI:37:LYS:C	7:BI:59:ARG:HA	2.42	0.45
34:B5:199:G:H2'	34:B5:200:A:C8	2.51	0.45
34:B5:887:A:H2'	34:B5:888:U:H6	1.82	0.45
82:B5:1801:HYG:O14	82:B5:1801:HYG:C19	2.52	0.45
38:A1:63:A:H5''	50:AN:174:ILE:HG21	1.99	0.45
38:A1:712:G:H5'	48:AL:174:ARG:NH1	2.32	0.45
38:A1:2737:C:O2'	64:Ab:36:ASP:OD1	2.31	0.45
38:A1:3110:C:H2'	38:A1:3111:U:C6	2.51	0.45
38:A1:3127:A:H2'	38:A1:3128:G:O4'	2.17	0.45
45:AH:91:ARG:NH1	45:AH:141:LYS:O	2.50	0.45
48:AL:123:ILE:HG22	70:Ah:118:ILE:HG12	1.99	0.45
58:AV:87:ARG:HB2	58:AV:89:ASP:OD2	2.17	0.45
80:EC:6924:G:O2'	80:EC:6925:C:H3'	2.17	0.45
1:BA:125:ASP:HB3	1:BA:128:SER:HB2	1.97	0.45
6:BH:107:ARG:NH2	34:B5:742:U:O2'	2.50	0.45
11:BO:17:ALA:N	11:BO:80:HIS:O	2.38	0.45
13:BW:52:TYR:CE1	13:BW:59:GLY:HA3	2.51	0.45
16:Ba:79:ILE:HD13	34:B5:1794:A:H1'	1.99	0.45
31:Bg:84:SER:O	31:Bg:110:VAL:HG12	2.17	0.45
31:Bg:133:VAL:HG11	31:Bg:186:PHE:CZ	2.52	0.45
32:Bf:119:ARG:HG3	32:Bf:120:GLU:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:830:U:H2'	34:B5:831:U:H6	1.80	0.45
36:AB:311:PHE:HB2	36:AB:315:GLY:O	2.17	0.45
38:A1:252:U:H4'	38:A1:253:A:C8	2.52	0.45
38:A1:1354:G:O2'	38:A1:1355:A:OP1	2.25	0.45
78:Ap:59:CYS:C	78:Ap:61:LYS:H	2.25	0.45
79:E:32:VAL:HG21	79:E:179:LEU:HD11	1.98	0.45
6:BH:139:ARG:HG2	13:BW:51:GLU:OE2	2.17	0.45
11:BO:16:VAL:HG12	11:BO:18:ARG:HG3	2.00	0.45
13:BW:101:TYR:HA	13:BW:113:HIS:CE1	2.52	0.45
15:BY:128:LYS:HG3	15:BY:131:ARG:HH21	1.81	0.45
34:B5:739:G:H3'	34:B5:741:C:O2'	2.17	0.45
34:B5:909:U:H2'	34:B5:910:C:C6	2.52	0.45
34:B5:1203:A:C2	34:B5:1556:A:C4	3.05	0.45
34:B5:1209:C:N3	34:B5:1455:G:N2	2.65	0.45
36:AB:188:ILE:O	36:AB:192:VAL:HG23	2.17	0.45
36:AB:256:HIS:HA	36:AB:257:PRO:C	2.42	0.45
36:AB:323:MET:HE1	36:AB:359:ILE:HD13	1.99	0.45
38:A1:1334:U:H5''	43:AF:206:LYS:HB3	1.99	0.45
38:A1:2426:U:H2'	38:A1:2427:U:C6	2.52	0.45
39:A3:38:U:N3	39:A3:41:G:OP2	2.46	0.45
39:A3:64:A:H5'	39:A3:65:G:H5''	1.98	0.45
47:AJ:52:TYR:HB2	47:AJ:60:ARG:O	2.17	0.45
47:AJ:60:ARG:NH1	80:EC:6798:C:H4'	2.32	0.45
56:AT:36:VAL:HA	56:AT:64:VAL:HG12	1.98	0.45
66:Ad:54:GLU:OE2	66:Ad:54:GLU:N	2.46	0.45
70:Ah:86:ARG:O	70:Ah:90:ARG:HG2	2.18	0.45
73:Ak:28:ASN:HB2	73:Ak:40:GLN:HB3	1.99	0.45
1:BA:182:LEU:HD11	1:BA:187:ALA:HB3	1.98	0.44
1:BA:184:LEU:O	1:BA:185:ARG:HG2	2.17	0.44
6:BH:113:PRO:HG2	6:BH:116:ARG:HD3	1.98	0.44
9:BL:4:GLU:HG2	9:BL:5:LEU:H	1.82	0.44
10:BN:42:ARG:HE	10:BN:80:LEU:HD11	1.82	0.44
15:BY:60:PHE:H	15:BY:71:GLY:HA2	1.82	0.44
20:BF:185:ARG:NH2	34:B5:1471:A:OP1	2.50	0.44
23:BQ:14:LYS:O	23:BQ:123:ARG:NH1	2.48	0.44
24:BR:70:SER:HA	24:BR:74:GLN:HE21	1.81	0.44
34:B5:201:G:H2'	34:B5:202:A:C8	2.52	0.44
34:B5:1017:U:H2'	34:B5:1018:U:C6	2.52	0.44
34:B5:1117:U:H2'	34:B5:1118:G:C8	2.51	0.44
34:B5:1164:G:H2'	34:B5:1165:G:C8	2.53	0.44
34:B5:1183:A:H2'	34:B5:1184:A:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:1322:A:H2'	34:B5:1323:C:C6	2.51	0.44
34:B5:1417:A:H2'	34:B5:1418:G:O4'	2.17	0.44
40:A4:37:A:OP2	70:Ah:86:ARG:HD2	2.16	0.44
44:AG:60:ARG:O	44:AG:64:ILE:HG12	2.17	0.44
46:AI:54:SER:OG	46:AI:130:ASP:O	2.35	0.44
58:AV:15:LEU:HD23	58:AV:53:SER:HB3	1.98	0.44
61:AY:63:LYS:HG3	61:AY:97:ILE:HD11	1.99	0.44
63:Aa:132:LYS:HG2	63:Aa:136:GLU:OE2	2.16	0.44
68:Af:103:TYR:HA	68:Af:104:PRO:C	2.42	0.44
4:BE:131:LEU:HD22	34:B5:251:A:H2	1.83	0.44
5:BG:21:GLU:OE2	5:BG:24:ILE:HD12	2.16	0.44
5:BG:31:ARG:HG2	5:BG:34:GLN:NE2	2.32	0.44
6:BH:23:ALA:HB1	6:BH:84:LYS:NZ	2.32	0.44
13:BW:95:PRO:HG2	13:BW:99:PHE:CE1	2.52	0.44
17:Bb:2:VAL:O	17:Bb:3:LEU:HG	2.17	0.44
19:BD:28:GLU:HG2	19:BD:29:LEU:N	2.32	0.44
21:BK:35:ILE:HG22	21:BK:37:THR:HG22	2.00	0.44
23:BQ:69:VAL:HG11	23:BQ:81:ILE:HD11	2.00	0.44
34:B5:293:U:H2'	34:B5:294:C:C6	2.52	0.44
34:B5:749:U:H2'	34:B5:750:U:C6	2.52	0.44
34:B5:1585:U:H3	34:B5:1611:A:H2	1.65	0.44
38:A1:2218:G:H2'	38:A1:2219:A:H8	1.81	0.44
38:A1:3231:U:H2'	38:A1:3232:G:C8	2.52	0.44
38:A1:3371:G:H2'	38:A1:3372:A:C8	2.53	0.44
62:AZ:27:LYS:HD2	62:AZ:42:LEU:HD12	1.98	0.44
79:E:182:GLN:O	79:E:186:SER:OG	2.29	0.44
80:EC:6796:C:H2'	80:EC:6797:U:C6	2.52	0.44
80:EC:6836:U:H1'	80:EC:6874:A:O2'	2.18	0.44
2:BB:32:ILE:HD11	2:BB:46:THR:OG1	2.17	0.44
11:BO:135:ARG:HD2	34:B5:1008:G:OP1	2.18	0.44
23:BQ:135:ARG:HH12	34:B5:1582:U:H3'	1.82	0.44
24:BR:14:LYS:O	24:BR:18:GLU:HG3	2.17	0.44
24:BR:55:THR:HG22	24:BR:59:LYS:HZ3	1.82	0.44
34:B5:93:A:H4'	34:B5:94:U:OP2	2.18	0.44
34:B5:649:U:HO2'	34:B5:650:U:H6	1.65	0.44
34:B5:850:A:OP1	54:AR:162:ARG:HG3	2.17	0.44
34:B5:889:U:H2'	34:B5:890:C:C6	2.53	0.44
34:B5:919:A:H2'	34:B5:920:U:C6	2.52	0.44
34:B5:1208:A:H5'	34:B5:1209:C:OP2	2.17	0.44
38:A1:377:A:H1'	38:A1:392:G:N2	2.33	0.44
38:A1:1404:G:N2	38:A1:1407:A:OP2	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AJ:157:GLU:OE2	47:AJ:157:GLU:N	2.49	0.44
55:AS:66:GLU:OE1	55:AS:98:SER:HA	2.16	0.44
2:BB:111:ARG:NH2	34:B5:930:A:O2'	2.46	0.44
2:BB:155:TYR:OH	34:B5:932:U:OP2	2.21	0.44
5:BG:85:ARG:HB3	5:BG:87:ARG:HH12	1.83	0.44
6:BH:30:SER:O	6:BH:33:GLU:HG3	2.17	0.44
22:BP:52:LYS:HB2	22:BP:53:PRO:HD3	1.99	0.44
31:Bg:91:LEU:HD22	31:Bg:101:GLN:HE22	1.81	0.44
31:Bg:212:ALA:HA	31:Bg:222:LEU:HA	2.00	0.44
34:B5:293:U:H2'	34:B5:294:C:H6	1.81	0.44
34:B5:1202:A:H1'	34:B5:1207:C:N4	2.33	0.44
34:B5:1261:G:H2'	34:B5:1262:U:C6	2.52	0.44
34:B5:1365:C:H2'	34:B5:1366:U:C6	2.52	0.44
38:A1:255:A:H2'	38:A1:256:G:C8	2.53	0.44
38:A1:570:A:H2'	38:A1:571:U:O4'	2.17	0.44
38:A1:1708:C:H2'	38:A1:1709:C:H6	1.81	0.44
38:A1:1909:A:H2'	38:A1:1910:A:C8	2.52	0.44
38:A1:2357:A:H2'	38:A1:2358:A:H8	1.80	0.44
54:AR:21:LYS:HE3	54:AR:55:VAL:HA	1.99	0.44
55:AS:93:GLU:HB2	55:AS:140:VAL:HG11	1.98	0.44
56:AT:123:GLY:O	56:AT:126:VAL:HG13	2.18	0.44
62:AZ:9:LYS:HB2	62:AZ:25:ILE:HD12	1.99	0.44
1:BA:79:ARG:HE	1:BA:81:PHE:HB2	1.82	0.44
8:BJ:7:THR:HG23	34:B5:771:A:H5'	2.00	0.44
19:BD:58:VAL:HG23	19:BD:88:ALA:HB1	2.00	0.44
19:BD:158:ILE:HD13	19:BD:202:LEU:HD11	1.98	0.44
20:BF:42:LEU:HG	20:BF:43:PHE:H	1.83	0.44
23:BQ:76:SER:N	34:B5:1609:U:OP1	2.47	0.44
27:BU:74:GLU:CD	34:B5:1429:G:H1'	2.43	0.44
33:BM:66:VAL:HG21	34:B5:1228:G:O6	2.18	0.44
34:B5:29:U:H2'	34:B5:30:G:H8	1.82	0.44
38:A1:184:U:H2'	38:A1:185:C:C6	2.53	0.44
38:A1:548:G:OP2	38:A1:549:U:H5'	2.16	0.44
38:A1:968:G:H2'	38:A1:969:C:H6	1.81	0.44
38:A1:1016:C:O2'	38:A1:1018:G:O5'	2.35	0.44
38:A1:2318:U:H2'	38:A1:2319:U:O4'	2.17	0.44
43:AF:35:ALA:O	43:AF:39:GLU:HG2	2.17	0.44
43:AF:48:ASN:ND2	43:AF:182:ASP:OD2	2.50	0.44
73:Ak:14:LEU:O	73:Ak:20:VAL:HG21	2.18	0.44
79:E:34:LEU:HD12	79:E:34:LEU:O	2.18	0.44
80:EC:6920:C:H2'	80:EC:6921:C:C5	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BE:247:SER:OG	4:BE:250:GLU:HG3	2.18	0.44
20:BF:104:ASN:OD1	34:B5:1587:A:O2'	2.25	0.44
20:BF:135:ASP:OD1	20:BF:139:ASN:ND2	2.51	0.44
22:BP:124:THR:CG2	34:B5:1182:U:H4'	2.47	0.44
24:BR:7:LYS:HA	24:BR:10:LYS:HB2	1.98	0.44
29:Bc:22:ARG:NE	34:B5:1619:C:O2	2.50	0.44
34:B5:208:U:H2'	34:B5:209:U:C6	2.52	0.44
34:B5:404:G:H2'	34:B5:405:C:C6	2.53	0.44
34:B5:607:G:H5'	34:B5:613:G:N2	2.33	0.44
34:B5:962:C:H2'	34:B5:963:A:O4'	2.18	0.44
34:B5:1237:G:N3	34:B5:1238:A:C8	2.86	0.44
34:B5:1668:G:H2'	34:B5:1669:U:C6	2.52	0.44
38:A1:93:C:C2	63:Aa:55:LYS:HE2	2.53	0.44
38:A1:426:G:H2'	38:A1:427:C:C6	2.53	0.44
38:A1:1046:A:H2'	38:A1:1049:C:C5	2.53	0.44
38:A1:1096:U:OP2	56:AT:116:ARG:NH2	2.51	0.44
38:A1:1340:G:H2'	38:A1:1341:U:H6	1.83	0.44
38:A1:1722:U:OP1	54:AR:100:ARG:NE	2.40	0.44
38:A1:1785:U:H2'	38:A1:1786:G:H8	1.82	0.44
38:A1:2736:A:H2'	38:A1:2737:C:O4'	2.18	0.44
38:A1:3068:U:OP2	54:AR:62:ARG:NH2	2.46	0.44
38:A1:3191:G:H2'	38:A1:3192:U:C6	2.53	0.44
38:A1:3205:G:O2'	55:AS:171:PHE:HZ	2.01	0.44
39:A3:71:G:H2'	39:A3:72:A:H8	1.82	0.44
43:AF:86:VAL:O	43:AF:114:GLY:HA2	2.18	0.44
2:BB:135:LEU:HA	2:BB:218:LEU:HG	2.00	0.44
8:BJ:175:ARG:HG2	8:BJ:179:ARG:NH1	2.33	0.44
15:BY:5:VAL:HG12	15:BY:7:ILE:HG13	2.00	0.44
21:BK:77:ARG:CZ	21:BK:85:HIS:H	2.31	0.44
26:BT:38:LYS:HD3	26:BT:43:ASN:O	2.18	0.44
34:B5:97:C:H2'	34:B5:98:U:C6	2.53	0.44
34:B5:126:A:H62	34:B5:291:G:N2	2.15	0.44
34:B5:585:A:H2'	34:B5:586:G:H8	1.82	0.44
34:B5:907:A:H2'	34:B5:908:U:C6	2.52	0.44
34:B5:1107:G:O2'	34:B5:1108:G:H5'	2.18	0.44
34:B5:1254:U:H2'	34:B5:1255:G:C5	2.52	0.44
34:B5:1775:U:OP1	76:An:11:ARG:NH2	2.49	0.44
36:AB:28:ARG:NH2	38:A1:3140:G:N7	2.66	0.44
37:AC:350:LYS:HD3	37:AC:351:PRO:O	2.18	0.44
38:A1:845:G:O2'	38:A1:847:A:N1	2.46	0.44
38:A1:1119:C:H2'	38:A1:1120:A:C8	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:2689:A:N3	38:A1:2689:A:H2'	2.32	0.44
43:AF:207:LEU:HB3	43:AF:243:MET:O	2.17	0.44
48:AL:126:PHE:CD2	70:Ah:115:LYS:HE2	2.53	0.44
62:AZ:34:LYS:HG3	62:AZ:35:SER:H	1.83	0.44
79:E:111:ILE:HA	79:E:135:PRO:HA	1.99	0.44
4:BE:181:VAL:HG12	4:BE:227:VAL:HG22	2.00	0.44
6:BH:39:ARG:O	6:BH:39:ARG:NE	2.50	0.44
23:BQ:143:ARG:HD3	23:BQ:143:ARG:HA	1.79	0.44
24:BR:34:LEU:O	24:BR:38:ILE:HG12	2.17	0.44
25:BS:16:ARG:C	25:BS:17:LEU:HD12	2.43	0.44
31:Bg:81:LEU:HD21	31:Bg:122:ILE:HG23	1.99	0.44
33:BM:84:ASN:OD1	33:BM:85:LYS:N	2.47	0.44
34:B5:480:G:C4	34:B5:509:G:N2	2.86	0.44
34:B5:528:U:H2'	34:B5:529:A:O4'	2.18	0.44
34:B5:1227:A:H61	34:B5:1256:A:H5''	1.82	0.44
35:AA:93:LYS:NZ	38:A1:2548:C:OP1	2.39	0.44
37:AC:212:ASP:OD2	37:AC:216:VAL:HG23	2.18	0.44
38:A1:297:G:OP2	38:A1:297:G:N2	2.42	0.44
38:A1:715:A:N1	38:A1:781:G:O2'	2.43	0.44
38:A1:1073:U:H2'	38:A1:1074:U:C6	2.53	0.44
38:A1:1128:U:H2'	38:A1:1129:A:O4'	2.17	0.44
38:A1:2270:A:H2'	38:A1:2271:A:C8	2.53	0.44
38:A1:3033:A:H2'	38:A1:3034:C:O2	2.18	0.44
41:AD:39:GLN:NE2	41:AD:46:THR:O	2.33	0.44
47:AJ:50:ALA:HB3	47:AJ:62:ASN:H	1.82	0.44
58:AV:104:ASN:HD21	58:AV:108:GLU:HB2	1.82	0.44
10:BN:26:PHE:CE2	10:BN:28:LEU:HB2	2.53	0.44
11:BO:123:SER:O	11:BO:124:ASP:C	2.61	0.44
15:BY:78:SER:HB3	15:BY:81:GLU:HG2	1.99	0.44
19:BD:67:ASN:HD21	21:BK:95:ARG:HH12	1.65	0.44
20:BF:88:PRO:HG2	20:BF:91:GLU:HB2	2.00	0.44
20:BF:187:ILE:HA	34:B5:1535:U:C4	2.53	0.44
23:BQ:143:ARG:C	34:B5:1195:C:H42	2.26	0.44
31:Bg:129:LYS:HA	31:Bg:150:TRP:HA	1.99	0.44
34:B5:1055:U:C2	34:B5:1064:G:O6	2.71	0.44
34:B5:1213:G:H1	34:B5:1450:U:H3	1.65	0.44
35:AA:219:ILE:HD13	35:AA:223:SER:OG	2.17	0.44
38:A1:594:U:H2'	38:A1:609:G:O6	2.17	0.44
38:A1:1662:G:H22	38:A1:1787:A:H2	1.66	0.44
38:A1:2106:A:H2'	38:A1:2107:A:C8	2.53	0.44
41:AD:177:GLU:HG3	41:AD:183:TRP:CZ3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:AG:170:CYS:SG	44:AG:177:TYR:HB3	2.58	0.44
80:EC:6884:G:H2'	80:EC:6885:G:C8	2.52	0.44
4:BE:102:VAL:CG2	4:BE:239:PRO:HG3	2.48	0.43
5:BG:38:GLY:HA2	5:BG:41:VAL:HG12	1.98	0.43
6:BH:178:GLY:HA3	34:B5:641:G:H21	1.83	0.43
17:Bb:36:LYS:HE2	17:Bb:43:ILE:HD11	2.00	0.43
19:BD:31:GLU:O	19:BD:54:ARG:NE	2.46	0.43
21:BK:77:ARG:O	21:BK:81:ASN:N	2.49	0.43
22:BP:78:THR:HA	34:B5:1241:G:H5'	2.00	0.43
34:B5:28:A2M:H2'	34:B5:29:U:C6	2.53	0.43
34:B5:841:U:H2'	34:B5:842:C:H6	1.82	0.43
34:B5:1120:U:H2'	34:B5:1121:C:H6	1.83	0.43
34:B5:1363:U:HO2'	34:B5:1364:G:H8	1.64	0.43
34:B5:1392:U:H2'	34:B5:1393:C:C6	2.52	0.43
34:B5:1512:G:H2'	34:B5:1513:G:O4'	2.18	0.43
34:B5:1532:U:H2'	34:B5:1533:C:O4'	2.18	0.43
38:A1:1167:U:H2'	38:A1:1168:U:O4'	2.17	0.43
39:A3:26:C:H2'	39:A3:27:A:O4'	2.18	0.43
41:AD:38:THR:O	41:AD:48:LYS:NZ	2.36	0.43
50:AN:183:THR:HG23	50:AN:183:THR:O	2.18	0.43
54:AR:97:ARG:O	54:AR:101:VAL:HG23	2.17	0.43
3:BC:235:LEU:HD23	12:BV:52:THR:HG22	1.99	0.43
5:BG:28:PHE:CE2	5:BG:104:PRO:HG3	2.53	0.43
9:BL:40:LEU:HG	34:B5:246:G:N3	2.33	0.43
12:BV:40:ASP:OD2	12:BV:41:GLU:N	2.47	0.43
28:BZ:95:HIS:NE2	34:B5:1529:C:OP1	2.51	0.43
34:B5:1240:U:H2'	34:B5:1242:A:OP2	2.18	0.43
34:B5:1732:A:H2'	34:B5:1733:C:C6	2.53	0.43
36:AB:50:LYS:NZ	36:AB:330:GLY:O	2.37	0.43
36:AB:236:LYS:HB2	36:AB:236:LYS:HE2	1.79	0.43
37:AC:227:THR:HG23	38:A1:689:U:H3	1.82	0.43
38:A1:637:C:H4'	67:Ae:24:ARG:HH12	1.83	0.43
38:A1:1208:U:O2'	38:A1:3115:C:N4	2.51	0.43
38:A1:1658:G:H2'	38:A1:1659:U:C6	2.53	0.43
38:A1:1950:U:H3	38:A1:2096:A:H62	1.64	0.43
38:A1:2376:G:H2'	38:A1:2377:G:C8	2.53	0.43
38:A1:2445:A:C6	38:A1:2503:G:C2	3.06	0.43
38:A1:2711:C:O2'	38:A1:2744:U:OP1	2.36	0.43
38:A1:2992:U:OP1	38:A1:3310:A:O2'	2.33	0.43
43:AF:165:ASP:OD1	43:AF:166:ASN:N	2.52	0.43
46:AI:31:ILE:HA	46:AI:66:GLU:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:AP:128:ARG:HE	52:AP:136:ILE:HG21	1.82	0.43
57:AU:84:LEU:O	57:AU:89:LEU:N	2.44	0.43
58:AV:54:LEU:HD21	58:AV:119:GLY:HA3	1.99	0.43
80:EC:6883:A:H2'	80:EC:6884:G:C8	2.53	0.43
5:BG:1:MET:HE1	5:BG:106:LEU:HB2	2.00	0.43
20:BF:125:THR:HG22	20:BF:125:THR:O	2.18	0.43
21:BK:46:LEU:O	21:BK:50:THR:OG1	2.31	0.43
26:BT:63:ARG:HH21	26:BT:67:MET:HE3	1.83	0.43
34:B5:778:G:H3'	34:B5:780:A:N1	2.33	0.43
34:B5:819:G:H4'	34:B5:820:U:O5'	2.17	0.43
34:B5:830:U:H2'	34:B5:831:U:C6	2.53	0.43
34:B5:1179:G:H21	34:B5:1460:A:N6	2.17	0.43
35:AA:7:ASN:O	38:A1:2163:C:H4'	2.19	0.43
37:AC:191:LYS:HG2	37:AC:194:TYR:OH	2.19	0.43
38:A1:149:U:P	50:AN:49:ARG:HH12	2.41	0.43
38:A1:701:G:H2'	38:A1:702:C:C6	2.53	0.43
38:A1:976:U:H2'	38:A1:977:C:O4'	2.18	0.43
38:A1:2218:G:H2'	38:A1:2219:A:C8	2.52	0.43
38:A1:2512:C:H2'	38:A1:2513:U:C6	2.53	0.43
38:A1:3066:U:H2'	38:A1:3067:C:C6	2.53	0.43
38:A1:3153:U:H5	38:A1:3293:U:H3	1.66	0.43
39:A3:76:A:H1'	55:AS:50:LYS:NZ	2.33	0.43
41:AD:123:GLU:HG2	41:AD:248:ARG:HH12	1.83	0.43
41:AD:194:LEU:O	41:AD:197:SER:OG	2.26	0.43
41:AD:211:LEU:HD12	41:AD:223:PHE:HE2	1.83	0.43
47:AJ:172:LEU:O	47:AJ:172:LEU:HD23	2.18	0.43
61:AY:3:LYS:HD2	61:AY:8:VAL:HG23	2.00	0.43
71:AI:75:LYS:HA	71:AI:75:LYS:HD2	1.89	0.43
77:Ao:4:VAL:O	77:Ao:94:GLY:N	2.51	0.43
5:BG:160:ARG:O	5:BG:171:LYS:N	2.36	0.43
6:BH:50:ASP:OD2	6:BH:56:LYS:NZ	2.48	0.43
6:BH:125:ILE:O	6:BH:129:LEU:N	2.48	0.43
6:BH:159:VAL:O	6:BH:163:ASP:N	2.51	0.43
20:BF:143:ARG:HE	20:BF:214:LYS:HZ1	1.65	0.43
32:Bf:135:HIS:C	32:Bf:136:LYS:HD3	2.43	0.43
33:BM:62:LEU:H	33:BM:86:VAL:HG22	1.83	0.43
34:B5:254:A:H2'	34:B5:255:U:H6	1.83	0.43
34:B5:1537:C:P	34:B5:1572:OMG:HN21	2.42	0.43
34:B5:1685:G:N1	34:B5:1717:G:C2	2.86	0.43
36:AB:158:VAL:HG23	36:AB:188:ILE:HD12	2.01	0.43
38:A1:75:G:H5'	48:AL:58:VAL:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:596:C:N3	38:A1:608:A:O2'	2.48	0.43
38:A1:797:U:O2	48:AL:12:ASN:ND2	2.51	0.43
38:A1:966:U:H2'	38:A1:967:A:H8	1.81	0.43
39:A3:73:C:N4	55:AS:19:VAL:HG11	2.33	0.43
40:A4:34:U:O2'	40:A4:35:C:OP2	2.33	0.43
42:AE:93:VAL:O	42:AE:93:VAL:HG12	2.18	0.43
44:AG:33:ASN:O	44:AG:39:ALA:HB3	2.17	0.43
45:AH:173:ARG:HB3	75:Am:127:LEU:HD21	2.00	0.43
47:AJ:26:SER:OG	47:AJ:27:GLY:N	2.51	0.43
47:AJ:82:ARG:HB3	47:AJ:112:LEU:HD22	2.00	0.43
55:AS:73:LYS:HE2	55:AS:75:PHE:CZ	2.53	0.43
64:Ab:5:LYS:HE3	64:Ab:8:THR:HB	2.00	0.43
66:Ad:80:ASN:OD1	66:Ad:81:GLU:N	2.51	0.43
69:Ag:22:VAL:HG12	69:Ag:30:LEU:HD22	2.00	0.43
80:EC:6828:G:H2'	80:EC:6829:A:C8	2.53	0.43
2:BB:153:HIS:NE2	34:B5:1045:C:OP1	2.51	0.43
11:BO:111:ARG:HH21	16:Ba:57:SER:C	2.27	0.43
15:BY:133:ASN:OD1	15:BY:134:ALA:N	2.52	0.43
20:BF:117:THR:HG21	20:BF:194:LEU:HD23	1.99	0.43
24:BR:48:ASN:ND2	34:B5:1388:A:H5''	2.33	0.43
31:Bg:20:VAL:HG23	31:Bg:35:SER:OG	2.18	0.43
34:B5:61:A:H8	34:B5:269:G:O2'	2.01	0.43
34:B5:842:C:H2'	34:B5:843:U:O4'	2.18	0.43
34:B5:1457:C:O2'	34:B5:1458:G:O5'	2.36	0.43
34:B5:1682:U:O4	34:B5:1720:G:N2	2.52	0.43
38:A1:640:U:H2'	38:A1:641:C:C6	2.53	0.43
38:A1:968:G:H2'	38:A1:969:C:C6	2.53	0.43
38:A1:1378:U:H2'	38:A1:1379:G:H8	1.84	0.43
44:AG:156:ASP:OD1	44:AG:156:ASP:N	2.52	0.43
79:E:130:LYS:HD2	80:EC:6774:U:H5	1.83	0.43
80:EC:6761:C:H2'	80:EC:6762:U:C6	2.53	0.43
7:BI:107:THR:HB	7:BI:108:PRO:HD3	1.99	0.43
7:BI:107:THR:HG22	7:BI:111:GLN:HE22	1.84	0.43
9:BL:21:ASN:OD1	9:BL:32:LYS:N	2.46	0.43
19:BD:115:ILE:H	19:BD:115:ILE:HD12	1.83	0.43
20:BF:116:HIS:O	20:BF:120:ILE:HD12	2.19	0.43
22:BP:51:SER:HB2	22:BP:54:ALA:HB2	1.99	0.43
27:BU:36:ASN:O	27:BU:40:ASN:N	2.38	0.43
34:B5:343:C:H2'	34:B5:344:A:H8	1.84	0.43
36:AB:94:GLU:HG3	51:AO:152[A]:VAL:CG2	2.49	0.43
37:AC:320:ASN:HD22	38:A1:505:G:P	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:385:A:H2'	38:A1:386:A:C8	2.54	0.43
38:A1:2106:A:H2'	38:A1:2107:A:H8	1.82	0.43
38:A1:2894:C:C5'	45:AH:168:ARG:HH21	2.32	0.43
39:A3:95:A:N3	55:AS:119:ARG:HD2	2.34	0.43
40:A4:16:G:O2'	40:A4:17:A:OP2	2.35	0.43
46:AI:52:LEU:HB3	46:AI:136:PHE:HB2	1.99	0.43
47:AJ:141:ARG:O	47:AJ:145:LYS:HD3	2.19	0.43
55:AS:93:GLU:CB	55:AS:140:VAL:HG11	2.49	0.43
3:BC:116:LYS:HG2	3:BC:127:ALA:HB3	2.00	0.43
4:BE:3:ARG:NH1	34:B5:401:A:O3'	2.51	0.43
5:BG:110:ALA:HB1	34:B5:163:G:O2'	2.19	0.43
6:BH:67:LEU:HG	6:BH:71:HIS:NE2	2.33	0.43
12:BV:80:LYS:HA	12:BV:80:LYS:HD3	1.87	0.43
16:Ba:2:PRO:HB3	34:B5:1142:A:H5''	1.99	0.43
27:BU:85:ARG:NH2	34:B5:1335:U:H5'	2.24	0.43
28:BZ:40:VAL:HG13	28:BZ:41:ILE:HG12	2.01	0.43
28:BZ:59:TYR:HD2	28:BZ:64:VAL:HG11	1.84	0.43
28:BZ:76:ALA:O	28:BZ:80:LEU:HB2	2.18	0.43
28:BZ:83:LEU:O	28:BZ:86:GLU:HG2	2.18	0.43
31:Bg:67:ILE:O	31:Bg:85:TRP:N	2.34	0.43
31:Bg:73:LEU:HD12	31:Bg:80:ALA:HB2	2.00	0.43
31:Bg:102:ARG:NH1	34:B5:1342:C:O5'	2.51	0.43
34:B5:107:C:H2'	34:B5:108:A:H8	1.84	0.43
34:B5:188:A:H2'	34:B5:189:C:O4'	2.19	0.43
34:B5:215:A:H2'	34:B5:216:U:O4'	2.17	0.43
34:B5:300:A:H2'	34:B5:301:A:C8	2.53	0.43
34:B5:1542:G:O2'	34:B5:1543:A:OP2	2.35	0.43
38:A1:384:A:H2'	38:A1:385:A:O4'	2.18	0.43
38:A1:981:U:H2'	38:A1:982:C:H5'	2.01	0.43
38:A1:1278:A:H3'	38:A1:1279:C:C6	2.54	0.43
38:A1:1942:U:H2'	38:A1:1943:C:O4'	2.18	0.43
38:A1:2927:C:H2'	38:A1:2928:C:C6	2.54	0.43
38:A1:3000:A:H2'	38:A1:3001:C:H6	1.84	0.43
38:A1:3165:A:H2'	38:A1:3166:C:H6	1.83	0.43
43:AF:96:PRO:HG2	43:AF:99:PRO:HG2	2.00	0.43
54:AR:173:ARG:O	54:AR:177:VAL:HG22	2.18	0.43
56:AT:102:ARG:HD2	56:AT:102:ARG:HA	1.88	0.43
58:AV:33:ASN:ND2	58:AV:64:LYS:HG2	2.34	0.43
61:AY:43:TYR:O	61:AY:124:GLY:HA2	2.17	0.43
67:Ae:32:TRP:CZ2	67:Ae:53:PRO:HD2	2.54	0.43
77:Ao:28:TYR:CZ	77:Ao:30:ALA:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:127:VAL:HG13	2:BB:176:VAL:HG11	2.00	0.43
3:BC:40:LYS:HE3	3:BC:40:LYS:HB2	1.92	0.43
5:BG:50:PHE:CD2	5:BG:111:LEU:HD23	2.54	0.43
17:Bb:3:LEU:HD12	17:Bb:4:VAL:HG23	1.99	0.43
26:BT:38:LYS:O	26:BT:39:THR:OG1	2.36	0.43
26:BT:87:GLY:C	34:B5:1542:G:H5''	2.43	0.43
29:Bc:21:SER:HB2	29:Bc:22:ARG:HD2	2.01	0.43
31:Bg:179:LYS:HZ2	31:Bg:190:ALA:H	1.64	0.43
34:B5:222:A:H2'	34:B5:223:U:N1	2.34	0.43
34:B5:780:A:H5''	34:B5:781:U:C5	2.54	0.43
34:B5:954:G:H2'	34:B5:955:A:C8	2.53	0.43
34:B5:973:A:H2'	34:B5:974:A2M:H8	2.01	0.43
34:B5:1302:U:H2'	34:B5:1303:U:H6	1.84	0.43
34:B5:1350:U:H2'	34:B5:1351:G:C8	2.54	0.43
35:AA:178:PRO:HG2	78:Ap:26:VAL:HG23	2.00	0.43
38:A1:273:A:H2'	38:A1:274:G:H8	1.83	0.43
38:A1:1460:A:H2'	38:A1:1461:A:H8	1.83	0.43
38:A1:2481:G:H8	38:A1:2482:U:C6	2.37	0.43
38:A1:2538:U:O2'	38:A1:2539:C:O5'	2.37	0.43
38:A1:2651:G:H5''	38:A1:2652:U:O4'	2.18	0.43
38:A1:3065:G:H2'	38:A1:3066:U:C6	2.54	0.43
38:A1:3066:U:H2'	38:A1:3067:C:H6	1.84	0.43
38:A1:3288:G:O2'	38:A1:3289:G:H8	2.02	0.43
41:AD:236:LEU:HD13	41:AD:239:ILE:HD11	2.01	0.43
58:AV:40:LYS:HE3	58:AV:40:LYS:HB3	1.87	0.43
2:BB:139:ALA:HB2	2:BB:172:LEU:HD11	1.99	0.43
5:BG:23:ARG:HH21	5:BG:42:GLY:HA2	1.84	0.43
7:BI:152:ILE:O	7:BI:153:GLU:HG3	2.19	0.43
8:BJ:149:ARG:HB2	34:B5:765:G:O6	2.18	0.43
11:BO:103:ARG:NH2	16:Ba:46:GLU:OE1	2.51	0.43
15:BY:61:ARG:HD2	15:BY:62:THR:H	1.84	0.43
16:Ba:18:VAL:O	16:Ba:19:LYS:HB2	2.19	0.43
16:Ba:46:GLU:HB3	16:Ba:48:ALA:H	1.83	0.43
20:BF:182:ALA:HB3	20:BF:193:THR:HB	2.01	0.43
21:BK:59:PHE:CZ	21:BK:62:GLN:HA	2.54	0.43
22:BP:89:MET:O	22:BP:89:MET:HG2	2.19	0.43
30:Bd:46:LYS:O	30:Bd:50:ILE:HG12	2.19	0.43
33:BM:119:SER:OG	34:B5:1228:G:N2	2.52	0.43
34:B5:887:A:H2'	34:B5:888:U:C6	2.54	0.43
34:B5:1433:G:H2'	34:B5:1434:U:O4'	2.19	0.43
34:B5:1508:U:H2'	34:B5:1509:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:AC:145:ILE:HD13	37:AC:148:ILE:HD11	1.99	0.43
38:A1:170:G:C6	38:A1:250:U:C2	3.06	0.43
38:A1:411:U:H2'	38:A1:412:G:H8	1.84	0.43
38:A1:656:A:H2'	38:A1:657:A:H8	1.84	0.43
38:A1:863:C:H2'	38:A1:864:G:O4'	2.19	0.43
38:A1:1248:C:H2'	38:A1:1249:G:H8	1.83	0.43
38:A1:1260:A:H4'	38:A1:1279:C:O2'	2.18	0.43
39:A3:44:C:O2'	41:AD:152:ARG:HD2	2.19	0.43
41:AD:262:LYS:HA	41:AD:265:TYR:HD2	1.84	0.43
47:AJ:60:ARG:NH2	80:EC:6798:C:H4'	2.34	0.43
48:AL:165:SER:O	48:AL:168:ARG:N	2.52	0.43
53:AQ:182:LYS:NZ	63:Aa:55:LYS:O	2.47	0.43
79:E:55:LEU:HD22	79:E:182:GLN:HG2	2.01	0.43
1:BA:88:LYS:HA	1:BA:88:LYS:HD3	1.85	0.43
1:BA:144:ILE:HG23	1:BA:158:VAL:HB	2.00	0.43
19:BD:9:ARG:HH11	30:Bd:34:TYR:HA	1.83	0.43
20:BF:69:PHE:HE1	23:BQ:53:LEU:HB3	1.82	0.43
21:BK:87:VAL:HG12	21:BK:89:GLY:N	2.32	0.43
34:B5:333:A:H2'	34:B5:334:G:C8	2.54	0.43
34:B5:450:U:H2'	34:B5:451:A:C8	2.54	0.43
34:B5:502:U:H3'	34:B5:503:G:H8	1.84	0.43
34:B5:1329:A:H2'	34:B5:1330:G:O4'	2.19	0.43
38:A1:8:C:H2'	38:A1:9:U:C6	2.53	0.43
38:A1:537:A:N6	38:A1:554:A:H1'	2.29	0.43
38:A1:2266:U:H2'	38:A1:2267:C:C6	2.53	0.43
38:A1:2932:U:O2'	38:A1:2934:A:N7	2.39	0.43
38:A1:3089:C:H2'	38:A1:3090:U:O4'	2.18	0.43
42:AE:51:ARG:O	42:AE:72:ASN:ND2	2.52	0.43
50:AN:28:TRP:O	50:AN:32:GLN:HG2	2.19	0.43
53:AQ:94:PHE:CZ	63:Aa:119:PRO:HD3	2.54	0.43
54:AR:132:PHE:CE2	54:AR:138:LEU:HD13	2.54	0.43
78:Ap:51:ALA:HB3	78:Ap:54:ILE:HD12	2.00	0.43
79:E:190:PHE:CE1	79:E:194:LEU:HD22	2.54	0.43
2:BB:32:ILE:HG12	2:BB:96:LEU:HD13	2.00	0.42
4:BE:56:LEU:HD23	15:BY:20:ARG:NH2	2.34	0.42
19:BD:5:ILE:HD12	34:B5:1514:U:C6	2.53	0.42
21:BK:62:GLN:HE22	30:Bd:25:SER:HB3	1.84	0.42
27:BU:77:LYS:NZ	34:B5:1195:C:OP1	2.36	0.42
34:B5:565:C:O2'	34:B5:577:G:N2	2.51	0.42
34:B5:792:U:H2'	34:B5:793:A:O4'	2.18	0.42
34:B5:898:A:N1	34:B5:911:U:O2'	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:1233:G:H2'	34:B5:1234:A:O4'	2.18	0.42
38:A1:94:G:H2'	38:A1:95:A:C8	2.54	0.42
38:A1:208:C:H2'	38:A1:209:A:O4'	2.19	0.42
38:A1:381:U:H2'	38:A1:382:U:C6	2.54	0.42
38:A1:649:A2M:OP2	38:A1:2868:U:O2'	2.37	0.42
38:A1:1497:C:H2'	38:A1:1498:A:C8	2.54	0.42
38:A1:2148:U:H2'	38:A1:2149:A:C8	2.54	0.42
38:A1:3297:U:H2'	38:A1:3298:C:H6	1.84	0.42
39:A3:64:A:H8	46:AI:204:GLY:O	2.02	0.42
45:AH:5:GLN:NE2	45:AH:7:GLU:HG2	2.30	0.42
56:AT:73:GLY:HA2	56:AT:89:LEU:O	2.19	0.42
70:Ah:9:LEU:HD23	70:Ah:12:LYS:NZ	2.34	0.42
79:E:67:ILE:HB	79:E:111:ILE:HD11	1.99	0.42
80:EC:6809:G:O2'	80:EC:6810:U:O4'	2.25	0.42
4:BE:11:ARG:NH1	4:BE:20:LEU:HB3	2.33	0.42
8:BJ:82:ARG:HD2	8:BJ:149:ARG:HG2	2.00	0.42
13:BW:83:ILE:HG12	34:B5:749:U:H5''	2.01	0.42
19:BD:64:ARG:C	19:BD:66:ILE:H	2.27	0.42
19:BD:101:GLN:O	19:BD:105:MET:HG2	2.19	0.42
20:BF:129:PRO:O	20:BF:133:VAL:HG23	2.18	0.42
21:BK:33:GLU:O	21:BK:34:GLU:HG2	2.19	0.42
21:BK:59:PHE:CZ	21:BK:62:GLN:HG2	2.54	0.42
26:BT:88:VAL:HG11	34:B5:1173:C:H1'	2.01	0.42
28:BZ:60:VAL:HG13	28:BZ:65:LEU:HD21	2.01	0.42
29:Bc:22:ARG:HG3	34:B5:1619:C:N3	2.34	0.42
34:B5:1216:C:H1'	34:B5:1217:A:C8	2.52	0.42
34:B5:1467:C:H2'	34:B5:1468:U:C6	2.54	0.42
34:B5:1647:U:H2'	34:B5:1648:A:H8	1.83	0.42
34:B5:1684:U:H2'	34:B5:1685:G:N7	2.34	0.42
36:AB:284:ARG:HB3	36:AB:323:MET:HB3	2.00	0.42
38:A1:784:A:H1'	53:AQ:65:SER:HB3	2.01	0.42
38:A1:1339:C:H2'	38:A1:1340:G:C8	2.54	0.42
38:A1:1895:A:O2'	38:A1:3053:G:H4'	2.18	0.42
38:A1:2615:G:H2'	38:A1:2616:C:H6	1.83	0.42
38:A1:2681:U:O2	47:AJ:20:ASN:ND2	2.51	0.42
40:A4:9:A:H2'	40:A4:10:A:H8	1.81	0.42
54:AR:37:SER:O	54:AR:41:ILE:HD12	2.19	0.42
59:AW:56:ARG:HB3	59:AW:61:LYS:HB2	2.00	0.42
65:Ac:16:LEU:HD23	65:Ac:98:SER:HA	2.00	0.42
65:Ac:60:ALA:O	65:Ac:64:LYS:N	2.52	0.42
79:E:31:THR:H	79:E:209:SER:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BE:166:SER:O	4:BE:168:LYS:N	2.51	0.42
5:BG:85:ARG:O	5:BG:87:ARG:NH1	2.52	0.42
10:BN:55:ARG:HH22	17:Bb:51:GLN:NE2	2.17	0.42
17:Bb:19:HIS:HB3	17:Bb:22:LYS:HG3	2.01	0.42
20:BF:146:THR:CG2	20:BF:157:ARG:HG3	2.49	0.42
22:BP:75:PRO:HA	22:BP:93:VAL:HG23	2.01	0.42
34:B5:882:U:H2'	34:B5:883:C:C6	2.54	0.42
34:B5:954:G:H2'	34:B5:955:A:H8	1.84	0.42
34:B5:1451:C:H2'	34:B5:1452:U:C6	2.55	0.42
38:A1:151:A:H4'	70:Ah:102:GLU:OE1	2.19	0.42
38:A1:235:A:H2'	38:A1:236:G:C8	2.55	0.42
38:A1:2482:U:C5	79:E:102:LYS:HD3	2.54	0.42
38:A1:2991:A:O2'	38:A1:3309:G:N7	2.50	0.42
38:A1:3159:C:H2'	38:A1:3160:U:C6	2.55	0.42
38:A1:3252:G:H2'	38:A1:3253:G:H8	1.81	0.42
38:A1:3296:A:H2'	38:A1:3297:U:H6	1.84	0.42
54:AR:170:ARG:HG2	54:AR:174:ALA:HB3	2.02	0.42
57:AU:54:VAL:HG12	57:AU:67:SER:HB2	2.01	0.42
61:AY:103:LYS:HD3	61:AY:103:LYS:HA	1.79	0.42
2:BB:125:VAL:HG21	2:BB:173:THR:HB	2.01	0.42
4:BE:77:ARG:HD3	4:BE:77:ARG:HA	1.76	0.42
8:BJ:169:PRO:HD2	8:BJ:174:ARG:HH11	1.83	0.42
19:BD:60:GLY:HA3	19:BD:64:ARG:O	2.20	0.42
30:Bd:14:TYR:HB2	34:B5:1597:A:H8	1.84	0.42
31:Bg:34:LEU:HD12	31:Bg:73:LEU:HB2	2.01	0.42
34:B5:752:A:O2'	34:B5:753:A:OP1	2.34	0.42
34:B5:1181:U:OP1	80:EC:6913:U:O2'	2.33	0.42
34:B5:1375:A:H2'	34:B5:1376:C:C6	2.54	0.42
35:AA:37:ARG:NH1	38:A1:2526:C:OP1	2.37	0.42
35:AA:52:SER:HB3	35:AA:191:LEU:HD12	2.01	0.42
35:AA:80:GLU:HG3	78:Ap:76:ALA:HB2	2.01	0.42
38:A1:3267:A:N6	42:AE:70:LYS:O	2.53	0.42
38:A1:3317:U:H1'	38:A1:3318:G:C5	2.55	0.42
45:AH:21:LYS:HG3	49:AM:8:LYS:HG3	2.01	0.42
53:AQ:80:THR:HB	53:AQ:137:THR:HG22	2.01	0.42
2:BB:133:TYR:HE1	2:BB:220:GLN:HG2	1.84	0.42
3:BC:53:ILE:HD12	3:BC:57:PHE:CE2	2.54	0.42
15:BY:41:ARG:NH2	15:BY:53:ASP:HA	2.35	0.42
23:BQ:47:LYS:HE2	23:BQ:79:TYR:CZ	2.55	0.42
25:BS:9:GLY:HA2	28:BZ:41:ILE:HG22	2.02	0.42
25:BS:141:THR:HG21	34:B5:1173:C:H5''	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:733:A:H5'	34:B5:734:A:N1	2.33	0.42
34:B5:1410:A:H2'	34:B5:1411:A:C8	2.54	0.42
36:AB:93:VAL:N	36:AB:100:ARG:O	2.52	0.42
38:A1:1252:A:C2	38:A1:1263:A:H2'	2.55	0.42
38:A1:2406:C:H2'	38:A1:2407:C:H6	1.84	0.42
38:A1:2902:A:H2'	38:A1:2903:A:O4'	2.19	0.42
38:A1:3101:G:H2'	38:A1:3102:G:H8	1.84	0.42
44:AG:105:LYS:HG3	44:AG:108:ARG:HH21	1.83	0.42
44:AG:185:ARG:O	44:AG:188:THR:HG22	2.20	0.42
46:AI:47:PRO:HB3	46:AI:171:TRP:CE2	2.55	0.42
46:AI:47:PRO:HB2	46:AI:178:ARG:HH12	1.84	0.42
55:AS:26:ARG:O	56:AT:150:THR:HB	2.19	0.42
62:AZ:95:VAL:O	62:AZ:100:THR:HG21	2.19	0.42
77:Ao:66:LYS:HE2	77:Ao:66:LYS:HB3	1.81	0.42
3:BC:89:GLN:OE1	3:BC:94:GLN:NE2	2.52	0.42
7:BI:69:SER:OG	9:BL:23:PRO:HD2	2.19	0.42
8:BJ:87:SER:OG	8:BJ:89:ASP:OD1	2.34	0.42
14:BX:97:ASP:HB2	14:BX:100:ASP:OD2	2.20	0.42
20:BF:99:MET:HE1	34:B5:1165:G:H5''	2.00	0.42
23:BQ:45:ARG:HG3	23:BQ:49:TYR:HE1	1.84	0.42
34:B5:892:A:H2'	34:B5:893:U:C6	2.54	0.42
34:B5:1071:U:H2'	34:B5:1072:C:C6	2.55	0.42
34:B5:1483:A:C2	34:B5:1607:G:H1'	2.54	0.42
38:A1:1680:G:H2'	38:A1:1681:U:H6	1.84	0.42
38:A1:2228:A:H2'	38:A1:2229:A:H8	1.84	0.42
38:A1:2656:A:OP2	77:Ao:97:LYS:HB2	2.20	0.42
46:AI:208:ASN:HA	46:AI:211:ARG:NH1	2.34	0.42
56:AT:75:ILE:HG23	56:AT:86:GLU:HG3	2.00	0.42
61:AY:67:GLU:O	61:AY:84:LYS:HE3	2.19	0.42
66:Ad:46:THR:OG1	66:Ad:91:SER:OG	2.26	0.42
79:E:194:LEU:HD21	79:E:200:ASN:HB2	2.01	0.42
4:BE:91:THR:HG23	4:BE:98:ASN:OD1	2.19	0.42
10:BN:34:ILE:HD11	10:BN:67:THR:HG23	2.00	0.42
13:BW:83:ILE:HD13	13:BW:122:SER:HB2	2.01	0.42
14:BX:79:ASN:OD1	14:BX:81:LYS:HG2	2.20	0.42
17:Bb:22:LYS:HD3	34:B5:864:U:C5	2.54	0.42
31:Bg:220:ILE:HB	31:Bg:234:LEU:HB2	2.01	0.42
34:B5:1202:A:H62	34:B5:1456:C:H3'	1.84	0.42
34:B5:1550:A:H2'	34:B5:1551:U:C6	2.54	0.42
34:B5:1688:U:H3'	34:B5:1689:A:H8	1.85	0.42
38:A1:1781:C:H2'	38:A1:1782:U:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:2660:G:OP1	38:A1:2750:U:O2'	2.33	0.42
40:A4:95:G:O2'	72:Aj:81:GLY:O	2.32	0.42
43:AF:239:LEU:O	43:AF:243:MET:HG2	2.19	0.42
50:AN:153:ASP:OD1	50:AN:154:PRO:HD2	2.20	0.42
55:AS:152:LEU:HB2	55:AS:172:TYR:CE2	2.54	0.42
58:AV:13:ILE:HD13	58:AV:54:LEU:HB3	2.02	0.42
70:Ah:9:LEU:HD23	70:Ah:12:LYS:HZ3	1.84	0.42
1:BA:198:MET:HB2	1:BA:199:PRO:HD2	2.00	0.42
2:BB:30:PHE:CZ	2:BB:91:VAL:HG13	2.55	0.42
2:BB:157:GLN:C	2:BB:159:SER:H	2.28	0.42
3:BC:200:SER:HB3	3:BC:204:THR:HG21	2.01	0.42
4:BE:19:LEU:HD13	34:B5:788:A:C6	2.54	0.42
4:BE:248:ILE:HD12	8:BJ:71:PHE:CD2	2.55	0.42
8:BJ:89:ASP:OD1	8:BJ:89:ASP:N	2.53	0.42
8:BJ:108:ARG:HE	8:BJ:110:GLN:HB3	1.85	0.42
15:BY:12:VAL:HG22	15:BY:23:PHE:HB3	2.00	0.42
20:BF:80:LYS:HB2	20:BF:83:ARG:HB2	2.01	0.42
24:BR:37:GLU:HG3	31:Bg:150:TRP:CZ3	2.38	0.42
26:BT:115:GLU:HG2	26:BT:116:ILE:N	2.34	0.42
34:B5:978:A:H2'	34:B5:979:A:O4'	2.19	0.42
35:AA:181:LYS:HB2	38:A1:860:G:C6	2.55	0.42
38:A1:273:A:H2'	38:A1:274:G:C8	2.54	0.42
38:A1:796:U:H2'	38:A1:797:U:C6	2.53	0.42
38:A1:2152:A:H2'	38:A1:2153:U:H6	1.85	0.42
38:A1:2407:C:H2'	38:A1:2408:U:H6	1.85	0.42
38:A1:2767:U:H2'	38:A1:2768:U:H6	1.84	0.42
38:A1:2829:U:C2	38:A1:2830:G:C8	3.07	0.42
38:A1:3283:U:H2'	38:A1:3284:G:C8	2.54	0.42
39:A3:48:U:OP1	41:AD:94:ASN:ND2	2.49	0.42
46:AI:189:GLU:HA	46:AI:200:LEU:HB3	2.02	0.42
51:AO:125[A]:ARG:HG3	51:AO:129[A]:LEU:HD12	2.02	0.42
53:AQ:94:PHE:CE2	63:Aa:119:PRO:HD3	2.55	0.42
67:Ae:64:LYS:HD3	67:Ae:65:PHE:CE2	2.54	0.42
79:E:10:ARG:NE	79:E:10:ARG:HA	2.35	0.42
80:EC:6844:A:H1'	80:EC:6845:G:N7	2.34	0.42
5:BG:192:ALA:O	5:BG:196:ARG:HG3	2.20	0.42
11:BO:125:SER:OG	11:BO:126:THR:N	2.43	0.42
18:Be:53:LYS:HG3	18:Be:54:ARG:N	2.35	0.42
20:BF:144:GLU:HA	20:BF:162:VAL:HG23	2.02	0.42
22:BP:79:HIS:HD2	34:B5:1241:G:C4	2.37	0.42
24:BR:17:ILE:HD12	24:BR:17:ILE:HA	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:16:G:H2'	34:B5:17:C:C6	2.55	0.42
34:B5:602:U:H2'	34:B5:603:U:C6	2.55	0.42
34:B5:1086:A:H2'	34:B5:1087:A:C8	2.55	0.42
38:A1:1072:G:H2'	38:A1:1073:U:C6	2.55	0.42
38:A1:1568:U:H4'	38:A1:1569:U:OP2	2.17	0.42
38:A1:1597:C:H5''	69:Ag:25:THR:HG23	2.01	0.42
38:A1:1682:U:O2	57:AU:82:LYS:HD2	2.20	0.42
38:A1:2273:G:N2	38:A1:2311:G:H2'	2.35	0.42
38:A1:2333:C:H2'	38:A1:2334:U:O4'	2.20	0.42
38:A1:2615:G:H2'	38:A1:2616:C:C6	2.54	0.42
38:A1:2772:C:H4'	38:A1:2773:C:H5'	2.02	0.42
41:AD:113:LEU:HD12	41:AD:115:LEU:HB2	2.02	0.42
43:AF:160:ARG:HG3	43:AF:203:TRP:CD2	2.55	0.42
53:AQ:79:LYS:HG2	53:AQ:136:ASN:OD1	2.20	0.42
54:AR:21:LYS:HE2	54:AR:55:VAL:HG12	2.01	0.42
61:AY:77:LYS:HD2	61:AY:98:ASN:OD1	2.20	0.42
6:BH:125:ILE:O	6:BH:129:LEU:HB2	2.20	0.42
6:BH:126:LEU:HD13	6:BH:152:VAL:HG11	2.02	0.42
8:BJ:169:PRO:HG2	8:BJ:174:ARG:HG3	2.02	0.42
14:BX:24:TRP:CE3	14:BX:30:LYS:HD2	2.52	0.42
23:BQ:13:LYS:NZ	23:BQ:120:ASP:OD2	2.53	0.42
23:BQ:75:VAL:HB	34:B5:1609:U:H5''	2.01	0.42
34:B5:566:C:H2'	34:B5:567:A:O4'	2.20	0.42
34:B5:602:U:H2'	34:B5:603:U:H6	1.84	0.42
34:B5:779:U:H3'	34:B5:780:A:H2	1.85	0.42
34:B5:1260:U:N3	34:B5:1261:G:N7	2.68	0.42
36:AB:130:PHE:H	38:A1:3150:A:H5'	1.85	0.42
38:A1:170:G:H5''	70:Ah:109:ILE:HD12	2.01	0.42
38:A1:604:G:H2'	38:A1:605:U:H6	1.85	0.42
38:A1:1747:G:N2	73:Ak:2:ALA:HB3	2.33	0.42
38:A1:2230:C:H2'	38:A1:2231:C:O4'	2.20	0.42
38:A1:2812:C:H2'	38:A1:2813:A:C8	2.55	0.42
38:A1:2881:C:H2'	38:A1:2882:U:C6	2.55	0.42
39:A3:67:G:H2'	39:A3:68:C:O4'	2.20	0.42
45:AH:93:VAL:HG22	75:Am:82:LEU:HB3	2.02	0.42
2:BB:26:ARG:O	2:BB:50:LYS:HG2	2.20	0.41
2:BB:31:ASP:O	2:BB:96:LEU:N	2.33	0.41
5:BG:78:THR:HG22	5:BG:92:ARG:HD2	2.01	0.41
6:BH:140:VAL:HG22	6:BH:150:GLN:HG2	2.00	0.41
7:BI:41:LYS:HA	7:BI:59:ARG:O	2.20	0.41
22:BP:73:PRO:HD2	22:BP:92:SER:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Bd:41:GLN:OE1	30:Bd:41:GLN:N	2.51	0.41
31:Bg:117:LYS:NZ	31:Bg:159:ASN:OD1	2.53	0.41
31:Bg:211:ILE:O	31:Bg:223:TRP:N	2.48	0.41
34:B5:94:U:H2'	34:B5:95:G:O4'	2.20	0.41
34:B5:1391:A:H2'	34:B5:1392:U:C6	2.55	0.41
34:B5:1550:A:H2'	34:B5:1551:U:H6	1.84	0.41
34:B5:1717:G:C2	34:B5:1718:G:C4	3.08	0.41
38:A1:830:A:H2'	38:A1:831:G:O4'	2.20	0.41
38:A1:1749:A:H5''	38:A1:1751:G:N7	2.34	0.41
38:A1:2723:U:H2'	38:A1:2724:OMU:C6	2.50	0.41
43:AF:203:TRP:CD1	43:AF:204:PRO:HD2	2.55	0.41
45:AH:96:HIS:O	45:AH:98:PRO:HD3	2.20	0.41
45:AH:168:ARG:HD2	45:AH:168:ARG:N	2.35	0.41
47:AJ:11:ASP:OD1	47:AJ:11:ASP:N	2.52	0.41
61:AY:17:LYS:O	61:AY:21:THR:OG1	2.23	0.41
61:AY:109:LEU:HD23	61:AY:109:LEU:H	1.84	0.41
79:E:17:LEU:HD11	79:E:179:LEU:HD23	2.01	0.41
6:BH:13:PRO:HB2	6:BH:14:THR:CG2	2.50	0.41
12:BV:9:VAL:HG23	12:BV:9:VAL:O	2.19	0.41
13:BW:101:TYR:HB3	13:BW:112:ASP:HB2	2.02	0.41
34:B5:225:A:H2'	34:B5:226:A:C8	2.55	0.41
34:B5:423:G:H8	34:B5:423:G:OP2	2.03	0.41
34:B5:522:U:H2'	34:B5:523:G:O4'	2.20	0.41
34:B5:696:C:O2'	34:B5:697:C:OP2	2.37	0.41
34:B5:781:U:H4'	34:B5:782:U:N1	2.34	0.41
34:B5:950:C:HO2'	34:B5:951:A:P	2.39	0.41
34:B5:980:G:H4'	34:B5:1776:A:H4'	2.02	0.41
34:B5:998:A:N6	34:B5:1004:U:OP2	2.53	0.41
38:A1:1483:G:O6	69:Ag:4:ARG:NH2	2.52	0.41
38:A1:1578:C:H2'	38:A1:1579:C:C6	2.54	0.41
38:A1:2611:U:H2'	38:A1:2612:U:C6	2.56	0.41
38:A1:2916:U:H2'	38:A1:2917:G:H8	1.84	0.41
40:A4:119:C:H2'	40:A4:120:C:C6	2.55	0.41
49:AM:57:ALA:HB2	55:AS:97:VAL:HG21	2.02	0.41
49:AM:108:ARG:O	49:AM:112:LEU:HD12	2.20	0.41
54:AR:21:LYS:HD2	54:AR:53:LYS:O	2.20	0.41
54:AR:134:HIS:CE1	54:AR:136:ARG:HB3	2.55	0.41
55:AS:19:VAL:HG13	55:AS:19:VAL:O	2.19	0.41
70:Ah:83:LYS:HG3	70:Ah:83:LYS:O	2.20	0.41
80:EC:6927:U:H5''	80:EC:6928:G:N7	2.35	0.41
80:EC:6938:A:H2'	80:EC:6939:C:O4'	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:43:VAL:HG13	2:BB:68:VAL:HG11	2.01	0.41
6:BH:159:VAL:HG12	6:BH:163:ASP:HB2	2.02	0.41
7:BI:38:ILE:HG12	7:BI:96:LEU:HD11	2.02	0.41
19:BD:32:GLU:HG2	19:BD:58:VAL:HG13	2.02	0.41
24:BR:55:THR:HG22	24:BR:59:LYS:NZ	2.34	0.41
25:BS:32:LEU:O	25:BS:35:ILE:HG22	2.20	0.41
30:Bd:14:TYR:HB2	34:B5:1597:A:C8	2.55	0.41
33:BM:114:LYS:O	33:BM:114:LYS:HG2	2.21	0.41
34:B5:326:G:H2'	34:B5:327:U:C6	2.55	0.41
34:B5:649:U:O2'	34:B5:650:U:H6	2.04	0.41
34:B5:831:U:H2'	34:B5:832:U:O4'	2.21	0.41
34:B5:989:U:H2'	34:B5:990:C:C6	2.55	0.41
37:AC:302:ALA:HB2	53:AQ:39:ARG:CZ	2.50	0.41
38:A1:679:U:O2'	38:A1:788:C:O2	2.36	0.41
38:A1:716:A:N6	63:Aa:117:ARG:HG3	2.35	0.41
38:A1:1037:C:H2'	38:A1:1038:C:C6	2.55	0.41
38:A1:3072:C:H2'	38:A1:3073:A:O4'	2.19	0.41
41:AD:65:ILE:CG2	41:AD:72:ASP:HB3	2.50	0.41
51:AO:23[A]:VAL:HG13	51:AO:33[A]:ILE:HG21	2.02	0.41
51:AO:42[A]:ASN:HA	51:AO:136[A]:THR:O	2.20	0.41
51:AO:54[A]:TYR:OH	51:AO:73[A]:PHE:O	2.35	0.41
56:AT:112:ASN:HB3	56:AT:128:LEU:HD12	2.02	0.41
73:Ak:19:ASP:OD1	73:Ak:20:VAL:HG23	2.20	0.41
79:E:4:ILE:HG13	79:E:198:TRP:HZ3	1.86	0.41
4:BE:192:ILE:HG13	4:BE:243:GLY:HA3	2.02	0.41
6:BH:24:PHE:CE1	6:BH:77:LEU:HD21	2.55	0.41
7:BI:31:ARG:HD2	34:B5:332:U:OP1	2.21	0.41
11:BO:80:HIS:ND1	11:BO:114:ARG:HB2	2.36	0.41
11:BO:122:PRO:HB3	34:B5:887:A:H1'	2.02	0.41
19:BD:120:TYR:HB3	19:BD:124:ARG:NH1	2.35	0.41
20:BF:43:PHE:CE1	20:BF:70:VAL:HA	2.56	0.41
22:BP:106:GLU:OE2	22:BP:108:ARG:NE	2.53	0.41
27:BU:61:LYS:HE3	27:BU:61:LYS:HB3	1.85	0.41
28:BZ:73:GLY:O	28:BZ:77:ARG:HG2	2.20	0.41
34:B5:953:G:H2'	34:B5:954:G:H8	1.85	0.41
34:B5:1172:G:H2'	34:B5:1173:C:H6	1.84	0.41
34:B5:1275:A:C6	34:B5:1438:G:C5	3.08	0.41
34:B5:1636:C:O2	34:B5:1765:A:N6	2.54	0.41
37:AC:3:ARG:HD2	37:AC:3:ARG:HA	1.82	0.41
38:A1:158:G:H2'	38:A1:159:A:C8	2.55	0.41
38:A1:871:U:H2'	38:A1:872:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:1114:U:OP1	63:Aa:23:GLY:N	2.42	0.41
38:A1:1659:U:H2'	38:A1:1660:C:H6	1.84	0.41
38:A1:2486:A:HO2'	38:A1:2487:U:H6	1.67	0.41
38:A1:2941:A:H8	38:A1:2941:A:OP2	2.03	0.41
38:A1:3186:A:N3	45:AH:44:THR:OG1	2.46	0.41
40:A4:149:A:H2'	40:A4:150:G:C8	2.55	0.41
40:A4:156:U:H2'	40:A4:157:U:C6	2.55	0.41
44:AG:78:PHE:CD1	44:AG:179:ILE:HG12	2.55	0.41
58:AV:67:PRO:HA	58:AV:70:ARG:HD3	2.01	0.41
59:AW:9:SER:HB2	59:AW:51:TRP:CZ3	2.55	0.41
63:Aa:117:ARG:HD3	63:Aa:117:ARG:HA	1.78	0.41
79:E:189:PHE:CE1	79:E:193:LEU:HD22	2.53	0.41
1:BA:205:ARG:HH21	24:BR:81:LYS:NZ	2.17	0.41
5:BG:64:LYS:HB2	5:BG:97:VAL:HG21	2.02	0.41
8:BJ:79:ARG:NH1	34:B5:762:A:OP1	2.49	0.41
22:BP:13:LYS:HA	22:BP:13:LYS:HD2	1.77	0.41
22:BP:121:ILE:HD12	22:BP:121:ILE:HA	1.93	0.41
23:BQ:9:THR:HG21	23:BQ:88:GLY:HA2	2.03	0.41
24:BR:70:SER:HA	24:BR:74:GLN:NE2	2.35	0.41
28:BZ:40:VAL:C	28:BZ:75:LEU:HD11	2.46	0.41
31:Bg:80:ALA:O	31:Bg:92:TRP:N	2.47	0.41
31:Bg:172:ALA:HB2	31:Bg:202:LEU:HD13	2.02	0.41
34:B5:702:G:HO2'	34:B5:703:G:H8	1.67	0.41
34:B5:1450:U:C2	34:B5:1451:C:C5	3.08	0.41
34:B5:1586:A:H2'	34:B5:1587:A:O4'	2.21	0.41
38:A1:1737:U:O2	69:Ag:52:GLN:NE2	2.54	0.41
38:A1:2612:U:H2'	38:A1:2613:U:O4'	2.20	0.41
49:AM:65:LEU:HD13	55:AS:172:TYR:OH	2.21	0.41
52:AP:56:ARG:NH2	52:AP:75:GLU:OE2	2.54	0.41
55:AS:81:TYR:HE2	55:AS:90:MET:HE3	1.84	0.41
1:BA:50:VAL:HG22	24:BR:109:LEU:HD21	2.02	0.41
15:BY:35:VAL:HG23	15:BY:36:SER:N	2.36	0.41
20:BF:207:THR:O	20:BF:212:LYS:NZ	2.53	0.41
22:BP:93:VAL:HA	22:BP:106:GLU:HA	2.03	0.41
23:BQ:25:GLY:HA3	23:BQ:64:ASP:OD2	2.21	0.41
25:BS:30:TYR:CE2	25:BS:40:ARG:HG2	2.56	0.41
27:BU:57:ARG:HD2	34:B5:1382:A:N3	2.35	0.41
28:BZ:86:GLU:HG3	28:BZ:88:ILE:HG12	2.01	0.41
30:Bd:5:ASN:OD1	30:Bd:8:PHE:HB2	2.21	0.41
34:B5:30:G:H2'	34:B5:31:C:C6	2.55	0.41
34:B5:301:A:H2'	34:B5:302:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B5:872:G:H2'	34:B5:873:U:O4'	2.20	0.41
34:B5:995:A:H2'	34:B5:996:U:O4'	2.21	0.41
34:B5:1451:C:H2'	34:B5:1452:U:H6	1.85	0.41
34:B5:1562:G:H2'	34:B5:1563:C:O4'	2.21	0.41
35:AA:166:ILE:H	35:AA:166:ILE:HG12	1.72	0.41
37:AC:128:ALA:CB	37:AC:244:LEU:HG	2.50	0.41
38:A1:71:A:OP1	63:Aa:67:HIS:NE2	2.53	0.41
38:A1:168:U:HO2'	38:A1:169:U:P	2.41	0.41
38:A1:1566:A:N6	38:A1:1574:C:H42	2.18	0.41
38:A1:1699:A:H2'	38:A1:1700:G:C8	2.55	0.41
38:A1:2291:A:H2'	38:A1:2292:U:C6	2.56	0.41
38:A1:2890:A:O2'	38:A1:2933:A:N3	2.47	0.41
38:A1:3129:A:H2'	38:A1:3130:A:H5''	2.02	0.41
40:A4:23:U:H5''	61:AY:13:ARG:HG3	2.02	0.41
41:AD:119:TYR:OH	41:AD:139:PRO:O	2.32	0.41
42:AE:82:ARG:HD2	42:AE:82:ARG:HA	1.84	0.41
45:AH:57:VAL:HG12	45:AH:68:LEU:HD22	2.02	0.41
46:AI:208:ASN:OD1	46:AI:211:ARG:NH1	2.33	0.41
51:AO:8[A]:VAL:O	51:AO:118[A]:VAL:HG22	2.20	0.41
51:AO:128[A]:ARG:HE	51:AO:128[A]:ARG:HB3	1.56	0.41
76:An:25:LYS:HB3	76:An:25:LYS:HE3	1.91	0.41
3:BC:54:GLU:OE1	12:BV:11:LEU:HB3	2.20	0.41
3:BC:90:THR:OG1	3:BC:93:GLY:O	2.27	0.41
11:BO:90:ARG:NH2	34:B5:902:G:OP1	2.51	0.41
14:BX:108:GLY:HA2	34:B5:600:U:OP2	2.21	0.41
31:Bg:206:PRO:HD3	31:Bg:245:PHE:HB3	2.02	0.41
34:B5:289:U:C2	34:B5:290:G:C8	3.09	0.41
34:B5:480:G:H1	34:B5:508:U:H3	1.68	0.41
34:B5:1564:U:H2'	34:B5:1565:C:H6	1.85	0.41
34:B5:1775:U:H2'	34:B5:1776:A:C8	2.56	0.41
35:AA:2:GLY:N	38:A1:2608:G:OP1	2.53	0.41
37:AC:312:VAL:HG23	37:AC:313:LEU:HD23	2.02	0.41
38:A1:86:G:O2'	38:A1:98:G:O6	2.34	0.41
38:A1:179:C:H2'	38:A1:180:C:H6	1.86	0.41
38:A1:393:U:H2'	38:A1:394:G:O4'	2.21	0.41
38:A1:1615:C:H2'	38:A1:1616:U:H6	1.84	0.41
38:A1:3015:G:H2'	38:A1:3016:A:H8	1.86	0.41
39:A3:59:U:C2	39:A3:60:G:C8	3.09	0.41
49:AM:32:LEU:HD11	49:AM:94:TRP:CG	2.54	0.41
50:AN:172:ARG:O	50:AN:183:THR:OG1	2.35	0.41
54:AR:70:LYS:NZ	54:AR:75:HIS:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:AV:87:ARG:HH22	58:AV:137:VAL:HG22	1.85	0.41
79:E:24:LYS:HE2	79:E:210:MET:O	2.20	0.41
1:BA:175:TYR:CD2	1:BA:199:PRO:HB3	2.56	0.41
9:BL:152:GLN:CD	10:BN:137:PRO:HD3	2.45	0.41
20:BF:144:GLU:HG2	20:BF:161:ASP:HA	2.03	0.41
27:BU:58:LEU:HD21	27:BU:90:TYR:HE1	1.85	0.41
31:Bg:273:ASP:OD1	31:Bg:275:ARG:NH1	2.53	0.41
34:B5:765:G:H1'	34:B5:768:C:OP1	2.21	0.41
36:AB:266:ARG:HG2	36:AB:266:ARG:HH11	1.85	0.41
38:A1:508:U:H2'	38:A1:509:U:C6	2.56	0.41
38:A1:537:A:C2	38:A1:538:G:H1'	2.56	0.41
38:A1:799:G:OP2	63:Aa:32:ARG:HD3	2.21	0.41
38:A1:872:U:H2'	38:A1:873:C:C6	2.55	0.41
38:A1:949:C:O2'	38:A1:971:G:OP1	2.25	0.41
38:A1:1694:U:O2'	38:A1:1695:U:H5'	2.20	0.41
38:A1:3045:G:H2'	38:A1:3046:A:O4'	2.20	0.41
38:A1:3132:C:H2'	38:A1:3133:C:C6	2.55	0.41
38:A1:3337:G:H2'	38:A1:3338:C:C6	2.56	0.41
40:A4:91:C:H2'	40:A4:92:A:H8	1.86	0.41
40:A4:102:U:H2'	40:A4:103:G:C8	2.56	0.41
41:AD:243:ALA:O	41:AD:247:ILE:HD12	2.20	0.41
47:AJ:87:LYS:HD3	47:AJ:87:LYS:HA	1.93	0.41
53:AQ:57:ILE:HG21	53:AQ:147:ARG:HH11	1.86	0.41
53:AQ:159:LYS:HD3	53:AQ:159:LYS:HA	1.90	0.41
60:AX:141:TYR:O	60:AX:142:ILE:HG22	2.21	0.41
80:EC:6921:C:N3	80:EC:6922:G:C8	2.89	0.41
2:BB:158:SER:HB3	34:B5:875:G:OP1	2.20	0.41
3:BC:228:ASN:C	3:BC:228:ASN:ND2	2.78	0.41
4:BE:141:THR:OG1	4:BE:143:ASP:OD1	2.32	0.41
5:BG:53:SER:OG	34:B5:163:G:O2'	2.36	0.41
7:BI:105:ASP:C	7:BI:107:THR:H	2.27	0.41
11:BO:17:ALA:HA	11:BO:30:VAL:HG22	2.02	0.41
11:BO:87:GLY:HA3	11:BO:120:PRO:HG2	2.03	0.41
15:BY:37:LYS:NZ	15:BY:93:ARG:HD3	2.36	0.41
18:Be:47:VAL:O	18:Be:47:VAL:HG13	2.20	0.41
19:BD:53:THR:OG1	19:BD:94:ARG:HD3	2.20	0.41
19:BD:202:LEU:HB3	19:BD:204:ASP:OD1	2.21	0.41
20:BF:72:HIS:NE2	34:B5:1610:G:OP1	2.39	0.41
23:BQ:46:PHE:O	23:BQ:50:GLU:HG2	2.20	0.41
27:BU:30:LYS:HD3	27:BU:33:GLN:NE2	2.36	0.41
28:BZ:80:LEU:O	28:BZ:84:GLU:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BZ:97:LYS:HE3	34:B5:1474:G:N7	2.36	0.41
33:BM:62:LEU:HD23	33:BM:63:VAL:N	2.36	0.41
34:B5:179:A:H3'	34:B5:180:A:H8	1.85	0.41
34:B5:190:C:O2'	34:B5:195:G:N1	2.53	0.41
34:B5:343:C:C2	34:B5:344:A:C8	3.09	0.41
34:B5:645:C:H2'	34:B5:646:C:C6	2.56	0.41
34:B5:1164:G:H2'	34:B5:1165:G:H8	1.85	0.41
34:B5:1179:G:H21	34:B5:1460:A:H62	1.69	0.41
34:B5:1225:U:O2	34:B5:1230:A:O2'	2.39	0.41
36:AB:10:ARG:NH1	36:AB:11:HIS:O	2.54	0.41
38:A1:34:A:H2'	38:A1:35:A:C8	2.56	0.41
38:A1:98:G:N7	48:AL:13:HIS:NE2	2.66	0.41
38:A1:156:G:OP2	71:AI:25:LYS:HB3	2.21	0.41
38:A1:1152:G:OP2	38:A1:1152:G:N2	2.51	0.41
38:A1:1213:G:H4'	55:AS:90:MET:HB2	2.01	0.41
38:A1:1423:C:H1'	42:AE:5:LYS:HD3	2.02	0.41
38:A1:1443:G:H2'	38:A1:1444:G:C8	2.56	0.41
38:A1:1497:C:O2'	38:A1:1602:A:N3	2.52	0.41
38:A1:1566:A:H62	38:A1:1574:C:H42	1.69	0.41
38:A1:1915:A:H2'	38:A1:1916:U:C6	2.56	0.41
38:A1:1945:A:H2'	38:A1:1946:A:C8	2.56	0.41
38:A1:2351:U:H2'	38:A1:2352:A:H8	1.86	0.41
38:A1:2684:C:H2'	38:A1:2685:C:H6	1.86	0.41
38:A1:2709:C:H2'	38:A1:2710:C:C6	2.55	0.41
38:A1:2780:A:H2'	38:A1:2781:U:C6	2.56	0.41
38:A1:3229:G:OP1	49:AM:137:LYS:NZ	2.54	0.41
38:A1:3232:G:C6	38:A1:3256:G:C6	3.08	0.41
39:A3:9:C:OP1	56:AT:26:HIS:HB2	2.21	0.41
40:A4:62:C:H4'	40:A4:63:G:O5'	2.20	0.41
40:A4:74:U:C4	61:AY:74:TYR:CD1	3.08	0.41
42:AE:54:TYR:OH	42:AE:57:HIS:HB2	2.21	0.41
42:AE:58:LEU:HD12	42:AE:78:ARG:HD3	2.03	0.41
42:AE:60:ASP:OD1	42:AE:62:THR:OG1	2.31	0.41
47:AJ:12:LEU:HD12	47:AJ:131:MET:HB3	2.02	0.41
53:AQ:40:THR:HG21	53:AQ:133:LYS:HG2	2.03	0.41
56:AT:151:LEU:HG	56:AT:152:ALA:H	1.84	0.41
60:AX:69:SER:O	60:AX:73:MET:HG2	2.20	0.41
61:AY:56:VAL:HG11	61:AY:104:LEU:HD13	2.02	0.41
62:AZ:133:LYS:HE3	62:AZ:135:ARG:NH1	2.36	0.41
70:Ah:45:LYS:O	70:Ah:49:LYS:HG2	2.21	0.41
72:Aj:43:LYS:HE3	72:Aj:43:LYS:HB2	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:EC:6890:A:H2'	80:EC:6891:G:H8	1.83	0.41
4:BE:174:LYS:HB2	4:BE:179:LYS:NZ	2.35	0.41
4:BE:182:TYR:N	4:BE:226:PHE:O	2.48	0.41
5:BG:3:LEU:O	5:BG:15:THR:HA	2.21	0.41
9:BL:53:TYR:CD1	9:BL:113:PRO:HG2	2.55	0.41
10:BN:132:VAL:HG23	10:BN:134:VAL:HG23	2.02	0.41
11:BO:136:ARG:HD3	11:BO:136:ARG:H	1.86	0.41
14:BX:107:PHE:CD2	14:BX:114:LYS:HG3	2.56	0.41
14:BX:107:PHE:CE1	14:BX:123:LYS:HB3	2.56	0.41
19:BD:70:THR:O	19:BD:74:GLN:HG3	2.21	0.41
23:BQ:6:SER:OG	23:BQ:22:VAL:O	2.21	0.41
26:BT:122:ARG:NH2	34:B5:1500:C:OP1	2.54	0.41
28:BZ:69:LEU:O	28:BZ:70:LYS:HD3	2.21	0.41
30:Bd:31:ILE:HG12	30:Bd:38:ILE:O	2.21	0.41
31:Bg:54:PHE:CE1	31:Bg:312:VAL:HG11	2.56	0.41
31:Bg:150:TRP:NE1	31:Bg:174:ASN:HD22	2.19	0.41
34:B5:296:U:H2'	34:B5:297:U:H6	1.86	0.41
34:B5:352:A:OP2	34:B5:352:A:H8	2.04	0.41
35:AA:179:LEU:O	35:AA:184:ARG:HD2	2.21	0.41
36:AB:227:GLU:HG2	36:AB:270:ARG:HD3	2.03	0.41
38:A1:1299:U:H2'	38:A1:1300:G:O4'	2.22	0.41
38:A1:1856:C:H2'	38:A1:1857:C:C6	2.56	0.41
39:A3:49:G:C8	41:AD:58:LYS:HG2	2.56	0.41
42:AE:40:LEU:HD11	42:AE:54:TYR:HB2	2.02	0.41
43:AF:102:VAL:HG13	43:AF:126:LEU:HD22	2.03	0.41
45:AH:57:VAL:HG11	45:AH:65:VAL:HG12	2.03	0.41
46:AI:75:TYR:CE2	46:AI:150:GLU:HB3	2.55	0.41
48:AL:80:VAL:HG13	48:AL:85:LEU:HD12	2.02	0.41
51:AO:41[A]:LEU:HB2	51:AO:138[A]:LEU:HD12	2.03	0.41
51:AO:60[A]:LYS:O	51:AO:72[A]:HIS:NE2	2.54	0.41
58:AV:104:ASN:ND2	58:AV:108:GLU:HB2	2.36	0.41
60:AX:64:GLU:OE1	60:AX:85:GLN:NE2	2.54	0.41
63:Aa:112:ILE:HB	63:Aa:130:VAL:HG23	2.02	0.41
79:E:169:VAL:HG11	79:E:183:ILE:HG22	2.03	0.41
5:BG:27:PHE:HZ	5:BG:111:LEU:HD21	1.86	0.40
7:BI:39:GLY:HA2	7:BI:61:GLU:HB3	2.02	0.40
8:BJ:40:LYS:HB2	34:B5:593:U:OP1	2.21	0.40
10:BN:54:LEU:HB3	10:BN:60:VAL:HB	2.02	0.40
13:BW:28:ARG:HD3	13:BW:60:LYS:HE2	2.02	0.40
21:BK:4:PRO:HG2	21:BK:7:ASP:HB2	2.03	0.40
27:BU:45:ALA:HB2	27:BU:93:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Bg:221:MET:HG2	31:Bg:233:THR:HG23	2.03	0.40
34:B5:649:U:O2'	34:B5:650:U:O5'	2.39	0.40
34:B5:1725:U:H2'	34:B5:1726:G:C8	2.56	0.40
34:B5:1767:G:H4'	34:B5:1768:G:C4	2.56	0.40
38:A1:127:G:H2'	38:A1:128:G:H8	1.86	0.40
38:A1:242:C:O2'	38:A1:243:G:H8	2.04	0.40
38:A1:1180:A:H5''	68:Af:77:ASN:HB2	2.02	0.40
38:A1:2561:A:O2'	38:A1:2562:A:H8	2.04	0.40
38:A1:2655:U:H4'	38:A1:2656:A:O4'	2.22	0.40
38:A1:3215:A:C2	42:AE:157:GLN:HB3	2.56	0.40
40:A4:8:C:H2'	40:A4:9:A:H8	1.86	0.40
40:A4:29:U:H5''	48:AL:27:ASP:HB3	2.03	0.40
41:AD:131:LEU:HD23	41:AD:172:TYR:HE1	1.86	0.40
47:AJ:32:ARG:HD3	47:AJ:118:PRO:HB2	2.02	0.40
54:AR:173:ARG:HG3	54:AR:174:ALA:H	1.87	0.40
55:AS:10:ILE:HG12	55:AS:26:ARG:HB2	2.03	0.40
55:AS:78:TRP:CZ3	55:AS:125:LYS:HD3	2.56	0.40
74:Al:23:LEU:HD12	74:Al:24:PRO:HD2	2.01	0.40
79:E:13:VAL:O	79:E:17:LEU:HG	2.21	0.40
79:E:98:LYS:HG2	79:E:102:LYS:HE2	2.03	0.40
80:EC:6777:C:H2'	80:EC:6778:C:C5	2.56	0.40
1:BA:76:ILE:HB	1:BA:123:VAL:HG12	2.02	0.40
2:BB:153:HIS:CD2	2:BB:155:TYR:CD2	3.10	0.40
9:BL:116:ARG:HH12	54:AR:151:ARG:NH1	2.19	0.40
17:Bb:2:VAL:C	17:Bb:4:VAL:H	2.30	0.40
20:BF:146:THR:HA	20:BF:159:ALA:HA	2.01	0.40
22:BP:77:ARG:HB2	22:BP:102:PHE:CD2	2.57	0.40
25:BS:88:ARG:HH22	34:B5:1546:G:H21	1.68	0.40
28:BZ:81:ARG:HA	28:BZ:84:GLU:HG2	2.04	0.40
31:Bg:13:LEU:HD12	31:Bg:310:ILE:HG13	2.03	0.40
31:Bg:54:PHE:HE1	31:Bg:312:VAL:HG11	1.86	0.40
31:Bg:106:HIS:CE1	31:Bg:132:LYS:HB2	2.56	0.40
31:Bg:214:ALA:HB2	31:Bg:243:LEU:HD21	2.03	0.40
31:Bg:239:GLU:HG2	31:Bg:241:PHE:CZ	2.56	0.40
33:BM:103:LEU:O	33:BM:106:ILE:HG23	2.22	0.40
34:B5:131:C:H2'	34:B5:132:U:H5'	2.03	0.40
34:B5:601:A:H2'	34:B5:602:U:C6	2.57	0.40
34:B5:629:U:H2'	34:B5:630:A:C8	2.55	0.40
34:B5:1386:G:H2'	34:B5:1387:G:O4'	2.20	0.40
34:B5:1524:A:N3	34:B5:1590:G:O2'	2.46	0.40
38:A1:207:U:H2'	38:A1:208:C:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:277:G:H2'	38:A1:278:U:C6	2.56	0.40
38:A1:655:C:OP2	67:Ae:27:ARG:HD3	2.22	0.40
38:A1:1347:U:H2'	38:A1:1355:A:H61	1.87	0.40
38:A1:2117:A:C8	38:A1:3064:U:H1'	2.56	0.40
38:A1:3176:G:N2	38:A1:3213:A:H1'	2.36	0.40
40:A4:27:U:H2'	40:A4:28:C:C6	2.57	0.40
41:AD:187:THR:OG1	41:AD:189:GLU:OE2	2.40	0.40
43:AF:138:TYR:CD2	43:AF:233:GLU:HB2	2.57	0.40
43:AF:160:ARG:HG3	43:AF:203:TRP:CG	2.57	0.40
72:Aj:27:PHE:HA	72:Aj:34:CYS:HA	2.03	0.40
80:EC:6781:U:H3	80:EC:6815:U:H3	1.69	0.40
7:BI:25:ARG:HA	34:B5:400:A:H5''	2.04	0.40
10:BN:112:LYS:HE2	34:B5:974:A2M:H4'	2.03	0.40
15:BY:112:LYS:HB3	15:BY:112:LYS:HE3	1.85	0.40
28:BZ:67:ASP:HB3	80:EC:6868:C:O2'	2.21	0.40
31:Bg:167:VAL:HB	31:Bg:183:LEU:HD21	2.03	0.40
31:Bg:294:TRP:CE2	31:Bg:301:LEU:HD21	2.57	0.40
34:B5:225:A:H2'	34:B5:226:A:N7	2.36	0.40
36:AB:106:TRP:O	36:AB:137:TYR:OH	2.39	0.40
37:AC:290:ILE:HD12	53:AQ:35:PHE:CD2	2.57	0.40
38:A1:728:G:H5''	53:AQ:43:PRO:HB2	2.04	0.40
38:A1:1021:G:N2	38:A1:1031:C:H2'	2.33	0.40
38:A1:1188:U:OP1	38:A1:1210:U:O2'	2.33	0.40
38:A1:1765:U:H2'	38:A1:1766:G:H4'	2.03	0.40
38:A1:1856:C:H2'	38:A1:1857:C:H6	1.86	0.40
38:A1:2152:A:H2'	38:A1:2153:U:C6	2.56	0.40
55:AS:45:LEU:HD12	55:AS:45:LEU:HA	1.92	0.40
62:AZ:60:LYS:HA	62:AZ:60:LYS:HD3	1.77	0.40
79:E:183:ILE:HG13	79:E:184:LEU:N	2.37	0.40
80:EC:6836:U:OP2	80:EC:6847:G:N2	2.54	0.40
3:BC:140:ARG:HB3	3:BC:221:THR:HB	2.02	0.40
11:BO:84:ARG:HG2	11:BO:85:ALA:O	2.22	0.40
23:BQ:72:GLY:N	34:B5:1483:A:H4'	2.37	0.40
25:BS:119:ILE:HD13	25:BS:119:ILE:HA	1.91	0.40
30:Bd:36:LEU:O	30:Bd:38:ILE:HG13	2.21	0.40
31:Bg:234:LEU:HD23	31:Bg:261:LYS:NZ	2.37	0.40
34:B5:684:A:H2'	34:B5:685:A:C8	2.56	0.40
34:B5:972:G:O2'	38:A1:847:A:N6	2.55	0.40
34:B5:1490:C:H1'	34:B5:1492:A:N1	2.36	0.40
34:B5:1659:A:H2'	34:B5:1660:A:C8	2.56	0.40
35:AA:192:LYS:HB3	35:AA:193:ARG:CZ	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A1:173:G:C6	38:A1:245:U:O2	2.74	0.40
38:A1:589:A:H8	38:A1:590:G:C8	2.39	0.40
38:A1:744:A:H2'	38:A1:745:C:O4'	2.22	0.40
38:A1:979:U:H4'	38:A1:980:A:O4'	2.22	0.40
38:A1:1463:U:H2'	38:A1:1464:G:O4'	2.22	0.40
38:A1:1573:G:H2'	38:A1:1574:C:O4'	2.20	0.40
38:A1:2508:U:H2'	38:A1:2509:U:C6	2.57	0.40
44:AG:140:VAL:HG21	50:AN:3:ALA:HB2	2.03	0.40
46:AI:68:ALA:HB1	46:AI:155:ALA:HB1	2.03	0.40
49:AM:46:ILE:HD11	49:AM:56:GLN:HE21	1.85	0.40
49:AM:127:LYS:O	49:AM:130:THR:OG1	2.38	0.40
54:AR:10:LEU:HD23	54:AR:10:LEU:HA	1.93	0.40
55:AS:13:ARG:O	55:AS:22:PRO:HG2	2.21	0.40
63:Aa:2:PRO:HG2	63:Aa:5:PHE:CD2	2.56	0.40
69:Ag:54:ILE:HG23	69:Ag:70:LYS:HA	2.04	0.40
80:EC:6853:G:H22	80:EC:6875:C:N4	2.10	0.40
1:BA:71:GLU:HG2	1:BA:96:THR:HG23	2.04	0.40
3:BC:45:VAL:HG21	3:BC:68:ILE:HG23	2.03	0.40
13:BW:6:VAL:HB	13:BW:29:PRO:HD2	2.04	0.40
20:BF:81:ARG:HE	34:B5:1615:C:P	2.44	0.40
20:BF:121:ILE:O	20:BF:121:ILE:HG22	2.22	0.40
21:BK:14:TYR:HA	21:BK:17:GLN:HG2	2.03	0.40
25:BS:118:LYS:HD3	25:BS:120:ARG:NH1	2.37	0.40
25:BS:126:ARG:NE	25:BS:132:ARG:O	2.51	0.40
26:BT:57:ARG:HH21	34:B5:1479:A:P	2.44	0.40
31:Bg:241:PHE:CE2	31:Bg:288:HIS:CD2	3.09	0.40
34:B5:631:G:H2'	34:B5:632:U:C6	2.56	0.40
38:A1:251:G:H1'	38:A1:253:A:C4	2.57	0.40
38:A1:293:C:H2'	38:A1:294:U:O4'	2.22	0.40
38:A1:716:A:C6	63:Aa:117:ARG:HG3	2.56	0.40
38:A1:2115:G:O2'	54:AR:82:LYS:HD3	2.22	0.40
38:A1:2419:A:H2'	38:A1:2420:C:C6	2.57	0.40
38:A1:2485:A:H5''	79:E:101:LYS:HD3	2.04	0.40
41:AD:107:ARG:HB3	41:AD:251:PRO:HG3	2.03	0.40
62:AZ:105:SER:O	62:AZ:108:GLU:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	
1	BA	204/252 (81%)	181 (89%)	23 (11%)	0	100	100
2	BB	212/255 (83%)	181 (85%)	31 (15%)	0	100	100
3	BC	215/254 (85%)	208 (97%)	7 (3%)	0	100	100
4	BE	258/261 (99%)	238 (92%)	20 (8%)	0	100	100
5	BG	224/236 (95%)	209 (93%)	15 (7%)	0	100	100
6	BH	182/190 (96%)	171 (94%)	11 (6%)	0	100	100
7	BI	184/200 (92%)	167 (91%)	17 (9%)	0	100	100
8	BJ	183/197 (93%)	170 (93%)	13 (7%)	0	100	100
9	BL	153/156 (98%)	139 (91%)	14 (9%)	0	100	100
10	BN	148/151 (98%)	139 (94%)	9 (6%)	0	100	100
11	BO	125/137 (91%)	110 (88%)	15 (12%)	0	100	100
12	BV	85/87 (98%)	77 (91%)	8 (9%)	0	100	100
13	BW	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
14	BX	142/145 (98%)	127 (89%)	15 (11%)	0	100	100
15	BY	132/135 (98%)	123 (93%)	9 (7%)	0	100	100
16	Ba	95/119 (80%)	78 (82%)	17 (18%)	0	100	100
17	Bb	79/82 (96%)	71 (90%)	8 (10%)	0	100	100
18	Be	58/63 (92%)	49 (84%)	8 (14%)	1 (2%)	7	13
19	BD	221/240 (92%)	207 (94%)	14 (6%)	0	100	100
20	BF	204/225 (91%)	190 (93%)	14 (7%)	0	100	100
21	BK	94/105 (90%)	80 (85%)	14 (15%)	0	100	100
22	BP	122/142 (86%)	112 (92%)	10 (8%)	0	100	100
23	BQ	139/143 (97%)	130 (94%)	9 (6%)	0	100	100
24	BR	117/136 (86%)	110 (94%)	7 (6%)	0	100	100
25	BS	143/146 (98%)	131 (92%)	12 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	BT	139/144 (96%)	124 (89%)	15 (11%)	0	100	100
27	BU	105/121 (87%)	98 (93%)	7 (7%)	0	100	100
28	BZ	67/108 (62%)	64 (96%)	3 (4%)	0	100	100
29	Bc	61/67 (91%)	56 (92%)	5 (8%)	0	100	100
30	Bd	51/56 (91%)	51 (100%)	0	0	100	100
31	Bg	310/319 (97%)	275 (89%)	35 (11%)	0	100	100
32	Bf	53/152 (35%)	36 (68%)	17 (32%)	0	100	100
33	BM	119/143 (83%)	95 (80%)	24 (20%)	0	100	100
35	AA	245/254 (96%)	236 (96%)	9 (4%)	0	100	100
36	AB	383/387 (99%)	371 (97%)	12 (3%)	0	100	100
37	AC	359/362 (99%)	337 (94%)	22 (6%)	0	100	100
41	AD	290/297 (98%)	274 (94%)	16 (6%)	0	100	100
42	AE	152/176 (86%)	140 (92%)	12 (8%)	0	100	100
43	AF	220/244 (90%)	213 (97%)	7 (3%)	0	100	100
44	AG	228/256 (89%)	212 (93%)	16 (7%)	0	100	100
45	AH	188/191 (98%)	173 (92%)	15 (8%)	0	100	100
46	AI	201/221 (91%)	195 (97%)	6 (3%)	0	100	100
47	AJ	167/174 (96%)	143 (86%)	24 (14%)	0	100	100
48	AL	191/199 (96%)	178 (93%)	13 (7%)	0	100	100
49	AM	134/138 (97%)	129 (96%)	5 (4%)	0	100	100
50	AN	201/204 (98%)	191 (95%)	10 (5%)	0	100	100
51	AO	195/199 (98%)	192 (98%)	3 (2%)	0	100	100
52	AP	171/184 (93%)	165 (96%)	6 (4%)	0	100	100
53	AQ	183/186 (98%)	180 (98%)	3 (2%)	0	100	100
54	AR	186/189 (98%)	178 (96%)	8 (4%)	0	100	100
55	AS	170/178 (96%)	157 (92%)	13 (8%)	0	100	100
56	AT	157/160 (98%)	146 (93%)	11 (7%)	0	100	100
57	AU	98/121 (81%)	95 (97%)	3 (3%)	0	100	100
58	AV	134/137 (98%)	130 (97%)	4 (3%)	0	100	100
59	AW	61/155 (39%)	61 (100%)	0	0	100	100
60	AX	119/142 (84%)	114 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	AY	124/127 (98%)	121 (98%)	3 (2%)	0	100	100
62	AZ	133/136 (98%)	125 (94%)	8 (6%)	0	100	100
63	Aa	146/149 (98%)	133 (91%)	13 (9%)	0	100	100
64	Ab	56/59 (95%)	50 (89%)	6 (11%)	0	100	100
65	Ac	95/105 (90%)	95 (100%)	0	0	100	100
66	Ad	107/113 (95%)	102 (95%)	5 (5%)	0	100	100
67	Ae	125/130 (96%)	120 (96%)	5 (4%)	0	100	100
68	Af	104/107 (97%)	98 (94%)	6 (6%)	0	100	100
69	Ag	110/121 (91%)	107 (97%)	3 (3%)	0	100	100
70	Ah	117/120 (98%)	111 (95%)	6 (5%)	0	100	100
71	Ai	97/100 (97%)	91 (94%)	6 (6%)	0	100	100
72	Aj	85/88 (97%)	81 (95%)	4 (5%)	0	100	100
73	Ak	75/78 (96%)	67 (89%)	8 (11%)	0	100	100
74	Al	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
75	Am	50/128 (39%)	47 (94%)	3 (6%)	0	100	100
76	An	23/25 (92%)	23 (100%)	0	0	100	100
77	Ao	103/106 (97%)	93 (90%)	10 (10%)	0	100	100
78	Ap	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
79	E	215/217 (99%)	201 (94%)	14 (6%)	0	100	100
All	All	11086/12103 (92%)	10325 (93%)	760 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	Be	54	ARG

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 PDB entries followed by that with respect to all EM entries.

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	
1	BA	173/210 (82%)	173 (100%)	0	100	100
2	BB	191/224 (85%)	191 (100%)	0	100	100
3	BC	176/205 (86%)	176 (100%)	0	100	100
4	BE	221/222 (100%)	221 (100%)	0	100	100
5	BG	193/201 (96%)	193 (100%)	0	100	100
6	BH	165/170 (97%)	165 (100%)	0	100	100
7	BI	150/161 (93%)	150 (100%)	0	100	100
8	BJ	158/166 (95%)	158 (100%)	0	100	100
9	BL	136/137 (99%)	136 (100%)	0	100	100
10	BN	127/128 (99%)	127 (100%)	0	100	100
11	BO	96/105 (91%)	96 (100%)	0	100	100
12	BV	74/74 (100%)	74 (100%)	0	100	100
13	BW	110/111 (99%)	110 (100%)	0	100	100
14	BX	119/120 (99%)	119 (100%)	0	100	100
15	BY	112/113 (99%)	112 (100%)	0	100	100
16	Ba	83/100 (83%)	83 (100%)	0	100	100
17	Bb	70/71 (99%)	70 (100%)	0	100	100
18	Be	51/54 (94%)	51 (100%)	0	100	100
19	BD	182/195 (93%)	182 (100%)	0	100	100
20	BF	173/191 (91%)	173 (100%)	0	100	100
21	BK	89/98 (91%)	89 (100%)	0	100	100
22	BP	104/118 (88%)	104 (100%)	0	100	100
23	BQ	117/119 (98%)	117 (100%)	0	100	100
24	BR	110/124 (89%)	110 (100%)	0	100	100
25	BS	128/129 (99%)	128 (100%)	0	100	100
26	BT	113/116 (97%)	113 (100%)	0	100	100
27	BU	100/114 (88%)	100 (100%)	0	100	100
28	BZ	61/89 (68%)	61 (100%)	0	100	100
29	Bc	56/60 (93%)	56 (100%)	0	100	100
30	Bd	47/49 (96%)	47 (100%)	0	100	100
31	Bg	256/262 (98%)	256 (100%)	0	100	100
32	Bf	49/135 (36%)	49 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	BM	98/119 (82%)	98 (100%)	0	100	100
35	AA	189/196 (96%)	189 (100%)	0	100	100
36	AB	320/322 (99%)	320 (100%)	0	100	100
37	AC	288/289 (100%)	288 (100%)	0	100	100
41	AD	241/245 (98%)	241 (100%)	0	100	100
42	AE	134/153 (88%)	134 (100%)	0	100	100
43	AF	186/205 (91%)	186 (100%)	0	100	100
44	AG	189/208 (91%)	189 (100%)	0	100	100
45	AH	170/171 (99%)	170 (100%)	0	100	100
46	AI	176/187 (94%)	176 (100%)	0	100	100
47	AJ	147/150 (98%)	147 (100%)	0	100	100
48	AL	154/159 (97%)	154 (100%)	0	100	100
49	AM	107/109 (98%)	107 (100%)	0	100	100
50	AN	175/176 (99%)	175 (100%)	0	100	100
51	AO	160/162 (99%)	160 (100%)	0	100	100
52	AP	141/146 (97%)	141 (100%)	0	100	100
53	AQ	150/151 (99%)	150 (100%)	0	100	100
54	AR	153/154 (99%)	153 (100%)	0	100	100
55	AS	156/162 (96%)	156 (100%)	0	100	100
56	AT	136/137 (99%)	136 (100%)	0	100	100
57	AU	87/107 (81%)	87 (100%)	0	100	100
58	AV	104/105 (99%)	104 (100%)	0	100	100
59	AW	55/129 (43%)	55 (100%)	0	100	100
60	AX	105/118 (89%)	105 (100%)	0	100	100
61	AY	109/110 (99%)	109 (100%)	0	100	100
62	AZ	115/116 (99%)	115 (100%)	0	100	100
63	Aa	118/119 (99%)	118 (100%)	0	100	100
64	Ab	46/47 (98%)	46 (100%)	0	100	100
65	Ac	81/88 (92%)	81 (100%)	0	100	100
66	Ad	96/97 (99%)	96 (100%)	0	100	100
67	Ae	109/111 (98%)	109 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	Af	90/91 (99%)	90 (100%)	0	100	100
69	Ag	95/103 (92%)	95 (100%)	0	100	100
70	Ah	104/105 (99%)	104 (100%)	0	100	100
71	Ai	81/82 (99%)	81 (100%)	0	100	100
72	Aj	70/71 (99%)	70 (100%)	0	100	100
73	Ak	68/69 (99%)	68 (100%)	0	100	100
74	Al	45/46 (98%)	45 (100%)	0	100	100
75	Am	47/116 (40%)	47 (100%)	0	100	100
76	An	23/23 (100%)	23 (100%)	0	100	100
77	Ao	90/91 (99%)	90 (100%)	0	100	100
78	Ap	71/72 (99%)	71 (100%)	0	100	100
79	E	198/198 (100%)	198 (100%)	0	100	100
All	All	9467/10186 (93%)	9467 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	BA	30	GLN
3	BC	152	HIS
5	BG	34	GLN
6	BH	174	ASN
7	BI	35	ASN
7	BI	111	GLN
8	BJ	131	GLN
8	BJ	176	ASN
9	BL	14	GLN
9	BL	81	HIS
9	BL	98	ASN
9	BL	127	GLN
11	BO	12	GLN
11	BO	99	GLN
12	BV	21	ASN
12	BV	75	ASN
13	BW	12	ASN
13	BW	39	GLN
14	BX	18	HIS

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Mol	Chain	Res	Type
15	BY	15	ASN
15	BY	77	ASN
16	Ba	94	ASN
17	Bb	9	HIS
17	Bb	49	HIS
19	BD	67	ASN
19	BD	159	HIS
20	BF	86	GLN
20	BF	100	ASN
20	BF	104	ASN
21	BK	28	ASN
24	BR	74	GLN
25	BS	8	GLN
25	BS	104	ASN
26	BT	77	ASN
27	BU	40	ASN
27	BU	105	GLN
29	Bc	43	ASN
30	Bd	53	ASN
31	Bg	29	GLN
32	Bf	123	ASN
32	Bf	135	HIS
36	AB	109	HIS
36	AB	182	GLN
36	AB	184	ASN
37	AC	5	GLN
37	AC	196	ASN
41	AD	40	HIS
41	AD	206	GLN
41	AD	296	GLN
42	AE	61	ASN
43	AF	157	ASN
43	AF	231	ASN
43	AF	244	ASN
44	AG	240	ASN
44	AG	252	ASN
45	AH	96	HIS
46	AI	23	ASN
46	AI	73	ASN
47	AJ	43	GLN
48	AL	114	GLN
48	AL	120	GLN

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Mol	Chain	Res	Type
49	AM	56	GLN
50	AN	138	GLN
51	AO	26[A]	GLN
51	AO	31[A]	GLN
51	AO	50[A]	ASN
52	AP	133	HIS
54	AR	141	HIS
55	AS	46	GLN
55	AS	49	HIS
55	AS	74	ASN
56	AT	5	HIS
56	AT	98	HIS
57	AU	101	ASN
59	AW	59	HIS
60	AX	65	GLN
60	AX	85	GLN
61	AY	98	ASN
62	AZ	78	ASN
62	AZ	103	GLN
62	AZ	122	HIS
63	Aa	14	HIS
63	Aa	62	HIS
63	Aa	89	GLN
64	Ab	43	HIS
65	Ac	11	ASN
66	Ad	21	HIS
67	Ae	21	HIS
69	Ag	98	GLN
72	Aj	13	ASN
77	Ao	99	GLN
79	E	182	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	B5	1780/1798 (98%)	405 (22%)	12 (0%)
38	A1	3194/3360 (95%)	580 (18%)	18 (0%)
39	A3	120/121 (99%)	10 (8%)	1 (0%)
40	A4	157/158 (99%)	29 (18%)	0
80	EC	190/202 (94%)	104 (54%)	6 (3%)
All	All	5441/5639 (96%)	1128 (20%)	37 (0%)

All (1128) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
34	B5	4	C
34	B5	5	U
34	B5	17	C
34	B5	25	C
34	B5	26	A
34	B5	34	G
34	B5	42	G
34	B5	45	U
34	B5	46	A
34	B5	47	A
34	B5	57	G
34	B5	60	U
34	B5	67	A
34	B5	68	A
34	B5	72	A
34	B5	73	U
34	B5	74	U
34	B5	76	A
34	B5	77	U
34	B5	81	G
34	B5	93	A
34	B5	104	A
34	B5	114	C
34	B5	116	U
34	B5	127	G
34	B5	130	C
34	B5	131	C
34	B5	132	U
34	B5	133	U
34	B5	134	U
34	B5	135	A
34	B5	136	C
34	B5	137	U
34	B5	138	A
34	B5	141	U
34	B5	145	A
34	B5	163	G
34	B5	166	C
34	B5	178	U
34	B5	179	A
34	B5	181	A
34	B5	182	A

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Mol	Chain	Res	Type
34	B5	188	A
34	B5	191	C
34	B5	192	U
34	B5	193	U
34	B5	194	U
34	B5	195	G
34	B5	198	A
34	B5	200	A
34	B5	201	G
34	B5	217	A
34	B5	218	A
34	B5	219	A
34	B5	221	A
34	B5	225	A
34	B5	227	U
34	B5	228	G
34	B5	230	C
34	B5	232	U
34	B5	233	C
34	B5	234	G
34	B5	238	U
34	B5	240	U
34	B5	241	U
34	B5	257	A
34	B5	261	U
34	B5	262	U
34	B5	265	A
34	B5	267	U
34	B5	272	U
34	B5	277	U
34	B5	280	U
34	B5	283	U
34	B5	287	G
34	B5	299	A
34	B5	314	C
34	B5	316	A
34	B5	320	U
34	B5	321	C
34	B5	322	G
34	B5	333	A
34	B5	337	G
34	B5	338	C

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Mol	Chain	Res	Type
34	B5	352	A
34	B5	353	A
34	B5	359	A
34	B5	360	A
34	B5	361	C
34	B5	390	G
34	B5	400	A
34	B5	401	A
34	B5	402	C
34	B5	417	A
34	B5	419	G
34	B5	423	G
34	B5	424	C
34	B5	425	A
34	B5	426	G
34	B5	434	G
34	B5	435	C
34	B5	439	U
34	B5	440	U
34	B5	444	C
34	B5	453	U
34	B5	459	G
34	B5	460	A
34	B5	475	A
34	B5	477	A
34	B5	484	C
34	B5	485	A
34	B5	486	G
34	B5	487	G
34	B5	489	C
34	B5	490	C
34	B5	491	C
34	B5	492	A
34	B5	493	U
34	B5	494	U
34	B5	495	C
34	B5	496	G
34	B5	497	G
34	B5	498	G
34	B5	499	U
34	B5	500	C
34	B5	501	U

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Mol	Chain	Res	Type
34	B5	502	U
34	B5	503	G
34	B5	506	A
34	B5	507	U
34	B5	514	G
34	B5	515	A
34	B5	527	A
34	B5	538	A
34	B5	539	G
34	B5	540	G
34	B5	541	A2M
34	B5	542	A
34	B5	544	A
34	B5	554	C
34	B5	555	A
34	B5	557	G
34	B5	558	U
34	B5	559	C
34	B5	565	C
34	B5	577	G
34	B5	580	A
34	B5	582	U
34	B5	594	A
34	B5	595	G
34	B5	606	A
34	B5	610	G
34	B5	611	U
34	B5	619	A2M
34	B5	620	A
34	B5	622	A
34	B5	623	A
34	B5	624	G
34	B5	638	U
34	B5	639	U
34	B5	650	U
34	B5	652	G
34	B5	655	G
34	B5	656	G
34	B5	657	U
34	B5	658	C
34	B5	677	G
34	B5	678	A

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Mol	Chain	Res	Type
34	B5	681	U
34	B5	683	C
34	B5	693	U
34	B5	694	U
34	B5	696	C
34	B5	697	C
34	B5	705	U
34	B5	706	A
34	B5	708	C
34	B5	709	C
34	B5	710	U
34	B5	712	G
34	B5	713	A
34	B5	715	U
34	B5	716	C
34	B5	717	C
34	B5	718	U
34	B5	719	U
34	B5	720	G
34	B5	722	G
34	B5	725	U
34	B5	726	C
34	B5	727	U
34	B5	729	G
34	B5	730	G
34	B5	731	C
34	B5	733	A
34	B5	735	C
34	B5	738	G
34	B5	740	A
34	B5	741	C
34	B5	742	U
34	B5	753	A
34	B5	765	G
34	B5	766	U
34	B5	774	A
34	B5	775	G
34	B5	778	G
34	B5	781	U
34	B5	782	U
34	B5	783	G
34	B5	784	C

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Mol	Chain	Res	Type
34	B5	789	A
34	B5	794	U
34	B5	811	A
34	B5	812	A
34	B5	814	A
34	B5	819	G
34	B5	820	U
34	B5	821	U
34	B5	823	G
34	B5	833	U
34	B5	840	U
34	B5	846	G
34	B5	848	C
34	B5	850	A
34	B5	851	U
34	B5	859	A
34	B5	863	A
34	B5	893	U
34	B5	895	G
34	B5	898	A
34	B5	906	A
34	B5	907	A
34	B5	923	A
34	B5	929	A
34	B5	933	A
34	B5	935	U
34	B5	951	A
34	B5	960	U
34	B5	966	A
34	B5	973	A
34	B5	987	G
34	B5	988	A
34	B5	992	A
34	B5	993	A
34	B5	1004	U
34	B5	1005	A
34	B5	1020	A
34	B5	1021	C
34	B5	1026	A
34	B5	1028	C
34	B5	1032	G
34	B5	1039	A

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Mol	Chain	Res	Type
34	B5	1040	G
34	B5	1052	U
34	B5	1054	U
34	B5	1056	U
34	B5	1057	U
34	B5	1058	U
34	B5	1060	U
34	B5	1061	A
34	B5	1062	A
34	B5	1083	G
34	B5	1092	A
34	B5	1093	A
34	B5	1097	U
34	B5	1100	G
34	B5	1126	OMG
34	B5	1138	A
34	B5	1150	G
34	B5	1158	C
34	B5	1159	C
34	B5	1173	C
34	B5	1185	U
34	B5	1194	A
34	B5	1196	A
34	B5	1199	G
34	B5	1200	G
34	B5	1201	G
34	B5	1202	A
34	B5	1203	A
34	B5	1214	U
34	B5	1217	A
34	B5	1218	G
34	B5	1226	A
34	B5	1227	A
34	B5	1228	G
34	B5	1230	A
34	B5	1234	A
34	B5	1235	C
34	B5	1244	A
34	B5	1245	G
34	B5	1246	C
34	B5	1249	U
34	B5	1251	U

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Mol	Chain	Res	Type
34	B5	1254	U
34	B5	1255	G
34	B5	1256	A
34	B5	1257	U
34	B5	1258	U
34	B5	1269	OMU
34	B5	1273	G
34	B5	1276	U
34	B5	1286	U
34	B5	1291	G
34	B5	1306	C
34	B5	1314	U
34	B5	1315	U
34	B5	1316	G
34	B5	1321	A
34	B5	1325	A
34	B5	1340	U
34	B5	1342	C
34	B5	1344	A
34	B5	1345	A
34	B5	1355	C
34	B5	1356	U
34	B5	1362	U
34	B5	1363	U
34	B5	1364	G
34	B5	1368	G
34	B5	1370	U
34	B5	1371	A
34	B5	1372	U
34	B5	1373	C
34	B5	1375	A
34	B5	1378	U
34	B5	1389	C
34	B5	1390	U
34	B5	1396	U
34	B5	1399	C
34	B5	1400	A
34	B5	1412	G
34	B5	1413	U
34	B5	1415	U
34	B5	1425	A
34	B5	1427	A

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Mol	Chain	Res	Type
34	B5	1428	OMG
34	B5	1436	A
34	B5	1444	A
34	B5	1445	G
34	B5	1446	A
34	B5	1447	C
34	B5	1458	G
34	B5	1459	C
34	B5	1461	C
34	B5	1471	A
34	B5	1486	G
34	B5	1491	U
34	B5	1492	A
34	B5	1493	A
34	B5	1494	C
34	B5	1506	G
34	B5	1516	A
34	B5	1521	G
34	B5	1523	G
34	B5	1524	A
34	B5	1537	C
34	B5	1540	G
34	B5	1542	G
34	B5	1557	U
34	B5	1559	A
34	B5	1568	C
34	B5	1572	OMG
34	B5	1573	A
34	B5	1575	G7M
34	B5	1576	A
34	B5	1577	A
34	B5	1584	G
34	B5	1590	G
34	B5	1601	G
34	B5	1616	G
34	B5	1619	C
34	B5	1634	C
34	B5	1635	A
34	B5	1638	G
34	B5	1657	U
34	B5	1658	G
34	B5	1667	A

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Mol	Chain	Res	Type
34	B5	1680	G
34	B5	1682	U
34	B5	1683	C
34	B5	1684	U
34	B5	1688	U
34	B5	1700	C
34	B5	1701	A
34	B5	1703	C
34	B5	1709	C
34	B5	1715	G
34	B5	1716	C
34	B5	1717	G
34	B5	1730	A
34	B5	1757	G
34	B5	1760	G
34	B5	1762	A
34	B5	1766	A
34	B5	1767	G
34	B5	1769	U
34	B5	1780	G
34	B5	1782	MA6
34	B5	1792	G
34	B5	1793	G
34	B5	1794	A
34	B5	1795	U
34	B5	1796	C
34	B5	1799	U
38	A1	26	A
38	A1	34	A
38	A1	40	A
38	A1	43	A
38	A1	49	A
38	A1	59	G
38	A1	60	A
38	A1	65	A
38	A1	66	A
38	A1	71	A
38	A1	77	A
38	A1	92	G
38	A1	99	A
38	A1	109	A
38	A1	110	G

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Mol	Chain	Res	Type
38	A1	111	C
38	A1	116	A
38	A1	118	U
38	A1	122	A
38	A1	133	U
38	A1	134	U
38	A1	136	G
38	A1	143	G
38	A1	156	G
38	A1	157	A
38	A1	165	A
38	A1	169	U
38	A1	173	G
38	A1	176	G
38	A1	187	A
38	A1	190	U
38	A1	191	U
38	A1	200	C
38	A1	210	U
38	A1	211	A
38	A1	219	A
38	A1	234	G
38	A1	240	U
38	A1	241	G
38	A1	243	G
38	A1	245	U
38	A1	248	U
38	A1	249	U
38	A1	250	U
38	A1	251	G
38	A1	252	U
38	A1	253	A
38	A1	269	G
38	A1	286	U
38	A1	295	A
38	A1	296	A
38	A1	305	U
38	A1	311	C
38	A1	329	U
38	A1	339	C
38	A1	349	A
38	A1	352	A

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Mol	Chain	Res	Type
38	A1	373	A
38	A1	374	A
38	A1	376	G
38	A1	387	A
38	A1	398	A
38	A1	399	A
38	A1	401	U
38	A1	402	A
38	A1	403	C
38	A1	420	G
38	A1	421	G
38	A1	422	A
38	A1	438	A
38	A1	440	A
38	A1	495	G
38	A1	510	G
38	A1	521	A
38	A1	523	A
38	A1	535	G
38	A1	540	U
38	A1	543	C
38	A1	545	U
38	A1	546	C
38	A1	547	G
38	A1	548	G
38	A1	551	A
38	A1	552	G
38	A1	554	A
38	A1	557	A
38	A1	558	U
38	A1	559	A
38	A1	560	G
38	A1	579	G
38	A1	589	A
38	A1	602	A
38	A1	604	G
38	A1	608	A
38	A1	611	A
38	A1	620	U
38	A1	621	A
38	A1	649	A2M
38	A1	660	A

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Mol	Chain	Res	Type
38	A1	677	A
38	A1	681	U
38	A1	691	A
38	A1	705	A
38	A1	715	A
38	A1	719	U
38	A1	736	A
38	A1	737	G
38	A1	758	C
38	A1	765	C
38	A1	766	U
38	A1	767	U
38	A1	774	G
38	A1	777	U
38	A1	781	G
38	A1	785	G
38	A1	786	A
38	A1	799	G
38	A1	806	A
38	A1	813	G
38	A1	817	A2M
38	A1	818	C
38	A1	830	A
38	A1	849	C
38	A1	861	C
38	A1	874	U
38	A1	879	U
38	A1	896	A
38	A1	897	U
38	A1	907	G
38	A1	908	OMG
38	A1	909	G
38	A1	914	A
38	A1	916	G
38	A1	917	A
38	A1	921	A
38	A1	923	C
38	A1	925	A
38	A1	934	G
38	A1	937	G
38	A1	943	U
38	A1	944	C

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Mol	Chain	Res	Type
38	A1	953	G
38	A1	959	C
38	A1	961	C
38	A1	964	G
38	A1	974	G
38	A1	980	A
38	A1	981	U
38	A1	982	C
38	A1	1002	A
38	A1	1010	G
38	A1	1015	U
38	A1	1016	C
38	A1	1017	C
38	A1	1018	G
38	A1	1019	G
38	A1	1020	G
38	A1	1021	G
38	A1	1022	U
38	A1	1032	C
38	A1	1033	U
38	A1	1034	U
38	A1	1035	G
38	A1	1047	A
38	A1	1064	A
38	A1	1072	G
38	A1	1081	U
38	A1	1082	U
38	A1	1093	A
38	A1	1094	U
38	A1	1095	U
38	A1	1097	G
38	A1	1098	A
38	A1	1103	A
38	A1	1117	G
38	A1	1131	G
38	A1	1144	U
38	A1	1145	G
38	A1	1152	G
38	A1	1153	A
38	A1	1155	C
38	A1	1159	A
38	A1	1160	C

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Mol	Chain	Res	Type
38	A1	1178	G
38	A1	1179	A
38	A1	1180	A
38	A1	1181	U
38	A1	1182	A
38	A1	1192	C
38	A1	1193	A
38	A1	1201	C
38	A1	1206	G
38	A1	1208	U
38	A1	1219	C
38	A1	1220	U
38	A1	1222	G
38	A1	1223	A
38	A1	1226	G
38	A1	1227	C
38	A1	1232	C
38	A1	1233	G
38	A1	1235	U
38	A1	1236	G
38	A1	1240	A
38	A1	1241	U
38	A1	1243	G
38	A1	1244	A
38	A1	1245	A
38	A1	1246	G
38	A1	1258	U
38	A1	1259	A
38	A1	1260	A
38	A1	1262	G
38	A1	1263	A
38	A1	1265	U
38	A1	1270	A
38	A1	1272	C
38	A1	1278	A
38	A1	1279	C
38	A1	1280	C
38	A1	1281	G
38	A1	1282	G
38	A1	1283	C
38	A1	1285	G
38	A1	1286	A

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Mol	Chain	Res	Type
38	A1	1287	A
38	A1	1292	C
38	A1	1293	U
38	A1	1305	U
38	A1	1307	G
38	A1	1309	U
38	A1	1317	A
38	A1	1318	A
38	A1	1330	A
38	A1	1331	U
38	A1	1348	U
38	A1	1349	G
38	A1	1350	A
38	A1	1351	U
38	A1	1352	A
38	A1	1353	U
38	A1	1355	A
38	A1	1356	U
38	A1	1357	G
38	A1	1386	A
38	A1	1392	G
38	A1	1399	A
38	A1	1400	G
38	A1	1418	A
38	A1	1419	A
38	A1	1434	G
38	A1	1437	OMC
38	A1	1446	A
38	A1	1455	U
38	A1	1468	A
38	A1	1481	A
38	A1	1496	C
38	A1	1508	C
38	A1	1523	U
38	A1	1555	U
38	A1	1556	C
38	A1	1562	C
38	A1	1564	U
38	A1	1565	G
38	A1	1567	U
38	A1	1568	U
38	A1	1569	U

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Mol	Chain	Res	Type
38	A1	1572	U
38	A1	1575	A
38	A1	1576	G
38	A1	1579	C
38	A1	1580	A
38	A1	1581	C
38	A1	1583	A
38	A1	1587	A
38	A1	1589	A
38	A1	1593	A
38	A1	1605	A
38	A1	1628	C
38	A1	1629	U
38	A1	1630	U
38	A1	1639	C
38	A1	1642	A
38	A1	1643	A
38	A1	1645	U
38	A1	1724	U
38	A1	1734	G
38	A1	1736	G
38	A1	1738	C
38	A1	1750	A
38	A1	1751	G
38	A1	1761	C
38	A1	1762	C
38	A1	1763	U
38	A1	1764	U
38	A1	1765	U
38	A1	1766	G
38	A1	1775	G
38	A1	1778	G
38	A1	1797	A
38	A1	1813	A
38	A1	1815	U
38	A1	1817	G
38	A1	1818	U
38	A1	1820	U
38	A1	1821	U
38	A1	1842	A
38	A1	1846	C
38	A1	1849	C

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Mol	Chain	Res	Type
38	A1	1851	G
38	A1	1866	C
38	A1	1878	G
38	A1	1880	U
38	A1	1893	A
38	A1	1906	G
38	A1	1932	A
38	A1	1948	G
38	A1	1952	G
38	A1	1953	G
38	A1	1954	G
38	A1	1955	U
38	A1	2112	U
38	A1	2114	C
38	A1	2117	A
38	A1	2122	G
38	A1	2131	A
38	A1	2140	U
38	A1	2144	A
38	A1	2145	A
38	A1	2158	A
38	A1	2169	G
38	A1	2188	A
38	A1	2192	C
38	A1	2197	OMC
38	A1	2201	G
38	A1	2206	G
38	A1	2207	A
38	A1	2210	G
38	A1	2242	A
38	A1	2249	G
38	A1	2256	A2M
38	A1	2257	C
38	A1	2258	U
38	A1	2259	A
38	A1	2260	U
38	A1	2262	A
38	A1	2269	U
38	A1	2270	A
38	A1	2272	G
38	A1	2273	G
38	A1	2278	5MC

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Mol	Chain	Res	Type
38	A1	2279	A
38	A1	2281	A2M
38	A1	2282	U
38	A1	2307	G
38	A1	2308	C
38	A1	2310	U
38	A1	2313	A
38	A1	2314	U
38	A1	2315	G
38	A1	2334	U
38	A1	2335	G
38	A1	2336	U
38	A1	2340	U
38	A1	2366	C
38	A1	2372	A
38	A1	2373	A
38	A1	2374	C
38	A1	2375	G
38	A1	2383	C
38	A1	2388	U
38	A1	2393	G
38	A1	2397	A
38	A1	2402	A
38	A1	2403	G
38	A1	2404	A
38	A1	2411	U
38	A1	2442	G
38	A1	2445	A
38	A1	2447	A
38	A1	2449	A
38	A1	2452	G
38	A1	2453	U
38	A1	2454	G
38	A1	2455	U
38	A1	2456	A
38	A1	2459	A
38	A1	2461	A
38	A1	2462	A
38	A1	2463	G
38	A1	2465	G
38	A1	2467	G
38	A1	2468	A

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Mol	Chain	Res	Type
38	A1	2469	G
38	A1	2471	U
38	A1	2472	U
38	A1	2474	G
38	A1	2480	A
38	A1	2483	G
38	A1	2484	A
38	A1	2485	A
38	A1	2486	A
38	A1	2487	U
38	A1	2490	C
38	A1	2491	A
38	A1	2492	C
38	A1	2493	U
38	A1	2494	A
38	A1	2495	C
38	A1	2496	C
38	A1	2497	U
38	A1	2498	U
38	A1	2500	A
38	A1	2505	U
38	A1	2506	U
38	A1	2507	C
38	A1	2514	U
38	A1	2515	A
38	A1	2522	G
38	A1	2523	A
38	A1	2524	A
38	A1	2537	U
38	A1	2538	U
38	A1	2539	C
38	A1	2540	A
38	A1	2541	U
38	A1	2544	U
38	A1	2549	G
38	A1	2552	C
38	A1	2554	A
38	A1	2561	A
38	A1	2568	C
38	A1	2569	A
38	A1	2570	U
38	A1	2571	U

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Mol	Chain	Res	Type
38	A1	2573	G
38	A1	2585	G
38	A1	2593	A
38	A1	2594	C
38	A1	2606	G
38	A1	2607	G
38	A1	2614	G
38	A1	2626	A
38	A1	2652	U
38	A1	2656	A
38	A1	2657	A
38	A1	2672	G
38	A1	2674	A
38	A1	2676	A
38	A1	2677	G
38	A1	2678	A
38	A1	2679	A
38	A1	2681	U
38	A1	2688	U
38	A1	2689	A
38	A1	2691	A
38	A1	2703	A
38	A1	2704	A
38	A1	2714	G
38	A1	2719	U
38	A1	2728	G
38	A1	2729	OMU
38	A1	2737	C
38	A1	2749	G
38	A1	2752	U
38	A1	2753	G
38	A1	2762	A
38	A1	2772	C
38	A1	2773	C
38	A1	2777	G
38	A1	2778	G
38	A1	2796	G
38	A1	2798	C
38	A1	2800	G
38	A1	2801	A
38	A1	2803	A
38	A1	2810	C

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Mol	Chain	Res	Type
38	A1	2814	G
38	A1	2817	A
38	A1	2842	U
38	A1	2843	U
38	A1	2845	A
38	A1	2860	U
38	A1	2864	A
38	A1	2871	G
38	A1	2872	A
38	A1	2875	U
38	A1	2887	A
38	A1	2894	C
38	A1	2898	G
38	A1	2923	U
38	A1	2933	A
38	A1	2935	U
38	A1	2936	A
38	A1	2942	C
38	A1	2943	G
38	A1	2947	G
38	A1	2954	U
38	A1	2977	G
38	A1	2983	C
38	A1	2990	G
38	A1	2997	G
38	A1	3011	A
38	A1	3012	A
38	A1	3022	G
38	A1	3032	A
38	A1	3056	U
38	A1	3059	G
38	A1	3078	U
38	A1	3079	U
38	A1	3086	A
38	A1	3092	C
38	A1	3101	G
38	A1	3109	G
38	A1	3122	A
38	A1	3129	A
38	A1	3131	U
38	A1	3142	A
38	A1	3143	C

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Mol	Chain	Res	Type
38	A1	3149	G
38	A1	3153	U
38	A1	3154	C
38	A1	3155	U
38	A1	3156	U
38	A1	3157	U
38	A1	3164	C
38	A1	3165	A
38	A1	3170	A
38	A1	3172	A
38	A1	3173	G
38	A1	3174	A
38	A1	3175	U
38	A1	3176	G
38	A1	3179	U
38	A1	3181	C
38	A1	3187	A
38	A1	3194	C
38	A1	3196	U
38	A1	3197	G
38	A1	3206	C
38	A1	3207	U
38	A1	3210	A
38	A1	3215	A
38	A1	3217	C
38	A1	3218	A
38	A1	3219	G
38	A1	3224	G
38	A1	3234	A
38	A1	3243	A
38	A1	3244	A
38	A1	3246	G
38	A1	3247	G
38	A1	3259	U
38	A1	3263	G
38	A1	3275	U
38	A1	3276	G
38	A1	3278	C
38	A1	3281	U
38	A1	3289	G
38	A1	3294	A
38	A1	3304	U

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Mol	Chain	Res	Type
38	A1	3314	A
38	A1	3316	A
38	A1	3317	U
38	A1	3319	U
38	A1	3335	A
38	A1	3342	A
38	A1	3345	G
38	A1	3350	C
38	A1	3351	U
38	A1	3352	U
38	A1	3353	G
38	A1	3354	U
38	A1	3355	U
38	A1	3356	G
38	A1	3369	G
38	A1	3378	C
38	A1	3382	U
38	A1	3389	U
38	A1	3390	G
39	A3	7	G
39	A3	41	G
39	A3	49	G
39	A3	53	U
39	A3	54	U
39	A3	65	G
39	A3	76	A
39	A3	99	G
39	A3	102	A
39	A3	112	G
40	A4	23	U
40	A4	34	U
40	A4	35	C
40	A4	38	U
40	A4	51	G
40	A4	52	A
40	A4	58	G
40	A4	59	A
40	A4	60	U
40	A4	62	C
40	A4	63	G
40	A4	75	G
40	A4	81	U

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Mol	Chain	Res	Type
40	A4	83	C
40	A4	86	U
40	A4	87	G
40	A4	90	U
40	A4	95	G
40	A4	104	A
40	A4	106	C
40	A4	107	G
40	A4	111	A
40	A4	113	U
40	A4	116	G
40	A4	125	U
40	A4	152	G
40	A4	156	U
40	A4	157	U
40	A4	158	U
80	EC	6762	U
80	EC	6767	G
80	EC	6768	U
80	EC	6769	A
80	EC	6770	U
80	EC	6771	U
80	EC	6772	G
80	EC	6773	G
80	EC	6774	U
80	EC	6775	U
80	EC	6776	A
80	EC	6777	C
80	EC	6778	C
80	EC	6779	C
80	EC	6780	A
80	EC	6781	U
80	EC	6782	C
80	EC	6787	U
80	EC	6788	C
80	EC	6789	G
80	EC	6790	A
80	EC	6791	A
80	EC	6792	A
80	EC	6793	A
80	EC	6794	C
80	EC	6795	U

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Mol	Chain	Res	Type
80	EC	6802	A
80	EC	6803	C
80	EC	6804	A
80	EC	6816	A
80	EC	6817	A
80	EC	6818	G
80	EC	6819	G
80	EC	6822	U
80	EC	6823	U
80	EC	6825	A
80	EC	6831	U
80	EC	6832	G
80	EC	6835	U
80	EC	6836	U
80	EC	6837	G
80	EC	6842	U
80	EC	6843	U
80	EC	6844	A
80	EC	6845	G
80	EC	6849	A
80	EC	6850	C
80	EC	6851	G
80	EC	6852	U
80	EC	6856	C
80	EC	6858	A
80	EC	6859	U
80	EC	6860	A
80	EC	6863	C
80	EC	6864	A
80	EC	6868	C
80	EC	6870	A
80	EC	6871	A
80	EC	6872	A
80	EC	6873	A
80	EC	6874	A
80	EC	6875	C
80	EC	6877	C
80	EC	6888	A
80	EC	6889	A
80	EC	6892	U
80	EC	6895	C
80	EC	6896	A

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Mol	Chain	Res	Type
80	EC	6897	G
80	EC	6898	U
80	EC	6901	C
80	EC	6902	U
80	EC	6903	U
80	EC	6904	U
80	EC	6907	G
80	EC	6908	C
80	EC	6909	A
80	EC	6910	A
80	EC	6913	U
80	EC	6914	A
80	EC	6915	G
80	EC	6916	A
80	EC	6918	A
80	EC	6919	G
80	EC	6920	C
80	EC	6921	C
80	EC	6922	G
80	EC	6923	C
80	EC	6924	G
80	EC	6926	U
80	EC	6927	U
80	EC	6928	G
80	EC	6935	G
80	EC	6937	G
80	EC	6938	A
80	EC	6940	U
80	EC	6941	U
80	EC	6942	A
80	EC	6943	A
80	EC	6945	U
80	EC	6946	A
80	EC	6949	G
80	EC	6950	C
80	EC	6954	A

All (37) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	B5	224	C
34	B5	486	G

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Mol	Chain	Res	Type
34	B5	741	C
34	B5	752	A
34	B5	819	G
34	B5	862	A
34	B5	950	C
34	B5	1057	U
34	B5	1226	A
34	B5	1285	U
34	B5	1344	A
34	B5	1458	G
38	A1	168	U
38	A1	873	C
38	A1	916	G
38	A1	1014	U
38	A1	1016	C
38	A1	1092	C
38	A1	1218	U
38	A1	1259	A
38	A1	1292	C
38	A1	1354	G
38	A1	1568	U
38	A1	1629	U
38	A1	1947	G
38	A1	2241	U
38	A1	2466	G
38	A1	2506	U
38	A1	2870	5MC
38	A1	3121	U
39	A3	52	G
80	EC	6844	A
80	EC	6851	G
80	EC	6857	C
80	EC	6858	A
80	EC	6876	A
80	EC	6934	U

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

67 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
34	XSX	B5	1191	34	24,28,29	0.98	0	30,40,43	5.15	4 (13%)
38	OMG	A1	2791	38	23,26,27	1.20	3 (13%)	32,38,41	1.99	6 (18%)
38	OMG	A1	908	38	23,26,27	1.21	3 (13%)	32,38,41	2.02	6 (18%)
38	A2M	A1	2256	38	22,25,26	1.52	4 (18%)	30,36,39	2.09	8 (26%)
38	A2M	A1	2281	38	22,25,26	1.42	5 (22%)	30,36,39	2.32	11 (36%)
38	OMG	A1	2815	38	23,26,27	1.20	3 (13%)	32,38,41	1.95	5 (15%)
38	OMU	A1	2724	38	19,22,23	1.25	3 (15%)	25,31,34	1.88	6 (24%)
38	OMG	A1	2922	38	23,26,27	1.20	3 (13%)	32,38,41	1.93	6 (18%)
38	OMU	A1	2729	38	19,22,23	1.28	3 (15%)	25,31,34	1.76	5 (20%)
34	G7M	B5	1575	34	23,26,27	2.36	5 (21%)	34,39,42	3.13	10 (29%)
34	A2M	B5	541	34	22,25,26	1.50	4 (18%)	30,36,39	2.10	7 (23%)
34	OMU	B5	1269	34	19,22,23	1.28	4 (21%)	25,31,34	1.89	5 (20%)
38	OMG	A1	2793	38	23,26,27	1.18	3 (13%)	32,38,41	1.99	6 (18%)
38	OMC	A1	2948	38	19,22,23	0.77	0	25,31,34	0.98	2 (8%)
34	A2M	B5	796	34	22,25,26	1.49	5 (22%)	30,36,39	2.18	10 (33%)
38	OMC	A1	650	38	19,22,23	0.79	0	25,31,34	0.86	0
38	1MA	A1	645	38,81	21,25,26	1.36	4 (19%)	30,37,40	1.71	6 (20%)
36	HIC	AB	243	36	10,11,12	1.42	1 (10%)	9,14,16	1.19	1 (11%)
38	1MA	A1	2142	38,81	21,25,26	1.33	4 (19%)	30,37,40	1.71	4 (13%)
34	OMC	B5	1007	34	19,22,23	0.76	0	25,31,34	0.80	0
34	OMG	B5	1126	34	23,26,27	1.17	3 (13%)	32,38,41	1.99	6 (18%)
38	OMG	A1	805	38	23,26,27	1.19	3 (13%)	32,38,41	2.00	7 (21%)
34	OMC	B5	1639	34	19,22,23	0.76	0	25,31,34	0.74	0
34	A2M	B5	436	34	22,25,26	1.51	4 (18%)	30,36,39	2.04	8 (26%)
38	OMC	A1	2197	38	19,22,23	0.79	0	25,31,34	0.88	0
34	OMC	B5	414	34	19,22,23	0.82	0	25,31,34	0.79	0
34	OMG	B5	1572	34	23,26,27	1.18	3 (13%)	32,38,41	1.95	6 (18%)
38	A2M	A1	817	38,81	22,25,26	1.50	4 (18%)	30,36,39	2.03	9 (30%)
38	OMC	A1	2337	38	19,22,23	0.78	0	25,31,34	0.76	0
38	A2M	A1	807	38	22,25,26	1.48	5 (22%)	30,36,39	2.10	10 (33%)
38	OMC	A1	1437	38,81	19,22,23	0.78	0	25,31,34	0.93	2 (8%)
34	OMU	B5	578	34	19,22,23	1.20	3 (15%)	25,31,34	1.85	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	A2M	A1	2946	38,81	22,25,26	1.47	5 (22%)	30,36,39	2.19	9 (30%)
34	A2M	B5	619	81,34	22,25,26	1.50	4 (18%)	30,36,39	2.05	8 (26%)
38	OMU	A1	1888	38	19,22,23	1.25	3 (15%)	25,31,34	1.89	5 (20%)
38	OMU	A1	2421	38	19,22,23	1.29	3 (15%)	25,31,34	1.79	4 (16%)
38	A2M	A1	876	38	22,25,26	1.47	3 (13%)	30,36,39	2.02	7 (23%)
34	MA6	B5	1782	34	23,26,27	1.48	5 (21%)	33,38,41	2.13	10 (30%)
38	OMU	A1	898	38	19,22,23	1.27	3 (15%)	25,31,34	1.75	4 (16%)
38	OMG	A1	2288	38	23,26,27	1.19	3 (13%)	32,38,41	1.97	6 (18%)
34	OMG	B5	1428	81,34	23,26,27	1.20	3 (13%)	32,38,41	1.97	6 (18%)
38	A2M	A1	649	38	22,25,26	1.46	5 (22%)	30,36,39	2.01	8 (26%)
34	A2M	B5	100	81,34	22,25,26	1.49	4 (18%)	30,36,39	2.07	7 (23%)
38	A2M	A1	2220	38	22,25,26	1.51	5 (22%)	30,36,39	1.96	8 (26%)
38	A2M	A1	2280	38	22,25,26	1.45	4 (18%)	30,36,39	2.08	8 (26%)
38	OMC	A1	2959	38	19,22,23	0.76	0	25,31,34	0.74	0
34	A2M	B5	28	81,34	22,25,26	1.48	4 (18%)	30,36,39	2.06	8 (26%)
38	A2M	A1	1449	38,81	22,25,26	1.46	4 (18%)	30,36,39	2.02	7 (23%)
38	5MC	A1	2870	38	19,22,23	1.48	3 (15%)	26,32,35	1.16	3 (11%)
38	OMG	A1	867	38	23,26,27	1.21	3 (13%)	32,38,41	1.98	6 (18%)
38	OMC	A1	663	38	19,22,23	0.77	0	25,31,34	0.80	0
34	OMG	B5	1271	34	23,26,27	1.19	3 (13%)	32,38,41	1.97	5 (15%)
34	A2M	B5	420	34	22,25,26	1.49	4 (18%)	30,36,39	2.10	10 (33%)
34	MA6	B5	1781	34	23,26,27	1.47	5 (21%)	33,38,41	2.11	10 (30%)
38	A2M	A1	1133	38,81	22,25,26	1.47	5 (22%)	30,36,39	2.15	10 (33%)
38	5MC	A1	2278	38,81	19,22,23	1.67	3 (15%)	26,32,35	1.51	4 (15%)
38	OMU	A1	2347	38	19,22,23	1.33	3 (15%)	25,31,34	1.86	5 (20%)
38	OMG	A1	2619	38	23,26,27	1.18	3 (13%)	32,38,41	2.01	6 (18%)
38	A2M	A1	2640	38	22,25,26	1.50	4 (18%)	30,36,39	2.00	8 (26%)
38	OMU	A1	2921	38,81	19,22,23	1.22	3 (15%)	25,31,34	1.86	5 (20%)
38	UR3	A1	2634	38	19,22,23	0.94	1 (5%)	26,32,35	1.73	2 (7%)
34	4AC	B5	1773	34	21,24,25	1.13	1 (4%)	28,34,37	1.20	3 (10%)
38	OMU	A1	2417	38	19,22,23	1.27	3 (15%)	25,31,34	1.80	4 (16%)
34	A2M	B5	974	34	22,25,26	1.49	5 (22%)	30,36,39	2.08	9 (30%)
34	OMG	B5	562	34	23,26,27	1.19	3 (13%)	32,38,41	1.97	6 (18%)
34	4AC	B5	1280	34	21,24,25	1.07	1 (4%)	28,34,37	1.11	2 (7%)
38	OMG	A1	1450	38	23,26,27	1.19	3 (13%)	32,38,41	1.99	6 (18%)

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
34	XSX	B5	1191	34	-	6/16/34/35	0/2/2/2
38	OMG	A1	2791	38	-	1/9/27/28	0/3/3/3
38	OMG	A1	908	38	-	0/9/27/28	0/3/3/3
38	A2M	A1	2256	38	-	4/9/27/28	0/3/3/3
38	A2M	A1	2281	38	-	1/9/27/28	0/3/3/3
38	OMG	A1	2815	38	-	0/9/27/28	0/3/3/3
38	OMU	A1	2724	38	-	1/9/27/28	0/2/2/2
38	OMG	A1	2922	38	-	1/9/27/28	0/3/3/3
38	OMU	A1	2729	38	-	2/9/27/28	0/2/2/2
34	G7M	B5	1575	34	3/3/5/5	2/7/25/26	0/3/3/3
34	A2M	B5	541	34	-	5/9/27/28	0/3/3/3
34	OMU	B5	1269	34	-	3/9/27/28	0/2/2/2
38	OMG	A1	2793	38	-	0/9/27/28	0/3/3/3
38	OMC	A1	2948	38	-	0/9/27/28	0/2/2/2
34	A2M	B5	796	34	-	0/9/27/28	0/3/3/3
38	OMC	A1	650	38	-	0/9/27/28	0/2/2/2
38	1MA	A1	645	38,81	-	2/7/25/26	0/3/3/3
36	HIC	AB	243	36	-	0/5/6/8	0/1/1/1
38	1MA	A1	2142	38,81	-	0/7/25/26	0/3/3/3
34	OMC	B5	1007	34	-	0/9/27/28	0/2/2/2
34	OMG	B5	1126	34	-	1/9/27/28	0/3/3/3
38	OMG	A1	805	38	-	1/9/27/28	0/3/3/3
34	OMC	B5	1639	34	-	0/9/27/28	0/2/2/2
34	A2M	B5	436	34	-	0/9/27/28	0/3/3/3
38	OMC	A1	2197	38	-	6/9/27/28	0/2/2/2
34	OMC	B5	414	34	-	1/9/27/28	0/2/2/2
34	OMG	B5	1572	34	-	3/9/27/28	0/3/3/3
38	A2M	A1	817	38,81	-	1/9/27/28	0/3/3/3
38	OMC	A1	2337	38	-	1/9/27/28	0/2/2/2
38	A2M	A1	807	38	-	0/9/27/28	0/3/3/3
38	OMC	A1	1437	38,81	-	2/9/27/28	0/2/2/2
34	OMU	B5	578	34	-	0/9/27/28	0/2/2/2
38	A2M	A1	2946	38,81	-	0/9/27/28	0/3/3/3
34	A2M	B5	619	81,34	-	4/9/27/28	0/3/3/3
38	OMU	A1	1888	38	-	0/9/27/28	0/2/2/2
38	OMU	A1	2421	38	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	A2M	A1	876	38	-	1/9/27/28	0/3/3/3
34	MA6	B5	1782	34	-	3/11/29/30	0/3/3/3
38	OMU	A1	898	38	-	0/9/27/28	0/2/2/2
38	OMG	A1	2288	38	-	0/9/27/28	0/3/3/3
34	OMG	B5	1428	81,34	-	3/9/27/28	0/3/3/3
38	A2M	A1	649	38	-	0/9/27/28	0/3/3/3
34	A2M	B5	100	81,34	-	1/9/27/28	0/3/3/3
38	A2M	A1	2220	38	-	1/9/27/28	0/3/3/3
38	A2M	A1	2280	38	-	1/9/27/28	0/3/3/3
38	OMC	A1	2959	38	-	0/9/27/28	0/2/2/2
34	A2M	B5	28	81,34	-	1/9/27/28	0/3/3/3
38	A2M	A1	1449	38,81	-	0/9/27/28	0/3/3/3
38	5MC	A1	2870	38	-	4/7/25/26	0/2/2/2
38	OMG	A1	867	38	-	1/9/27/28	0/3/3/3
38	OMC	A1	663	38	-	0/9/27/28	0/2/2/2
34	OMG	B5	1271	34	-	1/9/27/28	0/3/3/3
34	A2M	B5	420	34	-	1/9/27/28	0/3/3/3
34	MA6	B5	1781	34	-	0/11/29/30	0/3/3/3
38	A2M	A1	1133	38,81	-	0/9/27/28	0/3/3/3
38	5MC	A1	2278	38,81	-	0/7/25/26	0/2/2/2
38	OMU	A1	2347	38	-	0/9/27/28	0/2/2/2
38	OMG	A1	2619	38	-	1/9/27/28	0/3/3/3
38	A2M	A1	2640	38	-	0/9/27/28	0/3/3/3
38	OMU	A1	2921	38,81	-	0/9/27/28	0/2/2/2
38	UR3	A1	2634	38	-	0/7/25/26	0/2/2/2
34	4AC	B5	1773	34	-	2/11/29/30	0/2/2/2
38	OMU	A1	2417	38	-	1/9/27/28	0/2/2/2
34	A2M	B5	974	34	-	0/9/27/28	0/3/3/3
34	OMG	B5	562	34	-	1/9/27/28	0/3/3/3
34	4AC	B5	1280	34	-	2/11/29/30	0/2/2/2
38	OMG	A1	1450	38	-	1/9/27/28	0/3/3/3

All (196) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B5	1575	G7M	C8-N7	7.41	1.45	1.33
38	A1	2278	5MC	C5-C4	5.91	1.48	1.44
38	A1	2870	5MC	C5-C4	5.17	1.48	1.44
34	B5	1575	G7M	C5-N7	-4.85	1.33	1.39
38	A1	2256	A2M	C5-C4	4.78	1.47	1.39
34	B5	541	A2M	C5-C4	4.74	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B5	436	A2M	C5-C4	4.65	1.47	1.39
34	B5	28	A2M	C5-C4	4.57	1.47	1.39
38	A1	2640	A2M	C5-C4	4.54	1.47	1.39
34	B5	1781	MA6	C5-C4	4.52	1.47	1.39
34	B5	100	A2M	C5-C4	4.50	1.47	1.39
34	B5	1782	MA6	C5-C4	4.49	1.47	1.39
34	B5	420	A2M	C5-C4	4.48	1.47	1.39
38	A1	2220	A2M	C5-C4	4.46	1.47	1.39
38	A1	1449	A2M	C5-C4	4.46	1.47	1.39
34	B5	619	A2M	C5-C4	4.46	1.47	1.39
38	A1	876	A2M	C5-C4	4.45	1.47	1.39
38	A1	807	A2M	C5-C4	4.44	1.47	1.39
34	B5	796	A2M	C5-C4	4.43	1.47	1.39
38	A1	2946	A2M	C5-C4	4.40	1.46	1.39
38	A1	2280	A2M	C5-C4	4.40	1.46	1.39
38	A1	649	A2M	C5-C4	4.37	1.46	1.39
38	A1	817	A2M	C5-C4	4.33	1.46	1.39
34	B5	974	A2M	C5-C4	4.32	1.46	1.39
38	A1	1133	A2M	C5-C4	4.28	1.46	1.39
38	A1	2281	A2M	C5-C4	4.25	1.46	1.39
34	B5	1575	G7M	C8-N9	4.17	1.47	1.35
34	B5	1575	G7M	C5-C4	3.87	1.47	1.38
34	B5	1773	4AC	C4-N4	-3.59	1.34	1.39
34	B5	1271	OMG	C5-C4	3.18	1.47	1.38
38	A1	645	1MA	C6-N6	3.15	1.35	1.28
34	B5	1428	OMG	C5-C4	3.13	1.47	1.38
34	B5	562	OMG	C5-C4	3.11	1.47	1.38
38	A1	2347	OMU	C4-N3	-3.09	1.33	1.38
34	B5	1572	OMG	C5-C4	3.07	1.47	1.38
38	A1	2142	1MA	C5-C4	3.07	1.47	1.38
38	A1	2791	OMG	C5-C4	3.06	1.47	1.38
38	A1	908	OMG	C5-C4	3.05	1.47	1.38
34	B5	1782	MA6	C5-C6	3.05	1.49	1.41
38	A1	2288	OMG	C5-C4	3.05	1.47	1.38
38	A1	898	OMU	C4-N3	-3.03	1.33	1.38
38	A1	2729	OMU	C4-N3	-3.02	1.33	1.38
34	B5	1280	4AC	C4-N4	-3.01	1.35	1.39
38	A1	2793	OMG	C5-C4	3.01	1.47	1.38
38	A1	2417	OMU	C4-N3	-3.01	1.33	1.38
38	A1	2922	OMG	C5-C4	2.99	1.47	1.38
38	A1	2815	OMG	C5-C4	2.99	1.47	1.38
38	A1	2619	OMG	C5-C4	2.97	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A1	2421	OMU	C4-N3	-2.97	1.33	1.38
38	A1	645	1MA	C5-C4	2.97	1.46	1.38
38	A1	2142	1MA	C6-N6	2.96	1.35	1.28
34	B5	1781	MA6	C5-C6	2.96	1.49	1.41
38	A1	2278	5MC	C6-N1	-2.96	1.33	1.38
38	A1	867	OMG	C5-C4	2.94	1.46	1.38
38	A1	1450	OMG	C5-C4	2.93	1.46	1.38
34	B5	1126	OMG	C5-C4	2.89	1.46	1.38
38	A1	805	OMG	C5-C4	2.89	1.46	1.38
38	A1	2921	OMU	C4-N3	-2.88	1.33	1.38
38	A1	2724	OMU	C4-N3	-2.87	1.33	1.38
34	B5	1269	OMU	C4-N3	-2.85	1.33	1.38
38	A1	867	OMG	C6-N1	-2.85	1.33	1.38
36	AB	243	HIC	CD2-CG	2.82	1.41	1.36
38	A1	1888	OMU	C4-N3	-2.79	1.33	1.38
38	A1	2870	5MC	C6-C5	2.78	1.39	1.34
38	A1	2815	OMG	C6-N1	-2.77	1.33	1.38
38	A1	2220	A2M	C5-C6	2.76	1.48	1.41
38	A1	805	OMG	C6-N1	-2.75	1.33	1.38
34	B5	420	A2M	C5-C6	2.74	1.48	1.41
38	A1	1450	OMG	C6-N1	-2.73	1.33	1.38
38	A1	2791	OMG	C6-N1	-2.70	1.33	1.38
38	A1	2256	A2M	C5-C6	2.70	1.48	1.41
34	B5	28	A2M	C5-C6	2.68	1.48	1.41
38	A1	2946	A2M	C5-C6	2.67	1.48	1.41
34	B5	1428	OMG	C6-N1	-2.67	1.33	1.38
34	B5	974	A2M	C5-C6	2.66	1.48	1.41
34	B5	541	A2M	C5-C6	2.65	1.48	1.41
38	A1	908	OMG	C6-N1	-2.63	1.33	1.38
38	A1	2640	A2M	C5-C6	2.63	1.48	1.41
34	B5	436	A2M	C5-C6	2.63	1.48	1.41
38	A1	817	A2M	C5-N7	-2.62	1.34	1.39
38	A1	649	A2M	C5-N7	-2.62	1.34	1.39
34	B5	974	A2M	C5-N7	-2.62	1.34	1.39
38	A1	1449	A2M	C5-N7	-2.61	1.34	1.39
38	A1	2288	OMG	C6-N1	-2.61	1.34	1.38
38	A1	1133	A2M	C5-N7	-2.60	1.34	1.39
34	B5	619	A2M	C5-C6	2.60	1.48	1.41
38	A1	2922	OMG	C6-N1	-2.60	1.34	1.38
34	B5	100	A2M	C5-N7	-2.60	1.34	1.39
34	B5	619	A2M	C5-N7	-2.59	1.34	1.39
38	A1	817	A2M	C5-C6	2.59	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A1	2640	A2M	C5-N7	-2.58	1.34	1.39
34	B5	796	A2M	C5-C6	2.58	1.48	1.41
38	A1	876	A2M	C5-N7	-2.58	1.34	1.39
34	B5	1126	OMG	C6-N1	-2.58	1.34	1.38
38	A1	2619	OMG	C6-N1	-2.57	1.34	1.38
34	B5	578	OMU	C4-N3	-2.57	1.34	1.38
38	A1	807	A2M	C5-C6	2.56	1.48	1.41
38	A1	2793	OMG	C6-N1	-2.55	1.34	1.38
38	A1	649	A2M	C5-C6	2.55	1.48	1.41
34	B5	562	OMG	C6-N1	-2.55	1.34	1.38
38	A1	876	A2M	C5-C6	2.55	1.48	1.41
34	B5	100	A2M	C5-C6	2.54	1.48	1.41
38	A1	898	OMU	C2-N3	-2.54	1.33	1.38
34	B5	436	A2M	C5-N7	-2.54	1.34	1.39
38	A1	2280	A2M	C5-C6	2.53	1.48	1.41
38	A1	2921	OMU	C2-N3	-2.53	1.33	1.38
38	A1	2347	OMU	C2-N3	-2.52	1.33	1.38
38	A1	807	A2M	C5-N7	-2.52	1.34	1.39
38	A1	2280	A2M	C5-N7	-2.51	1.34	1.39
34	B5	796	A2M	C5-N7	-2.50	1.34	1.39
38	A1	2281	A2M	C5-C6	2.48	1.47	1.41
34	B5	1271	OMG	C6-N1	-2.48	1.34	1.38
38	A1	2417	OMU	C2-N3	-2.48	1.33	1.38
34	B5	1575	G7M	C6-N1	-2.47	1.34	1.38
38	A1	1133	A2M	C5-C6	2.47	1.47	1.41
38	A1	2421	OMU	C2-N3	-2.45	1.33	1.38
38	A1	1449	A2M	C5-C6	2.42	1.47	1.41
38	A1	2281	A2M	C5-N7	-2.41	1.34	1.39
38	A1	2946	A2M	C5-N7	-2.41	1.34	1.39
38	A1	2256	A2M	C5-N7	-2.41	1.34	1.39
38	A1	2724	OMU	C2-N3	-2.39	1.33	1.38
38	A1	2729	OMU	C2-N3	-2.38	1.33	1.38
34	B5	541	A2M	C5-N7	-2.38	1.34	1.39
38	A1	908	OMG	C5-N7	-2.38	1.34	1.39
38	A1	2347	OMU	C5-C4	-2.36	1.38	1.43
38	A1	645	1MA	C5-N7	-2.35	1.34	1.39
38	A1	2220	A2M	C5-N7	-2.34	1.34	1.39
34	B5	420	A2M	C5-N7	-2.34	1.34	1.39
38	A1	2142	1MA	C5-N7	-2.33	1.34	1.39
38	A1	2724	OMU	C5-C4	-2.32	1.38	1.43
34	B5	28	A2M	C5-N7	-2.31	1.34	1.39
38	A1	867	OMG	C5-N7	-2.30	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B5	1269	OMU	C2-N3	-2.30	1.34	1.38
38	A1	1888	OMU	C2-N3	-2.30	1.34	1.38
38	A1	898	OMU	C5-C4	-2.30	1.38	1.43
38	A1	2729	OMU	C5-C4	-2.29	1.38	1.43
34	B5	1572	OMG	C6-N1	-2.29	1.34	1.38
38	A1	2278	5MC	C6-C5	2.27	1.38	1.34
38	A1	2220	A2M	C8-N7	2.26	1.36	1.31
38	A1	2288	OMG	C5-N7	-2.25	1.34	1.39
38	A1	2619	OMG	C5-N7	-2.24	1.34	1.39
34	B5	1782	MA6	C5-N7	-2.24	1.35	1.39
34	B5	1269	OMU	C2-N1	2.24	1.42	1.38
34	B5	1781	MA6	C5-N7	-2.23	1.35	1.39
34	B5	1126	OMG	C5-N7	-2.23	1.34	1.39
38	A1	2256	A2M	C8-N7	2.23	1.36	1.31
38	A1	2815	OMG	C5-N7	-2.23	1.34	1.39
38	A1	817	A2M	C4-N9	-2.20	1.33	1.37
38	A1	2922	OMG	C5-N7	-2.20	1.34	1.39
38	A1	2417	OMU	C5-C4	-2.20	1.38	1.43
38	A1	2870	5MC	C6-N1	-2.18	1.34	1.38
38	A1	2791	OMG	C5-N7	-2.18	1.34	1.39
34	B5	1428	OMG	C5-N7	-2.17	1.34	1.39
34	B5	436	A2M	C8-N7	2.17	1.35	1.31
38	A1	1450	OMG	C5-N7	-2.17	1.34	1.39
38	A1	2220	A2M	C4-N9	-2.17	1.33	1.37
34	B5	619	A2M	C8-N7	2.17	1.35	1.31
38	A1	2421	OMU	C5-C4	-2.16	1.39	1.43
34	B5	541	A2M	C8-N7	2.16	1.35	1.31
38	A1	805	OMG	C5-N7	-2.15	1.34	1.39
38	A1	2793	OMG	C5-N7	-2.15	1.34	1.39
38	A1	2142	1MA	C2-N3	2.15	1.34	1.30
34	B5	796	A2M	C4-N9	-2.14	1.33	1.37
34	B5	420	A2M	C8-N7	2.14	1.35	1.31
34	B5	796	A2M	C8-N7	2.13	1.35	1.31
38	A1	2946	A2M	C8-N7	2.13	1.35	1.31
34	B5	578	OMU	C2-N3	-2.12	1.34	1.38
38	A1	1888	OMU	C5-C4	-2.11	1.39	1.43
38	A1	2281	A2M	C4-N9	-2.10	1.33	1.37
34	B5	974	A2M	C8-N7	2.10	1.35	1.31
34	B5	1782	MA6	C8-N7	2.10	1.35	1.31
38	A1	807	A2M	C8-N7	2.09	1.35	1.31
34	B5	562	OMG	C5-N7	-2.09	1.34	1.39
38	A1	807	A2M	C4-N9	-2.09	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A1	1449	A2M	C4-N9	-2.09	1.33	1.37
38	A1	1133	A2M	C4-N9	-2.08	1.33	1.37
38	A1	2921	OMU	C5-C4	-2.07	1.39	1.43
34	B5	28	A2M	C8-N7	2.07	1.35	1.31
34	B5	1269	OMU	C5-C4	-2.07	1.39	1.43
34	B5	1271	OMG	C5-N7	-2.07	1.34	1.39
34	B5	578	OMU	C5-C4	-2.07	1.39	1.43
38	A1	2640	A2M	C8-N7	2.07	1.35	1.31
34	B5	100	A2M	C8-N7	2.07	1.35	1.31
34	B5	1781	MA6	C8-N7	2.07	1.35	1.31
34	B5	974	A2M	C4-N9	-2.06	1.33	1.37
34	B5	1782	MA6	C4-N9	-2.06	1.33	1.37
38	A1	649	A2M	C4-N9	-2.05	1.33	1.37
38	A1	2946	A2M	C4-N9	-2.04	1.33	1.37
38	A1	2281	A2M	C8-N7	2.04	1.35	1.31
38	A1	645	1MA	C2-N3	2.04	1.34	1.30
38	A1	2634	UR3	C5-C4	-2.03	1.38	1.43
38	A1	2280	A2M	C4-N9	-2.03	1.33	1.37
38	A1	1133	A2M	C8-N7	2.02	1.35	1.31
34	B5	1781	MA6	C4-N9	-2.01	1.33	1.37
34	B5	1572	OMG	C5-N7	-2.01	1.35	1.39
38	A1	649	A2M	C8-N7	2.01	1.35	1.31

All (370) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B5	1191	XSX	C3-C1-N3	27.25	159.80	112.16
34	B5	1575	G7M	CN7-N7-C8	-8.03	112.63	124.79
38	A1	2634	UR3	C4-N3-C2	-6.89	119.03	124.58
34	B5	1575	G7M	N9-C4-N3	6.75	139.44	125.95
34	B5	1575	G7M	N9-C8-N7	-6.61	96.44	112.48
38	A1	908	OMG	C5-C4-N3	-6.43	118.15	128.39
34	B5	1428	OMG	C5-C4-N3	-6.33	118.32	128.39
34	B5	1575	G7M	C8-N7-C5	6.32	115.68	107.78
34	B5	541	A2M	C5-C4-N3	-6.32	118.01	126.72
38	A1	2619	OMG	C5-C4-N3	-6.30	118.36	128.39
38	A1	2791	OMG	C5-C4-N3	-6.30	118.37	128.39
38	A1	2815	OMG	C5-C4-N3	-6.25	118.44	128.39
34	B5	1271	OMG	C5-C4-N3	-6.25	118.44	128.39
34	B5	562	OMG	C5-C4-N3	-6.24	118.45	128.39
38	A1	867	OMG	C5-C4-N3	-6.24	118.46	128.39
38	A1	1450	OMG	C5-C4-N3	-6.22	118.50	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	2288	OMG	C5-C4-N3	-6.16	118.58	128.39
34	B5	100	A2M	C5-C4-N3	-6.10	118.32	126.72
34	B5	28	A2M	C5-C4-N3	-6.07	118.36	126.72
34	B5	1126	OMG	C5-C4-N3	-6.02	118.81	128.39
38	A1	2793	OMG	C5-C4-N3	-6.01	118.83	128.39
38	A1	2922	OMG	C5-C4-N3	-6.00	118.85	128.39
38	A1	876	A2M	C5-C4-N3	-5.97	118.49	126.72
34	B5	420	A2M	C5-C4-N3	-5.97	118.50	126.72
38	A1	2640	A2M	C5-C4-N3	-5.96	118.51	126.72
34	B5	436	A2M	C5-C4-N3	-5.93	118.55	126.72
34	B5	619	A2M	C5-C4-N3	-5.93	118.55	126.72
38	A1	2220	A2M	C5-C4-N3	-5.91	118.59	126.72
38	A1	2256	A2M	C5-C4-N3	-5.89	118.61	126.72
38	A1	1449	A2M	C5-C4-N3	-5.87	118.63	126.72
38	A1	649	A2M	C5-C4-N3	-5.85	118.67	126.72
38	A1	2946	A2M	C5-C4-N3	-5.80	118.73	126.72
38	A1	805	OMG	C5-C4-N3	-5.78	119.19	128.39
38	A1	807	A2M	C5-C4-N3	-5.78	118.76	126.72
38	A1	2280	A2M	C5-C4-N3	-5.76	118.79	126.72
34	B5	796	A2M	C5-C4-N3	-5.76	118.79	126.72
38	A1	817	A2M	C5-C4-N3	-5.70	118.87	126.72
34	B5	1575	G7M	C5-C4-N3	-5.70	117.38	128.15
38	A1	1133	A2M	C5-C4-N3	-5.66	118.93	126.72
34	B5	974	A2M	C5-C4-N3	-5.65	118.94	126.72
34	B5	1572	OMG	C5-C4-N3	-5.64	119.41	128.39
38	A1	2281	A2M	C5-C4-N3	-5.60	119.01	126.72
34	B5	1782	MA6	C5-C4-N3	-5.57	119.05	126.72
34	B5	1781	MA6	C5-C4-N3	-5.40	119.28	126.72
38	A1	2142	1MA	C5-C4-N3	-5.39	119.33	127.27
38	A1	645	1MA	C5-C4-N3	-5.39	119.34	127.27
38	A1	2619	OMG	C2-N3-C4	5.23	121.31	112.30
38	A1	1450	OMG	C2-N3-C4	5.19	121.23	112.30
38	A1	2791	OMG	C2-N3-C4	5.13	121.14	112.30
38	A1	2815	OMG	C2-N3-C4	5.13	121.13	112.30
38	A1	2793	OMG	C2-N3-C4	5.12	121.11	112.30
34	B5	541	A2M	N3-C4-N9	5.10	135.85	127.17
34	B5	562	OMG	C2-N3-C4	5.10	121.09	112.30
34	B5	1271	OMG	C2-N3-C4	5.06	121.02	112.30
38	A1	908	OMG	C2-N3-C4	5.06	121.01	112.30
38	A1	1888	OMU	C4-N3-C2	-5.05	120.34	126.61
38	A1	2921	OMU	C4-N3-C2	-5.03	120.37	126.61
34	B5	578	OMU	C4-N3-C2	-4.98	120.43	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	867	OMG	C2-N3-C4	4.97	120.87	112.30
38	A1	2288	OMG	C2-N3-C4	4.97	120.86	112.30
38	A1	908	OMG	N9-C4-N3	4.95	135.86	125.95
34	B5	1428	OMG	C2-N3-C4	4.95	120.83	112.30
34	B5	1126	OMG	C2-N3-C4	4.93	120.79	112.30
34	B5	1575	G7M	C1'-N9-C8	-4.91	110.16	126.74
38	A1	2922	OMG	C2-N3-C4	4.91	120.75	112.30
34	B5	100	A2M	N3-C4-N9	4.90	135.50	127.17
34	B5	1428	OMG	N9-C4-N3	4.90	135.75	125.95
38	A1	805	OMG	C2-N3-C4	4.88	120.70	112.30
38	A1	2288	OMG	N9-C4-N3	4.86	135.67	125.95
34	B5	1572	OMG	C2-N3-C4	4.85	120.66	112.30
38	A1	2724	OMU	C4-N3-C2	-4.85	120.59	126.61
38	A1	867	OMG	N9-C4-N3	4.82	135.59	125.95
38	A1	2347	OMU	C4-N3-C2	-4.81	120.64	126.61
34	B5	28	A2M	N3-C4-N9	4.80	135.34	127.17
34	B5	420	A2M	N3-C4-N9	4.75	135.25	127.17
38	A1	1449	A2M	N3-C4-N9	4.74	135.24	127.17
38	A1	2280	A2M	N3-C4-N9	4.74	135.22	127.17
34	B5	1269	OMU	C4-N3-C2	-4.73	120.75	126.61
38	A1	2421	OMU	C4-N3-C2	-4.73	120.75	126.61
38	A1	649	A2M	N3-C4-N9	4.71	135.18	127.17
38	A1	2417	OMU	C4-N3-C2	-4.71	120.77	126.61
38	A1	876	A2M	N3-C4-N9	4.70	135.17	127.17
38	A1	2791	OMG	N9-C4-N3	4.69	135.34	125.95
38	A1	2256	A2M	N3-C4-N9	4.68	135.13	127.17
34	B5	436	A2M	N3-C4-N9	4.66	135.09	127.17
38	A1	2619	OMG	N9-C4-N3	4.64	135.24	125.95
38	A1	2640	A2M	N3-C4-N9	4.61	135.01	127.17
34	B5	562	OMG	N9-C4-N3	4.61	135.16	125.95
38	A1	645	1MA	C2-N3-C4	4.60	121.55	112.53
34	B5	1126	OMG	N9-C4-N3	4.59	135.13	125.95
38	A1	1450	OMG	N9-C4-N3	4.59	135.13	125.95
34	B5	1271	OMG	N9-C4-N3	4.59	135.13	125.95
34	B5	619	A2M	N3-C4-N9	4.57	134.94	127.17
38	A1	2281	A2M	N3-C4-N9	4.55	134.90	127.17
38	A1	898	OMU	C4-N3-C2	-4.54	120.97	126.61
34	B5	796	A2M	N3-C4-N9	4.54	134.89	127.17
38	A1	2142	1MA	C2-N3-C4	4.51	121.38	112.53
38	A1	817	A2M	N3-C4-N9	4.51	134.83	127.17
34	B5	1191	XSX	C4-N3-C2	-4.50	119.38	124.66
38	A1	2793	OMG	N9-C4-N3	4.49	134.93	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	807	A2M	N3-C4-N9	4.48	134.79	127.17
38	A1	2815	OMG	N9-C4-N3	4.47	134.89	125.95
38	A1	2922	OMG	N9-C4-N3	4.45	134.85	125.95
38	A1	2729	OMU	C4-N3-C2	-4.45	121.09	126.61
34	B5	1575	G7M	C2-N3-C4	4.45	119.96	112.30
38	A1	2281	A2M	O4'-C1'-N9	4.44	116.62	108.09
34	B5	974	A2M	N3-C4-N9	4.44	134.72	127.17
38	A1	1888	OMU	N3-C2-N1	4.42	120.64	114.89
34	B5	1781	MA6	C2-N1-C6	4.40	122.57	111.83
34	B5	796	A2M	C2'-C1'-N9	-4.39	106.53	113.75
38	A1	1133	A2M	N3-C4-N9	4.39	134.63	127.17
38	A1	2421	OMU	N3-C2-N1	4.39	120.61	114.89
34	B5	1269	OMU	N3-C2-N1	4.36	120.57	114.89
38	A1	2946	A2M	N3-C4-N9	4.36	134.59	127.17
38	A1	2921	OMU	N3-C2-N1	4.35	120.55	114.89
38	A1	805	OMG	N9-C4-N3	4.30	134.55	125.95
38	A1	2724	OMU	N3-C2-N1	4.29	120.48	114.89
34	B5	1782	MA6	C2-N1-C6	4.27	122.26	111.83
38	A1	2417	OMU	N3-C2-N1	4.22	120.39	114.89
38	A1	2729	OMU	N3-C2-N1	4.22	120.38	114.89
34	B5	1575	G7M	C8-N9-C4	4.19	117.45	107.09
38	A1	2220	A2M	N3-C4-N9	4.18	134.28	127.17
34	B5	1781	MA6	N3-C4-N9	4.17	134.26	127.17
34	B5	1572	OMG	N9-C4-N3	4.13	134.22	125.95
34	B5	1782	MA6	C4-C5-N7	-4.13	105.86	110.58
34	B5	1782	MA6	N3-C4-N9	4.13	134.19	127.17
38	A1	2347	OMU	C5-C4-N3	4.10	120.54	114.80
38	A1	2417	OMU	C5-C4-N3	4.09	120.53	114.80
38	A1	2946	A2M	C2'-C1'-N9	-4.08	107.03	113.75
38	A1	2921	OMU	C5-C4-N3	4.08	120.52	114.80
34	B5	1781	MA6	C4-C5-N7	-4.08	105.92	110.58
34	B5	578	OMU	N3-C2-N1	4.04	120.16	114.89
38	A1	2278	5MC	C1'-N1-C6	-4.03	114.51	121.15
38	A1	898	OMU	N3-C2-N1	4.03	120.13	114.89
38	A1	2347	OMU	N3-C2-N1	4.00	120.10	114.89
38	A1	2724	OMU	C5-C4-N3	3.97	120.36	114.80
38	A1	2220	A2M	C4-C5-N7	-3.95	106.06	110.58
34	B5	1575	G7M	CN7-N7-C5	3.92	131.69	126.80
38	A1	898	OMU	C5-C4-N3	3.88	120.23	114.80
34	B5	541	A2M	C2-N3-C4	3.86	121.27	111.83
34	B5	578	OMU	C5-C4-N3	3.85	120.19	114.80
38	A1	1888	OMU	C5-C4-N3	3.81	120.13	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B5	1782	MA6	C2-N3-C4	3.80	121.12	111.83
34	B5	1269	OMU	C5-C4-N3	3.79	120.11	114.80
38	A1	649	A2M	C2-N3-C4	3.79	121.08	111.83
38	A1	2421	OMU	C5-C4-N3	3.78	120.09	114.80
38	A1	1449	A2M	C2-N3-C4	3.78	121.06	111.83
34	B5	420	A2M	C2-N3-C4	3.77	121.04	111.83
38	A1	2281	A2M	C2-N3-C4	3.76	121.03	111.83
38	A1	2729	OMU	C5-C4-N3	3.76	120.07	114.80
38	A1	1133	A2M	C2'-C1'-N9	-3.76	107.57	113.75
34	B5	28	A2M	C2-N3-C4	3.75	121.00	111.83
38	A1	2946	A2M	C2-N3-C4	3.75	120.99	111.83
38	A1	2946	A2M	C4-C5-N7	-3.72	106.33	110.58
34	B5	619	A2M	C2-N3-C4	3.72	120.91	111.83
34	B5	1781	MA6	C2-N3-C4	3.70	120.87	111.83
38	A1	876	A2M	C2-N3-C4	3.70	120.87	111.83
38	A1	2142	1MA	N9-C4-N3	3.70	135.33	126.90
38	A1	807	A2M	C2-N3-C4	3.68	120.83	111.83
34	B5	100	A2M	C2-N3-C4	3.67	120.80	111.83
34	B5	1773	4AC	N4-C4-N3	3.67	119.82	113.87
34	B5	436	A2M	C2-N3-C4	3.67	120.78	111.83
38	A1	817	A2M	C2-N3-C4	3.66	120.77	111.83
38	A1	1133	A2M	C2-N3-C4	3.66	120.76	111.83
34	B5	796	A2M	C2-N3-C4	3.65	120.75	111.83
38	A1	2256	A2M	C2-N3-C4	3.65	120.74	111.83
34	B5	619	A2M	C4-C5-N7	-3.64	106.42	110.58
38	A1	2640	A2M	C2-N3-C4	3.64	120.71	111.83
38	A1	2280	A2M	C2-N3-C4	3.62	120.68	111.83
34	B5	974	A2M	C2-N3-C4	3.61	120.65	111.83
34	B5	1280	4AC	N4-C4-N3	3.59	119.70	113.87
38	A1	2640	A2M	C4-C5-N7	-3.59	106.47	110.58
38	A1	807	A2M	C4-C5-N7	-3.55	106.52	110.58
34	B5	28	A2M	C4-C5-N7	-3.55	106.53	110.58
38	A1	2281	A2M	N3-C2-N1	-3.54	123.22	128.58
34	B5	420	A2M	C4-C5-N7	-3.54	106.53	110.58
38	A1	817	A2M	C4-C5-N7	-3.52	106.55	110.58
34	B5	1572	OMG	C6-C5-N7	3.50	136.67	130.29
38	A1	1133	A2M	C4-C5-N7	-3.50	106.58	110.58
34	B5	796	A2M	C4-C5-N7	-3.50	106.58	110.58
34	B5	1782	MA6	N1-C2-N3	-3.50	123.29	128.58
38	A1	805	OMG	C6-C5-N7	3.50	136.65	130.29
34	B5	1781	MA6	N1-C2-N3	-3.50	123.29	128.58
38	A1	2220	A2M	C2-N3-C4	3.45	120.27	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	2256	A2M	C4-C5-N7	-3.44	106.65	110.58
38	A1	1449	A2M	N3-C2-N1	-3.44	123.37	128.58
34	B5	974	A2M	C4-C5-N7	-3.44	106.65	110.58
34	B5	100	A2M	C4-C5-N7	-3.40	106.69	110.58
38	A1	2278	5MC	C5-C4-N3	-3.39	118.28	121.75
38	A1	645	1MA	N9-C4-N3	3.38	134.61	126.90
38	A1	2724	OMU	O4-C4-C5	-3.37	119.35	125.16
38	A1	2634	UR3	C5-C4-N3	3.34	119.44	115.04
38	A1	1133	A2M	N3-C2-N1	-3.34	123.53	128.58
38	A1	2793	OMG	C6-C5-N7	3.34	136.36	130.29
38	A1	876	A2M	C4-C5-N7	-3.34	106.77	110.58
38	A1	2281	A2M	C2'-C1'-N9	-3.33	108.27	113.75
34	B5	578	OMU	O4-C4-C5	-3.33	119.42	125.16
34	B5	436	A2M	C4-C5-N7	-3.31	106.79	110.58
38	A1	649	A2M	N3-C2-N1	-3.26	123.64	128.58
38	A1	2815	OMG	C6-C5-N7	3.26	136.22	130.29
38	A1	1450	OMG	C6-C5-N7	3.26	136.22	130.29
34	B5	1271	OMG	C6-C5-N7	3.25	136.21	130.29
38	A1	807	A2M	N3-C2-N1	-3.25	123.67	128.58
38	A1	2281	A2M	C4-C5-N7	-3.25	106.87	110.58
34	B5	974	A2M	N3-C2-N1	-3.24	123.68	128.58
34	B5	619	A2M	N3-C2-N1	-3.24	123.68	128.58
38	A1	817	A2M	N3-C2-N1	-3.24	123.68	128.58
34	B5	796	A2M	N3-C2-N1	-3.23	123.69	128.58
34	B5	541	A2M	C4-C5-N7	-3.23	106.89	110.58
38	A1	2946	A2M	N3-C2-N1	-3.23	123.70	128.58
38	A1	2280	A2M	N3-C2-N1	-3.23	123.70	128.58
38	A1	2280	A2M	C4-C5-N7	-3.22	106.90	110.58
38	A1	2278	5MC	C5-C6-N1	-3.22	119.82	123.31
34	B5	420	A2M	N3-C2-N1	-3.20	123.73	128.58
34	B5	562	OMG	C6-C5-N7	3.19	136.10	130.29
38	A1	2922	OMG	C6-C5-N7	3.19	136.10	130.29
38	A1	2619	OMG	C6-C5-N7	3.19	136.09	130.29
34	B5	541	A2M	N3-C2-N1	-3.19	123.76	128.58
38	A1	1449	A2M	C4-C5-N7	-3.17	106.96	110.58
34	B5	1126	OMG	C6-C5-N7	3.16	136.04	130.29
38	A1	2256	A2M	N3-C2-N1	-3.16	123.80	128.58
38	A1	649	A2M	C4-C5-N7	-3.15	106.99	110.58
38	A1	2347	OMU	O4-C4-C5	-3.13	119.76	125.16
34	B5	436	A2M	N3-C2-N1	-3.13	123.84	128.58
38	A1	876	A2M	N3-C2-N1	-3.13	123.85	128.58
34	B5	28	A2M	N3-C2-N1	-3.12	123.86	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	2791	OMG	C6-C5-N7	3.12	135.97	130.29
38	A1	1888	OMU	O4-C4-C5	-3.11	119.80	125.16
38	A1	2870	5MC	C5-C6-N1	-3.10	119.95	123.31
38	A1	898	OMU	O4-C4-C5	-3.04	119.93	125.16
38	A1	2417	OMU	O4-C4-C5	-3.03	119.94	125.16
38	A1	867	OMG	C6-C5-N7	3.00	135.76	130.29
34	B5	1781	MA6	C4-N9-C8	2.98	108.86	105.74
38	A1	2347	OMU	C1'-N1-C2	2.96	122.91	117.59
34	B5	974	A2M	C2'-C1'-N9	-2.95	108.89	113.75
38	A1	2640	A2M	N3-C2-N1	-2.95	124.11	128.58
38	A1	2921	OMU	O4-C4-C5	-2.95	120.07	125.16
38	A1	2870	5MC	C5-C4-N3	-2.94	118.74	121.75
34	B5	1781	MA6	C5-N7-C8	2.94	108.07	103.45
38	A1	2288	OMG	C6-C5-N7	2.93	135.63	130.29
34	B5	100	A2M	N3-C2-N1	-2.93	124.14	128.58
38	A1	2729	OMU	O4-C4-C5	-2.92	120.12	125.16
34	B5	1269	OMU	O4-C4-C5	-2.88	120.19	125.16
34	B5	1782	MA6	C5-N7-C8	2.88	107.98	103.45
38	A1	2281	A2M	C4-N9-C8	2.86	108.74	105.74
34	B5	1428	OMG	C6-C5-N7	2.85	135.48	130.29
38	A1	908	OMG	C6-C5-N7	2.77	135.34	130.29
38	A1	2421	OMU	O4-C4-C5	-2.76	120.39	125.16
34	B5	1269	OMU	C1'-N1-C2	2.74	122.52	117.59
34	B5	796	A2M	C4-N9-C8	2.73	108.61	105.74
34	B5	1575	G7M	O6-C6-C5	-2.73	121.92	128.01
38	A1	817	A2M	C4-N9-C8	2.71	108.59	105.74
38	A1	2280	A2M	C4-N9-C8	2.71	108.58	105.74
34	B5	420	A2M	C4-N9-C8	2.70	108.57	105.74
38	A1	2921	OMU	O2-C2-N1	-2.69	119.29	122.80
36	AB	243	HIC	NE2-CE1-ND1	-2.67	111.64	112.66
34	B5	1782	MA6	C4-N9-C8	2.66	108.53	105.74
34	B5	1271	OMG	C4-C5-N7	-2.65	106.48	110.67
34	B5	420	A2M	C5-N7-C8	2.64	107.60	103.45
34	B5	1191	XSX	C5-C4-N3	2.64	119.29	115.64
34	B5	619	A2M	C5-N7-C8	2.62	107.57	103.45
38	A1	805	OMG	C4-C5-N7	-2.61	106.53	110.67
38	A1	2946	A2M	C5-N7-C8	2.60	107.53	103.45
34	B5	1572	OMG	C4-C5-N7	-2.59	106.57	110.67
38	A1	2815	OMG	C4-C5-N7	-2.59	106.57	110.67
34	B5	562	OMG	C4-C5-N7	-2.58	106.59	110.67
34	B5	974	A2M	C4-N9-C8	2.57	108.44	105.74
38	A1	2256	A2M	C5-N7-C8	2.57	107.48	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	817	A2M	C5-N7-C8	2.56	107.47	103.45
38	A1	2948	OMC	O2-C2-N3	-2.55	118.31	122.33
38	A1	807	A2M	C5-N7-C8	2.55	107.46	103.45
38	A1	2220	A2M	C5-N7-C8	2.55	107.45	103.45
38	A1	2619	OMG	C4-C5-N7	-2.54	106.64	110.67
34	B5	100	A2M	C5-N7-C8	2.54	107.45	103.45
34	B5	28	A2M	C5-N7-C8	2.54	107.45	103.45
38	A1	2793	OMG	C4-C5-N7	-2.53	106.65	110.67
34	B5	796	A2M	C5-N7-C8	2.53	107.43	103.45
38	A1	2278	5MC	C1'-N1-C2	2.53	124.02	118.44
38	A1	1450	OMG	C4-C5-N7	-2.53	106.67	110.67
34	B5	100	A2M	C4-N9-C8	2.52	108.39	105.74
34	B5	1782	MA6	C6-C5-N7	2.52	137.45	133.43
38	A1	807	A2M	C4-N9-C8	2.52	108.38	105.74
34	B5	974	A2M	C5-N7-C8	2.52	107.40	103.45
38	A1	1133	A2M	C5-N7-C8	2.51	107.40	103.45
38	A1	2640	A2M	C5-N7-C8	2.51	107.40	103.45
34	B5	1280	4AC	C6-C5-C4	2.51	120.02	117.00
38	A1	2922	OMG	C4-C5-N7	-2.49	106.72	110.67
38	A1	645	1MA	C4-C5-N7	-2.49	106.73	110.67
38	A1	649	A2M	C4-N9-C8	2.48	108.34	105.74
38	A1	2791	OMG	C4-C5-N7	-2.47	106.75	110.67
38	A1	2280	A2M	C2'-C1'-N9	-2.46	109.70	113.75
38	A1	1133	A2M	C4-N9-C8	2.46	108.32	105.74
38	A1	1449	A2M	C4-N9-C8	2.46	108.32	105.74
34	B5	28	A2M	C4-N9-C8	2.45	108.31	105.74
34	B5	1781	MA6	C6-C5-N7	2.45	137.34	133.43
34	B5	1191	XSX	C6-N1-C2	-2.45	119.80	121.80
34	B5	1126	OMG	C4-C5-N7	-2.43	106.81	110.67
34	B5	619	A2M	C4-N9-C8	2.43	108.29	105.74
38	A1	2281	A2M	C5-N7-C8	2.43	107.26	103.45
38	A1	2256	A2M	C4-N9-C8	2.42	108.28	105.74
38	A1	2280	A2M	C5-N7-C8	2.42	107.25	103.45
38	A1	1437	OMC	O2-C2-N3	-2.39	118.56	122.33
38	A1	2946	A2M	C4-N9-C8	2.38	108.24	105.74
38	A1	876	A2M	C5-N7-C8	2.37	107.17	103.45
34	B5	541	A2M	C5-N7-C8	2.36	107.16	103.45
34	B5	1126	OMG	O6-C6-C5	-2.35	120.32	126.53
34	B5	1428	OMG	C4-C5-N7	-2.35	106.94	110.67
38	A1	867	OMG	C4-C5-N7	-2.34	106.95	110.67
38	A1	1449	A2M	C5-N7-C8	2.34	107.13	103.45
38	A1	649	A2M	C5-N7-C8	2.34	107.13	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A1	2946	A2M	C6-C5-N7	2.34	136.60	132.09
34	B5	436	A2M	C5-N7-C8	2.32	107.10	103.45
38	A1	908	OMG	O6-C6-C5	-2.32	120.42	126.53
38	A1	807	A2M	C2'-C1'-N9	-2.31	109.95	113.75
34	B5	1781	MA6	N9-C8-N7	-2.29	110.69	113.94
38	A1	2288	OMG	C4-C5-N7	-2.28	107.05	110.67
38	A1	2724	OMU	O2-C2-N1	-2.28	119.82	122.80
38	A1	908	OMG	C4-C5-N7	-2.28	107.06	110.67
38	A1	1888	OMU	O2-C2-N1	-2.28	119.83	122.80
34	B5	541	A2M	C4-N9-C8	2.27	108.12	105.74
38	A1	2870	5MC	O2-C2-N3	-2.27	118.75	122.33
38	A1	2288	OMG	O6-C6-C5	-2.26	120.57	126.53
34	B5	420	A2M	C2'-C1'-N9	-2.25	110.05	113.75
38	A1	876	A2M	C4-N9-C8	2.25	108.10	105.74
38	A1	2619	OMG	O6-C6-C5	-2.23	120.64	126.53
34	B5	1572	OMG	O6-C6-C5	-2.23	120.65	126.53
34	B5	1773	4AC	O2-C2-N3	-2.22	118.83	122.33
34	B5	436	A2M	C4-N9-C8	2.22	108.07	105.74
34	B5	578	OMU	O2-C2-N1	-2.21	119.92	122.80
38	A1	2220	A2M	C6-C5-N7	2.21	136.34	132.09
38	A1	807	A2M	C6-C5-N7	2.20	136.33	132.09
38	A1	2640	A2M	C4-N9-C8	2.20	108.05	105.74
38	A1	2948	OMC	C1'-N1-C2	2.20	123.30	118.44
34	B5	974	A2M	C6-C5-N7	2.19	136.31	132.09
38	A1	805	OMG	C2'-C1'-N9	-2.19	110.09	114.24
38	A1	2724	OMU	C1'-N1-C2	2.18	121.52	117.59
38	A1	2256	A2M	C2'-C1'-N9	-2.18	110.17	113.75
38	A1	817	A2M	C6-C5-N7	2.17	136.27	132.09
38	A1	2142	1MA	C4-C5-N7	-2.16	107.24	110.67
34	B5	1782	MA6	N9-C8-N7	-2.16	110.87	113.94
38	A1	805	OMG	O6-C6-C5	-2.16	120.83	126.53
34	B5	619	A2M	C6-C5-N7	2.14	136.21	132.09
38	A1	1133	A2M	C6-C5-N7	2.13	136.20	132.09
38	A1	2281	A2M	C6-C5-N7	2.12	136.17	132.09
38	A1	2220	A2M	C4-N9-C8	2.10	107.94	105.74
34	B5	436	A2M	C2'-C1'-N9	-2.09	110.31	113.75
38	A1	645	1MA	C6-C5-N7	2.09	135.86	132.16
38	A1	2729	OMU	C1'-N1-C2	2.08	121.34	117.59
38	A1	1450	OMG	O6-C6-C5	-2.07	121.08	126.53
34	B5	420	A2M	C6-C5-N7	2.06	136.07	132.09
38	A1	2791	OMG	O6-C6-C5	-2.06	121.09	126.53
38	A1	2640	A2M	C6-C5-N7	2.06	136.06	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B5	796	A2M	C6-C5-N7	2.06	136.06	132.09
38	A1	867	OMG	O6-C6-C5	-2.06	121.11	126.53
34	B5	28	A2M	C6-C5-N7	2.05	136.05	132.09
38	A1	2281	A2M	N9-C8-N7	-2.05	111.03	113.94
38	A1	2922	OMG	O6-C6-C5	-2.04	121.14	126.53
38	A1	649	A2M	C6-C5-N7	2.04	136.03	132.09
38	A1	1437	OMC	C1'-N1-C2	2.04	122.95	118.44
38	A1	1133	A2M	C2-N1-C6	2.04	122.08	118.73
34	B5	1428	OMG	O6-C6-C5	-2.04	121.15	126.53
38	A1	2793	OMG	O6-C6-C5	-2.04	121.15	126.53
34	B5	420	A2M	N9-C8-N7	-2.03	111.05	113.94
38	A1	807	A2M	O4'-C1'-N9	2.03	111.99	108.09
34	B5	1773	4AC	C6-C5-C4	2.03	119.44	117.00
34	B5	796	A2M	N9-C8-N7	-2.03	111.06	113.94
38	A1	2220	A2M	N3-C2-N1	-2.03	125.52	128.58
38	A1	645	1MA	N1-C2-N3	-2.02	123.59	126.00
34	B5	562	OMG	O6-C6-C5	-2.02	121.20	126.53
38	A1	817	A2M	N9-C8-N7	-2.01	111.08	113.94

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
34	B5	1575	G7M	C3'
34	B5	1575	G7M	C4'
34	B5	1575	G7M	C2'

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	B5	28	A2M	C1'-C2'-O2'-CM'
34	B5	100	A2M	C1'-C2'-O2'-CM'
34	B5	414	OMC	C1'-C2'-O2'-CM2
34	B5	420	A2M	C1'-C2'-O2'-CM'
34	B5	562	OMG	C1'-C2'-O2'-CM2
34	B5	619	A2M	C1'-C2'-O2'-CM'
34	B5	1191	XSX	C3-C1-N3-C2
34	B5	1191	XSX	C3-C1-N3-C4
34	B5	1271	OMG	C1'-C2'-O2'-CM2
34	B5	1280	4AC	N3-C4-N4-C7
34	B5	1280	4AC	C5-C4-N4-C7
34	B5	1428	OMG	C1'-C2'-O2'-CM2
34	B5	1572	OMG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
34	B5	1773	4AC	N3-C4-N4-C7
34	B5	1773	4AC	C5-C4-N4-C7
38	A1	867	OMG	C1'-C2'-O2'-CM2
38	A1	876	A2M	C1'-C2'-O2'-CM'
38	A1	1437	OMC	C1'-C2'-O2'-CM2
38	A1	2197	OMC	C2'-C1'-N1-C2
38	A1	2197	OMC	C2'-C1'-N1-C6
38	A1	2220	A2M	C1'-C2'-O2'-CM'
38	A1	2280	A2M	C1'-C2'-O2'-CM'
38	A1	2337	OMC	C1'-C2'-O2'-CM2
38	A1	2417	OMU	C1'-C2'-O2'-CM2
38	A1	2421	OMU	C1'-C2'-O2'-CM2
38	A1	2619	OMG	C1'-C2'-O2'-CM2
38	A1	2724	OMU	C1'-C2'-O2'-CM2
38	A1	2791	OMG	C1'-C2'-O2'-CM2
38	A1	2870	5MC	C2'-C1'-N1-C2
38	A1	2870	5MC	C2'-C1'-N1-C6
34	B5	1572	OMG	C3'-C4'-C5'-O5'
34	B5	1575	G7M	C3'-C4'-C5'-O5'
34	B5	1782	MA6	O4'-C4'-C5'-O5'
38	A1	2729	OMU	O4'-C4'-C5'-O5'
34	B5	619	A2M	O4'-C4'-C5'-O5'
38	A1	2197	OMC	O4'-C4'-C5'-O5'
38	A1	2256	A2M	O4'-C4'-C5'-O5'
38	A1	2729	OMU	C3'-C4'-C5'-O5'
34	B5	1191	XSX	N4-C7-C9-O10
34	B5	619	A2M	C3'-C4'-C5'-O5'
34	B5	1269	OMU	O4'-C1'-N1-C2
34	B5	1575	G7M	O4'-C4'-C5'-O5'
38	A1	2197	OMC	C3'-C4'-C5'-O5'
38	A1	2256	A2M	C3'-C4'-C5'-O5'
34	B5	1269	OMU	O4'-C1'-N1-C6
34	B5	1126	OMG	C3'-C4'-C5'-O5'
34	B5	1782	MA6	C3'-C4'-C5'-O5'
34	B5	541	A2M	C4'-C5'-O5'-P
38	A1	817	A2M	C4'-C5'-O5'-P
34	B5	1428	OMG	O4'-C4'-C5'-O5'
34	B5	1191	XSX	C1-C3-C7-C9
38	A1	2256	A2M	C2'-C1'-N9-C8
38	A1	645	1MA	C2'-C1'-N9-C8
38	A1	2922	OMG	C3'-C2'-O2'-CM2
38	A1	2256	A2M	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
34	B5	1191	XSX	C3-C7-C9-O10
34	B5	1782	MA6	C5-C6-N6-C9
34	B5	619	A2M	C2'-C1'-N9-C8
38	A1	2197	OMC	O4'-C1'-N1-C6
38	A1	2870	5MC	O4'-C1'-N1-C6
34	B5	1269	OMU	C4'-C5'-O5'-P
38	A1	1450	OMG	C4'-C5'-O5'-P
34	B5	1428	OMG	C4'-C5'-O5'-P
34	B5	1191	XSX	C3-C7-C9-O11
38	A1	645	1MA	C2'-C1'-N9-C4
34	B5	1572	OMG	C4'-C5'-O5'-P
34	B5	541	A2M	O4'-C1'-N9-C8
38	A1	805	OMG	C3'-C2'-O2'-CM2
34	B5	541	A2M	C2'-C1'-N9-C8
38	A1	1437	OMC	O4'-C4'-C5'-O5'
34	B5	541	A2M	C2'-C1'-N9-C4
34	B5	541	A2M	O4'-C4'-C5'-O5'
38	A1	2281	A2M	C2'-C1'-N9-C8
38	A1	2870	5MC	O4'-C1'-N1-C2
38	A1	2197	OMC	O4'-C1'-N1-C2

There are no ring outliers.

22 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	A1	2281	A2M	1	0
38	A1	2724	OMU	2	0
34	B5	1575	G7M	1	0
34	B5	1269	OMU	1	0
34	B5	796	A2M	1	0
38	A1	650	OMC	1	0
34	B5	436	A2M	1	0
38	A1	2197	OMC	1	0
34	B5	414	OMC	2	0
34	B5	1572	OMG	3	0
38	A1	876	A2M	1	0
34	B5	1428	OMG	1	0
38	A1	649	A2M	1	0
34	B5	100	A2M	1	0
38	A1	2220	A2M	4	0
34	B5	28	A2M	1	0
38	A1	1449	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	A1	663	OMC	1	0
38	A1	1133	A2M	1	0
34	B5	1773	4AC	2	0
38	A1	2417	OMU	1	0
34	B5	974	A2M	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 259 ligands modelled in this entry, 258 are monoatomic - leaving 1 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	$\# Z > 2$
82	HYG	B5	1801	81	36,39,39	4.33	15 (41%)	44,60,60	1.80	14 (31%)

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
82	HYG	B5	1801	81	-	5/12/87/87	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	B5	1801	HYG	O22-C17	-12.62	1.21	1.43
82	B5	1801	HYG	O29-C12	-12.50	1.21	1.43
82	B5	1801	HYG	O14-C15	7.88	1.63	1.44
82	B5	1801	HYG	C27-C33	-7.55	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	B5	1801	HYG	O28-C23	7.52	1.49	1.40
82	B5	1801	HYG	O28-C27	6.53	1.53	1.44
82	B5	1801	HYG	O35-C34	-5.49	1.19	1.42
82	B5	1801	HYG	O14-C13	5.30	1.55	1.41
82	B5	1801	HYG	C25-C24	-5.23	1.44	1.53
82	B5	1801	HYG	C17-C12	3.33	1.60	1.53
82	B5	1801	HYG	C34-C33	2.85	1.57	1.52
82	B5	1801	HYG	O30-C24	2.66	1.48	1.42
82	B5	1801	HYG	O31-C25	2.33	1.48	1.43
82	B5	1801	HYG	C26-C27	2.08	1.57	1.52
82	B5	1801	HYG	O18-C13	-2.06	1.36	1.41

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	B5	1801	HYG	O35-C34-C33	3.86	119.92	111.55
82	B5	1801	HYG	C10-N9-C4	-3.67	110.00	114.39
82	B5	1801	HYG	O14-C15-C16	3.09	115.28	109.70
82	B5	1801	HYG	C16-C17-C12	-3.06	106.18	113.50
82	B5	1801	HYG	O22-C17-C12	2.75	108.01	103.63
82	B5	1801	HYG	O22-C17-C16	2.75	117.77	111.22
82	B5	1801	HYG	C25-C26-C27	2.72	115.84	109.68
82	B5	1801	HYG	C6-C5-C4	2.64	116.30	109.93
82	B5	1801	HYG	C5-C6-C1	2.60	114.47	110.86
82	B5	1801	HYG	C13-C12-C17	-2.58	103.73	111.41
82	B5	1801	HYG	O28-C27-C26	2.38	111.82	108.50
82	B5	1801	HYG	C13-O18-C6	-2.38	112.34	117.98
82	B5	1801	HYG	C13-O14-C15	2.15	117.92	113.72
82	B5	1801	HYG	O29-C23-O22	-2.13	103.49	105.90

There are no chirality outliers.

All (5) torsion outliers are listed below:

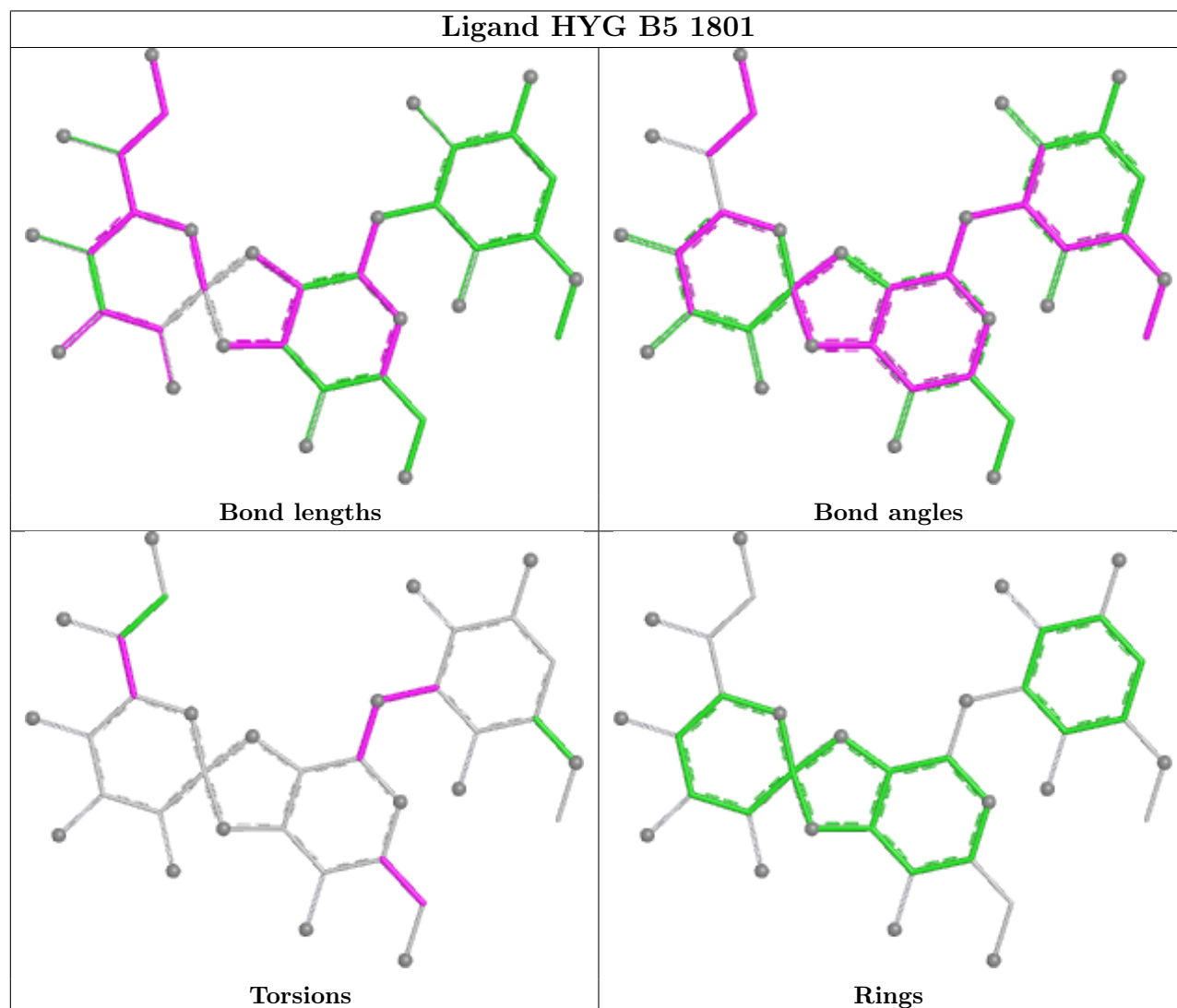
Mol	Chain	Res	Type	Atoms
82	B5	1801	HYG	O14-C13-O18-C6
82	B5	1801	HYG	O14-C15-C19-O20
82	B5	1801	HYG	O28-C27-C33-C34
82	B5	1801	HYG	C1-C6-O18-C13
82	B5	1801	HYG	C26-C27-C33-C34

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	B5	1801	HYG	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

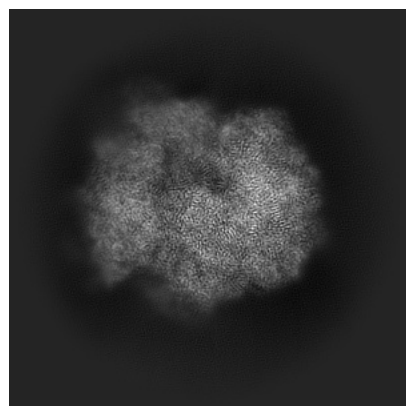
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47093. These allow visual inspection of the internal detail of the map and identification of artifacts.

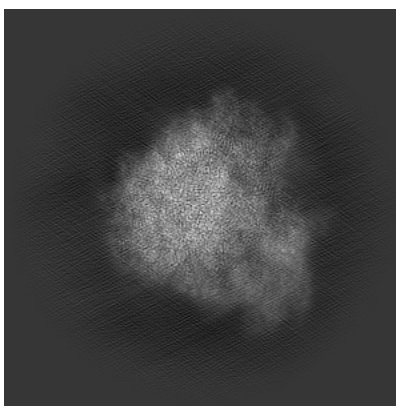
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

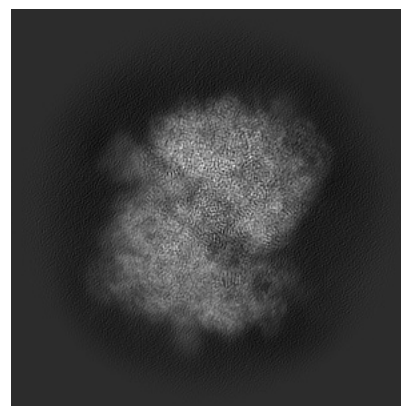
6.1.1 Primary map



X

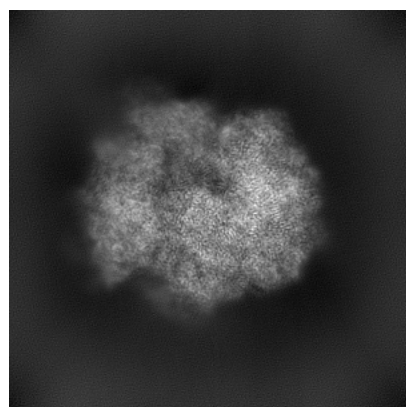


Y

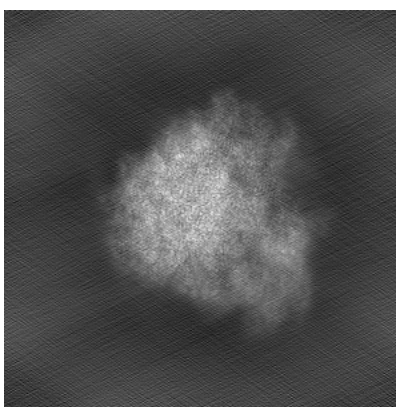


Z

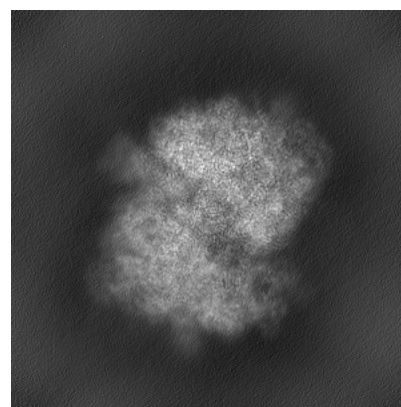
6.1.2 Raw map



X



Y

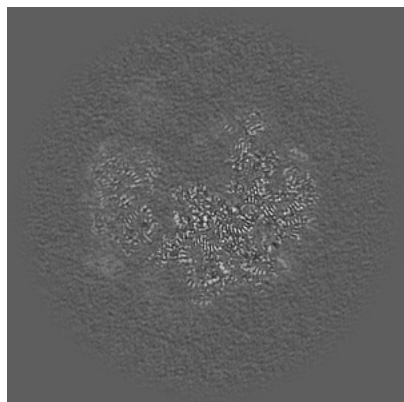


Z

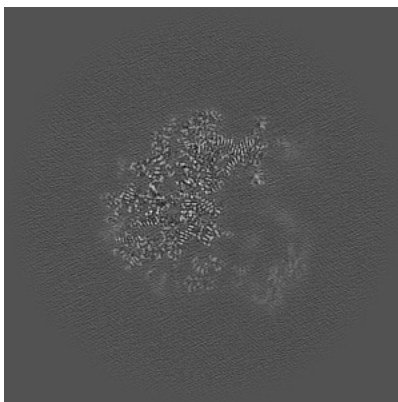
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

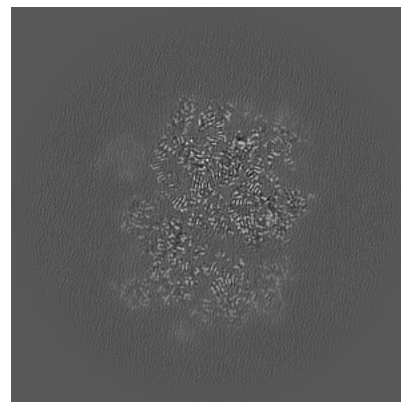
6.2.1 Primary map



X Index: 200

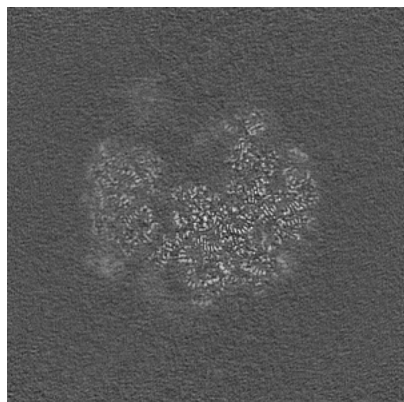


Y Index: 200

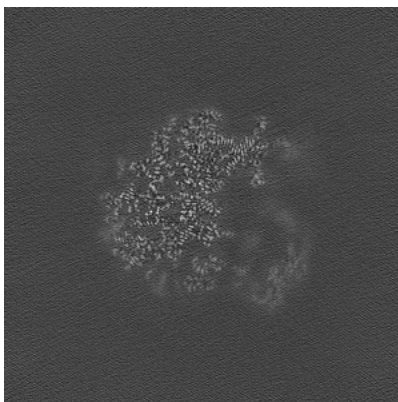


Z Index: 200

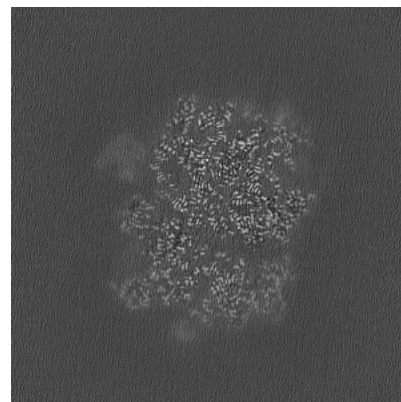
6.2.2 Raw map



X Index: 200



Y Index: 200

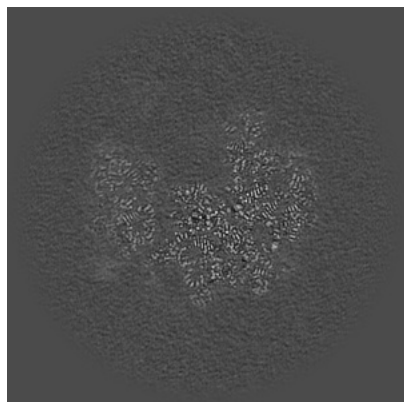


Z Index: 200

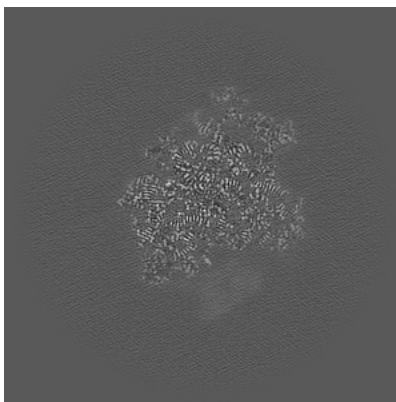
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

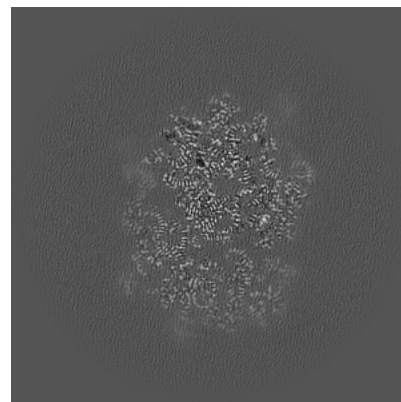
6.3.1 Primary map



X Index: 202

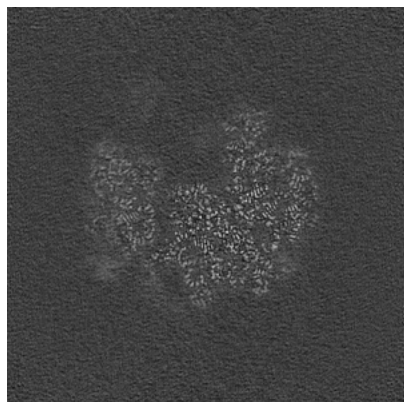


Y Index: 246

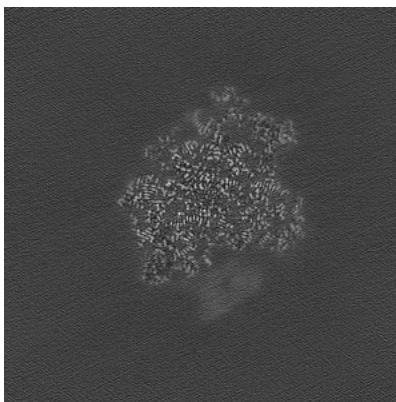


Z Index: 188

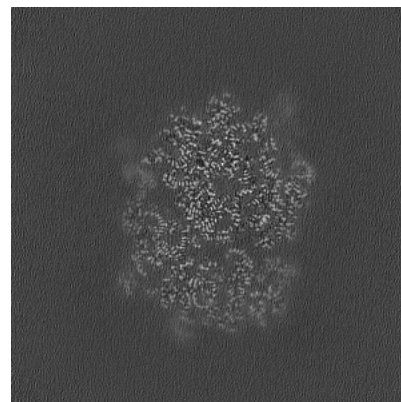
6.3.2 Raw map



X Index: 202



Y Index: 246

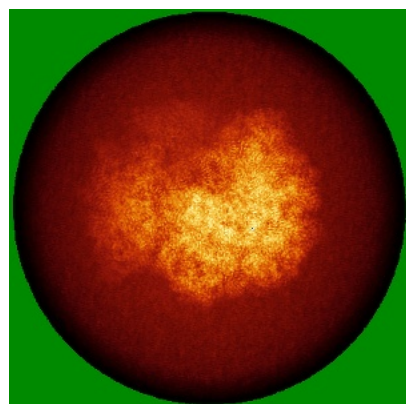


Z Index: 188

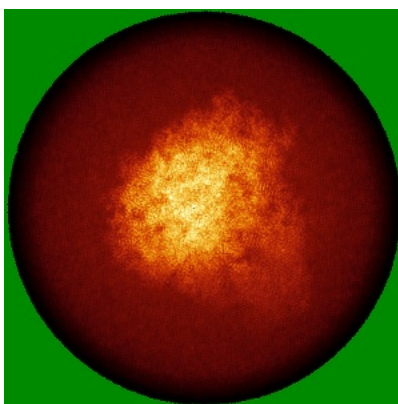
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

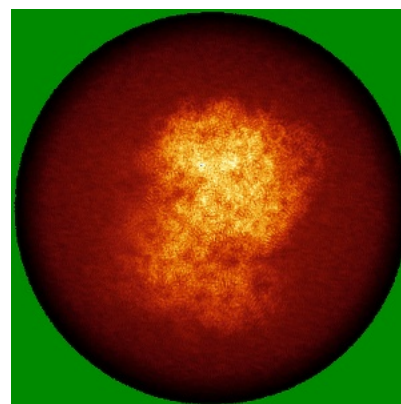
6.4.1 Primary map



X

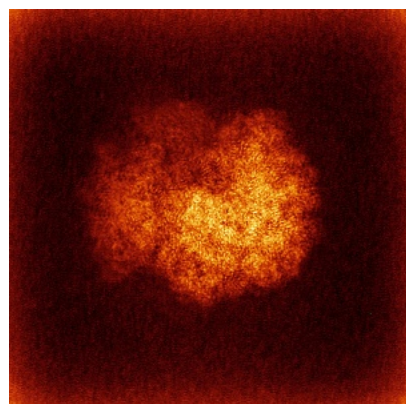


Y

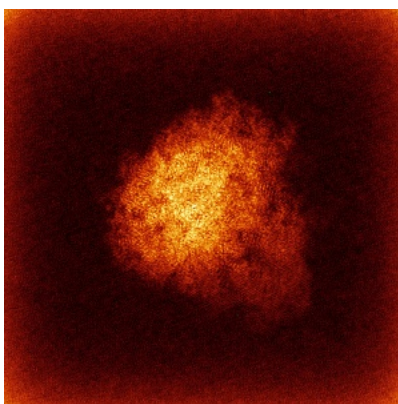


Z

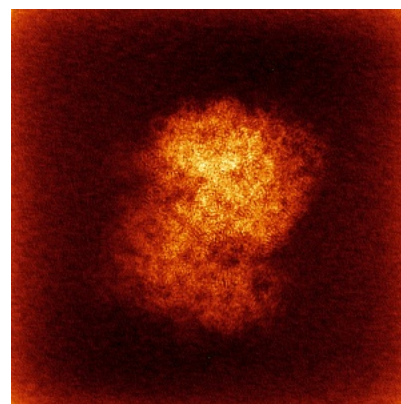
6.4.2 Raw map



X



Y

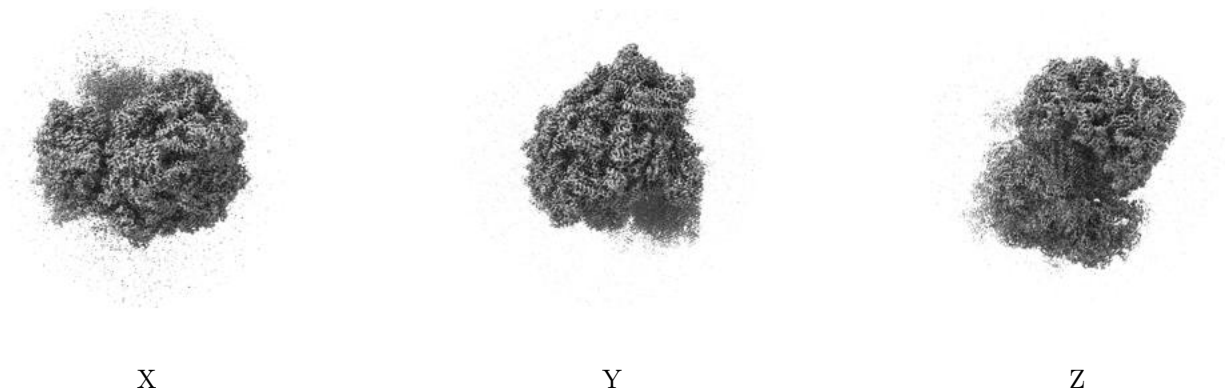


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

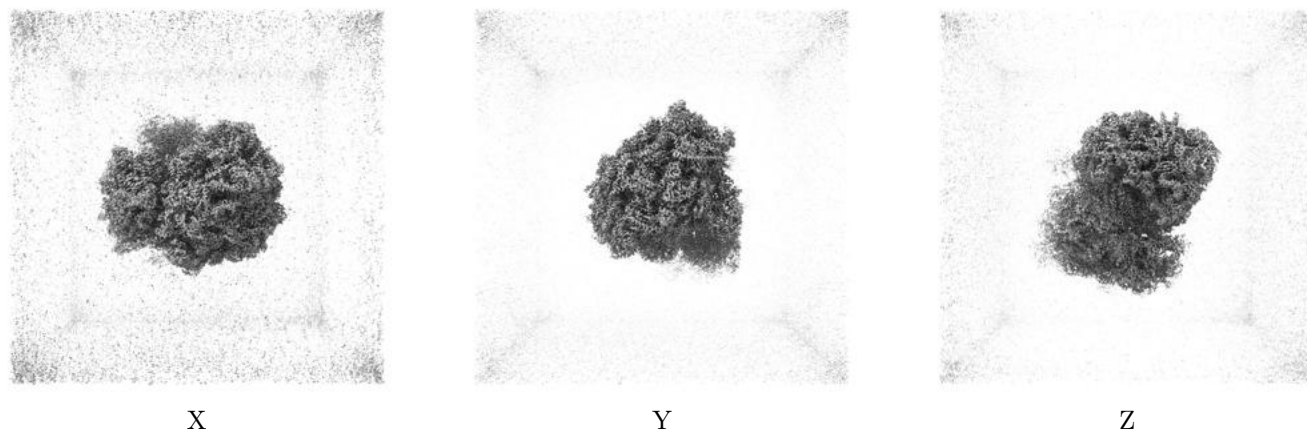
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

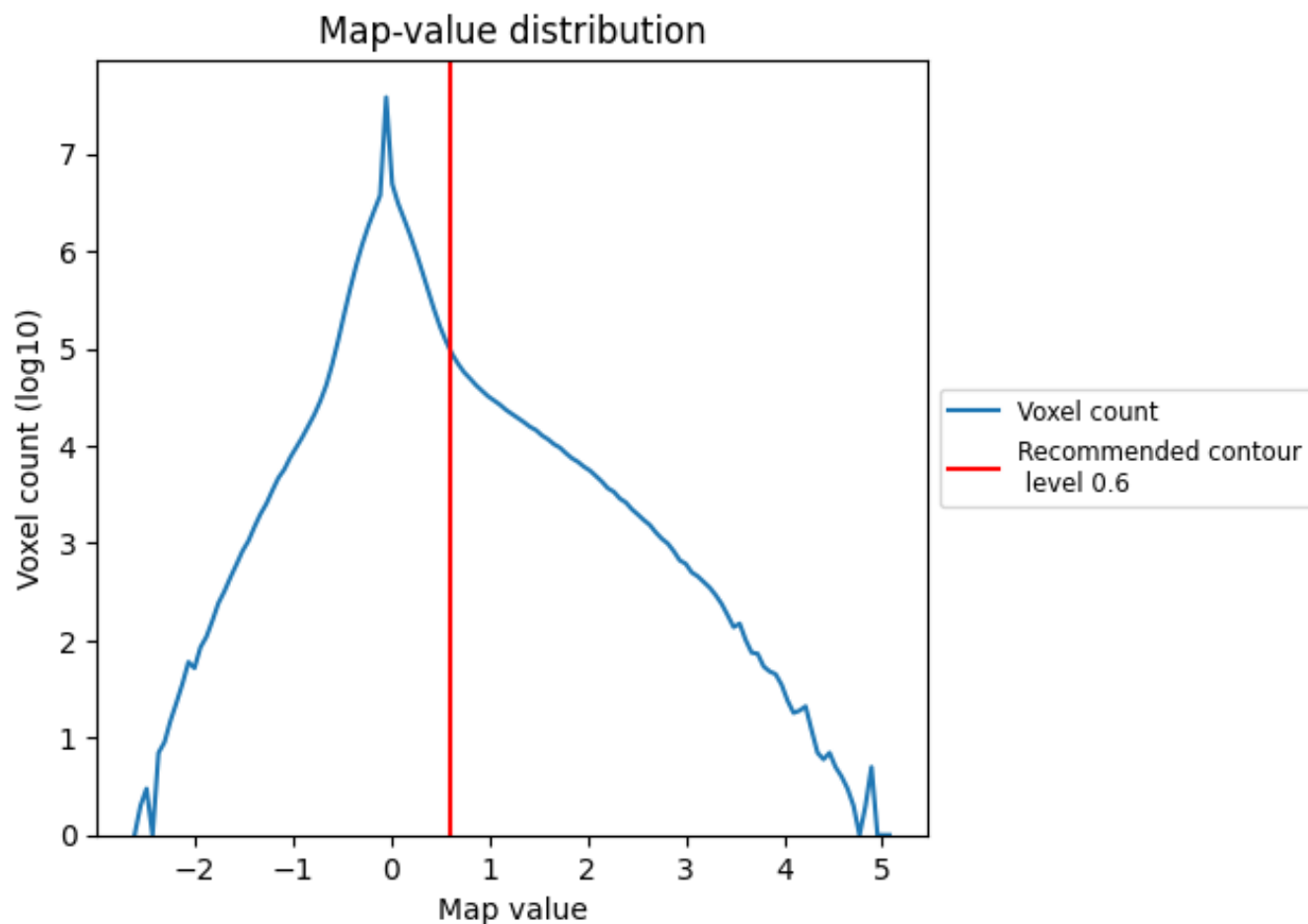
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

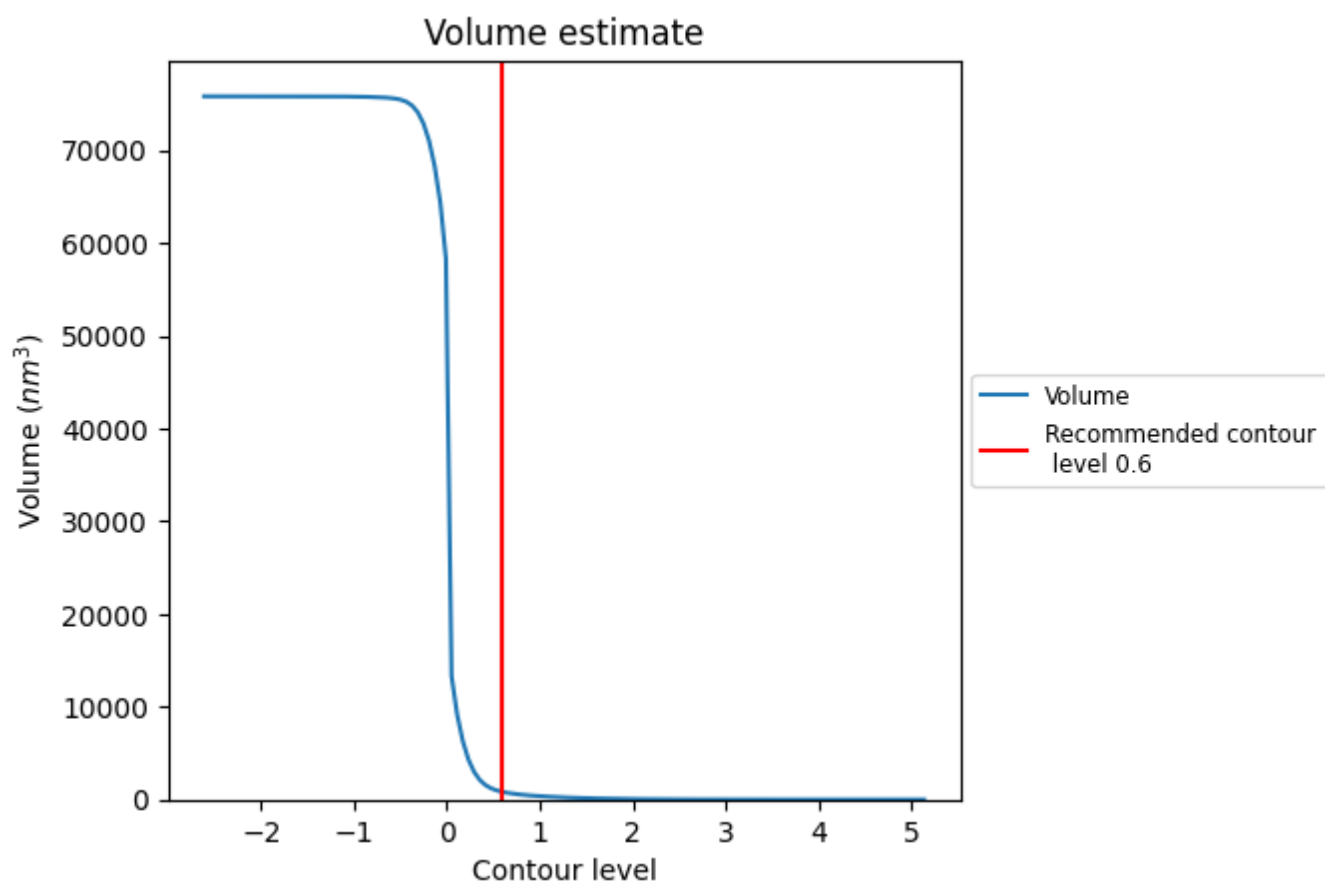
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

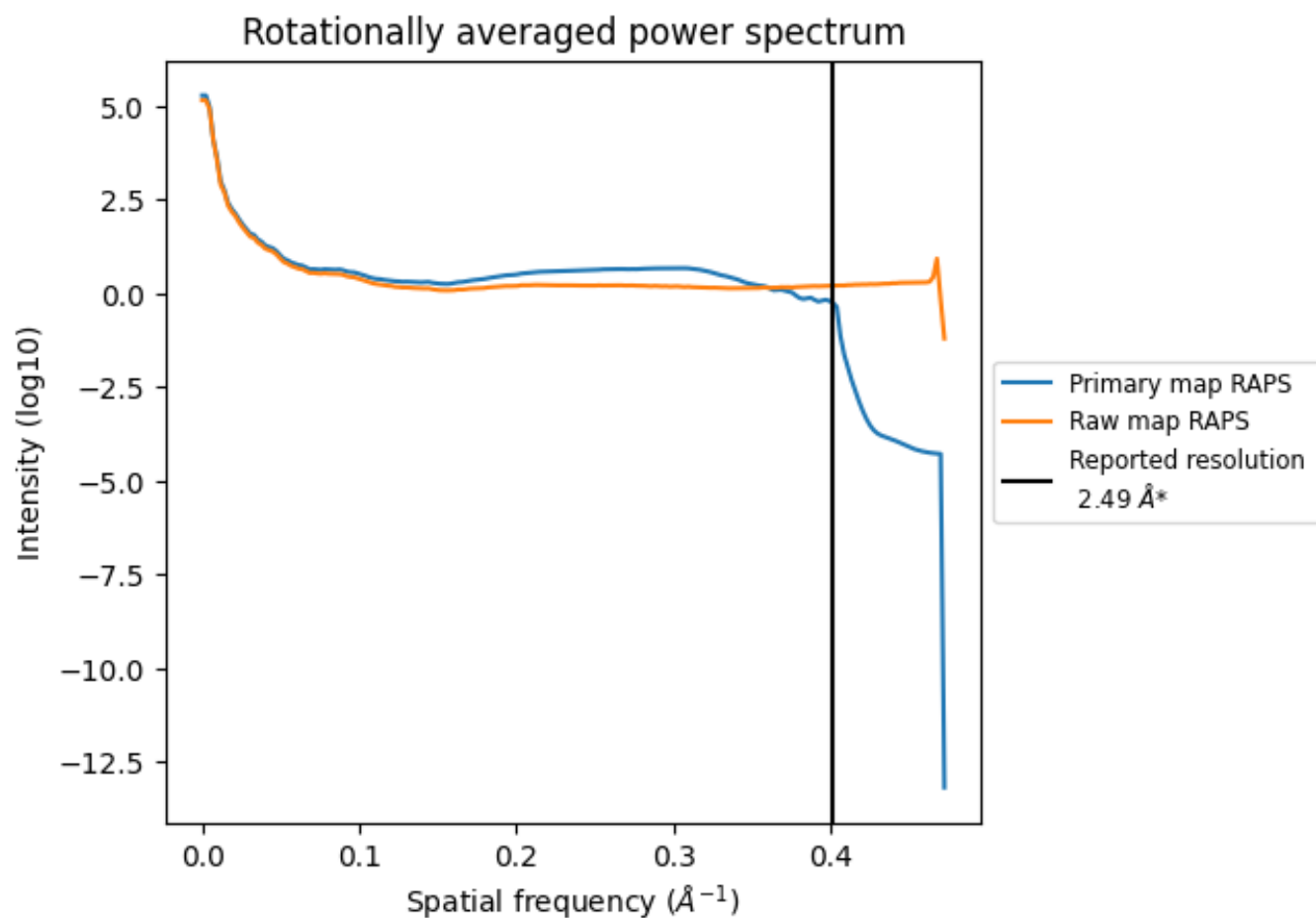
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 823 nm³; this corresponds to an approximate mass of 743 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

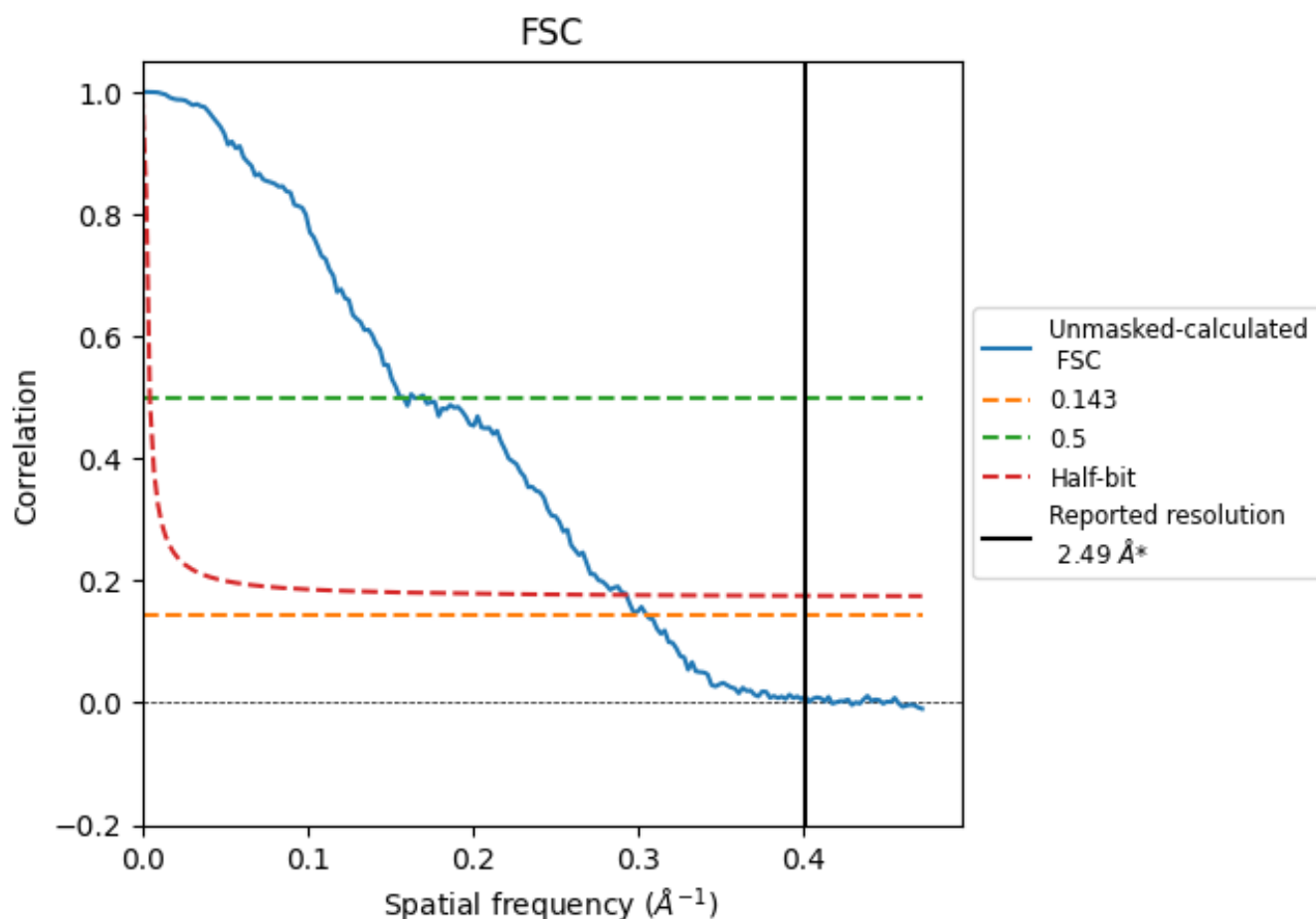


*Reported resolution corresponds to spatial frequency of 0.402 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.402 \AA^{-1}

8.2 Resolution estimates [i](#)

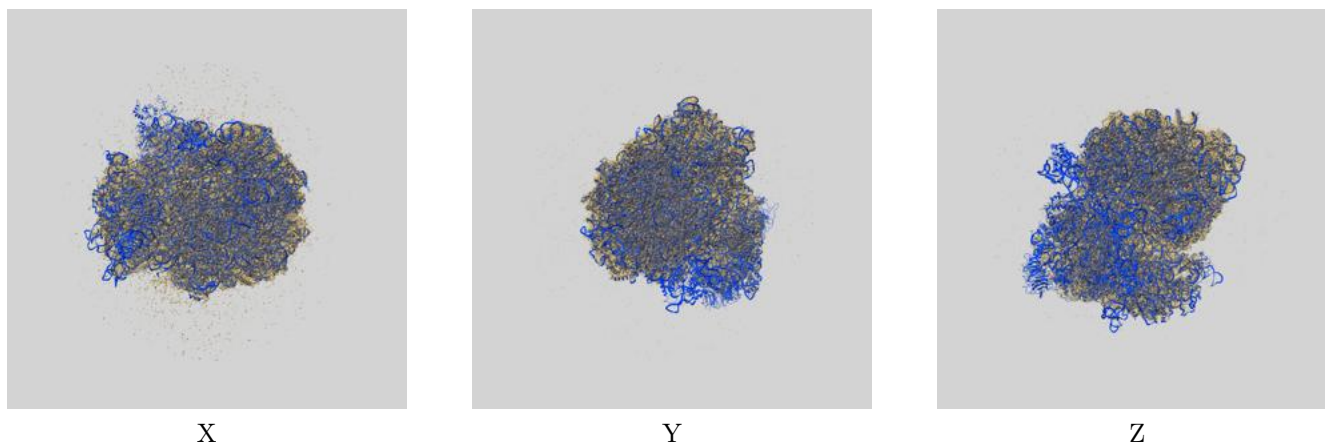
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.49	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.27	6.32	3.41

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.27 differs from the reported value 2.49 by more than 10 %

9 Map-model fit [i](#)

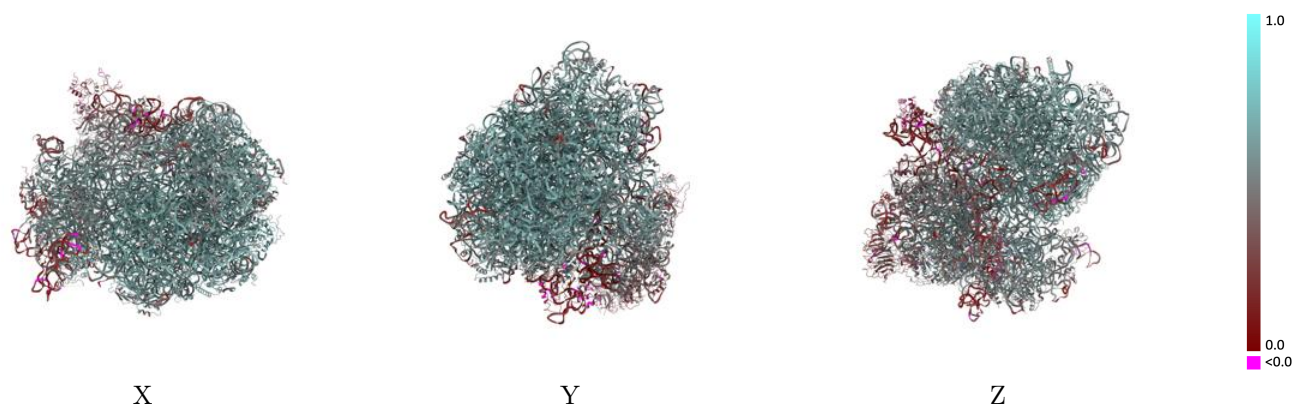
This section contains information regarding the fit between EMDB map EMD-47093 and PDB model 9DOV. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

9.1 Map-model overlay [i](#)



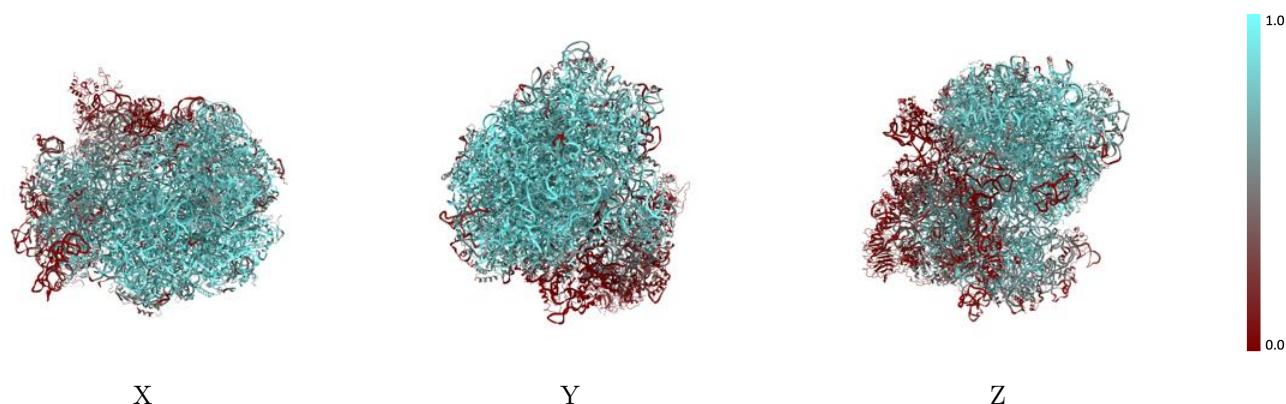
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



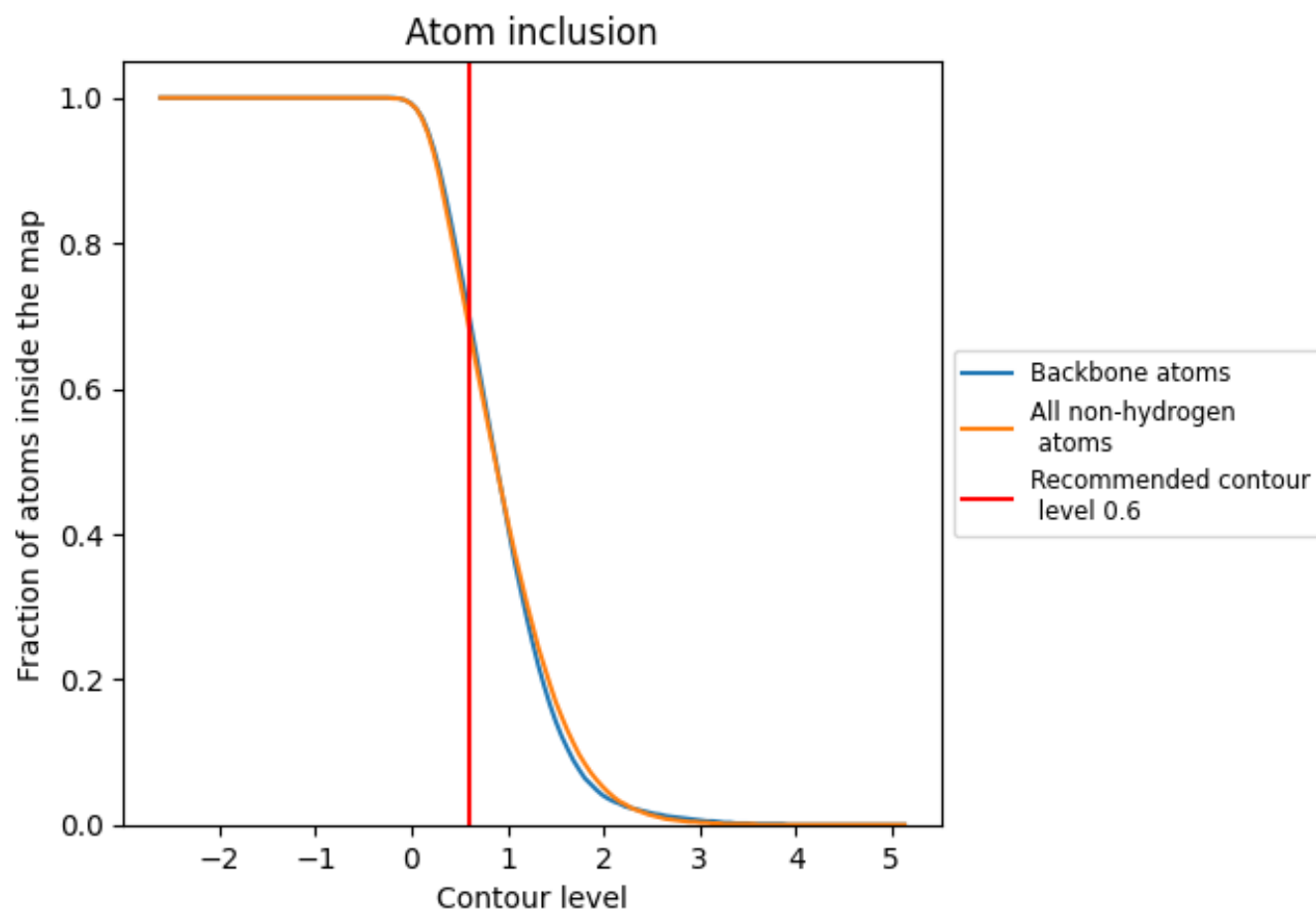
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.6).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6830	 0.5460
A1	 0.8450	 0.5960
A3	 0.8610	 0.5990
A4	 0.9150	 0.6310
AA	 0.9210	 0.6550
AB	 0.8570	 0.6260
AC	 0.8550	 0.6300
AD	 0.6040	 0.5490
AE	 0.6590	 0.5600
AF	 0.8400	 0.6160
AG	 0.6830	 0.5640
AH	 0.6690	 0.5530
AI	 0.7600	 0.5980
AJ	 0.3680	 0.4520
AL	 0.7990	 0.6100
AM	 0.6890	 0.5630
AN	 0.9380	 0.6520
AO	 0.8470	 0.6170
AP	 0.8590	 0.6390
AQ	 0.8950	 0.6450
AR	 0.7530	 0.5870
AS	 0.8000	 0.5990
AT	 0.7850	 0.6010
AU	 0.6180	 0.5580
AV	 0.8230	 0.6330
AW	 0.8520	 0.6340
AX	 0.8140	 0.6160
AY	 0.8130	 0.6190
AZ	 0.7670	 0.5870
Aa	 0.8790	 0.6310
Ab	 0.7460	 0.5870
Ac	 0.7510	 0.5960
Ad	 0.7670	 0.6010
Ae	 0.8680	 0.6430
Af	 0.8900	 0.6390











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Chain	Atom inclusion	Q-score
Ag	 0.8180	 0.6140
Ah	 0.8000	 0.6060
Ai	 0.7050	 0.5840
Aj	 0.9310	 0.6530
Ak	 0.5710	 0.5360
Al	 0.9160	 0.6460
Am	 0.6620	 0.5590
An	 0.7880	 0.5990
Ao	 0.7310	 0.5920
Ap	 0.8040	 0.6300
B5	 0.6200	 0.5040
BA	 0.4850	 0.5080
BB	 0.5330	 0.5360
BC	 0.6870	 0.5860
BD	 0.2460	 0.4160
BE	 0.5670	 0.5490
BF	 0.1700	 0.4030
BG	 0.3070	 0.4450
BH	 0.3620	 0.4630
BI	 0.6900	 0.5730
BJ	 0.5530	 0.5340
BK	 0.1000	 0.3260
BL	 0.7060	 0.5710
BM	 0.0030	 0.2070
BN	 0.7120	 0.5880
BO	 0.6510	 0.5700
BP	 0.0690	 0.3210
BQ	 0.1730	 0.4230
BR	 0.2420	 0.4440
BS	 0.1150	 0.3700
BT	 0.1410	 0.3850
BU	 0.1860	 0.3760
BV	 0.5530	 0.5460
BW	 0.8060	 0.6220
BX	 0.6970	 0.5850
BY	 0.3300	 0.4710
BZ	 0.0960	 0.3540
Ba	 0.7010	 0.5790
Bb	 0.5410	 0.5320
Bc	 0.1890	 0.4180
Bd	 0.3990	 0.4890
Be	 0.4140	 0.4910

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Chain	Atom inclusion	Q-score
Bf	 0.0020	 0.1850
Bg	 0.0430	 0.3080
E	 0.0050	 0.1770
EC	 0.0490	 0.2080