Full wwPDB EM Validation Report ⓘ

May 16, 2026 – 08:48 am BST

PDB ID	:	9RVU / pdb_00009rvu
EMDB ID	:	EMD-54290
Title	:	in situ S. pombe hibernating ribosome after 7 days of glucose depletion
Authors	:	Rosa, H.; Gluc, M.; Jomaa, A.; Mattei, S.
Deposited on	:	2025-07-09
Resolution	:	3.38 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:

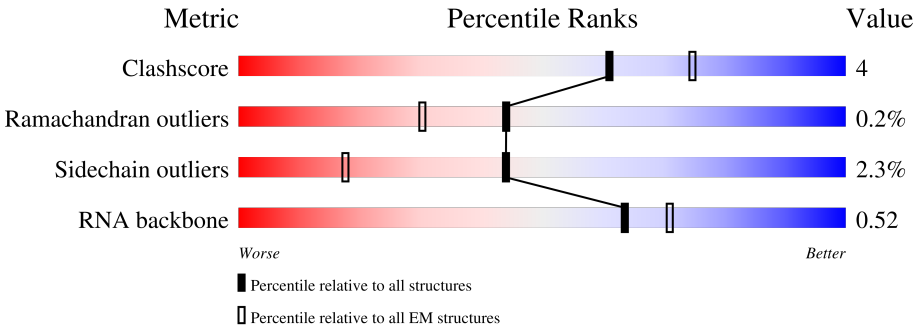
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

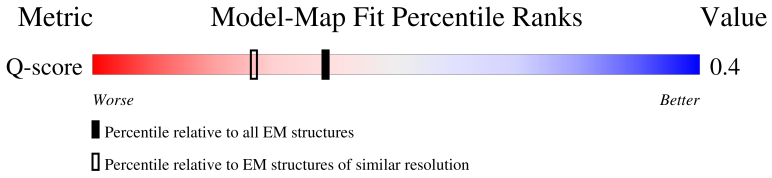
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.38 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	14261 (2.88 - 3.88)

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 <=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	AA	1842	12% 59% 30% • 7%
2	AD	292	23% 47% 20% • 30%
3	AE	252	50% 70% 15% 14%

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Mol	Chain	Length	Quality of chain
4	AF	253	64% 21% 15%
5	AG	249	33% 68% 18% 13%
6	AH	262	32% 70% 30%
7	AI	203	60% 74% 24%
8	AJ	239	50% 75% 17% 8%
9	AK	195	47% 75% 23%
10	AL	200	10% 82% 11% 6%
11	AM	192	20% 73% 19% 7%
12	AN	147	32% 48% 14% 37%
13	AO	152	14% 68% 24% 6%
14	AP	145	74% 69% 14% 17%
15	AQ	151	29% 81% 18%
16	AR	139	56% 63% 27% 8%
17	AS	154	39% 60% 16% 23%
18	AT	140	52% 70% 30%
19	AU	131	40% 61% 20% 19%
20	AV	152	48% 66% 26% 7%
21	AW	144	49% 72% 27%
22	Aa	118	47% 69% 15% 15%
23	Ab	87	25% 82% 18%
24	Ac	130	5% 80% 18%
25	Ad	143	10% 77% 22%
26	Ae	134	63% 71% 28%
27	Af	89	61% 66% 11% 22%
28	Ag	119	16% 68% 13% 18%

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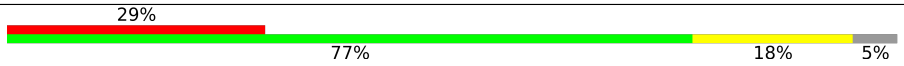
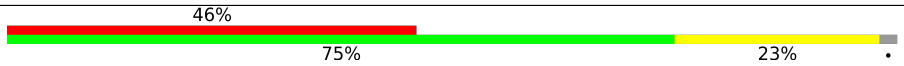
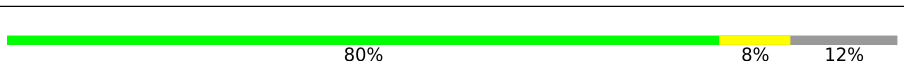
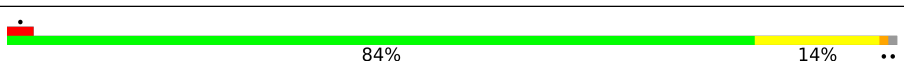
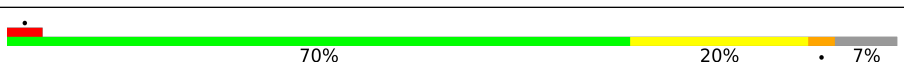
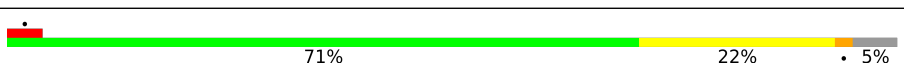
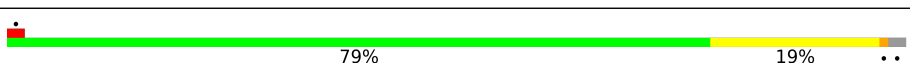
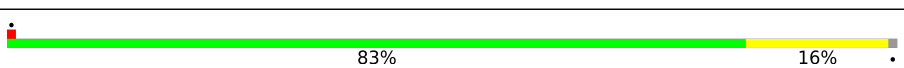
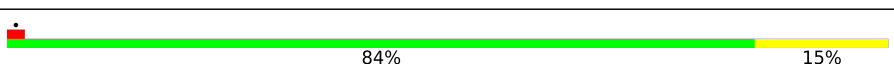
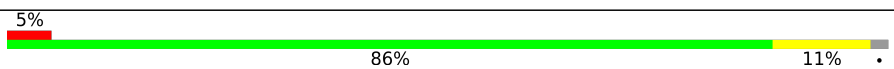
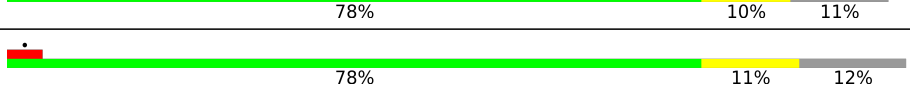
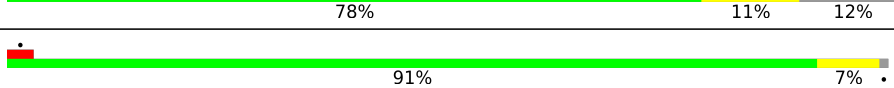
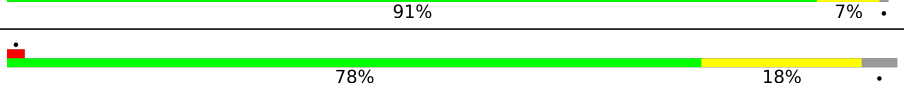
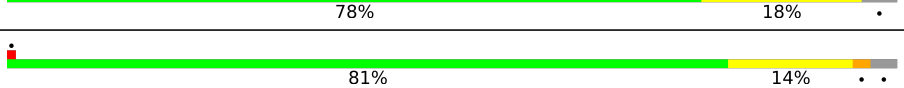
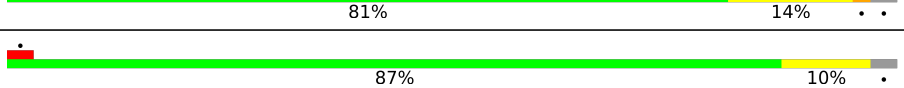
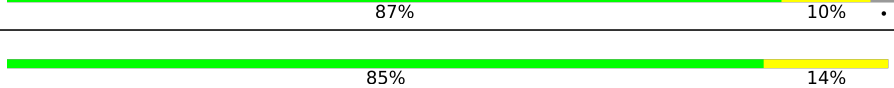
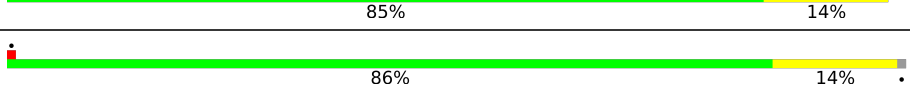
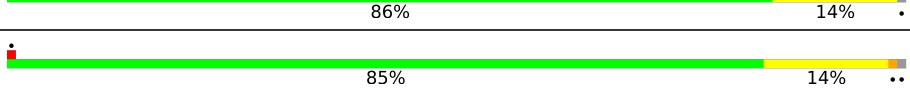
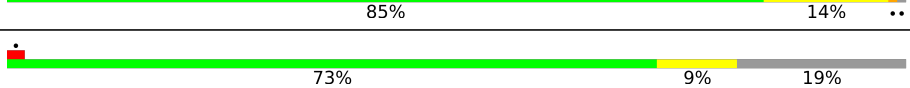
Mol	Chain	Length	Quality of chain
29	Ah	83	
30	Ai	68	
31	Aj	56	
32	Ak	61	
33	Am	314	
34	B0	106	
35	B1	94	
36	B2	3498	
37	B3	246	
38	B4	165	
39	BN	253	
40	BO	388	
41	BP	363	
42	BQ	294	
43	BR	195	
44	BS	251	
45	BT	259	
46	BV	221	
47	BW	174	
48	BX	208	
49	BY	134	
50	BZ	201	
51	Ba	197	
52	Bc	187	
53	Bd	193	

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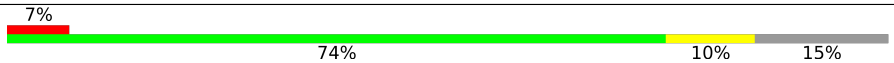
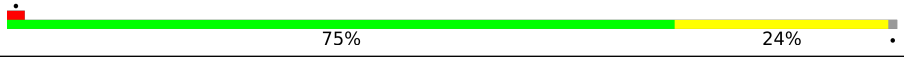
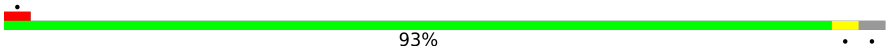
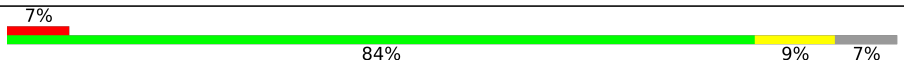
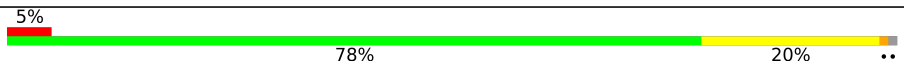
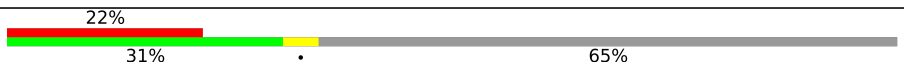
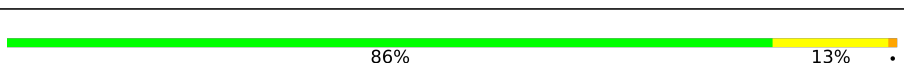
Mol	Chain	Length	Quality of chain
54	Be	176	
55	Bf	160	
56	Bg	117	
57	Bh	139	
58	Bi	149	
59	Bj	141	
60	Bk	126	
61	Bl	136	
62	Bm	148	
63	Bn	61	
64	Bo	109	
65	Bp	113	
66	Bq	127	
67	Br	108	
68	Bs	111	
69	Bt	122	
70	Bu	99	
71	Bv	91	
72	Bw	74	
73	Bx	51	
74	By	134	
75	H1	284	
76	HE	842	
77	HL	216	
78	HS	106	

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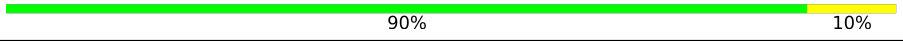
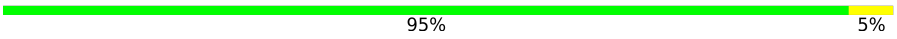
Mol	Chain	Length	Quality of chain
79	HI	157	
80	BA	51	
81	BU	189	
82	Bb	187	
83	A	20	

2 Entry composition (i)

There are 84 unique types of molecules in this entry. The entry contains 209623 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 RNA chain called 18S small subunit ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	AA	1705	36359	16255	6470	11929	1705	0	0

- Molecule 2 is a protein called Small ribosomal subunit protein uS2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	AD	205	1602	1016	294	287	5	0	0

- Molecule 3 is a protein called Small ribosomal subunit protein eS1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	AE	216	1733	1093	319	316	5	0	0

- Molecule 4 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	AF	216	1660	1072	289	292	7	0	0

- Molecule 5 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AG	216	1701	1080	308	305	8	0	0

- Molecule 6 is a protein called Small ribosomal subunit protein eS4C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	AH	261	2083	1330	391	356	6	0	0

- Molecule 7 is a protein called Small ribosomal subunit protein uS7A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AI	203	Total	C	N	O	S	0	0
			1559	972	291	290	6		

- Molecule 8 is a protein called Small ribosomal subunit protein eS6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AJ	221	Total	C	N	O	S	0	0
			1784	1123	352	302	7		

- Molecule 9 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AK	193	Total	C	N	O	S	0	0
			1530	967	284	276	3		

- Molecule 10 is a protein called Small ribosomal subunit protein eS8B.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AL	188	Total	C	N	O	S	0	0
			1506	936	303	264	3		

- Molecule 11 is a protein called Small ribosomal subunit protein uS4B.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AM	178	Total	C	N	O	S	0	0
			1462	928	291	241	2		

- Molecule 12 is a protein called Small ribosomal subunit protein eS10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AN	92	Total	C	N	O	S	0	0
			748	484	132	130	2		

- Molecule 13 is a protein called Small ribosomal subunit protein uS17A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AO	143	Total	C	N	O	S	0	0
			1164	743	222	196	3		

- Molecule 14 is a protein called Small ribosomal subunit protein eS12A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AP	121	Total 884	C 549	N 151	O 177	S 7	0	0

- Molecule 15 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AQ	150	Total 1184	C 754	N 222	O 204	S 4	0	0

- Molecule 16 is a protein called Small ribosomal subunit protein uS11A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AR	128	Total 949	C 587	N 184	O 174	S 4	0	0

- Molecule 17 is a protein called Small ribosomal subunit protein uS19B.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AS	119	Total 954	C 608	N 179	O 163	S 4	0	0

- Molecule 18 is a protein called Small ribosomal subunit protein uS9A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AT	140	Total 1082	C 688	N 203	O 186	S 5	0	0

- Molecule 19 is a protein called Small ribosomal subunit protein eS17A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AU	106	Total 879	C 546	N 169	O 162	S 2	0	0

- Molecule 20 is a protein called Small ribosomal subunit protein uS13A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AV	141	Total 1144	C 714	N 222	O 204	S 4	0	0

- Molecule 21 is a protein called Small ribosomal subunit protein eS19A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AW	142	Total	C	N	O	S	0	0
			1119	699	212	205	3		

- Molecule 22 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Aa	100	Total	C	N	O	S	0	0
			810	508	155	145	2		

- Molecule 23 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Ab	87	Total	C	N	O	S	0	0
			672	411	122	135	4		

- Molecule 24 is a protein called Small ribosomal subunit protein uS8A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Ac	129	Total	C	N	O	S	0	0
			1028	649	196	179	4		

- Molecule 25 is a protein called Small ribosomal subunit protein uS12A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Ad	142	Total	C	N	O	S	0	0
			1095	692	214	187	2		

- Molecule 26 is a protein called Small ribosomal subunit protein eS24A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Ae	133	Total	C	N	O	S	0	0
			1078	672	217	185	4		

- Molecule 27 is a protein called Small ribosomal subunit protein eS25A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Af	69	Total	C	N	O	S	0	0
			551	350	103	97	1		

- Molecule 28 is a protein called Small ribosomal subunit protein eS26B.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Ag	97	Total	C	N	O	S	0	0
			795	491	167	132	5		

- Molecule 29 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Ah	81	Total	C	N	O	S	0	0
			619	388	114	108	9		

- Molecule 30 is a protein called Small ribosomal subunit protein eS28A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Ai	63	Total	C	N	O	S	0	0
			498	308	99	90	1		

- Molecule 31 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Aj	53	Total	C	N	O	S	0	0
			447	282	91	73	1		

- Molecule 32 is a protein called Small ribosomal subunit protein eS30A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Ak	60	Total	C	N	O	S	0	0
			475	296	99	78	2		

- Molecule 33 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Am	314	Total	C	N	O	S	0	0
			2458	1549	422	478	9		

- Molecule 34 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	B0	93	Total	C	N	O	S	0	0
			758	479	152	122	5		

- Molecule 35 is a protein called Large ribosomal subunit protein eL43A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	B1	93	Total	C	N	O	S	0	0
			718	442	147	123	6		

- Molecule 36 is a RNA chain called 28S large subunit ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	B2	3249	Total	C	N	O	P	0	0
			69470	31043	12521	22657	3249		

- Molecule 37 is a RNA chain called 5S large subunit ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	B3	119	Total	C	N	O	P	0	0
			2539	1133	454	833	119		

- Molecule 38 is a RNA chain called 5.8S large subunit ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	B4	157	Total	C	N	O	P	0	0
			3332	1491	583	1101	157		

- Molecule 39 is a protein called Large ribosomal subunit protein uL2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BN	248	Total	C	N	O	S	0	0
			1872	1166	377	324	5		

- Molecule 40 is a protein called Large ribosomal subunit protein uL3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BO	384	Total	C	N	O	S	0	0
			3050	1929	576	535	10		

- Molecule 41 is a protein called Large ribosomal subunit protein uL4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BP	362	Total	C	N	O	S	0	0
			2799	1768	538	490	3		

- Molecule 42 is a protein called Large ribosomal subunit protein uL18B.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BQ	287	Total	C	N	O	S	0	0
			2312	1461	410	437	4		

- Molecule 43 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BR	171	Total	C	N	O	S	0	0
			1333	857	244	229	3		

- Molecule 44 is a protein called Large ribosomal subunit protein uL30C.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BS	223	Total	C	N	O	S	0	0
			1814	1158	334	319	3		

- Molecule 45 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BT	229	Total	C	N	O	S	0	0
			1772	1135	325	309	3		

- Molecule 46 is a protein called Large ribosomal subunit protein uL16A.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BV	219	Total	C	N	O	S	0	0
			1769	1114	340	305	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BW	167	Total	C	N	O	S	0	0
			1346	854	252	235	5		

- Molecule 48 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BX	201	Total	C	N	O	S	0	0
			1607	1005	320	281	1		

- Molecule 49 is a protein called Large ribosomal subunit protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BY	130	Total	C	N	O	S	0	0
			1038	662	198	174	4		

- Molecule 50 is a protein called Large ribosomal subunit protein eL15B.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BZ	200	Total	C	N	O	S	0	0
			1676	1050	348	275	3		

- Molecule 51 is a protein called Large ribosomal subunit protein uL13A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Ba	196	Total	C	N	O	S	0	0
			1545	991	294	256	4		

- Molecule 52 is a protein called Large ribosomal subunit protein eL18B.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	Bc	186	Total	C	N	O	0	0
			1487	937	300	250		

- Molecule 53 is a protein called Large ribosomal subunit protein eL19B.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Bd	157	Total	C	N	O	S	0	0
			1301	809	275	212	5		

- Molecule 54 is a protein called Large ribosomal subunit protein eL20A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Be	173	Total	C	N	O	S	0	0
			1423	916	268	234	5		

- Molecule 55 is a protein called Large ribosomal subunit protein eL21B.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Bf	159	Total	C	N	O	S	0	0
			1286	810	247	226	3		

- Molecule 56 is a protein called Large ribosomal subunit protein eL22.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	Bg	99	Total 798	C 518	N 138	O 142	0	0

- Molecule 57 is a protein called Large ribosomal subunit protein uL14A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Bh	134	Total 999	C 630	N 184	O 177	S 8	0	0

- Molecule 58 is a protein called Large ribosomal subunit protein eL24B.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Bi	63	Total 523	C 336	N 102	O 82	S 3	0	0

- Molecule 59 is a protein called Large ribosomal subunit protein uL23A.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Bj	118	Total 947	C 605	N 175	O 166	S 1	0	0

- Molecule 60 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Bk	125	Total 998	C 622	N 201	O 173	S 2	0	0

- Molecule 61 is a protein called Large ribosomal subunit protein eL27A.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Bl	135	Total 1078	C 698	N 200	O 178	S 2	0	0

- Molecule 62 is a protein called Large ribosomal subunit protein uL15B.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Bm	147	Total 1171	C 740	N 235	O 194	S 2	0	0

- Molecule 63 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms				AltConf	Trace
63	Bn	59	Total 495	C 299	N 112	O 84	0	0

- Molecule 64 is a protein called Large ribosomal subunit protein eL30A.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Bo	94	Total 705	C 450	N 121	O 130	S 4	0	0

- Molecule 65 is a protein called Large ribosomal subunit protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Bp	103	Total 857	C 538	N 167	O 149	S 3	0	0

- Molecule 66 is a protein called Large ribosomal subunit protein eL32A.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Bq	118	Total 944	C 591	N 191	O 157	S 5	0	0

- Molecule 67 is a protein called Large ribosomal subunit protein eL33A.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Br	104	Total 831	C 531	N 160	O 137	S 3	0	0

- Molecule 68 is a protein called Large ribosomal subunit protein eL34B.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Bs	106	Total 858	C 538	N 176	O 142	S 2	0	0

- Molecule 69 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms				AltConf	Trace
69	Bt	121	Total 999	C 629	N 194	O 176	0	0

- Molecule 70 is a protein called Large ribosomal subunit protein eL36B.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Bu	95	Total	C	N	O	S	0	0
			759	472	159	127	1		

- Molecule 71 is a protein called Large ribosomal subunit protein eL37B.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Bv	82	Total	C	N	O	S	0	0
			652	399	140	106	7		

- Molecule 72 is a protein called Large ribosomal subunit protein eL38A.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Bw	69	Total	C	N	O	S	0	0
			560	355	103	101	1		

- Molecule 73 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Bx	50	Total	C	N	O	S	0	0
			436	273	98	64	1		

- Molecule 74 is a protein called Large ribosomal subunit protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	By	133	Total	C	N	O	S	0	0
			1031	641	203	186	1		

- Molecule 75 is a protein called Ribosome-associated protein oga1.

Mol	Chain	Residues	Atoms				AltConf	Trace
75	H1	100	Total	C	N	O	0	0
			758	449	148	161		

- Molecule 76 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	HE	842	Total	C	N	O	S	0	0
			6544	4134	1132	1239	39		

- Molecule 77 is a protein called Large ribosomal subunit protein uL1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	HL	216	Total	C	N	O	S	0	0
			1679	1072	297	302	8		

- Molecule 78 is a protein called SDO1-like protein C21C3.19.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	HS	106	Total	C	N	O	S	0	0
			834	517	147	167	3		

- Molecule 79 is a protein called Eukaryotic translation initiation factor 5A-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	HI	138	Total	C	N	O	S	0	0
			1067	658	187	213	9		

- Molecule 80 is a protein called Large ribosomal subunit protein eL40A.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	BA	51	Total	C	N	O	S	0	0
			413	257	84	67	5		

- Molecule 81 is a protein called Large ribosomal subunit protein uL6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	BU	184	Total	C	N	O	S	0	0
			1461	922	267	267	5		

- Molecule 82 is a protein called Large ribosomal subunit protein uL22A.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Bb	152	Total	C	N	O	S	0	0
			1212	770	229	210	3		

- Molecule 83 is a protein called Large ribosomal subunit protein uL22A.

Mol	Chain	Residues	Atoms				AltConf	Trace
83	A	20	Total	C	N	O	0	0
			149	90	34	25		

- Molecule 84 is ZINC ION (CCD ID: ZN) (formula: Zn).

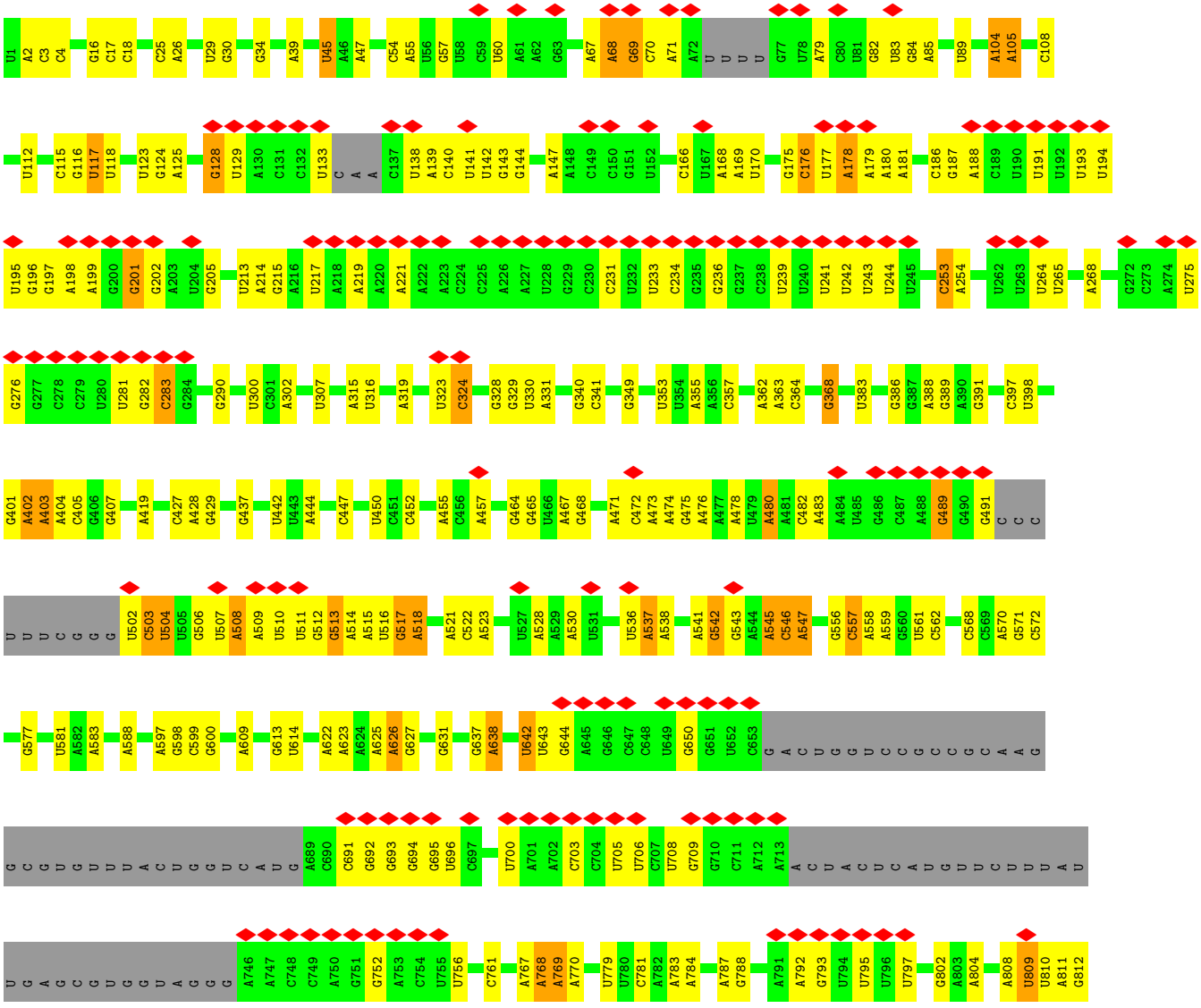
Mol	Chain	Residues	Atoms	AltConf
84	Ag	1	Total Zn 1 1	0
84	Ah	1	Total Zn 1 1	0
84	Aj	1	Total Zn 1 1	0
84	B0	1	Total Zn 1 1	0
84	B1	1	Total Zn 1 1	0
84	Bv	1	Total Zn 1 1	0

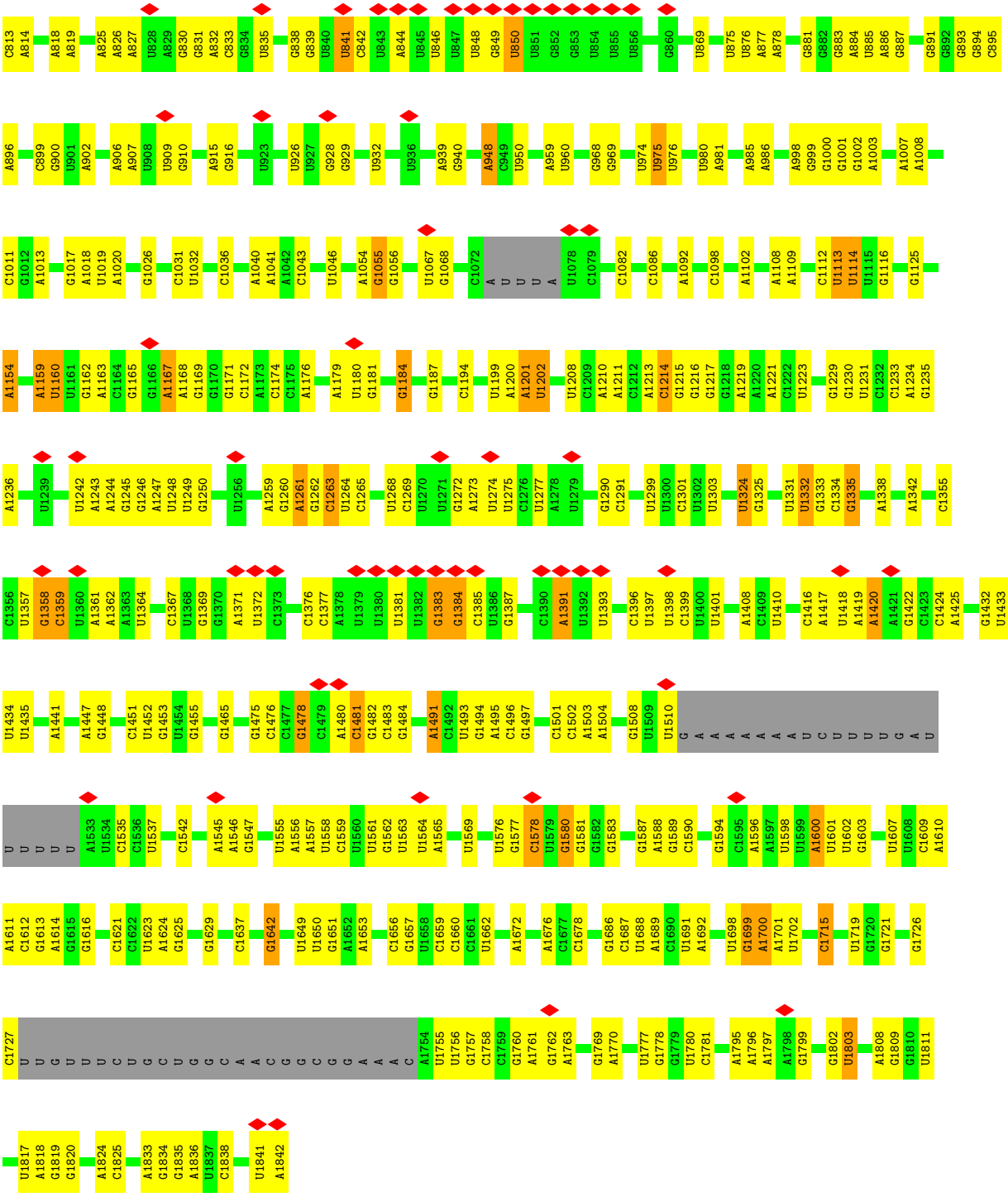
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: 18S small subunit ribosomal RNA

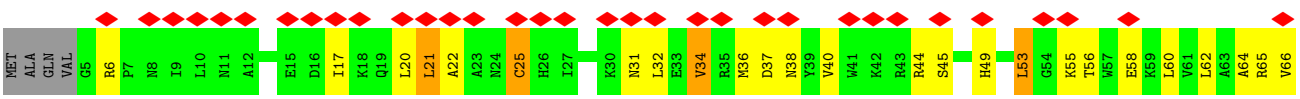
Chain AA:

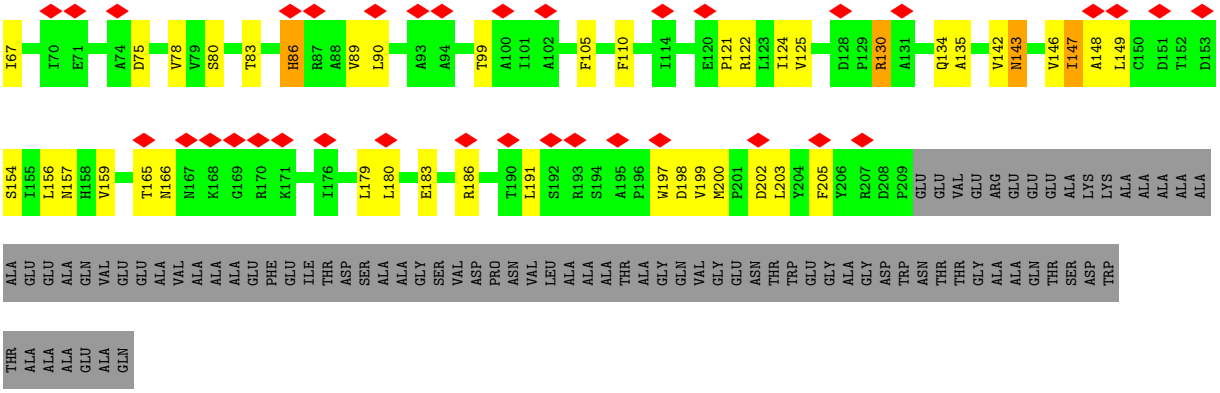




• Molecule 2: Small ribosomal subunit protein uS2A

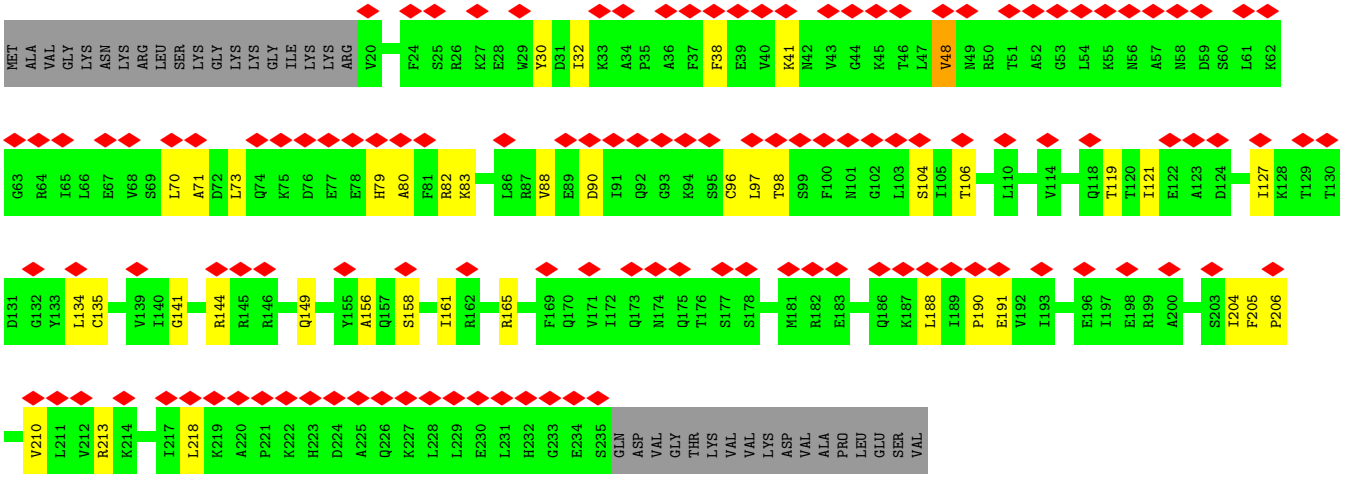
Chain AD:





• Molecule 3: Small ribosomal subunit protein eS1B

Chain AE:

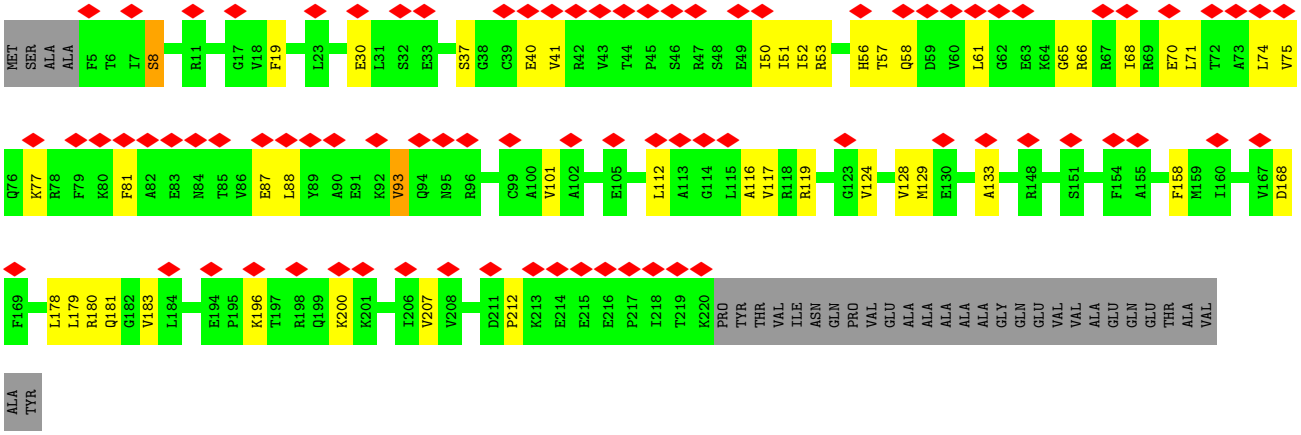


• Molecule 4: Small ribosomal subunit protein uS5

Chain AF:

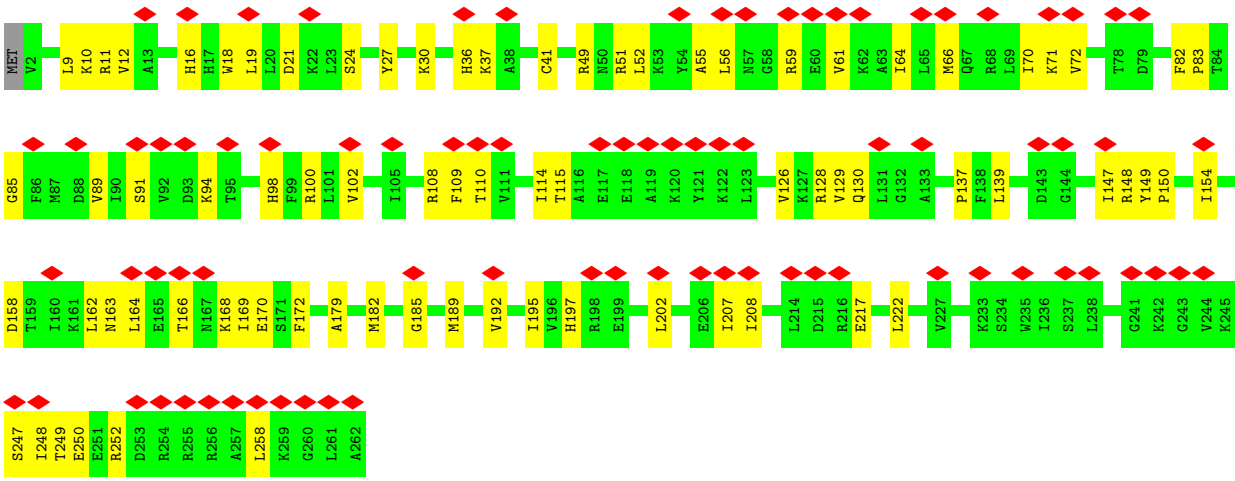
• Molecule 5: Small ribosomal subunit protein uS3

Chain AG:



• Molecule 6: Small ribosomal subunit protein eS4C

Chain AH:

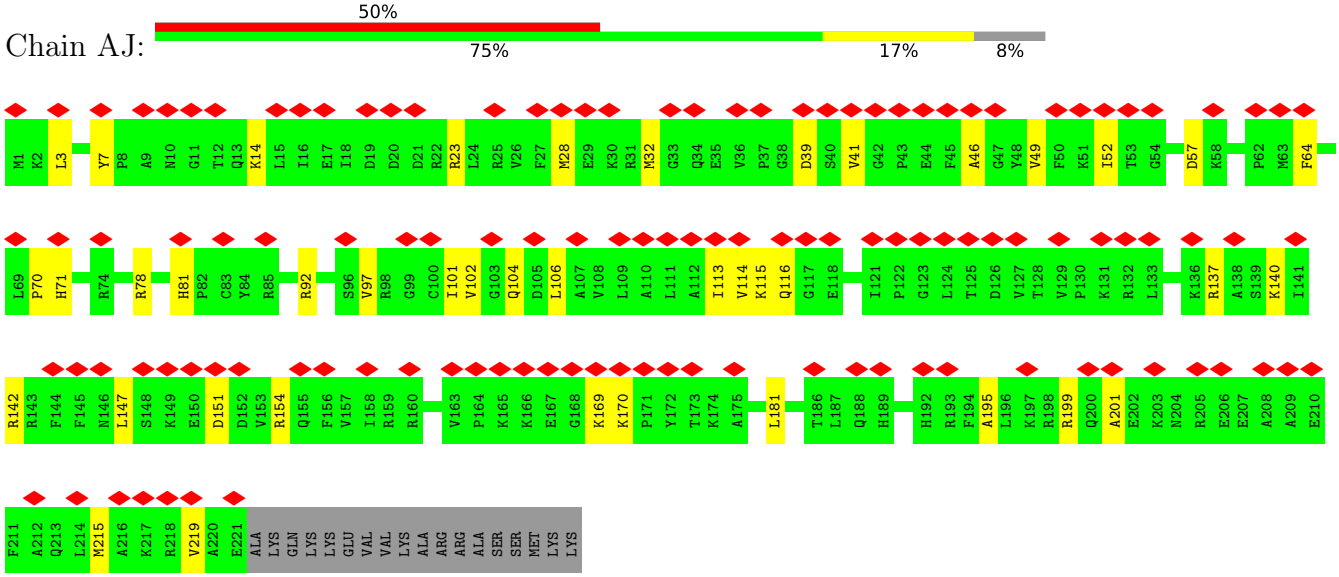


• Molecule 7: Small ribosomal subunit protein uS7A

Chain AI:

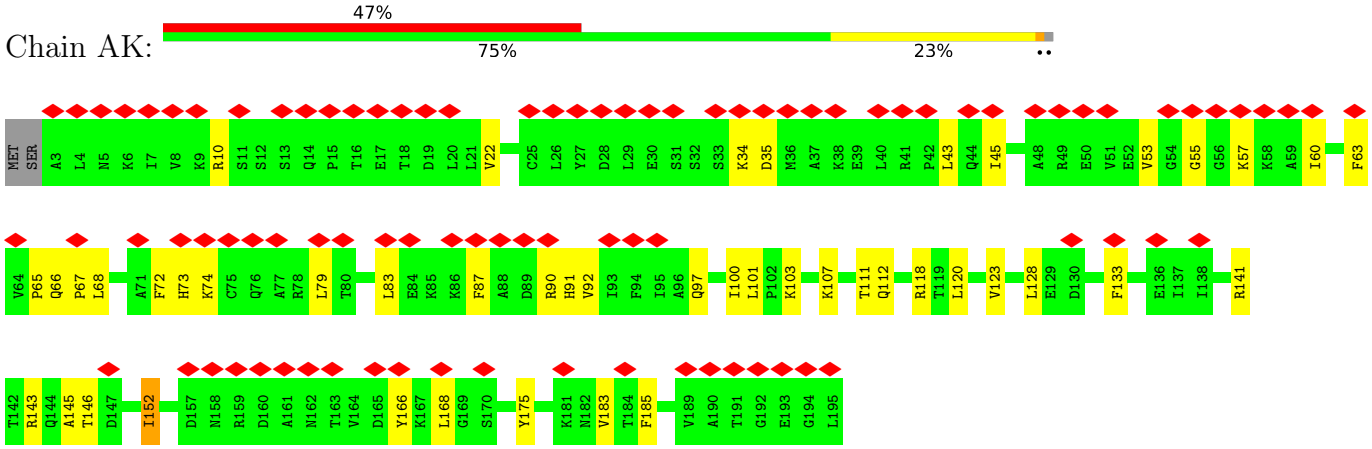
• Molecule 8: Small ribosomal subunit protein eS6B

Chain AJ:



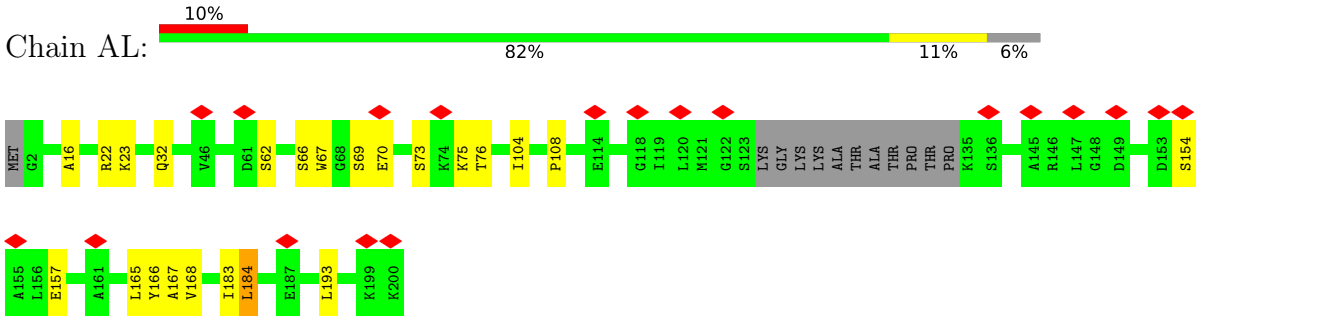
• Molecule 9: Small ribosomal subunit protein eS7

Chain AK:



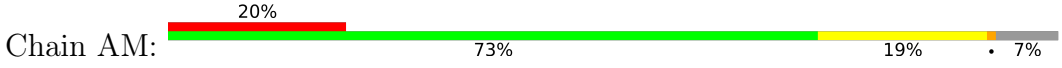
• Molecule 10: Small ribosomal subunit protein eS8B

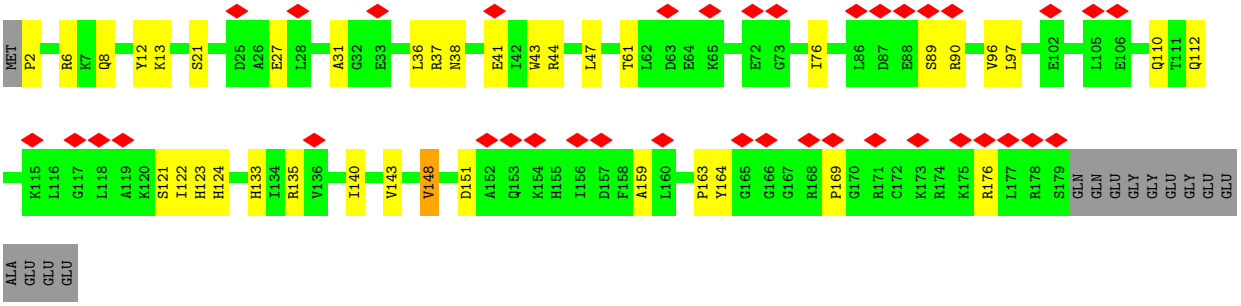
Chain AL:



• Molecule 11: Small ribosomal subunit protein uS4B

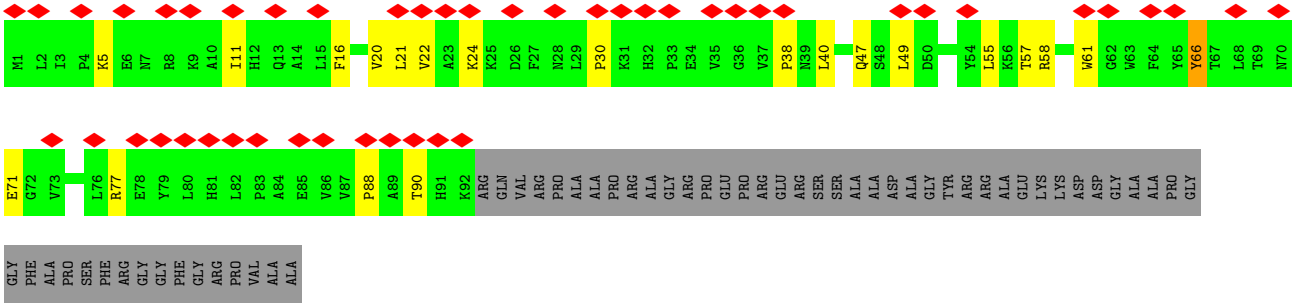
Chain AM:





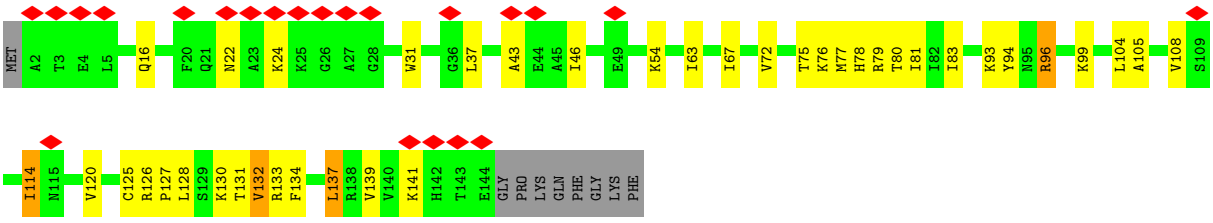
• Molecule 12: Small ribosomal subunit protein eS10B

Chain AN:



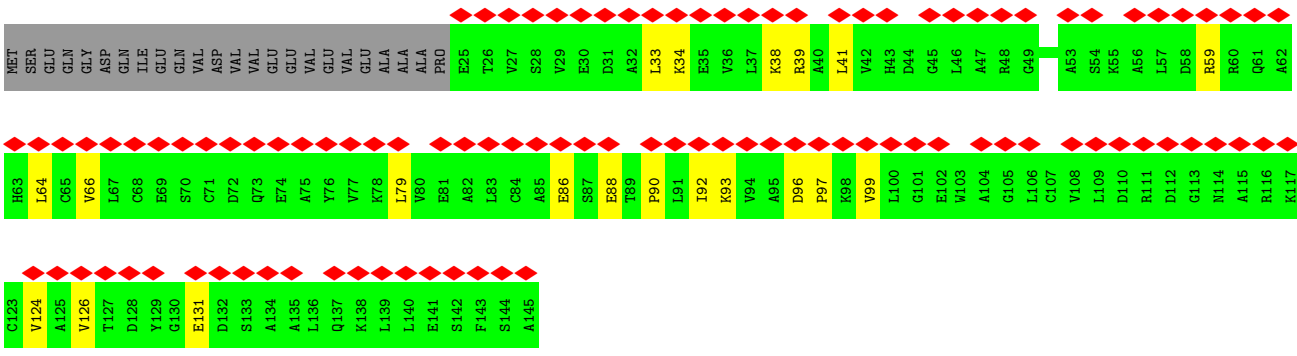
• Molecule 13: Small ribosomal subunit protein uS17A

Chain AO:



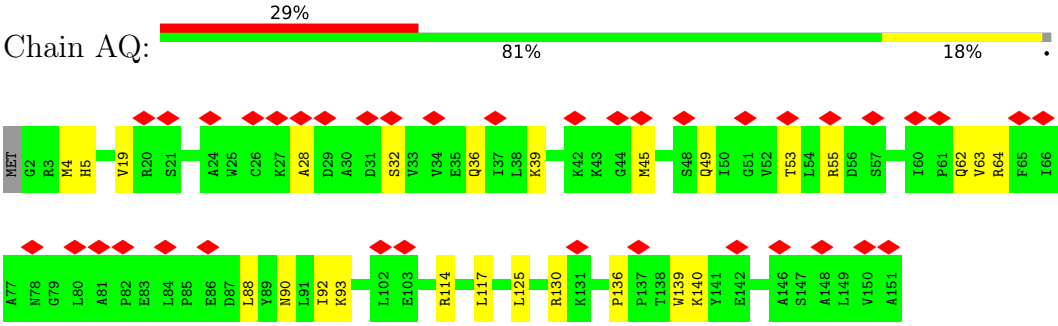
• Molecule 14: Small ribosomal subunit protein eS12A

Chain AP:



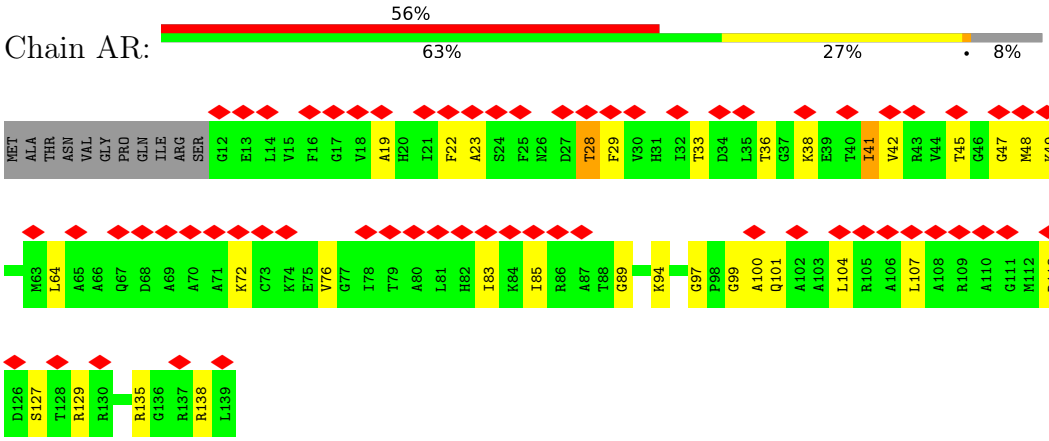
• Molecule 15: Small ribosomal subunit protein uS15

Chain AQ:



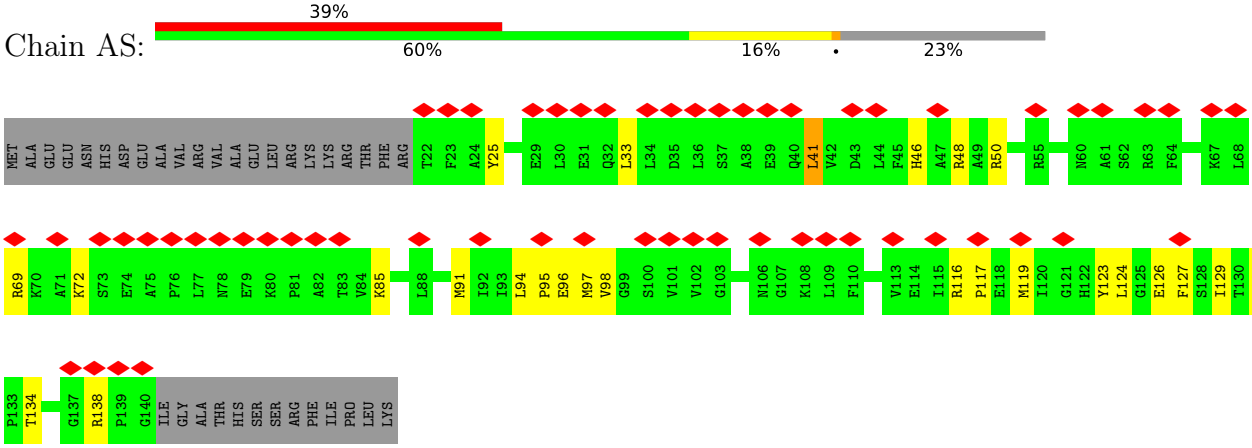
• Molecule 16: Small ribosomal subunit protein uS11A

Chain AR:



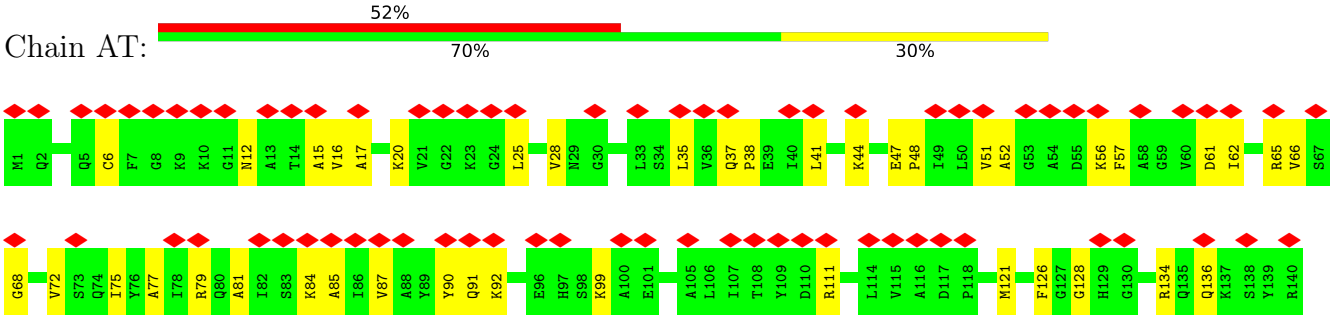
• Molecule 17: Small ribosomal subunit protein uS19B

Chain AS:



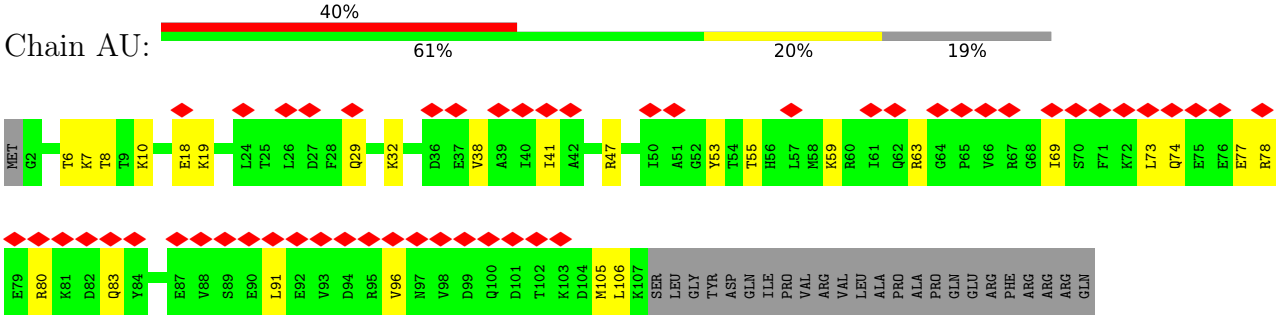
• Molecule 18: Small ribosomal subunit protein uS9A

Chain AT:



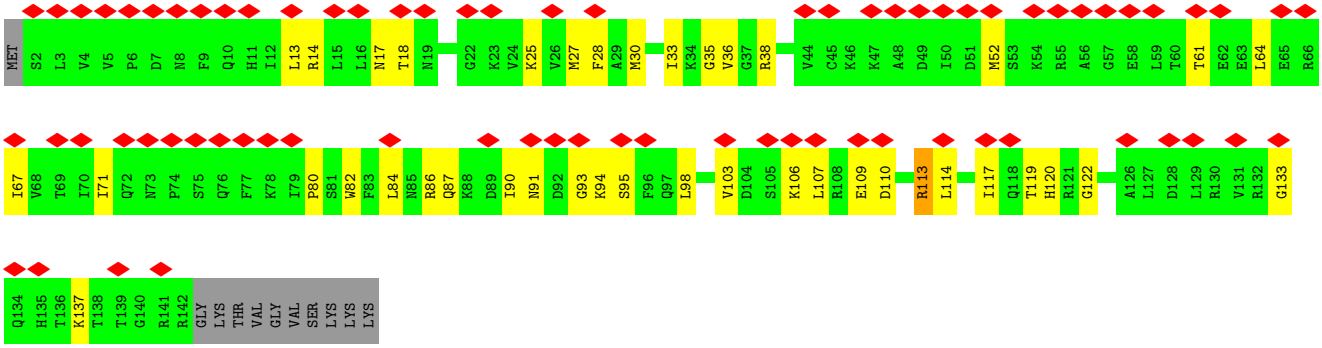
• Molecule 19: Small ribosomal subunit protein eS17A

Chain AU:



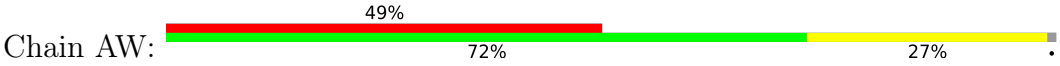
• Molecule 20: Small ribosomal subunit protein uS13A

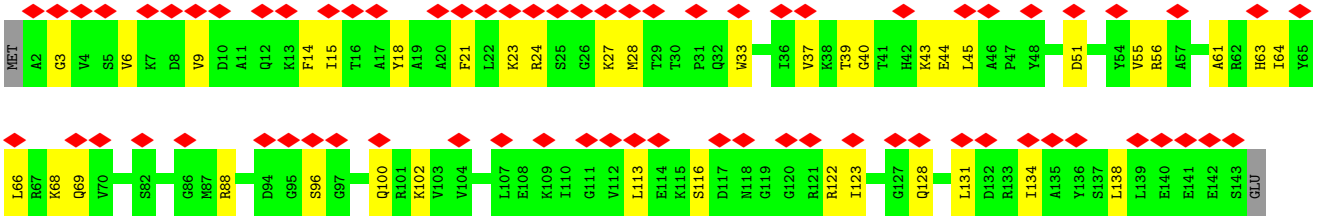
Chain AV:



• Molecule 21: Small ribosomal subunit protein eS19A

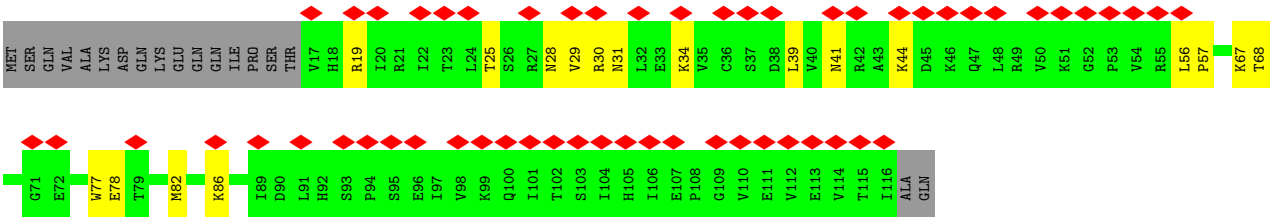
Chain AW:





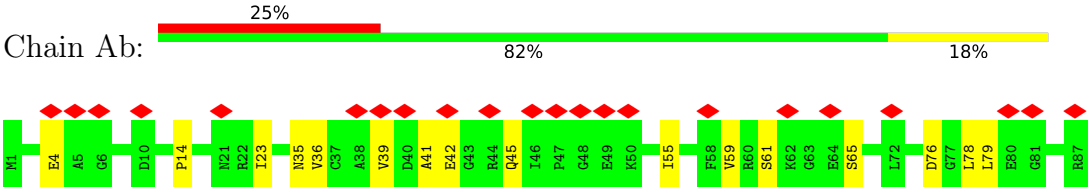
• Molecule 22: Small ribosomal subunit protein uS10

Chain Aa:



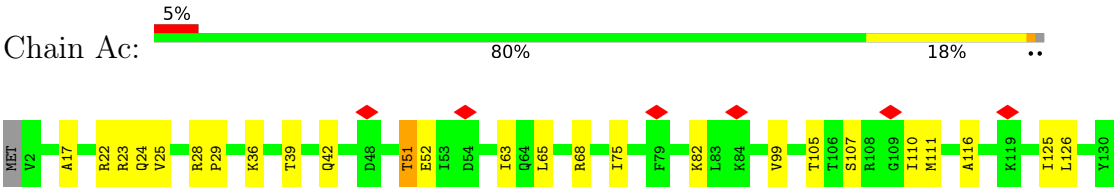
• Molecule 23: Small ribosomal subunit protein eS21

Chain Ab:



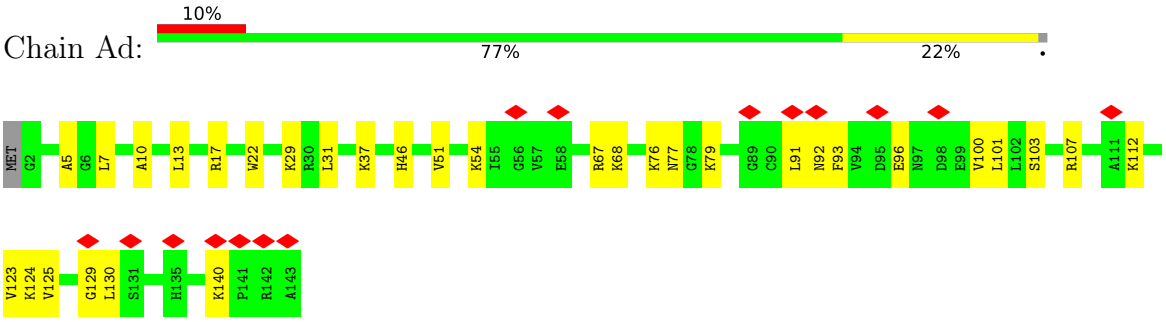
• Molecule 24: Small ribosomal subunit protein uS8A

Chain Ac:



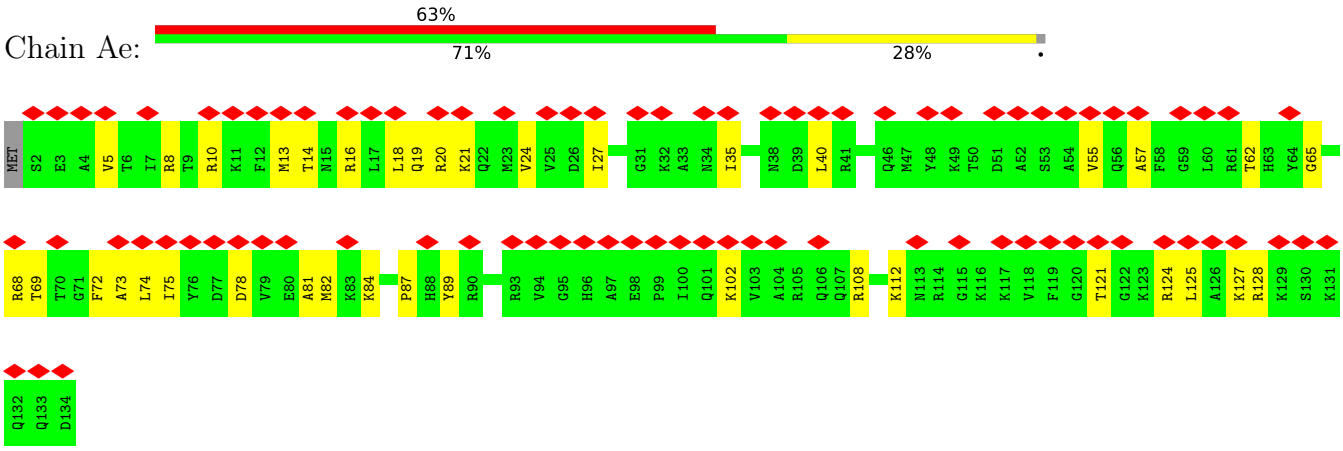
• Molecule 25: Small ribosomal subunit protein uS12A

Chain Ad:



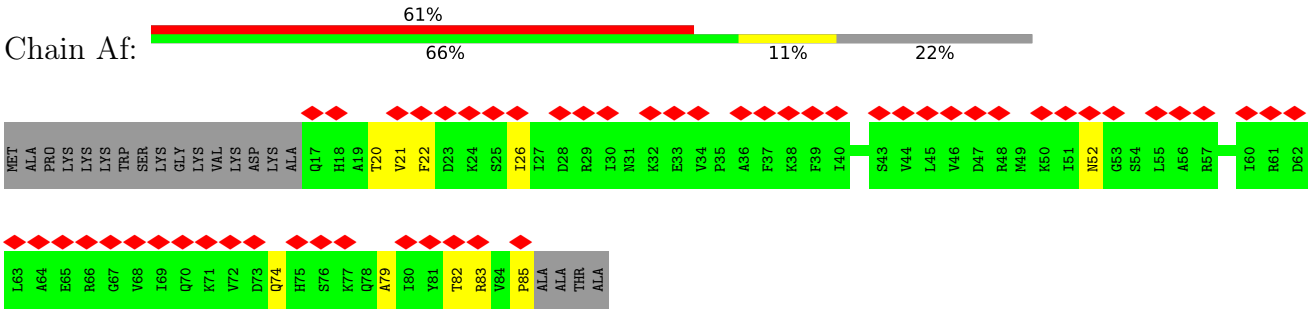
• Molecule 26: Small ribosomal subunit protein eS24A

Chain Ae:



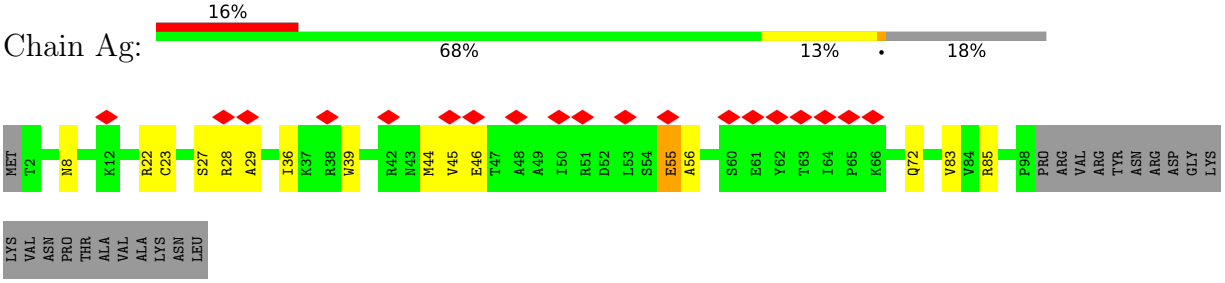
• Molecule 27: Small ribosomal subunit protein eS25A

Chain Af:



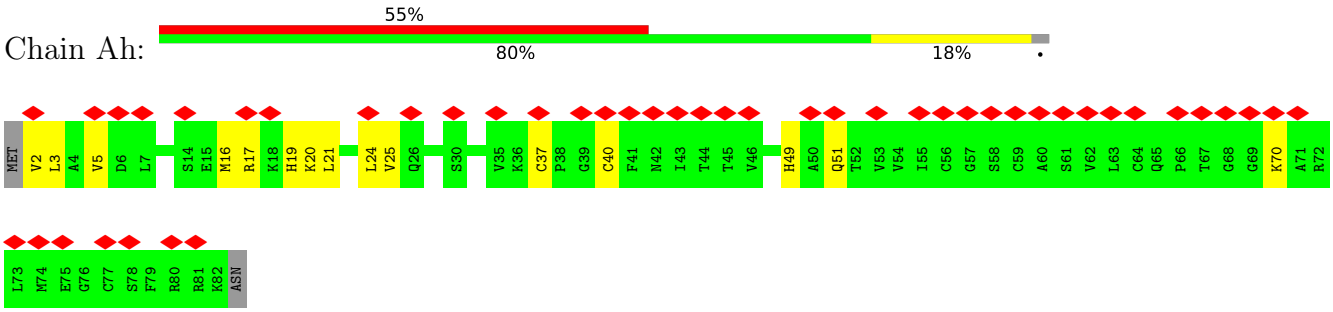
• Molecule 28: Small ribosomal subunit protein eS26B

Chain Ag:



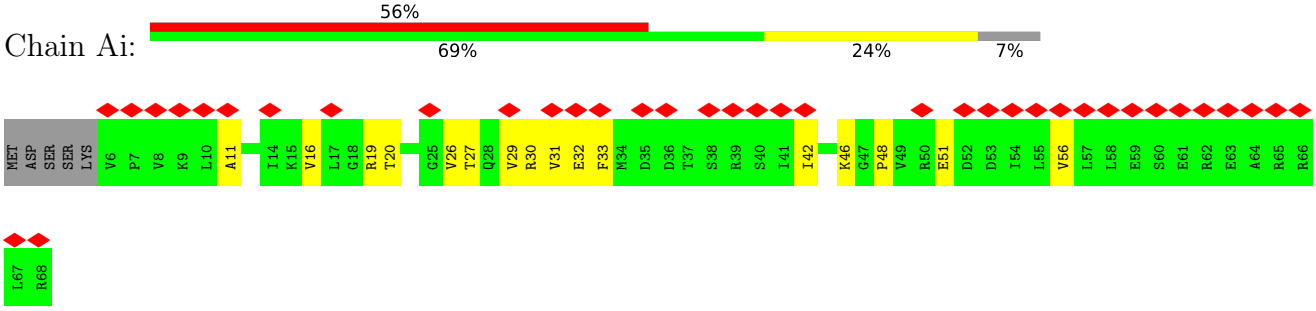
• Molecule 29: Small ribosomal subunit protein eS27

Chain Ah:



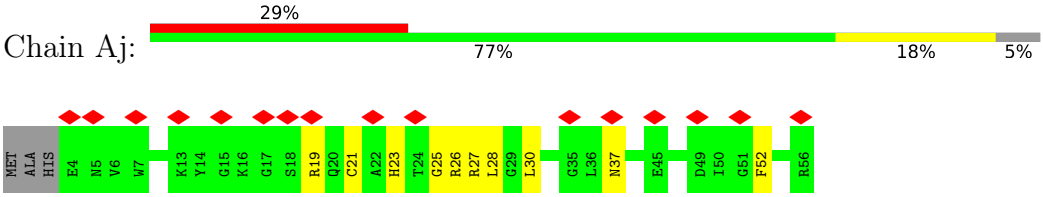
• Molecule 30: Small ribosomal subunit protein eS28A

Chain Ai:



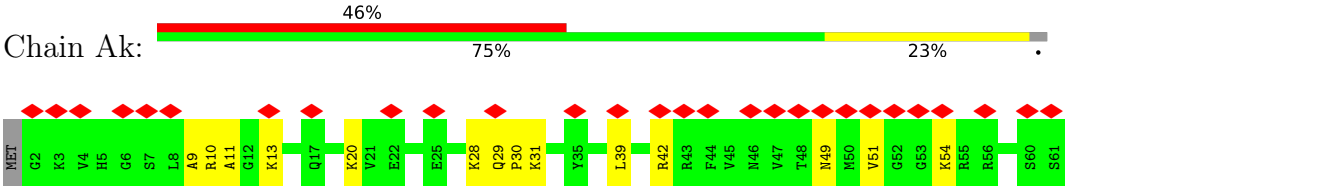
• Molecule 31: Small ribosomal subunit protein uS14

Chain Aj:



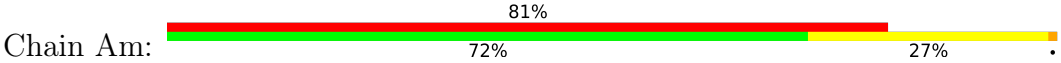
• Molecule 32: Small ribosomal subunit protein eS30A

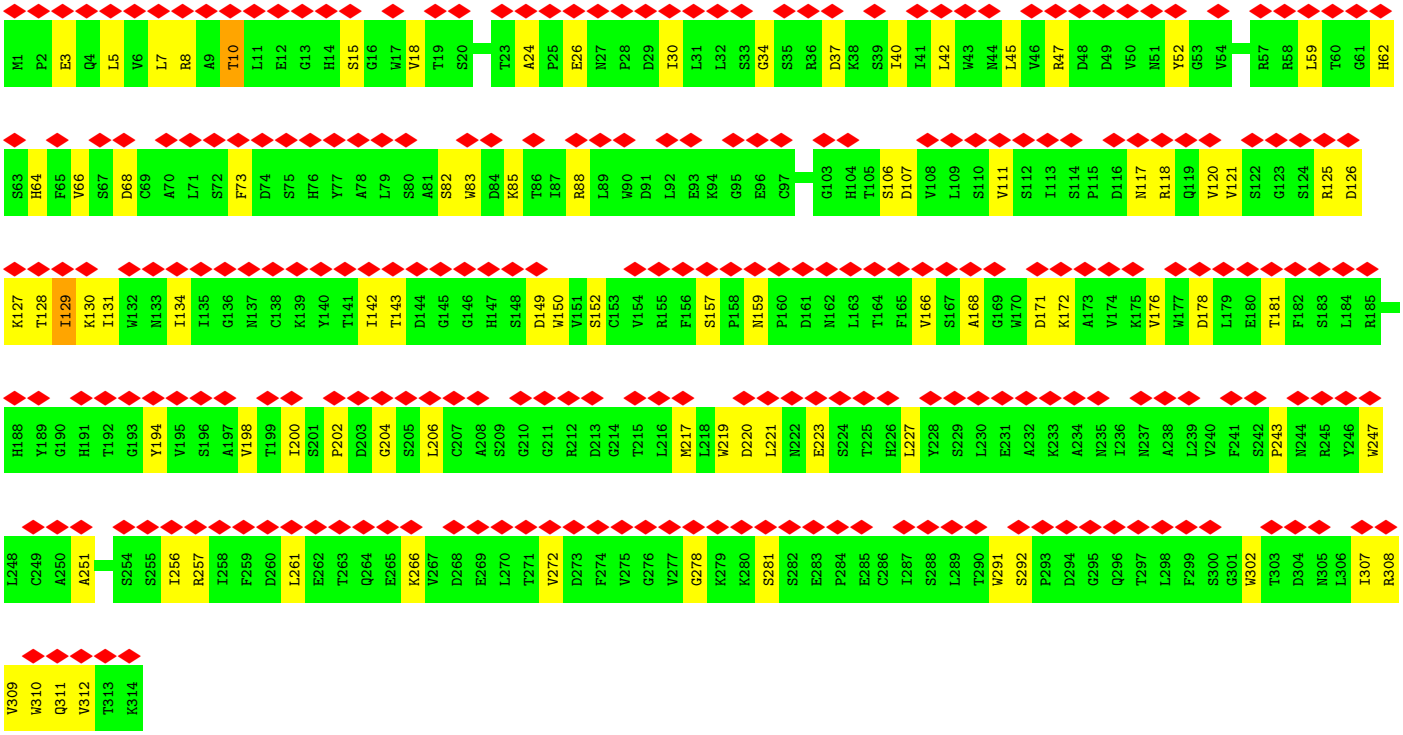
Chain Ak:



• Molecule 33: Small ribosomal subunit protein RACK1

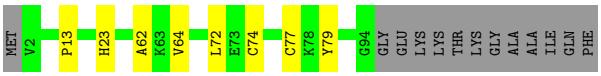
Chain Am:





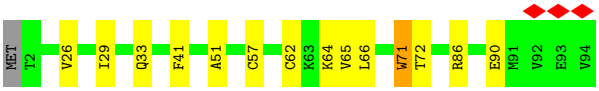
• Molecule 34: Large ribosomal subunit protein eL42

Chain B0:



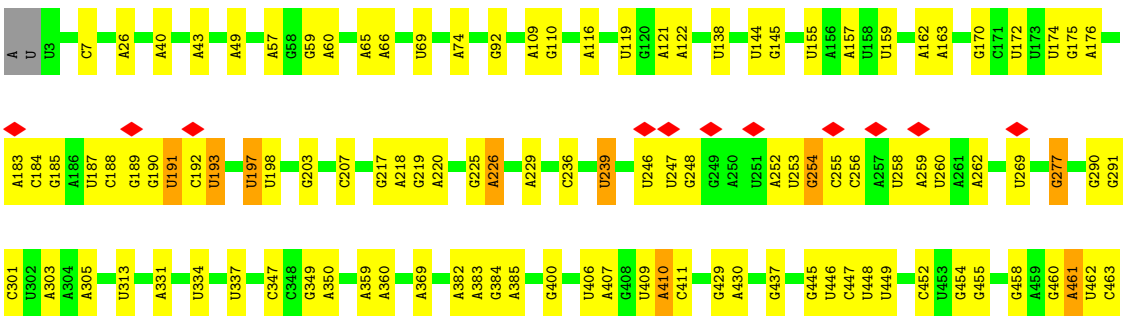
• Molecule 35: Large ribosomal subunit protein eL43A

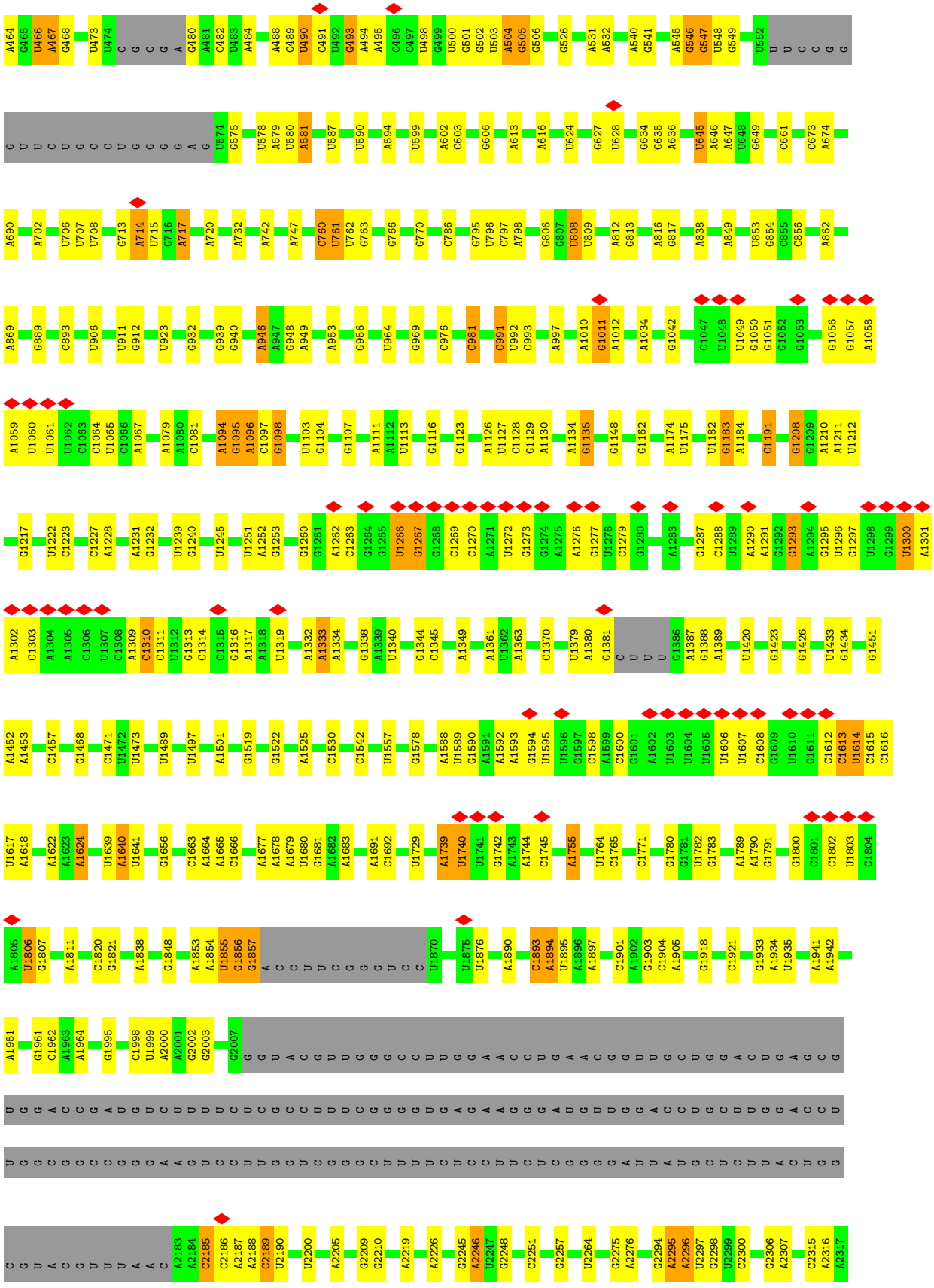
Chain B1:

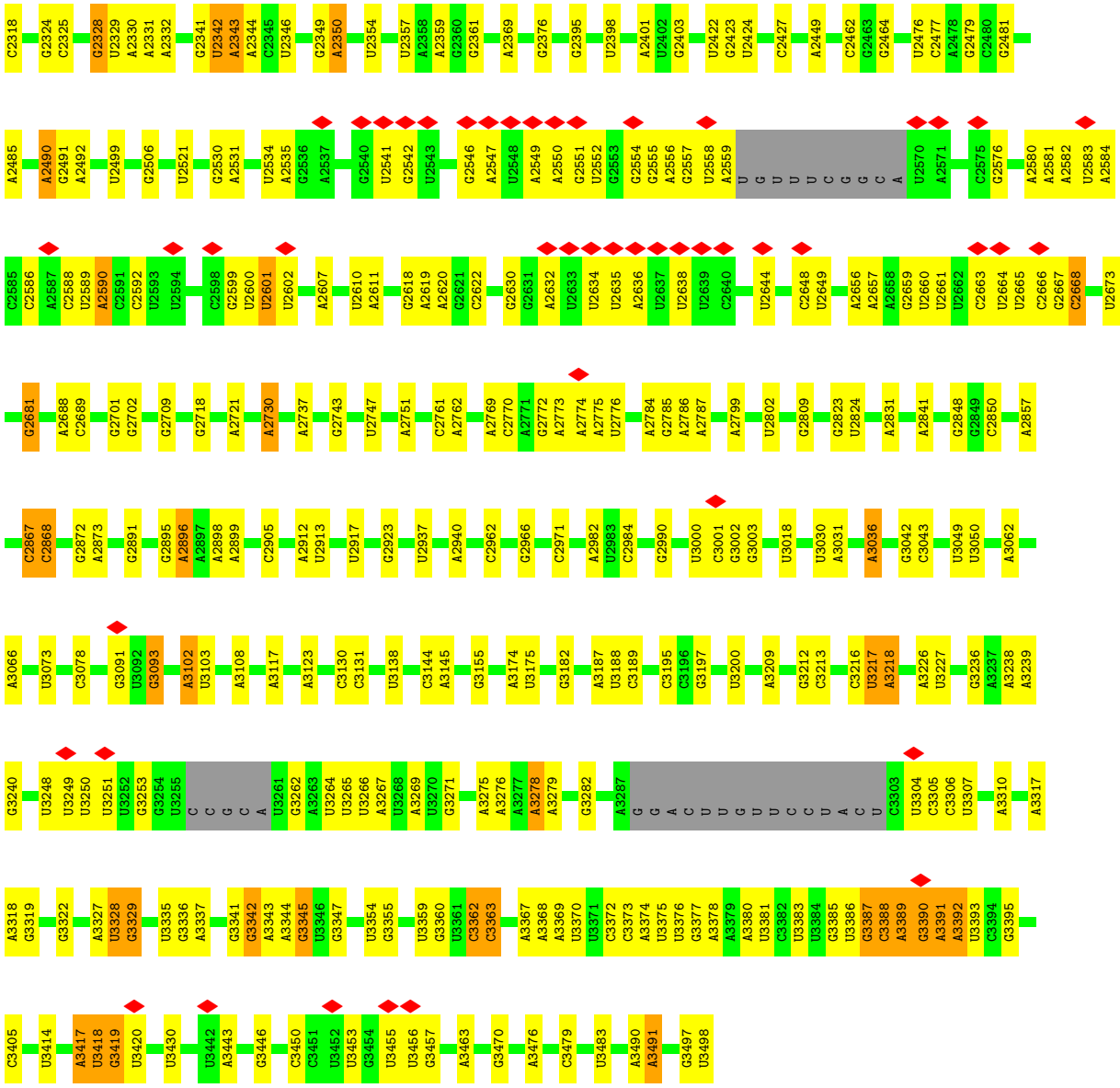


• Molecule 36: 28S large subunit ribosomal RNA

Chain B2:

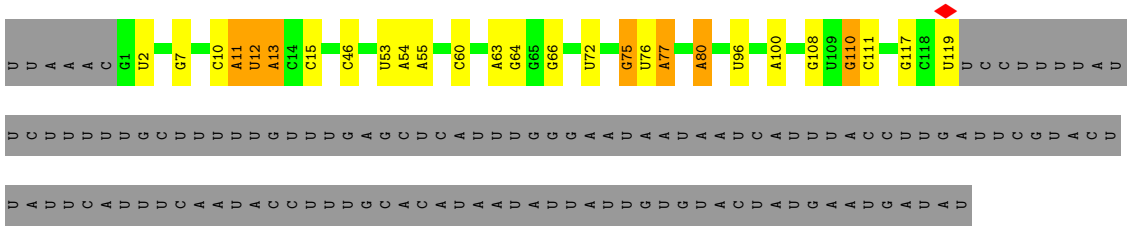






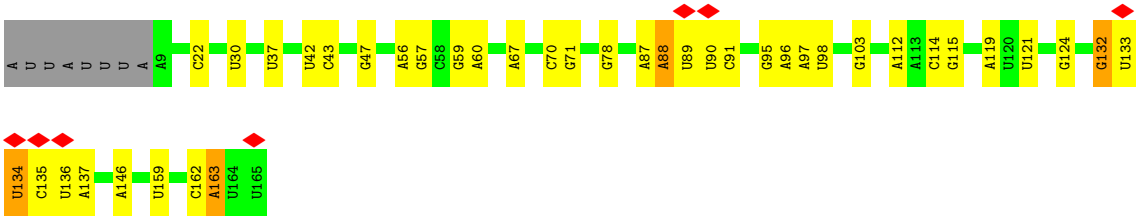
• Molecule 37: 5S large subunit ribosomal RNA

Chain B3:



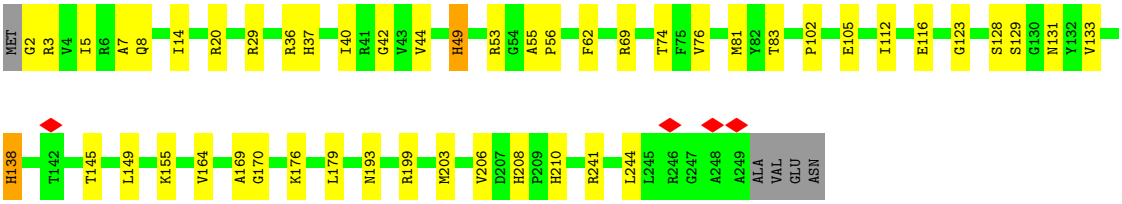
• Molecule 38: 5.8S large subunit ribosomal RNA

Chain B4:



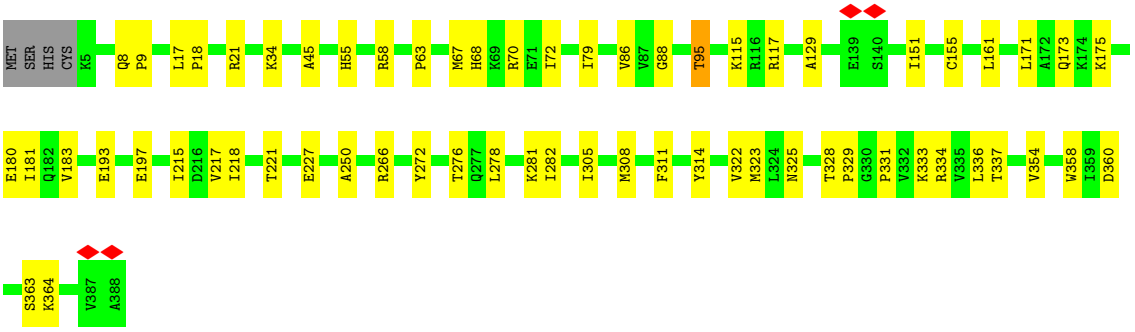
• Molecule 39: Large ribosomal subunit protein uL2A

Chain BN:



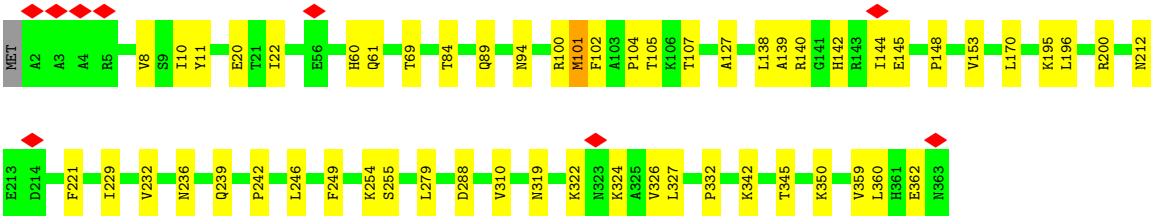
• Molecule 40: Large ribosomal subunit protein uL3A

Chain BO:



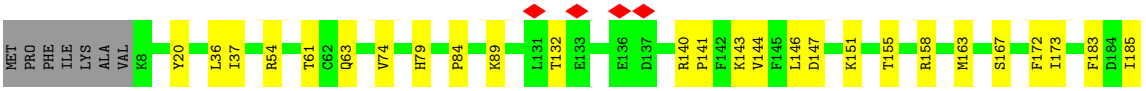
• Molecule 41: Large ribosomal subunit protein uL4A

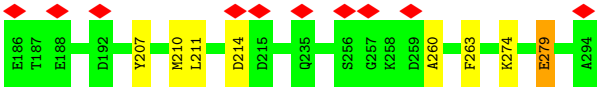
Chain BP:



• Molecule 42: Large ribosomal subunit protein uL18B

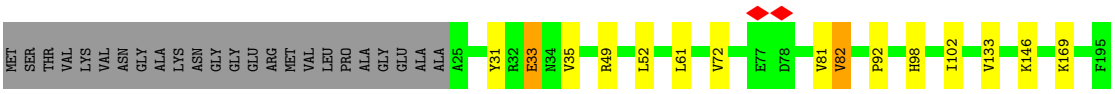
Chain BQ:





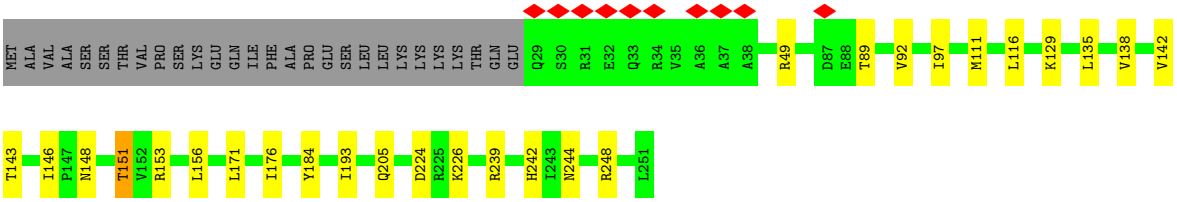
• Molecule 43: Large ribosomal subunit protein eL6

Chain BR:



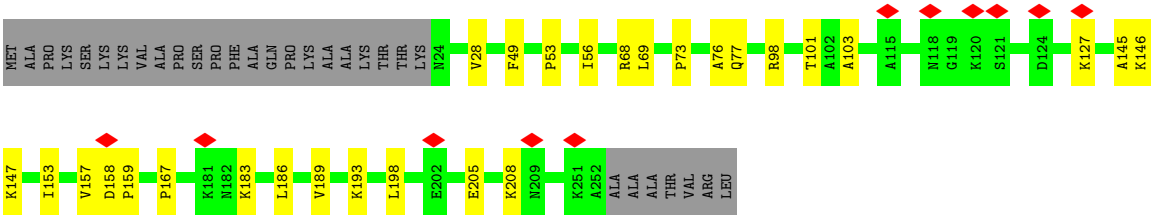
• Molecule 44: Large ribosomal subunit protein uL30C

Chain BS:



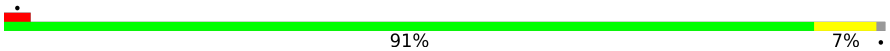
• Molecule 45: Large ribosomal subunit protein eL8

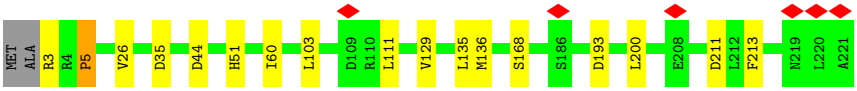
Chain BT:



• Molecule 46: Large ribosomal subunit protein uL16A

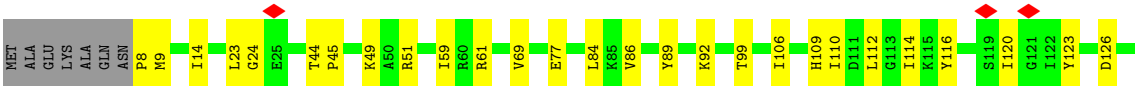
Chain BV:

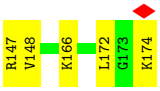




• Molecule 47: Large ribosomal subunit protein uL5A

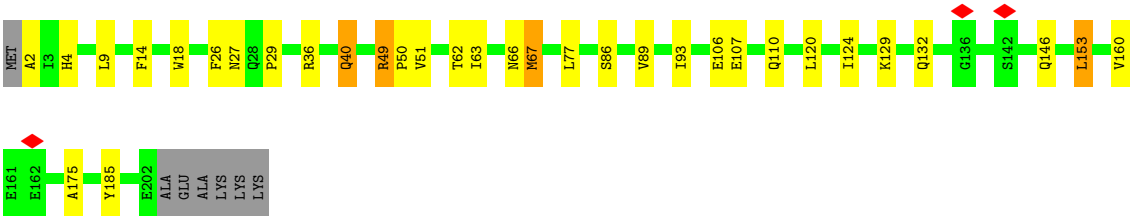
Chain BW:





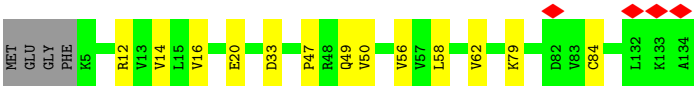
• Molecule 48: Large ribosomal subunit protein eL13

Chain BX:



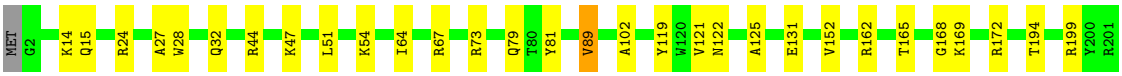
• Molecule 49: Large ribosomal subunit protein eL14

Chain BY:



• Molecule 50: Large ribosomal subunit protein eL15B

Chain BZ:

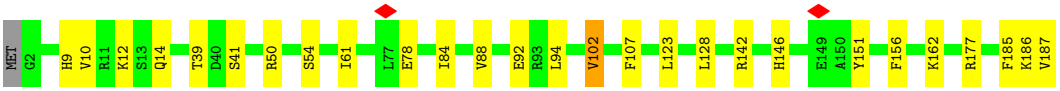


• Molecule 51: Large ribosomal subunit protein uL13A

Chain Ba:

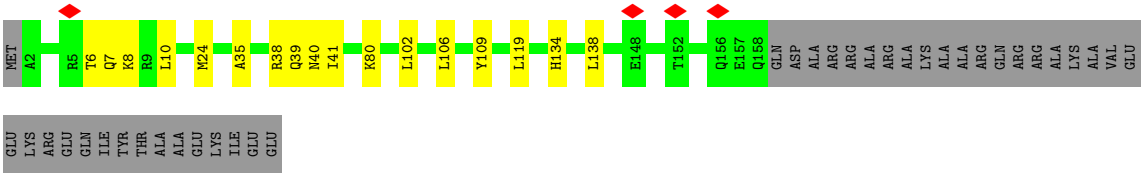
• Molecule 52: Large ribosomal subunit protein eL18B

Chain Bc:

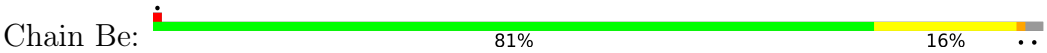


• Molecule 53: Large ribosomal subunit protein eL19B

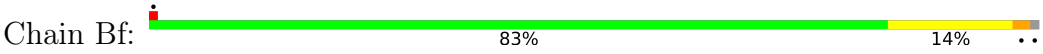
Chain Bd:

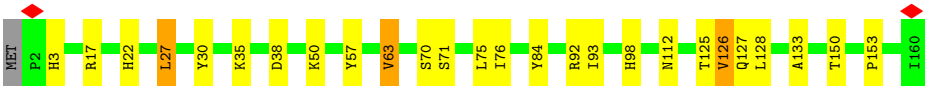


• Molecule 54: Large ribosomal subunit protein eL20A

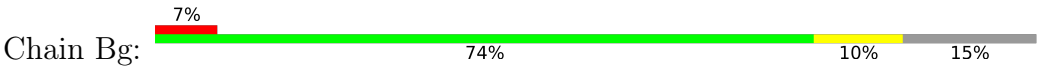


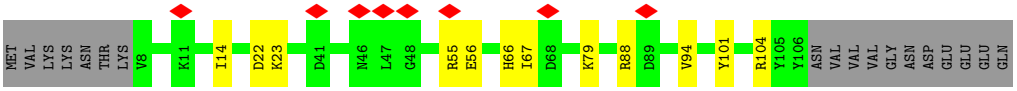
• Molecule 55: Large ribosomal subunit protein eL21B



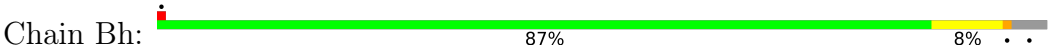


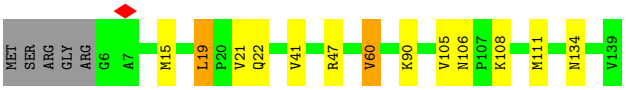
• Molecule 56: Large ribosomal subunit protein eL22



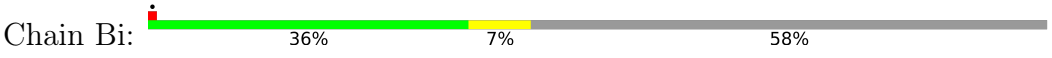


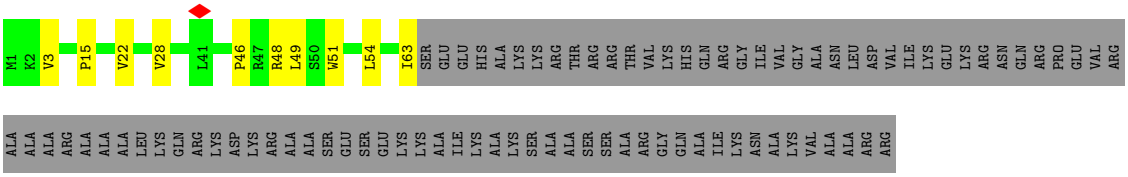
• Molecule 57: Large ribosomal subunit protein uL14A



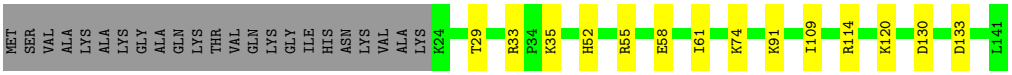


• Molecule 58: Large ribosomal subunit protein eL24B



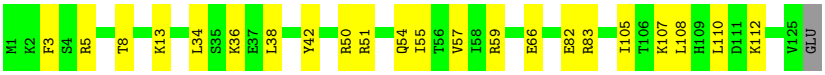


• Molecule 59: Large ribosomal subunit protein uL23A



• Molecule 60: Large ribosomal subunit protein uL24

Chain Bk:

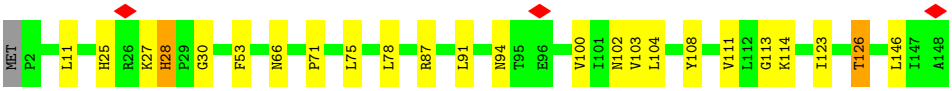


• Molecule 61: Large ribosomal subunit protein eL27A

Chain Bl:

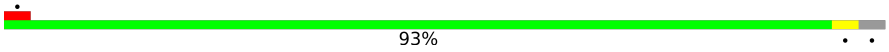
• Molecule 62: Large ribosomal subunit protein uL15B

Chain Bm:



• Molecule 63: Large ribosomal subunit protein eL29

Chain Bn:

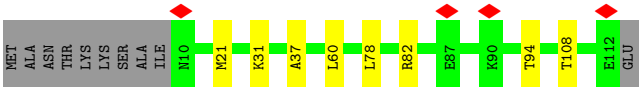


• Molecule 64: Large ribosomal subunit protein eL30A

Chain Bo:

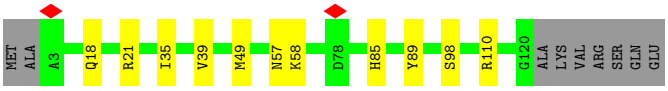
• Molecule 65: Large ribosomal subunit protein eL31

Chain Bp:



• Molecule 66: Large ribosomal subunit protein eL32A

Chain Bq:

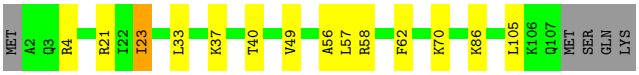


• Molecule 67: Large ribosomal subunit protein eL33A

Chain Br:

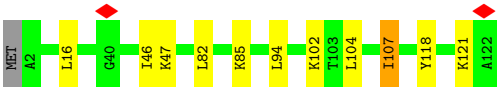
• Molecule 68: Large ribosomal subunit protein eL34B

Chain Bs:



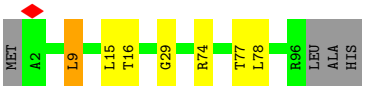
• Molecule 69: Large ribosomal subunit protein uL29

Chain Bt:



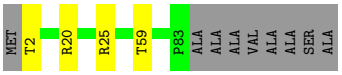
• Molecule 70: Large ribosomal subunit protein eL36B

Chain Bu:



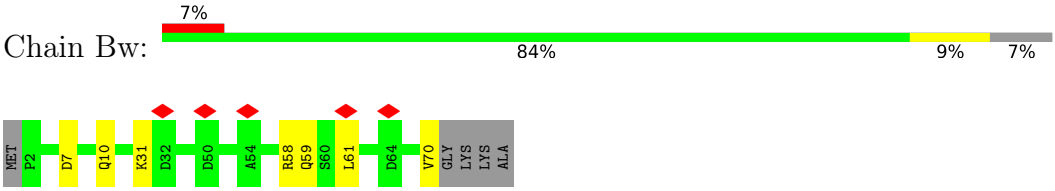
• Molecule 71: Large ribosomal subunit protein eL37B

Chain Bv:



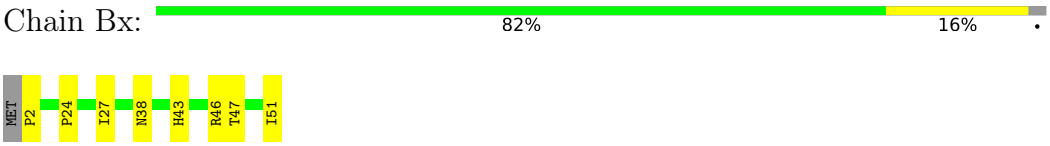
• Molecule 72: Large ribosomal subunit protein eL38A

Chain Bw:



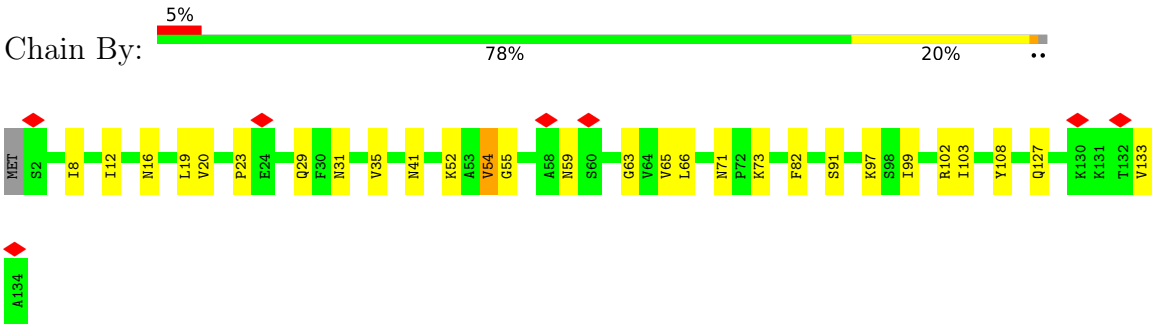
• Molecule 73: Large ribosomal subunit protein eL39

Chain Bx:



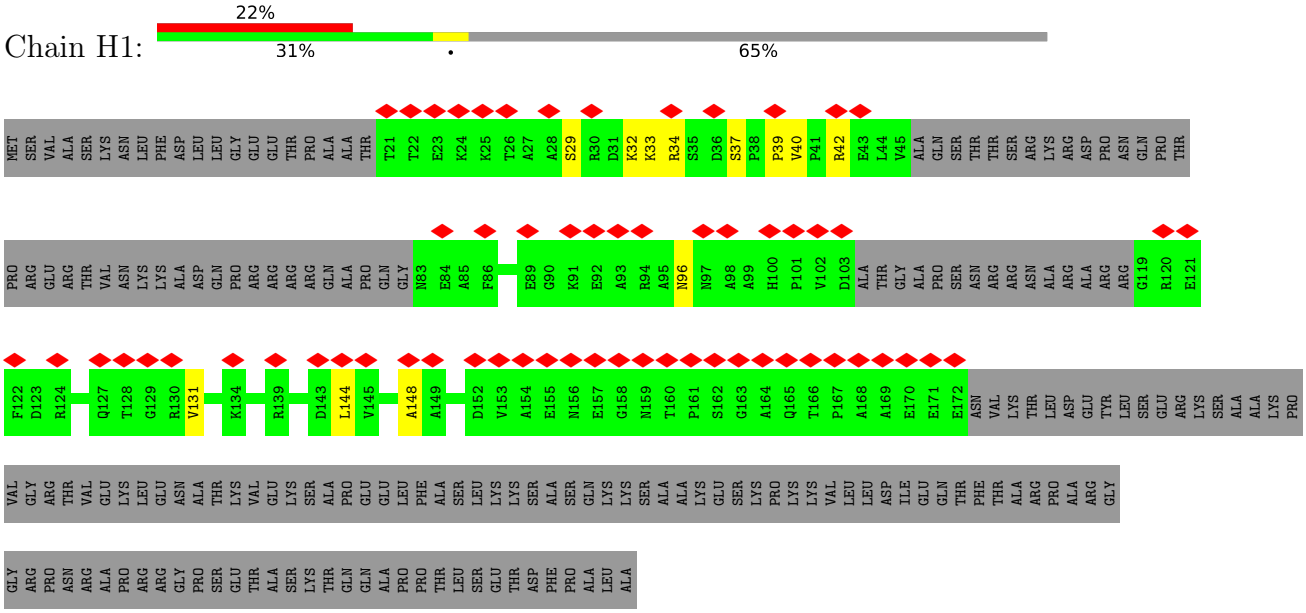
• Molecule 74: Large ribosomal subunit protein eL28

Chain By:



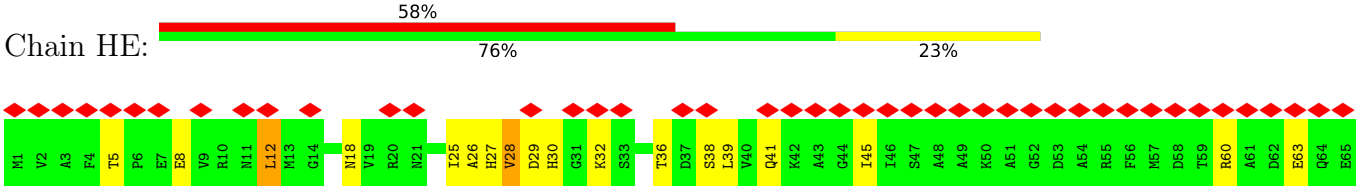
• Molecule 75: Ribosome-associated protein oga1

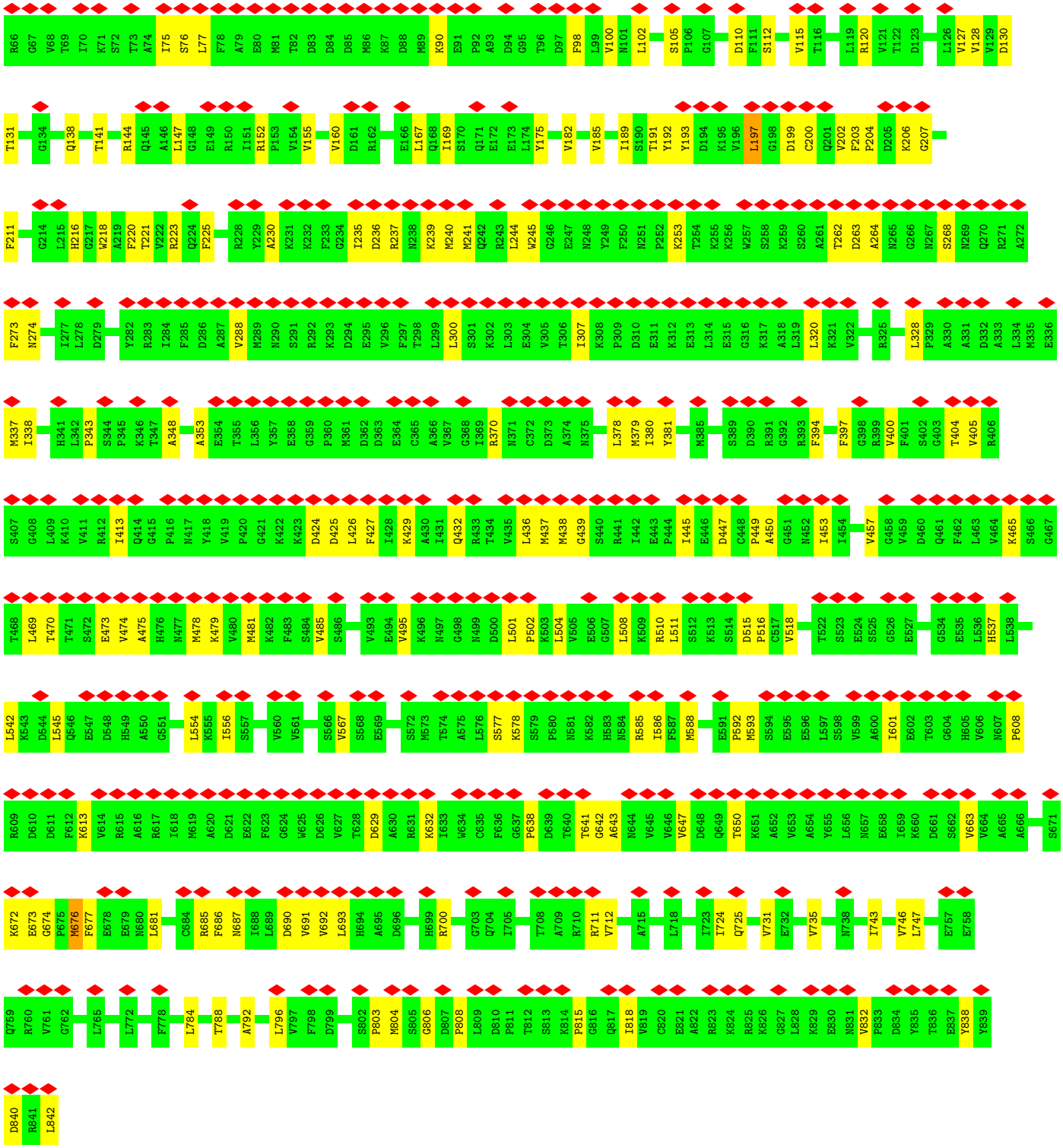
Chain H1:



• Molecule 76: Elongation factor 2

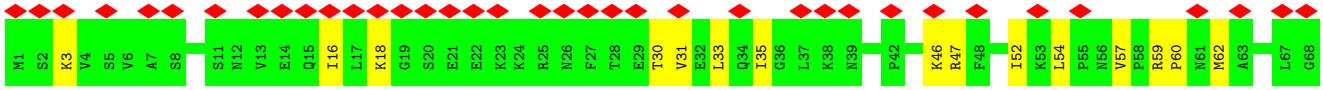
Chain HE:

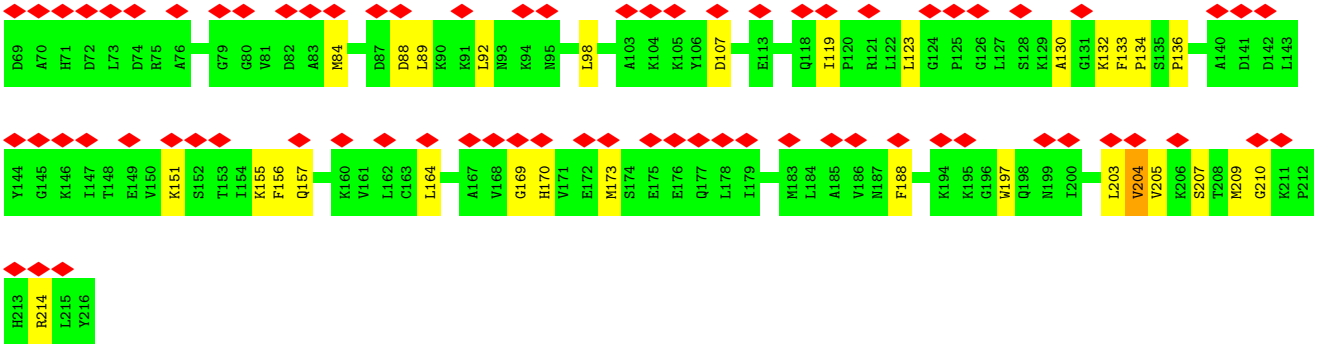




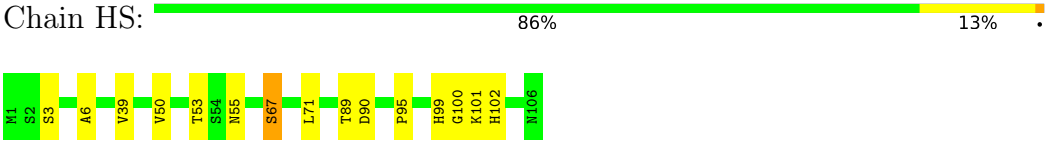
• Molecule 77: Large ribosomal subunit protein uL1B

Chain HL:

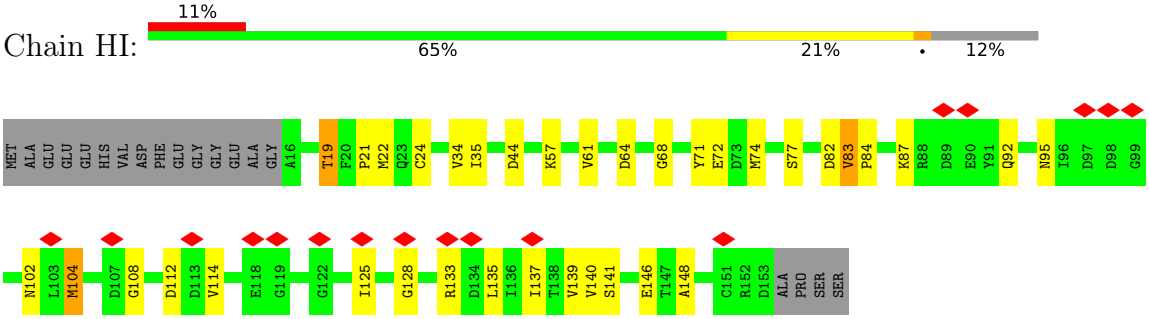




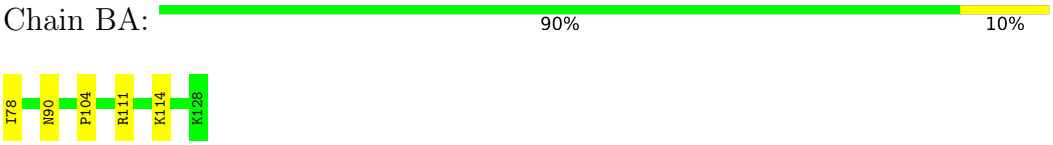
• Molecule 78: SDO1-like protein C21C3.19



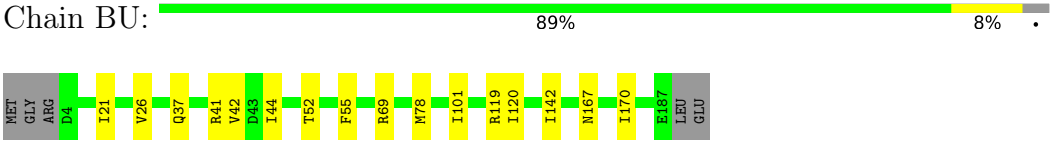
• Molecule 79: Eukaryotic translation initiation factor 5A-1



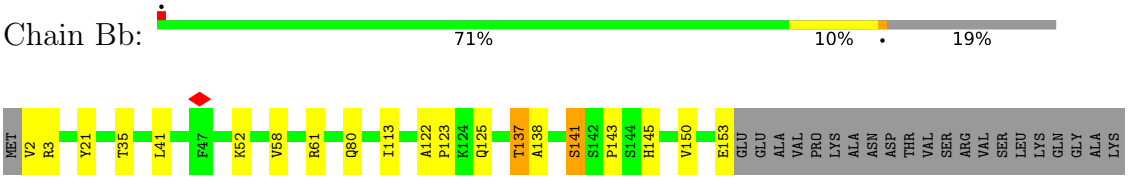
• Molecule 80: Large ribosomal subunit protein eL40A



• Molecule 81: Large ribosomal subunit protein uL6B



• Molecule 82: Large ribosomal subunit protein uL22A



• Molecule 83: Large ribosomal subunit protein uL22A

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	88206	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; 3D CTF Estimation done in Warp	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	140	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	81000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.004	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.000494	Depositor
Map size (Å)	585.8, 585.8, 585.8	wwPDB
Map dimensions	580, 580, 580	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.01, 1.01, 1.01	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 5CT

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	AA	0.06	0/40670	0.14	0/63362
2	AD	0.14	0/1635	0.44	0/2228
3	AE	0.08	0/1756	0.25	0/2358
4	AF	0.10	0/1695	0.29	0/2297
5	AG	0.11	0/1726	0.30	0/2316
6	AH	0.11	0/2125	0.33	0/2858
7	AI	0.12	0/1577	0.37	0/2123
8	AJ	0.08	0/1815	0.25	0/2428
9	AK	0.09	0/1554	0.28	0/2091
10	AL	0.08	0/1534	0.23	0/2050
11	AM	0.10	0/1487	0.30	0/1990
12	AN	0.11	0/769	0.33	0/1043
13	AO	0.09	0/1190	0.30	0/1602
14	AP	0.10	0/892	0.30	0/1208
15	AQ	0.12	0/1208	0.26	0/1624
16	AR	0.07	0/961	0.24	0/1293
17	AS	0.10	0/973	0.30	0/1307
18	AT	0.11	0/1100	0.35	0/1474
19	AU	0.12	0/888	0.39	0/1188
20	AV	0.18	0/1158	0.41	0/1552
21	AW	0.11	0/1139	0.28	0/1531
22	Aa	0.08	0/821	0.23	0/1107
23	Ab	0.09	0/680	0.24	0/918
24	Ac	0.14	0/1042	0.36	0/1399
25	Ad	0.11	0/1115	0.28	0/1489
26	Ae	0.11	0/1093	0.30	0/1453
27	Af	0.09	0/558	0.27	0/750
28	Ag	0.11	0/808	0.33	0/1083
29	Ah	0.07	0/630	0.20	0/845
30	Ai	0.21	0/500	0.44	0/669
31	Aj	0.08	0/458	0.24	0/610
32	Ak	0.13	0/482	0.44	0/639

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Am	0.09	0/2520	0.25	0/3434
34	B0	0.07	0/772	0.22	0/1025
35	B1	0.11	0/727	0.34	0/973
36	B2	0.07	0/77761	0.16	0/121212
37	B3	0.07	0/2838	0.13	0/4422
38	B4	0.06	0/3723	0.11	0/5796
39	BN	0.10	0/1910	0.27	0/2575
40	BO	0.10	0/3116	0.27	0/4190
41	BP	0.09	0/2852	0.26	0/3850
42	BQ	0.10	0/2361	0.28	0/3173
43	BR	0.13	0/1361	0.35	0/1836
44	BS	0.09	0/1846	0.23	0/2475
45	BT	0.10	0/1801	0.28	0/2430
46	BV	0.11	0/1804	0.34	1/2416 (0.0%)
47	BW	0.12	0/1369	0.30	0/1830
48	BX	0.08	0/1639	0.21	0/2208
49	BY	0.09	0/1054	0.24	0/1413
50	BZ	0.10	0/1717	0.24	0/2306
51	Ba	0.09	0/1575	0.24	0/2109
52	Bc	0.11	0/1511	0.28	0/2021
53	Bd	0.09	0/1320	0.25	0/1757
54	Be	0.10	0/1458	0.26	0/1961
55	Bf	0.11	0/1314	0.28	0/1771
56	Bg	0.10	0/812	0.31	0/1090
57	Bh	0.10	0/1015	0.27	0/1369
58	Bi	0.09	0/534	0.26	0/709
59	Bj	0.08	0/963	0.25	0/1296
60	Bk	0.11	0/1008	0.32	0/1341
61	Bl	0.12	0/1101	0.29	0/1477
62	Bm	0.10	0/1200	0.27	0/1611
63	Bn	0.07	0/503	0.21	0/664
64	Bo	0.09	0/714	0.25	0/961
65	Bp	0.09	0/872	0.25	0/1172
66	Bq	0.10	0/958	0.25	0/1278
67	Br	0.09	0/853	0.22	0/1146
68	Bs	0.08	0/870	0.20	0/1165
69	Bt	0.08	0/1008	0.20	0/1340
70	Bu	0.07	0/766	0.21	0/1017
71	Bv	0.10	0/666	0.30	0/881
72	Bw	0.07	0/566	0.22	0/757
73	Bx	0.08	0/447	0.26	0/597
74	By	0.10	0/1045	0.26	0/1404
75	H1	0.10	0/768	0.26	0/1035

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	HE	0.10	0/6670	0.29	0/9031
77	HL	0.10	0/1704	0.32	0/2285
78	HS	0.09	0/847	0.34	0/1144
79	HI	0.12	0/1066	0.32	0/1437
80	BA	0.09	0/419	0.23	0/554
81	BU	0.08	0/1479	0.24	0/1993
82	Bb	0.14	0/1237	0.42	0/1661
83	A	0.10	0/148	0.30	0/193
All	All	0.08	0/224627	0.22	1/328676 (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
20	AV	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	BV	5	PRO	N-CA-CB	7.06	110.66	103.25

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
20	AV	113	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	36359	0	18299	209	0
2	AD	1602	0	1625	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	AE	1733	0	1816	22	0
4	AF	1660	0	1736	31	0
5	AG	1701	0	1777	28	0
6	AH	2083	0	2192	51	0
7	AI	1559	0	1624	44	0
8	AJ	1784	0	1879	22	0
9	AK	1530	0	1609	29	0
10	AL	1506	0	1538	19	0
11	AM	1462	0	1562	21	0
12	AN	748	0	735	15	0
13	AO	1164	0	1201	34	0
14	AP	884	0	872	12	0
15	AQ	1184	0	1252	20	0
16	AR	949	0	986	26	0
17	AS	954	0	993	16	0
18	AT	1082	0	1142	31	0
19	AU	879	0	918	17	0
20	AV	1144	0	1197	32	0
21	AW	1119	0	1130	26	0
22	Aa	810	0	871	11	0
23	Ab	672	0	660	11	0
24	Ac	1028	0	1080	23	0
25	Ad	1095	0	1149	23	0
26	Ae	1078	0	1133	30	0
27	Af	551	0	583	6	0
28	Ag	795	0	832	11	0
29	Ah	619	0	635	12	0
30	Ai	498	0	539	11	0
31	Aj	447	0	443	9	0
32	Ak	475	0	517	9	0
33	Am	2458	0	2370	50	0
34	B0	758	0	815	4	0
35	B1	718	0	751	9	0
36	B2	69470	0	34918	185	0
37	B3	2539	0	1283	12	0
38	B4	3332	0	1684	10	0
39	BN	1872	0	1917	34	0
40	BO	3050	0	3125	35	0
41	BP	2799	0	2925	30	0
42	BQ	2312	0	2272	23	0
43	BR	1333	0	1413	9	0
44	BS	1814	0	1884	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	BT	1772	0	1866	16	0
46	BV	1769	0	1804	10	0
47	BW	1346	0	1397	23	0
48	BX	1607	0	1650	25	0
49	BY	1038	0	1115	5	0
50	BZ	1676	0	1712	20	0
51	Ba	1545	0	1641	17	0
52	Bc	1487	0	1597	15	0
53	Bd	1301	0	1393	8	0
54	Be	1423	0	1488	21	0
55	Bf	1286	0	1310	16	0
56	Bg	798	0	834	6	0
57	Bh	999	0	1047	9	0
58	Bi	523	0	555	5	0
59	Bj	947	0	1012	13	0
60	Bk	998	0	1090	13	0
61	Bl	1078	0	1154	20	0
62	Bm	1171	0	1215	17	0
63	Bn	495	0	504	2	0
64	Bo	705	0	746	6	0
65	Bp	857	0	891	4	0
66	Bq	944	0	1005	7	0
67	Br	831	0	858	14	0
68	Bs	858	0	925	8	0
69	Bt	999	0	1092	9	0
70	Bu	759	0	840	4	0
71	Bv	652	0	663	2	0
72	Bw	560	0	608	4	0
73	Bx	436	0	463	5	0
74	By	1031	0	1080	22	0
75	H1	758	0	712	11	0
76	HE	6544	0	6571	113	0
77	HL	1679	0	1795	27	0
78	HS	834	0	833	7	0
79	HI	1067	0	1056	20	0
80	BA	413	0	455	3	0
81	BU	1461	0	1527	9	0
82	Bb	1212	0	1239	13	0
83	A	149	0	169	2	0
84	Ag	1	0	0	0	0
84	Ah	1	0	0	0	0
84	Aj	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	B0	1	0	0	0	0
84	B1	1	0	0	0	0
84	Bv	1	0	0	0	0
All	All	209623	0	157794	1629	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 4.

All (1629) 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)
20:AV:110:ASP:HA	20:AV:113:ARG:HD2	1.49	0.91
18:AT:37:GLN:HG3	18:AT:38:PRO:HD3	1.54	0.89
1:AA:572:C:H41	25:Ad:67:ARG:HH12	1.30	0.80
76:HE:110:ASP:HB3	76:HE:537:HIS:HB2	1.64	0.79
1:AA:1102:A:H5'	4:AF:163:SER:HB3	1.65	0.79
36:B2:2589:U:H3'	36:B2:2590:A:H5"	1.66	0.78
16:AR:45:THR:HG23	16:AR:47:GLY:H	1.50	0.77
42:BQ:84:PRO:HB3	42:BQ:89:LYS:HE3	1.66	0.77
3:AE:144:ARG:HD3	3:AE:206:PRO:HG2	1.67	0.77
15:AQ:136:PRO:HG2	15:AQ:139:TRP:HB2	1.65	0.76
6:AH:139:LEU:HB3	6:AH:147:ILE:HB	1.68	0.76
68:Bs:23:ILE:HD13	68:Bs:33:LEU:HB2	1.65	0.76
1:AA:175:G:H21	1:AA:176:C:H41	1.34	0.76
36:B2:1951:A:H61	36:B2:2427:C:H42	1.35	0.75
49:BY:47:PRO:HG2	49:BY:49:GLN:HE22	1.50	0.75
1:AA:884:A:H5'	15:AQ:90:ASN:HD22	1.51	0.75
20:AV:98:LEU:HD13	20:AV:103:VAL:HB	1.68	0.75
43:BR:31:TYR:HD1	43:BR:33:GLU:H	1.32	0.75
1:AA:68:A:H62	1:AA:85:A:H61	1.35	0.75
6:AH:51:ARG:HH12	6:AH:109:PHE:HB2	1.51	0.74
1:AA:1401:U:H4'	22:Aa:57:PRO:HG3	1.68	0.74
36:B2:1183:G:H22	36:B2:1231:A:H61	1.34	0.73
8:AJ:169:LYS:HD3	8:AJ:170:LYS:HG2	1.71	0.72
26:Ae:8:ARG:HH12	26:Ae:68:ARG:HH22	1.34	0.72
6:AH:208:ILE:HD11	6:AH:222:LEU:HD23	1.72	0.72
37:B3:2:U:H3	37:B3:117:G:H1	1.39	0.71
76:HE:36:THR:HA	76:HE:39:LEU:HD23	1.71	0.71
16:AR:22:PHE:HB3	16:AR:29:PHE:HB2	1.72	0.71
77:HL:62:MET:HE2	77:HL:62:MET:HA	1.72	0.71
21:AW:15:ILE:HA	21:AW:18:TYR:HB3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Am:30:ILE:HD11	33:Am:42:LEU:HB3	1.72	0.71
26:Ae:62:THR:HG23	26:Ae:69:THR:HG22	1.73	0.70
1:AA:1496:C:H5"	21:AW:44:GLU:HG3	1.73	0.70
8:AJ:78:ARG:HH21	8:AJ:92:ARG:HD2	1.55	0.70
6:AH:49:ARG:HH11	6:AH:61:VAL:HG21	1.57	0.69
40:BO:331:PRO:HD2	40:BO:334:ARG:HD2	1.73	0.69
18:AT:17:ALA:HB1	18:AT:62:ILE:HD11	1.74	0.69
1:AA:1497:G:H5"	21:AW:43:LYS:HE3	1.74	0.69
1:AA:1231:U:H5"	1:AA:1263:C:H1'	1.74	0.69
5:AG:116:ALA:HB3	5:AG:119:ARG:HG2	1.75	0.69
76:HE:28:VAL:HG12	76:HE:29:ASP:H	1.58	0.69
76:HE:577:SER:HB3	76:HE:712:VAL:HG12	1.74	0.68
8:AJ:39:ASP:HA	8:AJ:46:ALA:HA	1.75	0.68
1:AA:1580:G:H5'	20:AV:38:ARG:HH12	1.59	0.67
36:B2:3344:A:H61	51:Ba:106:VAL:HG21	1.58	0.67
36:B2:2785:G:H21	36:B2:2786:A:H5"	1.58	0.67
18:AT:38:PRO:HG2	18:AT:75:ILE:HG13	1.77	0.67
22:Aa:56:LEU:HD21	22:Aa:86:LYS:HG2	1.76	0.67
9:AK:101:LEU:HD23	9:AK:118:ARG:HB3	1.76	0.67
45:BT:53:PRO:HD2	45:BT:56:ILE:HD12	1.77	0.67
76:HE:413:ILE:HG12	76:HE:469:LEU:HD22	1.76	0.67
36:B2:3253:G:H22	36:B2:3393:U:H3	1.43	0.66
1:AA:452:C:H5"	6:AH:30:LYS:HE2	1.76	0.66
2:AD:20:LEU:HD11	2:AD:53:LEU:HG	1.77	0.66
36:B2:359:A:H61	73:Bx:38:ASN:HA	1.60	0.66
1:AA:480:A:H61	1:AA:542:G:H21	1.44	0.66
43:BR:169:LYS:HE3	43:BR:169:LYS:HA	1.78	0.66
76:HE:380:ILE:HG22	76:HE:400:VAL:HA	1.77	0.66
44:BS:171:LEU:HA	44:BS:176:ILE:HD11	1.78	0.65
22:Aa:67:LYS:HE2	22:Aa:78:GLU:HG3	1.77	0.65
45:BT:101:THR:HG23	45:BT:103:ALA:H	1.61	0.65
74:By:16:ASN:HB2	74:By:19:LEU:HB2	1.77	0.65
5:AG:66:ARG:HD2	12:AN:90:THR:HG23	1.77	0.65
36:B2:2521:U:H1'	50:BZ:125:ALA:HB2	1.78	0.65
36:B2:2990:G:H1	36:B2:3000:U:H3	1.43	0.65
76:HE:672:LYS:HG2	76:HE:673:GLU:HG2	1.77	0.65
4:AF:169:VAL:HB	4:AF:196:TYR:HB2	1.79	0.65
21:AW:40:GLY:HA2	21:AW:96:SER:H	1.61	0.65
77:HL:31:VAL:HA	77:HL:207:SER:HA	1.79	0.65
16:AR:41:ILE:HD11	16:AR:76:VAL:HG11	1.78	0.65
35:B1:65:VAL:H	39:BN:83:THR:HG22	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:HE:804:MET:HG2	76:HE:806:GLY:H	1.62	0.65
79:HI:92:GLN:HB2	79:HI:104:MET:HB2	1.79	0.65
36:B2:1011:G:H22	36:B2:1135:G:H21	1.45	0.64
36:B2:2600:U:H3'	36:B2:2601:U:H5"	1.78	0.64
21:AW:56:ARG:HH12	21:AW:100:GLN:HE21	1.45	0.64
44:BS:151:THR:HG22	44:BS:248:ARG:HH22	1.61	0.64
41:BP:324:LYS:HG3	41:BP:327:LEU:HD23	1.78	0.64
54:Be:15:THR:HG23	54:Be:18:GLU:H	1.63	0.64
2:AD:44:ARG:HG2	2:AD:45:SER:H	1.62	0.64
4:AF:114:ILE:H	4:AF:130:MET:HE1	1.62	0.64
7:AI:48:LEU:HD22	18:AT:41:LEU:HD13	1.80	0.64
74:By:29:GLN:HE21	74:By:41:ASN:HD21	1.45	0.64
79:HI:114:VAL:HG12	79:HI:146:GLU:HG2	1.80	0.64
1:AA:357:C:H5"	10:AL:16:ALA:HB2	1.78	0.64
1:AA:650:G:H1	1:AA:692:G:H22	1.44	0.64
1:AA:1236:A:H4'	12:AN:47:GLN:HE22	1.63	0.64
6:AH:247:SER:HB3	6:AH:250:GLU:HG3	1.79	0.64
79:HI:24:CYS:HB3	79:HI:77:SER:HA	1.80	0.64
36:B2:7:C:H5"	45:BT:193:LYS:HB3	1.81	0.63
48:BX:36:ARG:HH21	48:BX:40:GLN:HE22	1.45	0.63
47:BW:92:LYS:HB3	47:BW:174:LYS:HG3	1.80	0.63
6:AH:249:THR:HA	6:AH:252:ARG:HD3	1.81	0.63
6:AH:9:LEU:HB2	6:AH:30:LYS:HB3	1.81	0.63
64:Bo:53:ASN:HB2	64:Bo:79:THR:HG22	1.81	0.63
71:Bv:25:ARG:HD2	73:Bx:51:ILE:HB	1.80	0.63
74:By:12:ILE:HB	74:By:16:ASN:HD21	1.63	0.63
27:Af:20:THR:HG23	27:Af:21:VAL:HG23	1.79	0.63
36:B2:473:U:H3	36:B2:480:G:H22	1.46	0.63
36:B2:494:A:H4'	74:By:91:SER:HB2	1.80	0.63
10:AL:62:SER:HB3	10:AL:75:LYS:HD3	1.81	0.63
33:Am:73:PHE:H	33:Am:117:ASN:HD21	1.47	0.63
74:By:66:LEU:HD21	74:By:99:ILE:HG12	1.80	0.63
1:AA:638:A:H61	1:AA:876:U:H3	1.47	0.62
14:AP:64:LEU:HA	14:AP:90:PRO:HG2	1.80	0.62
76:HE:235:ILE:HG21	76:HE:239:LYS:HB3	1.81	0.62
4:AF:141:GLY:HA3	4:AF:154:PRO:HB3	1.81	0.62
6:AH:148:ARG:HG2	6:AH:149:TYR:CD1	2.34	0.62
36:B2:461:A:H62	36:B2:495:A:H1'	1.64	0.62
39:BN:128:SER:HB3	39:BN:131:ASN:HD22	1.63	0.62
11:AM:133:HIS:HD2	11:AM:164:TYR:HB2	1.63	0.62
16:AR:28:THR:HG21	16:AR:99:GLY:HA3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Ae:24:VAL:HG23	26:Ae:73:ALA:H	1.64	0.62
36:B2:2185:C:H2'	36:B2:2186:C:C6	2.34	0.62
41:BP:10:ILE:HD11	41:BP:20:GLU:HB2	1.80	0.62
1:AA:915:A:H3'	1:AA:916:G:H21	1.64	0.62
32:Ak:10:ARG:HD3	32:Ak:10:ARG:H	1.63	0.62
36:B2:717:A:H5'	60:Bk:5:ARG:HH21	1.63	0.62
27:Af:20:THR:HA	27:Af:52:ASN:HD21	1.63	0.62
1:AA:67:A:H8	1:AA:84:G:H21	1.48	0.62
1:AA:187:G:H21	1:AA:199:A:H62	1.46	0.62
36:B2:3342:G:H5'	36:B2:3345:G:H8	1.63	0.62
36:B2:2490:A:H2'	41:BP:69:THR:HG21	1.80	0.61
60:Bk:36:LYS:HA	60:Bk:36:LYS:HE3	1.82	0.61
45:BT:77:GLN:HE22	45:BT:167:PRO:HG2	1.64	0.61
5:AG:40:GLU:HB3	5:AG:51:ILE:HG22	1.81	0.61
26:Ae:35:ILE:HG12	26:Ae:40:LEU:HD12	1.81	0.61
3:AE:121:ILE:HD11	3:AE:165:ARG:HD2	1.82	0.61
9:AK:87:PHE:HB3	9:AK:90:ARG:HB2	1.82	0.61
24:Ac:24:GLN:HE21	29:Ah:5:VAL:HG12	1.65	0.61
2:AD:149:LEU:HB3	2:AD:165:THR:HB	1.83	0.61
28:Ag:44:MET:HE3	28:Ag:45:VAL:HG23	1.81	0.61
33:Am:128:THR:HG22	33:Am:130:LYS:H	1.66	0.61
2:AD:199:VAL:HG21	2:AD:203:LEU:HD13	1.83	0.61
13:AO:104:LEU:HD12	13:AO:105:ALA:H	1.66	0.61
36:B2:301:C:H4'	70:Bu:74:ARG:HH21	1.65	0.61
7:AI:145:ARG:HH22	30:Ai:56:VAL:HB	1.66	0.61
20:AV:14:ARG:HH21	20:AV:17:ASN:HA	1.66	0.61
36:B2:2226:A:H1'	71:Bv:2:THR:HB	1.81	0.61
39:BN:53:ARG:HG2	39:BN:55:ALA:H	1.65	0.61
36:B2:460:G:H22	36:B2:493:G:H1	1.46	0.60
76:HE:394:PHE:HZ	76:HE:510:ARG:HG3	1.65	0.60
2:AD:83:THR:HA	2:AD:86:HIS:HE1	1.65	0.60
5:AG:74:LEU:HA	5:AG:77:LYS:HE3	1.83	0.60
20:AV:106:LYS:HA	20:AV:109:GLU:HB3	1.82	0.60
16:AR:113:ARG:HA	28:Ag:56:ALA:HB1	1.82	0.60
9:AK:83:LEU:HB3	9:AK:92:VAL:HG11	1.82	0.60
15:AQ:36:GLN:HA	15:AQ:39:LYS:HE2	1.83	0.60
79:HI:61:VAL:HG23	79:HI:72:GLU:HB3	1.84	0.60
22:Aa:41:ASN:HA	22:Aa:44:LYS:HE2	1.83	0.60
36:B2:489:C:H4'	36:B2:490:U:H5'	1.82	0.60
36:B2:1995:G:H21	36:B2:3463:A:H8	1.48	0.60
2:AD:197:TRP:CD1	2:AD:198:ASP:H	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:B2:1111:A:H5”	42:BQ:140:ARG:HD2	1.83	0.60
2:AD:200:MET:HE1	2:AD:202:ASP:HB2	1.82	0.60
45:BT:205:GLU:HA	45:BT:208:LYS:HE2	1.83	0.60
79:HI:22:MET:HE2	79:HI:83:VAL:HG11	1.83	0.60
6:AH:11:ARG:HH22	11:AM:2:PRO:HB2	1.67	0.60
7:AI:101:LEU:HD21	27:Af:82:THR:HB	1.84	0.60
2:AD:130:ARG:HH21	2:AD:154:SER:HA	1.66	0.60
76:HE:27:HIS:CG	76:HE:138:GLN:HB2	2.36	0.60
1:AA:976:U:H5”	15:AQ:71:ILE:HD11	1.82	0.59
17:AS:123:TYR:HB2	17:AS:126:GLU:HG2	1.84	0.59
36:B2:3414:U:H4’	40:BO:173:GLN:HG3	1.84	0.59
61:Bl:125:GLY:C	61:Bl:126:LYS:HD2	2.27	0.59
76:HE:343:PRO:HB2	76:HE:348:ALA:HB2	1.83	0.59
76:HE:638:PRO:HD2	76:HE:642:GLY:HA3	1.84	0.59
10:AL:154:SER:HA	10:AL:157:GLU:HB2	1.84	0.59
36:B2:190:G:H22	36:B2:239:U:H3	1.49	0.59
36:B2:482:C:H1’	74:By:102:ARG:HH21	1.67	0.59
72:Bw:7:ASP:HB3	72:Bw:10:GLN:HB3	1.84	0.59
82:Bb:137:THR:HG22	82:Bb:138:ALA:H	1.67	0.59
7:AI:152:LEU:HD23	7:AI:155:ILE:HD11	1.84	0.59
54:Be:109:MET:HE2	54:Be:120:ILE:HD11	1.83	0.59
13:AO:72:VAL:HG12	13:AO:83:ILE:HG22	1.84	0.59
17:AS:25:TYR:HB3	17:AS:33:LEU:HD11	1.84	0.59
7:AI:87:LEU:HA	7:AI:90:ARG:HE	1.67	0.59
18:AT:121:MET:HE2	18:AT:121:MET:HA	1.83	0.59
21:AW:21:PHE:HA	21:AW:24:ARG:HD3	1.84	0.59
43:BR:61:LEU:HD21	43:BR:102:ILE:HG23	1.84	0.59
77:HL:130:ALA:HB1	77:HL:132:LYS:HE3	1.85	0.59
6:AH:126:VAL:HG12	6:AH:158:ASP:H	1.67	0.59
46:BV:60:ILE:HD12	46:BV:129:VAL:HG21	1.84	0.59
6:AH:154:ILE:HD12	6:AH:172:PHE:HB2	1.83	0.59
18:AT:44:LYS:HE2	18:AT:79:ARG:HD3	1.84	0.59
20:AV:90:ILE:HG13	20:AV:91:ASN:N	2.18	0.59
36:B2:3388:C:H1’	36:B2:3389:A:O4’	2.02	0.59
9:AK:65:PRO:HD2	9:AK:68:LEU:HD11	1.84	0.59
13:AO:81:ILE:HG21	13:AO:114:ILE:HG21	1.83	0.59
14:AP:66:VAL:HG11	14:AP:124:VAL:H	1.68	0.59
25:Ad:124:LYS:HG2	25:Ad:129:GLY:HA2	1.85	0.59
26:Ae:55:VAL:HG13	26:Ae:57:ALA:H	1.66	0.59
36:B2:3145:A:H4’	40:BO:364:LYS:HE3	1.85	0.59
76:HE:495:VAL:HG12	76:HE:504:LEU:HD22	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:AW:131:LEU:HD13	21:AW:134:ILE:HD11	1.85	0.58
77:HL:204:VAL:HG12	77:HL:214:ARG:HA	1.84	0.58
61:Bl:70:PRO:HG3	61:Bl:115:LYS:HB2	1.85	0.58
67:Br:17:PHE:HD2	67:Br:24:ILE:HD11	1.69	0.58
77:HL:119:ILE:HG23	77:HL:123:LEU:HD23	1.86	0.58
33:Am:178:ASP:HB3	33:Am:181:THR:HG22	1.85	0.58
36:B2:1856:G:H1'	36:B2:1857:G:H4'	1.86	0.58
40:BO:217:VAL:HG21	40:BO:328:THR:HG22	1.85	0.58
1:AA:69:G:H1	1:AA:83:U:H3	1.51	0.58
1:AA:89:U:H3	1:AA:455:A:H61	1.52	0.58
10:AL:76:THR:HG22	10:AL:108:PRO:HG2	1.86	0.58
76:HE:650:THR:HG21	76:HE:691:VAL:HG12	1.85	0.58
1:AA:1194:C:H41	20:AV:137:LYS:HD3	1.69	0.58
6:AH:182:MET:HB2	6:AH:192:VAL:HG12	1.85	0.58
36:B2:2251:C:H4'	39:BN:8:GLN:HA	1.86	0.58
33:Am:157:SER:HA	33:Am:200:ILE:HG12	1.86	0.58
1:AA:642:U:H2'	9:AK:103:LYS:HD3	1.85	0.57
17:AS:69:ARG:HH11	17:AS:72:LYS:HE2	1.69	0.57
18:AT:128:GLY:HA3	18:AT:134:ARG:HA	1.85	0.57
39:BN:149:LEU:HD21	39:BN:155:LYS:HB3	1.85	0.57
73:Bx:43:HIS:HB3	73:Bx:46:ARG:HB2	1.85	0.57
40:BO:221:THR:HG22	40:BO:329:PRO:HB3	1.86	0.57
30:Ai:30:ARG:HE	30:Ai:42:ILE:HG12	1.68	0.57
36:B2:3391:A:H1'	36:B2:3392:A:H5'	1.86	0.57
42:BQ:163:MET:HG2	42:BQ:173:ILE:HD12	1.86	0.57
52:Bc:39:THR:HG22	52:Bc:41:SER:H	1.68	0.57
77:HL:30:THR:HA	77:HL:170:HIS:HA	1.86	0.57
82:Bb:21:TYR:H	82:Bb:145:HIS:HD2	1.52	0.57
82:Bb:113:ILE:HD13	82:Bb:153:GLU:HG2	1.86	0.57
1:AA:1162:G:H4'	4:AF:90:ARG:HB2	1.85	0.57
10:AL:22:ARG:HE	10:AL:23:LYS:H	1.53	0.57
59:Bj:91:LYS:HD3	59:Bj:109:ILE:HG22	1.87	0.57
76:HE:230:ALA:HB1	76:HE:236:ASP:HA	1.85	0.57
76:HE:436:LEU:HG	76:HE:445:ILE:HD11	1.85	0.57
1:AA:300:U:H5"	6:AH:37:LYS:HD3	1.86	0.57
16:AR:23:ALA:HB1	16:AR:97:GLY:H	1.69	0.57
33:Am:107:ASP:H	33:Am:125:ARG:HE	1.53	0.57
41:BP:236:ASN:HB3	41:BP:239:GLN:HE21	1.69	0.57
44:BS:239:ARG:HB2	44:BS:242:HIS:HB2	1.87	0.57
7:AI:62:LYS:HB3	7:AI:70:ARG:HH12	1.70	0.57
7:AI:120:PRO:HD2	7:AI:148:GLN:HE21	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:849:G:H2'	1:AA:850:U:H5	1.68	0.57
5:AG:50:ILE:H	5:AG:87:GLU:HB3	1.69	0.57
16:AR:107:LEU:HD12	16:AR:114:ILE:HD11	1.87	0.57
26:Ae:108:ARG:HG2	26:Ae:112:LYS:HZ2	1.69	0.57
36:B2:531:A:H3'	41:BP:350:LYS:HE2	1.86	0.57
36:B2:1578:G:H5'	50:BZ:67:ARG:HD2	1.87	0.57
47:BW:92:LYS:HG2	47:BW:174:LYS:HE3	1.86	0.57
48:BX:62:THR:HG21	62:Bm:66:ASN:HD22	1.69	0.57
41:BP:94:ASN:HD22	41:BP:102:PHE:HB2	1.69	0.57
39:BN:138:HIS:HB2	39:BN:145:THR:HG22	1.86	0.57
76:HE:5:THR:HG22	76:HE:8:GLU:H	1.69	0.57
5:AG:30:GLU:HA	12:AN:58:ARG:HG3	1.87	0.56
36:B2:455:G:H22	36:B2:498:U:H5	1.53	0.56
36:B2:3335:U:H3'	36:B2:3336:G:H21	1.68	0.56
76:HE:586:ILE:HG23	76:HE:712:VAL:HG11	1.86	0.56
1:AA:613:G:H5"	25:Ad:17:ARG:HH12	1.71	0.56
38:B4:78:G:H21	38:B4:96:A:H62	1.51	0.56
76:HE:175:TYR:HB2	76:HE:274:ASN:HD21	1.69	0.56
1:AA:1199:U:H2'	1:AA:1200:A:H2'	1.86	0.56
1:AA:1376:C:H42	1:AA:1385:C:H42	1.53	0.56
4:AF:68:VAL:HG21	4:AF:132:LYS:HB3	1.88	0.56
12:AN:77:ARG:HH12	12:AN:88:PRO:HA	1.71	0.56
36:B2:157:A:H4'	69:Bt:104:LEU:HD23	1.86	0.56
74:By:31:ASN:HD21	74:By:41:ASN:HB3	1.69	0.56
76:HE:470:THR:HG21	76:HE:475:ALA:HB3	1.88	0.56
82:Bb:21:TYR:H	82:Bb:145:HIS:CD2	2.23	0.56
24:Ac:22:ARG:NH2	24:Ac:23:ARG:H	2.04	0.56
44:BS:148:ASN:HB2	44:BS:244:ASN:HD21	1.69	0.56
16:AR:89:GLY:HA2	16:AR:94:LYS:HZ2	1.71	0.56
33:Am:206:LEU:HA	33:Am:221:LEU:H	1.70	0.56
76:HE:182:VAL:HG21	76:HE:204:PRO:HD3	1.87	0.56
21:AW:33:TRP:HZ2	21:AW:102:LYS:HE3	1.70	0.56
61:Bl:14:THR:HB	68:Bs:86:LYS:HG3	1.86	0.56
1:AA:522:C:H42	1:AA:536:U:H3	1.53	0.56
4:AF:35:VAL:HG22	4:AF:36:PRO:HD2	1.87	0.56
19:AU:105:MET:HG2	19:AU:106:LEU:HG	1.88	0.56
24:Ac:22:ARG:NE	24:Ac:22:ARG:HA	2.21	0.56
36:B2:3209:A:H4'	81:BU:69:ARG:HG2	1.88	0.56
39:BN:2:GLY:HA2	39:BN:206:VAL:HG23	1.86	0.56
50:BZ:28:TRP:NE1	50:BZ:32:GLN:HE22	2.03	0.56
76:HE:105:SER:HB2	76:HE:115:VAL:HG22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Am:15:SER:H	33:Am:37:ASP:HB3	1.71	0.56
36:B2:1473:U:H5"	41:BP:89:GLN:HE22	1.71	0.56
62:Bm:111:VAL:HG13	62:Bm:126:THR:HG21	1.88	0.56
39:BN:208:HIS:HD2	39:BN:210:HIS:H	1.52	0.56
1:AA:323:U:H2'	1:AA:324:C:H2'	1.88	0.55
1:AA:39:A:H5'	11:AM:6:ARG:HG3	1.87	0.55
47:BW:14:ILE:HD12	47:BW:77:GLU:HG3	1.86	0.55
1:AA:625:A:H4'	1:AA:626:A:H5"	1.88	0.55
2:AD:21:LEU:HD23	19:AU:96:VAL:HB	1.88	0.55
19:AU:29:GLN:HA	19:AU:32:LYS:HE3	1.87	0.55
1:AA:506:G:H2'	1:AA:508:A:H5"	1.87	0.55
1:AA:1651:G:H5"	7:AI:85:LYS:HD2	1.87	0.55
20:AV:107:LEU:HA	20:AV:110:ASP:OD2	2.07	0.55
61:Bl:42:VAL:HG12	61:Bl:74:VAL:HG22	1.88	0.55
16:AR:129:ARG:HB3	28:Ag:22:ARG:HH21	1.72	0.55
48:BX:160:VAL:HG23	62:Bm:102:ASN:HD22	1.71	0.55
1:AA:1504:A:H5'	18:AT:12:ASN:HD21	1.72	0.55
67:Br:14:HIS:HE1	67:Br:29:SER:HB3	1.72	0.55
3:AE:32:ILE:HA	3:AE:96:CYS:HB2	1.87	0.55
4:AF:155:VAL:HG11	4:AF:223:ILE:HG21	1.89	0.55
36:B2:2619:A:H3'	59:Bj:29:THR:HG21	1.88	0.55
40:BO:79:ILE:HD13	40:BO:336:LEU:HD11	1.89	0.55
64:Bo:23:THR:HG21	64:Bo:98:ILE:HD12	1.89	0.55
36:B2:1806:U:H5"	53:Bd:39:GLN:HE22	1.72	0.55
53:Bd:8:LYS:HD2	53:Bd:24:MET:HE3	1.88	0.55
76:HE:731:VAL:HG12	76:HE:796:LEU:HB3	1.88	0.55
19:AU:80:ARG:HA	19:AU:83:GLN:HG2	1.88	0.55
45:BT:98:ARG:HD2	45:BT:189:VAL:HG13	1.88	0.55
56:Bg:14:ILE:HG22	56:Bg:101:TYR:HD2	1.69	0.55
36:B2:504:A:H4'	36:B2:505:G:OP1	2.06	0.55
44:BS:153:ARG:HG2	44:BS:193:ILE:HD13	1.89	0.55
11:AM:135:ARG:HE	11:AM:159:ALA:HA	1.72	0.54
11:AM:163:PRO:HB3	11:AM:169:PRO:HB3	1.89	0.54
61:Bl:6:LYS:HG3	61:Bl:7:PRO:HD2	1.89	0.54
1:AA:467:A:H2'	1:AA:468:G:H8	1.73	0.54
4:AF:120:VAL:HG21	75:H1:148:ALA:HA	1.89	0.54
6:AH:12:VAL:HG12	6:AH:12:VAL:O	2.07	0.54
16:AR:124:PRO:HB2	16:AR:127:SER:HB3	1.90	0.54
17:AS:138:ARG:HB3	75:H1:96:ASN:HD22	1.71	0.54
36:B2:2770:C:C2	47:BW:24:GLY:HA3	2.42	0.54
56:Bg:94:VAL:HG21	56:Bg:104:ARG:HH21	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:BQ:37:ILE:HG13	42:BQ:37:ILE:O	2.08	0.54
76:HE:26:ALA:HB3	76:HE:32:LYS:HD2	1.87	0.54
6:AH:64:ILE:HD13	6:AH:70:ILE:HG13	1.90	0.54
7:AI:31:VAL:O	7:AI:32:LYS:HG3	2.08	0.54
7:AI:121:ARG:HA	7:AI:145:ARG:HH21	1.72	0.54
14:AP:86:GLU:HG3	14:AP:88:GLU:H	1.73	0.54
21:AW:15:ILE:HG21	21:AW:55:VAL:HA	1.89	0.54
21:AW:116:SER:HB3	21:AW:122:ARG:HB2	1.88	0.54
36:B2:2923:G:H4'	46:BV:3:ARG:HB2	1.88	0.54
76:HE:427:PHE:HB3	76:HE:429:LYS:HD3	1.89	0.54
1:AA:883:G:H22	1:AA:975:U:H3	1.54	0.54
16:AR:52:THR:HG23	16:AR:54:ARG:H	1.71	0.54
35:B1:26:VAL:HG21	39:BN:179:LEU:HD22	1.90	0.54
51:Ba:75:ARG:HG3	51:Ba:146:VAL:HG12	1.89	0.54
59:Bj:114:ARG:HD3	59:Bj:120:LYS:HG3	1.90	0.54
79:HI:34:VAL:HG23	79:HI:84:PRO:HD3	1.89	0.54
19:AU:6:THR:HG22	19:AU:8:THR:H	1.72	0.54
31:Aj:21:CYS:HB3	31:Aj:25:GLY:H	1.72	0.54
33:Am:121:VAL:HG22	33:Am:131:ILE:HG22	1.90	0.54
1:AA:631:G:H21	1:AA:986:A:H62	1.56	0.54
1:AA:968:G:H2'	1:AA:969:G:H8	1.73	0.54
27:Af:83:ARG:HE	27:Af:85:PRO:HG2	1.71	0.54
29:Ah:19:HIS:HE1	29:Ah:21:LEU:HD23	1.73	0.54
55:Bf:50:LYS:HB3	55:Bf:92:ARG:HH12	1.73	0.54
1:AA:1184:G:H21	18:AT:136:GLN:HE22	1.55	0.54
11:AM:13:LYS:HB2	11:AM:47:LEU:HD12	1.90	0.54
25:Ad:123:VAL:HG13	25:Ad:124:LYS:HG3	1.90	0.54
76:HE:77:LEU:HB3	76:HE:100:VAL:HB	1.90	0.54
23:Ab:14:PRO:HB2	23:Ab:23:ILE:HD11	1.90	0.54
23:Ab:39:VAL:HA	23:Ab:45:GLN:HG2	1.89	0.54
36:B2:3387:G:O2'	36:B2:3388:C:H5'	2.08	0.54
3:AE:204:ILE:HG22	3:AE:205:PHE:H	1.73	0.54
1:AA:1055:G:H4'	2:AD:34:VAL:HG22	1.90	0.53
6:AH:179:ALA:HB3	6:AH:195:ILE:HD12	1.90	0.53
8:AJ:154:ARG:HH22	8:AJ:181:LEU:HD13	1.73	0.53
36:B2:2718:G:H5"	78:HS:67:SER:HB3	1.90	0.53
41:BP:212:ASN:HD22	41:BP:255:SER:HB2	1.72	0.53
48:BX:50:PRO:HA	48:BX:146:GLN:HE22	1.73	0.53
54:Be:90:TYR:HD2	54:Be:136:ARG:HH21	1.55	0.53
54:Be:144:ASN:HB3	54:Be:147:LEU:HD13	1.90	0.53
36:B2:305:A:H8	70:Bu:29:GLY:HA2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:B2:467:A:H2'	36:B2:468:G:H8	1.73	0.53
58:Bi:49:LEU:HD12	58:Bi:51:TRP:HE1	1.73	0.53
13:AO:63:ILE:HG12	13:AO:125:CYS:HB3	1.90	0.53
1:AA:838:G:H2'	1:AA:839:G:H8	1.72	0.53
1:AA:886:A:H2'	1:AA:887:G:C8	2.43	0.53
19:AU:77:GLU:HB2	19:AU:80:ARG:HB2	1.89	0.53
36:B2:3102:A:H62	36:B2:3236:G:H21	1.56	0.53
50:BZ:121:VAL:HG21	50:BZ:131:GLU:HG3	1.90	0.53
13:AO:16:GLN:HE22	13:AO:31:TRP:HB3	1.74	0.53
48:BX:77:LEU:HD23	48:BX:77:LEU:H	1.73	0.53
9:AK:143:ARG:HH12	9:AK:145:ALA:HA	1.74	0.53
11:AM:31:ALA:HA	11:AM:36:LEU:HD12	1.90	0.53
36:B2:3387:G:H2'	36:B2:3388:C:C6	2.43	0.53
47:BW:120:ILE:H	47:BW:120:ILE:HD12	1.73	0.53
6:AH:163:ASN:HD21	6:AH:170:GLU:HG2	1.74	0.53
11:AM:112:GLN:HG3	11:AM:148:VAL:HG11	1.90	0.53
24:Ac:22:ARG:HE	29:Ah:3:LEU:HD13	1.74	0.53
30:Ai:19:ARG:HD3	30:Ai:27:THR:HG22	1.91	0.53
36:B2:467:A:H2'	36:B2:468:G:C8	2.43	0.53
39:BN:116:GLU:HG2	39:BN:123:GLY:H	1.74	0.53
76:HE:18:ASN:HB2	76:HE:98:PHE:HA	1.91	0.53
7:AI:61:ARG:HD3	7:AI:64:ARG:HH21	1.72	0.53
19:AU:10:LYS:HD3	19:AU:53:TYR:HE2	1.73	0.53
20:AV:86:ARG:HD2	20:AV:103:VAL:HG11	1.91	0.53
39:BN:36:ARG:HG3	39:BN:37:HIS:HD2	1.74	0.53
4:AF:39:LYS:HE2	4:AF:246:LEU:HD11	1.91	0.53
18:AT:41:LEU:HD12	18:AT:44:LYS:HD2	1.91	0.53
29:Ah:24:LEU:HG	29:Ah:25:VAL:HG23	1.89	0.53
36:B2:3003:G:H4'	80:BA:114:LYS:HE3	1.90	0.53
60:Bk:34:LEU:HD22	60:Bk:38:LEU:HD23	1.91	0.53
75:H1:40:VAL:HG22	75:H1:42:ARG:HG2	1.91	0.53
26:Ae:16:ARG:HD3	26:Ae:19:GLN:HA	1.91	0.53
48:BX:2:ALA:HB2	62:Bm:30:GLY:HA3	1.91	0.53
76:HE:515:ASP:HB3	76:HE:518:VAL:HG12	1.91	0.53
77:HL:46:LYS:O	77:HL:47:ARG:HG2	2.09	0.53
3:AE:90:ASP:HB3	3:AE:97:LEU:HB2	1.91	0.52
5:AG:68:ILE:HG23	5:AG:88:LEU:HD13	1.91	0.52
33:Am:45:LEU:HB2	33:Am:47:ARG:HE	1.74	0.52
36:B2:1095:G:H8	36:B2:1098:G:H1'	1.74	0.52
20:AV:119:THR:HG23	20:AV:122:GLY:H	1.74	0.52
26:Ae:78:ASP:HB3	26:Ae:81:ALA:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:BQ:167:SER:HB3	42:BQ:173:ILE:HD11	1.92	0.52
1:AA:70:C:H2'	1:AA:71:A:H8	1.74	0.52
6:AH:10:LYS:HA	6:AH:27:TYR:HA	1.90	0.52
6:AH:59:ARG:HD2	26:Ae:87:PRO:HG3	1.90	0.52
24:Ac:22:ARG:HH22	24:Ac:24:GLN:CD	2.18	0.52
25:Ad:54:LYS:HD3	25:Ad:91:LEU:HG	1.91	0.52
40:BO:117:ARG:HA	40:BO:175:LYS:HD3	1.90	0.52
57:Bh:105:VAL:HG12	57:Bh:111:MET:HA	1.91	0.52
1:AA:811:A:H2'	1:AA:812:G:H8	1.73	0.52
1:AA:1358:G:H4'	1:AA:1359:C:H5	1.74	0.52
24:Ac:22:ARG:HH22	24:Ac:24:GLN:NE2	2.08	0.52
34:B0:23:HIS:HD2	34:B0:74:CYS:HA	1.75	0.52
36:B2:1615:C:H5'	36:B2:2618:G:C8	2.43	0.52
36:B2:1663:C:H5"	36:B2:1664:A:H5'	1.90	0.52
42:BQ:63:GLN:HE21	42:BQ:74:VAL:HG21	1.74	0.52
33:Am:202:PRO:HG2	33:Am:243:PRO:HA	1.92	0.52
79:HI:64:ASP:HB3	79:HI:68:GLY:H	1.74	0.52
26:Ae:102:LYS:HB3	26:Ae:108:ARG:NH2	2.25	0.52
36:B2:1423:G:H5"	66:Bq:98:SER:HB3	1.91	0.52
40:BO:88:GLY:HA3	40:BO:161:LEU:HD12	1.90	0.52
45:BT:127:LYS:HD3	45:BT:127:LYS:N	2.24	0.52
76:HE:288:VAL:HG11	76:HE:320:LEU:HB2	1.90	0.52
1:AA:545:A:H3'	1:AA:546:C:H3'	1.92	0.52
1:AA:1290:G:H4'	1:AA:1291:C:H5"	1.91	0.52
4:AF:226:PRO:HA	4:AF:229:TRP:CD2	2.44	0.52
10:AL:167:ALA:HB2	10:AL:183:ILE:HG22	1.92	0.52
15:AQ:90:ASN:HA	15:AQ:93:LYS:HE2	1.92	0.52
28:Ag:55:GLU:HG2	28:Ag:56:ALA:H	1.74	0.52
1:AA:1607:U:H4'	20:AV:35:GLY:HA2	1.90	0.52
5:AG:129:MET:HA	5:AG:133:ALA:HB3	1.91	0.52
7:AI:29:VAL:HG12	7:AI:31:VAL:H	1.74	0.52
26:Ae:102:LYS:HB3	26:Ae:108:ARG:HH22	1.74	0.52
33:Am:106:SER:OG	33:Am:126:ASP:HB3	2.09	0.52
36:B2:547:G:H1'	36:B2:581:A:N6	2.25	0.52
40:BO:63:PRO:HA	40:BO:68:HIS:HD2	1.75	0.52
76:HE:155:VAL:HG11	76:HE:185:VAL:HG11	1.92	0.52
76:HE:650:THR:HG22	76:HE:690:ASP:HA	1.91	0.52
77:HL:33:LEU:HD13	77:HL:205:VAL:HG12	1.92	0.52
1:AA:1008:A:H62	1:AA:1026:G:H21	1.57	0.52
20:AV:61:THR:HA	20:AV:64:LEU:HB2	1.92	0.52
27:Af:74:GLN:HG2	27:Af:79:ALA:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:HE:197:LEU:HD23	76:HE:199:ASP:H	1.74	0.52
76:HE:244:LEU:HD23	76:HE:245:TRP:N	2.25	0.52
76:HE:725:GLN:HE21	76:HE:803:PRO:HB3	1.74	0.52
77:HL:35:ILE:HD12	77:HL:203:LEU:HD22	1.92	0.52
6:AH:162:LEU:HG	6:AH:164:LEU:H	1.75	0.52
15:AQ:49:GLN:HE22	15:AQ:53:THR:HG23	1.75	0.52
36:B2:57:A:H1'	50:BZ:162:ARG:HH12	1.74	0.52
76:HE:437:MET:HE3	76:HE:437:MET:HA	1.92	0.52
33:Am:129:ILE:HB	33:Am:142:ILE:HD11	1.91	0.51
40:BO:308:MET:HB2	40:BO:363:SER:HB2	1.92	0.51
58:Bi:48:ARG:HD2	58:Bi:49:LEU:H	1.75	0.51
62:Bm:71:PRO:HG2	62:Bm:108:TYR:HA	1.92	0.51
21:AW:68:LYS:HG2	21:AW:69:GLN:HG2	1.92	0.51
36:B2:2590:A:OP1	36:B2:2590:A:H4'	2.10	0.51
62:Bm:100:VAL:HG12	62:Bm:123:ILE:HB	1.93	0.51
76:HE:404:THR:HA	76:HE:449:PRO:HA	1.90	0.51
2:AD:183:GLU:HA	2:AD:186:ARG:HG2	1.92	0.51
36:B2:3354:U:H2'	36:B2:3355:G:C8	2.45	0.51
42:BQ:36:LEU:HD11	42:BQ:147:ASP:HB3	1.92	0.51
60:Bk:55:ILE:HG22	60:Bk:105:ILE:HA	1.92	0.51
61:Bl:9:LYS:HD2	61:Bl:86:ALA:HB2	1.92	0.51
76:HE:191:THR:HG23	76:HE:192:TYR:HD1	1.74	0.51
7:AI:1:MET:HA	21:AW:3:GLY:HA3	1.92	0.51
44:BS:129:LYS:HB2	55:Bf:133:ALA:HB3	1.93	0.51
6:AH:179:ALA:H	6:AH:195:ILE:HB	1.76	0.51
13:AO:81:ILE:HG12	13:AO:108:VAL:HB	1.92	0.51
67:Br:19:ARG:HD2	67:Br:24:ILE:HD12	1.92	0.51
1:AA:513:G:H3'	11:AM:176:ARG:HG3	1.93	0.51
1:AA:1833:A:H5"	28:Ag:8:ASN:HD21	1.76	0.51
36:B2:409:U:H5"	36:B2:410:A:H5"	1.91	0.51
47:BW:109:HIS:ND1	47:BW:114:ILE:HD11	2.26	0.51
54:Be:5:GLU:HG2	54:Be:63:ILE:HB	1.92	0.51
77:HL:47:ARG:HH12	77:HL:157:GLN:HE22	1.59	0.51
8:AJ:28:MET:HE2	8:AJ:104:GLN:HE21	1.76	0.51
8:AJ:57:ASP:HA	8:AJ:106:LEU:HA	1.93	0.51
10:AL:67:TRP:HE1	10:AL:70:GLU:HG2	1.75	0.51
18:AT:25:LEU:HD23	18:AT:61:ASP:HB3	1.93	0.51
36:B2:546:G:N2	54:Be:131:LYS:HD2	2.25	0.51
40:BO:218:ILE:HG23	40:BO:276:THR:HG22	1.93	0.51
76:HE:400:VAL:HG12	76:HE:450:ALA:HA	1.91	0.51
1:AA:902:A:H5"	16:AR:122:PRO:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AE:38:PHE:CG	3:AE:73:LEU:HD11	2.46	0.51
5:AG:75:VAL:HG22	5:AG:81:PHE:HE2	1.76	0.51
5:AG:212:PRO:HD2	19:AU:19:LYS:HE3	1.92	0.51
36:B2:2003:G:H1	36:B2:2186:C:H42	1.59	0.51
41:BP:319:ASN:HD21	41:BP:322:LYS:HD3	1.75	0.51
45:BT:145:ALA:O	45:BT:146:LYS:HG2	2.11	0.51
50:BZ:64:ILE:HG21	50:BZ:102:ALA:HB1	1.93	0.51
2:AD:64:ALA:HA	2:AD:67:ILE:HG22	1.92	0.51
9:AK:79:LEU:HB2	9:AK:83:LEU:HD23	1.93	0.51
26:Ae:125:LEU:HA	26:Ae:128:ARG:HE	1.76	0.51
36:B2:1096:A:H4'	36:B2:1097:C:H3'	1.92	0.51
38:B4:134:U:H2'	38:B4:137:A:C6	2.46	0.51
55:Bf:63:VAL:HG13	55:Bf:75:LEU:HB2	1.93	0.51
9:AK:43:LEU:HD13	9:AK:72:PHE:HE1	1.76	0.51
15:AQ:114:ARG:HA	15:AQ:117:LEU:HD12	1.92	0.51
37:B3:75:G:H5"	54:Be:49:LYS:HG2	1.93	0.51
51:Ba:157:LEU:HD23	51:Ba:160:ARG:HH21	1.76	0.51
60:Bk:8:THR:HG21	60:Bk:13:LYS:HD2	1.92	0.51
9:AK:53:VAL:HG23	9:AK:55:GLY:H	1.74	0.50
23:Ab:55:ILE:HD12	23:Ab:65:SER:HB2	1.92	0.50
33:Am:7:LEU:HD13	33:Am:272:VAL:HG21	1.94	0.50
36:B2:2802:U:H5'	75:H1:34:ARG:HH12	1.76	0.50
67:Br:46:LEU:HD21	67:Br:75:PRO:HD3	1.92	0.50
74:By:12:ILE:HB	74:By:16:ASN:ND2	2.26	0.50
14:AP:92:ILE:HG13	14:AP:93:LYS:N	2.26	0.50
36:B2:981:C:OP1	52:Bc:9:HIS:HB2	2.11	0.50
66:Bq:39:VAL:HG12	66:Bq:49:MET:HE2	1.92	0.50
74:By:35:VAL:HG11	74:By:82:PHE:HE2	1.76	0.50
51:Ba:56:LEU:HA	51:Ba:59:LEU:HD12	1.92	0.50
60:Bk:42:TYR:HE2	60:Bk:108:LEU:HD21	1.76	0.50
4:AF:52:ILE:HG23	4:AF:55:ILE:HD11	1.93	0.50
33:Am:168:ALA:HB2	33:Am:198:VAL:HG21	1.94	0.50
1:AA:475:G:H2'	1:AA:476:A:H8	1.76	0.50
1:AA:1587:G:H2'	1:AA:1588:A:H8	1.76	0.50
44:BS:135:LEU:HA	44:BS:138:VAL:HG12	1.94	0.50
52:Bc:50:ARG:HH12	52:Bc:142:ARG:HG2	1.76	0.50
66:Bq:18:GLN:HG2	66:Bq:21:ARG:HH11	1.77	0.50
3:AE:134:LEU:HD22	3:AE:218:LEU:HB2	1.93	0.50
5:AG:68:ILE:HG12	5:AG:88:LEU:HD22	1.94	0.50
6:AH:169:ILE:H	6:AH:169:ILE:HD12	1.77	0.50
7:AI:18:ILE:HG13	7:AI:19:LYS:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AI:24:PHE:H	7:AI:25:PRO:CD	2.23	0.50
39:BN:112:ILE:HG13	39:BN:133:VAL:HG13	1.92	0.50
61:Bl:70:PRO:HG2	61:Bl:111:ARG:HG3	1.94	0.50
67:Br:53:VAL:HG22	67:Br:67:VAL:HG22	1.92	0.50
77:HL:16:ILE:HD11	77:HL:210:GLY:HA3	1.94	0.50
2:AD:65:ARG:HG2	23:Ab:36:VAL:HG13	1.93	0.50
33:Am:257:ARG:HH11	33:Am:266:LYS:HE3	1.76	0.50
1:AA:1715:C:H42	1:AA:1769:G:H1	1.60	0.50
9:AK:63:PHE:HB3	9:AK:97:GLN:HB2	1.94	0.50
26:Ae:82:MET:N	26:Ae:82:MET:HE2	2.27	0.50
36:B2:1210:A:H5'	67:Br:76:HIS:HE1	1.77	0.50
36:B2:2681:G:H22	45:BT:68:ARG:HH12	1.59	0.50
61:Bl:5:LEU:HD12	64:Bo:41:ARG:HD2	1.93	0.50
1:AA:1194:C:H5'	1:AA:1214:C:H41	1.77	0.50
33:Am:62:HIS:HD2	33:Am:88:ARG:HD3	1.77	0.50
36:B2:253:U:H3'	36:B2:254:G:C8	2.46	0.50
36:B2:856:C:H5"	39:BN:20:ARG:HD3	1.94	0.50
36:B2:3369:A:H4'	36:B2:3370:U:H3'	1.93	0.50
36:B2:3430:U:H5"	40:BO:308:MET:HE3	1.93	0.50
74:By:54:VAL:HG21	74:By:103:ILE:HG13	1.92	0.50
76:HE:378:LEU:HD13	76:HE:405:VAL:HG22	1.93	0.50
1:AA:349:G:H5'	13:AO:76:LYS:HG3	1.94	0.49
1:AA:1383:G:H1'	1:AA:1384:G:H5'	1.93	0.49
1:AA:1569:U:H5"	7:AI:90:ARG:NH2	2.27	0.49
5:AG:124:VAL:O	5:AG:128:VAL:HG12	2.11	0.49
16:AR:36:THR:HG22	16:AR:38:LYS:H	1.77	0.49
36:B2:2002:G:H1	36:B2:2189:C:H42	1.60	0.49
40:BO:55:HIS:HB2	40:BO:360:ASP:HB2	1.94	0.49
47:BW:109:HIS:CD2	47:BW:123:TYR:H	2.30	0.49
77:HL:107:ASP:HA	77:HL:132:LYS:HD3	1.94	0.49
1:AA:330:U:H2'	1:AA:331:A:C8	2.47	0.49
1:AA:1417:A:H2'	1:AA:1420:A:N6	2.26	0.49
25:Ad:93:PHE:HZ	25:Ad:140:LYS:HB3	1.76	0.49
36:B2:1208:G:H5'	67:Br:19:ARG:HH22	1.77	0.49
36:B2:3042:G:C2	40:BO:250:ALA:HB1	2.47	0.49
9:AK:128:LEU:HD21	9:AK:175:TYR:CE1	2.48	0.49
42:BQ:132:THR:HB	42:BQ:172:PHE:HA	1.95	0.49
54:Be:11:ARG:HG3	54:Be:23:LEU:HD23	1.94	0.49
2:AD:78:VAL:HA	2:AD:125:VAL:HG22	1.94	0.49
6:AH:49:ARG:HA	6:AH:55:ALA:HB3	1.95	0.49
16:AR:85:ILE:HG22	16:AR:119:ASP:HA	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:B2:1592:A:H1'	59:Bj:33:ARG:HB2	1.94	0.49
43:BR:72:VAL:HA	43:BR:82:VAL:HG23	1.94	0.49
77:HL:3:LYS:HZ3	77:HL:197:TRP:CD1	2.31	0.49
7:AI:181:LYS:HE3	7:AI:183:SER:HB2	1.94	0.49
13:AO:126:ARG:HE	13:AO:127:PRO:HD2	1.77	0.49
17:AS:116:ARG:HG2	17:AS:117:PRO:HD2	1.94	0.49
30:Ai:16:VAL:HA	30:Ai:29:VAL:HG12	1.93	0.49
33:Am:128:THR:HG23	33:Am:143:THR:HG22	1.94	0.49
36:B2:2831:A:H4'	55:Bf:71:SER:HB2	1.94	0.49
36:B2:3430:U:H4'	40:BO:308:MET:HB3	1.94	0.49
1:AA:368:G:H5'	1:AA:770:A:H61	1.78	0.49
32:Ak:49:ASN:HD22	32:Ak:54:LYS:HE2	1.77	0.49
36:B2:466:U:H2'	36:B2:467:A:C5	2.47	0.49
51:Ba:143:SER:HA	51:Ba:146:VAL:HB	1.94	0.49
1:AA:761:C:H5"	24:Ac:82:LYS:HG3	1.95	0.49
16:AR:33:THR:HA	16:AR:41:ILE:HG22	1.93	0.49
25:Ad:100:VAL:HG12	25:Ad:125:VAL:HA	1.95	0.49
26:Ae:127:LYS:HE3	26:Ae:127:LYS:HA	1.95	0.49
36:B2:690:A:H1'	48:BX:14:PHE:HE2	1.77	0.49
42:BQ:260:ALA:HA	42:BQ:263:PHE:HD2	1.78	0.49
44:BS:143:THR:HG21	44:BS:239:ARG:HH21	1.78	0.49
76:HE:120:ARG:HH22	76:HE:481:MET:HE3	1.77	0.49
76:HE:473:GLU:HG3	76:HE:474:VAL:HG22	1.95	0.49
1:AA:1491:A:H5'	7:AI:163:ARG:CZ	2.42	0.49
6:AH:89:VAL:HG22	6:AH:100:ARG:HD3	1.95	0.49
13:AO:93:LYS:HG3	13:AO:94:TYR:HD1	1.78	0.49
36:B2:3093:G:H1'	36:B2:3498:U:H5'	1.94	0.49
38:B4:87:A:N6	38:B4:88:A:H61	2.11	0.49
45:BT:73:PRO:HA	45:BT:76:ALA:HB3	1.94	0.49
49:BY:12:ARG:HH11	49:BY:62:VAL:HG22	1.77	0.49
1:AA:1417:A:H2'	1:AA:1420:A:H61	1.78	0.49
7:AI:105:GLN:HB2	7:AI:109:GLN:HE22	1.77	0.49
20:AV:14:ARG:NH2	20:AV:17:ASN:HA	2.28	0.49
42:BQ:146:LEU:HD22	42:BQ:163:MET:HB2	1.93	0.49
76:HE:578:LYS:HZ3	76:HE:842:LEU:HD22	1.77	0.49
1:AA:178:A:H4'	1:AA:179:A:H5'	1.95	0.49
1:AA:1769:G:H2'	1:AA:1770:A:C8	2.48	0.49
8:AJ:23:ARG:HG2	8:AJ:41:VAL:HG13	1.93	0.49
9:AK:22:VAL:HG12	9:AK:87:PHE:HZ	1.78	0.49
24:Ac:25:VAL:HG22	24:Ac:63:ILE:HB	1.94	0.49
36:B2:808:U:H3'	63:Bn:40:ARG:HH21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:B4:132:G:H1	38:B4:137:A:H61	1.59	0.49
41:BP:22:ILE:HD11	41:BP:254:LYS:HG3	1.95	0.49
41:BP:107:THR:HG22	48:BX:26:PHE:HE2	1.77	0.49
1:AA:838:G:H2'	1:AA:839:G:C8	2.48	0.48
4:AF:224:LEU:HD12	24:Ac:68:ARG:HA	1.95	0.48
36:B2:1613:C:H5'	36:B2:1614:U:H5	1.77	0.48
37:B3:12:U:H1'	37:B3:108:G:H21	1.78	0.48
41:BP:11:TYR:CZ	41:BP:148:PRO:HB2	2.48	0.48
79:HI:19:THR:HG21	79:HI:82:ASP:HB3	1.95	0.48
81:BU:21:ILE:HG22	81:BU:26:VAL:HG22	1.95	0.48
1:AA:89:U:H3	1:AA:455:A:N6	2.12	0.48
1:AA:700:U:H1'	9:AK:100:ILE:HG21	1.94	0.48
7:AI:190:LYS:HE2	7:AI:191:LYS:HE2	1.94	0.48
8:AJ:142:ARG:HA	8:AJ:147:LEU:HD13	1.94	0.48
33:Am:34:GLY:HA2	33:Am:40:ILE:HG22	1.95	0.48
55:Bf:17:ARG:HD3	55:Bf:22:HIS:HA	1.95	0.48
3:AE:30:TYR:CE1	3:AE:48:VAL:HG22	2.48	0.48
4:AF:78:GLU:HG3	4:AF:185:ARG:HH11	1.78	0.48
8:AJ:137:ARG:HB2	8:AJ:140:LYS:HG2	1.95	0.48
26:Ae:57:ALA:HB1	26:Ae:73:ALA:HA	1.93	0.48
62:Bm:27:LYS:HE2	62:Bm:28:HIS:ND1	2.28	0.48
76:HE:815:PRO:HA	76:HE:818:ILE:HG12	1.94	0.48
6:AH:19:LEU:HD21	6:AH:108:ARG:HH11	1.77	0.48
13:AO:104:LEU:HD12	13:AO:105:ALA:N	2.26	0.48
17:AS:97:MET:HE2	17:AS:97:MET:N	2.29	0.48
36:B2:1457:C:OP1	74:By:23:PRO:HG3	2.13	0.48
56:Bg:22:ASP:O	56:Bg:23:LYS:HG2	2.12	0.48
1:AA:201:G:H2'	1:AA:202:G:C8	2.48	0.48
1:AA:213:U:H2'	1:AA:214:A:H8	1.78	0.48
18:AT:15:ALA:HA	18:AT:66:VAL:HG12	1.94	0.48
19:AU:41:ILE:HG13	19:AU:47:ARG:HB3	1.96	0.48
33:Am:68:ASP:HB3	33:Am:111:VAL:HG12	1.95	0.48
36:B2:1739:A:H4'	36:B2:1740:U:H5"	1.94	0.48
48:BX:63:ILE:HA	48:BX:66:ASN:ND2	2.28	0.48
49:BY:58:LEU:HD23	49:BY:58:LEU:H	1.77	0.48
55:Bf:126:VAL:HG23	55:Bf:127:GLN:H	1.79	0.48
56:Bg:66:HIS:C	56:Bg:67:ILE:HD13	2.38	0.48
7:AI:61:ARG:HE	7:AI:64:ARG:HE	1.61	0.48
44:BS:184:TYR:CZ	44:BS:205:GLN:HG2	2.49	0.48
53:Bd:35:ALA:HA	53:Bd:40:ASN:HD22	1.79	0.48
77:HL:169:GLY:HA3	77:HL:173:MET:HE1	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:HS:6:ALA:HB2	78:HS:95:PRO:HB3	1.95	0.48
1:AA:1332:U:H2'	1:AA:1333:G:C8	2.48	0.48
5:AG:57:THR:HG23	5:AG:61:LEU:HG	1.95	0.48
7:AI:47:PRO:HG3	18:AT:47:GLU:OE1	2.13	0.48
21:AW:63:HIS:O	21:AW:66:LEU:HD23	2.13	0.48
39:BN:208:HIS:CD2	39:BN:210:HIS:H	2.31	0.48
77:HL:89:LEU:HD11	77:HL:123:LEU:HD11	1.96	0.48
1:AA:570:A:H5'	32:Ak:10:ARG:HH21	1.79	0.48
1:AA:884:A:H5'	15:AQ:90:ASN:ND2	2.25	0.48
36:B2:1893:C:H4'	36:B2:1894:A:O5'	2.14	0.48
76:HE:189:ILE:O	76:HE:193:TYR:HB2	2.14	0.48
2:AD:53:LEU:HA	2:AD:56:THR:HB	1.96	0.48
8:AJ:7:TYR:HD1	8:AJ:113:ILE:HG23	1.78	0.48
9:AK:73:HIS:HA	9:AK:133:PHE:HZ	1.79	0.48
14:AP:97:PRO:HB3	14:AP:122:SER:HB3	1.95	0.48
16:AR:135:ARG:HE	16:AR:138:ARG:NH1	2.12	0.48
51:Ba:176:GLN:HA	51:Ba:179:ILE:HG22	1.96	0.48
3:AE:71:ALA:HB2	3:AE:80:ALA:HA	1.96	0.48
6:AH:56:LEU:HD22	26:Ae:20:ARG:HD2	1.96	0.48
6:AH:166:THR:H	6:AH:168:LYS:NZ	2.11	0.48
33:Am:220:ASP:HB3	33:Am:223:GLU:HB3	1.94	0.48
33:Am:278:GLY:H	33:Am:281:SER:HB2	1.78	0.48
36:B2:2730:A:H2	36:B2:2737:A:H62	1.62	0.48
48:BX:129:LYS:HE2	48:BX:132:GLN:HG3	1.95	0.48
76:HE:203:PHE:HB2	76:HE:206:LYS:HD3	1.96	0.48
76:HE:225:PHE:HE1	76:HE:328:LEU:HD11	1.78	0.48
20:AV:110:ASP:CA	20:AV:113:ARG:HD2	2.34	0.47
28:Ag:28:ARG:HE	28:Ag:29:ALA:H	1.62	0.47
79:HI:95:ASN:HB3	79:HI:102:ASN:HD22	1.79	0.47
1:AA:599:C:H2'	1:AA:600:G:H8	1.79	0.47
7:AI:178:ASN:HB3	7:AI:186:SER:HB3	1.95	0.47
11:AM:96:VAL:HG13	11:AM:97:LEU:HD22	1.96	0.47
18:AT:81:ALA:HA	18:AT:84:LYS:HE3	1.97	0.47
33:Am:66:VAL:HA	33:Am:82:SER:HA	1.96	0.47
36:B2:1300:U:H1'	36:B2:1303:C:H5	1.79	0.47
40:BO:21:ARG:HG2	40:BO:272:TYR:HD2	1.79	0.47
72:Bw:58:ARG:HH11	72:Bw:59:GLN:HG2	1.77	0.47
74:By:63:GLY:H	74:By:127:GLN:HE22	1.61	0.47
1:AA:1555:U:O2'	5:AG:8:SER:HA	2.15	0.47
1:AA:1802:G:H1'	1:AA:1803:U:H5'	1.96	0.47
5:AG:37:SER:HB3	5:AG:101:VAL:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AK:152:ILE:HG23	9:AK:183:VAL:HG23	1.94	0.47
10:AL:104:ILE:HG22	10:AL:165:LEU:HB3	1.97	0.47
26:Ae:5:VAL:HG21	26:Ae:27:ILE:HG23	1.95	0.47
36:B2:1310:C:H2'	36:B2:1311:C:C6	2.49	0.47
36:B2:2300:C:H2'	36:B2:2318:C:H42	1.79	0.47
61:Bl:72:ILE:HG22	61:Bl:101:PHE:HE2	1.78	0.47
74:By:52:LYS:HE2	74:By:108:TYR:HA	1.96	0.47
76:HE:26:ALA:HB2	76:HE:128:VAL:HB	1.96	0.47
76:HE:438:MET:HG2	76:HE:439:GLY:H	1.79	0.47
4:AF:109:HIS:HB3	4:AF:135:ILE:HD11	1.95	0.47
8:AJ:64:PHE:HB2	8:AJ:97:VAL:HG21	1.96	0.47
20:AV:27:MET:HB2	20:AV:52:MET:HE1	1.95	0.47
24:Ac:36:LYS:HA	24:Ac:39:THR:HG22	1.96	0.47
39:BN:5:ILE:HG13	39:BN:7:ALA:H	1.79	0.47
50:BZ:165:THR:HG23	50:BZ:168:GLY:H	1.80	0.47
60:Bk:82:GLU:OE1	60:Bk:83:ARG:HG2	2.14	0.47
73:Bx:24:PRO:HG2	73:Bx:27:ILE:HG13	1.96	0.47
82:Bb:2:VAL:HG22	82:Bb:3:ARG:H	1.79	0.47
1:AA:792:A:H61	26:Ae:8:ARG:HH11	1.62	0.47
1:AA:1699:G:O2'	1:AA:1700:A:H8	1.98	0.47
2:AD:124:ILE:HG23	2:AD:146:VAL:HG23	1.96	0.47
13:AO:126:ARG:NE	13:AO:127:PRO:HD2	2.29	0.47
33:Am:251:ALA:HA	33:Am:256:ILE:HD12	1.96	0.47
38:B4:57:G:H5'	69:Bt:46:ILE:HD11	1.96	0.47
59:Bj:58:GLU:HA	59:Bj:61:ILE:HD12	1.97	0.47
76:HE:25:ILE:HD11	76:HE:127:VAL:HG22	1.96	0.47
76:HE:593:MET:HE3	76:HE:685:ARG:HB2	1.95	0.47
1:AA:708:U:H2'	1:AA:709:G:C8	2.49	0.47
6:AH:185:GLY:HA2	6:AH:189:MET:HE3	1.96	0.47
18:AT:56:LYS:HE3	18:AT:90:TYR:CE2	2.50	0.47
36:B2:2341:G:H2'	36:B2:2342:U:H5'	1.96	0.47
40:BO:281:LYS:HD3	40:BO:325:ASN:ND2	2.30	0.47
1:AA:813:C:H2'	1:AA:814:A:C8	2.50	0.47
1:AA:1508:G:H3'	1:AA:1556:A:H61	1.79	0.47
7:AI:50:HIS:CE1	7:AI:89:THR:HG21	2.50	0.47
22:Aa:28:ASN:HB3	22:Aa:31:ASN:HB2	1.96	0.47
25:Ad:76:LYS:HG3	25:Ad:77:ASN:OD1	2.15	0.47
30:Ai:11:ALA:HB1	30:Ai:31:VAL:HB	1.96	0.47
36:B2:2618:G:H1	39:BN:69:ARG:HH21	1.62	0.47
36:B2:2776:U:OP1	47:BW:51:ARG:HD3	2.15	0.47
36:B2:2802:U:H5'	75:H1:34:ARG:NH1	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:BP:324:LYS:HA	41:BP:327:LEU:HB3	1.97	0.47
45:BT:157:VAL:HG12	45:BT:183:LYS:HD3	1.96	0.47
51:Ba:4:PHE:HE2	67:Br:34:GLU:HB3	1.78	0.47
14:AP:96:ASP:HB3	14:AP:99:VAL:HG23	1.97	0.47
41:BP:142:HIS:HB3	41:BP:144:ILE:HD12	1.97	0.47
76:HE:465:LYS:HD2	76:HE:516:PRO:HA	1.96	0.47
78:HS:53:THR:HG22	78:HS:55:ASN:H	1.79	0.47
1:AA:253:C:H2'	1:AA:254:A:C8	2.49	0.47
1:AA:643:U:H2'	1:AA:644:G:C8	2.49	0.47
1:AA:1817:U:H2'	1:AA:1818:A:C8	2.50	0.47
6:AH:128:ARG:HB2	6:AH:130:GLN:HE22	1.80	0.47
13:AO:96:ARG:HB3	25:Ad:10:ALA:HB2	1.96	0.47
15:AQ:88:LEU:O	15:AQ:92:ILE:HG13	2.14	0.47
16:AR:49:LYS:HG2	16:AR:64:LEU:HB3	1.96	0.47
21:AW:51:ASP:O	21:AW:55:VAL:HG22	2.15	0.47
29:Ah:20:LYS:HE2	29:Ah:21:LEU:HD22	1.97	0.47
33:Am:40:ILE:HG13	33:Am:59:LEU:HB2	1.96	0.47
33:Am:159:ASN:HB3	33:Am:204:GLY:HA3	1.96	0.47
36:B2:1497:U:H3	36:B2:1501:A:H62	1.63	0.47
36:B2:3343:A:H4'	40:BO:95:THR:HB	1.96	0.47
1:AA:307:U:H5"	13:AO:133:ARG:HG3	1.97	0.47
2:AD:105:PHE:HE2	2:AD:135:ALA:HA	1.79	0.47
4:AF:95:THR:HG21	75:H1:144:LEU:HD13	1.97	0.47
27:Af:22:PHE:HA	27:Af:26:ILE:HD12	1.96	0.47
36:B2:1525:A:N7	73:Bx:2:PRO:HB3	2.30	0.47
59:Bj:130:ASP:HB3	59:Bj:133:ASP:HB3	1.97	0.47
76:HE:725:GLN:HG3	76:HE:803:PRO:HG3	1.96	0.47
1:AA:489:G:H1	1:AA:504:U:H3	1.63	0.46
6:AH:41:CYS:HB2	6:AH:83:PRO:HB2	1.96	0.46
7:AI:29:VAL:HG12	7:AI:31:VAL:N	2.31	0.46
17:AS:91:MET:HB3	17:AS:124:LEU:HD22	1.96	0.46
36:B2:742:A:C8	62:Bm:114:LYS:HD2	2.50	0.46
55:Bf:38:ASP:OD1	55:Bf:38:ASP:C	2.58	0.46
55:Bf:70:SER:O	55:Bf:93:ILE:HG23	2.15	0.46
76:HE:300:LEU:HD11	76:HE:307:ILE:HD12	1.97	0.46
76:HE:676:MET:HG2	76:HE:832:VAL:HG21	1.98	0.46
1:AA:1481:C:H2'	1:AA:1482:G:C8	2.51	0.46
2:AD:75:ASP:HB2	2:AD:122:ARG:HB2	1.97	0.46
5:AG:70:GLU:HG3	12:AN:20:VAL:HG22	1.95	0.46
9:AK:66:GLN:N	9:AK:67:PRO:HD2	2.30	0.46
13:AO:54:LYS:HD2	13:AO:128:LEU:HG	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:B2:547:G:H4'	36:B2:547:G:OP2	2.13	0.46
36:B2:645:U:H4'	83:A:166:ARG:HH22	1.81	0.46
81:BU:37:GLN:HB3	81:BU:78:MET:HE1	1.97	0.46
7:AI:66:PHE:O	7:AI:70:ARG:HG2	2.15	0.46
21:AW:61:ALA:O	21:AW:64:ILE:HG22	2.15	0.46
36:B2:191:U:H2'	36:B2:193:U:C4	2.50	0.46
36:B2:3389:A:C2'	36:B2:3390:G:H2'	2.46	0.46
1:AA:1086:C:H4'	29:Ah:17:ARG:HG3	1.96	0.46
2:AD:60:LEU:HD11	2:AD:180:LEU:HG	1.98	0.46
8:AJ:49:VAL:HG23	8:AJ:114:VAL:HB	1.98	0.46
9:AK:146:THR:HA	24:Ac:42:GLN:HE21	1.81	0.46
32:Ak:29:GLN:HG2	32:Ak:30:PRO:HD2	1.97	0.46
36:B2:277:G:H1	50:BZ:15:GLN:HE21	1.64	0.46
36:B2:2770:C:H1'	47:BW:23:LEU:HD12	1.97	0.46
37:B3:12:U:H4'	37:B3:13:A:OP2	2.16	0.46
46:BV:51:HIS:CD2	46:BV:168:SER:HB2	2.50	0.46
76:HE:221:THR:HG23	76:HE:223:ARG:H	1.79	0.46
76:HE:711:ARG:HH21	76:HE:838:TYR:HA	1.81	0.46
78:HS:99:HIS:CD2	78:HS:100:GLY:H	2.33	0.46
1:AA:16:G:H21	1:AA:1154:A:H62	1.63	0.46
2:AD:202:ASP:HA	2:AD:205:PHE:CD2	2.50	0.46
6:AH:98:HIS:HB2	6:AH:114:ILE:O	2.15	0.46
13:AO:130:LYS:HG3	13:AO:131:THR:HG23	1.97	0.46
16:AR:113:ARG:HE	28:Ag:56:ALA:HA	1.81	0.46
55:Bf:125:THR:HG22	55:Bf:126:VAL:H	1.80	0.46
76:HE:613:LYS:HD2	76:HE:613:LYS:HA	1.66	0.46
2:AD:180:LEU:HA	2:AD:183:GLU:HG2	1.97	0.46
13:AO:22:ASN:HD21	13:AO:24:LYS:HB2	1.80	0.46
23:Ab:76:ASP:HB3	23:Ab:78:LEU:HD12	1.98	0.46
33:Am:166:VAL:HG22	33:Am:176:VAL:HG22	1.97	0.46
36:B2:997:A:H5"	48:BX:4:HIS:HB3	1.98	0.46
36:B2:1683:A:H62	36:B2:1848:G:H21	1.64	0.46
46:BV:200:LEU:HB2	46:BV:213:PHE:HE2	1.80	0.46
1:AA:885:U:H2'	1:AA:886:A:C8	2.51	0.46
1:AA:1332:U:H2'	1:AA:1333:G:H8	1.81	0.46
9:AK:141:ARG:HD3	24:Ac:51:THR:OG1	2.15	0.46
11:AM:140:ILE:HG21	26:Ae:65:GLY:HA3	1.98	0.46
17:AS:129:ILE:HD11	17:AS:131:TYR:CE2	2.51	0.46
19:AU:69:ILE:HB	19:AU:74:GLN:HB2	1.95	0.46
20:AV:18:THR:HG21	20:AV:33:ILE:HB	1.98	0.46
61:Bl:61:ARG:HG2	61:Bl:64:ARG:HH22	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:Bm:75:LEU:HG	62:Bm:113:GLY:HA2	1.98	0.46
7:AI:71:LEU:HD11	7:AI:92:VAL:HG21	1.98	0.46
9:AK:34:LYS:HG3	9:AK:35:ASP:H	1.80	0.46
9:AK:91:HIS:HE1	9:AK:166:TYR:HE2	1.64	0.46
19:AU:69:ILE:HG21	19:AU:73:LEU:HD22	1.98	0.46
24:Ac:75:ILE:HG13	24:Ac:125:ILE:HG22	1.98	0.46
68:Bs:37:LYS:HG3	68:Bs:58:ARG:HH12	1.81	0.46
75:H1:37:SER:O	75:H1:39:PRO:HD3	2.16	0.46
76:HE:131:THR:HG21	76:HE:160:VAL:HA	1.97	0.46
82:Bb:35:THR:HG21	82:Bb:58:VAL:HG13	1.97	0.46
1:AA:104:A:H4'	1:AA:105:A:O5'	2.15	0.46
4:AF:128:ILE:O	4:AF:132:LYS:HG3	2.15	0.46
17:AS:94:LEU:HD13	17:AS:95:PRO:HD2	1.98	0.46
29:Ah:2:VAL:HG22	29:Ah:3:LEU:HD23	1.97	0.46
30:Ai:32:GLU:CD	30:Ai:33:PHE:N	2.74	0.46
40:BO:171:LEU:HD21	40:BO:333:LYS:HB2	1.96	0.46
50:BZ:73:ARG:H	50:BZ:89:VAL:HG23	1.81	0.46
51:Ba:52:LYS:HB3	51:Ba:52:LYS:HE3	1.57	0.46
57:Bh:21:VAL:HG12	57:Bh:22:GLN:HG2	1.98	0.46
82:Bb:52:LYS:HB3	82:Bb:52:LYS:HE2	1.78	0.46
1:AA:457:A:H61	26:Ae:84:LYS:HE2	1.80	0.46
29:Ah:19:HIS:CE1	29:Ah:21:LEU:HB2	2.50	0.46
39:BN:29:ARG:HH21	39:BN:40:ILE:HD13	1.80	0.46
40:BO:8:GLN:HG2	40:BO:9:PRO:HD2	1.97	0.46
44:BS:111:MET:HG3	44:BS:116:LEU:HB2	1.99	0.46
76:HE:432:GLN:HB3	76:HE:457:VAL:HG23	1.98	0.46
1:AA:809:U:H5"	1:AA:810:U:H5	1.81	0.45
6:AH:21:ASP:HB2	6:AH:24:SER:HB3	1.98	0.45
23:Ab:78:LEU:HD12	23:Ab:78:LEU:H	1.81	0.45
25:Ad:77:ASN:HB2	25:Ad:79:LYS:HG3	1.99	0.45
42:BQ:61:THR:HG22	42:BQ:79:HIS:CD2	2.51	0.45
46:BV:103:LEU:HD23	46:BV:103:LEU:HA	1.75	0.45
55:Bf:126:VAL:HB	55:Bf:128:LEU:HD23	1.97	0.45
57:Bh:41:VAL:HG13	57:Bh:60:VAL:HG12	1.98	0.45
79:HI:57:LYS:HD3	79:HI:74:MET:HE2	1.96	0.45
1:AA:650:G:H22	1:AA:692:G:H22	1.64	0.45
6:AH:114:ILE:HG13	6:AH:115:THR:N	2.31	0.45
14:AP:64:LEU:HD22	14:AP:126:VAL:HG12	1.97	0.45
17:AS:48:ARG:HA	17:AS:48:ARG:HD2	1.74	0.45
24:Ac:36:LYS:HD3	24:Ac:110:ILE:HB	1.97	0.45
26:Ae:20:ARG:HE	26:Ae:74:LEU:HB2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:BO:311:PHE:HB2	40:BO:314:TYR:HB3	1.97	0.45
54:Be:131:LYS:HG2	54:Be:131:LYS:O	2.16	0.45
76:HE:501:LEU:N	76:HE:502:PRO:HD2	2.31	0.45
76:HE:567:VAL:HG23	76:HE:592:PRO:HB3	1.98	0.45
81:BU:44:ILE:HD11	81:BU:55:PHE:HB3	1.98	0.45
7:AI:81:ASN:HD22	7:AI:158:ARG:HH22	1.63	0.45
22:Aa:30:ARG:HH21	22:Aa:34:LYS:HB3	1.82	0.45
36:B2:991:C:H41	36:B2:2896:A:H5"	1.81	0.45
36:B2:1370:C:H5'	66:Bq:57:ASN:HA	1.98	0.45
36:B2:2479:G:N2	40:BO:266:ARG:HH21	2.14	0.45
51:Ba:114:ASP:OD2	51:Ba:114:ASP:C	2.59	0.45
52:Bc:78:GLU:HA	52:Bc:78:GLU:OE1	2.16	0.45
53:Bd:38:ARG:HA	53:Bd:41:ILE:HB	1.98	0.45
54:Be:131:LYS:HG3	54:Be:143:LEU:HD12	1.97	0.45
65:Bp:21:MET:HE1	65:Bp:37:ALA:HA	1.98	0.45
65:Bp:60:LEU:HD11	65:Bp:78:LEU:HD22	1.99	0.45
68:Bs:37:LYS:H	68:Bs:37:LYS:HG2	1.47	0.45
76:HE:27:HIS:HD2	76:HE:28:VAL:HG23	1.81	0.45
76:HE:30:HIS:HE2	76:HE:130:ASP:HB2	1.81	0.45
76:HE:424:ASP:CG	76:HE:425:ASP:H	2.24	0.45
1:AA:70:C:H2'	1:AA:71:A:C8	2.51	0.45
1:AA:475:G:H2'	1:AA:476:A:C8	2.51	0.45
6:AH:94:LYS:HB3	6:AH:94:LYS:HE3	1.68	0.45
15:AQ:4:MET:HG3	15:AQ:5:HIS:CE1	2.52	0.45
36:B2:1942:A:H4'	40:BO:227:GLU:HA	1.97	0.45
38:B4:22:C:H5"	82:Bb:123:PRO:HG3	1.98	0.45
40:BO:58:ARG:HH21	40:BO:72:ILE:HD11	1.81	0.45
42:BQ:140:ARG:HG2	42:BQ:141:PRO:HD2	1.99	0.45
42:BQ:143:LYS:HG2	42:BQ:172:PHE:HD2	1.81	0.45
43:BR:146:LYS:H	43:BR:146:LYS:HG2	1.55	0.45
46:BV:103:LEU:HD11	46:BV:111:LEU:HD22	1.98	0.45
77:HL:209:MET:HE3	77:HL:209:MET:HA	1.99	0.45
1:AA:1699:G:HO2'	1:AA:1700:A:H8	1.63	0.45
4:AF:158:SER:HB3	4:AF:167:ARG:HD2	1.98	0.45
20:AV:113:ARG:O	20:AV:117:ILE:HG23	2.16	0.45
36:B2:2328:G:O2'	39:BN:241:ARG:HG2	2.17	0.45
40:BO:161:LEU:HD23	40:BO:180:GLU:HG2	1.98	0.45
44:BS:97:ILE:HG23	44:BS:226:LYS:HE2	1.99	0.45
51:Ba:77:PRO:HA	51:Ba:80:ILE:HD12	1.98	0.45
53:Bd:119:LEU:HD12	53:Bd:119:LEU:O	2.17	0.45
58:Bi:46:PRO:HB2	58:Bi:54:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:Br:49:ARG:HG3	67:Br:105:PRO:HD3	1.98	0.45
76:HE:647:VAL:HB	76:HE:687:ASN:HB3	1.97	0.45
76:HE:735:VAL:HG11	76:HE:743:ILE:HG21	1.99	0.45
81:BU:101:ILE:HG13	81:BU:142:ILE:HD11	1.98	0.45
1:AA:401:G:O2'	1:AA:402:A:H5"	2.17	0.45
1:AA:556:G:H3'	1:AA:557:C:H2'	1.97	0.45
1:AA:706:U:H3	1:AA:752:G:H1	1.63	0.45
1:AA:895:C:H2'	1:AA:896:A:C8	2.52	0.45
4:AF:56:TYR:CZ	4:AF:137:PRO:HD3	2.52	0.45
7:AI:178:ASN:HD21	7:AI:185:ASN:HB3	1.82	0.45
8:AJ:14:LYS:HD3	8:AJ:14:LYS:HA	1.80	0.45
10:AL:22:ARG:HE	10:AL:23:LYS:N	2.15	0.45
21:AW:37:VAL:HG12	21:AW:39:THR:H	1.81	0.45
24:Ac:22:ARG:HA	24:Ac:22:ARG:HE	1.80	0.45
28:Ag:72:GLN:OE1	28:Ag:72:GLN:HA	2.16	0.45
36:B2:1755:A:C8	64:Bo:90:LEU:HD13	2.52	0.45
36:B2:2589:U:H3'	36:B2:2590:A:C5'	2.42	0.45
47:BW:172:LEU:HD23	47:BW:172:LEU:HA	1.81	0.45
1:AA:1819:G:H2'	1:AA:1820:G:C8	2.51	0.45
2:AD:40:VAL:HG23	2:AD:49:HIS:HD2	1.82	0.45
2:AD:80:SER:HB2	2:AD:89:VAL:HG21	1.98	0.45
9:AK:10:ARG:HB3	9:AK:45:ILE:HB	1.97	0.45
11:AM:110:GLN:HB3	11:AM:122:ILE:HD11	1.98	0.45
17:AS:96:GLU:C	17:AS:97:MET:HE2	2.41	0.45
41:BP:101:MET:SD	41:BP:104:PRO:HA	2.57	0.45
41:BP:127:ALA:HA	41:BP:246:LEU:HD23	1.99	0.45
48:BX:89:VAL:O	48:BX:93:ILE:HG12	2.17	0.45
48:BX:124:ILE:HD11	69:Bt:121:LYS:HB3	1.98	0.45
51:Ba:138:THR:HG22	51:Ba:140:GLY:H	1.82	0.45
54:Be:158:VAL:HG23	54:Be:159:VAL:HG12	1.99	0.45
69:Bt:47:LYS:HE3	69:Bt:47:LYS:HB2	1.75	0.45
1:AA:1249:U:H2'	1:AA:1250:G:C8	2.52	0.45
1:AA:1324:U:H5	1:AA:1335:G:H21	1.65	0.45
4:AF:224:LEU:HD21	23:Ab:23:ILE:HD13	1.99	0.45
7:AI:19:LYS:HD3	7:AI:20:LEU:H	1.80	0.45
11:AM:76:ILE:HD12	11:AM:76:ILE:HA	1.82	0.45
13:AO:79:ARG:HD3	13:AO:79:ARG:HA	1.74	0.45
21:AW:27:LYS:HD2	21:AW:27:LYS:HA	1.71	0.45
24:Ac:24:GLN:NE2	29:Ah:5:VAL:HG12	2.31	0.45
28:Ag:23:CYS:HB3	28:Ag:27:SER:N	2.31	0.45
33:Am:8:ARG:HG3	33:Am:311:GLN:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:B1:29:ILE:HG21	39:BN:176:LYS:HG3	1.98	0.45
36:B2:197:U:H2'	60:Bk:59:ARG:HH22	1.82	0.45
39:BN:129:SER:HB2	39:BN:170:GLY:HA3	1.99	0.45
40:BO:68:HIS:O	40:BO:70:ARG:HG2	2.17	0.45
50:BZ:14:LYS:HA	50:BZ:14:LYS:HD3	1.76	0.45
1:AA:315:A:H4'	1:AA:316:U:H3'	1.97	0.45
1:AA:328:G:H2'	1:AA:329:G:H8	1.81	0.45
1:AA:999:G:H2'	1:AA:1000:G:H8	1.82	0.45
2:AD:147:ILE:HD12	2:AD:147:ILE:HA	1.80	0.45
7:AI:187:TYR:HA	7:AI:190:LYS:HG2	1.99	0.45
10:AL:168:VAL:HG23	10:AL:184:LEU:HD23	1.99	0.45
15:AQ:88:LEU:HD21	15:AQ:125:LEU:HD13	1.98	0.45
35:B1:51:ALA:HB1	39:BN:49:HIS:HB3	1.99	0.45
36:B2:1345:C:H5'	51:Ba:18:GLY:HA3	1.98	0.45
36:B2:1999:U:H2'	36:B2:2000:A:C8	2.52	0.45
36:B2:3217:U:H1'	36:B2:3218:A:H5"	1.99	0.45
40:BO:358:TRP:HZ3	58:Bi:15:PRO:HG2	1.81	0.45
69:Bt:85:LYS:HD2	69:Bt:85:LYS:HA	1.79	0.45
1:AA:546:C:H5"	1:AA:547:A:OP2	2.15	0.45
1:AA:693:G:H2'	1:AA:694:G:H8	1.82	0.45
3:AE:82:ARG:HH12	3:AE:213:ARG:HA	1.82	0.45
10:AL:193:LEU:HD23	10:AL:193:LEU:HA	1.82	0.45
17:AS:41:LEU:HD11	17:AS:95:PRO:HG3	2.00	0.45
36:B2:946:A:N1	39:BN:203:MET:HE2	2.31	0.45
36:B2:2668:C:H5'	61:Bl:61:ARG:HH11	1.82	0.45
40:BO:215:ILE:HD13	40:BO:282:ILE:HD11	1.99	0.45
47:BW:8:PRO:HB2	47:BW:9:MET:H	1.61	0.45
51:Ba:59:LEU:HA	51:Ba:73:HIS:CD2	2.52	0.45
76:HE:220:PHE:HB3	76:HE:328:LEU:HD13	1.99	0.45
81:BU:41:ARG:HG2	81:BU:42:VAL:HG13	1.98	0.45
1:AA:1165:G:H2'	1:AA:1167:A:H8	1.83	0.44
1:AA:1600:A:H5"	20:AV:133:GLY:H	1.82	0.44
2:AD:55:LYS:HA	2:AD:58:GLU:HG2	1.98	0.44
2:AD:65:ARG:HD3	23:Ab:45:GLN:HE22	1.82	0.44
4:AF:44:VAL:HG21	4:AF:67:ILE:HG23	1.98	0.44
4:AF:204:LYS:HB2	4:AF:204:LYS:HE3	1.73	0.44
8:AJ:147:LEU:HD23	8:AJ:151:ASP:HB3	1.98	0.44
9:AK:168:LEU:HB2	9:AK:185:PHE:HD2	1.82	0.44
17:AS:85:LYS:HD2	17:AS:85:LYS:HA	1.74	0.44
19:AU:59:LYS:O	19:AU:63:ARG:HD3	2.17	0.44
20:AV:38:ARG:HB3	21:AW:45:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Am:3:GLU:HB3	33:Am:312:VAL:HG12	1.98	0.44
46:BV:211:ASP:C	46:BV:211:ASP:OD2	2.60	0.44
52:Bc:186:LYS:HD2	52:Bc:187:VAL:HG23	1.99	0.44
76:HE:380:ILE:HD11	76:HE:469:LEU:HD12	2.00	0.44
1:AA:117:U:H2'	1:AA:118:U:C6	2.52	0.44
1:AA:613:G:H21	25:Ad:17:ARG:HH21	1.64	0.44
1:AA:939:A:H2'	1:AA:940:G:C8	2.52	0.44
1:AA:1653:A:H5"	7:AI:70:ARG:HH21	1.82	0.44
5:AG:41:VAL:HG12	5:AG:50:ILE:HD12	1.99	0.44
5:AG:53:ARG:CZ	5:AG:93:VAL:HG22	2.48	0.44
13:AO:77:MET:SD	13:AO:80:THR:HB	2.57	0.44
20:AV:38:ARG:N	20:AV:38:ARG:HD2	2.32	0.44
25:Ad:68:LYS:HG3	25:Ad:91:LEU:HD22	2.00	0.44
36:B2:203:G:H21	36:B2:226:A:H61	1.65	0.44
36:B2:463:C:H2'	36:B2:464:A:C8	2.52	0.44
36:B2:1287:G:H2'	36:B2:1288:C:C6	2.52	0.44
36:B2:1639:U:H2'	36:B2:1639:U:O2	2.15	0.44
36:B2:2550:A:H5"	36:B2:2580:A:H2	1.83	0.44
36:B2:3138:U:O3'	57:Bh:47:ARG:HD3	2.16	0.44
36:B2:3336:G:H2'	36:B2:3337:A:C8	2.52	0.44
37:B3:60:C:H5"	42:BQ:274:LYS:HG2	1.99	0.44
39:BN:102:PRO:HG2	39:BN:105:GLU:HB2	1.99	0.44
40:BO:193:GLU:O	40:BO:197:GLU:HG2	2.17	0.44
50:BZ:152:VAL:HG21	69:Bt:94:LEU:HD13	2.00	0.44
60:Bk:50:ARG:HG2	60:Bk:51:ARG:N	2.31	0.44
76:HE:585:ARG:HB2	76:HE:692:VAL:HB	2.00	0.44
76:HE:788:THR:HG21	76:HE:792:ALA:HB3	1.98	0.44
1:AA:282:G:H2'	1:AA:283:C:H4'	1.98	0.44
6:AH:56:LEU:HD21	26:Ae:18:LEU:HD22	1.99	0.44
8:AJ:70:PRO:HB3	8:AJ:101:ILE:HD11	1.98	0.44
25:Ad:107:ARG:HD3	25:Ad:112:LYS:HB3	2.00	0.44
30:Ai:26:VAL:HG12	30:Ai:46:LYS:HA	1.99	0.44
36:B2:546:G:H22	54:Be:143:LEU:HB3	1.81	0.44
36:B2:1855:U:O2	36:B2:1855:U:H2'	2.18	0.44
36:B2:3328:U:H4'	36:B2:3329:G:O5'	2.16	0.44
48:BX:67:MET:HG2	62:Bm:104:LEU:HG	1.99	0.44
72:Bw:31:LYS:HB2	72:Bw:31:LYS:HE2	1.83	0.44
1:AA:781:C:C2	11:AM:143:VAL:HG21	2.52	0.44
1:AA:906:A:H2'	1:AA:907:A:H8	1.82	0.44
1:AA:1165:G:H2'	1:AA:1167:A:C8	2.53	0.44
16:AR:85:ILE:HD12	16:AR:85:ILE:HA	1.87	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Am:149:ASP:HB3	33:Am:171:ASP:HB3	1.98	0.44
36:B2:2555:G:H21	36:B2:2584:A:H62	1.66	0.44
36:B2:2867:C:H4'	36:B2:2868:C:OP2	2.17	0.44
37:B3:80:A:H61	37:B3:96:U:H3	1.65	0.44
39:BN:241:ARG:HH22	39:BN:244:LEU:C	2.25	0.44
52:Bc:102:VAL:HG13	52:Bc:107:PHE:HZ	1.83	0.44
54:Be:11:ARG:HH12	54:Be:14:PRO:HG3	1.81	0.44
1:AA:1602:U:H2'	1:AA:1603:G:C8	2.52	0.44
36:B2:713:G:H4'	36:B2:714:A:H2'	2.00	0.44
75:H1:33:LYS:HE3	75:H1:33:LYS:HB3	1.68	0.44
76:HE:112:SER:HB2	76:HE:485:VAL:HB	1.99	0.44
76:HE:508:LEU:HD13	76:HE:511:LEU:HD21	1.99	0.44
77:HL:84:MET:HE3	77:HL:88:ASP:HB3	1.98	0.44
1:AA:388:A:H5"	10:AL:22:ARG:NH1	2.32	0.44
1:AA:875:U:H2'	1:AA:876:U:C6	2.53	0.44
1:AA:1168:A:H2'	1:AA:1169:G:C8	2.52	0.44
1:AA:1589:G:H4'	20:AV:87:GLN:HB2	1.99	0.44
3:AE:83:LYS:HG3	3:AE:104:SER:HB3	2.00	0.44
4:AF:136:MET:HE3	4:AF:218:SER:HB2	1.99	0.44
4:AF:187:LEU:HD12	4:AF:192:ILE:HB	2.00	0.44
7:AI:47:PRO:HG2	7:AI:48:LEU:HD12	1.99	0.44
10:AL:104:ILE:HD12	10:AL:104:ILE:HA	1.89	0.44
12:AN:21:LEU:HD23	12:AN:66:TYR:CD2	2.53	0.44
36:B2:3362:C:H3'	36:B2:3363:C:H5"	1.99	0.44
52:Bc:177:ARG:HG2	62:Bm:53:PHE:O	2.17	0.44
55:Bf:112:ASN:OD1	55:Bf:128:LEU:HD12	2.18	0.44
21:AW:14:PHE:HB2	21:AW:138:LEU:HD21	1.99	0.44
33:Am:149:ASP:CG	33:Am:150:TRP:H	2.25	0.44
36:B2:946:A:C6	39:BN:203:MET:HE2	2.53	0.44
37:B3:76:U:O2'	37:B3:77:A:H8	2.01	0.44
39:BN:116:GLU:HG2	39:BN:123:GLY:N	2.33	0.44
66:Bq:85:HIS:HB3	66:Bq:89:TYR:HD1	1.82	0.44
72:Bw:58:ARG:HA	72:Bw:61:LEU:HD23	1.99	0.44
76:HE:438:MET:CG	76:HE:439:GLY:H	2.31	0.44
76:HE:545:LEU:HD22	76:HE:554:LEU:HD13	2.00	0.44
1:AA:45:U:H3	1:AA:437:G:H1'	1.82	0.44
1:AA:1621:C:H4'	18:AT:134:ARG:HG2	1.99	0.44
1:AA:1777:U:H2'	1:AA:1778:G:C8	2.53	0.44
2:AD:25:CYS:HA	2:AD:166:ASN:OD1	2.18	0.44
3:AE:141:GLY:HA2	3:AE:210:VAL:HG22	1.99	0.44
4:AF:110:VAL:HG21	4:AF:186:PHE:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AF:226:PRO:HA	4:AF:229:TRP:CE2	2.53	0.44
5:AG:196:LYS:HA	5:AG:196:LYS:HD3	1.73	0.44
10:AL:67:TRP:NE1	10:AL:69:SER:HB2	2.33	0.44
25:Ad:37:LYS:HB3	25:Ad:37:LYS:HE2	1.66	0.44
26:Ae:21:LYS:H	26:Ae:21:LYS:HG2	1.65	0.44
33:Am:118:ARG:HA	33:Am:134:ILE:HG12	1.99	0.44
36:B2:236:C:H5"	60:Bk:3:PHE:HB2	2.00	0.44
36:B2:445:G:C5	36:B2:446:U:H5	2.36	0.44
47:BW:61:ARG:HE	75:H1:33:LYS:NZ	2.16	0.44
50:BZ:169:LYS:HA	50:BZ:172:ARG:HB3	2.00	0.44
62:Bm:87:ARG:O	62:Bm:91:LEU:HB2	2.18	0.44
74:By:59:ASN:HB3	74:By:63:GLY:C	2.43	0.44
76:HE:32:LYS:HB2	76:HE:32:LYS:HE2	1.82	0.44
76:HE:674:GLY:HA3	76:HE:681:LEU:HD21	1.98	0.44
1:AA:899:C:H2'	1:AA:900:G:H8	1.83	0.44
2:AD:37:ASP:O	2:AD:40:VAL:HG12	2.18	0.44
2:AD:110:PHE:CZ	2:AD:121:PRO:HG3	2.52	0.44
4:AF:184:LYS:O	4:AF:188:GLN:HG3	2.18	0.44
7:AI:24:PHE:H	7:AI:25:PRO:HD3	1.83	0.44
13:AO:94:TYR:CE2	25:Ad:13:LEU:HB3	2.53	0.44
15:AQ:62:GLN:HE21	15:AQ:64:ARG:HH11	1.66	0.44
18:AT:87:VAL:HG12	18:AT:99:LYS:HZ3	1.82	0.44
20:AV:120:HIS:C	20:AV:120:HIS:CD2	2.95	0.44
33:Am:5:LEU:HG	33:Am:312:VAL:HG22	1.99	0.44
33:Am:64:HIS:HD2	33:Am:83:TRP:HB3	1.83	0.44
36:B2:760:C:H3'	36:B2:761:U:O4'	2.17	0.44
36:B2:932:G:H1'	36:B2:1624:A:N6	2.33	0.44
53:Bd:102:LEU:HD22	53:Bd:138:LEU:HD22	2.00	0.44
54:Be:32:ASN:HB2	54:Be:35:VAL:HG23	2.00	0.44
77:HL:98:LEU:HD23	77:HL:98:LEU:H	1.83	0.44
78:HS:101:LYS:HB2	78:HS:101:LYS:HE3	1.72	0.44
82:Bb:41:LEU:HD22	82:Bb:150:VAL:HG11	2.00	0.44
1:AA:1656:C:H5'	30:Ai:19:ARG:HH22	1.82	0.43
10:AL:67:TRP:CE2	10:AL:69:SER:HB2	2.53	0.43
13:AO:104:LEU:HD21	13:AO:134:PHE:CE2	2.53	0.43
18:AT:6:CYS:HB2	18:AT:84:LYS:HZ3	1.82	0.43
20:AV:67:ILE:O	20:AV:71:ILE:HG13	2.17	0.43
39:BN:56:PRO:HD2	39:BN:169:ALA:HB3	2.00	0.43
40:BO:34:LYS:HD2	40:BO:34:LYS:HA	1.62	0.43
68:Bs:56:ALA:O	68:Bs:57:LEU:HD23	2.18	0.43
1:AA:1113:U:H4'	1:AA:1114:U:O5'	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1201:A:H2'	1:AA:1202:U:H4'	2.00	0.43
1:AA:1555:U:H5"	1:AA:1556:A:O4'	2.19	0.43
3:AE:88:VAL:HB	3:AE:98:THR:HG22	2.00	0.43
15:AQ:90:ASN:OD1	15:AQ:90:ASN:N	2.51	0.43
16:AR:101:GLN:HB3	28:Ag:46:GLU:OE1	2.18	0.43
33:Am:217:MET:HE1	33:Am:219:TRP:NE1	2.33	0.43
36:B2:3418:U:H1'	36:B2:3419:G:OP2	2.18	0.43
40:BO:151:ILE:HA	40:BO:155:CYS:SG	2.58	0.43
48:BX:18:TRP:CD1	48:BX:18:TRP:H	2.35	0.43
61:Bl:10:VAL:HG23	61:Bl:83:THR:OG1	2.18	0.43
61:Bl:61:ARG:O	61:Bl:65:ARG:HG2	2.18	0.43
76:HE:141:THR:HA	76:HE:144:ARG:HD3	2.01	0.43
6:AH:71:LYS:HG2	6:AH:91:SER:O	2.17	0.43
12:AN:30:PRO:HA	12:AN:38:PRO:HB3	2.00	0.43
17:AS:46:HIS:O	17:AS:50:ARG:HG3	2.17	0.43
33:Am:206:LEU:HD11	33:Am:261:LEU:HD11	1.99	0.43
57:Bh:106:ASN:HD21	57:Bh:108:LYS:HB3	1.84	0.43
59:Bj:52:HIS:CG	59:Bj:55:ARG:HH21	2.36	0.43
1:AA:1578:C:H1'	1:AA:1612:C:N4	2.33	0.43
1:AA:1650:U:H5"	18:AT:72:VAL:HB	2.00	0.43
9:AK:60:ILE:HG22	9:AK:92:VAL:HA	2.00	0.43
11:AM:41:GLU:HA	11:AM:44:ARG:HG2	2.01	0.43
12:AN:40:LEU:HA	12:AN:40:LEU:HD23	1.86	0.43
14:AP:39:ARG:HE	14:AP:131:GLU:HA	1.83	0.43
20:AV:25:LYS:HB3	20:AV:28:PHE:HD2	1.84	0.43
36:B2:3144:C:H5	36:B2:3187:A:H62	1.64	0.43
45:BT:158:ASP:HB3	45:BT:159:PRO:HD3	2.00	0.43
47:BW:51:ARG:HH21	75:H1:29:SER:HB2	1.83	0.43
51:Ba:131:LYS:HD2	51:Ba:132:PRO:HD2	2.00	0.43
53:Bd:106:LEU:HD23	53:Bd:106:LEU:HA	1.85	0.43
76:HE:264:ALA:HB3	76:HE:268:SER:HA	2.00	0.43
1:AA:1769:G:H21	10:AL:32:GLN:NE2	2.16	0.43
3:AE:41:LYS:HA	3:AE:41:LYS:HD3	1.90	0.43
8:AJ:32:MET:HA	8:AJ:52:ILE:HB	2.01	0.43
8:AJ:140:LYS:HB3	8:AJ:140:LYS:HE2	1.75	0.43
36:B2:816:A:H2	52:Bc:94:LEU:HD13	1.83	0.43
36:B2:1332:A:H4'	36:B2:1333:A:H5'	2.01	0.43
36:B2:2534:U:H2'	36:B2:2535:A:C8	2.53	0.43
40:BO:115:LYS:HD3	40:BO:129:ALA:HB3	2.00	0.43
42:BQ:279:GLU:H	42:BQ:279:GLU:HG2	1.59	0.43
45:BT:69:LEU:HD21	50:BZ:24:ARG:HH12	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:BX:49:ARG:HD3	69:Bt:118:TYR:H	1.84	0.43
57:Bh:134:ASN:OD1	57:Bh:134:ASN:C	2.61	0.43
67:Br:102:MET:HE2	67:Br:102:MET:HB3	1.89	0.43
74:By:35:VAL:HA	74:By:55:GLY:HA3	2.00	0.43
76:HE:75:ILE:HG22	76:HE:102:LEU:HB3	2.00	0.43
76:HE:207:GLY:O	76:HE:337:MET:HE1	2.17	0.43
76:HE:676:MET:HB2	76:HE:677:PHE:H	1.73	0.43
3:AE:70:LEU:HB2	3:AE:82:ARG:HB2	2.01	0.43
29:Ah:49:HIS:NE2	29:Ah:70:LYS:HD2	2.34	0.43
30:Ai:51:GLU:N	30:Ai:51:GLU:OE1	2.51	0.43
32:Ak:10:ARG:HG3	32:Ak:13:LYS:HG2	2.00	0.43
36:B2:155:U:H5”	50:BZ:54:LYS:HG2	1.99	0.43
37:B3:10:C:C4	42:BQ:20:TYR:HD2	2.36	0.43
39:BN:42:GLY:HA3	39:BN:62:PHE:CE1	2.53	0.43
41:BP:195:LYS:HB3	41:BP:200:ARG:HD2	2.01	0.43
42:BQ:210:MET:O	42:BQ:214:ASP:HB2	2.19	0.43
54:Be:105:MET:HE1	54:Be:122:ILE:HD12	2.00	0.43
67:Br:14:HIS:CE1	67:Br:29:SER:HB3	2.53	0.43
67:Br:60:VAL:HG22	67:Br:61:ARG:HG2	2.00	0.43
76:HE:353:ALA:HB3	76:HE:370:ARG:HH21	1.83	0.43
80:BA:104:PRO:HD3	80:BA:111:ARG:NH2	2.34	0.43
1:AA:502:U:C2	1:AA:503:C:H5	2.37	0.43
1:AA:752:G:H5”	6:AH:197:HIS:NE2	2.33	0.43
1:AA:893:G:H2’	1:AA:894:G:C8	2.53	0.43
2:AD:32:LEU:HA	2:AD:36:MET:SD	2.59	0.43
2:AD:66:VAL:HA	23:Ab:35:ASN:O	2.19	0.43
5:AG:178:LEU:HG	5:AG:183:VAL:HG12	2.01	0.43
11:AM:37:ARG:HE	11:AM:38:ASN:HB2	1.83	0.43
13:AO:128:LEU:HB2	13:AO:132:VAL:HG13	1.99	0.43
18:AT:35:LEU:HD23	18:AT:35:LEU:HA	1.87	0.43
25:Ad:22:TRP:CH2	25:Ad:31:LEU:HD22	2.53	0.43
26:Ae:10:ARG:HB2	26:Ae:24:VAL:O	2.18	0.43
31:Aj:26:ARG:HG2	31:Aj:28:LEU:H	1.84	0.43
33:Am:7:LEU:HD12	33:Am:310:TRP:HE1	1.84	0.43
33:Am:227:LEU:HD23	33:Am:227:LEU:HA	1.83	0.43
38:B4:115:G:H4’	38:B4:146:A:H5’	2.01	0.43
61:Bl:23:VAL:HG12	61:Bl:45:GLY:HA3	2.01	0.43
65:Bp:31:LYS:HA	65:Bp:31:LYS:HD3	1.76	0.43
1:AA:769:A:H5’	6:AH:16:HIS:NE2	2.34	0.43
1:AA:893:G:H2’	1:AA:894:G:H8	1.83	0.43
6:AH:202:LEU:HD12	13:AO:37:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AM:121:SER:OG	11:AM:124:HIS:HB3	2.19	0.43
13:AO:137:LEU:HD23	13:AO:137:LEU:HA	1.81	0.43
15:AQ:45:MET:HE2	15:AQ:45:MET:HB2	1.81	0.43
23:Ab:41:ALA:O	23:Ab:42:GLU:HG2	2.19	0.43
24:Ac:28:ARG:HB3	24:Ac:29:PRO:HD3	2.00	0.43
33:Am:10:THR:HG23	33:Am:308:ARG:HB3	2.01	0.43
37:B3:11:A:H2	37:B3:66:G:H21	1.67	0.43
44:BS:148:ASN:CB	44:BS:244:ASN:HD21	2.32	0.43
82:Bb:122:ALA:HB3	82:Bb:143:PRO:HG2	2.01	0.43
1:AA:650:G:H22	1:AA:692:G:N2	2.16	0.43
1:AA:691:C:H2'	1:AA:692:G:C8	2.54	0.43
1:AA:1167:A:H2'	1:AA:1168:A:C8	2.54	0.43
1:AA:1168:A:H2'	1:AA:1169:G:H8	1.84	0.43
7:AI:46:GLN:HG3	18:AT:111:ARG:HH22	1.84	0.43
7:AI:191:LYS:HA	7:AI:191:LYS:HD3	1.74	0.43
12:AN:22:VAL:CG1	12:AN:24:LYS:HG2	2.49	0.43
16:AR:23:ALA:HB2	16:AR:100:ALA:HB2	2.01	0.43
18:AT:16:VAL:HB	18:AT:65:ARG:HG3	2.00	0.43
34:B0:77:CYS:SG	34:B0:79:TYR:HB2	2.59	0.43
35:B1:33:GLN:HG2	35:B1:71:TRP:HB3	2.00	0.43
36:B2:1293:G:C6	36:B2:1309:A:H1'	2.53	0.43
37:B3:15:C:H5"	47:BW:147:ARG:HH22	1.84	0.43
38:B4:37:U:H5"	48:BX:27:ASN:HB3	2.00	0.43
48:BX:86:SER:HB3	48:BX:89:VAL:HG23	2.01	0.43
76:HE:724:ILE:HD11	76:HE:808:PRO:HB3	2.01	0.43
1:AA:1159:A:H2'	1:AA:1160:U:C6	2.54	0.43
1:AA:1569:U:H5"	7:AI:90:ARG:HH22	1.84	0.43
2:AD:142:VAL:HG13	2:AD:143:ASN:H	1.84	0.43
12:AN:57:THR:HG23	12:AN:66:TYR:HD1	1.84	0.43
21:AW:123:ILE:HG12	21:AW:128:GLN:HG3	2.01	0.43
25:Ad:29:LYS:HB2	25:Ad:29:LYS:HE2	1.82	0.43
35:B1:64:LYS:H	35:B1:64:LYS:HG2	1.59	0.43
36:B2:2477:C:H5'	82:Bb:80:GLN:NE2	2.33	0.43
36:B2:2554:G:H4'	77:HL:59:ARG:HH22	1.83	0.43
44:BS:89:THR:HG21	44:BS:146:ILE:HG23	2.01	0.43
46:BV:60:ILE:HD13	46:BV:135:LEU:HD21	1.99	0.43
47:BW:86:VAL:HG11	47:BW:106:ILE:HD13	1.99	0.43
76:HE:578:LYS:HE2	76:HE:840:ASP:HB3	2.01	0.43
76:HE:693:LEU:HB3	76:HE:700:ARG:NH1	2.33	0.43
1:AA:841:U:H2'	1:AA:842:C:C6	2.54	0.42
1:AA:1031:C:H2'	1:AA:1032:U:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AG:168:ASP:HB3	5:AG:196:LYS:HE2	2.00	0.42
18:AT:15:ALA:HB2	18:AT:77:ALA:HB1	2.01	0.42
20:AV:94:LYS:HD3	20:AV:94:LYS:N	2.34	0.42
22:Aa:39:LEU:HD12	22:Aa:39:LEU:HA	1.93	0.42
24:Ac:111:MET:SD	24:Ac:116:ALA:HB2	2.59	0.42
26:Ae:124:ARG:O	26:Ae:128:ARG:HD3	2.20	0.42
36:B2:1266:U:H4'	36:B2:1267:G:H3'	2.01	0.42
41:BP:279:LEU:HD23	41:BP:279:LEU:HA	1.90	0.42
42:BQ:183:PHE:HD2	42:BQ:185:ILE:HB	1.84	0.42
45:BT:186:LEU:HD22	45:BT:198:LEU:HD12	2.01	0.42
50:BZ:27:ALA:HB2	50:BZ:122:ASN:ND2	2.34	0.42
50:BZ:44:ARG:HG2	50:BZ:47:LYS:HB2	2.00	0.42
74:By:59:ASN:HB2	74:By:65:VAL:HG23	2.00	0.42
6:AH:82:PHE:CD1	6:AH:82:PHE:C	2.97	0.42
18:AT:20:LYS:HD3	18:AT:20:LYS:HA	1.88	0.42
19:AU:91:LEU:H	19:AU:91:LEU:HD23	1.84	0.42
25:Ad:22:TRP:HH2	25:Ad:31:LEU:HD22	1.84	0.42
49:BY:14:VAL:HG12	49:BY:58:LEU:HA	2.01	0.42
76:HE:263:ASP:HA	76:HE:268:SER:HB3	2.01	0.42
79:HI:35:ILE:HG21	79:HI:71:TYR:HB3	2.01	0.42
1:AA:29:U:H2'	1:AA:30:G:C8	2.55	0.42
15:AQ:130:ARG:HH12	15:AQ:140:LYS:H	1.66	0.42
25:Ad:46:HIS:HD2	25:Ad:103:SER:HB2	1.84	0.42
33:Am:302:TRP:CD1	33:Am:308:ARG:HE	2.37	0.42
36:B2:1116:G:H5"	55:Bf:35:LYS:HE3	2.01	0.42
36:B2:1210:A:H5'	67:Br:76:HIS:CE1	2.54	0.42
40:BO:67:MET:HG3	40:BO:70:ARG:HB2	2.02	0.42
76:HE:237:ARG:HH11	76:HE:241:MET:HE3	1.84	0.42
1:AA:128:G:H8	8:AJ:201:ALA:HB3	1.85	0.42
25:Ad:76:LYS:H	25:Ad:76:LYS:HG2	1.65	0.42
33:Am:62:HIS:CD2	33:Am:88:ARG:HD3	2.54	0.42
35:B1:41:PHE:HE2	35:B1:66:LEU:HD21	1.84	0.42
36:B2:3490:A:H5"	36:B2:3491:A:H5"	2.01	0.42
39:BN:3:ARG:HG2	39:BN:206:VAL:HG22	2.02	0.42
51:Ba:51:ASN:ND2	51:Ba:142:LEU:HD12	2.34	0.42
55:Bf:84:TYR:HB2	63:Bn:24:PRO:HD3	2.00	0.42
61:Bl:22:LYS:HE2	61:Bl:129:TRP:CH2	2.54	0.42
61:Bl:100:THR:HG22	61:Bl:106:GLN:HG2	2.01	0.42
62:Bm:103:VAL:HG12	62:Bm:108:TYR:HB2	2.00	0.42
64:Bo:37:LEU:HD11	64:Bo:65:TYR:CD2	2.54	0.42
67:Br:20:SER:HB3	67:Br:23:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:HL:92:LEU:HD12	77:HL:92:LEU:O	2.20	0.42
1:AA:642:U:H5'	9:AK:120:LEU:HB3	2.00	0.42
1:AA:1229:G:H2'	1:AA:1230:G:H8	1.84	0.42
1:AA:1777:U:H2'	1:AA:1778:G:H8	1.84	0.42
5:AG:56:HIS:CD2	5:AG:58:GLN:HB2	2.54	0.42
7:AI:32:LYS:HD2	7:AI:33:ASP:N	2.33	0.42
15:AQ:71:ILE:O	15:AQ:74:ILE:HG12	2.20	0.42
20:AV:30:MET:O	20:AV:36:VAL:HG11	2.19	0.42
24:Ac:17:ALA:HB1	24:Ac:22:ARG:HB2	2.01	0.42
24:Ac:25:VAL:HG13	24:Ac:65:LEU:HD11	1.99	0.42
25:Ad:101:LEU:HB3	25:Ad:124:LYS:HB2	2.02	0.42
34:B0:13:PRO:HG2	34:B0:79:TYR:CE2	2.55	0.42
36:B2:645:U:H4'	83:A:166:ARG:HH12	1.84	0.42
40:BO:45:ALA:HB3	40:BO:181:ILE:HG23	2.02	0.42
57:Bh:90:LYS:HD2	57:Bh:90:LYS:HA	1.79	0.42
64:Bo:53:ASN:HD22	64:Bo:80:ASN:ND2	2.17	0.42
76:HE:60:ARG:O	76:HE:63:GLU:HG3	2.19	0.42
76:HE:608:PRO:HG2	76:HE:641:THR:HA	2.02	0.42
80:BA:90:ASN:HB3	81:BU:170:ILE:HG13	2.00	0.42
1:AA:1223:U:H4'	31:Aj:27:ARG:HD2	2.01	0.42
1:AA:1272:G:H4'	12:AN:5:LYS:HZ3	1.84	0.42
1:AA:1367:C:H4'	18:AT:65:ARG:HH12	1.84	0.42
5:AG:88:LEU:HD23	5:AG:88:LEU:HA	1.90	0.42
9:AK:73:HIS:HD2	9:AK:133:PHE:HE1	1.67	0.42
9:AK:74:LYS:HD3	9:AK:74:LYS:HA	1.91	0.42
19:AU:55:THR:O	19:AU:59:LYS:HG2	2.19	0.42
33:Am:152:SER:HB3	33:Am:168:ALA:HB3	2.02	0.42
36:B2:144:U:H2'	36:B2:145:G:C8	2.55	0.42
43:BR:169:LYS:HA	43:BR:169:LYS:CE	2.49	0.42
47:BW:116:TYR:O	47:BW:116:TYR:CG	2.73	0.42
54:Be:65:GLU:HG3	54:Be:97:THR:HG22	2.01	0.42
77:HL:136:PRO:HG3	79:HI:108:GLY:HA3	2.01	0.42
79:HI:125:ILE:HD12	79:HI:125:ILE:HA	1.79	0.42
8:AJ:78:ARG:H	8:AJ:81:HIS:CD2	2.37	0.42
13:AO:75:THR:HG22	13:AO:81:ILE:HG22	2.02	0.42
16:AR:42:VAL:HG21	16:AR:72:LYS:HG2	2.01	0.42
20:AV:25:LYS:HD2	20:AV:52:MET:HE3	2.01	0.42
20:AV:114:LEU:O	20:AV:117:ILE:HG12	2.19	0.42
35:B1:62:CYS:C	35:B1:64:LYS:H	2.27	0.42
36:B2:2659:G:H22	36:B2:2673:U:H1'	1.85	0.42
36:B2:3036:A:H8	36:B2:3036:A:OP2	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:B2:3103:U:H5"	51:Ba:73:HIS:O	2.20	0.42
36:B2:3417:A:N3	36:B2:3490:A:H4'	2.34	0.42
48:BX:107:GLU:HG3	70:Bu:15:LEU:HD22	2.00	0.42
48:BX:175:ALA:HB1	62:Bm:146:LEU:HD21	2.00	0.42
50:BZ:79:GLN:HB3	50:BZ:81:TYR:CZ	2.55	0.42
54:Be:6:TYR:CE1	54:Be:62:GLU:HG3	2.55	0.42
59:Bj:114:ARG:H	59:Bj:114:ARG:HG2	1.63	0.42
76:HE:629:ASP:HA	76:HE:632:LYS:HE3	2.02	0.42
76:HE:747:LEU:HD23	76:HE:747:LEU:HA	1.92	0.42
77:HL:133:PHE:CD1	77:HL:134:PRO:HD2	2.54	0.42
1:AA:1494:G:H2'	1:AA:1495:A:C8	2.55	0.42
1:AA:1587:G:H2'	1:AA:1588:A:C8	2.55	0.42
16:AR:55:ASP:HB3	16:AR:58:SER:HB2	2.02	0.42
26:Ae:125:LEU:HA	26:Ae:128:ARG:NE	2.34	0.42
32:Ak:20:LYS:HE3	32:Ak:20:LYS:HA	2.01	0.42
38:B4:30:U:OP2	41:BP:196:LEU:HD22	2.20	0.42
39:BN:42:GLY:HA3	39:BN:62:PHE:CD1	2.54	0.42
41:BP:61:GLN:HE21	41:BP:61:GLN:HB2	1.61	0.42
41:BP:221:PHE:HB3	41:BP:229:ILE:HD11	2.02	0.42
52:Bc:92:GLU:CD	52:Bc:92:GLU:H	2.27	0.42
57:Bh:15:MET:H	57:Bh:15:MET:HG2	1.66	0.42
62:Bm:75:LEU:HA	62:Bm:78:LEU:HD23	2.00	0.42
65:Bp:82:ARG:HA	65:Bp:94:THR:HA	2.01	0.42
76:HE:8:GLU:O	76:HE:12:LEU:HD23	2.20	0.42
76:HE:191:THR:HG23	76:HE:192:TYR:CD1	2.53	0.42
76:HE:578:LYS:HE3	76:HE:578:LYS:HB2	1.94	0.42
79:HI:135:LEU:H	79:HI:135:LEU:HD12	1.84	0.42
1:AA:1769:G:H21	10:AL:32:GLN:HE22	1.66	0.42
2:AD:157:ASN:H	2:AD:159:VAL:HG23	1.85	0.42
2:AD:191:LEU:HD23	2:AD:191:LEU:HA	1.83	0.42
5:AG:53:ARG:HG3	5:AG:93:VAL:HG21	2.01	0.42
6:AH:102:VAL:O	6:AH:110:THR:HG22	2.20	0.42
45:BT:147:LYS:HE2	45:BT:147:LYS:HB2	1.69	0.42
57:Bh:19:LEU:HD13	57:Bh:19:LEU:HA	1.94	0.42
76:HE:185:VAL:O	76:HE:189:ILE:HG23	2.20	0.42
76:HE:588:MET:HE2	76:HE:686:PHE:HB3	2.02	0.42
14:AP:38:LYS:HE2	14:AP:41:LEU:HD21	2.01	0.42
15:AQ:55:ARG:HH22	29:Ah:51:GLN:NE2	2.18	0.42
16:AR:45:THR:O	16:AR:48:MET:HE3	2.20	0.42
17:AS:119:MET:HG2	17:AS:127:PHE:CZ	2.54	0.42
25:Ad:92:ASN:HD22	32:Ak:11:ALA:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Ae:13:MET:HG2	26:Ae:14:THR:N	2.35	0.42
39:BN:138:HIS:HA	39:BN:145:THR:HA	2.02	0.42
48:BX:106:GLU:O	48:BX:110:GLN:HG2	2.20	0.42
51:Ba:192:LEU:HD23	51:Ba:192:LEU:HA	1.93	0.42
52:Bc:12:LYS:HE3	52:Bc:12:LYS:HB2	1.84	0.42
60:Bk:112:LYS:HB3	60:Bk:112:LYS:HE3	1.85	0.42
76:HE:381:TYR:HD2	76:HE:478:MET:HG3	1.85	0.42
79:HI:44:ASP:HB3	79:HI:61:VAL:HG12	2.02	0.42
82:Bb:2:VAL:HG22	82:Bb:3:ARG:N	2.34	0.42
1:AA:517:G:O2'	1:AA:518:A:H8	2.02	0.41
3:AE:79:HIS:HD2	3:AE:82:ARG:HG3	1.83	0.41
4:AF:51:SER:HB3	4:AF:53:GLU:OE1	2.20	0.41
5:AG:71:LEU:HA	5:AG:74:LEU:HB3	2.02	0.41
6:AH:10:LYS:HE2	6:AH:10:LYS:HB3	1.98	0.41
8:AJ:195:ALA:O	8:AJ:199:ARG:HG2	2.20	0.41
20:AV:84:LEU:HD12	20:AV:95:SER:HB3	2.02	0.41
33:Am:73:PHE:N	33:Am:117:ASN:HD21	2.14	0.41
41:BP:139:ALA:HB1	74:By:16:ASN:HD22	1.85	0.41
41:BP:140:ARG:NH2	41:BP:242:PRO:HG2	2.35	0.41
41:BP:359:VAL:HA	41:BP:362:GLU:HG2	2.01	0.41
43:BR:49:ARG:HD2	43:BR:52:LEU:HG	2.02	0.41
47:BW:106:ILE:HG12	47:BW:112:LEU:HD11	2.02	0.41
48:BX:29:PRO:HD3	50:BZ:199:ARG:NH2	2.35	0.41
59:Bj:52:HIS:CD2	59:Bj:55:ARG:HH21	2.38	0.41
74:By:8:ILE:O	74:By:12:ILE:HG12	2.19	0.41
1:AA:123:U:H2'	1:AA:124:G:C8	2.55	0.41
1:AA:768:A:H2'	1:AA:769:A:C8	2.55	0.41
1:AA:1424:C:H2'	1:AA:1425:A:C8	2.55	0.41
2:AD:134:GLN:H	2:AD:134:GLN:CD	2.28	0.41
6:AH:148:ARG:HG2	6:AH:149:TYR:CE1	2.54	0.41
9:AK:107:LYS:HE3	9:AK:107:LYS:HB2	1.85	0.41
13:AO:22:ASN:ND2	13:AO:24:LYS:HB2	2.35	0.41
20:AV:93:GLY:C	20:AV:94:LYS:HD3	2.45	0.41
21:AW:43:LYS:HB3	21:AW:43:LYS:HE2	1.75	0.41
34:B0:62:ALA:HA	79:HI:21:PRO:HG3	2.01	0.41
36:B2:1370:C:OP1	66:Bq:58:LYS:HB2	2.20	0.41
36:B2:1664:A:H2'	61:Bl:115:LYS:HE2	2.02	0.41
40:BO:17:LEU:HG	40:BO:18:PRO:HA	2.01	0.41
42:BQ:151:LYS:HD2	42:BQ:151:LYS:HA	1.83	0.41
45:BT:49:PHE:O	59:Bj:29:THR:HG23	2.20	0.41
52:Bc:146:HIS:HA	52:Bc:151:TYR:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:Bl:93:LYS:HE2	61:Bl:93:LYS:HB2	1.69	0.41
69:Bt:16:LEU:HD23	69:Bt:16:LEU:HA	1.92	0.41
77:HL:52:ILE:HD11	77:HL:188:PHE:CE2	2.55	0.41
1:AA:474:A:H2'	1:AA:475:G:H8	1.84	0.41
1:AA:909:U:H2'	1:AA:910:G:C8	2.56	0.41
1:AA:1699:G:H1'	1:AA:1700:A:O5'	2.20	0.41
2:AD:142:VAL:O	4:AF:61:PRO:HG3	2.19	0.41
12:AN:58:ARG:HA	12:AN:58:ARG:HD3	1.62	0.41
13:AO:141:LYS:HD2	13:AO:141:LYS:HA	1.91	0.41
18:AT:6:CYS:SG	18:AT:85:ALA:HA	2.60	0.41
21:AW:64:ILE:HG21	21:AW:113:LEU:HD21	2.02	0.41
33:Am:8:ARG:HH21	33:Am:52:TYR:HB2	1.85	0.41
36:B2:2785:G:N2	36:B2:2786:A:H5"	2.32	0.41
46:BV:193:ASP:OD1	46:BV:193:ASP:C	2.63	0.41
76:HE:253:LYS:HA	76:HE:253:LYS:HD3	1.92	0.41
1:AA:108:C:H5"	1:AA:386:G:O2'	2.21	0.41
1:AA:537:A:H3'	1:AA:538:A:H8	1.85	0.41
3:AE:188:LEU:HD23	3:AE:188:LEU:HA	1.85	0.41
13:AO:67:ILE:N	13:AO:67:ILE:HD12	2.36	0.41
36:B2:3335:U:H3'	36:B2:3336:G:N2	2.35	0.41
47:BW:126:ASP:OD1	47:BW:126:ASP:N	2.53	0.41
48:BX:185:TYR:CD1	70:Bu:9:LEU:HD11	2.55	0.41
58:Bi:22:VAL:HG22	58:Bi:28:VAL:HG12	2.01	0.41
61:Bl:116:LYS:HE3	61:Bl:116:LYS:HB3	1.95	0.41
68:Bs:62:PHE:O	68:Bs:70:LYS:HD3	2.20	0.41
74:By:71:ASN:ND2	74:By:73:LYS:HD3	2.35	0.41
76:HE:38:SER:HA	76:HE:41:GLN:HB2	2.03	0.41
76:HE:601:ILE:HD12	76:HE:643:ALA:HB2	2.02	0.41
9:AK:111:THR:HG23	9:AK:112:GLN:HG2	2.03	0.41
10:AL:166:TYR:HE2	10:AL:193:LEU:HD21	1.85	0.41
13:AO:93:LYS:HG3	13:AO:94:TYR:CD1	2.55	0.41
13:AO:120:VAL:HG13	13:AO:139:VAL:HG12	2.02	0.41
14:AP:79:LEU:HD23	14:AP:79:LEU:HA	1.89	0.41
21:AW:134:ILE:O	21:AW:138:LEU:HD12	2.20	0.41
36:B2:526:G:H1	36:B2:599:U:H3	1.68	0.41
36:B2:1519:G:N2	68:Bs:4:ARG:HH11	2.19	0.41
36:B2:3278:A:H2'	36:B2:3279:A:C8	2.56	0.41
38:B4:162:C:H2'	38:B4:163:A:C8	2.56	0.41
46:BV:51:HIS:HD2	46:BV:168:SER:HB2	1.83	0.41
47:BW:84:LEU:HB3	47:BW:89:TYR:HE1	1.84	0.41
53:Bd:80:LYS:HE3	53:Bd:80:LYS:HB3	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:Bf:27:LEU:HD23	55:Bf:30:TYR:HD2	1.86	0.41
59:Bj:74:LYS:HE2	59:Bj:74:LYS:HB2	1.57	0.41
60:Bk:54:GLN:HB2	60:Bk:107:LYS:HB3	2.02	0.41
66:Bq:110:ARG:HH12	74:By:133:VAL:HG22	1.85	0.41
74:By:97:LYS:HD2	74:By:97:LYS:HA	1.95	0.41
76:HE:152:ARG:HG2	76:HE:200:CYS:SG	2.60	0.41
76:HE:542:LEU:HD13	76:HE:556:ILE:HG21	2.02	0.41
79:HI:139:VAL:HG12	79:HI:148:ALA:HB2	2.01	0.41
1:AA:403:A:H4'	1:AA:404:A:H5'	2.02	0.41
1:AA:474:A:H2'	1:AA:475:G:C8	2.56	0.41
1:AA:1055:G:H2'	1:AA:1056:G:C8	2.55	0.41
1:AA:1629:G:H1	1:AA:1649:U:H3	1.67	0.41
2:AD:142:VAL:O	2:AD:143:ASN:HB2	2.21	0.41
2:AD:200:MET:CE	2:AD:202:ASP:HB2	2.50	0.41
7:AI:143:LEU:HD23	30:Ai:48:PRO:HG2	2.03	0.41
13:AO:96:ARG:HH21	25:Ad:5:ALA:HA	1.85	0.41
18:AT:91:GLN:NE2	18:AT:92:LYS:HG3	2.36	0.41
18:AT:126:PHE:CD2	22:Aa:77:TRP:HB2	2.55	0.41
36:B2:1291:A:O2'	36:B2:1310:C:H1'	2.21	0.41
36:B2:1640:A:O2'	36:B2:1641:U:H5"	2.20	0.41
36:B2:3131:C:H42	81:BU:119:ARG:HH11	1.69	0.41
36:B2:3368:A:H1'	43:BR:92:PRO:HG3	2.02	0.41
39:BN:14:ILE:HG22	39:BN:193:ASN:HD21	1.86	0.41
47:BW:120:ILE:HD12	47:BW:120:ILE:N	2.35	0.41
50:BZ:51:LEU:HD11	50:BZ:119:TYR:HB3	2.02	0.41
55:Bf:57:TYR:HE1	55:Bf:76:ILE:HG21	1.85	0.41
76:HE:167:LEU:HB3	76:HE:169:ILE:HD11	2.03	0.41
76:HE:216:HIS:HB3	76:HE:218:TRP:CD1	2.55	0.41
76:HE:239:LYS:O	76:HE:240:MET:HG2	2.21	0.41
79:HI:128:GLY:HA2	79:HI:133:ARG:HH21	1.85	0.41
1:AA:17:C:H2'	1:AA:18:C:C6	2.56	0.41
1:AA:1261:A:N3	1:AA:1261:A:H2'	2.35	0.41
2:AD:40:VAL:HG23	2:AD:49:HIS:CD2	2.56	0.41
2:AD:62:LEU:HD22	23:Ab:79:LEU:HD22	2.02	0.41
6:AH:59:ARG:HH12	26:Ae:89:TYR:HB3	1.85	0.41
18:AT:52:ALA:HB3	18:AT:57:PHE:HZ	1.85	0.41
24:Ac:52:GLU:N	24:Ac:52:GLU:OE1	2.54	0.41
36:B2:853:U:H2'	36:B2:854:G:C8	2.55	0.41
36:B2:2343:A:H4'	36:B2:2350:A:C6	2.56	0.41
36:B2:3342:G:H5'	36:B2:3345:G:C8	2.50	0.41
47:BW:45:PRO:HA	47:BW:69:VAL:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:Bc:61:ILE:HG22	52:Bc:84:ILE:HD13	2.02	0.41
52:Bc:177:ARG:HH21	52:Bc:185:PHE:HE1	1.68	0.41
59:Bj:109:ILE:HD13	59:Bj:109:ILE:HA	1.84	0.41
69:Bt:102:LYS:HG3	69:Bt:107:ILE:HG22	2.02	0.41
76:HE:120:ARG:HH12	76:HE:481:MET:HG2	1.85	0.41
76:HE:746:VAL:HG21	76:HE:784:LEU:HD12	2.02	0.41
1:AA:910:G:H22	1:AA:932:U:H3	1.69	0.41
1:AA:1001:G:C2	1:AA:1002:G:H1'	2.55	0.41
1:AA:1082:C:H4'	3:AE:149:GLN:HG2	2.01	0.41
1:AA:1168:A:O2'	28:Ag:85:ARG:HD3	2.21	0.41
1:AA:1503:A:H4'	18:AT:68:GLY:HA2	2.02	0.41
3:AE:190:PRO:O	3:AE:191:GLU:HG3	2.21	0.41
16:AR:83:ILE:HD13	16:AR:104:LEU:HD13	2.03	0.41
33:Am:24:ALA:HB1	33:Am:26:GLU:CD	2.45	0.41
36:B2:3131:C:H1'	81:BU:120:ILE:HG22	2.02	0.41
54:Be:122:ILE:O	55:Bf:153:PRO:HG2	2.20	0.41
56:Bg:79:LYS:HD2	56:Bg:88:ARG:HH12	1.85	0.41
60:Bk:110:LEU:HD12	60:Bk:110:LEU:HA	1.91	0.41
76:HE:90:LYS:HA	76:HE:90:LYS:HD2	1.88	0.41
79:HI:137:ILE:HD13	79:HI:137:ILE:HA	1.91	0.41
82:Bb:125:GLN:HB2	82:Bb:141:SER:HB3	2.03	0.41
1:AA:215:G:H21	1:AA:254:A:H62	1.68	0.41
1:AA:881:G:N2	1:AA:980:U:H3	2.19	0.41
1:AA:1333:G:H4'	19:AU:10:LYS:HE3	2.03	0.41
1:AA:1642:G:C5	21:AW:88:ARG:HG2	2.56	0.41
6:AH:36:HIS:CE1	6:AH:85:GLY:HA3	2.56	0.41
6:AH:147:ILE:HD12	6:AH:169:ILE:HD11	2.02	0.41
6:AH:207:ILE:HD12	6:AH:207:ILE:HA	1.91	0.41
7:AI:94:HIS:O	7:AI:98:ILE:HD12	2.20	0.41
7:AI:190:LYS:HG3	7:AI:191:LYS:N	2.35	0.41
8:AJ:115:LYS:HD3	8:AJ:116:GLN:O	2.21	0.41
11:AM:12:TYR:HB2	11:AM:43:TRP:HB2	2.03	0.41
13:AO:78:HIS:HD2	13:AO:79:ARG:HB2	1.86	0.41
14:AP:59:ARG:HA	14:AP:59:ARG:HD3	1.93	0.41
20:AV:13:LEU:HD13	20:AV:13:LEU:HA	1.93	0.41
21:AW:6:VAL:O	21:AW:9:VAL:HG12	2.21	0.41
21:AW:23:LYS:HA	21:AW:28:MET:HE1	2.02	0.41
22:Aa:82:MET:HB2	31:Aj:52:PHE:HD1	1.86	0.41
26:Ae:55:VAL:HG22	26:Ae:57:ALA:HB3	2.03	0.41
29:Ah:37:CYS:HB3	29:Ah:40:CYS:HB3	2.03	0.41
31:Aj:21:CYS:HB3	31:Aj:25:GLY:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Ak:28:LYS:HE2	32:Ak:31:LYS:HE2	2.03	0.41
32:Ak:39:LEU:HD13	32:Ak:42:ARG:HH11	1.86	0.41
35:B1:86:ARG:O	35:B1:90:GLU:HG2	2.21	0.41
36:B2:1094:A:H4'	36:B2:1095:G:OP2	2.20	0.41
39:BN:29:ARG:NH2	39:BN:40:ILE:HD13	2.35	0.41
41:BP:142:HIS:CE1	41:BP:249:PHE:H	2.38	0.41
42:BQ:54:ARG:HA	42:BQ:54:ARG:HD3	1.72	0.41
47:BW:166:LYS:HE2	47:BW:166:LYS:HB3	1.83	0.41
49:BY:79:LYS:HA	49:BY:79:LYS:HD3	1.83	0.41
56:Bg:55:ARG:HE	56:Bg:56:GLU:H	1.68	0.41
76:HE:211:PHE:HE2	76:HE:273:PHE:HZ	1.69	0.41
78:HS:50:VAL:HG11	78:HS:71:LEU:HD21	2.02	0.41
78:HS:89:THR:HG23	78:HS:90:ASP:OD1	2.20	0.41
1:AA:708:U:H2'	1:AA:709:G:H8	1.85	0.41
1:AA:1325:G:H1	1:AA:1334:C:H42	1.69	0.41
1:AA:1358:G:H1'	1:AA:1397:U:H5"	2.02	0.41
1:AA:1688:U:H2'	1:AA:1689:A:C8	2.55	0.41
1:AA:1691:U:H2'	1:AA:1692:A:C8	2.56	0.41
4:AF:77:ASP:HB3	4:AF:103:ILE:HG13	2.03	0.41
5:AG:196:LYS:HB3	5:AG:200:LYS:HB3	2.03	0.41
6:AH:137:PRO:HB2	6:AH:150:PRO:HD2	2.02	0.41
7:AI:101:LEU:HD12	7:AI:101:LEU:HA	1.89	0.41
8:AJ:215:MET:O	8:AJ:219:VAL:HG12	2.20	0.41
11:AM:151:ASP:OD2	11:AM:151:ASP:C	2.65	0.41
12:AN:61:TRP:CD2	31:Aj:23:HIS:HB3	2.55	0.41
36:B2:1191:C:OP1	36:B2:1363:A:H5"	2.21	0.41
36:B2:2588:C:H2'	36:B2:2589:U:C2	2.56	0.41
41:BP:138:LEU:HD21	41:BP:145:GLU:HA	2.02	0.41
61:Bl:29:ILE:HD11	61:Bl:40:HIS:CE1	2.56	0.41
62:Bm:94:ASN:OD1	62:Bm:94:ASN:C	2.63	0.41
68:Bs:21:ARG:CZ	68:Bs:23:ILE:HD11	2.51	0.41
1:AA:1478:G:H21	17:AS:134:THR:HG23	1.86	0.40
1:AA:1818:A:H2'	1:AA:1819:G:H8	1.86	0.40
4:AF:89:THR:HG23	4:AF:92:GLY:H	1.86	0.40
11:AM:89:SER:O	11:AM:90:ARG:HG2	2.21	0.40
12:AN:49:LEU:HB2	12:AN:55:LEU:HD23	2.03	0.40
13:AO:99:LYS:HE2	13:AO:99:LYS:HB3	1.88	0.40
13:AO:130:LYS:HE3	13:AO:130:LYS:HB2	1.85	0.40
15:AQ:130:ARG:HH22	15:AQ:140:LYS:HA	1.86	0.40
19:AU:18:GLU:HG2	19:AU:19:LYS:N	2.35	0.40
31:Aj:30:LEU:HD21	31:Aj:37:ASN:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Am:127:LYS:HE3	33:Am:149:ASP:C	2.46	0.40
36:B2:1134:A:H2'	36:B2:1135:G:H4'	2.03	0.40
37:B3:46:C:H5"	42:BQ:158:ARG:HE	1.84	0.40
42:BQ:144:VAL:O	42:BQ:173:ILE:HG22	2.21	0.40
48:BX:120:LEU:HD23	48:BX:120:LEU:HA	1.91	0.40
52:Bc:156:PHE:HD1	52:Bc:162:LYS:HB2	1.86	0.40
76:HE:216:HIS:HB3	76:HE:218:TRP:HD1	1.86	0.40
76:HE:479:LYS:HA	76:HE:479:LYS:HD3	1.84	0.40
77:HL:155:LYS:HE2	77:HL:155:LYS:HB2	1.76	0.40
1:AA:54:C:H2'	1:AA:55:A:C8	2.55	0.40
1:AA:180:A:H2'	1:AA:181:A:C8	2.55	0.40
1:AA:457:A:C4	6:AH:66:MET:HE1	2.56	0.40
1:AA:489:G:H22	1:AA:504:U:H3	1.69	0.40
1:AA:849:G:H2'	1:AA:850:U:C5	2.54	0.40
1:AA:906:A:H2'	1:AA:907:A:C8	2.55	0.40
1:AA:1780:U:H2'	1:AA:1781:C:C6	2.55	0.40
7:AI:20:LEU:HD12	7:AI:21:PHE:H	1.87	0.40
10:AL:66:SER:HB2	10:AL:73:SER:HB3	2.03	0.40
15:AQ:28:ALA:O	15:AQ:32:SER:HB2	2.21	0.40
16:AR:19:ALA:HB3	16:AR:83:ILE:HA	2.03	0.40
20:AV:80:PRO:HB2	20:AV:82:TRP:HD1	1.85	0.40
22:Aa:82:MET:HB2	31:Aj:52:PHE:CD1	2.56	0.40
31:Aj:19:ARG:NE	31:Aj:37:ASN:HD21	2.19	0.40
33:Am:172:LYS:HE3	33:Am:194:TYR:HE1	1.86	0.40
36:B2:385:A:H1'	36:B2:400:G:N2	2.37	0.40
36:B2:2611:A:H5"	50:BZ:28:TRP:CD1	2.56	0.40
39:BN:199:ARG:HE	39:BN:199:ARG:HB2	1.54	0.40
41:BP:332:PRO:HG3	44:BS:49:ARG:NH1	2.37	0.40
41:BP:360:LEU:HG	54:Be:63:ILE:HD11	2.02	0.40
52:Bc:12:LYS:HG2	52:Bc:14:GLN:HG2	2.01	0.40
59:Bj:35:LYS:HD3	59:Bj:35:LYS:HA	1.72	0.40
62:Bm:11:LEU:HD23	62:Bm:11:LEU:HA	1.88	0.40
75:H1:32:LYS:HA	75:H1:32:LYS:HD3	1.72	0.40
1:AA:464:G:H2'	1:AA:465:G:H8	1.86	0.40
1:AA:1391:A:N6	22:Aa:19:ARG:HH22	2.19	0.40
2:AD:156:LEU:HG	2:AD:159:VAL:HG21	2.04	0.40
5:AG:112:LEU:HD23	5:AG:112:LEU:HA	1.87	0.40
6:AH:10:LYS:H	6:AH:10:LYS:HG2	1.67	0.40
11:AM:27:GLU:H	11:AM:27:GLU:HG3	1.58	0.40
12:AN:11:ILE:HD12	12:AN:11:ILE:HA	1.97	0.40
18:AT:48:PRO:HA	18:AT:51:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Ae:75:ILE:HD12	26:Ae:75:ILE:HA	1.88	0.40
33:Am:18:VAL:HG21	33:Am:307:ILE:HB	2.04	0.40
33:Am:85:LYS:HB2	33:Am:85:LYS:HE3	1.90	0.40
36:B2:1457:C:H5'	74:By:23:PRO:HD3	2.03	0.40
36:B2:2245:G:H4'	36:B2:2246:A:H5'	2.03	0.40
41:BP:60:HIS:HE1	41:BP:100:ARG:HE	1.68	0.40
41:BP:342:LYS:HD3	41:BP:345:THR:HG23	2.04	0.40
43:BR:49:ARG:HH11	43:BR:52:LEU:HD11	1.87	0.40
76:HE:397:PHE:CZ	76:HE:453:ILE:HD12	2.56	0.40
79:HI:87:LYS:HB3	79:HI:141:SER:HB3	2.03	0.40
1:AA:819:A:C5	24:Ac:107:SER:HA	2.56	0.40
1:AA:948:A:H61	1:AA:959:A:H61	1.70	0.40
1:AA:1264:U:H2'	1:AA:1265:C:C6	2.56	0.40
3:AE:119:THR:HG21	3:AE:156:ALA:HB3	2.04	0.40
3:AE:127:ILE:HD12	3:AE:127:ILE:HA	1.97	0.40
19:AU:7:LYS:H	19:AU:7:LYS:HG3	1.66	0.40
30:Ai:46:LYS:HB3	30:Ai:46:LYS:HE2	1.90	0.40
36:B2:546:G:H21	54:Be:131:LYS:HD2	1.86	0.40
36:B2:3470:G:N3	36:B2:3470:G:H2'	2.37	0.40
37:B3:110:G:H2'	37:B3:111:C:C6	2.56	0.40
42:BQ:207:TYR:CZ	42:BQ:211:LEU:HD22	2.57	0.40
47:BW:77:GLU:H	47:BW:77:GLU:CD	2.30	0.40
1:AA:1054:A:O2'	1:AA:1055:G:H8	2.05	0.40
2:AD:21:LEU:HD12	2:AD:22:ALA:N	2.37	0.40
2:AD:44:ARG:HG2	2:AD:45:SER:N	2.34	0.40
3:AE:158:SER:HA	3:AE:161:ILE:HD12	2.04	0.40
5:AG:65:GLY:O	5:AG:68:ILE:HG22	2.21	0.40
7:AI:18:ILE:HG13	7:AI:19:LYS:N	2.35	0.40
9:AK:57:LYS:HZ3	9:AK:90:ARG:HA	1.86	0.40
13:AO:43:ALA:O	13:AO:46:ILE:HG22	2.22	0.40
14:AP:33:LEU:HD21	14:AP:34:LYS:HZ2	1.86	0.40
15:AQ:4:MET:HA	15:AQ:4:MET:HE2	2.04	0.40
24:Ac:105:THR:OG1	24:Ac:126:LEU:HD11	2.21	0.40
33:Am:291:TRP:HD1	33:Am:292:SER:H	1.69	0.40
36:B2:2295:A:H5'	36:B2:2296:A:C8	2.57	0.40
36:B2:3390:G:O2'	36:B2:3391:A:H5"	2.21	0.40
48:BX:153:LEU:HD13	48:BX:153:LEU:HA	1.97	0.40
54:Be:69:LEU:HA	54:Be:69:LEU:HD12	1.91	0.40
77:HL:18:LYS:HD2	77:HL:18:LYS:HA	1.80	0.40
77:HL:60:PRO:HA	77:HL:151:LYS:HE3	2.04	0.40
77:HL:156:PHE:HB3	77:HL:164:LEU:HD21	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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
2	AD	203/292 (70%)	165 (81%)	34 (17%)	4 (2%)	6 24
3	AE	214/252 (85%)	203 (95%)	11 (5%)	0	100 100
4	AF	214/253 (85%)	205 (96%)	8 (4%)	1 (0%)	24 53
5	AG	214/249 (86%)	192 (90%)	20 (9%)	2 (1%)	14 41
6	AH	259/262 (99%)	235 (91%)	23 (9%)	1 (0%)	30 58
7	AI	201/203 (99%)	179 (89%)	15 (8%)	7 (4%)	3 16
8	AJ	219/239 (92%)	212 (97%)	7 (3%)	0	100 100
9	AK	191/195 (98%)	180 (94%)	11 (6%)	0	100 100
10	AL	184/200 (92%)	179 (97%)	5 (3%)	0	100 100
11	AM	176/192 (92%)	163 (93%)	13 (7%)	0	100 100
12	AN	90/147 (61%)	82 (91%)	8 (9%)	0	100 100
13	AO	141/152 (93%)	130 (92%)	11 (8%)	0	100 100
14	AP	119/145 (82%)	106 (89%)	13 (11%)	0	100 100
15	AQ	148/151 (98%)	142 (96%)	6 (4%)	0	100 100
16	AR	126/139 (91%)	117 (93%)	9 (7%)	0	100 100
17	AS	117/154 (76%)	110 (94%)	6 (5%)	1 (1%)	14 41
18	AT	138/140 (99%)	132 (96%)	6 (4%)	0	100 100
19	AU	104/131 (79%)	92 (88%)	11 (11%)	1 (1%)	12 39
20	AV	139/152 (91%)	132 (95%)	7 (5%)	0	100 100
21	AW	140/144 (97%)	134 (96%)	6 (4%)	0	100 100
22	Aa	98/118 (83%)	93 (95%)	5 (5%)	0	100 100
23	Ab	85/87 (98%)	83 (98%)	2 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	Ac	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
25	Ad	140/143 (98%)	132 (94%)	8 (6%)	0	100	100
26	Ae	131/134 (98%)	119 (91%)	12 (9%)	0	100	100
27	Af	67/89 (75%)	62 (92%)	5 (8%)	0	100	100
28	Ag	95/119 (80%)	93 (98%)	1 (1%)	1 (1%)	11	37
29	Ah	79/83 (95%)	75 (95%)	4 (5%)	0	100	100
30	Ai	61/68 (90%)	56 (92%)	5 (8%)	0	100	100
31	Aj	51/56 (91%)	51 (100%)	0	0	100	100
32	Ak	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	3	16
33	Am	312/314 (99%)	294 (94%)	18 (6%)	0	100	100
34	B0	91/106 (86%)	87 (96%)	4 (4%)	0	100	100
35	B1	91/94 (97%)	83 (91%)	8 (9%)	0	100	100
39	BN	246/253 (97%)	232 (94%)	14 (6%)	0	100	100
40	BO	382/388 (98%)	363 (95%)	19 (5%)	0	100	100
41	BP	360/363 (99%)	345 (96%)	15 (4%)	0	100	100
42	BQ	285/294 (97%)	264 (93%)	21 (7%)	0	100	100
43	BR	169/195 (87%)	151 (89%)	17 (10%)	1 (1%)	21	49
44	BS	221/251 (88%)	216 (98%)	5 (2%)	0	100	100
45	BT	227/259 (88%)	217 (96%)	10 (4%)	0	100	100
46	BV	217/221 (98%)	204 (94%)	12 (6%)	1 (0%)	24	53
47	BW	165/174 (95%)	153 (93%)	12 (7%)	0	100	100
48	BX	199/208 (96%)	198 (100%)	1 (0%)	0	100	100
49	BY	128/134 (96%)	127 (99%)	1 (1%)	0	100	100
50	BZ	198/201 (98%)	191 (96%)	7 (4%)	0	100	100
51	Ba	194/197 (98%)	192 (99%)	2 (1%)	0	100	100
52	Bc	184/187 (98%)	179 (97%)	5 (3%)	0	100	100
53	Bd	155/193 (80%)	152 (98%)	3 (2%)	0	100	100
54	Be	171/176 (97%)	167 (98%)	4 (2%)	0	100	100
55	Bf	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
56	Bg	97/117 (83%)	85 (88%)	12 (12%)	0	100	100
57	Bh	132/139 (95%)	131 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	Bi	61/149 (41%)	55 (90%)	6 (10%)	0	100	100
59	Bj	116/141 (82%)	115 (99%)	1 (1%)	0	100	100
60	Bk	123/126 (98%)	122 (99%)	1 (1%)	0	100	100
61	Bl	133/136 (98%)	124 (93%)	9 (7%)	0	100	100
62	Bm	145/148 (98%)	142 (98%)	3 (2%)	0	100	100
63	Bn	57/61 (93%)	56 (98%)	1 (2%)	0	100	100
64	Bo	92/109 (84%)	90 (98%)	2 (2%)	0	100	100
65	Bp	101/113 (89%)	100 (99%)	1 (1%)	0	100	100
66	Bq	116/127 (91%)	110 (95%)	6 (5%)	0	100	100
67	Br	102/108 (94%)	95 (93%)	7 (7%)	0	100	100
68	Bs	104/111 (94%)	102 (98%)	2 (2%)	0	100	100
69	Bt	119/122 (98%)	116 (98%)	3 (2%)	0	100	100
70	Bu	93/99 (94%)	92 (99%)	1 (1%)	0	100	100
71	Bv	80/91 (88%)	75 (94%)	5 (6%)	0	100	100
72	Bw	67/74 (90%)	66 (98%)	1 (2%)	0	100	100
73	Bx	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
74	By	131/134 (98%)	126 (96%)	5 (4%)	0	100	100
75	H1	94/284 (33%)	86 (92%)	7 (7%)	1 (1%)	11	37
76	HE	840/842 (100%)	783 (93%)	54 (6%)	3 (0%)	30	58
77	HL	214/216 (99%)	204 (95%)	10 (5%)	0	100	100
78	HS	104/106 (98%)	92 (88%)	11 (11%)	1 (1%)	12	39
79	HI	135/157 (86%)	119 (88%)	16 (12%)	0	100	100
80	BA	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
81	BU	182/189 (96%)	180 (99%)	2 (1%)	0	100	100
82	Bb	150/187 (80%)	141 (94%)	9 (6%)	0	100	100
83	A	18/20 (90%)	18 (100%)	0	0	100	100
All	All	12184/13456 (90%)	11513 (94%)	644 (5%)	27 (0%)	44	70

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AD	143	ASN
7	AI	24	PHE

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Mol	Chain	Res	Type
28	Ag	55	GLU
46	BV	5	PRO
76	HE	28	VAL
2	AD	34	VAL
7	AI	29	VAL
7	AI	31	VAL
7	AI	32	LYS
19	AU	78	ARG
75	H1	131	VAL
76	HE	45	ILE
2	AD	148	ALA
7	AI	7	THR
7	AI	17	SER
17	AS	98	VAL
32	Ak	9	ALA
43	BR	33	GLU
78	HS	3	SER
5	AG	180	ARG
2	AD	86	HIS
4	AF	223	ILE
5	AG	93	VAL
6	AH	217	GLU
32	Ak	51	VAL
7	AI	135	ARG
76	HE	676	MET

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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
2	AD	170/228 (75%)	158 (93%)	12 (7%)	13 39
3	AE	193/223 (86%)	190 (98%)	3 (2%)	55 68
4	AF	175/199 (88%)	169 (97%)	6 (3%)	32 58
5	AG	181/203 (89%)	173 (96%)	8 (4%)	25 51
6	AH	226/227 (100%)	220 (97%)	6 (3%)	39 61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	AI	169/169 (100%)	168 (99%)	1 (1%)	78	80
8	AJ	188/204 (92%)	185 (98%)	3 (2%)	55	68
9	AK	169/171 (99%)	167 (99%)	2 (1%)	63	72
10	AL	157/166 (95%)	156 (99%)	1 (1%)	78	80
11	AM	155/165 (94%)	150 (97%)	5 (3%)	34	59
12	AN	77/116 (66%)	74 (96%)	3 (4%)	28	53
13	AO	124/131 (95%)	120 (97%)	4 (3%)	34	59
14	AP	92/118 (78%)	92 (100%)	0	100	100
15	AQ	127/128 (99%)	125 (98%)	2 (2%)	55	68
16	AR	95/104 (91%)	93 (98%)	2 (2%)	47	64
17	AS	101/131 (77%)	100 (99%)	1 (1%)	68	75
18	AT	111/111 (100%)	110 (99%)	1 (1%)	70	76
19	AU	97/120 (81%)	96 (99%)	1 (1%)	68	75
20	AV	127/136 (93%)	127 (100%)	0	100	100
21	AW	117/119 (98%)	117 (100%)	0	100	100
22	Aa	95/111 (86%)	92 (97%)	3 (3%)	34	59
23	Ab	73/73 (100%)	70 (96%)	3 (4%)	27	52
24	Ac	114/115 (99%)	112 (98%)	2 (2%)	51	67
25	Ad	112/113 (99%)	108 (96%)	4 (4%)	31	56
26	Ae	112/113 (99%)	110 (98%)	2 (2%)	51	67
27	Af	61/75 (81%)	61 (100%)	0	100	100
28	Ag	87/106 (82%)	84 (97%)	3 (3%)	32	58
29	Ah	71/73 (97%)	70 (99%)	1 (1%)	59	70
30	Ai	56/61 (92%)	55 (98%)	1 (2%)	51	67
31	Aj	45/47 (96%)	45 (100%)	0	100	100
32	Ak	51/52 (98%)	51 (100%)	0	100	100
33	Am	276/276 (100%)	271 (98%)	5 (2%)	51	67
34	B0	84/93 (90%)	82 (98%)	2 (2%)	43	62
35	B1	74/75 (99%)	71 (96%)	3 (4%)	27	52
39	BN	188/192 (98%)	181 (96%)	7 (4%)	30	55
40	BO	318/326 (98%)	309 (97%)	9 (3%)	38	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	BP	293/294 (100%)	283 (97%)	10 (3%)	32	58
42	BQ	235/241 (98%)	233 (99%)	2 (1%)	70	76
43	BR	139/155 (90%)	134 (96%)	5 (4%)	31	56
44	BS	188/213 (88%)	183 (97%)	5 (3%)	39	61
45	BT	182/212 (86%)	180 (99%)	2 (1%)	65	74
46	BV	185/187 (99%)	181 (98%)	4 (2%)	45	63
47	BW	141/146 (97%)	135 (96%)	6 (4%)	26	51
48	BX	162/167 (97%)	156 (96%)	6 (4%)	30	55
49	BY	110/113 (97%)	104 (94%)	6 (6%)	19	46
50	BZ	175/176 (99%)	173 (99%)	2 (1%)	65	74
51	Ba	159/160 (99%)	156 (98%)	3 (2%)	50	66
52	Bc	157/158 (99%)	151 (96%)	6 (4%)	29	54
53	Bd	136/163 (83%)	131 (96%)	5 (4%)	30	55
54	Be	151/154 (98%)	146 (97%)	5 (3%)	33	58
55	Bf	138/139 (99%)	132 (96%)	6 (4%)	26	51
56	Bg	86/103 (84%)	86 (100%)	0	100	100
57	Bh	103/107 (96%)	101 (98%)	2 (2%)	50	66
58	Bi	57/121 (47%)	55 (96%)	2 (4%)	32	56
59	Bj	105/122 (86%)	105 (100%)	0	100	100
60	Bk	110/111 (99%)	108 (98%)	2 (2%)	51	67
61	Bl	114/115 (99%)	111 (97%)	3 (3%)	40	61
62	Bm	122/123 (99%)	119 (98%)	3 (2%)	42	62
63	Bn	50/51 (98%)	50 (100%)	0	100	100
64	Bo	75/87 (86%)	70 (93%)	5 (7%)	15	41
65	Bp	94/102 (92%)	93 (99%)	1 (1%)	65	74
66	Bq	100/107 (94%)	99 (99%)	1 (1%)	68	75
67	Br	91/94 (97%)	88 (97%)	3 (3%)	33	58
68	Bs	91/96 (95%)	87 (96%)	4 (4%)	25	51
69	Bt	106/107 (99%)	104 (98%)	2 (2%)	50	66
70	Bu	81/84 (96%)	77 (95%)	4 (5%)	22	49
71	Bv	68/71 (96%)	66 (97%)	2 (3%)	37	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
72	Bw	63/66 (96%)	62 (98%)	1 (2%)	55	68
73	Bx	46/47 (98%)	45 (98%)	1 (2%)	45	63
74	By	112/113 (99%)	110 (98%)	2 (2%)	51	67
75	H1	78/230 (34%)	78 (100%)	0	100	100
76	HE	720/720 (100%)	709 (98%)	11 (2%)	57	69
77	HL	188/188 (100%)	185 (98%)	3 (2%)	55	68
78	HS	97/97 (100%)	94 (97%)	3 (3%)	35	59
79	HI	118/131 (90%)	113 (96%)	5 (4%)	26	52
80	BA	46/46 (100%)	45 (98%)	1 (2%)	45	63
81	BU	164/168 (98%)	162 (99%)	2 (1%)	63	72
82	Bb	124/149 (83%)	121 (98%)	3 (2%)	43	62
83	A	14/14 (100%)	14 (100%)	0	100	100
All	All	10442/11318 (92%)	10197 (98%)	245 (2%)	44	63

All (245) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AD	6	ARG
2	AD	17	ILE
2	AD	21	LEU
2	AD	25	CYS
2	AD	31	ASN
2	AD	38	ASN
2	AD	53	LEU
2	AD	90	LEU
2	AD	99	THR
2	AD	130	ARG
2	AD	147	ILE
2	AD	179	LEU
3	AE	48	VAL
3	AE	106	THR
3	AE	135	CYS
4	AF	35	VAL
4	AF	60	LEU
4	AF	72	LEU
4	AF	82	VAL
4	AF	83	VAL
4	AF	182	VAL

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Mol	Chain	Res	Type
5	AG	8	SER
5	AG	19	PHE
5	AG	52	ILE
5	AG	117	VAL
5	AG	158	PHE
5	AG	179	LEU
5	AG	181	GLN
5	AG	207	VAL
6	AH	18	TRP
6	AH	52	LEU
6	AH	72	VAL
6	AH	129	VAL
6	AH	248	ILE
6	AH	258	LEU
7	AI	154	THR
8	AJ	3	LEU
8	AJ	71	HIS
8	AJ	102	VAL
9	AK	123	VAL
9	AK	152	ILE
10	AL	184	LEU
11	AM	8	GLN
11	AM	21	SER
11	AM	61	THR
11	AM	123	HIS
11	AM	148	VAL
12	AN	16	PHE
12	AN	66	TYR
12	AN	71	GLU
13	AO	96	ARG
13	AO	114	ILE
13	AO	132	VAL
13	AO	137	LEU
15	AQ	19	VAL
15	AQ	63	VAL
16	AR	28	THR
16	AR	41	ILE
17	AS	41	LEU
18	AT	28	VAL
19	AU	38	VAL
22	Aa	25	THR
22	Aa	29	VAL

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Mol	Chain	Res	Type
22	Aa	68	THR
23	Ab	4	GLU
23	Ab	59	VAL
23	Ab	61	SER
24	Ac	51	THR
24	Ac	99	VAL
25	Ad	7	LEU
25	Ad	51	VAL
25	Ad	96	GLU
25	Ad	130	LEU
26	Ae	72	PHE
26	Ae	121	THR
28	Ag	36	ILE
28	Ag	39	TRP
28	Ag	83	VAL
29	Ah	16	MET
30	Ai	20	THR
33	Am	10	THR
33	Am	120	VAL
33	Am	129	ILE
33	Am	247	TRP
33	Am	309	VAL
34	B0	64	VAL
34	B0	72	LEU
35	B1	57	CYS
35	B1	71	TRP
35	B1	72	THR
39	BN	44	VAL
39	BN	49	HIS
39	BN	74	THR
39	BN	76	VAL
39	BN	81	MET
39	BN	138	HIS
39	BN	164	VAL
40	BO	86	VAL
40	BO	95	THR
40	BO	183	VAL
40	BO	278	LEU
40	BO	305	ILE
40	BO	322	VAL
40	BO	323	MET
40	BO	337	THR

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Mol	Chain	Res	Type
40	BO	354	VAL
41	BP	8	VAL
41	BP	84	THR
41	BP	101	MET
41	BP	105	THR
41	BP	153	VAL
41	BP	170	LEU
41	BP	232	VAL
41	BP	288	ASP
41	BP	310	VAL
41	BP	326	VAL
42	BQ	155	THR
42	BQ	279	GLU
43	BR	35	VAL
43	BR	81	VAL
43	BR	82	VAL
43	BR	98	HIS
43	BR	133	VAL
44	BS	92	VAL
44	BS	142	VAL
44	BS	151	THR
44	BS	156	LEU
44	BS	224	ASP
45	BT	28	VAL
45	BT	153	ILE
46	BV	26	VAL
46	BV	35	ASP
46	BV	44	ASP
46	BV	136	MET
47	BW	44	THR
47	BW	49	LYS
47	BW	59	ILE
47	BW	99	THR
47	BW	110	ILE
47	BW	148	VAL
48	BX	9	LEU
48	BX	40	GLN
48	BX	49	ARG
48	BX	51	VAL
48	BX	67	MET
48	BX	153	LEU
49	BY	16	VAL

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Mol	Chain	Res	Type
49	BY	20	GLU
49	BY	33	ASP
49	BY	50	VAL
49	BY	56	VAL
49	BY	84	CYS
50	BZ	89	VAL
50	BZ	194	THR
51	Ba	35	VAL
51	Ba	49	PHE
51	Ba	102	HIS
52	Bc	10	VAL
52	Bc	54	SER
52	Bc	88	VAL
52	Bc	102	VAL
52	Bc	123	LEU
52	Bc	128	LEU
53	Bd	6	THR
53	Bd	7	GLN
53	Bd	10	LEU
53	Bd	109	TYR
53	Bd	134	HIS
54	Be	69	LEU
54	Be	86	THR
54	Be	87	HIS
54	Be	146	HIS
54	Be	159	VAL
55	Bf	3	HIS
55	Bf	27	LEU
55	Bf	63	VAL
55	Bf	98	HIS
55	Bf	126	VAL
55	Bf	150	THR
57	Bh	19	LEU
57	Bh	60	VAL
58	Bi	3	VAL
58	Bi	63	ILE
60	Bk	57	VAL
60	Bk	66	GLU
61	Bl	97	THR
61	Bl	102	LYS
61	Bl	105	THR
62	Bm	25	HIS

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Mol	Chain	Res	Type
62	Bm	28	HIS
62	Bm	126	THR
64	Bo	65	TYR
64	Bo	80	ASN
64	Bo	93	VAL
64	Bo	95	VAL
64	Bo	98	ILE
65	Bp	108	THR
66	Bq	35	ILE
67	Br	72	VAL
67	Br	81	VAL
67	Br	103	LEU
68	Bs	23	ILE
68	Bs	40	THR
68	Bs	49	VAL
68	Bs	105	LEU
69	Bt	82	LEU
69	Bt	107	ILE
70	Bu	9	LEU
70	Bu	16	THR
70	Bu	77	THR
70	Bu	78	LEU
71	Bv	20	ARG
71	Bv	59	THR
72	Bw	70	VAL
73	Bx	47	THR
74	By	20	VAL
74	By	54	VAL
76	HE	12	LEU
76	HE	76	SER
76	HE	147	LEU
76	HE	197	LEU
76	HE	202	VAL
76	HE	262	THR
76	HE	338	ILE
76	HE	379	MET
76	HE	426	LEU
76	HE	447	ASP
76	HE	663	VAL
77	HL	54	LEU
77	HL	57	VAL
77	HL	204	VAL

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Mol	Chain	Res	Type
78	HS	39	VAL
78	HS	67	SER
78	HS	102	HIS
79	HI	19	THR
79	HI	83	VAL
79	HI	104	MET
79	HI	112	ASP
79	HI	140	VAL
80	BA	78	ILE
81	BU	52	THR
81	BU	167	ASN
82	Bb	61	ARG
82	Bb	137	THR
82	Bb	141	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (189) such sidechains are listed below:

Mol	Chain	Res	Type
2	AD	26	HIS
2	AD	49	HIS
2	AD	86	HIS
2	AD	112	ASN
2	AD	157	ASN
2	AD	158	HIS
3	AE	42	ASN
3	AE	101	ASN
3	AE	125	GLN
3	AE	209	ASN
5	AG	24	ASN
5	AG	161	HIS
5	AG	199	GLN
6	AH	8	HIS
6	AH	67	GLN
6	AH	112	HIS
6	AH	163	ASN
7	AI	22	ASN
7	AI	46	GLN
7	AI	78	ASN
7	AI	148	GLN
8	AJ	34	GLN
8	AJ	65	GLN
8	AJ	81	HIS

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Mol	Chain	Res	Type
8	AJ	104	GLN
8	AJ	116	GLN
8	AJ	189	HIS
9	AK	73	HIS
9	AK	91	HIS
9	AK	125	ASN
11	AM	8	GLN
11	AM	112	GLN
12	AN	7	ASN
12	AN	39	ASN
12	AN	47	GLN
13	AO	16	GLN
13	AO	60	GLN
13	AO	78	HIS
13	AO	89	HIS
13	AO	95	ASN
13	AO	107	HIS
13	AO	115	ASN
13	AO	124	GLN
15	AQ	49	GLN
15	AQ	62	GLN
15	AQ	123	HIS
16	AR	101	GLN
17	AS	136	HIS
18	AT	12	ASN
18	AT	80	GLN
19	AU	83	GLN
20	AV	101	ASN
20	AV	118	GLN
20	AV	120	HIS
21	AW	128	GLN
23	Ab	7	GLN
23	Ab	70	ASN
24	Ac	24	GLN
24	Ac	42	GLN
25	Ad	46	HIS
25	Ad	87	HIS
25	Ad	92	ASN
25	Ad	97	ASN
26	Ae	88	HIS
27	Af	52	ASN
28	Ag	13	HIS

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Mol	Chain	Res	Type
28	Ag	80	HIS
29	Ah	19	HIS
32	Ak	58	ASN
33	Am	117	ASN
33	Am	162	ASN
33	Am	235	ASN
33	Am	264	GLN
34	B0	47	GLN
39	BN	8	GLN
39	BN	37	HIS
39	BN	67	HIS
39	BN	131	ASN
39	BN	208	HIS
39	BN	210	HIS
39	BN	232	GLN
40	BO	109	HIS
40	BO	165	GLN
40	BO	182	GLN
40	BO	212	ASN
40	BO	243	HIS
40	BO	367	HIS
41	BP	60	HIS
41	BP	118	ASN
41	BP	162	GLN
41	BP	201	HIS
41	BP	239	GLN
42	BQ	17	GLN
42	BQ	63	GLN
42	BQ	79	HIS
43	BR	75	GLN
43	BR	89	ASN
44	BS	46	GLN
44	BS	112	GLN
44	BS	118	GLN
44	BS	121	ASN
44	BS	202	ASN
44	BS	244	ASN
45	BT	77	GLN
45	BT	131	ASN
45	BT	137	ASN
45	BT	192	GLN
46	BV	100	ASN

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Mol	Chain	Res	Type
46	BV	133	GLN
47	BW	109	HIS
48	BX	28	GLN
48	BX	40	GLN
48	BX	132	GLN
48	BX	146	GLN
49	BY	49	GLN
50	BZ	32	GLN
50	BZ	34	ASN
50	BZ	37	HIS
50	BZ	57	GLN
50	BZ	95	GLN
50	BZ	139	HIS
50	BZ	186	HIS
50	BZ	193	ASN
51	Ba	116	GLN
51	Ba	189	ASN
52	Bc	153	HIS
52	Bc	159	HIS
53	Bd	39	GLN
53	Bd	40	ASN
53	Bd	55	ASN
53	Bd	67	HIS
54	Be	32	ASN
58	Bi	59	HIS
59	Bj	110	ASN
60	Bk	18	HIS
61	Bl	40	HIS
62	Bm	62	HIS
62	Bm	66	ASN
62	Bm	102	ASN
62	Bm	125	GLN
63	Bn	6	ASN
63	Bn	7	HIS
63	Bn	27	HIS
64	Bo	74	HIS
64	Bo	80	ASN
65	Bp	103	ASN
66	Bq	18	GLN
67	Br	14	HIS
67	Br	76	HIS
67	Br	89	ASN

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Mol	Chain	Res	Type
68	Bs	3	GLN
68	Bs	73	GLN
68	Bs	98	GLN
69	Bt	99	GLN
70	Bu	61	ASN
70	Bu	63	GLN
72	Bw	10	GLN
73	Bx	4	HIS
73	Bx	11	GLN
74	By	16	ASN
74	By	29	GLN
74	By	59	ASN
74	By	76	GLN
74	By	127	GLN
75	H1	125	HIS
76	HE	251	ASN
76	HE	274	ASN
76	HE	290	ASN
76	HE	350	GLN
76	HE	497	ASN
76	HE	537	HIS
76	HE	584	ASN
76	HE	644	ASN
76	HE	694	HIS
76	HE	725	GLN
76	HE	775	ASN
77	HL	157	GLN
78	HS	99	HIS
79	HI	59	HIS
79	HI	67	ASN
79	HI	102	ASN
80	BA	117	HIS
81	BU	49	GLN
81	BU	59	HIS
81	BU	184	ASN
82	Bb	25	HIS
82	Bb	28	ASN
82	Bb	56	GLN
82	Bb	145	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1696/1842 (92%)	410 (24%)	14 (0%)
36	B2	3240/3498 (92%)	635 (19%)	21 (0%)
37	B3	118/246 (47%)	16 (13%)	1 (0%)
38	B4	156/165 (94%)	28 (17%)	1 (0%)
All	All	5210/5751 (90%)	1089 (20%)	37 (0%)

All (1089) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	2	A
1	AA	3	C
1	AA	4	C
1	AA	25	C
1	AA	26	A
1	AA	34	G
1	AA	45	U
1	AA	47	A
1	AA	57	G
1	AA	60	U
1	AA	68	A
1	AA	69	G
1	AA	79	A
1	AA	82	G
1	AA	105	A
1	AA	112	U
1	AA	115	C
1	AA	116	G
1	AA	117	U
1	AA	125	A
1	AA	128	G
1	AA	129	U
1	AA	133	U
1	AA	138	U
1	AA	139	A
1	AA	141	U
1	AA	142	U
1	AA	143	G
1	AA	144	G
1	AA	147	A
1	AA	166	C
1	AA	168	A
1	AA	169	A
1	AA	170	U

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Mol	Chain	Res	Type
1	AA	176	C
1	AA	177	U
1	AA	178	A
1	AA	186	C
1	AA	188	A
1	AA	191	U
1	AA	193	U
1	AA	194	U
1	AA	195	U
1	AA	196	G
1	AA	197	G
1	AA	198	A
1	AA	201	G
1	AA	205	G
1	AA	217	U
1	AA	219	A
1	AA	221	A
1	AA	231	C
1	AA	233	U
1	AA	234	C
1	AA	236	G
1	AA	239	U
1	AA	241	U
1	AA	242	U
1	AA	243	U
1	AA	244	U
1	AA	253	C
1	AA	264	U
1	AA	265	U
1	AA	268	A
1	AA	275	U
1	AA	276	G
1	AA	281	U
1	AA	283	C
1	AA	290	G
1	AA	302	A
1	AA	319	A
1	AA	324	C
1	AA	340	G
1	AA	341	C
1	AA	353	U
1	AA	355	A

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Mol	Chain	Res	Type
1	AA	362	A
1	AA	363	A
1	AA	364	C
1	AA	368	G
1	AA	383	U
1	AA	389	G
1	AA	391	G
1	AA	397	C
1	AA	398	U
1	AA	402	A
1	AA	403	A
1	AA	405	C
1	AA	407	G
1	AA	419	A
1	AA	427	C
1	AA	428	A
1	AA	429	G
1	AA	442	U
1	AA	444	A
1	AA	447	C
1	AA	450	U
1	AA	471	A
1	AA	472	C
1	AA	473	A
1	AA	478	A
1	AA	480	A
1	AA	482	C
1	AA	483	A
1	AA	489	G
1	AA	491	G
1	AA	503	C
1	AA	504	U
1	AA	507	U
1	AA	508	A
1	AA	509	A
1	AA	510	U
1	AA	511	U
1	AA	512	G
1	AA	513	G
1	AA	514	A
1	AA	515	A
1	AA	516	U

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Mol	Chain	Res	Type
1	AA	517	G
1	AA	518	A
1	AA	521	A
1	AA	523	A
1	AA	528	A
1	AA	530	A
1	AA	537	A
1	AA	541	A
1	AA	542	G
1	AA	543	G
1	AA	545	A
1	AA	546	C
1	AA	547	A
1	AA	557	C
1	AA	558	A
1	AA	559	A
1	AA	561	U
1	AA	562	C
1	AA	568	C
1	AA	571	G
1	AA	577	G
1	AA	581	U
1	AA	583	A
1	AA	588	A
1	AA	597	A
1	AA	598	G
1	AA	609	A
1	AA	614	U
1	AA	622	A
1	AA	623	A
1	AA	626	A
1	AA	627	G
1	AA	637	G
1	AA	638	A
1	AA	642	U
1	AA	695	G
1	AA	696	U
1	AA	703	C
1	AA	705	U
1	AA	756	U
1	AA	767	A
1	AA	768	A

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Mol	Chain	Res	Type
1	AA	769	A
1	AA	779	U
1	AA	783	A
1	AA	784	A
1	AA	787	A
1	AA	788	G
1	AA	793	G
1	AA	795	U
1	AA	797	U
1	AA	802	G
1	AA	804	A
1	AA	808	A
1	AA	809	U
1	AA	818	A
1	AA	825	A
1	AA	826	A
1	AA	827	A
1	AA	830	G
1	AA	831	G
1	AA	832	A
1	AA	833	C
1	AA	835	U
1	AA	841	U
1	AA	844	A
1	AA	846	U
1	AA	848	U
1	AA	850	U
1	AA	869	U
1	AA	877	A
1	AA	878	A
1	AA	891	G
1	AA	926	U
1	AA	928	G
1	AA	929	G
1	AA	948	A
1	AA	950	U
1	AA	960	U
1	AA	974	U
1	AA	975	U
1	AA	981	A
1	AA	985	A
1	AA	998	A

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Mol	Chain	Res	Type
1	AA	1003	A
1	AA	1007	A
1	AA	1011	C
1	AA	1013	A
1	AA	1017	G
1	AA	1018	A
1	AA	1019	U
1	AA	1020	A
1	AA	1036	C
1	AA	1040	A
1	AA	1041	A
1	AA	1043	C
1	AA	1046	U
1	AA	1055	G
1	AA	1067	U
1	AA	1068	G
1	AA	1092	A
1	AA	1098	C
1	AA	1108	A
1	AA	1109	A
1	AA	1112	C
1	AA	1113	U
1	AA	1114	U
1	AA	1116	G
1	AA	1125	G
1	AA	1154	A
1	AA	1160	U
1	AA	1163	A
1	AA	1167	A
1	AA	1171	G
1	AA	1172	C
1	AA	1174	C
1	AA	1176	A
1	AA	1179	A
1	AA	1180	U
1	AA	1181	G
1	AA	1184	G
1	AA	1187	G
1	AA	1201	A
1	AA	1202	U
1	AA	1208	U
1	AA	1210	A

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Mol	Chain	Res	Type
1	AA	1211	A
1	AA	1213	A
1	AA	1214	C
1	AA	1215	G
1	AA	1216	G
1	AA	1217	G
1	AA	1219	A
1	AA	1221	A
1	AA	1233	C
1	AA	1234	A
1	AA	1235	G
1	AA	1242	U
1	AA	1243	A
1	AA	1244	A
1	AA	1245	G
1	AA	1246	G
1	AA	1247	A
1	AA	1248	U
1	AA	1259	A
1	AA	1260	G
1	AA	1261	A
1	AA	1262	G
1	AA	1263	C
1	AA	1268	U
1	AA	1269	C
1	AA	1273	A
1	AA	1274	U
1	AA	1275	U
1	AA	1277	U
1	AA	1299	U
1	AA	1301	C
1	AA	1303	U
1	AA	1324	U
1	AA	1331	U
1	AA	1332	U
1	AA	1335	G
1	AA	1338	A
1	AA	1342	A
1	AA	1355	C
1	AA	1357	U
1	AA	1358	G
1	AA	1359	C

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Mol	Chain	Res	Type
1	AA	1361	A
1	AA	1362	A
1	AA	1364	U
1	AA	1369	G
1	AA	1371	A
1	AA	1372	U
1	AA	1377	C
1	AA	1381	U
1	AA	1383	G
1	AA	1384	G
1	AA	1387	G
1	AA	1391	A
1	AA	1393	U
1	AA	1396	C
1	AA	1398	U
1	AA	1399	C
1	AA	1408	A
1	AA	1410	U
1	AA	1416	C
1	AA	1418	U
1	AA	1419	A
1	AA	1420	A
1	AA	1422	G
1	AA	1432	G
1	AA	1433	U
1	AA	1434	U
1	AA	1435	U
1	AA	1441	A
1	AA	1447	A
1	AA	1448	G
1	AA	1451	C
1	AA	1452	U
1	AA	1453	G
1	AA	1455	G
1	AA	1465	G
1	AA	1475	G
1	AA	1476	C
1	AA	1478	G
1	AA	1480	A
1	AA	1481	C
1	AA	1484	G
1	AA	1491	A

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Mol	Chain	Res	Type
1	AA	1493	U
1	AA	1502	C
1	AA	1510	U
1	AA	1535	C
1	AA	1537	U
1	AA	1542	C
1	AA	1545	A
1	AA	1546	A
1	AA	1547	G
1	AA	1557	A
1	AA	1558	U
1	AA	1559	C
1	AA	1561	U
1	AA	1562	G
1	AA	1563	U
1	AA	1564	U
1	AA	1565	A
1	AA	1576	U
1	AA	1577	G
1	AA	1578	C
1	AA	1581	G
1	AA	1583	G
1	AA	1590	C
1	AA	1594	G
1	AA	1596	A
1	AA	1598	U
1	AA	1600	A
1	AA	1601	U
1	AA	1609	C
1	AA	1610	A
1	AA	1611	A
1	AA	1613	G
1	AA	1614	A
1	AA	1616	G
1	AA	1623	U
1	AA	1624	A
1	AA	1625	G
1	AA	1637	C
1	AA	1642	G
1	AA	1657	G
1	AA	1659	C
1	AA	1660	C

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Mol	Chain	Res	Type
1	AA	1662	U
1	AA	1672	A
1	AA	1676	A
1	AA	1678	C
1	AA	1686	G
1	AA	1687	C
1	AA	1698	U
1	AA	1699	G
1	AA	1700	A
1	AA	1701	A
1	AA	1702	U
1	AA	1715	C
1	AA	1719	U
1	AA	1721	G
1	AA	1726	G
1	AA	1727	C
1	AA	1755	U
1	AA	1756	U
1	AA	1757	G
1	AA	1758	C
1	AA	1760	G
1	AA	1761	A
1	AA	1762	G
1	AA	1763	A
1	AA	1795	A
1	AA	1796	A
1	AA	1797	A
1	AA	1799	G
1	AA	1803	U
1	AA	1808	A
1	AA	1809	G
1	AA	1811	U
1	AA	1824	A
1	AA	1825	C
1	AA	1834	G
1	AA	1835	G
1	AA	1836	A
1	AA	1838	C
1	AA	1841	U
1	AA	1842	A
36	B2	26	A
36	B2	40	A

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Mol	Chain	Res	Type
36	B2	43	A
36	B2	49	A
36	B2	59	G
36	B2	60	A
36	B2	65	A
36	B2	66	A
36	B2	69	U
36	B2	74	A
36	B2	92	G
36	B2	109	A
36	B2	110	G
36	B2	116	A
36	B2	119	U
36	B2	121	A
36	B2	122	A
36	B2	138	U
36	B2	159	U
36	B2	162	A
36	B2	163	A
36	B2	170	G
36	B2	172	U
36	B2	174	U
36	B2	175	G
36	B2	176	A
36	B2	183	A
36	B2	184	C
36	B2	185	G
36	B2	187	U
36	B2	188	C
36	B2	189	G
36	B2	191	U
36	B2	192	C
36	B2	193	U
36	B2	197	U
36	B2	198	U
36	B2	207	C
36	B2	217	G
36	B2	218	A
36	B2	219	G
36	B2	220	A
36	B2	225	G
36	B2	226	A

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Mol	Chain	Res	Type
36	B2	229	A
36	B2	239	U
36	B2	246	U
36	B2	247	U
36	B2	248	G
36	B2	252	A
36	B2	254	G
36	B2	255	C
36	B2	256	C
36	B2	258	U
36	B2	259	A
36	B2	260	U
36	B2	262	A
36	B2	269	U
36	B2	277	G
36	B2	291	G
36	B2	292	A
36	B2	293	A
36	B2	303	A
36	B2	313	U
36	B2	331	A
36	B2	334	U
36	B2	337	U
36	B2	347	C
36	B2	350	A
36	B2	360	A
36	B2	369	A
36	B2	383	A
36	B2	384	G
36	B2	406	U
36	B2	407	A
36	B2	410	A
36	B2	411	C
36	B2	429	G
36	B2	430	A
36	B2	437	G
36	B2	447	C
36	B2	448	U
36	B2	449	U
36	B2	452	C
36	B2	454	G
36	B2	458	G

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Mol	Chain	Res	Type
36	B2	461	A
36	B2	462	U
36	B2	466	U
36	B2	467	A
36	B2	484	A
36	B2	488	A
36	B2	490	U
36	B2	491	C
36	B2	493	G
36	B2	500	U
36	B2	501	G
36	B2	502	G
36	B2	503	U
36	B2	504	A
36	B2	505	G
36	B2	506	G
36	B2	532	A
36	B2	540	A
36	B2	541	G
36	B2	545	A
36	B2	546	G
36	B2	547	G
36	B2	548	U
36	B2	549	G
36	B2	575	G
36	B2	578	U
36	B2	579	A
36	B2	580	U
36	B2	581	A
36	B2	587	U
36	B2	590	U
36	B2	594	A
36	B2	602	A
36	B2	603	C
36	B2	606	G
36	B2	613	A
36	B2	616	A
36	B2	624	U
36	B2	627	G
36	B2	628	U
36	B2	634	G
36	B2	635	G

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Mol	Chain	Res	Type
36	B2	636	A
36	B2	645	U
36	B2	646	A
36	B2	647	A
36	B2	649	G
36	B2	661	C
36	B2	673	C
36	B2	674	A
36	B2	702	A
36	B2	706	U
36	B2	707	U
36	B2	708	U
36	B2	714	A
36	B2	715	U
36	B2	717	A
36	B2	720	A
36	B2	732	A
36	B2	747	A
36	B2	760	C
36	B2	761	U
36	B2	762	U
36	B2	763	G
36	B2	766	G
36	B2	770	G
36	B2	786	C
36	B2	795	G
36	B2	796	U
36	B2	797	C
36	B2	798	A
36	B2	806	G
36	B2	808	U
36	B2	809	U
36	B2	812	A
36	B2	813	G
36	B2	817	G
36	B2	838	A
36	B2	849	A
36	B2	862	A
36	B2	869	A
36	B2	889	G
36	B2	893	C
36	B2	906	U

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Mol	Chain	Res	Type
36	B2	911	U
36	B2	912	G
36	B2	923	U
36	B2	939	G
36	B2	940	G
36	B2	946	A
36	B2	948	G
36	B2	949	A
36	B2	953	A
36	B2	956	G
36	B2	964	U
36	B2	969	G
36	B2	976	C
36	B2	981	C
36	B2	991	C
36	B2	992	U
36	B2	993	C
36	B2	1010	A
36	B2	1011	G
36	B2	1012	A
36	B2	1034	A
36	B2	1042	G
36	B2	1049	U
36	B2	1050	G
36	B2	1051	G
36	B2	1056	G
36	B2	1057	G
36	B2	1058	A
36	B2	1059	A
36	B2	1060	U
36	B2	1061	U
36	B2	1064	C
36	B2	1065	U
36	B2	1067	A
36	B2	1079	A
36	B2	1081	C
36	B2	1095	G
36	B2	1096	A
36	B2	1098	G
36	B2	1104	G
36	B2	1107	G
36	B2	1113	U

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Mol	Chain	Res	Type
36	B2	1123	G
36	B2	1126	A
36	B2	1127	U
36	B2	1128	C
36	B2	1129	G
36	B2	1130	A
36	B2	1135	G
36	B2	1148	G
36	B2	1162	G
36	B2	1174	A
36	B2	1175	U
36	B2	1183	G
36	B2	1184	A
36	B2	1191	C
36	B2	1208	G
36	B2	1211	A
36	B2	1212	U
36	B2	1217	G
36	B2	1222	U
36	B2	1223	C
36	B2	1227	C
36	B2	1228	A
36	B2	1232	G
36	B2	1239	U
36	B2	1240	G
36	B2	1245	U
36	B2	1251	U
36	B2	1252	A
36	B2	1253	G
36	B2	1260	G
36	B2	1262	A
36	B2	1263	C
36	B2	1266	U
36	B2	1267	G
36	B2	1270	C
36	B2	1272	U
36	B2	1273	G
36	B2	1276	A
36	B2	1277	G
36	B2	1279	C
36	B2	1290	A
36	B2	1293	G

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Mol	Chain	Res	Type
36	B2	1295	G
36	B2	1296	U
36	B2	1297	G
36	B2	1300	U
36	B2	1301	A
36	B2	1302	A
36	B2	1310	C
36	B2	1313	G
36	B2	1314	C
36	B2	1316	G
36	B2	1317	A
36	B2	1319	U
36	B2	1333	A
36	B2	1334	A
36	B2	1338	G
36	B2	1340	U
36	B2	1344	G
36	B2	1349	A
36	B2	1361	A
36	B2	1379	U
36	B2	1380	A
36	B2	1381	G
36	B2	1387	A
36	B2	1388	G
36	B2	1389	A
36	B2	1420	U
36	B2	1426	G
36	B2	1433	U
36	B2	1434	G
36	B2	1451	G
36	B2	1452	A
36	B2	1453	A
36	B2	1468	G
36	B2	1471	C
36	B2	1489	U
36	B2	1522	G
36	B2	1530	C
36	B2	1542	C
36	B2	1557	U
36	B2	1588	A
36	B2	1589	U
36	B2	1590	G

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Mol	Chain	Res	Type
36	B2	1593	A
36	B2	1594	G
36	B2	1595	U
36	B2	1598	C
36	B2	1600	C
36	B2	1606	U
36	B2	1607	U
36	B2	1608	C
36	B2	1612	C
36	B2	1613	C
36	B2	1614	U
36	B2	1616	C
36	B2	1617	U
36	B2	1618	A
36	B2	1622	A
36	B2	1624	A
36	B2	1640	A
36	B2	1656	G
36	B2	1665	A
36	B2	1666	C
36	B2	1677	A
36	B2	1678	A
36	B2	1679	A
36	B2	1680	U
36	B2	1681	G
36	B2	1691	A
36	B2	1692	C
36	B2	1729	U
36	B2	1739	A
36	B2	1740	U
36	B2	1742	G
36	B2	1744	A
36	B2	1745	C
36	B2	1755	A
36	B2	1764	U
36	B2	1765	C
36	B2	1771	C
36	B2	1780	G
36	B2	1782	U
36	B2	1783	G
36	B2	1789	A
36	B2	1790	A

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Mol	Chain	Res	Type
36	B2	1791	G
36	B2	1800	G
36	B2	1802	C
36	B2	1803	U
36	B2	1806	U
36	B2	1807	G
36	B2	1811	A
36	B2	1820	C
36	B2	1821	G
36	B2	1838	A
36	B2	1853	A
36	B2	1854	A
36	B2	1855	U
36	B2	1856	G
36	B2	1857	G
36	B2	1876	U
36	B2	1890	A
36	B2	1894	A
36	B2	1895	U
36	B2	1897	A
36	B2	1901	C
36	B2	1903	G
36	B2	1904	C
36	B2	1905	A
36	B2	1918	G
36	B2	1921	C
36	B2	1933	G
36	B2	1934	A
36	B2	1935	U
36	B2	1941	A
36	B2	1961	G
36	B2	1962	C
36	B2	1964	A
36	B2	1998	C
36	B2	2185	C
36	B2	2187	A
36	B2	2188	A
36	B2	2189	C
36	B2	2190	U
36	B2	2200	U
36	B2	2205	A
36	B2	2209	G

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Mol	Chain	Res	Type
36	B2	2210	G
36	B2	2219	A
36	B2	2246	A
36	B2	2248	G
36	B2	2257	G
36	B2	2264	U
36	B2	2275	G
36	B2	2276	A
36	B2	2294	G
36	B2	2295	A
36	B2	2296	A
36	B2	2297	U
36	B2	2298	G
36	B2	2306	G
36	B2	2307	A
36	B2	2315	C
36	B2	2316	A
36	B2	2324	G
36	B2	2325	C
36	B2	2328	G
36	B2	2329	U
36	B2	2330	A
36	B2	2331	A
36	B2	2332	A
36	B2	2342	U
36	B2	2343	A
36	B2	2344	A
36	B2	2346	U
36	B2	2349	G
36	B2	2350	A
36	B2	2354	U
36	B2	2357	U
36	B2	2359	A
36	B2	2361	G
36	B2	2369	A
36	B2	2376	G
36	B2	2395	G
36	B2	2398	U
36	B2	2401	A
36	B2	2403	G
36	B2	2422	U
36	B2	2423	G

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Mol	Chain	Res	Type
36	B2	2424	U
36	B2	2449	A
36	B2	2462	C
36	B2	2464	G
36	B2	2476	U
36	B2	2481	G
36	B2	2485	A
36	B2	2490	A
36	B2	2491	G
36	B2	2492	A
36	B2	2499	U
36	B2	2506	G
36	B2	2530	G
36	B2	2531	A
36	B2	2541	U
36	B2	2542	G
36	B2	2546	G
36	B2	2547	A
36	B2	2549	A
36	B2	2551	G
36	B2	2552	U
36	B2	2556	A
36	B2	2557	G
36	B2	2558	U
36	B2	2559	A
36	B2	2576	G
36	B2	2581	A
36	B2	2582	A
36	B2	2583	U
36	B2	2586	C
36	B2	2590	A
36	B2	2592	C
36	B2	2599	G
36	B2	2601	U
36	B2	2602	U
36	B2	2607	A
36	B2	2610	U
36	B2	2620	A
36	B2	2622	C
36	B2	2630	G
36	B2	2632	A
36	B2	2634	U

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Mol	Chain	Res	Type
36	B2	2635	U
36	B2	2636	A
36	B2	2638	U
36	B2	2644	U
36	B2	2648	C
36	B2	2649	U
36	B2	2656	A
36	B2	2657	A
36	B2	2660	U
36	B2	2661	U
36	B2	2663	C
36	B2	2664	U
36	B2	2665	U
36	B2	2666	C
36	B2	2667	G
36	B2	2668	C
36	B2	2681	G
36	B2	2688	A
36	B2	2689	C
36	B2	2701	G
36	B2	2702	G
36	B2	2709	G
36	B2	2721	A
36	B2	2730	A
36	B2	2743	G
36	B2	2747	U
36	B2	2751	A
36	B2	2761	C
36	B2	2762	A
36	B2	2769	A
36	B2	2772	G
36	B2	2773	A
36	B2	2774	A
36	B2	2775	A
36	B2	2784	A
36	B2	2787	A
36	B2	2799	A
36	B2	2809	G
36	B2	2823	G
36	B2	2824	U
36	B2	2841	A
36	B2	2848	G

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Mol	Chain	Res	Type
36	B2	2850	C
36	B2	2857	A
36	B2	2868	C
36	B2	2872	G
36	B2	2873	A
36	B2	2891	G
36	B2	2895	G
36	B2	2896	A
36	B2	2898	A
36	B2	2899	A
36	B2	2905	C
36	B2	2912	A
36	B2	2913	U
36	B2	2917	U
36	B2	2937	U
36	B2	2940	A
36	B2	2962	C
36	B2	2966	G
36	B2	2971	C
36	B2	2982	A
36	B2	2984	C
36	B2	3001	C
36	B2	3002	G
36	B2	3018	U
36	B2	3030	U
36	B2	3031	A
36	B2	3036	A
36	B2	3043	C
36	B2	3049	U
36	B2	3050	U
36	B2	3062	A
36	B2	3066	A
36	B2	3073	U
36	B2	3078	C
36	B2	3091	G
36	B2	3093	G
36	B2	3102	A
36	B2	3108	A
36	B2	3117	A
36	B2	3123	A
36	B2	3130	C
36	B2	3155	G

Continued on next page...

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Mol	Chain	Res	Type
36	B2	3174	A
36	B2	3175	U
36	B2	3182	G
36	B2	3188	U
36	B2	3189	C
36	B2	3195	C
36	B2	3197	G
36	B2	3200	U
36	B2	3212	G
36	B2	3213	C
36	B2	3216	C
36	B2	3218	A
36	B2	3226	A
36	B2	3227	U
36	B2	3238	A
36	B2	3239	A
36	B2	3240	G
36	B2	3248	U
36	B2	3249	U
36	B2	3250	U
36	B2	3251	U
36	B2	3262	G
36	B2	3264	U
36	B2	3265	U
36	B2	3266	U
36	B2	3267	A
36	B2	3269	A
36	B2	3271	G
36	B2	3275	A
36	B2	3276	A
36	B2	3278	A
36	B2	3282	G
36	B2	3304	U
36	B2	3305	C
36	B2	3306	C
36	B2	3307	U
36	B2	3310	A
36	B2	3317	A
36	B2	3318	A
36	B2	3319	G
36	B2	3322	G
36	B2	3327	A

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Mol	Chain	Res	Type
36	B2	3329	G
36	B2	3341	G
36	B2	3342	G
36	B2	3345	G
36	B2	3347	G
36	B2	3359	U
36	B2	3360	G
36	B2	3362	C
36	B2	3363	C
36	B2	3367	A
36	B2	3372	C
36	B2	3373	C
36	B2	3374	A
36	B2	3375	U
36	B2	3376	U
36	B2	3377	G
36	B2	3378	A
36	B2	3380	A
36	B2	3381	U
36	B2	3383	U
36	B2	3385	G
36	B2	3386	U
36	B2	3387	G
36	B2	3388	C
36	B2	3389	A
36	B2	3390	G
36	B2	3391	A
36	B2	3392	A
36	B2	3395	G
36	B2	3405	C
36	B2	3417	A
36	B2	3419	G
36	B2	3420	U
36	B2	3443	A
36	B2	3446	G
36	B2	3450	C
36	B2	3453	U
36	B2	3455	U
36	B2	3456	U
36	B2	3457	G
36	B2	3476	A
36	B2	3479	C

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Mol	Chain	Res	Type
36	B2	3483	U
36	B2	3491	A
36	B2	3497	G
37	B3	7	G
37	B3	11	A
37	B3	12	U
37	B3	13	A
37	B3	53	U
37	B3	54	A
37	B3	55	A
37	B3	63	A
37	B3	64	G
37	B3	72	U
37	B3	75	G
37	B3	77	A
37	B3	80	A
37	B3	100	A
37	B3	110	G
37	B3	119	U
38	B4	42	U
38	B4	43	C
38	B4	47	G
38	B4	56	A
38	B4	59	G
38	B4	60	A
38	B4	67	A
38	B4	70	C
38	B4	71	G
38	B4	88	A
38	B4	89	U
38	B4	90	U
38	B4	91	C
38	B4	95	G
38	B4	98	U
38	B4	103	G
38	B4	112	A
38	B4	114	C
38	B4	119	A
38	B4	121	U
38	B4	124	G
38	B4	132	G
38	B4	133	U

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Mol	Chain	Res	Type
38	B4	134	U
38	B4	135	C
38	B4	136	U
38	B4	159	U
38	B4	163	A

All (37) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	104	A
1	AA	140	C
1	AA	275	U
1	AA	546	C
1	AA	558	A
1	AA	768	A
1	AA	1113	U
1	AA	1159	A
1	AA	1361	A
1	AA	1383	G
1	AA	1483	C
1	AA	1501	C
1	AA	1580	G
1	AA	1699	G
36	B2	290	G
36	B2	349	G
36	B2	382	A
36	B2	502	G
36	B2	504	A
36	B2	545	A
36	B2	948	G
36	B2	1094	A
36	B2	1103	U
36	B2	1182	U
36	B2	1269	C
36	B2	1272	U
36	B2	1893	C
36	B2	2867	C
36	B2	3001	C
36	B2	3217	U
36	B2	3249	U
36	B2	3265	U
36	B2	3328	U

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Mol	Chain	Res	Type
36	B2	3390	G
36	B2	3418	U
37	B3	12	U
38	B4	97	A

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
79	5CT	HI	52	79	13,14,15	0.49	0	9,15,17	0.49	0

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
79	5CT	HI	52	79	-	8/13/14/16	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
79	HI	52	5CT	C2-C1-NZ-CE
79	HI	52	5CT	NZ-C1-C2-C3
79	HI	52	5CT	C-CA-CB-CG
79	HI	52	5CT	N-CA-CB-CG
79	HI	52	5CT	CD-CE-NZ-C1

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Mol	Chain	Res	Type	Atoms
79	HI	52	5CT	CE-CD-CG-CB
79	HI	52	5CT	NZ-C1-C2-O1
79	HI	52	5CT	O1-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

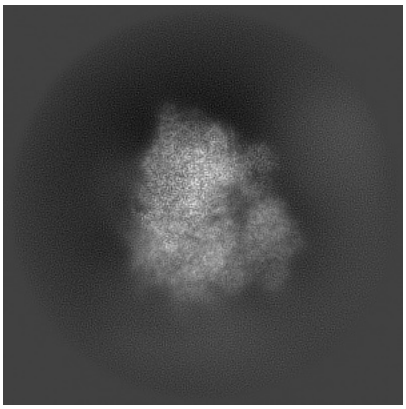
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-54290. These allow visual inspection of the internal detail of the map and identification of artifacts.

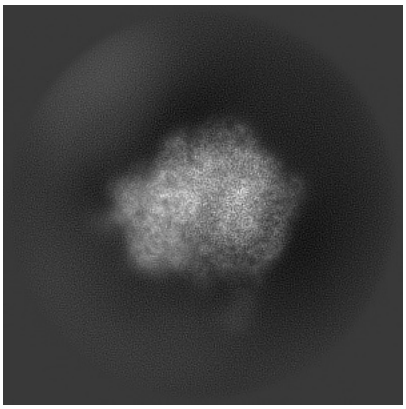
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

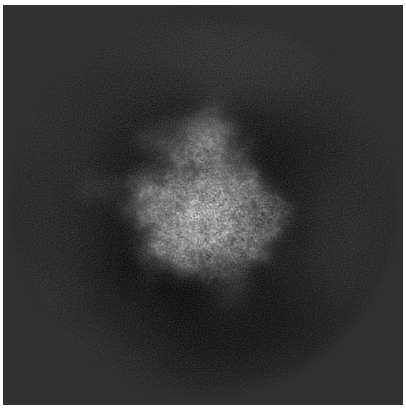
6.1.1 Primary map



X

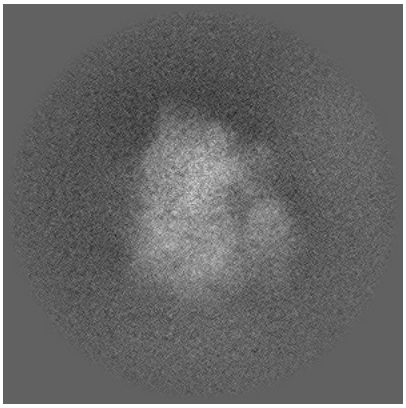


Y

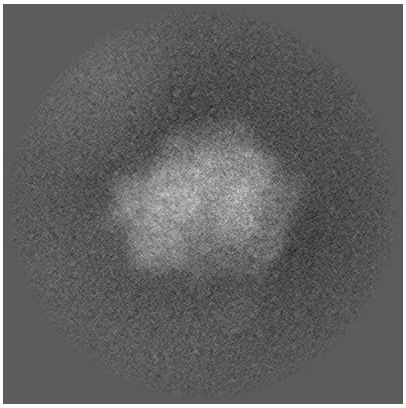


Z

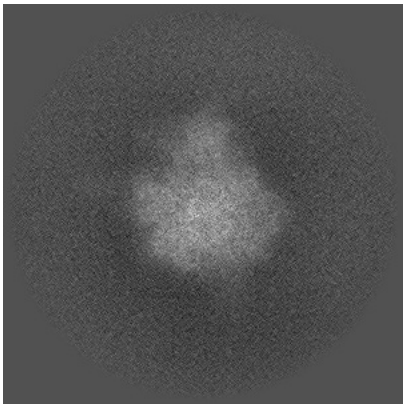
6.1.2 Raw map



X



Y

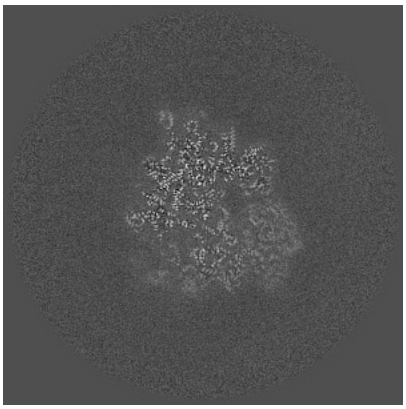


Z

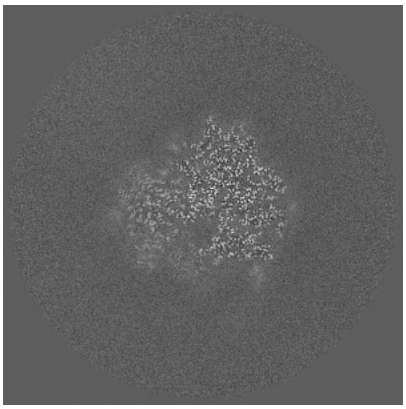
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

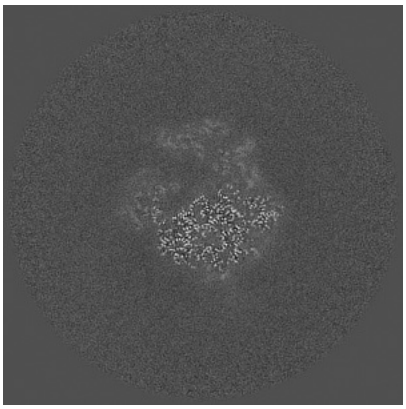
6.2.1 Primary map



X Index: 290

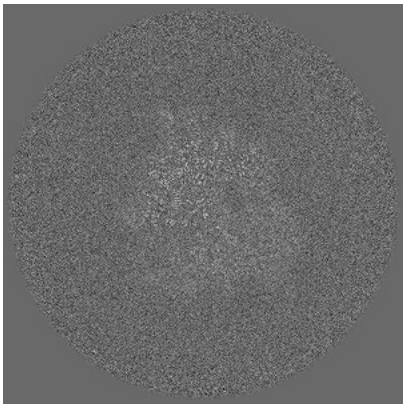


Y Index: 290

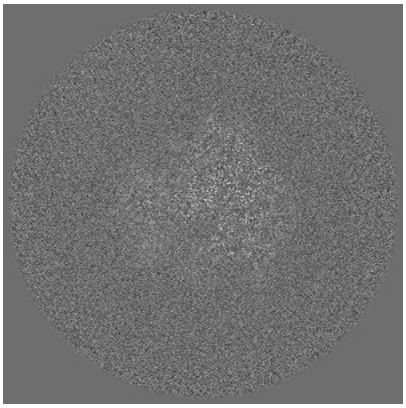


Z Index: 290

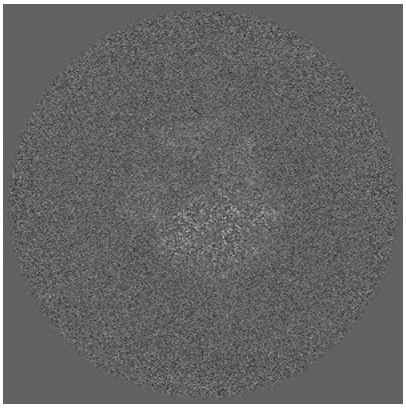
6.2.2 Raw map



X Index: 290



Y Index: 290

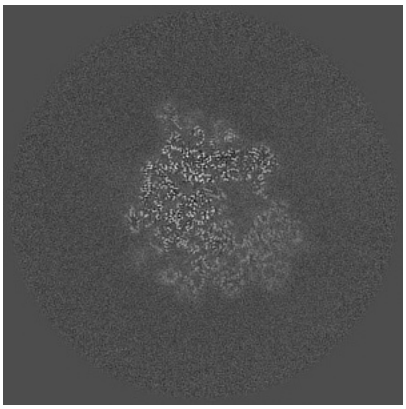


Z Index: 290

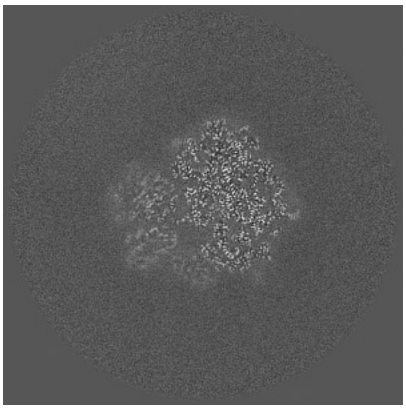
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

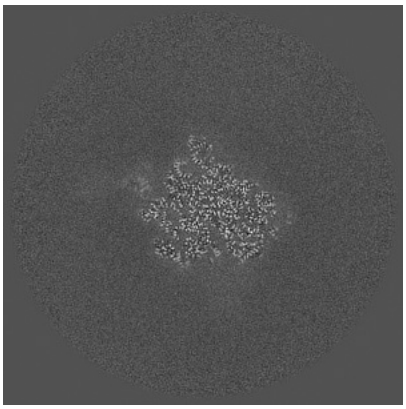
6.3.1 Primary map



X Index: 301

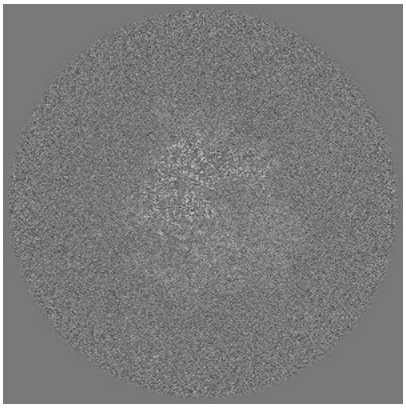


Y Index: 280

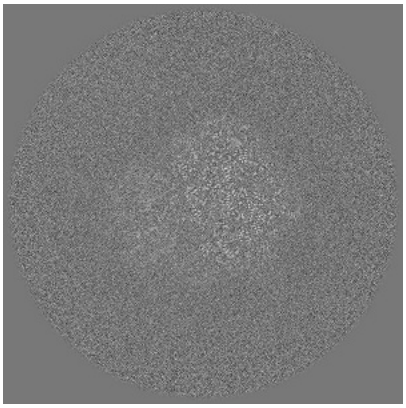


Z Index: 327

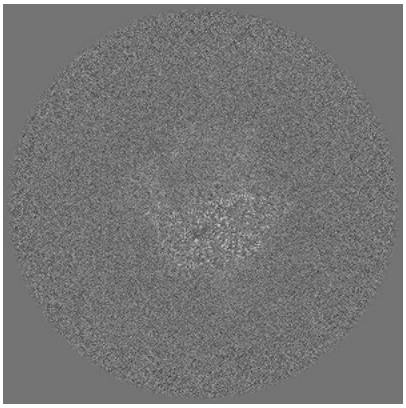
6.3.2 Raw map



X Index: 297



Y Index: 280

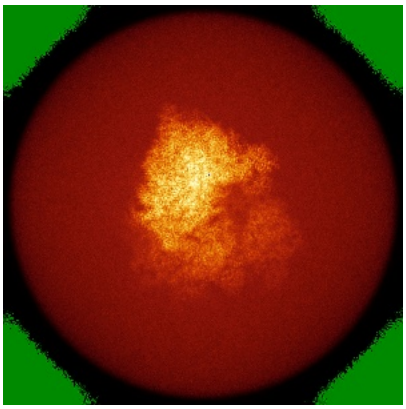


Z Index: 300

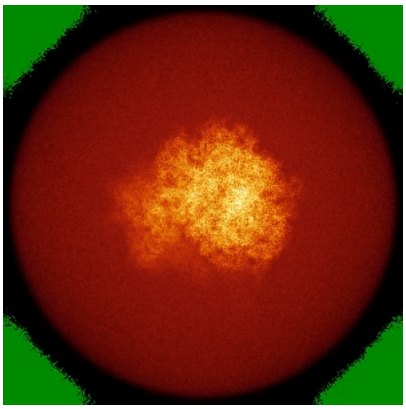
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

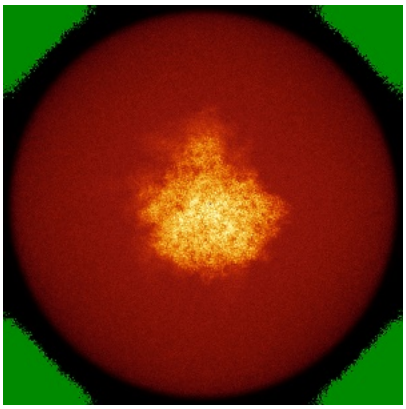
6.4.1 Primary map



X

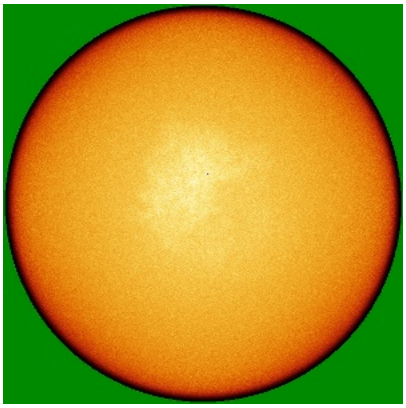


Y

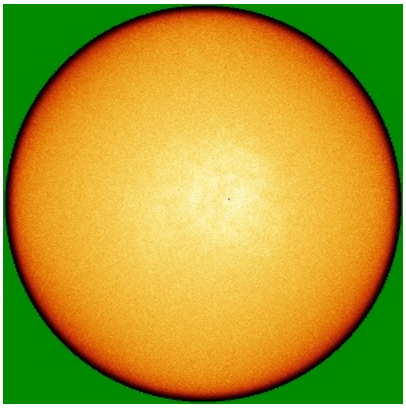


Z

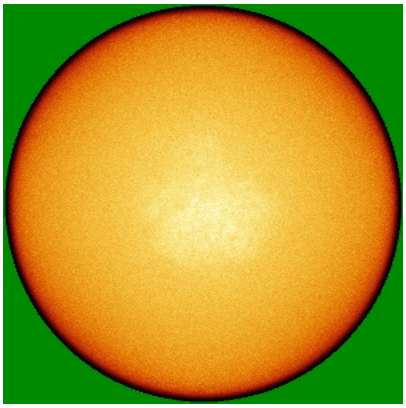
6.4.2 Raw map



X



Y

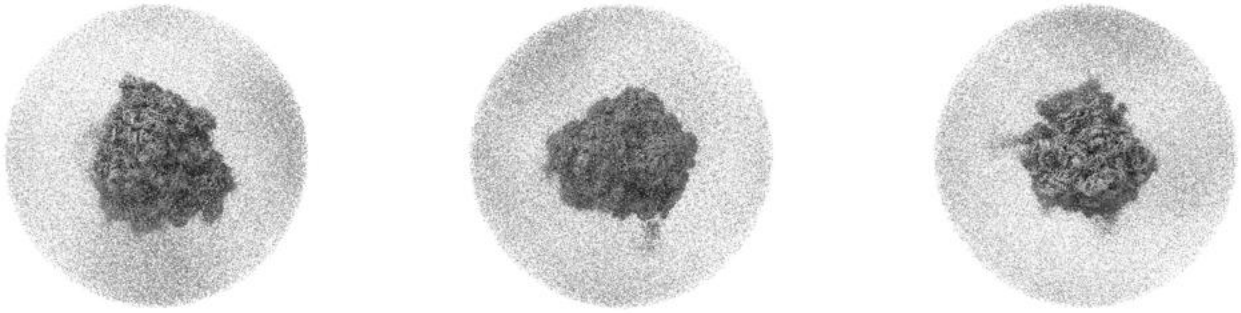


Z

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)

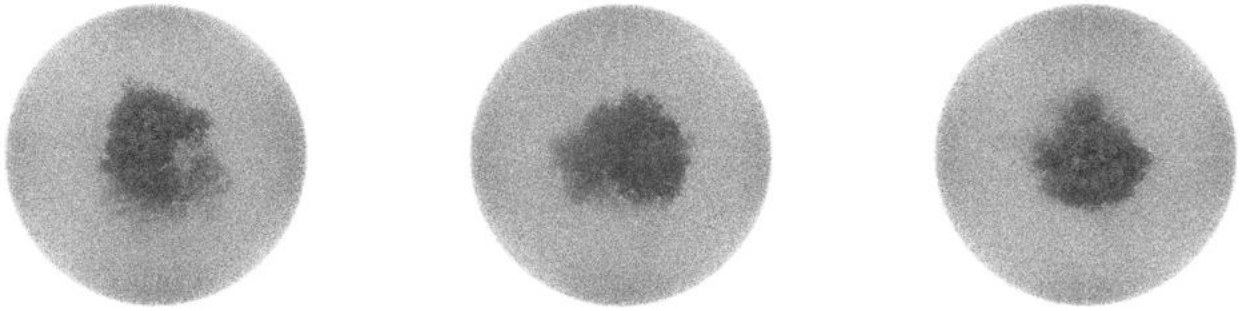
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.000494. 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



X Y Z

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.

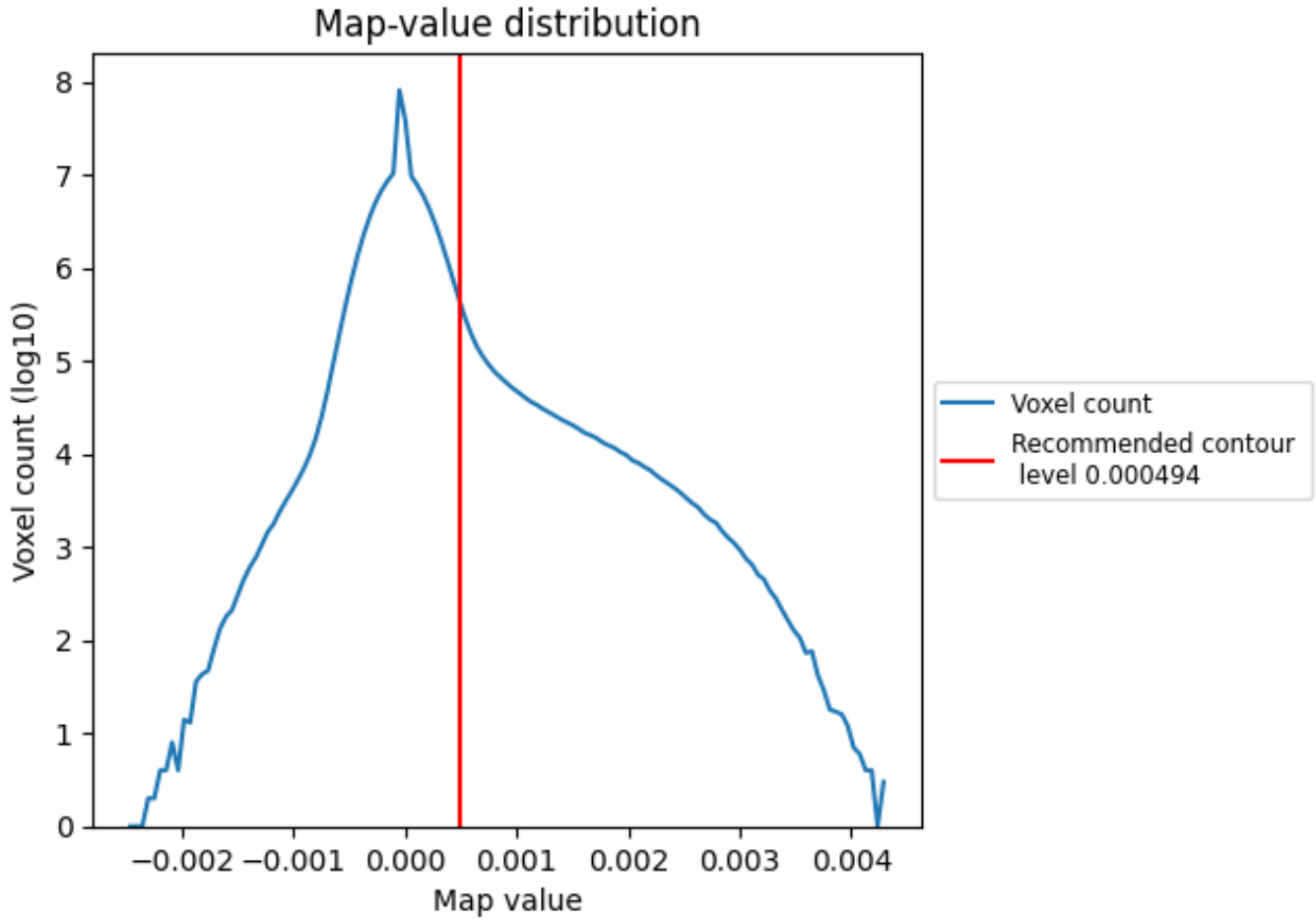
6.6 Mask visualisation (i)

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

7 Map analysis

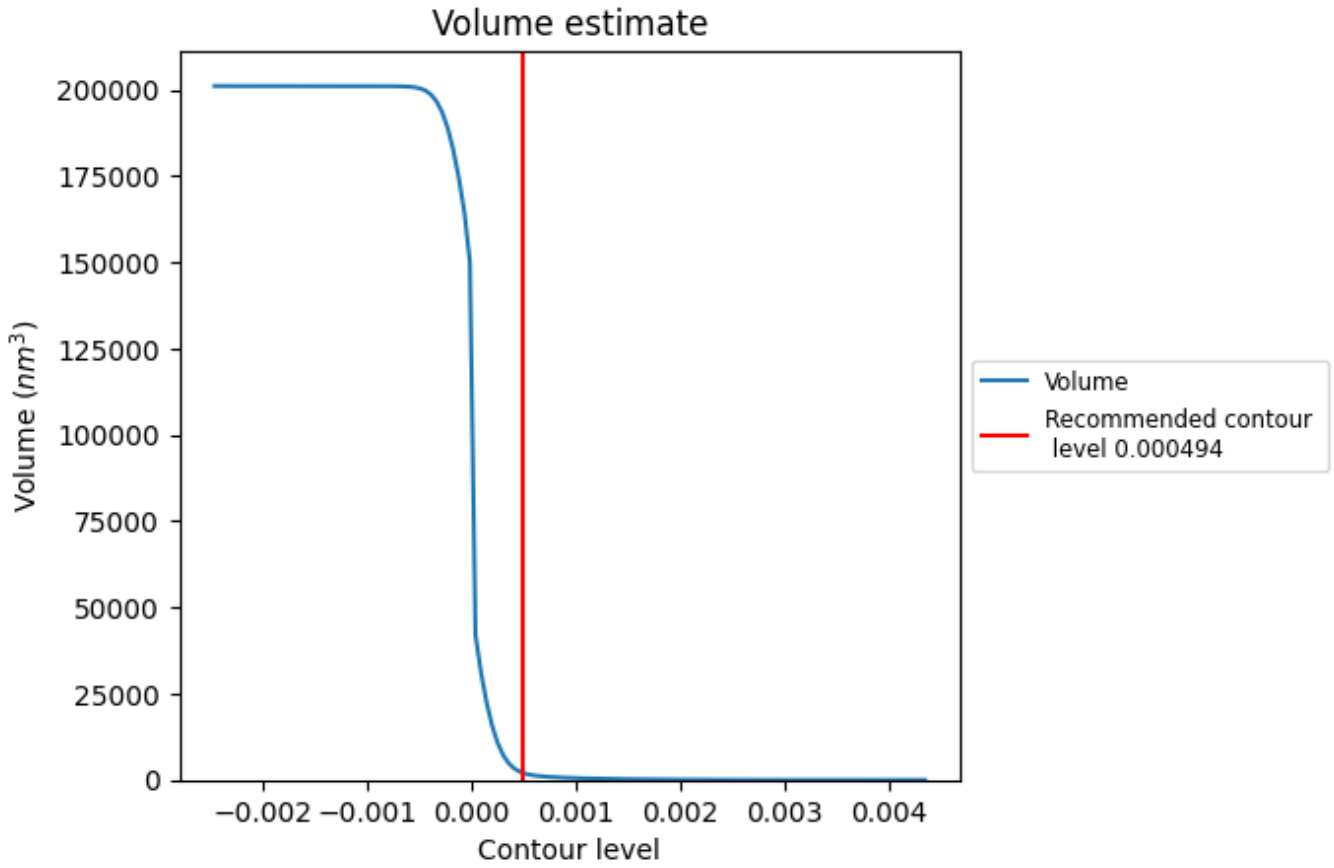
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

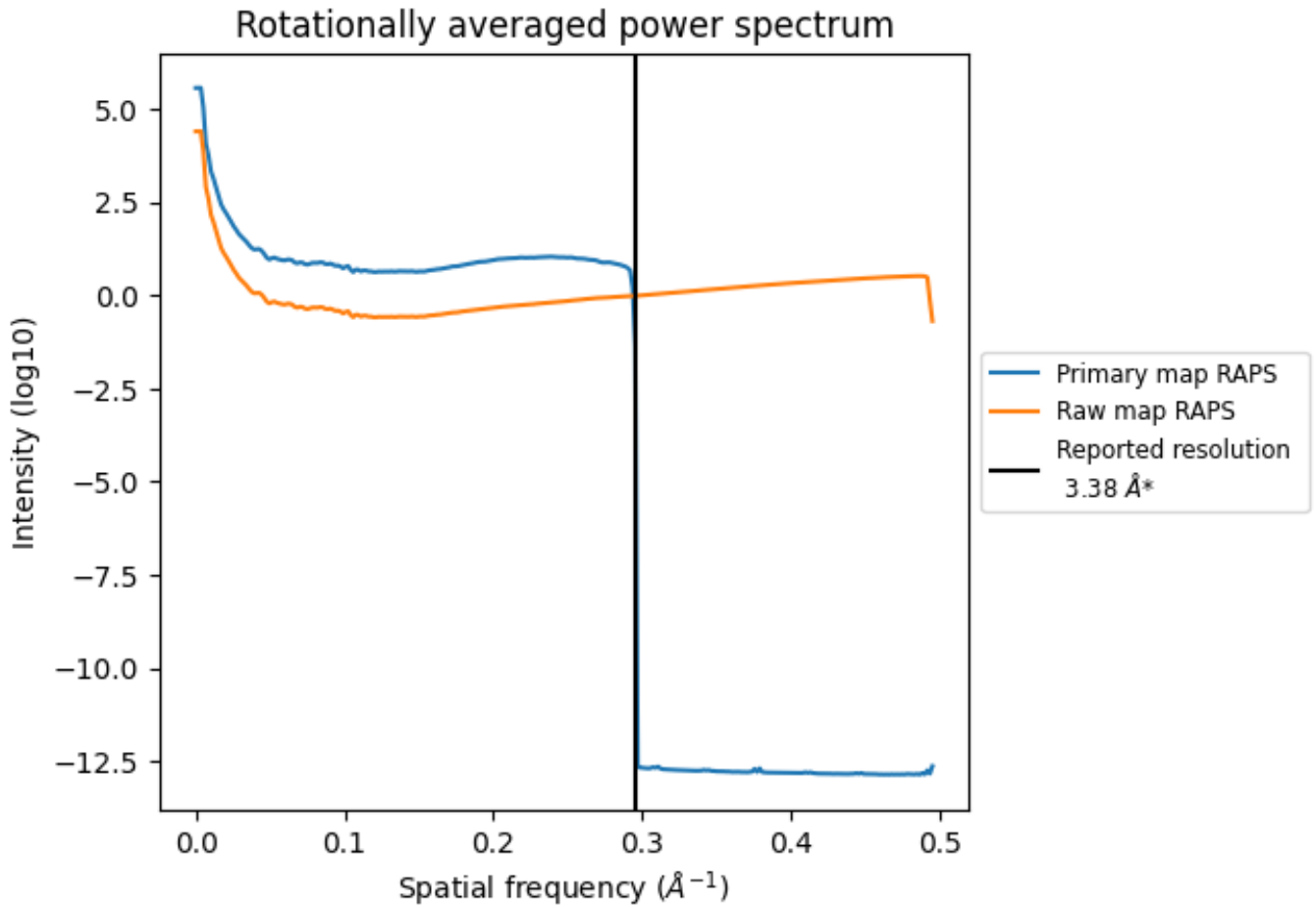
7.2 Volume estimate



The volume at the recommended contour level is 2034 nm^3; this corresponds to an approximate mass of 1837 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 (i)

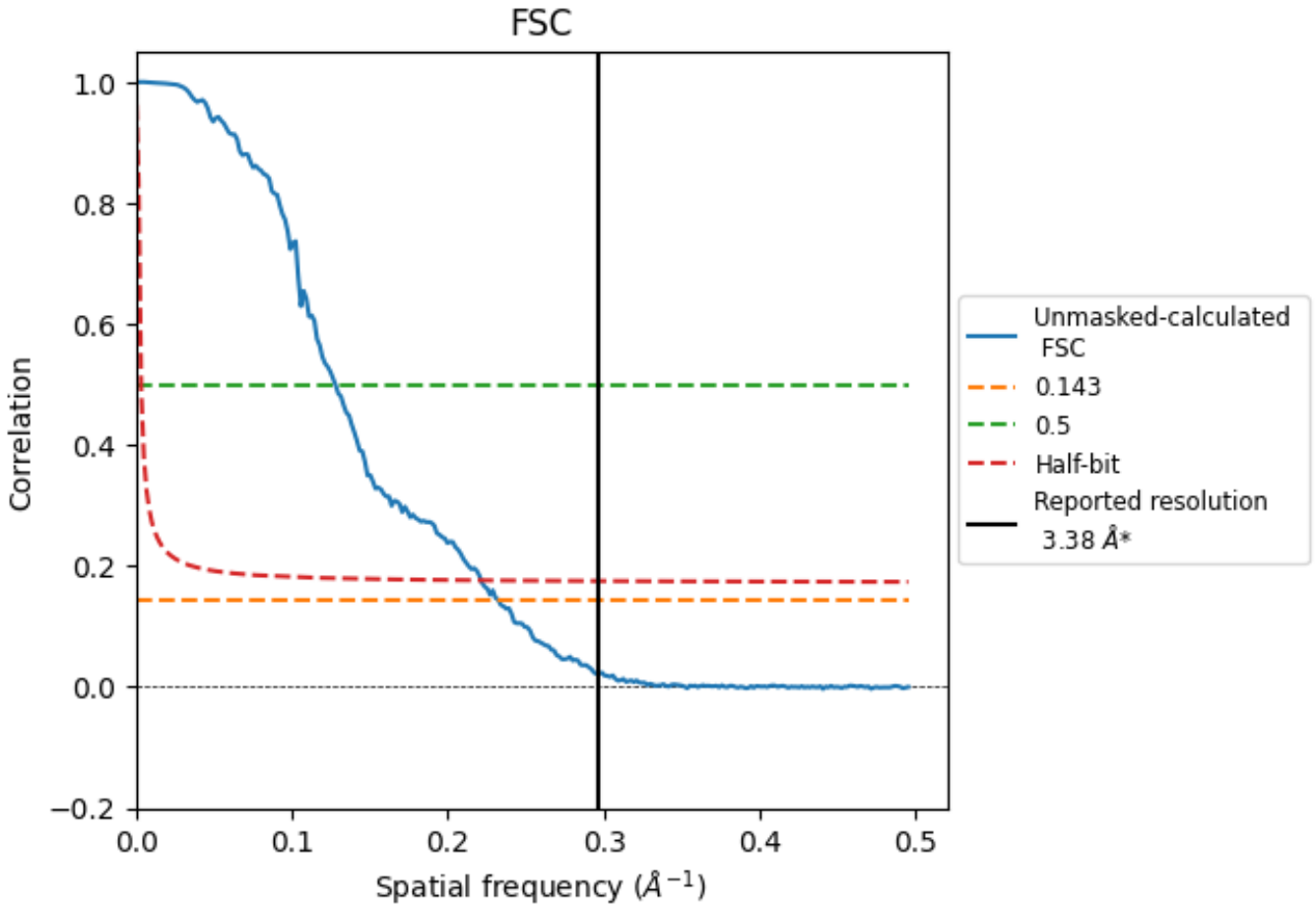


*Reported resolution corresponds to spatial frequency of 0.296 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.296 Å^{-1}

8.2 Resolution estimates (i)

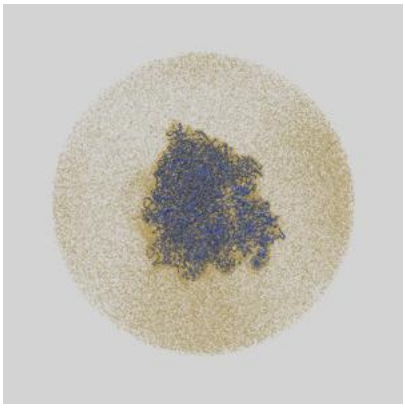
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.38	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.30	7.82	4.52

*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 4.30 differs from the reported value 3.38 by more than 10 %

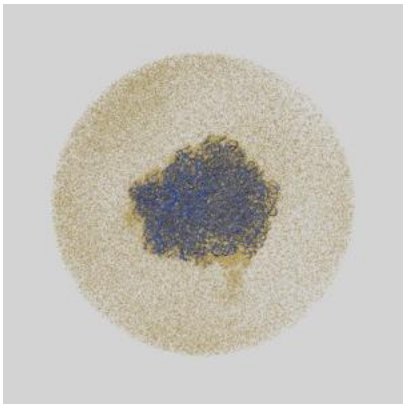
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-54290 and PDB model 9RVU. Per-residue inclusion information can be found in section 3 on page 20.

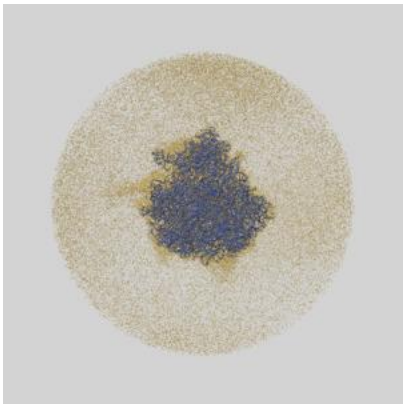
9.1 Map-model overlay



X



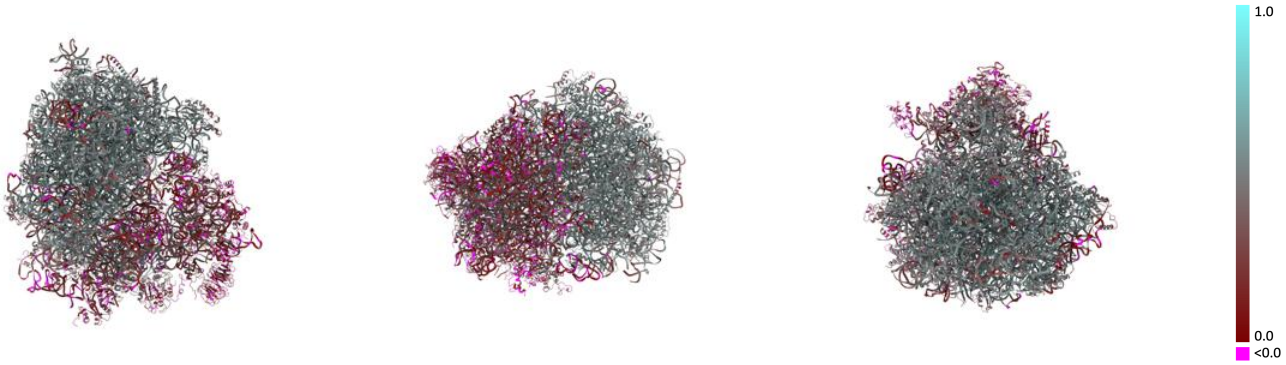
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.000494 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.

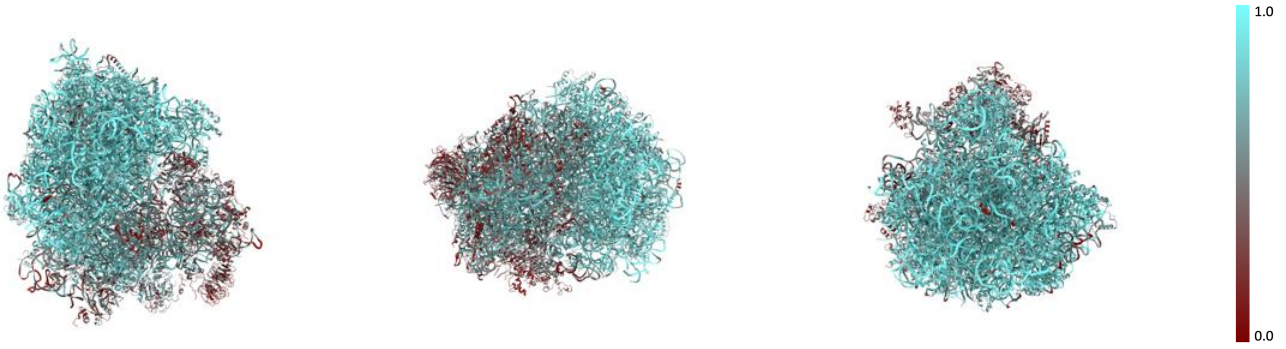
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

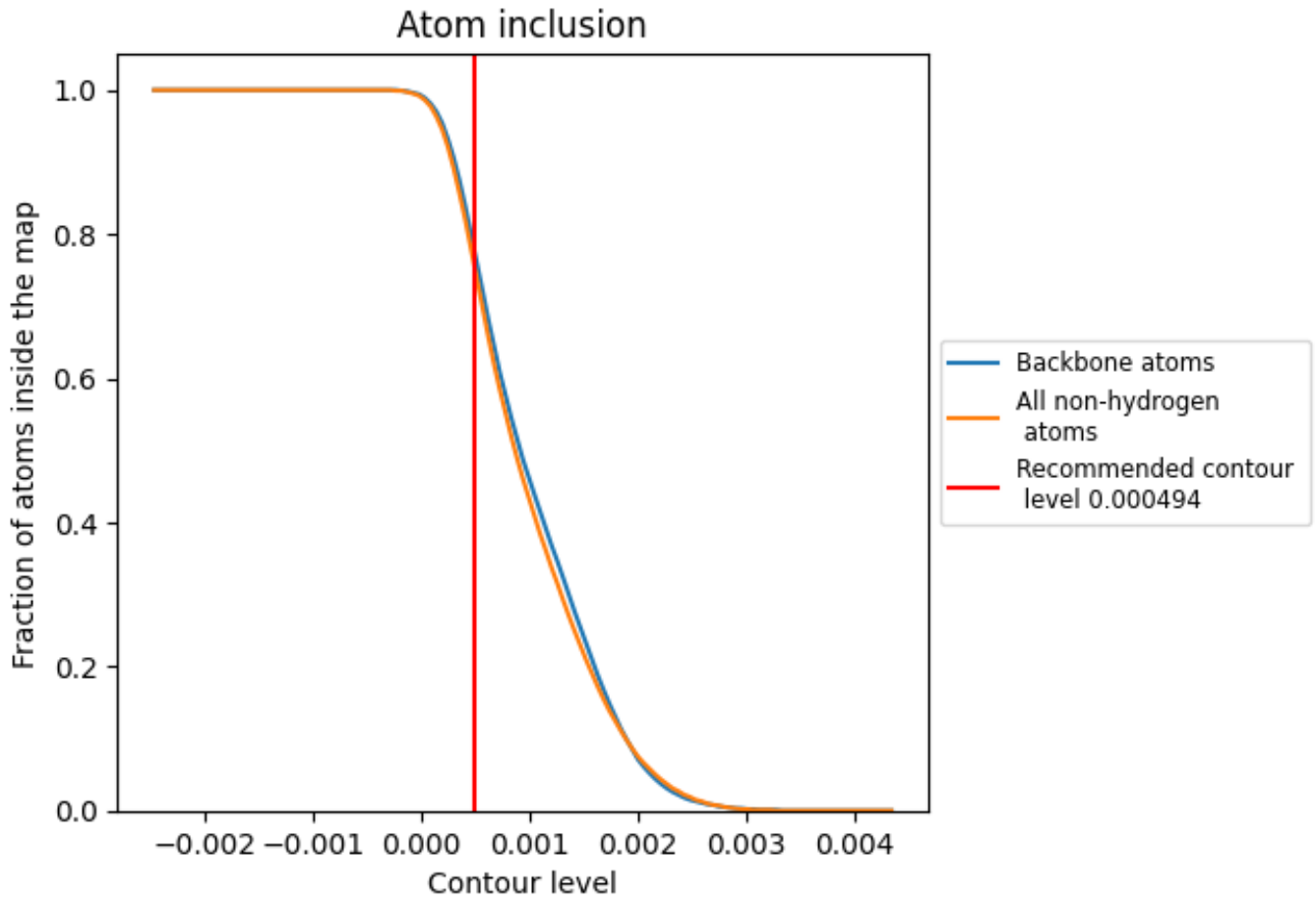
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.000494).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 76% 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 (0.000494) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7550	0.4000
A	0.8250	0.4990
AA	0.7160	0.2870
AD	0.5460	0.2730
AE	0.3620	0.1780
AF	0.7230	0.4160
AG	0.4830	0.2590
AH	0.5200	0.2760
AI	0.3650	0.2010
AJ	0.4050	0.2170
AK	0.4320	0.2470
AL	0.6880	0.3720
AM	0.5970	0.3080
AN	0.4080	0.1860
AO	0.6930	0.3810
AP	0.1480	0.0160
AQ	0.5660	0.2630
AR	0.3710	0.1420
AS	0.4160	0.1770
AT	0.3940	0.2050
AU	0.3940	0.2020
AV	0.4010	0.1960
AW	0.4190	0.1910
Aa	0.3910	0.1510
Ab	0.5980	0.3230
Ac	0.7060	0.4000
Ad	0.7140	0.3940
Ae	0.3460	0.1360
Af	0.2570	0.1260
Ag	0.6470	0.2980
Ah	0.3700	0.1850
Ai	0.3290	0.2080
Aj	0.5860	0.2720
Ak	0.4340	0.2020
Am	0.2330	0.1420

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Chain	Atom inclusion	Q-score
B0	0.8940	0.5230
B1	0.8420	0.4930
B2	0.8950	0.4800
B3	0.9350	0.5010
B4	0.9100	0.4940
BA	0.9080	0.5500
BN	0.8790	0.5210
BO	0.8690	0.5190
BP	0.8620	0.5130
BQ	0.8030	0.4640
BR	0.8260	0.5010
BS	0.8170	0.5060
BT	0.7980	0.4550
BU	0.8510	0.5290
BV	0.8620	0.5000
BW	0.8010	0.4820
BX	0.8470	0.5030
BY	0.8230	0.4780
BZ	0.9040	0.5400
Ba	0.8750	0.5230
Bb	0.8940	0.5560
Bc	0.8760	0.5250
Bd	0.8740	0.4990
Be	0.8720	0.5340
Bf	0.8520	0.5100
Bg	0.7070	0.3690
Bh	0.8600	0.5140
Bi	0.8770	0.4930
Bj	0.8420	0.5070
Bk	0.8510	0.5060
Bl	0.8170	0.4800
Bm	0.8690	0.5140
Bn	0.8850	0.5330
Bo	0.8390	0.4820
Bp	0.8480	0.5010
Bq	0.8790	0.5100
Br	0.8910	0.5290
Bs	0.8870	0.5300
Bt	0.8240	0.5010
Bu	0.8490	0.5150
Bv	0.9270	0.5400
Bw	0.7450	0.4450

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Chain	Atom inclusion	Q-score
Bx	0.8460	0.4940
By	0.7700	0.4780
H1	0.3320	0.1500
HE	0.3530	0.2500
HI	0.7170	0.4550
HL	0.3990	0.2320
HS	0.8270	0.5210