



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:44 PM UTC

PDB ID : 6GZ3 / pdb_00006gz3
EMDB ID : EMD-0098
Title : tRNA translocation by the eukaryotic 80S ribosome and the impact of GTP hydrolysis, Translocation-intermediate-POST-1 (TI-POST-1)
Authors : Flis, J.; Holm, M.; Rundlet, E.J.; Loerke, J.; Hilal, T.; Dabrowski, M.; Buerger, J.; Mielke, T.; Blanchard, S.C.; Spahn, C.M.T.; Budkevich, T.V.
Deposited on : 2018-07-03
Resolution : 3.60 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

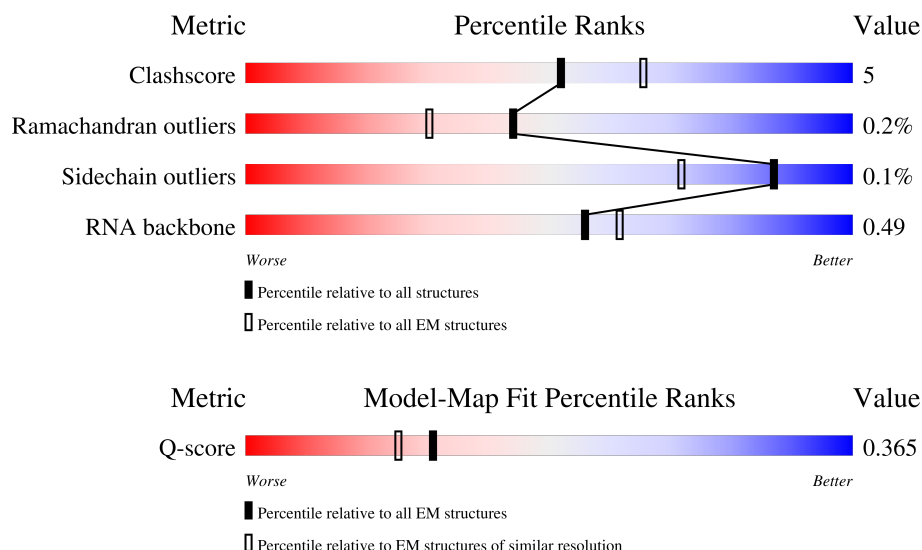
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A2	3612	9% 62% 33% 5%
2	Bv	76	24% 75% 25%
3	Bx	12	25% 42% 50% 8%

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Mol	Chain	Length	Quality of chain
4	Bw	76	
5	B1	1708	
6	BD	220	
7	BF	190	
8	BK	98	
9	BM	120	
10	BP	120	
11	BQ	139	
12	BR	125	
13	BS	139	
14	BT	143	
15	BU	97	
16	BZ	86	
17	Bc	62	
18	Bd	51	
19	Bf	73	
20	Bg	314	
21	BA	215	
22	BB	212	
23	BC	222	
24	BE	257	
25	BG	232	
26	BH	183	
27	BI	207	
28	BJ	179	

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Mol	Chain	Length	Quality of chain
29	BL	153	35% 84% 16%
30	BN	149	26% 87% 13%
31	BO	136	22% 88% 12%
32	BV	81	30% 83% 17%
33	BW	129	17% 86% 14%
34	BX	141	22% 79% 21%
35	BY	125	43% 88% 12%
36	Ba	97	19% 73% 27%
37	Bb	80	44% 78% 22%
38	Be	55	38% 80% 20%
39	A3	157	10% 59% 34% 7%
40	A4	119	65% 30% 5%
41	AA	252	6% 79% 21%
42	AB	394	10% 81% 19%
43	AC	363	10% 85% 14%
44	AD	294	13% 85% 15%
45	AE	194	29% 80% 19%
46	AF	234	10% 85% 15%
47	AG	234	21% 82% 18%
48	AH	191	9% 81% 19%
49	AI	211	11% 82% 17%
50	AJ	169	19% 91% 9%
51	AL	205	19% 78% 22%
52	AM	139	13% 78% 22%
53	AN	203	77% 23%

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Mol	Chain	Length	Quality of chain
54	AO	195	
55	AP	153	
56	AQ	187	
57	AR	181	
58	AS	175	
59	AT	157	
60	AU	99	
61	AV	129	
62	AW	121	
63	AX	117	
64	AY	127	
65	AZ	134	
66	Aa	147	
67	Ab	68	
68	Ac	103	
69	Ad	106	
70	Ae	129	
71	Af	109	
72	Ag	114	
73	Ah	122	
74	Ai	97	
75	Aj	84	
76	Ak	69	
77	Al	50	
78	Am	50	

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Mol	Chain	Length	Quality of chain
79	An	25	
80	Ao	105	
81	Ap	91	
82	At	122	
83	Au	217	
84	Aq	151	
85	AK	202	
86	Ct	853	

2 Entry composition [i](#)

There are 89 unique types of molecules in this entry. The entry contains 225624 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 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A2	3612	Total	C	N	O	P	0	0
			77427	34482	14158	25175	3612		

- Molecule 2 is a RNA chain called ap/P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Bv	76	Total	C	N	O	P	0	0
			1620	723	290	531	76		

- Molecule 3 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Bx	12	Total	C	N	O	P	0	0
			257	115	46	84	12		

- Molecule 4 is a RNA chain called pe/E-site-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Bw	76	Total	C	N	O	P	0	0
			1627	725	294	532	76		

- Molecule 5 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B1	1708	Total	C	N	O	P	0	0
			36456	16274	6546	11928	1708		

- Molecule 6 is a protein called ribosomal protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BD	220	Total	C	N	O	S	0	0
			1709	1090	308	304	7		

- Molecule 7 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BF	190	Total	C	N	O	S	0	0
			1502	939	285	271	7		

- Molecule 8 is a protein called ribosomal protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BK	98	Total	C	N	O	S	0	0
			827	539	148	134	6		

- Molecule 9 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BM	120	Total	C	N	O	S	0	0
			931	584	164	174	9		

- Molecule 10 is a protein called ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	BP	120	Total	C	N	O	S	0	0
			999	636	188	168	7		

- Molecule 11 is a protein called ribosomal protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BQ	139	Total	C	N	O	S	0	0
			1109	704	210	192	3		

- Molecule 12 is a protein called ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BR	125	Total	C	N	O	S	0	0
			1011	634	187	186	4		

- Molecule 13 is a protein called ribosomal protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BS	139	Total	C	N	O	S	0	0
			1154	725	233	195	1		

- Molecule 14 is a protein called ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BT	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 15 is a protein called ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BU	97	Total	C	N	O	S	0	0
			769	483	144	138	4		

- Molecule 16 is a protein called ribosomal protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BZ	86	Total	C	N	O	S	0	0
			688	442	129	116	1		

- Molecule 17 is a protein called Ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Bc	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 18 is a protein called ribosomal protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Bd	51	Total	C	N	O	S	0	0
			427	269	87	66	5		

- Molecule 19 is a protein called Ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Bf	73	Total	C	N	O	S	0	0
			601	379	115	100	7		

- Molecule 20 is a protein called ribosomal protein RACK 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Bg	314	Total	C	N	O	S	0	0
			2440	1537	425	466	12		

- Molecule 21 is a protein called ribosomal protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BA	215	Total	C	N	O	S	0	0
			1704	1083	298	315	8		

- Molecule 22 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BB	212	Total	C	N	O	S	0	0
			1722	1093	308	307	14		

- Molecule 23 is a protein called ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BC	222	Total	C	N	O	S	0	0
			1724	1114	296	304	10		

- Molecule 24 is a protein called ribosomal protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BE	257	Total	C	N	O	S	0	0
			2031	1298	381	344	8		

- Molecule 25 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BG	232	Total	C	N	O	S	0	0
			1884	1176	379	322	7		

- Molecule 26 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BH	183	Total	C	N	O	S	0	0
			1479	941	272	265	1		

- Molecule 27 is a protein called ribosomal protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BI	207	Total	C	N	O	S	0	0
			1696	1064	334	293	5		

- Molecule 28 is a protein called Ribosomal protein S9 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BJ	179	Total	C	N	O	S	0	0
			1495	953	299	241	2		

- Molecule 29 is a protein called Ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BL	153	Total	C	N	O	S	0	0
			1258	804	235	213	6		

- Molecule 30 is a protein called ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BN	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 31 is a protein called ribosomal protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BO	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 32 is a protein called ribosomal protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BV	81	Total	C	N	O	S	0	0
			617	380	114	118	5		

- Molecule 33 is a protein called Ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BW	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 34 is a protein called Ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BX	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 35 is a protein called ribosomal protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BY	125	Total	C	N	O	S	0	0
			1015	642	199	169	5		

- Molecule 36 is a protein called ribosomal protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Ba	97	Total	C	N	O	S	0	0
			774	481	160	128	5		

- Molecule 37 is a protein called ribosomal protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Bb	80	Total	C	N	O	S	0	0
			625	391	116	111	7		

- Molecule 38 is a protein called ribosomal protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Be	55	Total	C	N	O	S	0	0
			437	272	96	68	1		

- Molecule 39 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	A3	157	Total	C	N	O	P	0	0
			3337	1489	587	1104	157		

- Molecule 40 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	A4	119	Total	C	N	O	P	0	0
			2541	1132	454	836	119		

- Molecule 41 is a protein called Ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AA	252	Total	C	N	O	S	0	0
			1930	1209	395	320	6		

- Molecule 42 is a protein called ribosomal protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	AB	394	Total	C	N	O	S	0	0
			3178	2024	596	544	14		

- Molecule 43 is a protein called ribosomal protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	AC	363	Total	C	N	O	S	0	0
			2888	1817	577	480	14		

- Molecule 44 is a protein called ribosomal protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	AD	294	Total	C	N	O	S	0	0
			2392	1510	436	432	14		

- Molecule 45 is a protein called ribosomal protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	AE	194	Total	C	N	O	S	0	0
			1571	1013	294	263	1		

- Molecule 46 is a protein called ribosomal protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	AF	234	Total	C	N	O	S	0	0
			1950	1252	376	313	9		

- Molecule 47 is a protein called ribosomal protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	AG	234	Total	C	N	O	S	0	0
			1880	1197	362	317	4		

- Molecule 48 is a protein called ribosomal protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AH	191	Total	C	N	O	S	0	0
			1526	960	285	275	6		

- Molecule 49 is a protein called Ribosomal protein L10 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AI	208	Total	C	N	O	S	0	0
			1692	1074	327	278	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	149	ILE	VAL	conflict	UNP B7NZQ2

- Molecule 50 is a protein called Ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	AJ	169	Total	C	N	O	S	0	0
			1353	855	252	240	6		

- Molecule 51 is a protein called ribosomal protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AL	205	Total	C	N	O	S	0	0
			1657	1036	344	273	4		

- Molecule 52 is a protein called ribosomal protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	AM	139	Total	C	N	O	S	0	0
			1138	730	218	183	7		

- Molecule 53 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	AN	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 54 is a protein called ribosomal protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AO	195	Total	C	N	O	S	0	0
			1606	1034	315	252	5		

- Molecule 55 is a protein called ribosomal protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	AP	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 56 is a protein called ribosomal protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AQ	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 57 is a protein called ribosomal protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	AR	181	Total	C	N	O	S	0	0
			1517	938	329	241	9		

- Molecule 58 is a protein called ribosomal protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AS	175	Total	C	N	O	S	0	0
			1449	921	283	234	11		

- Molecule 59 is a protein called ribosomal protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AT	157	Total	C	N	O	S	0	0
			1284	815	250	214	5		

- Molecule 60 is a protein called ribosomal protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AU	99	Total	C	N	O	S	0	0
			808	518	141	147	2		

- Molecule 61 is a protein called Ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AV	129	Total	C	N	O	S	0	0
			969	613	182	169	5		

- Molecule 62 is a protein called ribosomal protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AW	121	Total	C	N	O	S	0	0
			989	617	202	167	3		

- Molecule 63 is a protein called ribosomal protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AX	117	Total	C	N	O	S	0	0
			958	612	180	165	1		

- Molecule 64 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	AY	127	Total	C	N	O	S	0	0
			1064	668	216	177	3		

- Molecule 65 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AZ	134	Total	C	N	O	S	0	0
			1103	712	207	181	3		

- Molecule 66 is a protein called ribosomal protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Aa	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 67 is a protein called ribosomal protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Ab	68	Total	C	N	O	S	0	0
			559	344	122	90	3		

- Molecule 68 is a protein called ribosomal protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Ac	103	Total	C	N	O	S	0	0
			801	508	141	145	7		

- Molecule 69 is a protein called ribosomal protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Ad	106	Total	C	N	O	S	0	0
			879	555	170	152	2		

- Molecule 70 is a protein called ribosomal protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Ae	129	Total	C	N	O	S	0	0
			1064	673	220	166	5		

- Molecule 71 is a protein called ribosomal protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Af	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 72 is a protein called ribosomal protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Ag	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 73 is a protein called ribosomal protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Ah	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 74 is a protein called ribosomal protein eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Ai	97	Total	C	N	O	S	0	0
			794	497	168	124	5		

- Molecule 75 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Aj	84	Total	C	N	O	S	0	0
			689	423	152	109	5		

- Molecule 76 is a protein called ribosomal protein eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Ak	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 77 is a protein called ribosomal protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Al	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 78 is a protein called ribosomal protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Am	50	Total	C	N	O	S	0	0
			411	254	87	64	6		

- Molecule 79 is a protein called ribosomal protein eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	An	25	Total	C	N	O	S	0	0
			240	145	64	28	3		

- Molecule 80 is a protein called ribosomal protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Ao	105	Total	C	N	O	S	0	0
			863	542	175	140	6		

- Molecule 81 is a protein called ribosomal protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Ap	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 82 is a protein called ribosomal protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	At	122	Total	C	N	O	S	0	0
			980	607	204	165	4		

- Molecule 83 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Au	217	Total	C	N	O	S	0	0
			1744	1114	314	307	9		

- Molecule 84 is a protein called Ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Aq	151	Total	C	N	O	S	0	0
			1140	708	215	213	4		

- Molecule 85 is a protein called ribosomal protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	AK	202	Total	C	N	O	S	0	0
			1556	989	272	286	9		

- Molecule 86 is a protein called eukaryotic elongation factor 2 (eEF2).

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Ct	853	Total	C	N	O	S	0	0
			6659	4226	1146	1243	44		

- Molecule 87 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
87	A2	231	Total	Mg	0
			231	231	
87	Bx	1	Total	Mg	0
			1	1	
87	B1	68	Total	Mg	0
			68	68	
87	BD	4	Total	Mg	0
			4	4	
87	BS	1	Total	Mg	0
			1	1	
87	Bd	1	Total	Mg	0
			1	1	
87	Ba	1	Total	Mg	0
			1	1	
87	A3	6	Total	Mg	0
			6	6	
87	A4	8	Total	Mg	0
			8	8	

Continued on next page...

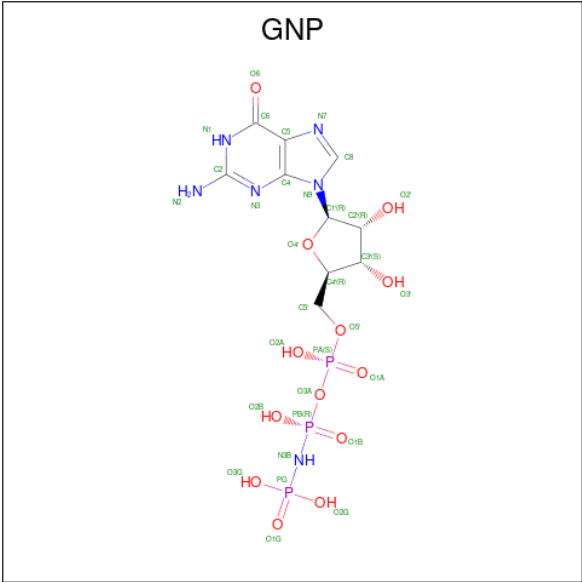
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
87	AA	1	Total 1	Mg 1	0
87	AL	1	Total 1	Mg 1	0
87	AN	1	Total 1	Mg 1	0
87	AY	1	Total 1	Mg 1	0
87	Al	1	Total 1	Mg 1	0
87	An	1	Total 1	Mg 1	0

- Molecule 88 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
88	Bd	1	Total 1	Zn 1	0
88	Ba	1	Total 1	Zn 1	0
88	Aj	1	Total 1	Zn 1	0
88	Ao	1	Total 1	Zn 1	0
88	Ap	1	Total 1	Zn 1	0

- Molecule 89 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

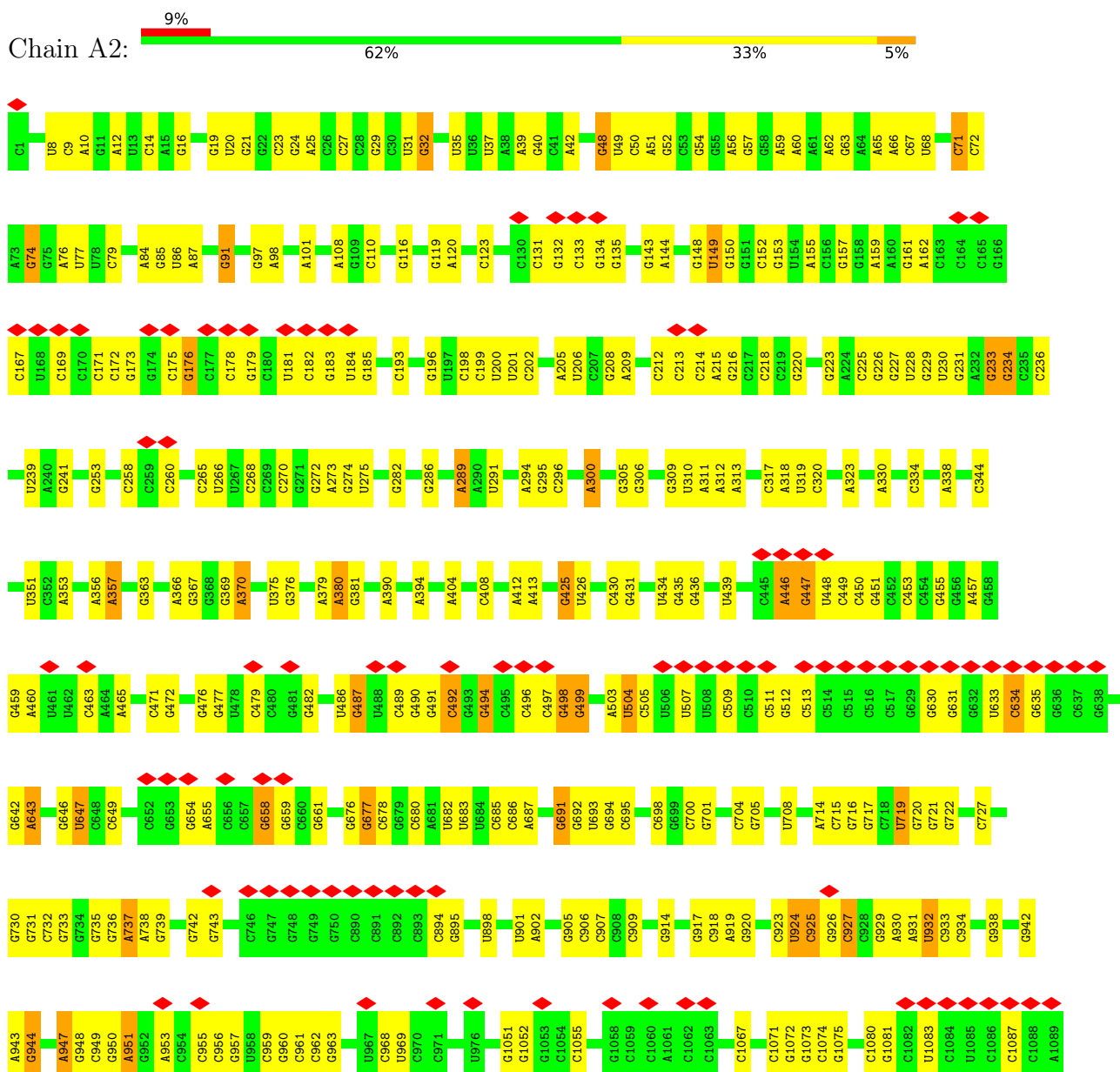


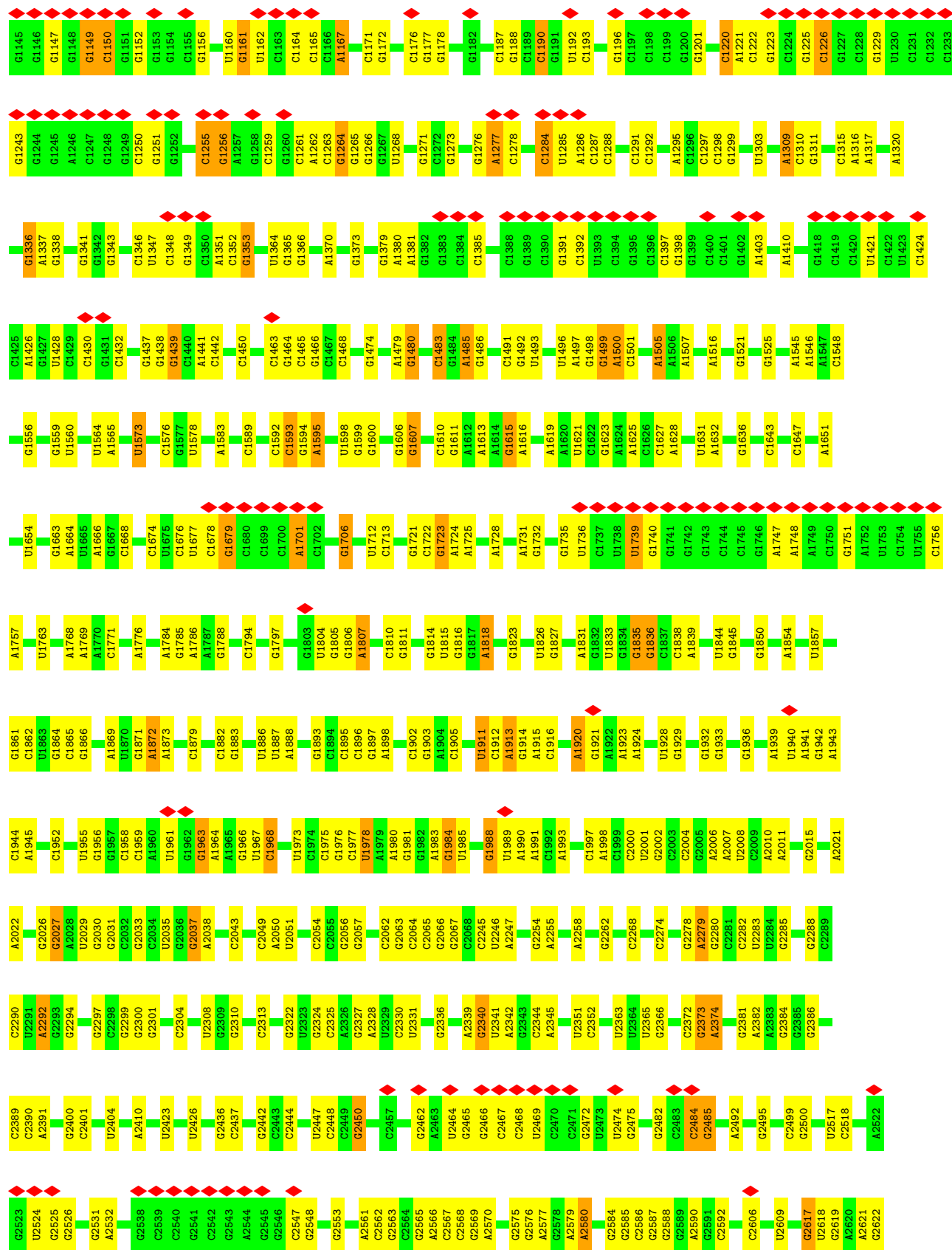
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
89	Ct	1	32	10	6	13	3	0

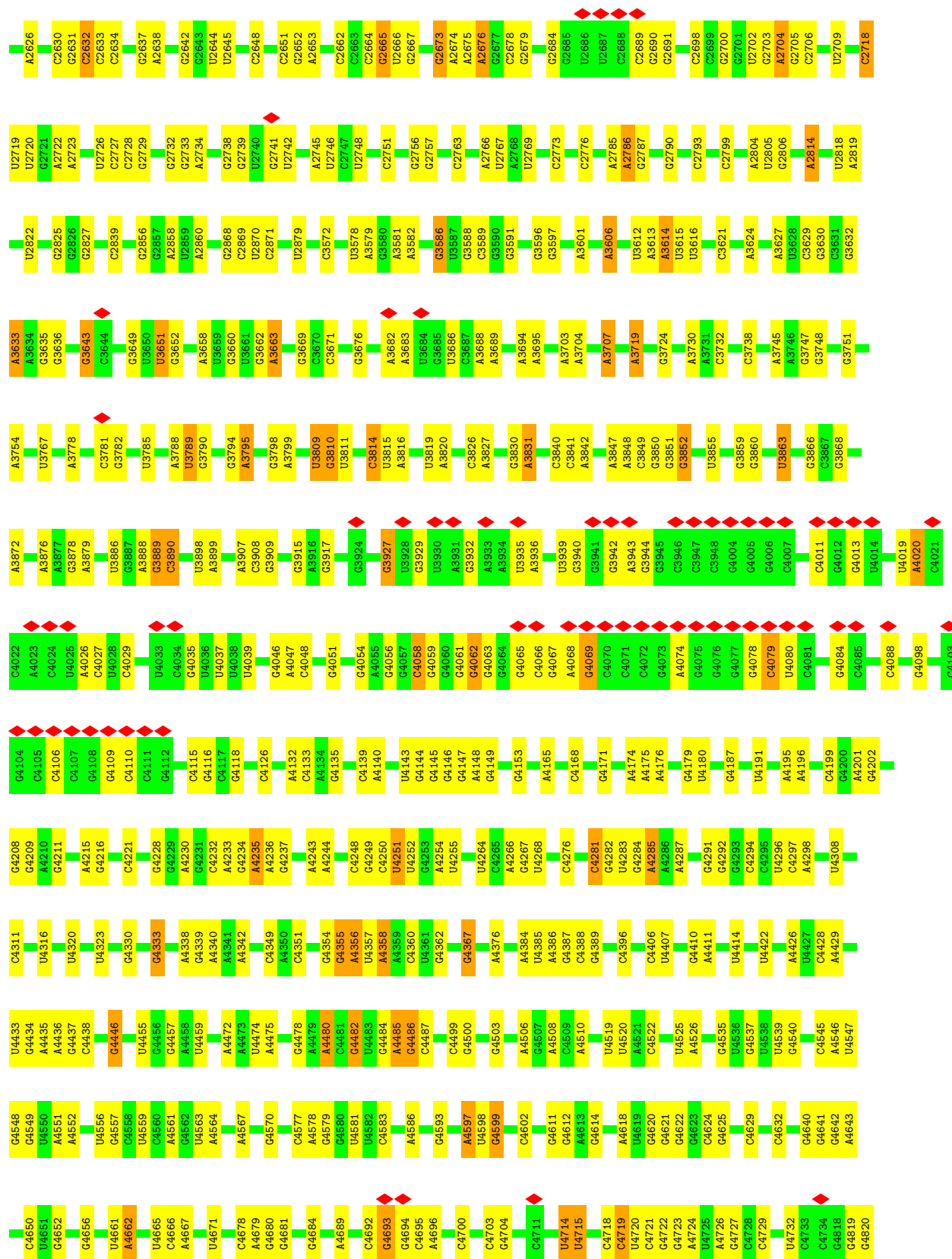
3 Residue-property plots

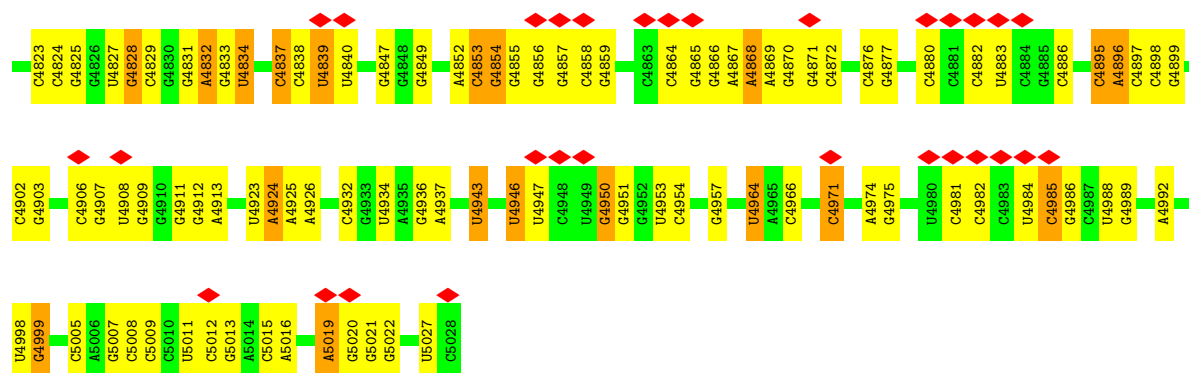
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 28S ribosomal RNA

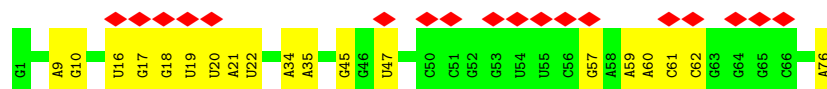
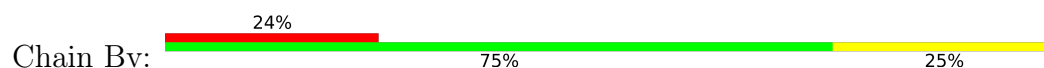




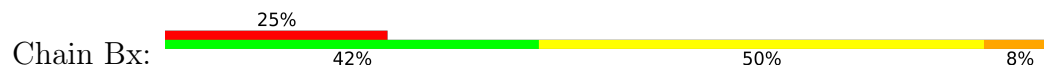




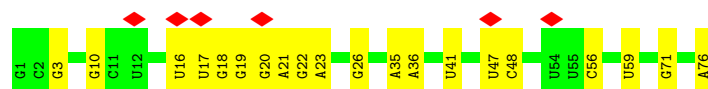
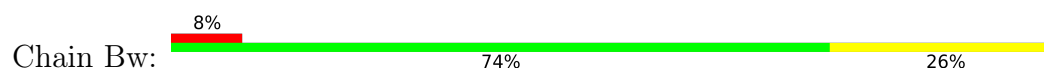
• Molecule 2: ap/P-site tRNA



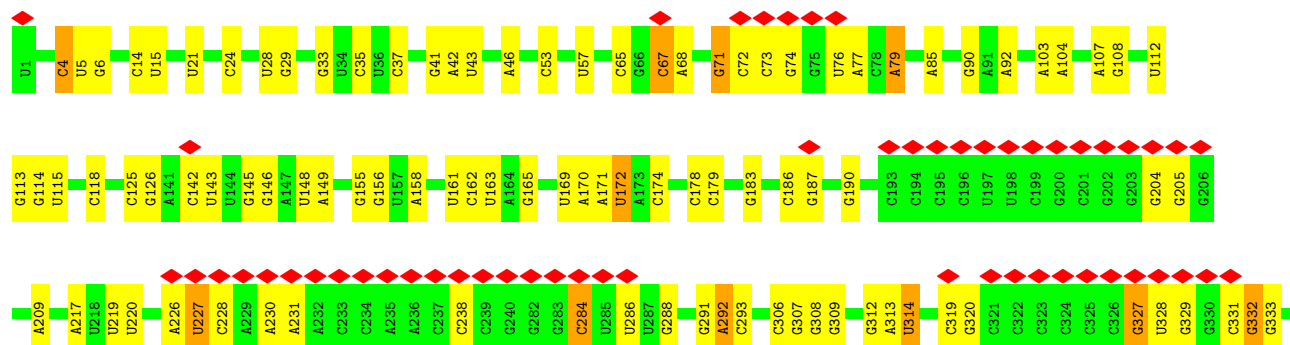
• Molecule 3: mRNA

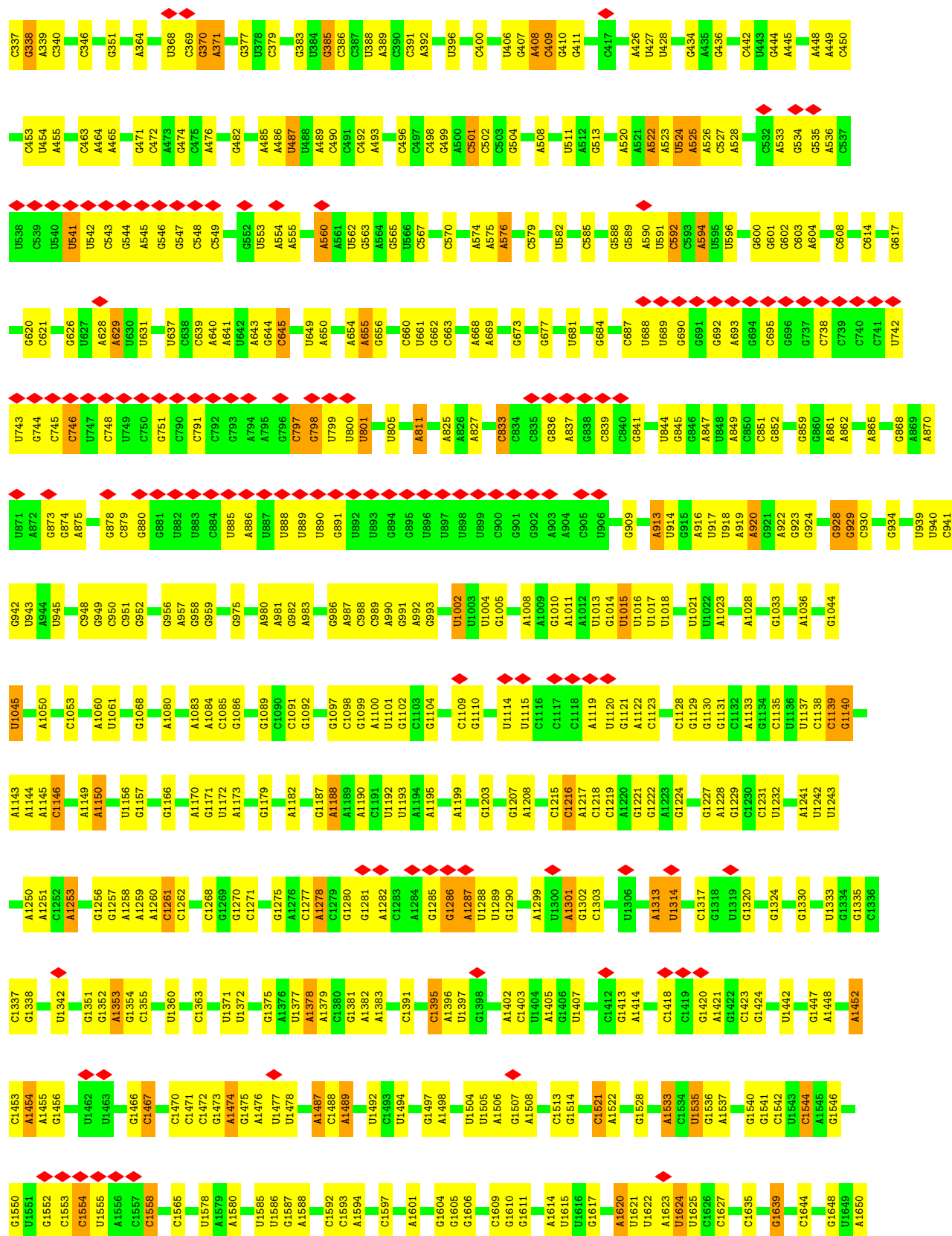


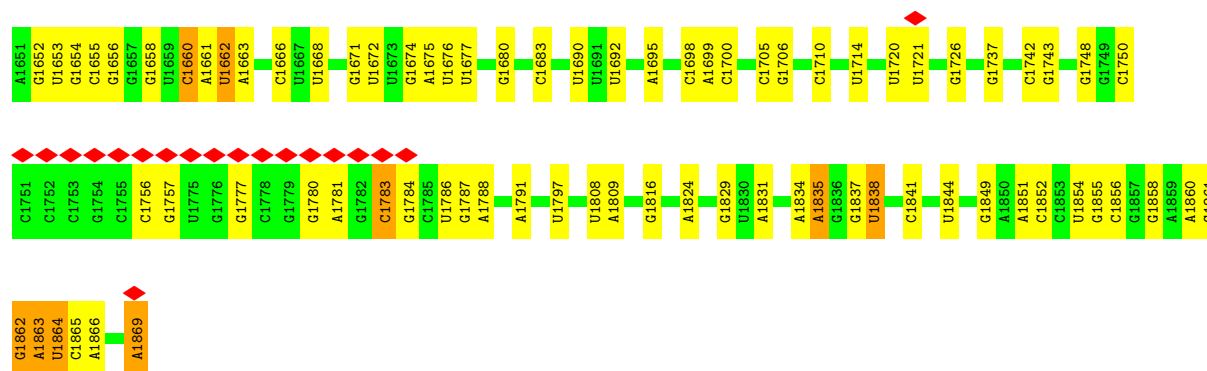
• Molecule 4: pe/E-site-tRNA



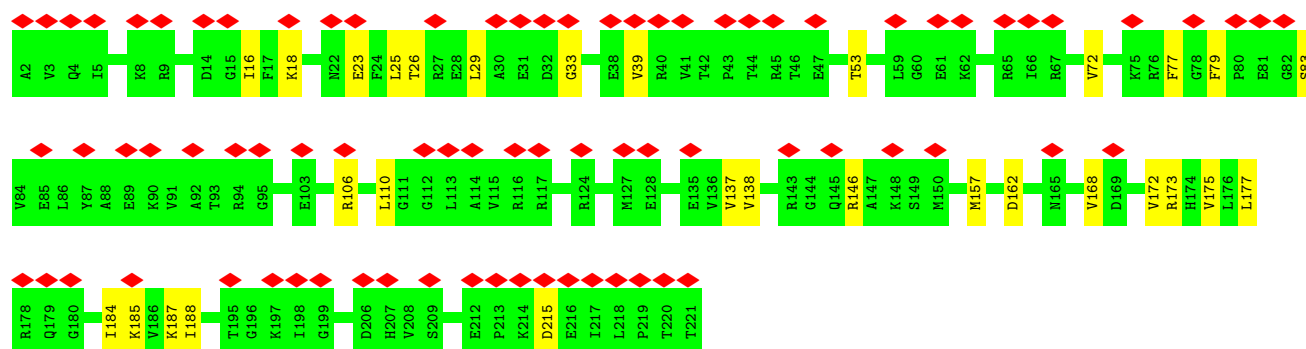
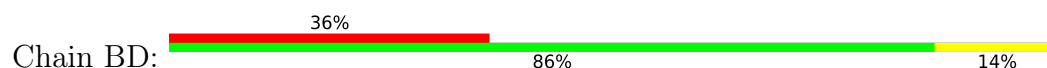
• Molecule 5: 18S ribosomal RNA



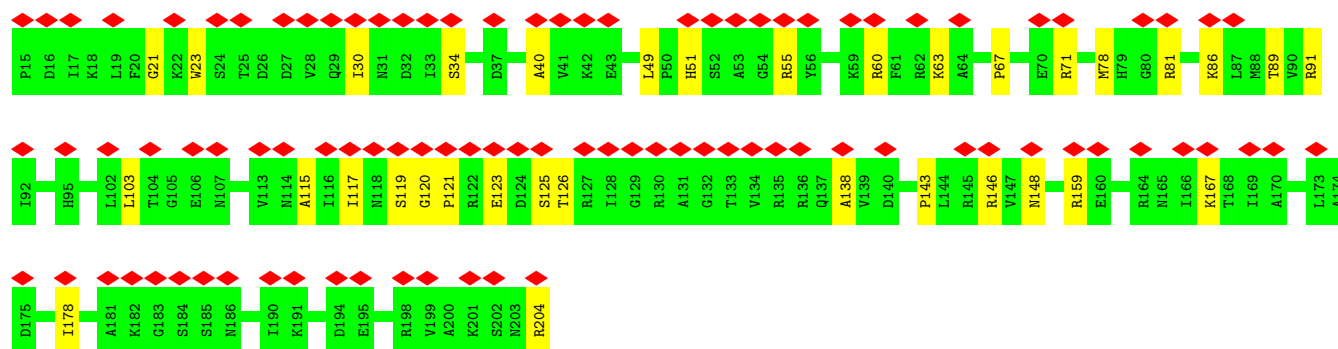
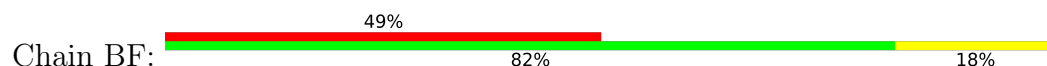




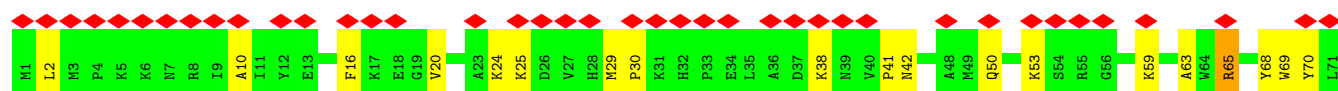
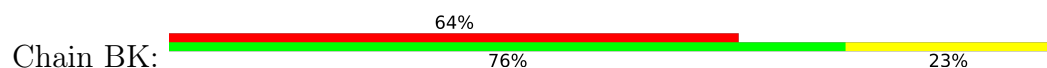
• Molecule 6: ribosomal protein uS3



• Molecule 7: Ribosomal protein S5



• Molecule 8: ribosomal protein eS10

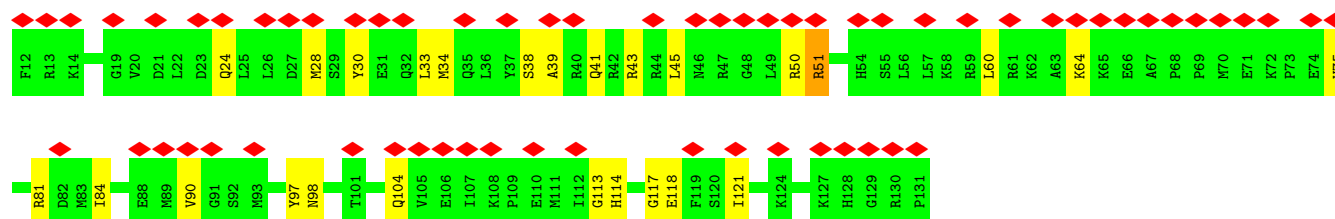
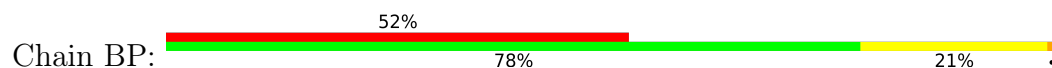




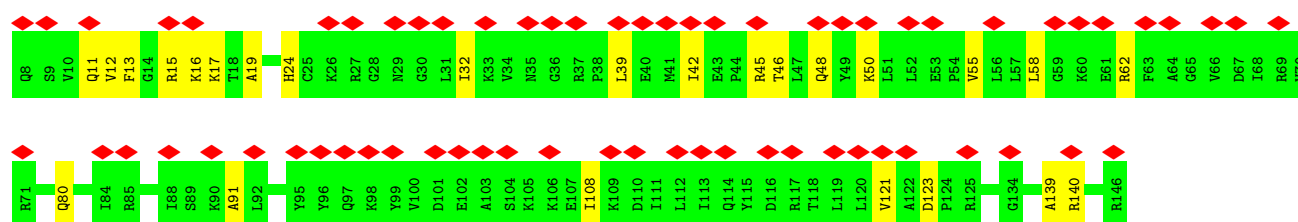
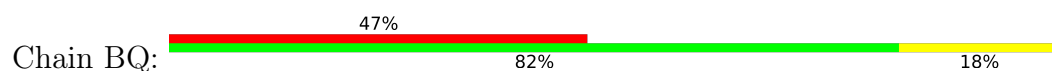
- Molecule 9: 40S ribosomal protein S12



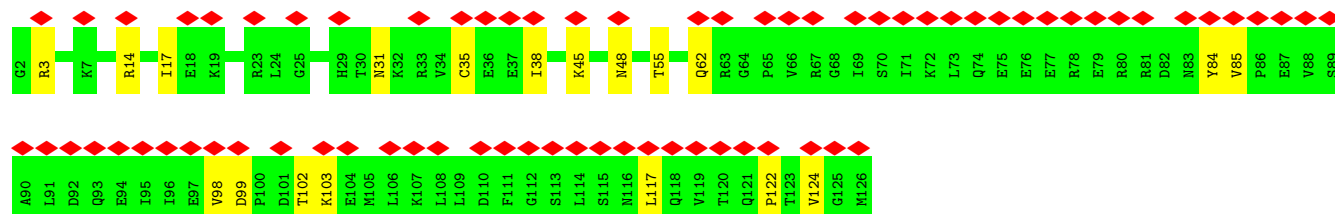
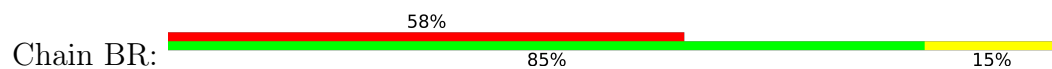
- Molecule 10: ribosomal protein uS19



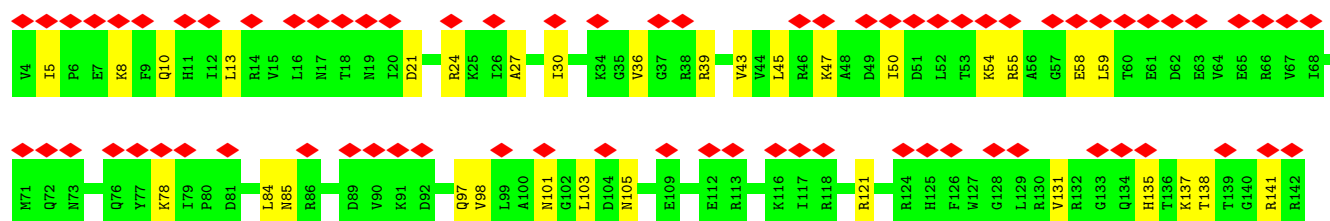
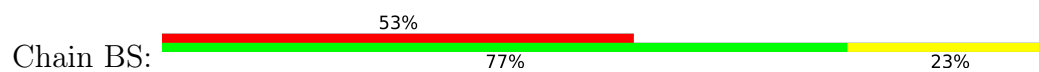
- Molecule 11: ribosomal protein uS9



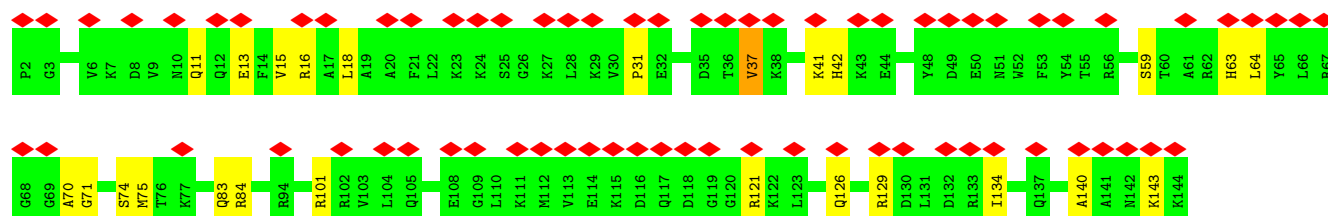
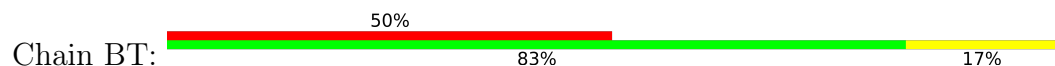
- Molecule 12: ribosomal protein eS17



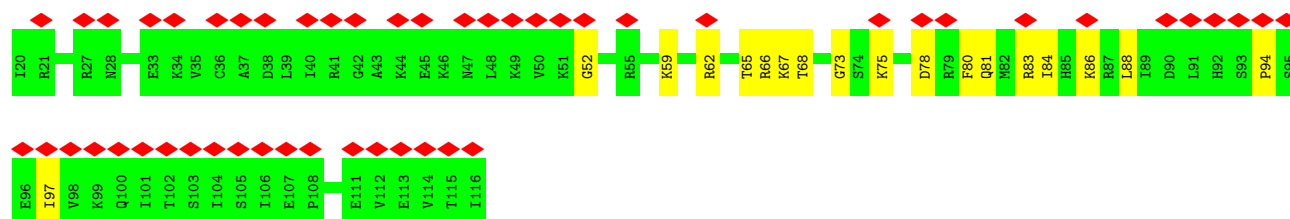
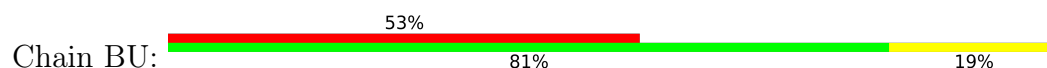
- Molecule 13: ribosomal protein uS13



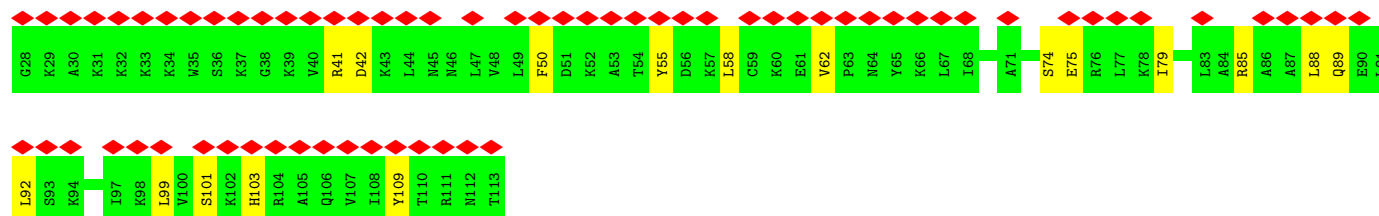
• Molecule 14: ribosomal protein eS19



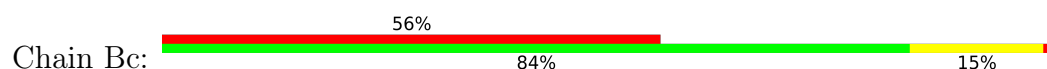
• Molecule 15: ribosomal protein uS10



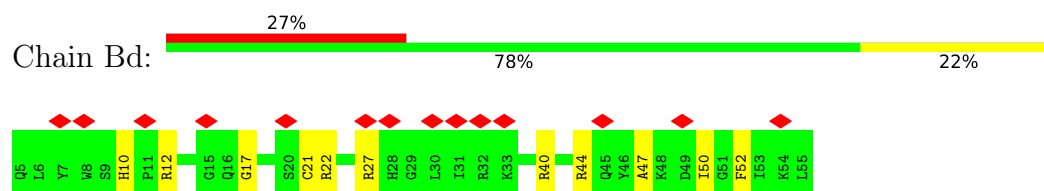
• Molecule 16: ribosomal protein eS25



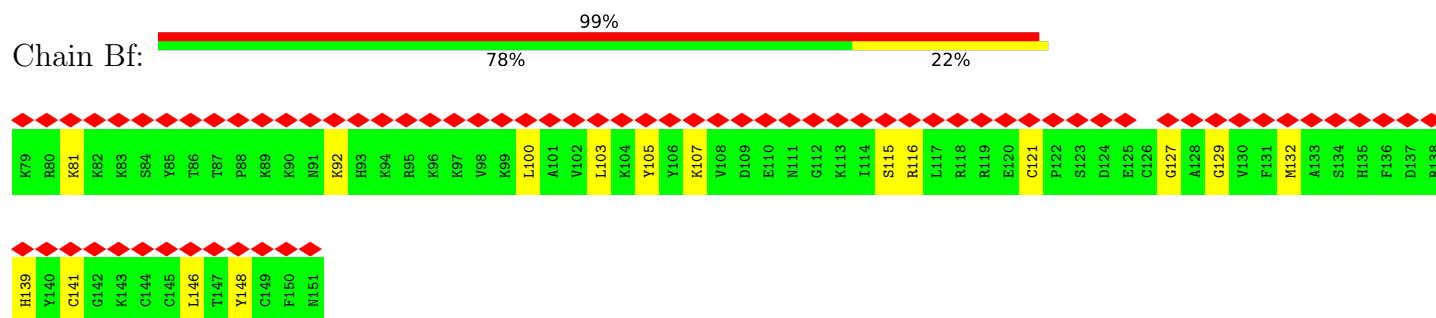
• Molecule 17: Ribosomal protein S28



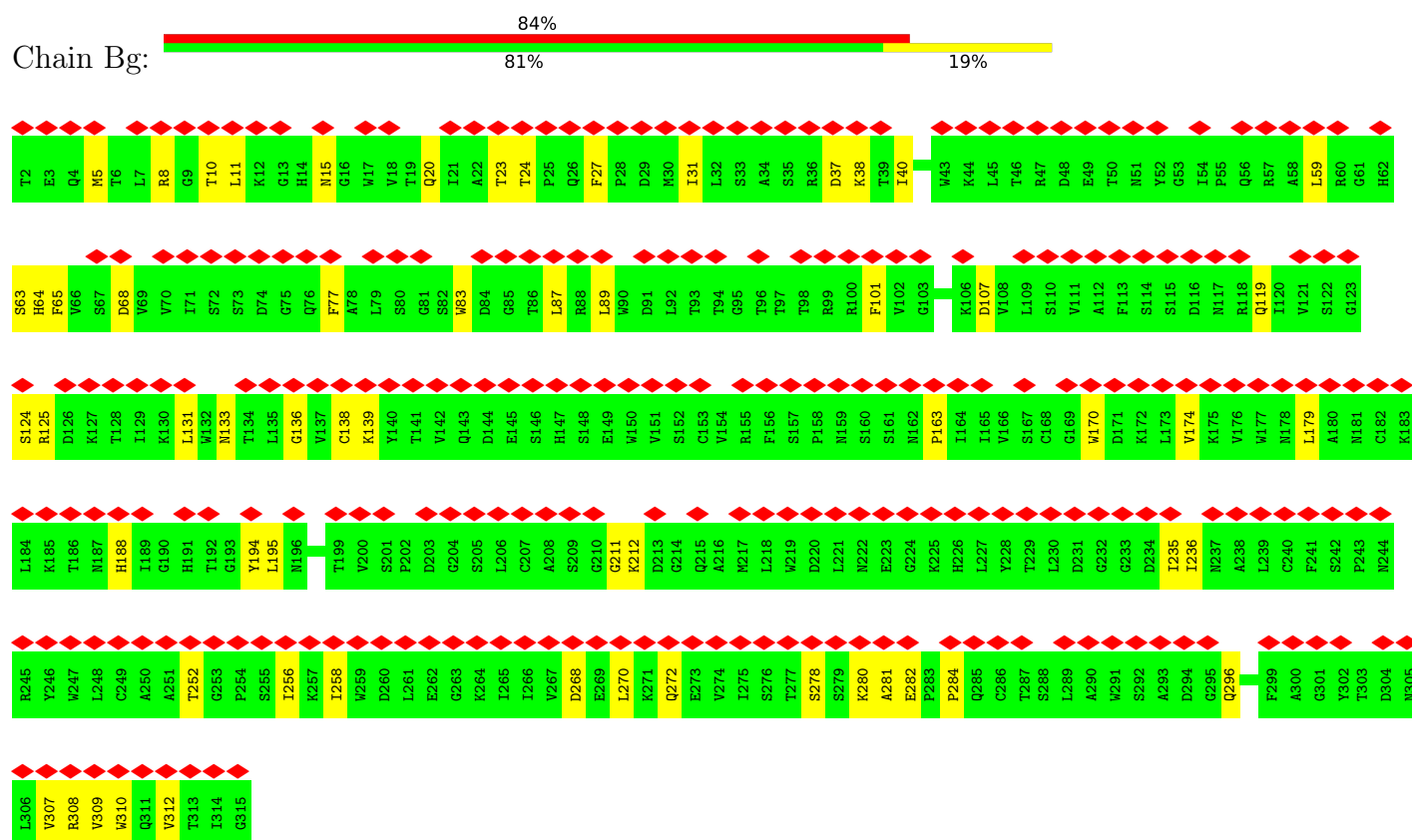
- Molecule 18: ribosomal protein uS14



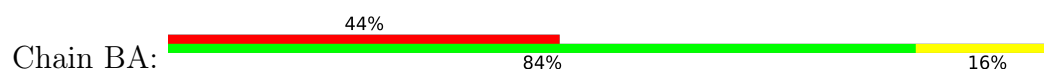
- Molecule 19: Ribosomal protein S27a

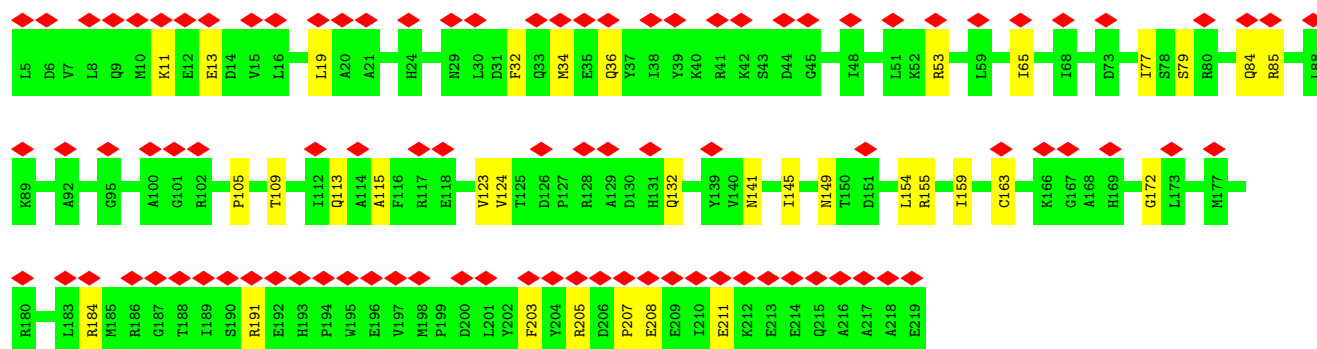


- Molecule 20: ribosomal protein RACK 1

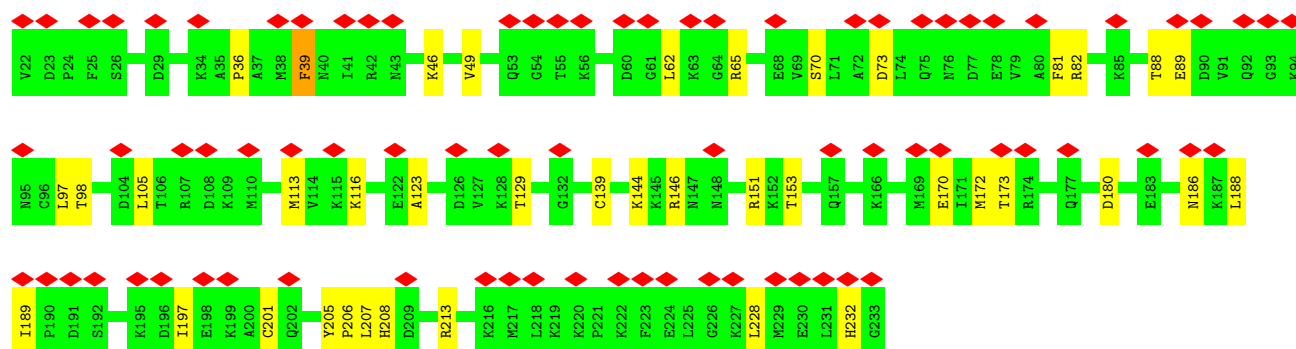
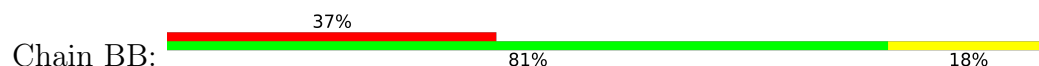


- Molecule 21: ribosomal protein uS2

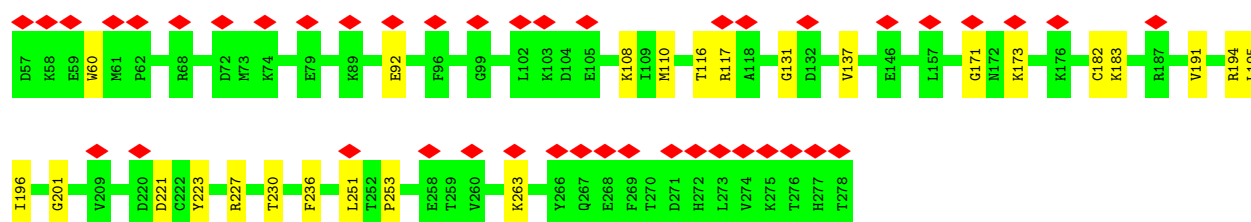




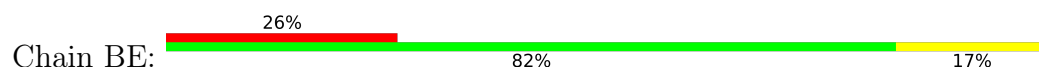
• Molecule 22: 40S ribosomal protein S3a

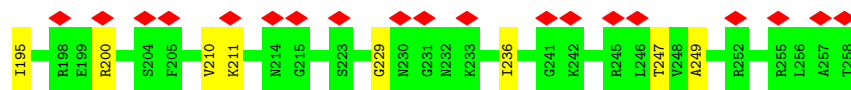


• Molecule 23: ribosomal protein uS5



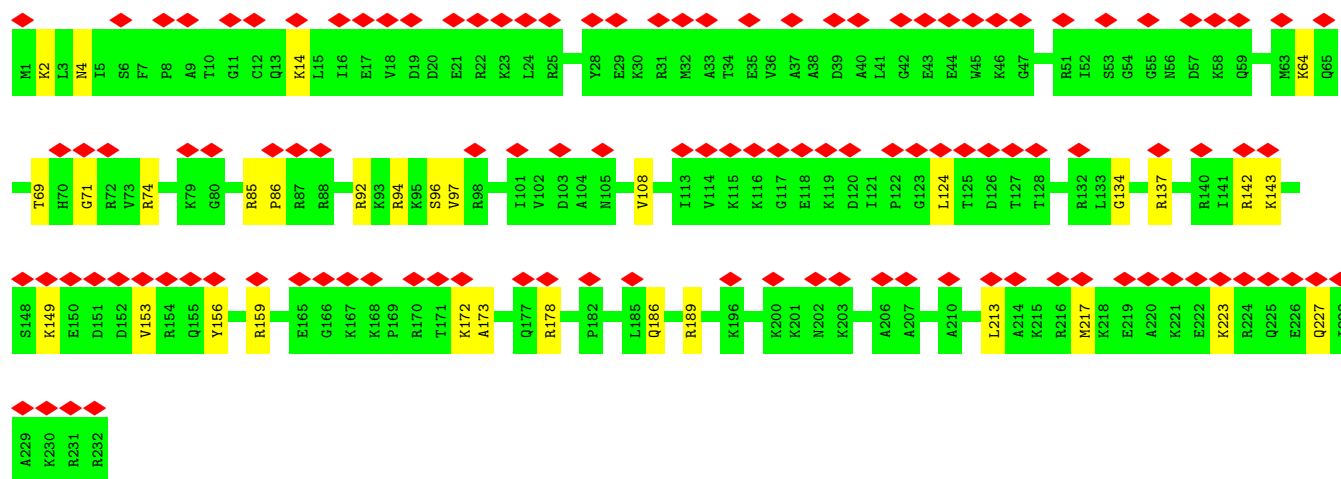
• Molecule 24: ribosomal protein eS4





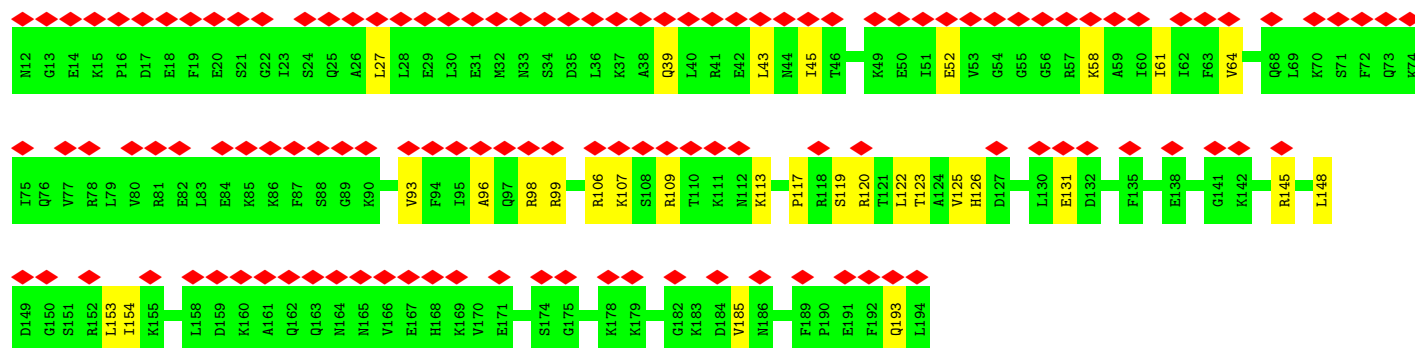
- Molecule 25: 40S ribosomal protein S6

Chain BG: 50%
86% 14%



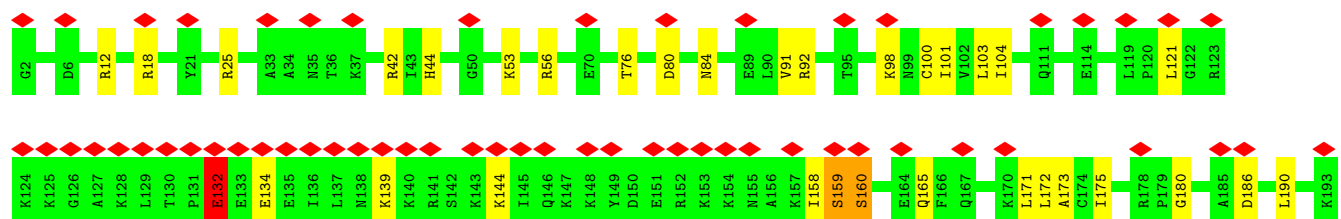
- Molecule 26: 40S ribosomal protein S7

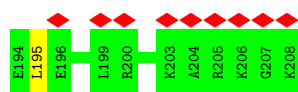
Chain BH: 67%
84% 16%



- Molecule 27: ribosomal protein eS8

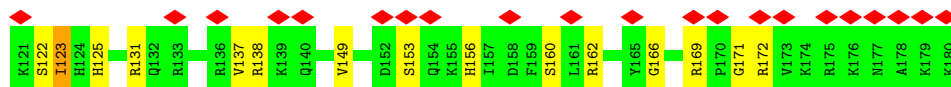
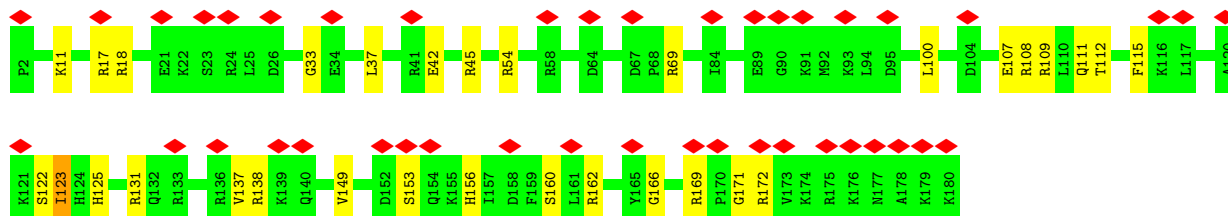
Chain BI: 32%
84% 15%





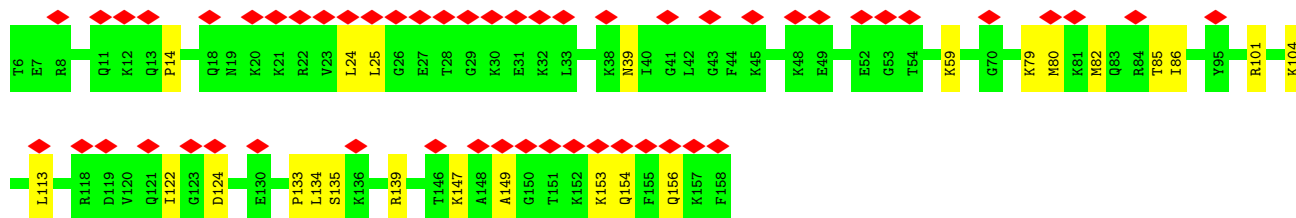
- Molecule 28: Ribosomal protein S9 (Predicted)

Chain BJ: 23% 83% 17%



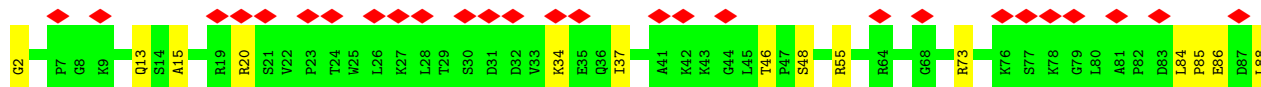
- Molecule 29: Ribosomal protein S11

Chain BL: 35% 84% 16%



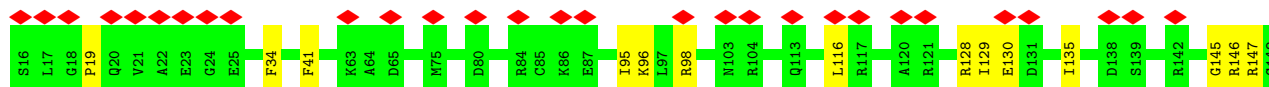
- Molecule 30: ribosomal protein uS15

Chain BN: 26% 87% 13%

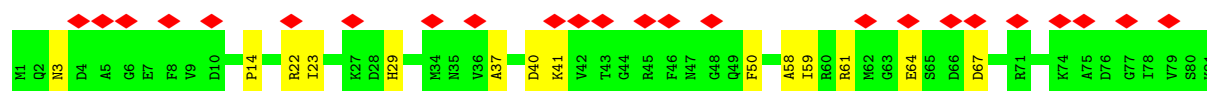
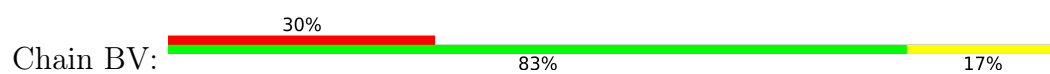


- Molecule 31: ribosomal protein uS11

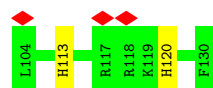
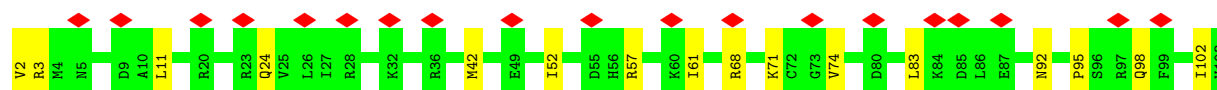
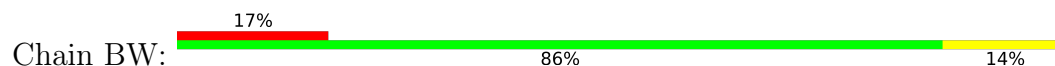
Chain BO: 22% 88% 12%



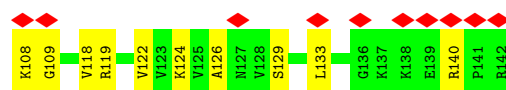
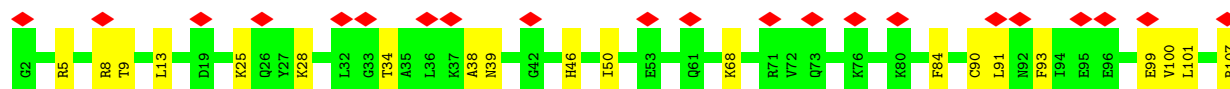
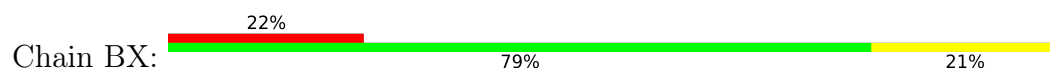
- Molecule 32: ribosomal protein eS21



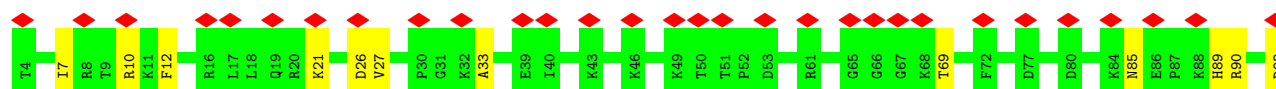
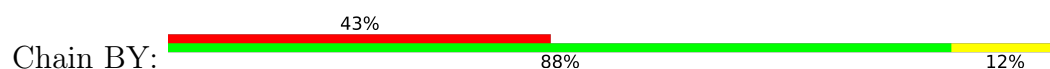
• Molecule 33: Ribosomal protein S15a



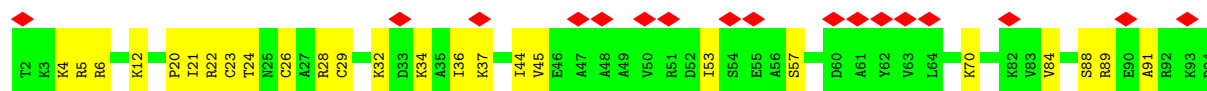
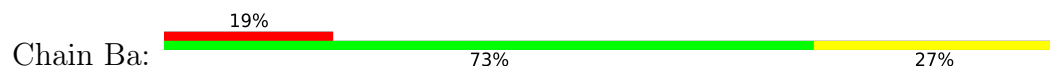
• Molecule 34: Ribosomal protein S23



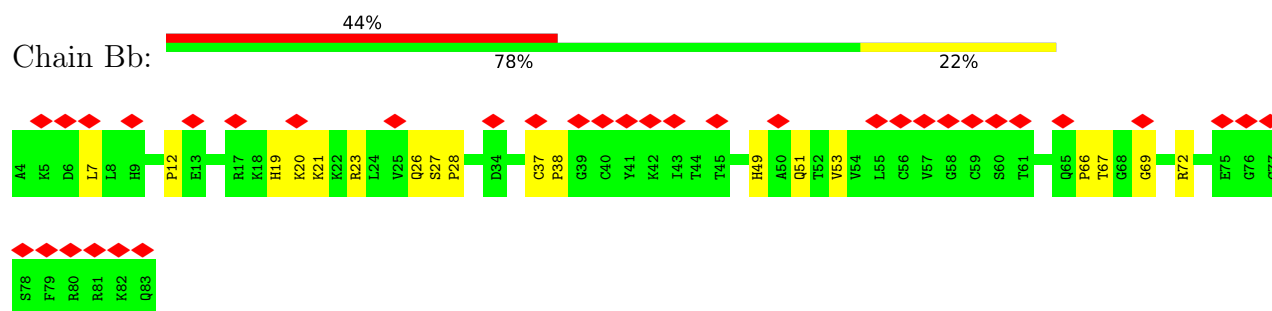
• Molecule 35: ribosomal protein eS24



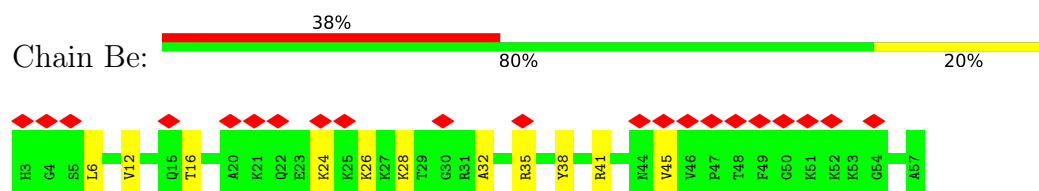
• Molecule 36: ribosomal protein eS26



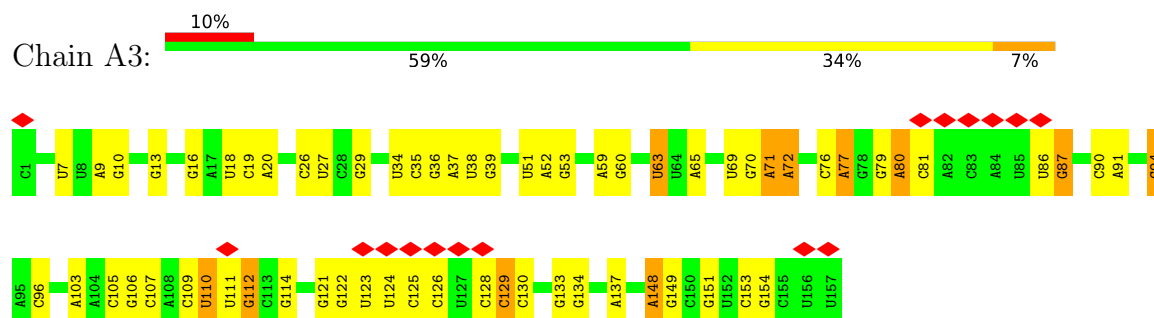
- Molecule 37: ribosomal protein eS27



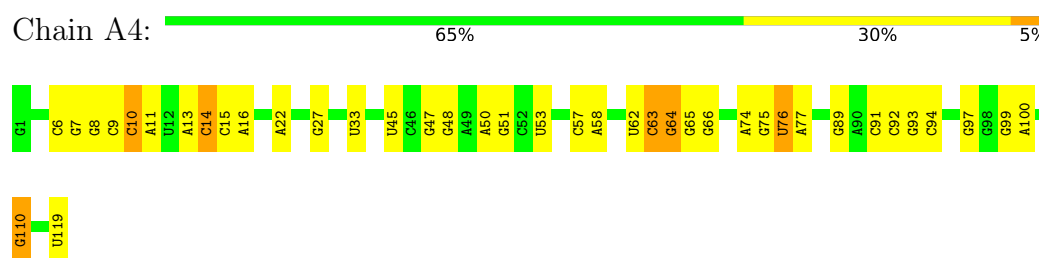
- Molecule 38: ribosomal protein eS30



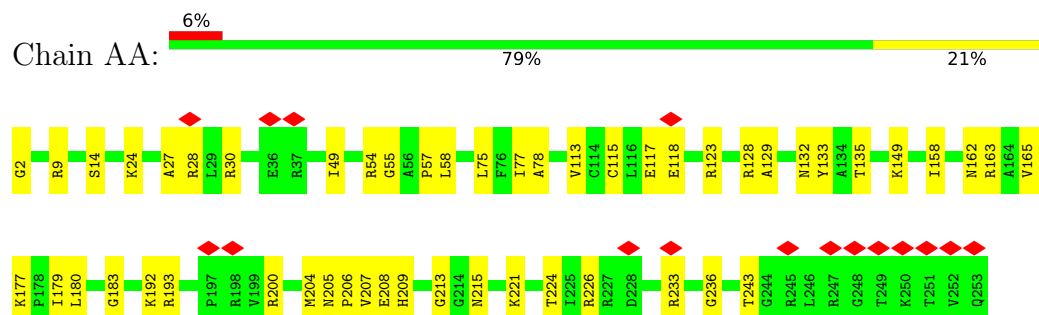
- Molecule 39: 5.8S ribosomal RNA



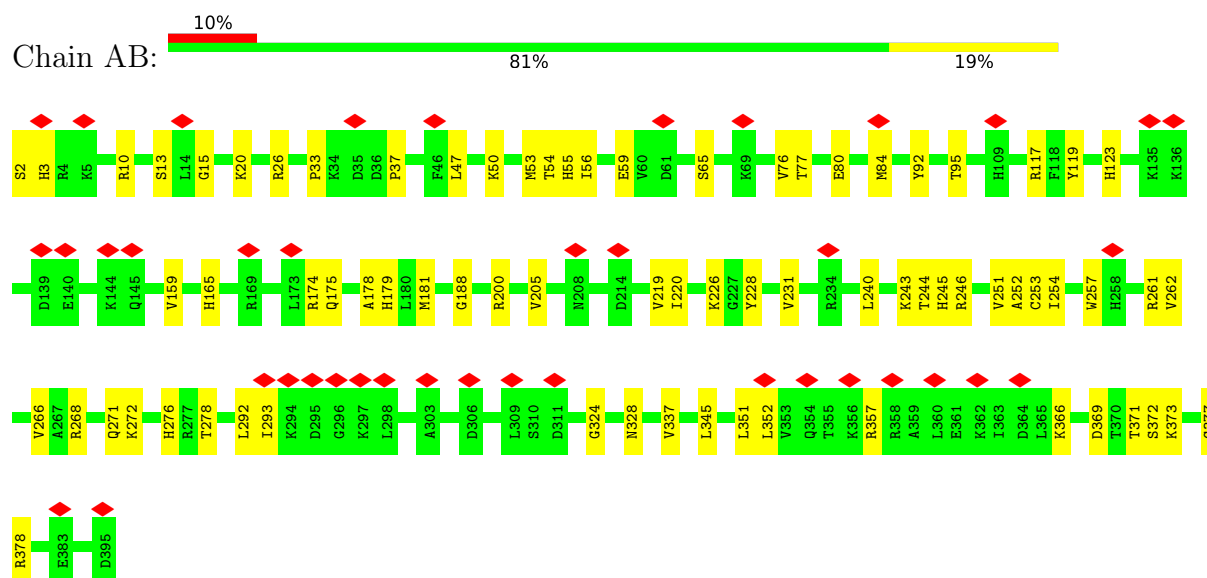
- Molecule 40: 5S ribosomal RNA



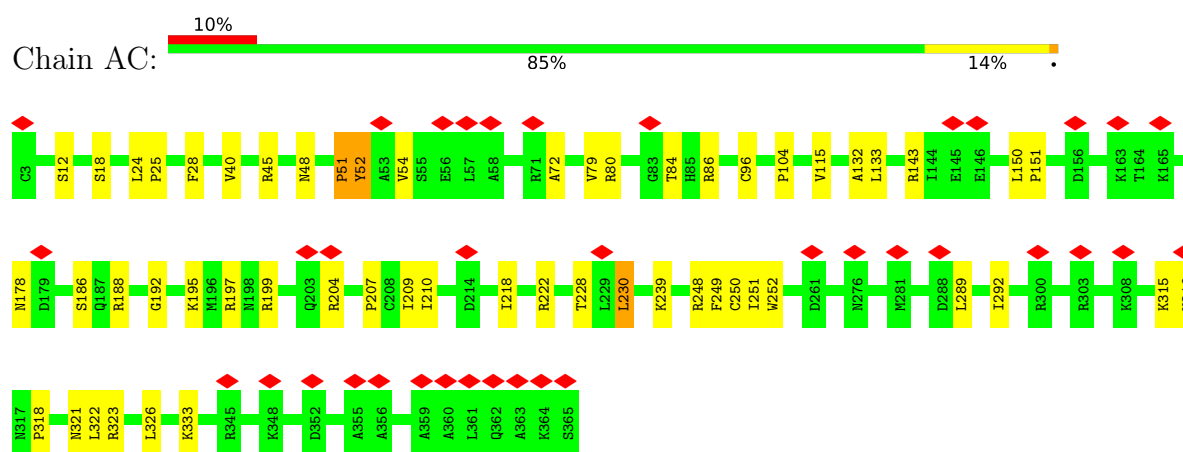
- Molecule 41: Ribosomal protein L8



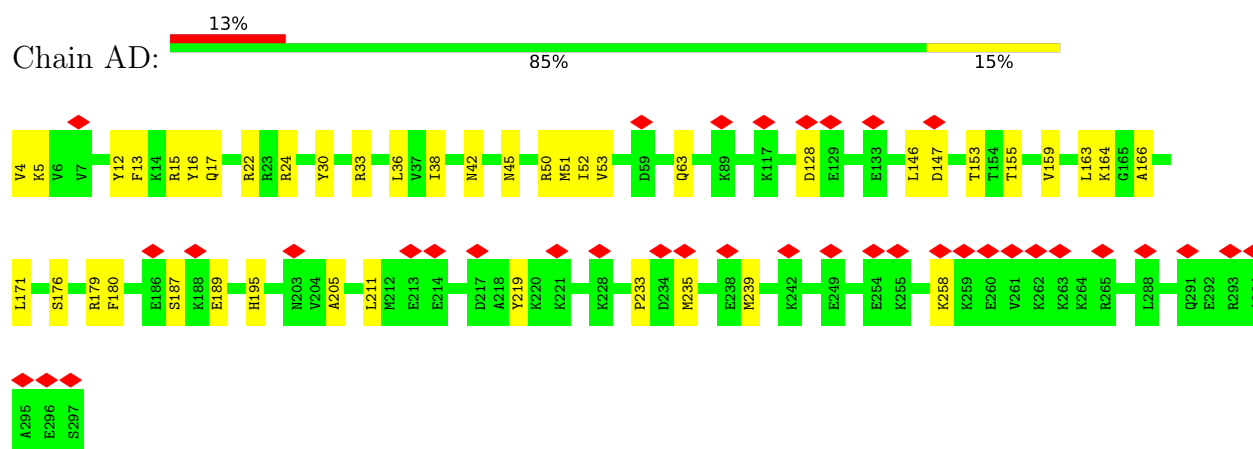
- Molecule 42: ribosomal protein uL3



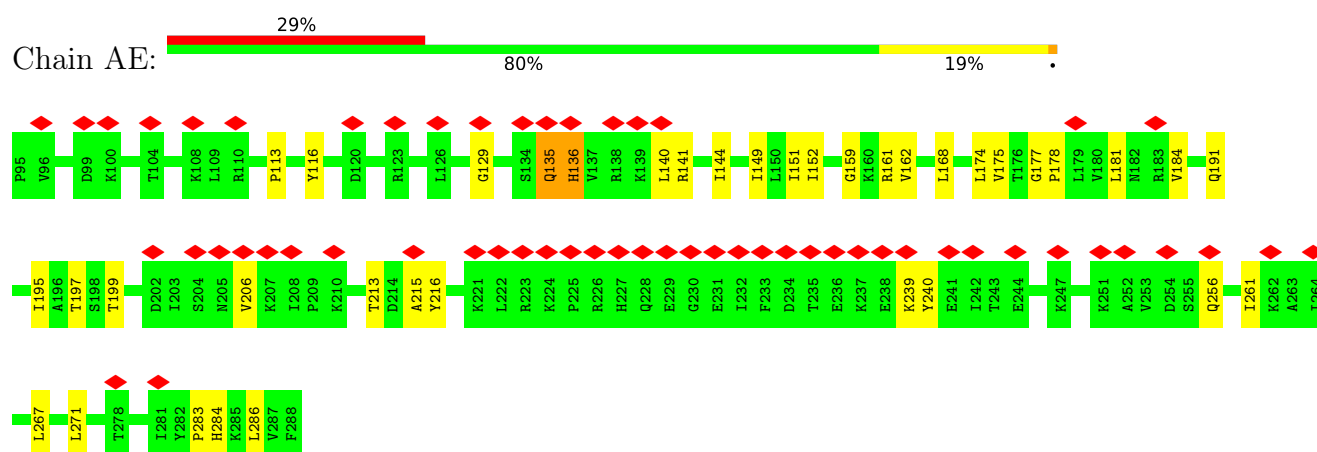
- Molecule 43: ribosomal protein uL4



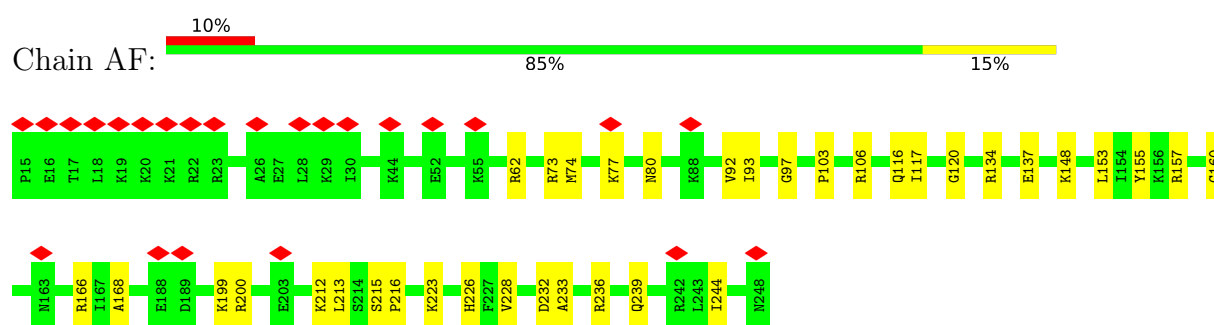
- Molecule 44: ribosomal protein uL18



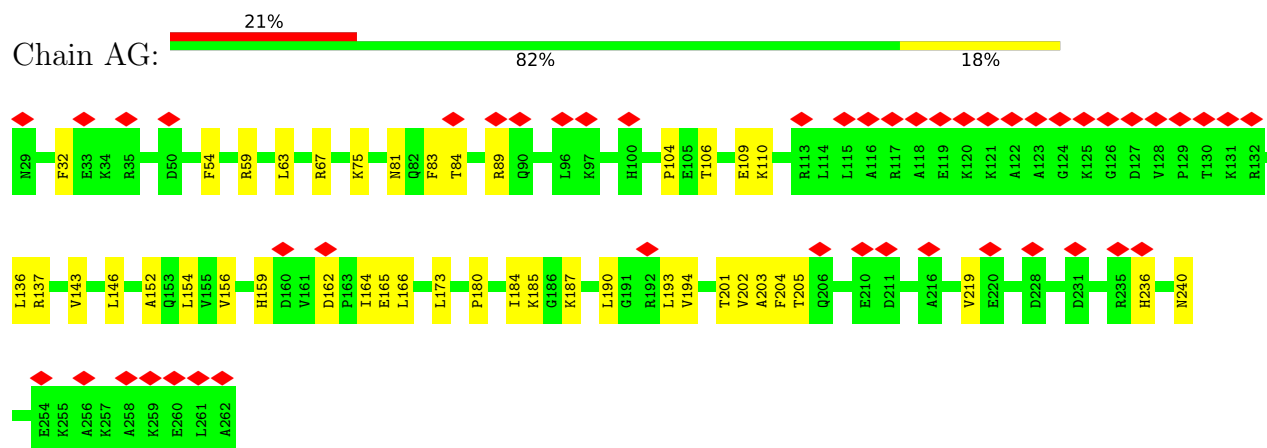
- Molecule 45: ribosomal protein eL6



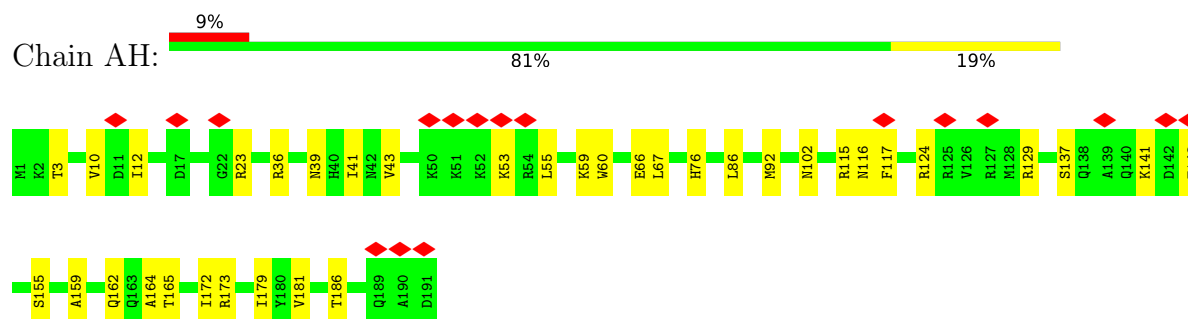
• Molecule 46: ribosomal protein uL30



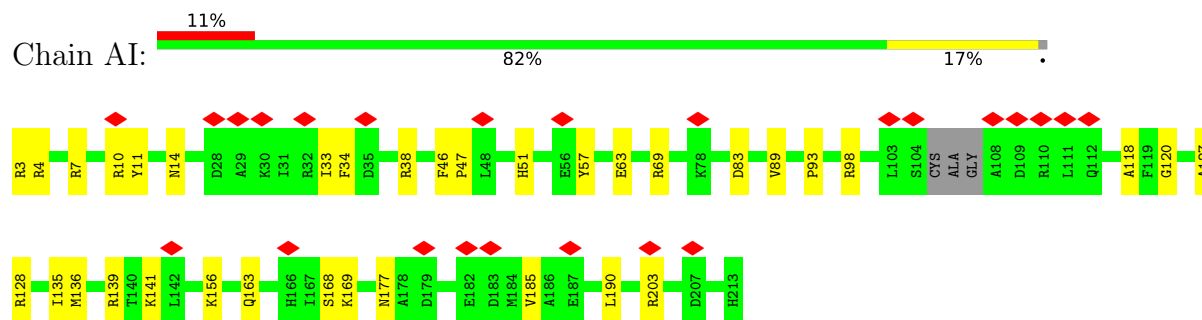
• Molecule 47: ribosomal protein eL8



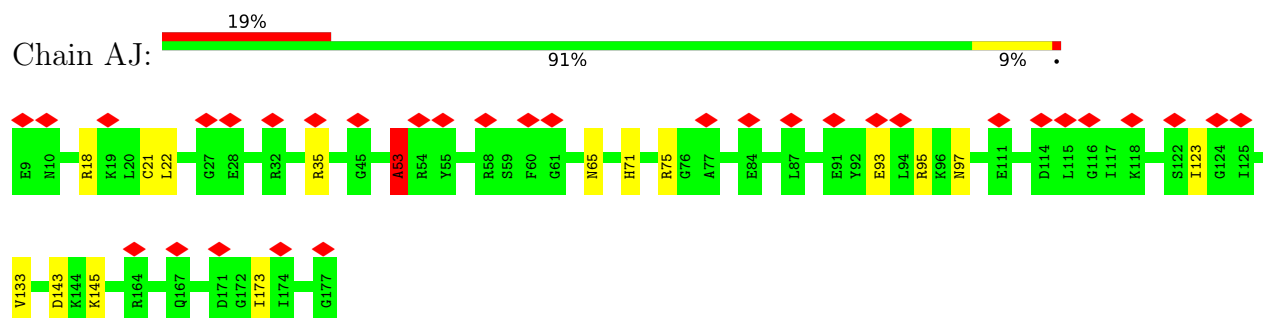
• Molecule 48: ribosomal protein uL6



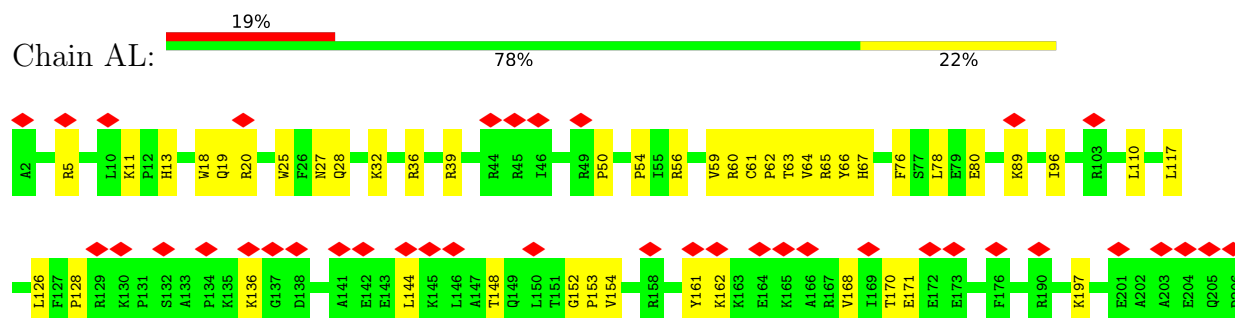
- Molecule 49: Ribosomal protein L10 (Predicted)



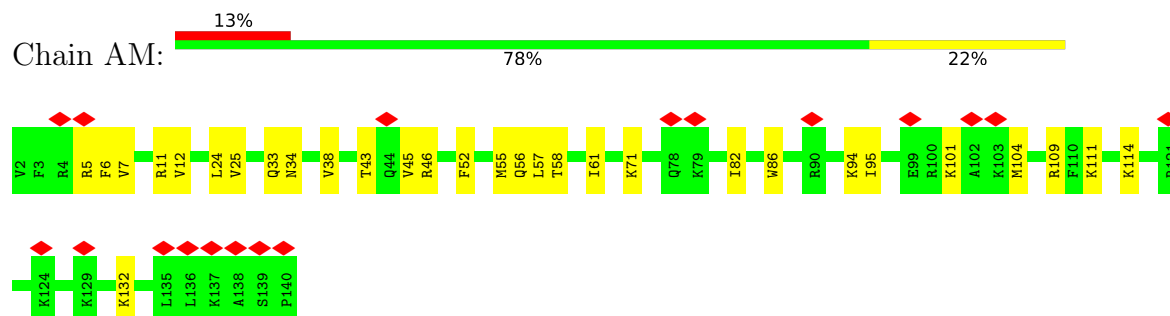
- Molecule 50: Ribosomal protein L11



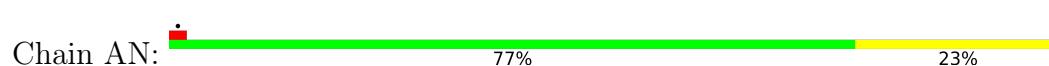
- Molecule 51: ribosomal protein eL13

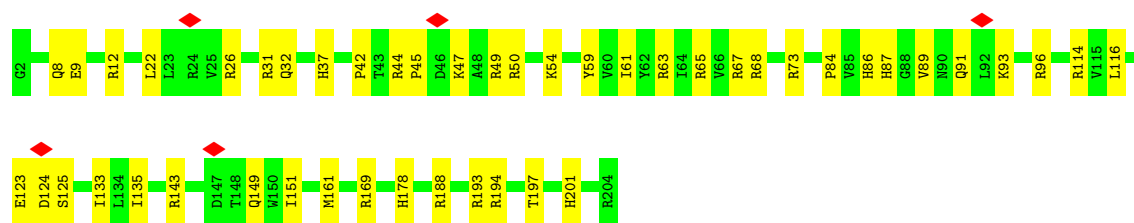


- Molecule 52: ribosomal protein eL14

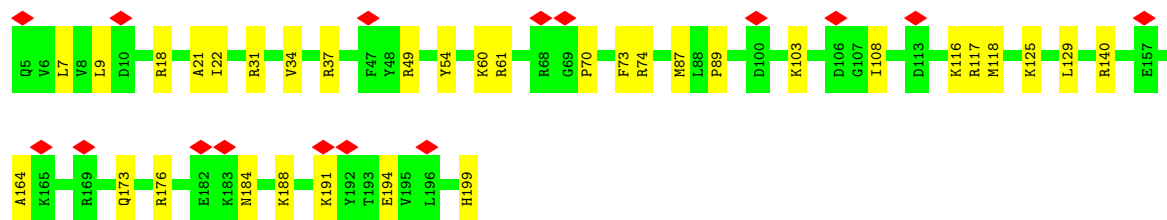
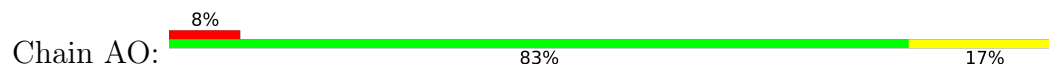


- Molecule 53: Ribosomal protein L15

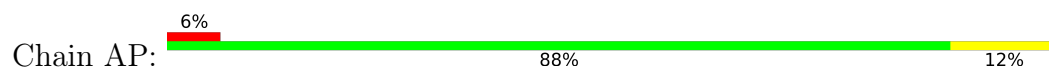




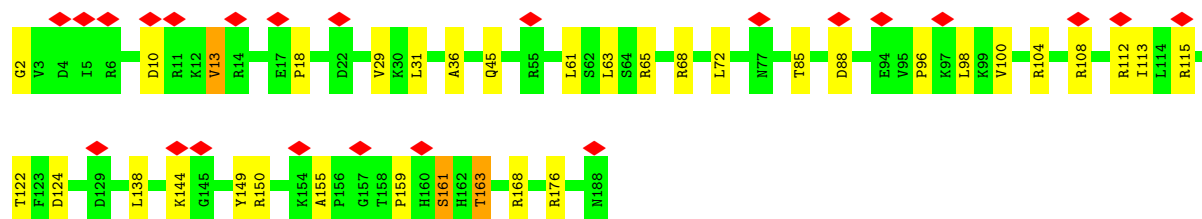
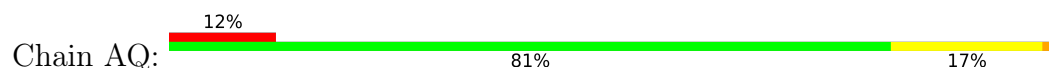
- Molecule 54: ribosomal protein uL13



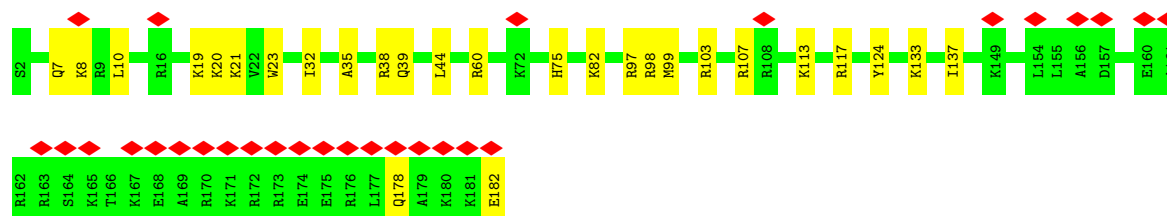
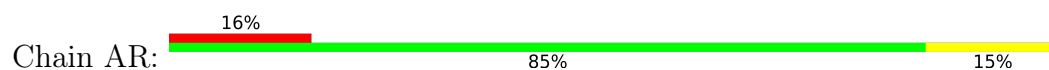
- Molecule 55: ribosomal protein uL22



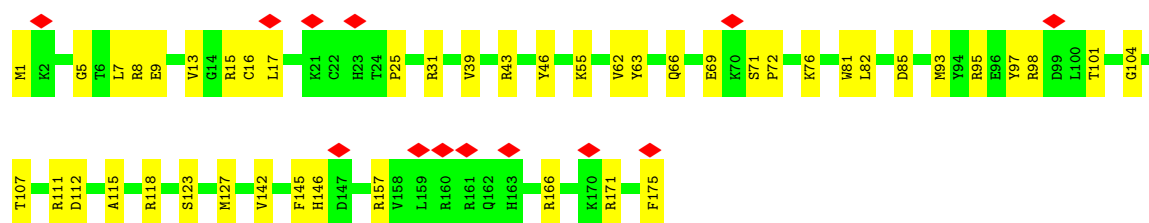
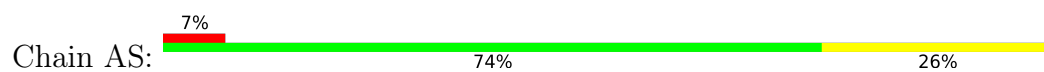
- Molecule 56: ribosomal protein eL18



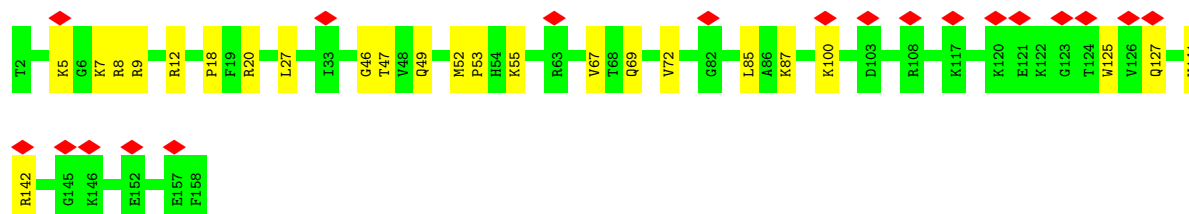
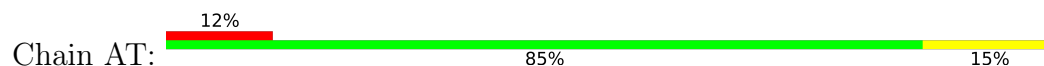
- Molecule 57: ribosomal protein eL19



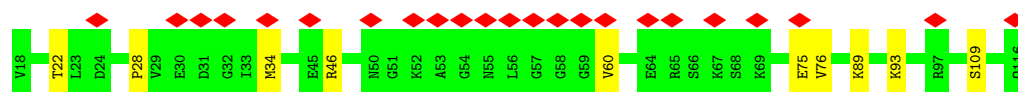
- Molecule 58: ribosomal protein eL20



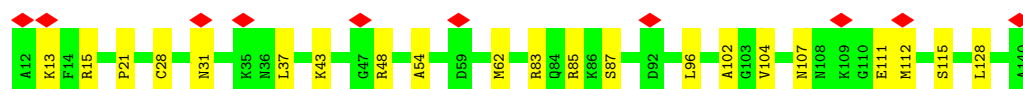
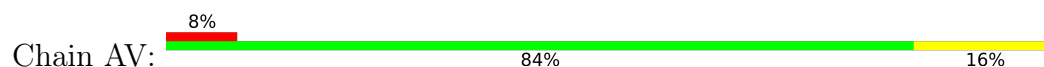
- Molecule 59: ribosomal protein eL21



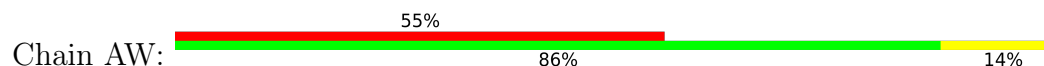
- Molecule 60: ribosomal protein eL22



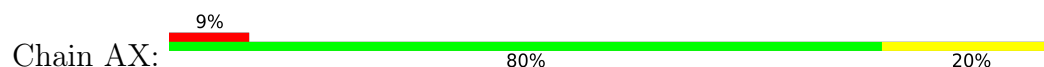
- Molecule 61: Ribosomal protein L23

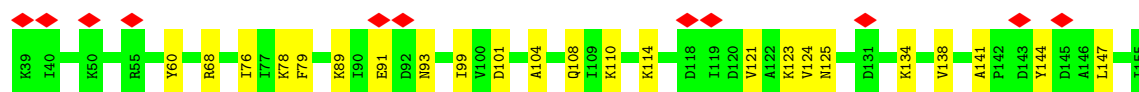


- Molecule 62: ribosomal protein eL24

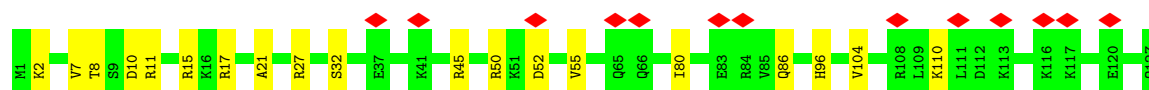
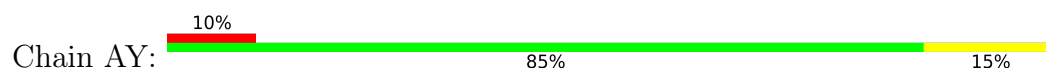


- Molecule 63: ribosomal protein uL23

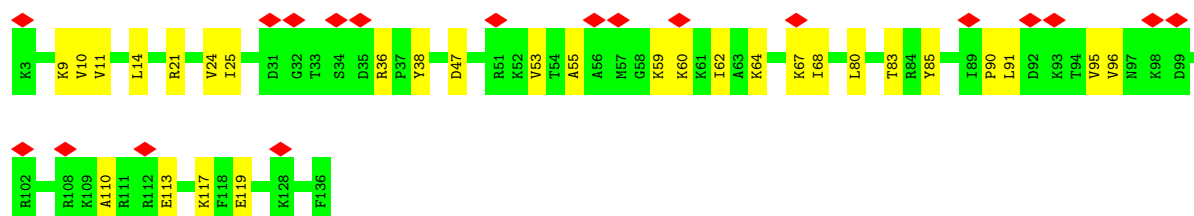
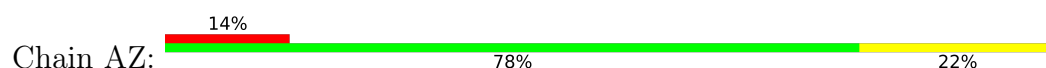




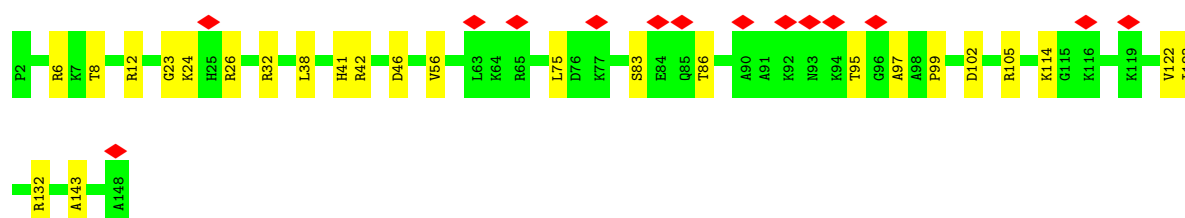
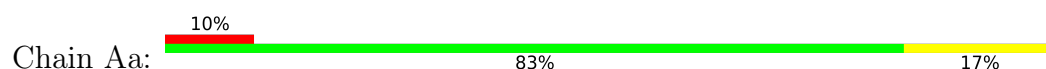
- Molecule 64: Ribosomal protein L26



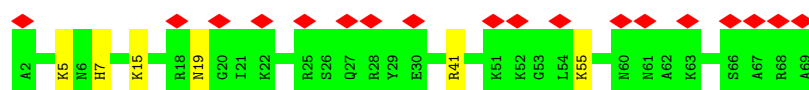
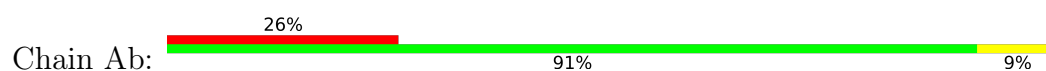
- Molecule 65: 60S ribosomal protein L27



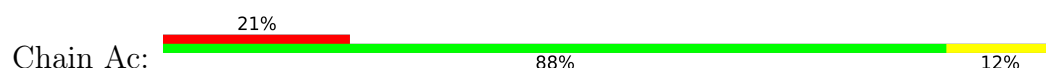
- Molecule 66: ribosomal protein uL15



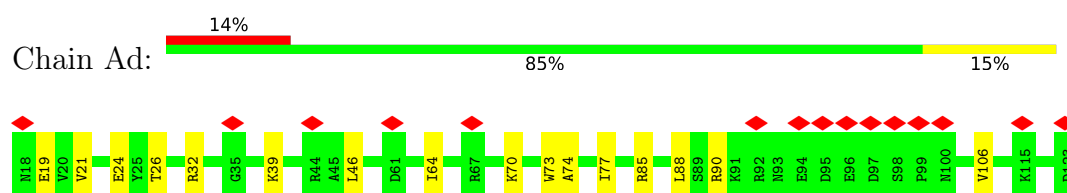
- Molecule 67: ribosomal protein eL29



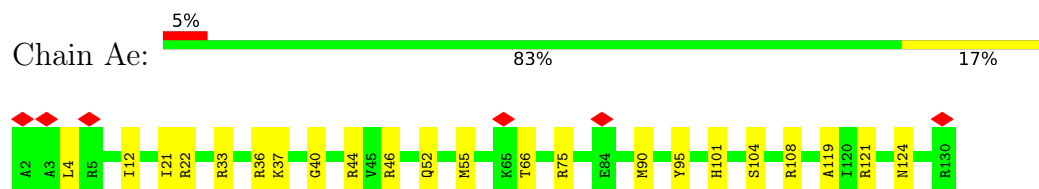
- Molecule 68: ribosomal protein eL30



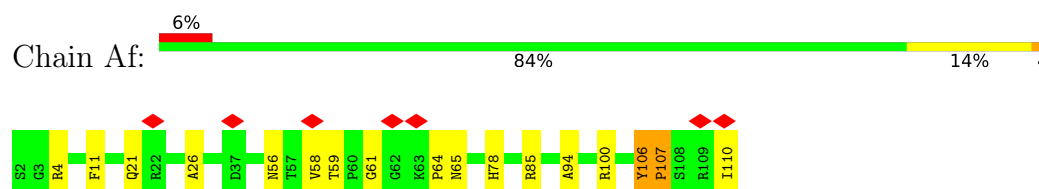
- Molecule 69: ribosomal protein eL31



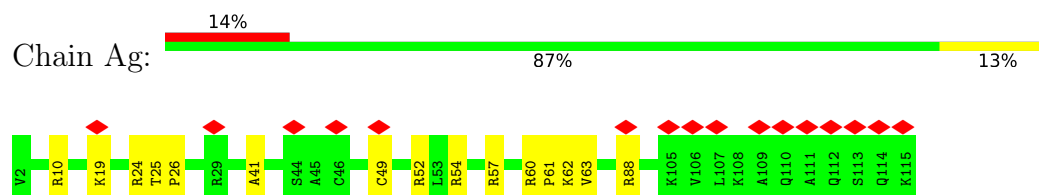
- Molecule 70: ribosomal protein eL32



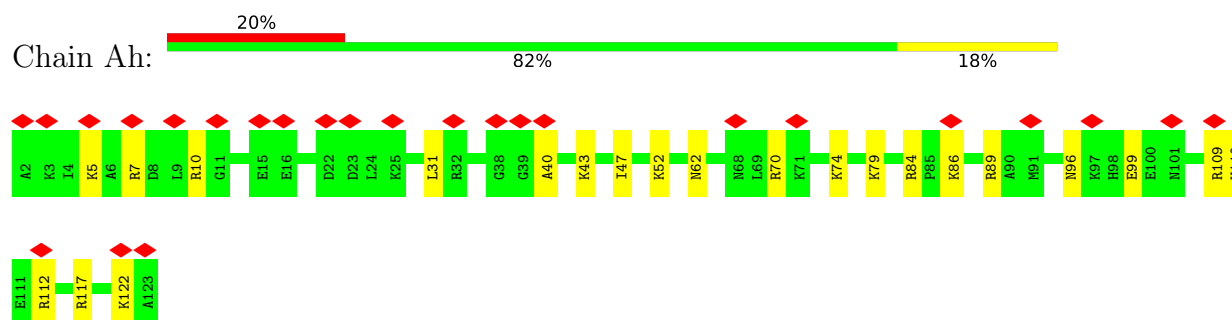
- Molecule 71: ribosomal protein eL33



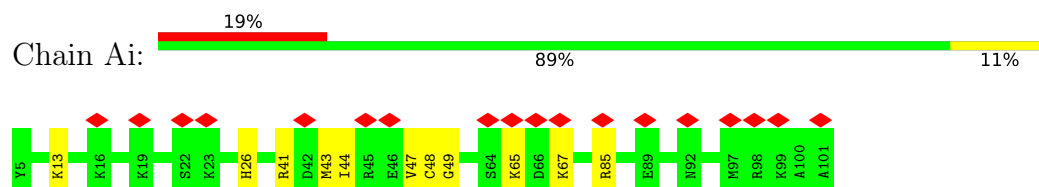
- Molecule 72: ribosomal protein eL34



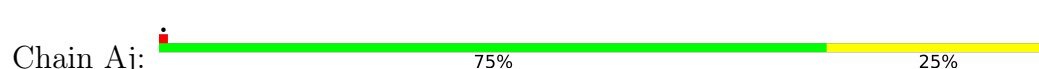
- Molecule 73: ribosomal protein uL29

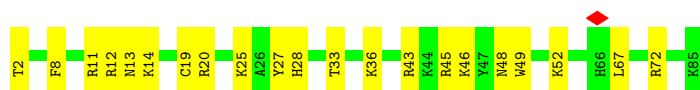


- Molecule 74: ribosomal protein eL36

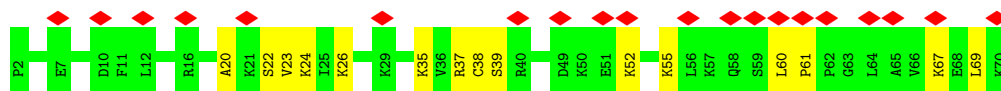
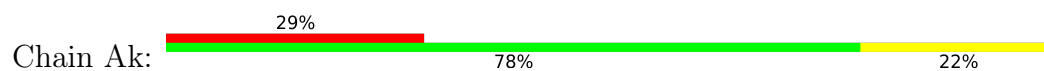


- Molecule 75: Ribosomal protein L37

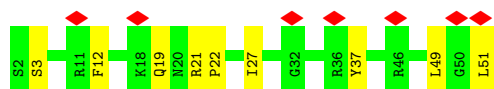
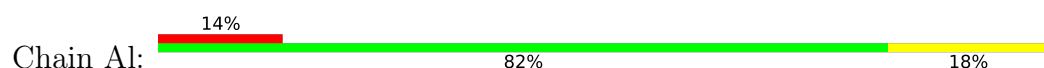




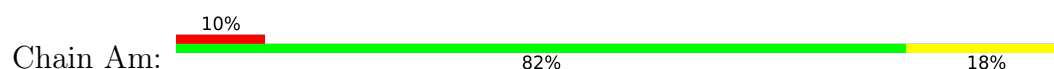
- Molecule 76: ribosomal protein eL38



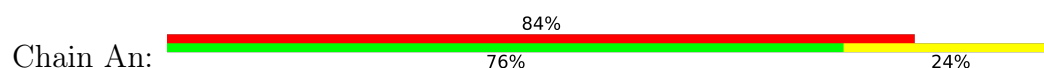
- Molecule 77: ribosomal protein eL39



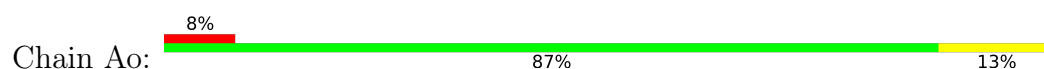
- Molecule 78: ribosomal protein eL40



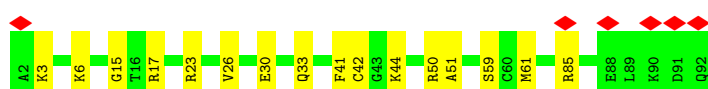
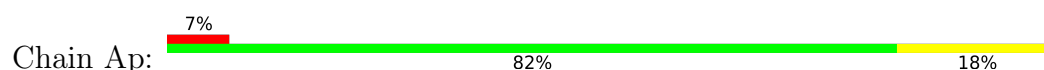
- Molecule 79: ribosomal protein eL41



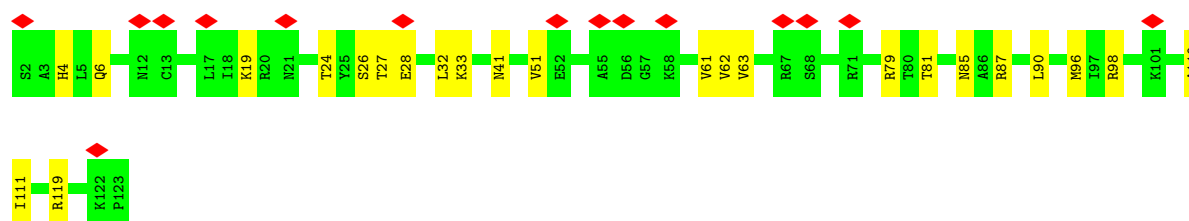
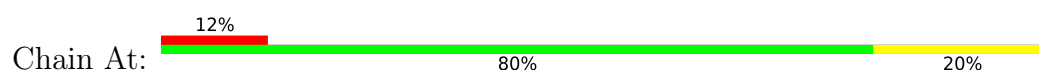
- Molecule 80: ribosomal protein eL42



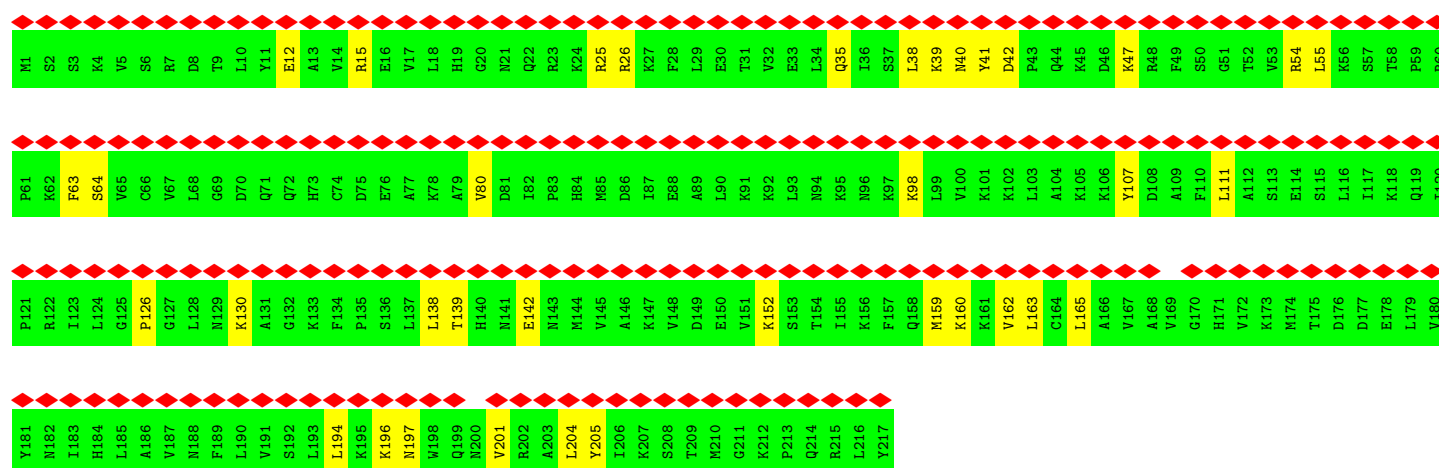
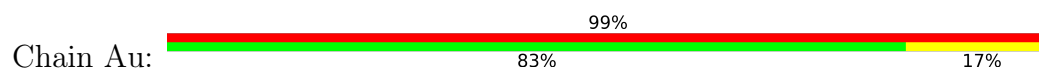
- Molecule 81: ribosomal protein eL43



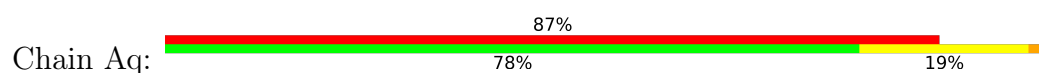
- Molecule 82: ribosomal protein eL28



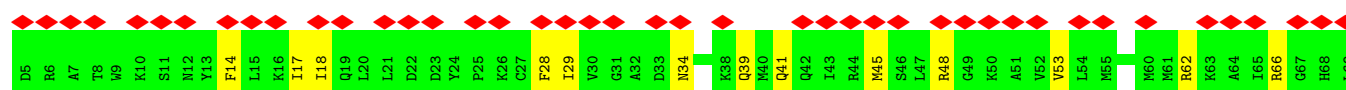
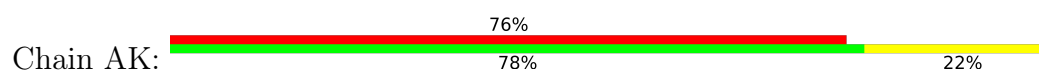
• Molecule 83: Ribosomal protein



• Molecule 84: Ribosomal protein L12

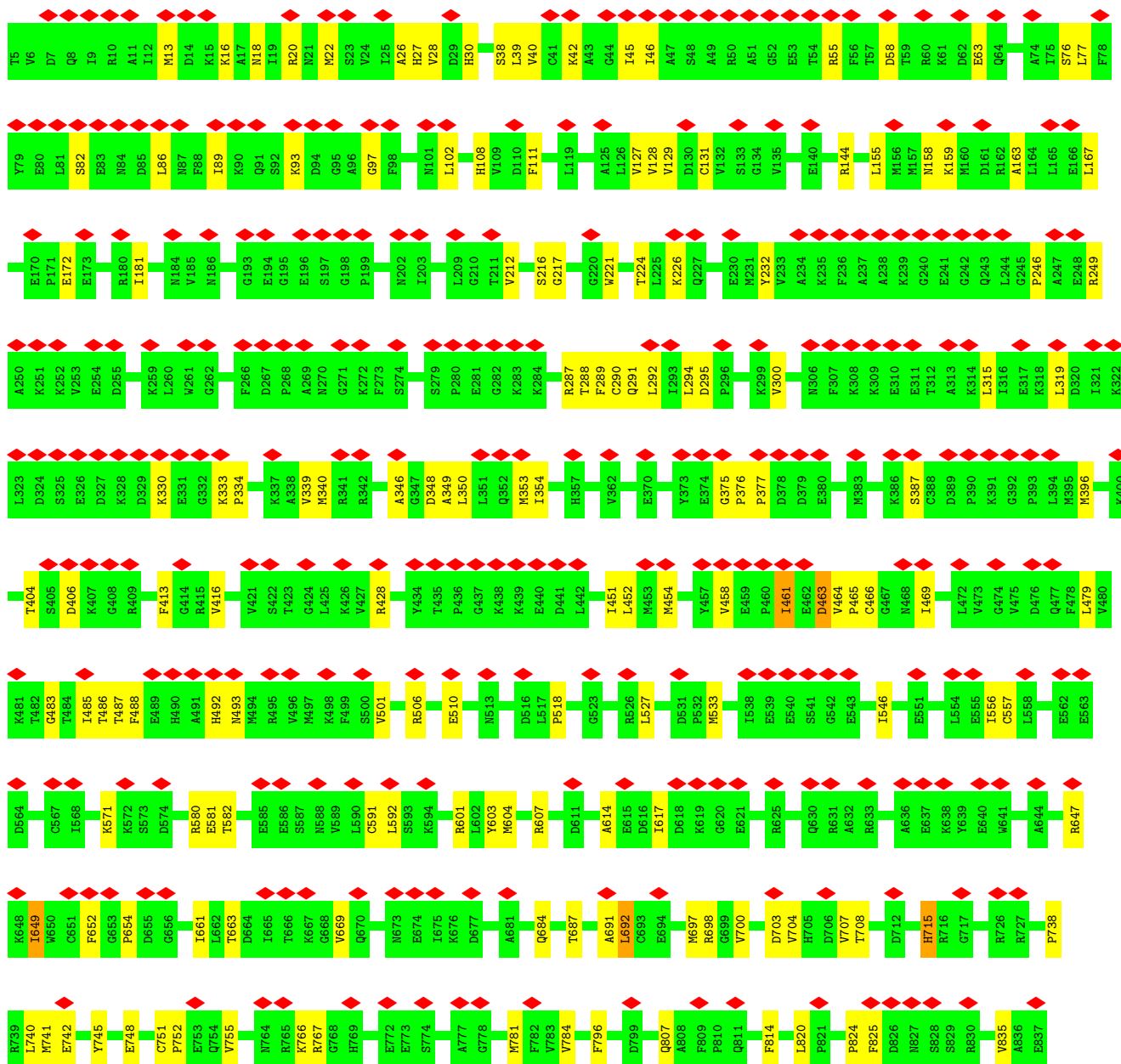
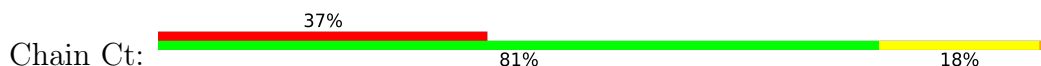


• Molecule 85: ribosomal protein uL10





- Molecule 86: eukaryotic elongation factor 2 (eEF2)



R841	K845	E846	I847	P848	A849	L850	D851	N852	F853	L854	D855	K856	L857
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	32386	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	11.639	Depositor
Minimum map value	-3.647	Depositor
Average map value	0.347	Depositor
Map value standard deviation	0.655	Depositor
Recommended contour level	2.5	Depositor
Map size ($\text{\AA}$)	394.875, 394.875, 394.875	wwPDB
Map dimensions	405, 405, 405	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.975, 0.975, 0.975	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	A2	0.16	0/86613	0.32	1/135108 (0.0%)
2	Bv	0.14	0/1810	0.28	0/2817
3	Bx	0.15	0/287	0.45	0/445
4	Bw	0.13	0/1819	0.26	0/2833
5	B1	0.15	0/40767	0.33	2/63536 (0.0%)
6	BD	0.24	1/1736 (0.1%)	0.49	0/2338
7	BF	0.21	0/1524	0.58	0/2048
8	BK	0.23	0/851	0.63	0/1147
9	BM	0.18	0/941	0.53	0/1264
10	BP	0.26	0/1019	0.70	3/1361 (0.2%)
11	BQ	0.20	0/1126	0.55	0/1506
12	BR	0.20	0/1023	0.54	0/1373
13	BS	0.20	0/1172	0.56	0/1570
14	BT	0.20	0/1131	0.56	0/1515
15	BU	0.17	0/778	0.49	0/1045
16	BZ	0.21	0/696	0.57	0/929
17	Bc	0.19	0/490	0.55	2/656 (0.3%)
18	Bd	0.22	0/437	0.59	0/580
19	Bf	0.14	0/613	0.45	0/811
20	Bg	0.17	0/2497	0.43	0/3399
21	BA	0.20	0/1741	0.51	0/2366
22	BB	0.21	0/1749	0.62	0/2340
23	BC	0.20	0/1761	0.52	0/2379
24	BE	0.19	0/2072	0.54	0/2793
25	BG	0.17	0/1907	0.49	0/2538
26	BH	0.17	0/1501	0.51	0/2009
27	BI	0.21	0/1725	0.60	2/2298 (0.1%)
28	BJ	0.21	0/1520	0.57	0/2030
29	BL	0.20	0/1281	0.51	0/1710
30	BN	0.19	0/1226	0.52	0/1649
31	BO	0.16	0/1029	0.50	0/1380
32	BV	0.18	0/623	0.49	0/833

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BW	0.20	0/1051	0.54	0/1406
34	BX	0.20	0/1116	0.52	0/1490
35	BY	0.17	0/1032	0.49	0/1371
36	Ba	0.19	0/786	0.52	0/1053
37	Bb	0.16	0/637	0.45	0/854
38	Be	0.20	0/443	0.60	0/583
39	A3	0.16	0/3726	0.33	0/5804
40	A4	0.17	0/2839	0.34	0/4425
41	AA	0.20	0/1968	0.51	0/2639
42	AB	0.20	0/3246	0.52	0/4345
43	AC	0.19	0/2942	0.55	0/3951
44	AD	0.20	0/2437	0.56	0/3262
45	AE	0.22	0/1603	0.65	2/2153 (0.1%)
46	AF	0.20	0/1986	0.55	0/2644
47	AG	0.22	0/1913	0.58	2/2576 (0.1%)
48	AH	0.21	0/1545	0.60	2/2077 (0.1%)
49	AI	0.17	0/1730	0.50	0/2311
50	AJ	0.19	0/1376	0.55	2/1841 (0.1%)
51	AL	0.22	0/1688	0.61	0/2260
52	AM	0.22	0/1161	0.51	0/1554
53	AN	0.19	0/1746	0.52	0/2338
54	AO	0.20	0/1638	0.50	0/2191
55	AP	0.17	0/1268	0.46	0/1701
56	AQ	0.21	0/1537	0.61	2/2052 (0.1%)
57	AR	0.18	0/1533	0.53	0/2025
58	AS	0.19	0/1488	0.49	0/1997
59	AT	0.17	0/1312	0.45	0/1753
60	AU	0.17	0/822	0.46	0/1103
61	AV	0.15	0/983	0.41	0/1319
62	AW	0.18	0/1004	0.54	0/1332
63	AX	0.16	0/975	0.46	0/1312
64	AY	0.17	0/1081	0.45	0/1439
65	AZ	0.19	0/1126	0.56	0/1502
66	Aa	0.18	0/1191	0.48	0/1591
67	Ab	0.23	0/569	0.69	0/750
68	Ac	0.18	0/812	0.48	0/1089
69	Ad	0.18	0/894	0.50	0/1204
70	Ae	0.20	0/1082	0.58	0/1443
71	Af	0.20	0/895	0.58	1/1198 (0.1%)
72	Ag	0.20	0/916	0.57	0/1220
73	Ah	0.20	0/1023	0.54	0/1351
74	Ai	0.19	0/805	0.54	0/1065
75	Aj	0.21	0/703	0.57	0/929

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	Ak	0.17	0/575	0.48	0/761
77	Al	0.19	0/454	0.53	0/599
78	Am	0.18	0/417	0.50	0/553
79	An	0.16	0/241	0.55	0/305
80	Ao	0.21	0/877	0.54	0/1156
81	Ap	0.20	0/718	0.59	0/953
82	At	0.27	0/995	0.73	4/1334 (0.3%)
83	Au	0.21	0/1772	0.55	1/2375 (0.0%)
84	Aq	0.29	0/1155	0.83	2/1558 (0.1%)
85	AK	0.21	0/1580	0.62	2/2133 (0.1%)
86	Ct	0.26	0/6767	0.69	10/9139 (0.1%)
All	All	0.18	1/241644 (0.0%)	0.43	40/353975 (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
8	BK	0	1
11	BQ	0	1
17	Bc	0	1
21	BA	0	1
22	BB	0	1
24	BE	0	1
27	BI	0	2
28	BJ	0	1
43	AC	0	2
44	AD	0	1
45	AE	0	3
48	AH	0	2
56	AQ	0	2
57	AR	0	1
71	Af	0	1
73	Ah	0	1
82	At	0	1
84	Aq	0	2
85	AK	0	1
86	Ct	0	4
All	All	0	30

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	BD	162	ASP	C-N	6.74	1.39	1.33

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	AK	94	ASP	CA-C-N	7.12	134.51	121.70
85	AK	94	ASP	C-N-CA	7.12	134.51	121.70
47	AG	83	PHE	CA-C-N	6.47	133.89	121.54
47	AG	83	PHE	C-N-CA	6.47	133.89	121.54
86	Ct	463	ASP	CA-C-N	6.14	133.48	122.13
86	Ct	463	ASP	C-N-CA	6.14	133.48	122.13
84	Aq	154	ASP	CA-C-N	6.00	129.46	120.69
84	Aq	154	ASP	C-N-CA	6.00	129.46	120.69
83	Au	80	VAL	N-CA-C	-5.99	106.58	111.91
71	Af	107	PRO	N-CA-C	5.74	124.29	112.47
86	Ct	288	THR	CA-C-N	5.64	132.32	121.54
86	Ct	288	THR	C-N-CA	5.64	132.32	121.54
27	BI	132	GLU	CA-C-N	5.58	132.20	121.54
27	BI	132	GLU	C-N-CA	5.58	132.20	121.54
10	BP	50	ARG	CA-C-N	5.55	132.15	121.54
10	BP	50	ARG	C-N-CA	5.55	132.15	121.54
17	Bc	32	VAL	CA-C-N	5.53	132.10	121.54
17	Bc	32	VAL	C-N-CA	5.53	132.10	121.54
86	Ct	158	ASN	CA-C-N	5.49	132.02	121.54
86	Ct	158	ASN	C-N-CA	5.49	132.02	121.54
82	At	26	SER	CA-C-N	5.42	131.90	121.54
82	At	26	SER	C-N-CA	5.42	131.90	121.54
5	B1	797	C	P-O3'-C3'	5.41	128.32	120.20
56	AQ	159	PRO	CA-C-N	5.41	131.87	121.54
56	AQ	159	PRO	C-N-CA	5.41	131.87	121.54
45	AE	135	GLN	CA-C-N	5.39	131.84	121.54
45	AE	135	GLN	C-N-CA	5.39	131.84	121.54
86	Ct	387	SER	CA-C-N	5.36	131.78	121.54
86	Ct	387	SER	C-N-CA	5.36	131.78	121.54
5	B1	227	U	P-O3'-C3'	5.33	128.19	120.20
50	AJ	53	ALA	CA-C-N	5.32	135.58	126.32
50	AJ	53	ALA	C-N-CA	5.32	135.58	126.32
86	Ct	488	PHE	CA-C-N	5.18	131.44	121.54
86	Ct	488	PHE	C-N-CA	5.18	131.44	121.54
10	BP	50	ARG	CA-CB-CG	5.18	124.46	114.10
1	A2	4946	U	P-O3'-C3'	5.08	127.82	120.20
82	At	85	ASN	CA-C-N	5.06	131.21	121.54
82	At	85	ASN	C-N-CA	5.06	131.21	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	AH	141	LYS	CA-C-N	5.00	129.51	122.46
48	AH	141	LYS	C-N-CA	5.00	129.51	122.46

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
43	AC	150	LEU	Peptide
43	AC	51	PRO	Peptide
44	AD	258	LYS	Peptide
45	AE	129	GLY	Peptide
45	AE	135	GLN	Peptide
45	AE	136	HIS	Peptide
48	AH	116	ASN	Peptide
48	AH	60	TRP	Peptide
85	AK	149	ARG	Peptide
56	AQ	13	VAL	Peptide
56	AQ	163	THR	Peptide
57	AR	113	LYS	Peptide
71	Af	106	TYR	Peptide
73	Ah	86	LYS	Peptide
84	Aq	29	ALA	Peptide
84	Aq	30	PRO	Peptide
82	At	27	THR	Peptide
21	BA	207	PRO	Peptide
22	BB	39	PHE	Peptide
24	BE	92	ILE	Peptide
27	BI	132	GLU	Peptide
27	BI	159	SER	Peptide
28	BJ	137	VAL	Peptide
8	BK	65	ARG	Peptide
11	BQ	13	PHE	Peptide
17	Bc	32	VAL	Peptide
86	Ct	333	LYS	Peptide
86	Ct	461	ILE	Peptide
86	Ct	463	ASP	Peptide
86	Ct	493	ASN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A2	77427	0	39115	665	0
2	Bv	1620	0	821	6	0
3	Bx	257	0	128	2	0
4	Bw	1627	0	821	5	0
5	B1	36456	0	18411	337	0
6	BD	1709	0	1803	18	0
7	BF	1502	0	1557	26	0
8	BK	827	0	854	15	0
9	BM	931	0	961	9	0
10	BP	999	0	1046	16	0
11	BQ	1109	0	1174	20	0
12	BR	1011	0	1063	15	0
13	BS	1154	0	1210	21	0
14	BT	1112	0	1146	17	0
15	BU	769	0	837	12	0
16	BZ	688	0	766	11	0
17	Bc	488	0	514	6	0
18	Bd	427	0	428	12	0
19	Bf	601	0	623	11	0
20	Bg	2440	0	2396	33	0
21	BA	1704	0	1704	23	0
22	BB	1722	0	1794	28	0
23	BC	1724	0	1808	18	0
24	BE	2031	0	2138	25	0
25	BG	1884	0	2044	22	0
26	BH	1479	0	1564	20	0
27	BI	1696	0	1785	24	0
28	BJ	1495	0	1615	20	0
29	BL	1258	0	1334	17	0
30	BN	1202	0	1289	15	0
31	BO	1016	0	1039	14	0
32	BV	617	0	622	12	0
33	BW	1034	0	1080	16	0
34	BX	1098	0	1167	20	0
35	BY	1015	0	1086	12	0
36	Ba	774	0	821	22	0
37	Bb	625	0	646	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	Be	437	0	483	9	0
39	A3	3337	0	1692	35	0
40	A4	2541	0	1285	22	0
41	AA	1930	0	2030	40	0
42	AB	3178	0	3314	54	0
43	AC	2888	0	3064	43	0
44	AD	2392	0	2425	31	0
45	AE	1571	0	1701	22	0
46	AF	1950	0	2093	30	0
47	AG	1880	0	2018	28	0
48	AH	1526	0	1605	21	0
49	AI	1692	0	1744	21	0
50	AJ	1353	0	1386	10	0
51	AL	1657	0	1764	33	0
52	AM	1138	0	1204	22	0
53	AN	1701	0	1749	42	0
54	AO	1606	0	1745	23	0
55	AP	1242	0	1269	12	0
56	AQ	1513	0	1628	27	0
57	AR	1517	0	1670	20	0
58	AS	1449	0	1493	31	0
59	AT	1284	0	1352	20	0
60	AU	808	0	831	6	0
61	AV	969	0	1031	13	0
62	AW	989	0	1041	12	0
63	AX	958	0	1029	14	0
64	AY	1064	0	1145	14	0
65	AZ	1103	0	1179	18	0
66	Aa	1162	0	1213	22	0
67	Ab	559	0	590	7	0
68	Ac	801	0	845	6	0
69	Ad	879	0	924	11	0
70	Ae	1064	0	1160	16	0
71	Af	876	0	912	12	0
72	Ag	906	0	1002	14	0
73	Ah	1015	0	1148	17	0
74	Ai	794	0	870	8	0
75	Aj	689	0	717	20	0
76	Ak	569	0	637	10	0
77	Al	444	0	483	8	0
78	Am	411	0	443	10	0
79	An	240	0	289	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	Ao	863	0	931	11	0
81	Ap	708	0	758	12	0
82	At	980	0	1041	16	0
83	Au	1744	0	1859	20	0
84	Aq	1140	0	1191	21	0
85	AK	1556	0	1612	24	0
86	Ct	6659	0	6744	93	0
87	A2	231	0	0	0	0
87	A3	6	0	0	0	0
87	A4	8	0	0	0	0
87	AA	1	0	0	0	0
87	AL	1	0	0	0	0
87	AN	1	0	0	0	0
87	AY	1	0	0	0	0
87	Al	1	0	0	0	0
87	An	1	0	0	0	0
87	B1	68	0	0	0	0
87	BD	4	0	0	0	0
87	BS	1	0	0	0	0
87	Ba	1	0	0	0	0
87	Bd	1	0	0	0	0
87	Bx	1	0	0	0	0
88	Aj	1	0	0	0	0
88	Ao	1	0	0	0	0
88	Ap	1	0	0	0	0
88	Ba	1	0	0	0	0
88	Bd	1	0	0	0	0
89	Ct	32	0	13	1	0
All	All	225624	0	169562	2067	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 5.

All (2067) 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)
5:B1:1652:G:H1	5:B1:1672:U:H3	1.00	0.97
1:A2:3942:G:N2	1:A2:4020:A:H62	1.61	0.97
5:B1:677:G:N2	5:B1:1028:A:H62	1.62	0.97
5:B1:442:C:H42	5:B1:449:A:H62	1.14	0.95
5:B1:1351:G:H1	5:B1:1360:U:H3	1.07	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:1871:G:H1	1:A2:1920:A:H61	1.07	0.94
5:B1:677:G:H21	5:B1:1028:A:N6	1.64	0.93
5:B1:1656:G:H1	5:B1:1668:U:H3	1.08	0.93
1:A2:465:A:H62	1:A2:677:G:H21	1.11	0.93
1:A2:3942:G:H21	1:A2:4020:A:N6	1.67	0.93
5:B1:1743:G:H21	5:B1:1791:A:H62	1.04	0.92
1:A2:1871:G:H1	1:A2:1920:A:N6	1.67	0.91
1:A2:708:U:H3	1:A2:938:G:H1	0.99	0.91
1:A2:161:G:H1	1:A2:266:U:H3	1.16	0.91
1:A2:465:A:H62	1:A2:677:G:N2	1.69	0.90
1:A2:3927:G:H1	1:A2:4026:A:H61	1.17	0.90
1:A2:499:G:H1	1:A2:647:U:H3	0.93	0.88
1:A2:2462:G:H1	1:A2:2474:U:H3	1.19	0.86
1:A2:3942:G:H21	1:A2:4020:A:H62	0.86	0.85
5:B1:1743:G:N2	5:B1:1791:A:H62	1.74	0.85
43:AC:218:ILE:O	43:AC:222:ARG:HB2	1.76	0.84
86:Ct:315:LEU:O	86:Ct:319:LEU:HB2	1.78	0.83
5:B1:1050:A:H62	5:B1:1068:G:H21	1.24	0.81
5:B1:677:G:H21	5:B1:1028:A:H62	0.85	0.81
1:A2:1977:C:H42	1:A2:1981:G:N2	1.78	0.80
1:A2:1977:C:H42	1:A2:1981:G:H22	1.28	0.80
1:A2:465:A:N6	1:A2:677:G:H21	1.80	0.79
5:B1:1743:G:H21	5:B1:1791:A:N6	1.79	0.78
1:A2:2617:G:H21	1:A2:2676:A:H62	1.35	0.73
1:A2:1977:C:N4	1:A2:1981:G:H22	1.87	0.73
10:BP:24:GLN:O	10:BP:28:MET:HB2	1.88	0.73
1:A2:455:G:H1	1:A2:687:A:H2	1.37	0.72
1:A2:1073:G:H22	1:A2:1188:G:H22	1.36	0.72
5:B1:1260:A:C2	5:B1:1617:G:N2	2.57	0.71
1:A2:4069:G:H1	1:A2:4080:U:H3	1.37	0.70
5:B1:442:C:N4	5:B1:449:A:H62	1.88	0.70
20:Bg:87:LEU:HB2	20:Bg:101:PHE:HB2	1.74	0.70
48:AH:173:ARG:HH22	78:Am:127:VAL:HG13	1.57	0.69
1:A2:3927:G:H1	1:A2:4026:A:N6	1.88	0.69
85:AK:66:ARG:HG3	85:AK:72:ASN:HD21	1.58	0.69
1:A2:1160:U:H3	1:A2:1167:A:H61	1.41	0.68
1:A2:272:G:H5''	53:AN:8:GLN:HE22	1.58	0.68
1:A2:4715:U:N3	1:A2:4837:C:N4	2.41	0.68
1:A2:2825:G:H5''	61:AV:85:ARG:HE	1.59	0.68
1:A2:2274:C:H5''	43:AC:199:ARG:HH12	1.59	0.67
5:B1:851:C:H5''	5:B1:852:G:H5'	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:3663:A:H62	1:A2:3794:G:H21	1.44	0.66
69:Ad:46:LEU:HD11	69:Ad:73:TRP:HE1	1.59	0.66
1:A2:2618:U:HO2'	1:A2:2673:G:H1	1.43	0.66
83:Au:159:MET:HA	83:Au:165:LEU:HD22	1.77	0.66
22:BB:197:ILE:O	22:BB:201:CYS:HB2	1.96	0.66
35:BY:104:ARG:HG3	35:BY:105:LYS:HG2	1.77	0.66
1:A2:1988:G:H21	1:A2:1993:A:N6	1.94	0.66
5:B1:383:G:H21	29:BL:133:PRO:HG2	1.59	0.66
58:AS:81:TRP:HB3	58:AS:127:MET:HE3	1.78	0.65
5:B1:1166:G:H1	5:B1:1193:U:H3	1.44	0.65
1:A2:4234:G:N1	1:A2:4298:A:C2	2.64	0.65
44:AD:235:MET:O	44:AD:239:MET:HB2	1.96	0.65
1:A2:4692:C:H1'	1:A2:4693:G:H2'	1.79	0.65
24:BE:31:PRO:HG3	24:BE:43:PRO:HG3	1.79	0.65
1:A2:451:G:H1	1:A2:691:G:H1	1.44	0.65
70:Ae:22:ARG:HE	70:Ae:36:ARG:HB3	1.61	0.65
48:AH:172:ILE:HD11	78:Am:102:ARG:HH22	1.61	0.64
28:BJ:37:LEU:HD23	28:BJ:42:GLU:HG3	1.77	0.64
58:AS:101:THR:HG23	58:AS:104:GLY:H	1.62	0.64
1:A2:1083:U:O2	1:A2:1178:G:N2	2.31	0.64
1:A2:24:G:N7	75:Aj:46:LYS:NZ	2.46	0.64
1:A2:123:C:H42	1:A2:144:A:H61	1.44	0.64
1:A2:1441:A:OP1	56:AQ:65:ARG:NH2	2.30	0.64
1:A2:3917:G:H1	1:A2:4037:U:H3	1.44	0.64
5:B1:1260:A:H2	5:B1:1617:G:H21	1.43	0.64
1:A2:200:U:O2	1:A2:208:G:C2	2.50	0.64
25:BG:137:ARG:HG3	25:BG:178:ARG:HG3	1.78	0.64
48:AH:59:LYS:HE2	48:AH:66:GLU:HB3	1.79	0.64
9:BM:55:ASN:HD22	9:BM:81:ASP:HB3	1.62	0.63
14:BT:71:GLY:H	14:BT:74:SER:HB2	1.64	0.63
74:Ai:48:CYS:SG	74:Ai:49:GLY:N	2.70	0.63
57:AR:133:LYS:H	57:AR:137:ILE:HD11	1.62	0.63
1:A2:289:A:H5'	80:Ao:39:ARG:HD2	1.80	0.63
1:A2:1073:G:H1	1:A2:1188:G:H1	1.47	0.63
1:A2:737:A:N1	58:AS:98:ARG:NH2	2.45	0.63
5:B1:924:G:H1	5:B1:1018:U:H3	1.45	0.63
1:A2:457:A:H61	1:A2:685:C:H42	1.45	0.63
66:Aa:42:ARG:O	66:Aa:46:ASP:HB2	1.98	0.63
51:AL:63:THR:HB	51:AL:65:ARG:H	1.63	0.62
1:A2:159:A:H61	1:A2:268:C:H42	1.46	0.62
1:A2:199:C:N3	1:A2:209:A:N6	2.45	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:Ct:40:VAL:HG23	86:Ct:77:LEU:HD21	1.79	0.62
5:B1:377:G:H5''	27:BI:98:LYS:HB3	1.80	0.62
5:B1:1748:G:H1	5:B1:1786:U:H3	1.48	0.62
16:BZ:58:LEU:O	16:BZ:62:VAL:HB	1.99	0.62
7:BF:143:PRO:HB3	7:BF:146:ARG:HH21	1.65	0.62
13:BS:47:LYS:HE3	13:BS:78:LYS:HD2	1.81	0.62
75:Aj:36:LYS:HA	75:Aj:45:ARG:HH21	1.64	0.62
10:BP:98:ASN:ND2	10:BP:121:ILE:O	2.32	0.62
20:Bg:5:MET:HB3	20:Bg:310:TRP:HB3	1.81	0.62
1:A2:1921:G:H22	1:A2:4396:C:H5''	1.65	0.62
1:A2:2569:G:H21	1:A2:2734:A:H62	1.48	0.62
64:AY:52:ASP:HB2	64:AY:110:LYS:HD2	1.82	0.62
1:A2:1320:A:H62	1:A2:2325:C:H5	1.47	0.62
34:BX:50:ILE:HD12	86:Ct:518:PRO:HB3	1.81	0.61
1:A2:1353:G:OP1	43:AC:48:ASN:ND2	2.32	0.61
1:A2:2645:U:OP2	57:AR:107:ARG:NH2	2.33	0.61
5:B1:391:C:H2'	5:B1:392:A:H8	1.66	0.61
1:A2:4650:C:HO2'	48:AH:155:SER:HG	1.46	0.61
49:AI:33:ILE:O	49:AI:69:ARG:NH1	2.33	0.61
71:Af:78:HIS:HB2	71:Af:85:ARG:HG3	1.83	0.61
86:Ct:601:ARG:HB3	86:Ct:708:THR:HB	1.81	0.61
1:A2:4508:A:N7	41:AA:215:ASN:ND2	2.47	0.61
7:BF:34:SER:HB3	7:BF:146:ARG:HH22	1.65	0.61
1:A2:2756:G:H5''	1:A2:2757:G:H5'	1.82	0.61
1:A2:4577:C:H5''	42:AB:357:ARG:HE	1.64	0.61
29:BL:101:ARG:HH22	34:BX:5:ARG:HA	1.64	0.61
56:AQ:18:PRO:HG3	56:AQ:29:VAL:HG21	1.82	0.61
28:BJ:162:ARG:H	28:BJ:166:GLY:HA3	1.64	0.61
66:Aa:24:LYS:HD3	66:Aa:26:ARG:HH21	1.66	0.61
80:Ao:71:GLU:HG2	80:Ao:80:LYS:HG2	1.83	0.61
1:A2:1721:G:N3	1:A2:1724:A:N6	2.47	0.61
1:A2:1933:G:H4'	58:AS:93:MET:HG3	1.82	0.61
5:B1:1144:A:H5'	5:B1:1355:C:H41	1.66	0.61
83:Au:139:THR:HB	83:Au:142:GLU:HB2	1.83	0.61
2:Bv:10:G:O6	2:Bv:45:G:N2	2.34	0.61
27:BI:165:GLN:HE22	27:BI:195:LEU:HD11	1.66	0.61
1:A2:682:U:OP1	82:At:87:ARG:NH1	2.34	0.60
1:A2:2618:U:O2'	1:A2:2673:G:N1	2.34	0.60
53:AN:68:ARG:NH2	53:AN:123:GLU:OE1	2.34	0.60
1:A2:2279:A:N7	43:AC:143:ARG:NH1	2.48	0.60
1:A2:4209:G:H4'	44:AD:5:LYS:HD3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BF:91:ARG:NH2	11:BQ:46:THR:OG1	2.35	0.60
69:Ad:39:LYS:HA	69:Ad:77:ILE:HD12	1.84	0.60
86:Ct:39:LEU:HB2	86:Ct:350:LEU:HD13	1.82	0.60
86:Ct:291:GLN:HA	86:Ct:295:ASP:HB2	1.83	0.60
1:A2:3606:A:H61	81:Ap:17:ARG:HB2	1.66	0.60
1:A2:3908:C:H1'	53:AN:125:SER:HB3	1.82	0.60
5:B1:639:C:H2'	5:B1:640:A:H8	1.66	0.60
13:BS:43:VAL:HG22	14:BT:37:VAL:HG21	1.82	0.60
39:A3:27:U:H4'	43:AC:54:VAL:HB	1.84	0.60
7:BF:71:ARG:NH2	7:BF:148:ASN:OD1	2.34	0.60
1:A2:412:A:H4'	1:A2:2290:C:H5'	1.84	0.60
5:B1:600:G:H2'	5:B1:601:G:H8	1.66	0.60
20:Bg:258:ILE:HD12	20:Bg:268:ASP:HB3	1.84	0.60
22:BB:82:ARG:NH2	22:BB:188:LEU:O	2.35	0.60
23:BC:60:TRP:HE1	23:BC:92:GLU:HB2	1.66	0.60
48:AH:12:ILE:HB	48:AH:53:LYS:HB3	1.83	0.60
51:AL:54:PRO:HB2	51:AL:56:ARG:HH12	1.66	0.60
28:BJ:153:SER:HB2	28:BJ:156:HIS:HD2	1.66	0.60
29:BL:104:LYS:HZ1	34:BX:8:ARG:HH11	1.48	0.60
41:AA:117:GLU:HB2	41:AA:162:ASN:HB2	1.83	0.60
1:A2:2065:C:H2'	1:A2:2066:G:H8	1.67	0.60
1:A2:4078:G:H21	1:A2:4079:C:H41	1.49	0.60
5:B1:411:G:H21	5:B1:811:A:H61	1.50	0.60
1:A2:2444:C:H1'	1:A2:3643:G:H1	1.66	0.60
1:A2:3915:G:H1	1:A2:4039:U:H3	1.49	0.60
1:A2:4895:C:N3	45:AE:239:LYS:NZ	2.50	0.59
5:B1:1050:A:H62	5:B1:1068:G:N2	1.97	0.59
40:A4:105:C:OP2	49:AI:203:ARG:NH1	2.34	0.59
82:At:63:VAL:HG22	82:At:79:ARG:HG2	1.83	0.59
21:BA:141:ASN:ND2	32:BV:29:HIS:O	2.35	0.59
83:Au:42:ASP:H	83:Au:47:LYS:HD2	1.67	0.59
1:A2:1600:G:OP1	75:Aj:13:ASN:ND2	2.36	0.59
1:A2:1988:G:N2	1:A2:1993:A:H62	2.00	0.59
5:B1:1854:U:H2'	5:B1:1855:G:H8	1.67	0.59
13:BS:50:ILE:HD13	13:BS:59:LEU:HD11	1.84	0.59
21:BA:34:MET:HE2	21:BA:154:LEU:HD11	1.85	0.59
53:AN:37:HIS:HE1	53:AN:63:ARG:HH11	1.49	0.59
1:A2:1725:A:N1	1:A2:1771:C:O2'	2.35	0.59
21:BA:11:LYS:HE3	21:BA:13:GLU:HB3	1.84	0.59
27:BI:101:ILE:HA	27:BI:173:ALA:O	2.02	0.59
36:Ba:23:CYS:SG	36:Ba:24:THR:N	2.75	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B1:601:G:H1	5:B1:621:C:H5	1.50	0.59
6:BD:18:LYS:HE2	6:BD:39:VAL:HB	1.83	0.59
6:BD:16:ILE:HG21	18:Bd:22:ARG:HH11	1.67	0.59
14:BT:11:GLN:HE21	14:BT:15:VAL:HB	1.67	0.59
34:BX:68:LYS:NZ	38:Be:6:LEU:O	2.34	0.59
1:A2:19:G:OP1	73:Ah:89:ARG:NH2	2.35	0.59
1:A2:1611:G:N7	41:AA:9:ARG:NH1	2.45	0.59
1:A2:2664:C:OP1	72:Ag:57:ARG:NH1	2.34	0.59
1:A2:2001:U:H2'	1:A2:2002:G:H8	1.68	0.59
1:A2:4180:U:OP2	59:AT:9:ARG:NH2	2.35	0.59
1:A2:4643:A:H4'	54:AO:140:ARG:HH22	1.66	0.59
5:B1:875:A:O2'	26:BH:113:LYS:NZ	2.36	0.59
42:AB:26:ARG:NH1	42:AB:181:MET:SD	2.75	0.59
1:A2:4062:G:H3'	1:A2:4063:G:H21	1.67	0.59
56:AQ:96:PRO:HG2	56:AQ:98:LEU:HD22	1.84	0.59
14:BT:75:MET:SD	14:BT:121:ARG:NH1	2.76	0.59
15:BU:59:LYS:HB2	15:BU:84:ILE:HB	1.84	0.59
33:BW:52:ILE:HG12	33:BW:61:ILE:HG12	1.84	0.59
48:AH:10:VAL:HB	48:AH:55:LEU:HB3	1.84	0.59
85:AK:18:ILE:HD12	85:AK:62:ARG:HH22	1.68	0.59
1:A2:4583:C:OP1	61:AV:48:ARG:NH1	2.35	0.58
86:Ct:506:ARG:HA	86:Ct:546:ILE:O	2.02	0.58
45:AE:149:ILE:HD12	45:AE:271:LEU:HD21	1.85	0.58
85:AK:119:CYS:SG	85:AK:120:GLU:N	2.73	0.58
1:A2:658:G:N2	1:A2:659:G:O6	2.35	0.58
1:A2:742:G:N2	1:A2:743:G:N7	2.46	0.58
1:A2:4602:C:N3	1:A2:4622:G:N2	2.51	0.58
29:BL:147:LYS:HG2	29:BL:149:ALA:H	1.68	0.58
42:AB:351:LEU:HD12	42:AB:352:LEU:HG	1.85	0.58
68:Ac:21:VAL:HG11	68:Ac:96:ILE:HD12	1.85	0.58
1:A2:2279:A:N6	43:AC:178:ASN:OD1	2.37	0.58
5:B1:1414:A:H61	5:B1:1423:C:H42	1.51	0.58
13:BS:30:ILE:HG22	13:BS:36:VAL:HG11	1.84	0.58
57:AR:98:ARG:HH21	57:AR:133:LYS:HA	1.68	0.58
5:B1:104:A:OP1	27:BI:12:ARG:NH1	2.37	0.58
5:B1:1123:C:OP1	22:BB:151:ARG:NH2	2.37	0.58
23:BC:196:ILE:HB	23:BC:223:TYR:HB2	1.85	0.58
29:BL:59:LYS:HD3	29:BL:134:LEU:HD23	1.84	0.58
34:BX:93:PHE:HB3	34:BX:133:LEU:HD23	1.85	0.58
36:Ba:44:ILE:HG13	36:Ba:45:VAL:HG23	1.84	0.58
82:At:90:LEU:HD11	82:At:111:ILE:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:AX:91:GLU:HG3	63:AX:147:LEU:HD21	1.85	0.58
1:A2:97:G:N7	51:AL:13:HIS:NE2	2.51	0.58
1:A2:722:G:H21	58:AS:72:PRO:HG2	1.66	0.58
1:A2:1997:C:H2'	1:A2:1998:A:H8	1.67	0.58
1:A2:3819:U:H2'	1:A2:3820:A:H8	1.69	0.58
1:A2:4333:G:N2	4:Bw:76:A:O2'	2.36	0.58
1:A2:4679:A:H4'	42:AB:20:LYS:HB3	1.85	0.58
26:BH:61:ILE:HG22	26:BH:93:VAL:HB	1.86	0.58
86:Ct:221:TRP:HB3	86:Ct:340:MET:HB3	1.86	0.58
1:A2:3863:U:O2'	55:AP:80:GLN:NE2	2.37	0.58
5:B1:190:G:O2'	5:B1:209:A:N6	2.37	0.58
5:B1:1280:G:H1	5:B1:1317:C:H42	1.52	0.58
39:A3:69:U:O2'	64:AY:27:ARG:NH2	2.37	0.58
42:AB:10:ARG:HH22	42:AB:13:SER:HA	1.69	0.58
5:B1:1231:C:O2'	5:B1:1253:A:N6	2.37	0.57
76:Ak:23:VAL:HA	76:Ak:35:LYS:O	2.04	0.57
1:A2:1498:G:H2'	1:A2:1500:A:H62	1.67	0.57
8:BK:53:LYS:HE2	8:BK:69:TRP:HE1	1.70	0.57
1:A2:2662:C:O2	72:Ag:54:ARG:NH2	2.33	0.57
1:A2:4936:G:OP1	42:AB:271:GLN:NE2	2.37	0.57
5:B1:442:C:H42	5:B1:449:A:N6	1.94	0.57
5:B1:986:G:OP2	5:B1:988:C:N4	2.37	0.57
5:B1:1844:U:H3	5:B1:1855:G:H1	1.51	0.57
20:Bg:163:PRO:HB2	20:Bg:179:LEU:HB2	1.86	0.57
44:AD:38:ILE:HD11	59:AT:27:LEU:HD22	1.86	0.57
83:Au:54:ARG:NH1	83:Au:55:LEU:O	2.37	0.57
5:B1:879:C:H3'	5:B1:880:G:H21	1.70	0.57
44:AD:128:ASP:O	44:AD:164:LYS:NZ	2.38	0.57
1:A2:2645:U:OP2	57:AR:103:ARG:NH2	2.37	0.57
5:B1:1592:C:H5''	7:BF:91:ARG:HH22	1.69	0.57
8:BK:29:MET:HG3	8:BK:30:PRO:HD3	1.87	0.57
24:BE:100:ARG:HH12	24:BE:236:ILE:HD12	1.69	0.57
1:A2:1722:C:O2	1:A2:1768:A:N6	2.38	0.57
5:B1:1171:G:N2	5:B1:1188:A:OP2	2.38	0.57
47:AG:89:ARG:HH22	47:AG:185:LYS:HD3	1.68	0.57
1:A2:1607:G:N2	1:A2:3890:C:OP2	2.37	0.57
32:BV:59:ILE:HG23	32:BV:64:GLU:HB3	1.85	0.57
40:A4:14:C:OP1	44:AD:24:ARG:NH1	2.37	0.57
82:At:28:GLU:OE2	82:At:41:ASN:ND2	2.38	0.57
1:A2:223:G:N2	64:AY:8:THR:O	2.37	0.57
1:A2:1952:C:O2	85:AK:41:GLN:NE2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B1:649:U:H2'	5:B1:650:A:H8	1.70	0.57
23:BC:171:GLY:HA2	33:BW:98:GLN:HE21	1.70	0.57
30:BN:15:ALA:HB3	37:Bb:20:LYS:HE2	1.87	0.57
45:AE:151:ILE:HB	45:AE:195:ILE:HB	1.87	0.57
69:Ad:88:LEU:HG	69:Ad:106:VAL:HG22	1.86	0.57
84:Aq:57:ARG:NH1	84:Aq:83:LYS:O	2.38	0.57
86:Ct:404:THR:HG23	86:Ct:406:ASP:H	1.70	0.57
18:Bd:47:ALA:HB1	18:Bd:52:PHE:HB2	1.85	0.57
27:BI:104:ILE:HB	27:BI:171:LEU:HB3	1.87	0.57
46:AF:93:ILE:HD13	46:AF:213:LEU:HD12	1.87	0.57
5:B1:309:G:H21	5:B1:340:C:H1'	1.70	0.57
5:B1:924:G:N2	5:B1:1018:U:O2	2.35	0.57
15:BU:66:ARG:HH12	15:BU:75:LYS:HG2	1.70	0.57
28:BJ:160:SER:O	28:BJ:162:ARG:NH1	2.38	0.57
42:AB:53:MET:HG2	42:AB:77:THR:HG22	1.86	0.57
50:AJ:53:ALA:HB2	50:AJ:65:ASN:H	1.70	0.57
86:Ct:396:MET:HB2	86:Ct:485:ILE:HB	1.87	0.57
1:A2:453:C:OP1	82:At:87:ARG:NH2	2.37	0.56
1:A2:1905:C:OP1	52:AM:34:ASN:ND2	2.38	0.56
1:A2:4478:G:OP2	42:AB:3:HIS:ND1	2.36	0.56
1:A2:4854:G:N7	1:A2:4882:C:N4	2.51	0.56
5:B1:527:C:OP1	38:Be:35:ARG:NH1	2.38	0.56
5:B1:1271:C:OP1	19:Bf:92:LYS:NZ	2.38	0.56
6:BD:79:PHE:HB3	6:BD:83:SER:HB2	1.87	0.56
40:A4:75:G:N2	40:A4:100:A:OP2	2.38	0.56
43:AC:209:ILE:HG13	43:AC:251:ILE:HB	1.87	0.56
86:Ct:580:ARG:HB2	86:Ct:741:MET:HB2	1.87	0.56
1:A2:1988:G:H21	1:A2:1993:A:H62	1.51	0.56
5:B1:434:G:OP2	27:BI:25:ARG:NH2	2.37	0.56
5:B1:639:C:OP1	38:Be:41:ARG:NH2	2.38	0.56
68:Ac:47:ILE:HB	68:Ac:94:LEU:HB2	1.86	0.56
1:A2:2372:C:OP2	1:A2:2373:G:N2	2.39	0.56
1:A2:2474:U:H2'	1:A2:2475:G:H8	1.70	0.56
1:A2:4320:U:H4'	51:AL:197:LYS:HD3	1.87	0.56
4:Bw:41:U:H1'	5:B1:1639:G:H21	1.70	0.56
5:B1:90:G:OP1	5:B1:445:A:N6	2.38	0.56
5:B1:1143:A:O3'	5:B1:1355:C:N4	2.37	0.56
5:B1:1533:A:O2'	7:BF:81:ARG:NH2	2.38	0.56
5:B1:1869:A:H61	22:BB:113:MET:H	1.53	0.56
49:AI:3:ARG:NH1	49:AI:4:ARG:O	2.38	0.56
51:AL:60:ARG:NH2	51:AL:67:HIS:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:AL:89:LYS:HZ3	73:Ah:110:LYS:HG2	1.70	0.56
51:AL:128:PRO:HD2	51:AL:136:LYS:HD3	1.87	0.56
86:Ct:18:ASN:ND2	86:Ct:97:GLY:O	2.39	0.56
86:Ct:155:LEU:HB3	86:Ct:212:VAL:HG12	1.86	0.56
1:A2:920:G:N2	1:A2:925:C:O2'	2.38	0.56
1:A2:1176:C:H2'	1:A2:1177:G:H8	1.70	0.56
1:A2:1724:A:N3	44:AD:15:ARG:NH2	2.54	0.56
5:B1:522:A:OP2	28:BJ:45:ARG:NH1	2.34	0.56
5:B1:1658:G:OP2	5:B1:1660:C:N4	2.38	0.56
37:Bb:20:LYS:HE3	37:Bb:28:PRO:HA	1.87	0.56
46:AF:80:ASN:ND2	59:AT:141:VAL:O	2.36	0.56
54:AO:125:LYS:HG3	54:AO:129:LEU:HD12	1.88	0.56
1:A2:1627:C:OP1	43:AC:80:ARG:NH1	2.37	0.56
1:A2:4829:C:OP2	52:AM:94:LYS:NZ	2.37	0.56
5:B1:1467:C:H5	12:BR:3:ARG:HH22	1.51	0.56
10:BP:114:HIS:ND1	10:BP:118:GLU:OE1	2.39	0.56
20:Bg:256:ILE:HB	20:Bg:270:LEU:HB2	1.88	0.56
27:BI:121:LEU:HD21	27:BI:158:ILE:HD11	1.88	0.56
1:A2:3613:A:HO2'	75:Aj:2:THR:N	2.04	0.56
29:BL:135:SER:O	29:BL:139:ARG:NH1	2.38	0.56
68:Ac:48:LEU:HD13	68:Ac:57:LYS:HG3	1.87	0.56
1:A2:2580:A:N6	1:A2:2723:A:OP2	2.39	0.56
5:B1:43:U:OP2	5:B1:485:A:N6	2.34	0.56
6:BD:172:VAL:HG22	6:BD:185:LYS:HG2	1.88	0.56
20:Bg:212:LYS:HA	20:Bg:235:ILE:HG13	1.87	0.56
25:BG:142:ARG:HH22	25:BG:149:LYS:HA	1.70	0.56
58:AS:15:ARG:HB2	58:AS:25:PRO:HB2	1.86	0.56
1:A2:1651:A:H5''	67:Ab:15:LYS:HD3	1.88	0.56
1:A2:3932:G:O2'	1:A2:4013:G:N2	2.38	0.56
1:A2:4410:G:H5''	1:A2:4411:A:H5''	1.88	0.56
36:Ba:20:PRO:HB2	36:Ba:29:CYS:HB2	1.86	0.56
47:AG:164:ILE:HD12	53:AN:22:LEU:HD11	1.88	0.56
5:B1:801:U:O4	26:BH:106:ARG:NH2	2.39	0.56
7:BF:143:PRO:HA	7:BF:146:ARG:HE	1.71	0.56
22:BB:123:ALA:HB3	22:BB:139:CYS:HB3	1.87	0.56
84:Aq:76:SER:OG	84:Aq:117:ARG:NH2	2.39	0.56
1:A2:1295:A:O2'	70:Ae:52:GLN:NE2	2.39	0.56
5:B1:661:U:O2'	33:BW:92:ASN:ND2	2.39	0.56
5:B1:1808:U:H2'	5:B1:1809:A:H8	1.71	0.56
22:BB:151:ARG:NH1	22:BB:153:THR:OG1	2.38	0.56
40:A4:13:A:OP2	40:A4:66:G:N2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:AC:318:PRO:HB2	46:AF:155:TYR:HB3	1.88	0.56
49:AI:47:PRO:HD2	49:AI:141:LYS:HA	1.87	0.56
57:AR:103:ARG:NH2	57:AR:124:TYR:OH	2.39	0.56
58:AS:71:SER:O	58:AS:76:LYS:NZ	2.39	0.56
85:AK:100:ASP:O	85:AK:104:ALA:HB2	2.05	0.56
1:A2:727:C:OP2	52:AM:71:LYS:NZ	2.39	0.55
1:A2:4482:G:N2	42:AB:253:CYS:SG	2.79	0.55
1:A2:4715:U:H3	1:A2:4837:C:N4	2.02	0.55
5:B1:745:C:H1'	26:BH:109:ARG:HD2	1.88	0.55
5:B1:1320:G:OP2	86:Ct:647:ARG:NH2	2.38	0.55
8:BK:50:GLN:HA	8:BK:53:LYS:HG2	1.87	0.55
20:Bg:107:ASP:OD2	20:Bg:125:ARG:NH1	2.39	0.55
82:At:51:VAL:HG12	82:At:62:VAL:HG22	1.88	0.55
86:Ct:13:MET:HA	86:Ct:465:PRO:HB3	1.87	0.55
86:Ct:58:ASP:HB2	86:Ct:63:GLU:HB3	1.87	0.55
86:Ct:654:PRO:HA	86:Ct:684:GLN:HG2	1.88	0.55
86:Ct:692:LEU:HD11	86:Ct:740:LEU:HD21	1.86	0.55
1:A2:294:A:H2'	1:A2:295:G:H8	1.71	0.55
1:A2:717:G:OP1	46:AF:73:ARG:NH2	2.39	0.55
1:A2:1285:U:O4	1:A2:1287:C:N4	2.39	0.55
1:A2:5019:A:OP1	42:AB:123:HIS:NE2	2.39	0.55
5:B1:53:C:OP1	35:BY:112:ASN:ND2	2.39	0.55
9:BM:32:ALA:HB3	9:BM:110:VAL:HB	1.88	0.55
33:BW:68:ARG:O	33:BW:68:ARG:NH1	2.39	0.55
42:AB:240:LEU:HB3	42:AB:244:THR:HG21	1.87	0.55
13:BS:98:VAL:HG21	13:BS:103:LEU:HD13	1.89	0.55
57:AR:8:LYS:HE3	57:AR:19:LYS:HG2	1.87	0.55
1:A2:476:G:H2'	1:A2:477:G:H8	1.70	0.55
7:BF:115:ALA:O	7:BF:119:SER:OG	2.22	0.55
26:BH:98:ARG:NH2	26:BH:125:VAL:O	2.39	0.55
28:BJ:108:ARG:NH2	28:BJ:149:VAL:O	2.39	0.55
1:A2:1498:G:O2'	51:AL:18:TRP:NE1	2.39	0.55
2:Bv:10:G:C6	2:Bv:45:G:N2	2.74	0.55
5:B1:833:C:N4	35:BY:10:ARG:O	2.40	0.55
5:B1:913:A:OP2	26:BH:99:ARG:NH1	2.39	0.55
5:B1:1396:A:OP2	11:BQ:15:ARG:NH1	2.40	0.55
39:A3:110:U:OP2	75:Aj:20:ARG:NH2	2.37	0.55
51:AL:11:LYS:H	56:AQ:168:ARG:HH22	1.55	0.55
57:AR:7:GLN:NE2	57:AR:35:ALA:O	2.39	0.55
5:B1:4:C:H5'	23:BC:230:THR:HG21	1.89	0.55
33:BW:57:ARG:NH2	37:Bb:26:GLN:OE1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:Ak:20:ALA:HA	76:Ak:38:CYS:HA	1.88	0.55
83:Au:201:VAL:HG11	83:Au:204:LEU:HD23	1.88	0.55
1:A2:2410:A:H5''	77:Al:22:PRO:HG3	1.88	0.55
5:B1:409:C:N4	5:B1:427:U:OP1	2.39	0.55
5:B1:1597:C:OP2	16:BZ:85:ARG:NH2	2.39	0.55
11:BQ:16:LYS:HB3	11:BQ:19:ALA:HB3	1.88	0.55
47:AG:143:VAL:HG22	47:AG:203:ALA:HB2	1.88	0.55
48:AH:124:ARG:HD3	48:AH:164:ALA:HB1	1.89	0.55
83:Au:25:ARG:NH1	83:Au:26:ARG:O	2.40	0.55
1:A2:305:G:OP1	74:Al:85:ARG:NH1	2.40	0.55
1:A2:1273:G:O2'	1:A2:4899:G:N7	2.40	0.55
1:A2:1615:G:H5'	41:AA:205:ASN:HD21	1.71	0.55
1:A2:4482:G:OP2	42:AB:2:SER:N	2.40	0.55
1:A2:4520:U:OP2	42:AB:246:ARG:NH2	2.39	0.55
1:A2:4729:C:H42	1:A2:4823:C:H42	1.54	0.55
23:BC:131:GLY:HA3	23:BC:137:VAL:HG12	1.88	0.55
39:A3:122:G:N2	39:A3:129:C:O2'	2.37	0.55
58:AS:69:GLU:HB3	58:AS:72:PRO:HG3	1.88	0.55
84:Aq:91:ASP:O	84:Aq:95:GLN:NE2	2.39	0.55
5:B1:1086:G:OP2	36:Ba:12:LYS:NZ	2.40	0.55
21:BA:36:GLN:O	21:BA:53:ARG:NH1	2.39	0.55
26:BH:131:GLU:OE1	30:BN:20:ARG:NH1	2.40	0.55
39:A3:29:G:H5''	51:AL:27:ASN:HB3	1.89	0.55
80:Ao:21:HIS:HA	80:Ao:71:GLU:O	2.07	0.55
86:Ct:76:SER:H	86:Ct:454:MET:HB3	1.72	0.55
1:A2:4943:U:OP1	42:AB:117:ARG:NH1	2.40	0.55
5:B1:379:C:OP1	27:BI:56:ARG:NH1	2.39	0.55
8:BK:65:ARG:NH2	18:Bd:21:CYS:O	2.40	0.55
30:BN:46:THR:HG23	30:BN:86:GLU:HG2	1.88	0.55
42:AB:33:PRO:HB3	42:AB:351:LEU:HA	1.89	0.55
61:AV:87:SER:HB3	62:AW:19:ARG:HH21	1.72	0.55
1:A2:2374:A:N6	1:A2:2799:C:O2	2.39	0.54
1:A2:2484:C:O2'	1:A2:2485:G:N2	2.41	0.54
5:B1:562:U:H2'	5:B1:563:G:H8	1.71	0.54
32:BV:37:ALA:HA	32:BV:50:PHE:HA	1.89	0.54
64:AY:8:THR:HB	64:AY:10:ASP:H	1.71	0.54
5:B1:385:G:N2	5:B1:388:U:OP2	2.41	0.54
19:Bf:107:LYS:HB3	19:Bf:115:SER:HB3	1.88	0.54
24:BE:80:VAL:HG13	24:BE:81:THR:HG23	1.89	0.54
65:AZ:90:PRO:HB2	65:AZ:117:LYS:HD2	1.87	0.54
1:A2:1879:C:OP1	56:AQ:2:GLY:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B1:1335:G:H1	5:B1:1492:U:H3	1.55	0.54
29:BL:80:MET:HE3	29:BL:122:ILE:HG13	1.90	0.54
63:AX:79:PHE:HB2	63:AX:99:ILE:HB	1.88	0.54
1:A2:944:G:N2	1:A2:2056:G:O2'	2.41	0.54
1:A2:1505:A:N3	1:A2:4351:C:O2'	2.40	0.54
1:A2:2313:C:OP2	43:AC:195:LYS:NZ	2.40	0.54
5:B1:1627:C:OP1	14:BT:83:GLN:NE2	2.39	0.54
7:BF:123:GLU:OE2	7:BF:204:ARG:NH2	2.40	0.54
39:A3:52:A:OP1	77:Al:21:ARG:NH1	2.40	0.54
42:AB:231:VAL:HG11	42:AB:251:VAL:HG23	1.89	0.54
45:AE:283:PRO:O	45:AE:284:HIS:ND1	2.40	0.54
59:AT:125:TRP:NE1	59:AT:127:GLN:OE1	2.39	0.54
66:Aa:95:THR:HG23	66:Aa:97:ALA:H	1.71	0.54
82:At:62:VAL:HG11	82:At:96:MET:HE1	1.89	0.54
83:Au:35:GLN:HB2	83:Au:205:TYR:HB2	1.88	0.54
1:A2:4287:A:H1'	44:AD:36:LEU:HD23	1.89	0.54
5:B1:1036:A:N3	5:B1:1844:U:O2'	2.40	0.54
5:B1:1413:G:H21	5:B1:1424:G:H1	1.56	0.54
20:Bg:296:GLN:NE2	20:Bg:312:VAL:O	2.40	0.54
37:Bb:23:ARG:NH2	37:Bb:27:SER:O	2.40	0.54
39:A3:52:A:H62	77:Al:27:ILE:HD13	1.73	0.54
49:AI:3:ARG:NE	49:AI:63:GLU:OE1	2.39	0.54
84:Aq:76:SER:O	84:Aq:117:ARG:NH2	2.41	0.54
1:A2:234:G:OP2	64:AY:45:ARG:NH2	2.41	0.54
1:A2:1385:C:OP1	67:Ab:55:LYS:NZ	2.41	0.54
15:BU:62:ARG:HG2	15:BU:81:GLN:HG2	1.89	0.54
20:Bg:11:LEU:HB2	20:Bg:307:VAL:HB	1.89	0.54
86:Ct:20:ARG:HB3	86:Ct:22:MET:HE3	1.89	0.54
34:BX:93:PHE:O	34:BX:140:ARG:NH1	2.40	0.54
56:AQ:88:ASP:OD1	56:AQ:112:ARG:NH2	2.41	0.54
58:AS:115:ALA:O	58:AS:118:ARG:NH1	2.41	0.54
83:Au:64:SER:HB3	83:Au:107:TYR:HD1	1.72	0.54
1:A2:1149:G:N3	1:A2:1150:C:O2'	2.40	0.54
1:A2:1450:C:OP1	66:Aa:132:ARG:NH2	2.40	0.54
1:A2:1483:C:H2'	56:AQ:68:ARG:HH22	1.73	0.54
1:A2:4720:U:H4'	54:AO:164:ALA:HB1	1.90	0.54
5:B1:560:A:H3'	28:BJ:171:GLY:HA3	1.90	0.54
1:A2:943:A:H5''	1:A2:944:G:H5'	1.90	0.54
2:Bv:18:G:O2'	2:Bv:57:G:N2	2.41	0.54
5:B1:1542:C:H5'	14:BT:11:GLN:HG2	1.90	0.54
19:Bf:105:TYR:O	19:Bf:116:ARG:NH2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:AB:59:GLU:HB2	42:AB:366:LYS:HE3	1.89	0.54
44:AD:155:THR:HG22	44:AD:179:ARG:HA	1.90	0.54
86:Ct:86:LEU:O	86:Ct:93:LYS:NZ	2.40	0.54
1:A2:369:G:OP2	75:Aj:52:LYS:NZ	2.41	0.54
1:A2:2245:C:O2	1:A2:2247:A:N6	2.41	0.54
5:B1:1261:C:O2	18:Bd:10:HIS:NE2	2.39	0.54
5:B1:1615:U:OP2	10:BP:43:ARG:NH2	2.37	0.54
5:B1:1783:C:N3	62:AW:73:ARG:NH2	2.56	0.54
14:BT:13:GLU:OE1	14:BT:16:ARG:NH2	2.40	0.54
63:AX:104:ALA:O	63:AX:134:LYS:NZ	2.41	0.54
83:Au:194:LEU:HD13	83:Au:196:LYS:H	1.72	0.54
1:A2:48:G:O6	53:AN:188:ARG:NH1	2.41	0.53
1:A2:67:C:N4	1:A2:319:U:O2'	2.39	0.53
1:A2:404:A:HO2'	1:A2:408:C:HO2'	1.57	0.53
1:A2:4264:U:H5''	59:AT:5:LYS:HE2	1.88	0.53
5:B1:641:A:O2'	5:B1:645:C:OP1	2.25	0.53
5:B1:1156:U:O4	23:BC:194:ARG:NH1	2.41	0.53
5:B1:1488:C:H3'	5:B1:1489:A:H4'	1.90	0.53
34:BX:25:LYS:HA	34:BX:28:LYS:HE2	1.90	0.53
1:A2:2365:U:H2'	1:A2:2366:G:H8	1.73	0.53
1:A2:4581:U:OP1	61:AV:15:ARG:NH1	2.41	0.53
5:B1:156:G:OP1	25:BG:2:LYS:NZ	2.42	0.53
5:B1:1474:A:H5''	11:BQ:121:VAL:HG13	1.90	0.53
1:A2:148:G:O6	47:AG:187:LYS:NZ	2.41	0.53
1:A2:2590:A:H5'	1:A2:2667:G:H4'	1.90	0.53
8:BK:25:LYS:H	8:BK:65:ARG:HG2	1.72	0.53
49:AI:98:ARG:HB3	49:AI:120:GLY:HA3	1.91	0.53
53:AN:116:LEU:HB3	53:AN:133:ILE:HG23	1.89	0.53
86:Ct:289:PHE:HA	86:Ct:292:LEU:HB2	1.91	0.53
1:A2:430:C:H2'	1:A2:431:G:H8	1.74	0.53
1:A2:654:G:H2'	1:A2:655:A:H8	1.73	0.53
1:A2:1309:A:OP2	1:A2:4407:U:O2'	2.25	0.53
1:A2:1831:A:N3	1:A2:2262:G:O2'	2.40	0.53
5:B1:165:G:H21	25:BG:4:ASN:HD21	1.57	0.53
14:BT:126:GLN:OE1	14:BT:129:ARG:NH2	2.42	0.53
43:AC:228:THR:OG1	43:AC:248:ARG:NH2	2.41	0.53
1:A2:646:G:O2'	56:AQ:115:ARG:NH2	2.42	0.53
1:A2:924:U:H5'	52:AM:46:ARG:HD2	1.90	0.53
27:BI:132:GLU:HB3	27:BI:134:GLU:HG2	1.89	0.53
42:AB:37:PRO:HA	42:AB:188:GLY:HA2	1.90	0.53
76:Ak:38:CYS:SG	76:Ak:39:SER:N	2.82	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:Ak:60:LEU:HD22	76:Ak:61:PRO:HD2	1.91	0.53
1:A2:29:G:O2'	53:AN:96:ARG:NH1	2.42	0.53
1:A2:1888:A:H4'	46:AF:223:LYS:HD2	1.89	0.53
1:A2:2382:A:OP1	72:Ag:10:ARG:NH1	2.42	0.53
1:A2:2450:G:H5''	47:AG:59:ARG:HE	1.74	0.53
5:B1:454:U:H5''	25:BG:94:ARG:HB2	1.89	0.53
5:B1:939:U:OP1	81:Ap:85:ARG:NH2	2.42	0.53
41:AA:221:LYS:HE2	41:AA:233:ARG:HH12	1.73	0.53
1:A2:2674:A:H5''	76:Ak:26:LYS:HE3	1.91	0.53
1:A2:4354:G:N2	1:A2:4357:U:O2	2.42	0.53
1:A2:4563:U:H2'	1:A2:4564:A:H8	1.74	0.53
5:B1:35:C:H5''	5:B1:579:C:H5''	1.90	0.53
5:B1:498:C:H5'	24:BE:7:LYS:HD3	1.91	0.53
12:BR:98:VAL:HG21	21:BA:19:LEU:HD12	1.90	0.53
53:AN:59:TYR:HB3	53:AN:133:ILE:HD11	1.91	0.53
1:A2:2569:G:N2	1:A2:2734:A:H62	2.06	0.53
1:A2:4714:U:H3'	71:Af:4:ARG:HD3	1.91	0.53
39:A3:63:U:O2'	73:Ah:52:LYS:NZ	2.41	0.53
44:AD:30:TYR:HA	44:AD:33:ARG:HB3	1.91	0.53
48:AH:92:MET:HG2	48:AH:181:VAL:HA	1.91	0.53
51:AL:25:TRP:HB3	51:AL:28:GLN:HB2	1.91	0.53
58:AS:1:MET:HG3	58:AS:43:ARG:HH21	1.74	0.53
66:Aa:6:ARG:HG3	66:Aa:8:THR:H	1.74	0.53
1:A2:274:G:OP2	53:AN:44:ARG:NH2	2.40	0.53
1:A2:3890:C:H4'	41:AA:207:VAL:HG12	1.90	0.53
5:B1:186:C:H2'	5:B1:187:G:H8	1.72	0.53
7:BF:21:GLY:H	7:BF:23:TRP:HD1	1.56	0.53
17:Bc:37:ASP:OD2	17:Bc:40:ARG:NH2	2.42	0.53
19:Bf:141:CYS:HB3	19:Bf:146:LEU:H	1.72	0.53
41:AA:158:ILE:HD12	41:AA:162:ASN:HD21	1.73	0.53
47:AG:32:PHE:HE1	65:AZ:55:ALA:HA	1.74	0.53
70:Ae:37:LYS:NZ	70:Ae:55:MET:SD	2.79	0.53
76:Ak:22:SER:HB3	76:Ak:37:ARG:HB3	1.91	0.53
83:Au:39:LYS:HD2	83:Au:40:ASN:HB2	1.89	0.53
1:A2:413:A:N3	1:A2:1315:C:O2'	2.39	0.53
1:A2:4056:G:H5'	47:AG:54:PHE:HB3	1.90	0.53
5:B1:1216:C:N4	5:B1:1342:U:OP1	2.42	0.53
6:BD:215:ASP:OD2	20:Bg:194:TYR:OH	2.25	0.53
11:BQ:58:LEU:HD22	11:BQ:108:ILE:HD11	1.91	0.53
20:Bg:24:THR:OG1	20:Bg:27:PHE:O	2.27	0.53
80:Ao:9:ARG:HG2	80:Ao:18:HIS:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:Ct:607:ARG:NH2	86:Ct:703:ASP:OD2	2.41	0.53
1:A2:932:U:OP2	46:AF:62:ARG:NH1	2.42	0.52
1:A2:2704:A:H5'	57:AR:97:ARG:HH21	1.74	0.52
5:B1:65:C:N4	25:BG:134:GLY:O	2.42	0.52
5:B1:104:A:H4'	27:BI:18:ARG:HH21	1.73	0.52
5:B1:681:U:H4'	34:BX:9:THR:HG22	1.91	0.52
5:B1:1010:G:H2'	5:B1:1011:A:H8	1.74	0.52
29:BL:85:THR:HA	29:BL:113:LEU:H	1.73	0.52
76:Ak:24:LYS:HB2	76:Ak:35:LYS:HB2	1.91	0.52
1:A2:1284:C:N4	1:A2:2294:G:OP1	2.36	0.52
1:A2:1864:G:N2	1:A2:2051:U:O2'	2.40	0.52
1:A2:1939:A:O2'	1:A2:2006:A:N1	2.41	0.52
5:B1:1092:G:OP1	30:BN:2:GLY:N	2.42	0.52
7:BF:40:ALA:HB3	7:BF:67:PRO:HA	1.90	0.52
22:BB:70:SER:OG	31:BO:128:ARG:NH1	2.38	0.52
84:Aq:14:TYR:O	84:Aq:62:LEU:HA	2.09	0.52
1:A2:1264:G:O2'	43:AC:322:LEU:O	2.28	0.52
1:A2:4255:U:O2'	80:Ao:81:ARG:NH2	2.42	0.52
5:B1:1378:A:H61	21:BA:109:THR:HG21	1.74	0.52
13:BS:10:GLN:HE21	13:BS:13:LEU:HD21	1.74	0.52
23:BC:182:CYS:HB2	33:BW:95:PRO:HB2	1.91	0.52
24:BE:100:ARG:NH2	24:BE:118:GLU:O	2.42	0.52
24:BE:100:ARG:HH21	24:BE:119:ALA:HA	1.75	0.52
46:AF:137:GLU:HB3	46:AF:226:HIS:HE1	1.74	0.52
59:AT:46:GLY:O	59:AT:49:GLN:NE2	2.42	0.52
85:AK:141:LEU:HD21	85:AK:171:GLU:HG3	1.91	0.52
1:A2:289:A:N6	1:A2:4323:U:O2'	2.38	0.52
1:A2:1666:A:OP2	51:AL:5:ARG:NH1	2.42	0.52
1:A2:4666:C:H4'	48:AH:129:ARG:HH22	1.74	0.52
1:A2:4722:G:H2'	1:A2:4723:G:H8	1.73	0.52
5:B1:1403:C:OP2	5:B1:1405:A:N6	2.42	0.52
39:A3:60:G:O6	73:Ah:62:ASN:ND2	2.43	0.52
42:AB:53:MET:O	42:AB:373:LYS:NZ	2.42	0.52
47:AG:180:PRO:HG3	47:AG:219:VAL:HG13	1.90	0.52
50:AJ:18:ARG:NH2	50:AJ:143:ASP:OD2	2.43	0.52
58:AS:82:LEU:HB2	58:AS:93:MET:HB3	1.91	0.52
86:Ct:451:ILE:HG23	86:Ct:458:VAL:HG13	1.92	0.52
1:A2:171:C:O2	73:Ah:112:ARG:NH1	2.42	0.52
1:A2:1739:U:H2'	1:A2:1740:G:H8	1.74	0.52
5:B1:943:U:O2'	31:BO:135:ILE:O	2.28	0.52
86:Ct:452:LEU:HD13	86:Ct:461:ILE:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:4147:G:OP1	41:AA:2:GLY:N	2.43	0.52
1:A2:4171:G:H4'	59:AT:12:ARG:HD2	1.91	0.52
1:A2:4549:G:N2	42:AB:15:GLY:O	2.37	0.52
5:B1:327:G:H3'	62:AW:120:GLN:HG3	1.92	0.52
5:B1:916:A:O2'	30:BN:73:ARG:NH1	2.43	0.52
39:A3:153:C:H2'	39:A3:154:G:H8	1.75	0.52
45:AE:140:LEU:HA	45:AE:191:GLN:HE22	1.75	0.52
68:Ac:50:ASN:HB2	68:Ac:76:GLY:H	1.74	0.52
1:A2:71:C:H5''	74:Ai:13:LYS:HE3	1.92	0.52
1:A2:193:C:O2	1:A2:218:C:O2'	2.28	0.52
1:A2:715:C:H2'	1:A2:716:G:H8	1.73	0.52
1:A2:1298:C:OP1	70:Ae:44:ARG:NH2	2.42	0.52
1:A2:2322:G:OP1	43:AC:52:TYR:OH	2.25	0.52
5:B1:1286:G:H22	9:BM:36:ARG:HB2	1.75	0.52
5:B1:1324:G:H1	5:B1:1504:U:H3	1.55	0.52
5:B1:1698:C:O2	6:BD:146:ARG:NH1	2.43	0.52
22:BB:88:THR:HA	22:BB:98:THR:HA	1.91	0.52
24:BE:247:THR:HG22	24:BE:249:ALA:H	1.74	0.52
34:BX:34:THR:O	34:BX:38:ALA:HB3	2.10	0.52
68:Ac:42:LYS:HG3	68:Ac:97:ILE:HB	1.91	0.52
73:Ah:79:LYS:HE3	73:Ah:84:ARG:HA	1.92	0.52
85:AK:28:PHE:HB2	85:AK:89:VAL:HB	1.92	0.52
1:A2:2386:G:N2	1:A2:2386:G:OP2	2.40	0.52
1:A2:2553:G:OP2	65:AZ:67:LYS:NZ	2.41	0.52
16:BZ:50:PHE:HB2	16:BZ:55:TYR:HB2	1.90	0.52
20:Bg:272:GLN:HE21	20:Bg:284:PRO:HG3	1.75	0.52
22:BB:105:LEU:HD13	22:BB:213:ARG:HA	1.91	0.52
24:BE:126:VAL:HG22	24:BE:139:LEU:HD21	1.91	0.52
31:BO:34:PHE:HB3	31:BO:41:PHE:HB2	1.91	0.52
39:A3:13:G:O2'	55:AP:121:LYS:O	2.28	0.52
69:Ad:64:ILE:HG22	69:Ad:106:VAL:HB	1.91	0.52
5:B1:1453:C:OP1	12:BR:48:ASN:ND2	2.42	0.52
5:B1:1680:G:OP1	7:BF:60:ARG:NH1	2.43	0.52
15:BU:68:THR:O	18:Bd:40:ARG:NH1	2.39	0.52
28:BJ:115:PHE:HB2	28:BJ:123:ILE:HD11	1.92	0.52
30:BN:13:GLN:OE1	37:Bb:21:LYS:NZ	2.43	0.52
39:A3:86:U:H3	73:Ah:7:ARG:HB2	1.75	0.52
55:AP:116:HIS:HB3	55:AP:149:ILE:HB	1.91	0.52
83:Au:63:PHE:HB2	83:Au:152:LYS:HA	1.92	0.52
84:Aq:151:ILE:HA	84:Aq:154:ASP:HB2	1.91	0.52
4:Bw:20:G:N2	4:Bw:59:U:OP1	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B1:957:A:H3'	5:B1:958:G:H21	1.74	0.52
5:B1:1139:C:O2'	5:B1:1140:G:O4'	2.27	0.52
5:B1:1270:G:O2'	5:B1:1301:A:N6	2.41	0.52
7:BF:63:LYS:HG2	7:BF:71:ARG:HH12	1.75	0.52
9:BM:89:VAL:HG21	9:BM:109:VAL:HG21	1.92	0.52
14:BT:59:SER:O	14:BT:63:HIS:ND1	2.41	0.52
20:Bg:20:GLN:HG3	20:Bg:68:ASP:HA	1.91	0.52
60:AU:22:THR:O	60:AU:109:SER:HA	2.10	0.52
64:AY:80:ILE:HD11	64:AY:104:VAL:HG21	1.92	0.52
65:AZ:10:VAL:HG22	65:AZ:24:VAL:HG12	1.92	0.52
86:Ct:751:CYS:HB3	86:Ct:755:VAL:HG23	1.92	0.52
1:A2:20:U:H3'	1:A2:21:G:H8	1.75	0.51
1:A2:370:A:H4'	43:AC:86:ARG:HD2	1.92	0.51
1:A2:4011:C:OP1	83:Au:98:LYS:NZ	2.43	0.51
1:A2:4048:C:OP1	53:AN:32:GLN:NE2	2.41	0.51
1:A2:4179:G:OP1	59:AT:55:LYS:NZ	2.41	0.51
21:BA:79:SER:O	21:BA:84:GLN:NE2	2.43	0.51
53:AN:73:ARG:HB3	53:AN:89:VAL:HG13	1.92	0.51
86:Ct:752:PRO:HA	86:Ct:781:MET:HA	1.92	0.51
1:A2:2278:G:O6	43:AC:188:ARG:NH2	2.44	0.51
1:A2:2609:U:OP2	60:AU:46:ARG:NH2	2.43	0.51
1:A2:2787:G:O2'	57:AR:60:ARG:NH1	2.43	0.51
5:B1:524:U:H3	5:B1:594:A:H62	1.56	0.51
30:BN:84:LEU:HD11	30:BN:88:LEU:HD23	1.91	0.51
39:A3:94:G:OP2	75:Aj:72:ARG:NH1	2.44	0.51
1:A2:1978:U:OP1	85:AK:48:ARG:NH2	2.42	0.51
1:A2:2278:G:OP2	43:AC:204:ARG:NH1	2.42	0.51
1:A2:2592:C:OP1	72:Ag:24:ARG:NH2	2.43	0.51
1:A2:2709:U:H5''	72:Ag:19:LYS:HD2	1.92	0.51
1:A2:2790:G:H4'	57:AR:82:LYS:HD3	1.91	0.51
5:B1:1587:G:OP1	5:B1:1587:G:N2	2.39	0.51
15:BU:65:THR:HB	15:BU:78:ASP:HB2	1.91	0.51
44:AD:52:ILE:HA	44:AD:147:ASP:HB3	1.92	0.51
48:AH:92:MET:HE2	48:AH:179:ILE:HG22	1.91	0.51
1:A2:379:A:H4'	1:A2:380:A:H5'	1.93	0.51
1:A2:2331:U:H1'	43:AC:96:CYS:HA	1.92	0.51
1:A2:3581:A:H2'	1:A2:3582:A:H8	1.75	0.51
5:B1:4:C:O2'	28:BJ:18:ARG:NH2	2.44	0.51
27:BI:76:THR:HG21	27:BI:104:ILE:HG12	1.93	0.51
41:AA:77:ILE:HD11	41:AA:128:ARG:HE	1.75	0.51
61:AV:13:LYS:HB2	61:AV:128:LEU:HD21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:Ad:24:GLU:OE1	69:Ad:85:ARG:NH2	2.43	0.51
86:Ct:27:HIS:HB3	86:Ct:30:HIS:CE1	2.45	0.51
1:A2:471:C:N4	1:A2:472:G:O6	2.43	0.51
1:A2:1493:U:OP2	66:Aa:6:ARG:NH1	2.43	0.51
1:A2:1668:C:OP1	67:Ab:19:ASN:ND2	2.42	0.51
5:B1:541:U:O4	5:B1:543:C:N4	2.44	0.51
42:AB:92:TYR:HB2	42:AB:159:VAL:HB	1.91	0.51
42:AB:254:ILE:HG23	42:AB:266:VAL:HG11	1.92	0.51
54:AO:37:ARG:HE	54:AO:108:ILE:HD11	1.76	0.51
79:An:22:GLN:OE1	79:An:25:LYS:NZ	2.42	0.51
1:A2:1491:C:H2'	1:A2:1492:G:H8	1.74	0.51
1:A2:3719:A:OP1	41:AA:243:THR:OG1	2.28	0.51
1:A2:4355:G:N2	1:A2:4358:A:OP2	2.41	0.51
1:A2:4547:U:H2'	1:A2:4548:G:H8	1.76	0.51
6:BD:23:GLU:HA	6:BD:26:THR:HG22	1.91	0.51
20:Bg:174:VAL:HB	20:Bg:188:HIS:HB2	1.92	0.51
23:BC:173:LYS:HB3	32:BV:3:ASN:HA	1.93	0.51
42:AB:378:ARG:HG3	62:AW:32:LEU:HD21	1.92	0.51
43:AC:84:THR:HG22	43:AC:86:ARG:H	1.75	0.51
51:AL:162:LYS:O	66:Aa:105:ARG:NH2	2.43	0.51
57:AR:178:GLN:NE2	57:AR:182:GLU:OE1	2.43	0.51
1:A2:447:G:O6	1:A2:1277:A:N6	2.43	0.51
1:A2:2868:G:OP1	57:AR:75:HIS:ND1	2.44	0.51
4:Bw:22:G:H2'	4:Bw:23:A:H8	1.75	0.51
5:B1:563:G:H1	5:B1:592:C:H5	1.59	0.51
5:B1:1528:G:O2'	5:B1:1666:C:OP1	2.28	0.51
20:Bg:195:LEU:HA	20:Bg:211:GLY:HA3	1.91	0.51
53:AN:42:PRO:HG3	53:AN:61:ILE:HG13	1.92	0.51
86:Ct:582:THR:HB	86:Ct:741:MET:HE2	1.93	0.51
1:A2:4187:G:HO2'	1:A2:4235:A:HO2'	1.59	0.51
1:A2:4954:C:OP1	69:Ad:32:ARG:NH1	2.43	0.51
5:B1:511:U:O2'	5:B1:576:A:N6	2.43	0.51
7:BF:167:LYS:NZ	16:BZ:75:GLU:OE1	2.41	0.51
10:BP:41:GLN:HE22	10:BP:113:GLY:HA2	1.75	0.51
58:AS:16:CYS:SG	58:AS:17:LEU:N	2.83	0.51
1:A2:220:G:O2'	1:A2:239:U:O2	2.27	0.51
1:A2:274:G:N2	1:A2:300:A:OP2	2.40	0.51
1:A2:1975:C:H2'	1:A2:1976:G:H8	1.76	0.51
12:BR:84:TYR:O	21:BA:205:ARG:NH2	2.44	0.51
21:BA:85:ARG:HH22	21:BA:205:ARG:HE	1.58	0.51
25:BG:159:ARG:HG2	25:BG:173:ALA:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BH:154:ILE:HB	26:BH:185:VAL:HG12	1.91	0.51
34:BX:46:HIS:HB3	34:BX:101:LEU:HD11	1.92	0.51
60:AU:60:VAL:HG21	60:AU:76:VAL:H	1.76	0.51
1:A2:200:U:C2	1:A2:208:G:N1	2.79	0.51
1:A2:2644:U:H5''	57:AR:107:ARG:HH21	1.75	0.51
1:A2:2652:G:H5''	1:A2:2653:A:H3'	1.93	0.51
1:A2:4143:U:O2'	41:AA:226:ARG:NH2	2.44	0.51
10:BP:81:ARG:NH2	10:BP:117:GLY:O	2.44	0.51
31:BO:96:LYS:NZ	31:BO:130:GLU:OE1	2.44	0.51
42:AB:262:VAL:HG11	42:AB:268:ARG:HE	1.76	0.51
58:AS:8:ARG:HD3	58:AS:66:GLN:HE22	1.74	0.51
81:Ap:15:GLY:O	81:Ap:23:ARG:NH1	2.44	0.51
1:A2:21:G:H5''	75:Aj:43:ARG:HG2	1.93	0.50
1:A2:1712:U:H4'	59:AT:100:LYS:HB2	1.92	0.50
1:A2:2856:G:N2	1:A2:3795:A:O2'	2.44	0.50
1:A2:4868:A:H5''	42:AB:95:THR:HG22	1.93	0.50
5:B1:602:G:H3'	5:B1:603:C:H2'	1.92	0.50
13:BS:138:THR:HA	13:BS:141:ARG:HE	1.76	0.50
28:BJ:122:SER:O	28:BJ:125:HIS:N	2.42	0.50
46:AF:116:GLN:HE22	46:AF:212:LYS:HG2	1.76	0.50
1:A2:54:G:OP1	75:Aj:43:ARG:NH1	2.44	0.50
1:A2:947:A:N6	1:A2:1266:G:O6	2.45	0.50
1:A2:4897:C:O2	45:AE:239:LYS:NZ	2.44	0.50
5:B1:453:C:O2'	25:BG:92:ARG:O	2.28	0.50
5:B1:663:C:O2'	23:BC:227:ARG:NH2	2.44	0.50
13:BS:54:LYS:NZ	13:BS:58:GLU:O	2.42	0.50
28:BJ:54:ARG:NH2	28:BJ:100:LEU:O	2.44	0.50
43:AC:133:LEU:HD13	82:At:6:GLN:HE21	1.76	0.50
47:AG:190:LEU:HD13	47:AG:193:LEU:HD21	1.93	0.50
57:AR:20:LYS:HG3	57:AR:21:LYS:HG3	1.93	0.50
61:AV:21:PRO:HA	61:AV:54:ALA:HA	1.92	0.50
65:AZ:83:THR:HG23	65:AZ:85:TYR:H	1.77	0.50
1:A2:1292:C:O2'	71:Af:21:GLN:NE2	2.35	0.50
1:A2:2499:C:H2'	1:A2:2500:G:H8	1.76	0.50
5:B1:525:A:H2'	5:B1:526:A:H8	1.74	0.50
7:BF:55:ARG:NE	11:BQ:123:ASP:OD2	2.45	0.50
40:A4:76:U:H2'	40:A4:77:A:H8	1.76	0.50
46:AF:232:ASP:OD1	46:AF:236:ARG:NH2	2.44	0.50
60:AU:89:LYS:HG2	60:AU:93:LYS:HE2	1.92	0.50
1:A2:296:C:OP1	53:AN:68:ARG:NH1	2.39	0.50
1:A2:1836:G:O6	1:A2:1861:G:N2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:2340:G:N2	1:A2:3831:A:OP2	2.40	0.50
21:BA:77:ILE:HB	21:BA:124:VAL:HG12	1.93	0.50
39:A3:19:C:H2'	39:A3:20:A:H8	1.77	0.50
50:AJ:18:ARG:HB3	50:AJ:133:VAL:HG23	1.94	0.50
85:AK:122:THR:HG22	85:AK:159:GLN:HG2	1.93	0.50
86:Ct:745:TYR:HB2	86:Ct:814:PHE:HA	1.93	0.50
1:A2:2288:G:O2'	39:A3:18:U:O2	2.29	0.50
1:A2:3586:G:OP2	62:AW:48:GLN:NE2	2.44	0.50
5:B1:1473:G:N2	5:B1:1473:G:OP2	2.45	0.50
8:BK:24:LYS:O	8:BK:42:ASN:ND2	2.37	0.50
12:BR:62:GLN:HE21	20:Bg:280:LYS:HD3	1.76	0.50
19:Bf:139:HIS:HB2	19:Bf:148:TYR:HB3	1.93	0.50
42:AB:165:HIS:HB2	42:AB:178:ALA:HB1	1.94	0.50
45:AE:261:ILE:HA	45:AE:267:LEU:HD23	1.94	0.50
58:AS:9:GLU:OE2	58:AS:31:ARG:NE	2.45	0.50
68:Ac:51:ASN:ND2	68:Ac:77:ASN:OD1	2.40	0.50
1:A2:446:A:O2'	1:A2:1276:G:N2	2.44	0.50
1:A2:1647:C:O2'	56:AQ:10:ASP:OD2	2.29	0.50
1:A2:4932:C:O2'	42:AB:174:ARG:NH2	2.44	0.50
5:B1:28:U:H2'	5:B1:29:G:H8	1.77	0.50
5:B1:308:G:OP1	27:BI:53:LYS:NZ	2.43	0.50
22:BB:46:LYS:NZ	31:BO:19:PRO:O	2.44	0.50
48:AH:23:ARG:HE	48:AH:39:ASN:HA	1.76	0.50
52:AM:111:LYS:HA	52:AM:114:LYS:HE3	1.94	0.50
56:AQ:122:THR:OG1	56:AQ:124:ASP:OD1	2.26	0.50
1:A2:1298:C:N4	1:A2:1299:G:O6	2.44	0.50
1:A2:3939:U:H2'	1:A2:3940:G:H8	1.77	0.50
5:B1:522:A:O3'	28:BJ:131:ARG:NH2	2.41	0.50
5:B1:1611:G:OP2	13:BS:121:ARG:NH2	2.44	0.50
5:B1:1655:C:H2'	5:B1:1656:G:H8	1.77	0.50
19:Bf:121:CYS:HA	19:Bf:132:MET:HE3	1.93	0.50
22:BB:62:LEU:HD13	22:BB:65:ARG:HD2	1.93	0.50
22:BB:129:THR:HB	22:BB:180:ASP:HA	1.93	0.50
41:AA:207:VAL:HG23	41:AA:208:GLU:HG3	1.93	0.50
44:AD:146:LEU:HD11	44:AD:163:LEU:HG	1.92	0.50
51:AL:126:LEU:HD13	73:Ah:117:ARG:HH21	1.75	0.50
70:Ae:40:GLY:O	70:Ae:46:ARG:NE	2.43	0.50
85:AK:39:GLN:HE22	85:AK:186:GLY:HA2	1.76	0.50
1:A2:63:G:OP2	53:AN:169:ARG:NH1	2.44	0.50
1:A2:2340:G:O2'	1:A2:3830:G:O6	2.28	0.50
1:A2:4367:G:OP2	49:AI:7:ARG:NH2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B1:406:U:O2'	5:B1:408:A:OP1	2.29	0.50
5:B1:1544:C:O2'	11:BQ:80:GLN:NE2	2.45	0.50
43:AC:315:LYS:HD2	46:AF:168:ALA:HB1	1.93	0.50
45:AE:177:GLY:HA3	45:AE:184:VAL:HB	1.94	0.50
52:AM:82:ILE:O	52:AM:86:TRP:HB2	2.12	0.50
54:AO:173:GLN:OE1	54:AO:176:ARG:NH2	2.41	0.50
69:Ad:70:LYS:O	69:Ad:74:ALA:HB2	2.11	0.50
1:A2:1619:A:H1'	75:Aj:11:ARG:HH21	1.77	0.50
1:A2:4876:C:H2'	1:A2:4877:G:C8	2.46	0.50
20:Bg:8:ARG:HB3	20:Bg:309:VAL:HG23	1.93	0.50
22:BB:49:VAL:HG22	22:BB:62:LEU:HD21	1.94	0.50
24:BE:195:ILE:HA	24:BE:210:VAL:HG12	1.94	0.50
53:AN:116:LEU:HD22	53:AN:135:ILE:HD11	1.93	0.50
62:AW:96:GLN:O	62:AW:101:ARG:NH1	2.44	0.50
1:A2:1347:U:O4	51:AL:36:ARG:NH2	2.45	0.49
1:A2:1499:G:OP1	51:AL:19:GLN:NE2	2.45	0.49
1:A2:2500:G:H4'	72:Ag:26:PRO:HD2	1.93	0.49
5:B1:1863:A:OP2	36:Ba:4:LYS:NZ	2.41	0.49
7:BF:126:THR:OG1	17:Bc:26:GLN:NE2	2.45	0.49
13:BS:101:ASN:O	13:BS:105:ASN:ND2	2.44	0.49
26:BH:193:GLN:HE22	37:Bb:12:PRO:HB3	1.77	0.49
47:AG:136:LEU:HD13	47:AG:202:VAL:HG13	1.94	0.49
49:AI:57:TYR:OH	49:AI:128:ARG:NH2	2.44	0.49
84:Aq:108:GLU:HA	84:Aq:111:ASN:HD22	1.77	0.49
1:A2:1338:G:OP1	56:AQ:108:ARG:NH1	2.43	0.49
1:A2:4567:A:O2'	86:Ct:27:HIS:NE2	2.35	0.49
5:B1:67:C:OP2	25:BG:172:LYS:NZ	2.43	0.49
21:BA:36:GLN:NE2	32:BV:67:ASP:OD1	2.44	0.49
21:BA:184:ARG:HD3	21:BA:191:ARG:HD2	1.94	0.49
45:AE:197:THR:HG22	45:AE:199:THR:H	1.77	0.49
48:AH:23:ARG:NH2	48:AH:39:ASN:OD1	2.37	0.49
52:AM:24:LEU:HB2	52:AM:43:THR:HG21	1.93	0.49
86:Ct:413:PHE:HZ	86:Ct:469:ILE:HD12	1.76	0.49
1:A2:1071:C:O2'	46:AF:74:MET:SD	2.70	0.49
1:A2:1315:C:H2'	1:A2:1316:A:H8	1.77	0.49
1:A2:2626:A:H62	1:A2:2665:G:H8	1.61	0.49
1:A2:4943:U:H4'	42:AB:175:GLN:HG3	1.93	0.49
47:AG:165:GLU:OE1	53:AN:26:ARG:NH2	2.45	0.49
53:AN:31:ARG:NH1	53:AN:124:ASP:OD2	2.45	0.49
1:A2:153:G:OP1	73:Ah:109:ARG:NH1	2.36	0.49
1:A2:2336:G:OP1	55:AP:121:LYS:NZ	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B1:148:U:H2'	5:B1:149:A:H8	1.77	0.49
5:B1:292:A:O2'	29:BL:39:ASN:O	2.30	0.49
5:B1:1172:U:H4'	79:An:10:MET:HE2	1.94	0.49
5:B1:1222:G:H5''	7:BF:78:MET:HE3	1.95	0.49
27:BI:100:CYS:HB3	27:BI:175:ILE:HD12	1.94	0.49
50:AJ:95:ARG:HH12	50:AJ:97:ASN:HD21	1.59	0.49
73:Ah:96:ASN:HB3	73:Ah:99:GLU:H	1.77	0.49
1:A2:16:G:H5''	63:AX:60:TYR:HE1	1.77	0.49
1:A2:1923:A:OP2	1:A2:2021:A:N6	2.40	0.49
15:BU:67:LYS:HA	18:Bd:44:ARG:HD2	1.93	0.49
44:AD:42:ASN:ND2	59:AT:69:GLN:OE1	2.37	0.49
46:AF:199:LYS:HG3	46:AF:200:ARG:HG2	1.94	0.49
51:AL:144:LEU:HD21	73:Ah:122:LYS:H	1.77	0.49
1:A2:951:A:H5''	82:At:98:ARG:HH11	1.78	0.49
5:B1:1192:U:OP2	34:BX:119:ARG:NH2	2.39	0.49
5:B1:1275:G:N1	5:B1:1506:A:OP2	2.43	0.49
5:B1:1454:A:H2'	12:BR:3:ARG:HD3	1.93	0.49
5:B1:1472:C:OP2	5:B1:1473:G:N1	2.46	0.49
6:BD:138:VAL:HG22	6:BD:184:ILE:HG22	1.94	0.49
8:BK:30:PRO:HB3	18:Bd:12:ARG:HD2	1.95	0.49
21:BA:184:ARG:HD3	21:BA:191:ARG:HA	1.94	0.49
35:BY:7:ILE:HG12	35:BY:27:VAL:HG22	1.95	0.49
1:A2:1845:G:OP2	49:AI:14:ASN:ND2	2.45	0.49
5:B1:941:C:H2'	5:B1:942:G:H8	1.76	0.49
5:B1:989:C:O2	36:Ba:32:LYS:NZ	2.46	0.49
5:B1:1241:A:OP1	19:Bf:81:LYS:NZ	2.44	0.49
41:AA:113:VAL:HG12	41:AA:166:VAL:HA	1.94	0.49
1:A2:3841:C:H2'	1:A2:3842:A:H8	1.78	0.49
5:B1:745:C:N3	5:B1:746:C:N4	2.61	0.49
39:A3:26:C:O2'	43:AC:54:VAL:O	2.27	0.49
1:A2:4061:G:H2'	1:A2:4062:G:H8	1.78	0.49
5:B1:1864:U:H3'	36:Ba:5:ARG:HH21	1.77	0.49
20:Bg:119:GLN:HB3	20:Bg:131:LEU:HD21	1.94	0.49
40:A4:64:G:H2'	40:A4:65:G:H8	1.78	0.49
52:AM:33:GLN:HB2	58:AS:145:PHE:HZ	1.78	0.49
65:AZ:95:VAL:HG11	65:AZ:113:GLU:HG3	1.94	0.49
86:Ct:16:LYS:HE2	86:Ct:466:CYS:H	1.78	0.49
86:Ct:163:ALA:HA	86:Ct:167:LEU:HB3	1.95	0.49
86:Ct:580:ARG:HB3	86:Ct:698:ARG:HB3	1.94	0.49
1:A2:306:G:H1	1:A2:319:U:H3	1.59	0.49
1:A2:920:G:H21	1:A2:926:G:H5''	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B1:913:A:N6	26:BH:119:SER:O	2.42	0.49
7:BF:125:SER:HA	7:BF:138:ALA:HA	1.94	0.49
11:BQ:58:LEU:HB3	11:BQ:62:ARG:HH11	1.78	0.49
28:BJ:169:ARG:HG2	28:BJ:172:ARG:HE	1.76	0.49
40:A4:99:G:OP2	58:AS:55:LYS:NZ	2.45	0.49
42:AB:56:ILE:HD12	42:AB:76:VAL:HG21	1.94	0.49
42:AB:292:LEU:HD13	42:AB:293:ILE:HG13	1.95	0.49
49:AI:185:VAL:HG12	49:AI:190:LEU:HB2	1.95	0.49
53:AN:73:ARG:HH12	53:AN:86:HIS:HB3	1.78	0.49
53:AN:193:ARG:NH1	53:AN:197:THR:OG1	2.45	0.49
66:Aa:99:PRO:HG2	66:Aa:122:VAL:HG12	1.94	0.49
71:Af:11:PHE:HE1	71:Af:26:ALA:HB1	1.78	0.49
1:A2:1805:G:O3'	44:AD:45:ASN:ND2	2.43	0.48
1:A2:1913:A:H61	1:A2:2037:G:H22	1.61	0.48
1:A2:4612:G:H4'	1:A2:4966:C:H4'	1.94	0.48
12:BR:85:VAL:HA	21:BA:205:ARG:HH22	1.78	0.48
25:BG:2:LYS:O	25:BG:108:VAL:HA	2.13	0.48
36:Ba:53:ILE:O	36:Ba:57:SER:HB2	2.13	0.48
52:AM:11:ARG:HE	52:AM:61:ILE:HG22	1.77	0.48
65:AZ:68:ILE:HG21	65:AZ:119:GLU:HB2	1.94	0.48
66:Aa:24:LYS:HB3	66:Aa:26:ARG:HE	1.78	0.48
80:Ao:44:LYS:HE2	80:Ao:52:THR:HB	1.94	0.48
83:Au:12:GLU:OE1	83:Au:15:ARG:NH2	2.46	0.48
85:AK:111:ALA:HB2	85:AK:182:PRO:HG3	1.96	0.48
1:A2:66:A:O2'	1:A2:320:C:O2	2.31	0.48
1:A2:957:G:N2	1:A2:1262:A:OP2	2.46	0.48
1:A2:1966:G:N2	1:A2:1984:G:O2'	2.43	0.48
5:B1:291:G:OP2	24:BE:200:ARG:NH2	2.45	0.48
5:B1:1203:G:O2'	23:BC:116:THR:O	2.31	0.48
5:B1:1216:C:H5''	5:B1:1217:A:H5''	1.95	0.48
7:BF:86:LYS:HA	7:BF:89:THR:HG22	1.96	0.48
16:BZ:89:GLN:NE2	16:BZ:109:TYR:OH	2.47	0.48
20:Bg:170:TRP:NE1	20:Bg:195:LEU:O	2.46	0.48
29:BL:24:LEU:HD12	29:BL:25:LEU:HG	1.94	0.48
31:BO:146:ARG:NH1	36:Ba:29:CYS:SG	2.86	0.48
40:A4:89:G:N2	49:AI:11:TYR:OH	2.46	0.48
86:Ct:22:MET:O	86:Ct:102:LEU:HA	2.13	0.48
86:Ct:144:ARG:NH1	86:Ct:781:MET:SD	2.87	0.48
1:A2:1914:G:H2'	1:A2:1915:A:C8	2.48	0.48
1:A2:2531:G:N2	1:A2:2746:U:O4	2.46	0.48
20:Bg:10:THR:HG22	20:Bg:308:ARG:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AG:152:ALA:HA	47:AG:205:THR:HG22	1.95	0.48
49:AI:38:ARG:HE	49:AI:83:ASP:HB3	1.78	0.48
1:A2:1291:C:O2'	71:Af:94:ALA:O	2.31	0.48
1:A2:3810:G:N2	1:A2:3814:C:O2'	2.45	0.48
1:A2:4208:G:H2'	1:A2:4209:G:H8	1.79	0.48
33:BW:2:VAL:HG12	33:BW:3:ARG:HG2	1.94	0.48
40:A4:6:C:OP2	44:AD:22:ARG:NH2	2.47	0.48
65:AZ:21:ARG:NH1	65:AZ:47:ASP:O	2.46	0.48
1:A2:1564:U:H2'	1:A2:1565:A:H8	1.79	0.48
5:B1:988:C:H5''	22:BB:116:LYS:HA	1.96	0.48
5:B1:1218:C:O2'	17:Bc:24:GLN:NE2	2.46	0.48
26:BH:64:VAL:HB	26:BH:96:ALA:HA	1.96	0.48
40:A4:9:C:OP2	40:A4:10:C:N4	2.36	0.48
54:AO:54:TYR:OH	54:AO:73:PHE:O	2.30	0.48
56:AQ:155:ALA:O	56:AQ:163:THR:OG1	2.31	0.48
86:Ct:349:ALA:O	86:Ct:353:MET:CB	2.61	0.48
1:A2:494:G:O2'	1:A2:498:G:OP1	2.31	0.48
5:B1:486:A:O2'	5:B1:487:U:O2	2.28	0.48
5:B1:1135:C:OP2	36:Ba:6:ARG:NH1	2.46	0.48
5:B1:1260:A:H2	5:B1:1617:G:N2	2.04	0.48
39:A3:86:U:O2'	73:Ah:5:LYS:NZ	2.46	0.48
47:AG:156:VAL:HB	47:AG:202:VAL:HB	1.95	0.48
52:AM:101:LYS:HA	52:AM:104:MET:HG3	1.96	0.48
73:Ah:40:ALA:HB1	73:Ah:43:LYS:HD2	1.94	0.48
86:Ct:604:MET:HG2	86:Ct:704:VAL:HG22	1.95	0.48
1:A2:693:U:H3'	1:A2:694:G:H21	1.79	0.48
1:A2:1706:G:N2	1:A2:1857:U:OP1	2.45	0.48
1:A2:2437:C:OP1	53:AN:67:ARG:NH2	2.46	0.48
1:A2:2642:G:H4'	57:AR:117:ARG:HE	1.78	0.48
5:B1:878:G:H1	5:B1:909:G:H1	1.61	0.48
27:BI:100:CYS:SG	27:BI:101:ILE:N	2.86	0.48
41:AA:30:ARG:O	41:AA:163:ARG:NH2	2.47	0.48
42:AB:200:ARG:HH22	42:AB:205:VAL:HG22	1.78	0.48
63:AX:110:LYS:NZ	63:AX:121:VAL:O	2.46	0.48
80:Ao:36:GLN:HE21	80:Ao:40:ARG:HH22	1.62	0.48
1:A2:3863:U:O2	55:AP:69:ARG:NH2	2.47	0.48
21:BA:65:ILE:HD11	21:BA:123:VAL:HG21	1.95	0.48
25:BG:2:LYS:HB2	25:BG:108:VAL:HG22	1.96	0.48
25:BG:223:LYS:O	25:BG:227:GLN:NE2	2.47	0.48
54:AO:9:LEU:HD23	54:AO:118:MET:HB2	1.95	0.48
61:AV:43:LYS:HD3	61:AV:62:MET:HE2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:AX:89:LYS:HD2	63:AX:93:ASN:HD22	1.79	0.48
1:A2:1599:G:O3'	75:Aj:12:ARG:NH2	2.47	0.48
1:A2:1723:G:O6	40:A4:103:A:O2'	2.26	0.48
1:A2:4436:A:OP2	1:A2:4438:C:N4	2.47	0.48
1:A2:4689:A:HO2'	1:A2:4924:A:HO2'	1.62	0.48
5:B1:5:U:H2'	5:B1:6:G:H8	1.79	0.48
5:B1:107:A:H2'	5:B1:108:G:H8	1.79	0.48
5:B1:520:A:O2'	5:B1:825:A:N3	2.45	0.48
5:B1:574:A:H4'	35:BY:89:HIS:HB2	1.96	0.48
5:B1:1156:U:OP1	33:BW:71:LYS:NZ	2.43	0.48
16:BZ:92:LEU:HD11	16:BZ:99:LEU:HD23	1.95	0.48
47:AG:143:VAL:HG21	47:AG:201:THR:HB	1.96	0.48
48:AH:36:ARG:HH12	48:AH:76:HIS:CD2	2.32	0.48
70:Ae:12:ILE:HG23	70:Ae:66:THR:HB	1.96	0.48
81:Ap:42:CYS:SG	81:Ap:59:SER:OG	2.72	0.48
85:AK:120:GLU:HG2	85:AK:162:LYS:HA	1.96	0.48
1:A2:62:A:N3	1:A2:77:U:O2'	2.39	0.48
1:A2:455:G:O6	1:A2:687:A:N1	2.46	0.48
1:A2:2653:A:N6	81:Ap:41:PHE:O	2.47	0.48
1:A2:2827:G:O2'	1:A2:3809:U:O4	2.30	0.48
5:B1:1139:C:O2'	5:B1:1140:G:O5'	2.30	0.48
5:B1:1281:G:H2'	5:B1:1282:A:H8	1.79	0.48
5:B1:1452:A:H61	5:B1:1473:G:H8	1.62	0.48
15:BU:94:PRO:HD2	15:BU:97:ILE:HD12	1.95	0.48
20:Bg:77:PHE:HB3	20:Bg:89:LEU:HD11	1.95	0.48
24:BE:87:MET:HE2	24:BE:123:LEU:H	1.77	0.48
40:A4:92:C:H2'	40:A4:93:G:H8	1.79	0.48
41:AA:57:PRO:HG2	41:AA:78:ALA:HB3	1.94	0.48
50:AJ:35:ARG:HD3	50:AJ:123:ILE:HA	1.96	0.48
64:AY:17:ARG:O	64:AY:21:ALA:HB2	2.14	0.48
69:Ad:19:GLU:HB2	69:Ad:90:ARG:HH21	1.77	0.48
1:A2:35:U:H4'	1:A2:1507:A:H2	1.79	0.47
1:A2:225:C:OP1	64:AY:11:ARG:NH1	2.47	0.47
1:A2:1845:G:O2'	49:AI:118:ALA:O	2.26	0.47
5:B1:1015:U:O2	37:Bb:51:GLN:NE2	2.46	0.47
5:B1:1157:G:O2'	33:BW:74:VAL:O	2.32	0.47
5:B1:1455:A:N6	5:B1:1456:G:O6	2.46	0.47
25:BG:14:LYS:HD3	25:BG:124:LEU:HD21	1.95	0.47
25:BG:143:LYS:HD2	62:AW:80:ARG:HD3	1.96	0.47
41:AA:28:ARG:HB3	41:AA:123:ARG:HB3	1.96	0.47
60:AU:60:VAL:HB	60:AU:75:GLU:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:At:61:VAL:HG21	82:At:79:ARG:HH21	1.79	0.47
1:A2:1303:U:O2'	1:A2:1872:A:N1	2.37	0.47
1:A2:1663:G:H2'	1:A2:1664:A:H8	1.79	0.47
1:A2:1911:U:OP2	54:AO:49:ARG:NH2	2.39	0.47
1:A2:2002:G:H4'	85:AK:85:ASN:H	1.79	0.47
1:A2:2274:C:O2'	43:AC:45:ARG:NH2	2.47	0.47
1:A2:2304:C:O2'	70:Ae:124:ASN:ND2	2.47	0.47
1:A2:3635:G:H2'	1:A2:3636:G:H8	1.79	0.47
5:B1:692:G:H2'	5:B1:693:A:H8	1.78	0.47
5:B1:1391:C:O2'	15:BU:83:ARG:NH2	2.47	0.47
5:B1:1624:U:N3	5:B1:1662:U:O2	2.47	0.47
14:BT:18:LEU:HD13	14:BT:134:ILE:HG21	1.96	0.47
18:Bd:21:CYS:SG	18:Bd:22:ARG:N	2.87	0.47
22:BB:170:GLU:O	22:BB:173:THR:OG1	2.31	0.47
23:BC:183:LYS:HA	23:BC:195:LEU:O	2.14	0.47
41:AA:55:GLY:HA3	41:AA:174:ARG:HH11	1.79	0.47
43:AC:186:SER:HB2	43:AC:204:ARG:HE	1.78	0.47
46:AF:92:VAL:O	46:AF:120:GLY:HA2	2.14	0.47
56:AQ:63:LEU:HG	56:AQ:112:ARG:HH22	1.80	0.47
85:AK:66:ARG:HH12	85:AK:71:ASN:HB2	1.79	0.47
85:AK:101:MET:HG3	85:AK:206:ILE:HG21	1.95	0.47
85:AK:107:VAL:HB	85:AK:184:SER:HB2	1.96	0.47
86:Ct:216:SER:OG	86:Ct:217:GLY:N	2.47	0.47
1:A2:1621:U:N3	1:A2:1625:A:O2'	2.48	0.47
1:A2:1895:C:H4'	54:AO:89:PRO:HD3	1.97	0.47
1:A2:2004:C:O2'	1:A2:4656:G:N2	2.44	0.47
1:A2:2054:C:H5''	46:AF:212:LYS:HB3	1.96	0.47
1:A2:4139:C:H2'	1:A2:4140:A:H8	1.79	0.47
5:B1:1535:U:O4	7:BF:159:ARG:NE	2.44	0.47
5:B1:1536:G:H4'	7:BF:81:ARG:HH21	1.78	0.47
5:B1:1552:G:OP2	5:B1:1578:U:N3	2.42	0.47
5:B1:1862:G:O6	36:Ba:34:LYS:NZ	2.44	0.47
6:BD:106:ARG:HG3	6:BD:175:VAL:HG22	1.95	0.47
9:BM:45:ARG:HE	9:BM:72:HIS:HD2	1.60	0.47
20:Bg:38:LYS:HE2	20:Bg:64:HIS:HA	1.96	0.47
40:A4:15:C:H2'	40:A4:16:A:H8	1.78	0.47
41:AA:192:LYS:HB3	41:AA:193:ARG:HE	1.78	0.47
45:AE:162:VAL:HG12	45:AE:175:VAL:HG12	1.97	0.47
80:Ao:22:LYS:HG3	80:Ao:73:VAL:HG22	1.95	0.47
85:AK:132:PRO:HA	85:AK:133:GLU:HA	1.54	0.47
1:A2:1654:U:OP1	67:Ab:7:HIS:ND1	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:2390:C:H2'	1:A2:2391:A:H8	1.79	0.47
1:A2:2718:C:N4	41:AA:177:LYS:O	2.47	0.47
1:A2:3660:G:O2'	1:A2:3789:U:OP2	2.33	0.47
1:A2:3686:U:OP1	4:Bw:3:G:O2'	2.31	0.47
1:A2:4385:U:H2'	78:Am:97:ARG:HD3	1.96	0.47
5:B1:284:C:OP1	5:B1:891:G:O2'	2.30	0.47
5:B1:486:A:H1'	5:B1:513:G:H22	1.79	0.47
10:BP:41:GLN:HG2	10:BP:84:ILE:HG21	1.97	0.47
11:BQ:32:ILE:HD12	11:BQ:39:LEU:HD22	1.95	0.47
14:BT:70:ALA:HB3	14:BT:121:ARG:HE	1.79	0.47
38:Be:28:LYS:HE3	38:Be:32:ALA:HB1	1.96	0.47
53:AN:73:ARG:NH1	53:AN:86:HIS:O	2.48	0.47
64:AY:2:LYS:HD2	64:AY:7:VAL:HG13	1.96	0.47
64:AY:32:SER:OG	64:AY:104:VAL:O	2.31	0.47
1:A2:4387:G:OP1	78:Am:100:TYR:OH	2.32	0.47
2:Bv:9:A:O2'	2:Bv:45:G:N2	2.47	0.47
5:B1:1277:C:H2'	5:B1:1278:A:H8	1.79	0.47
5:B1:1550:G:O2'	5:B1:1558:C:O2	2.28	0.47
34:BX:39:ASN:HD22	34:BX:108:LYS:HE2	1.79	0.47
44:AD:211:LEU:HB3	44:AD:219:TYR:HB2	1.96	0.47
85:AK:161:ILE:HD13	85:AK:167:VAL:HG22	1.95	0.47
1:A2:270:C:O2	74:Ai:26:HIS:NE2	2.42	0.47
1:A2:2763:C:N4	77:Al:3:SER:OG	2.47	0.47
1:A2:4722:G:N7	58:AS:171:ARG:NH1	2.62	0.47
5:B1:1648:G:N2	5:B1:1675:A:OP2	2.37	0.47
43:AC:326:LEU:HD21	43:AC:333:LYS:HB2	1.96	0.47
59:AT:85:LEU:HB2	59:AT:87:LYS:HE3	1.96	0.47
69:Ad:19:GLU:HB3	69:Ad:21:VAL:HG13	1.97	0.47
86:Ct:479:LEU:HD22	86:Ct:483:GLY:HA3	1.95	0.47
1:A2:317:C:H2'	1:A2:318:A:H8	1.78	0.47
1:A2:353:A:N3	1:A2:357:A:O2'	2.47	0.47
1:A2:633:U:H4'	1:A2:634:C:H5'	1.95	0.47
1:A2:1958:C:H5'	84:Aq:83:LYS:HD3	1.96	0.47
1:A2:2365:U:H2'	1:A2:2366:G:C8	2.49	0.47
1:A2:3815:U:H2'	1:A2:3816:A:H8	1.80	0.47
5:B1:1013:U:OP1	5:B1:1129:G:O2'	2.31	0.47
5:B1:1314:U:N3	8:BK:2:LEU:HB2	2.30	0.47
24:BE:64:ILE:HA	24:BE:67:GLN:HB2	1.97	0.47
33:BW:102:ILE:HB	33:BW:113:HIS:HB2	1.96	0.47
39:A3:154:G:OP1	47:AG:89:ARG:NE	2.39	0.47
40:A4:94:C:OP1	58:AS:46:TYR:OH	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:AC:250:CYS:SG	43:AC:252:TRP:NE1	2.88	0.47
44:AD:36:LEU:HB3	44:AD:50:ARG:HE	1.78	0.47
47:AG:184:ILE:HD13	47:AG:190:LEU:HD21	1.96	0.47
63:AX:89:LYS:O	63:AX:93:ASN:HB3	2.14	0.47
85:AK:14:PHE:HA	85:AK:17:ILE:HG22	1.97	0.47
85:AK:45:MET:HA	85:AK:48:ARG:HG2	1.96	0.47
1:A2:1315:C:H2'	1:A2:1316:A:C8	2.49	0.47
1:A2:1610:C:OP1	41:AA:14:SER:OG	2.30	0.47
1:A2:1838:C:H2'	1:A2:1839:A:H8	1.80	0.47
1:A2:2324:G:OP2	66:Aa:12:ARG:NH1	2.47	0.47
1:A2:4433:U:H3	1:A2:4446:G:H1	1.61	0.47
1:A2:4548:G:O6	1:A2:4679:A:N6	2.47	0.47
5:B1:920:A:O2'	5:B1:922:A:O5'	2.33	0.47
5:B1:1644:C:H4'	11:BQ:140:ARG:HB2	1.96	0.47
5:B1:1674:G:OP1	7:BF:51:HIS:NE2	2.43	0.47
5:B1:1737:G:H1	5:B1:1797:U:H3	1.62	0.47
11:BQ:42:ILE:HD12	11:BQ:48:GLN:HG2	1.97	0.47
58:AS:142:VAL:O	58:AS:146:HIS:ND1	2.44	0.47
1:A2:2027:G:O5'	54:AO:60:LYS:NZ	2.47	0.47
1:A2:2448:C:N4	1:A2:2450:G:O6	2.48	0.47
1:A2:3652:G:N1	41:AA:118:GLU:OE2	2.47	0.47
5:B1:1208:A:O2'	5:B1:1835:A:N1	2.41	0.47
13:BS:24:ARG:O	13:BS:55:ARG:NH1	2.46	0.47
36:Ba:21:ILE:HD12	36:Ba:32:LYS:HB3	1.96	0.47
65:AZ:9:LYS:HB3	65:AZ:25:ILE:HD12	1.95	0.47
66:Aa:38:LEU:O	66:Aa:42:ARG:NH2	2.48	0.47
86:Ct:649:ILE:HD11	86:Ct:661:ILE:HD12	1.97	0.47
86:Ct:663:THR:OG1	86:Ct:703:ASP:OD1	2.26	0.47
1:A2:50:C:H5''	51:AL:20:ARG:HH12	1.80	0.47
1:A2:1410:A:H2	56:AQ:138:LEU:HD23	1.79	0.47
1:A2:3614:A:OP1	75:Aj:2:THR:N	2.47	0.47
1:A2:3621:C:OP1	41:AA:200:ARG:NH2	2.48	0.47
5:B1:454:U:H2'	5:B1:455:A:C8	2.50	0.47
5:B1:1091:C:N4	5:B1:1092:G:O6	2.48	0.47
5:B1:1286:G:H4'	5:B1:1313:A:H62	1.80	0.47
40:A4:6:C:H4'	44:AD:52:ILE:HD13	1.96	0.47
50:AJ:22:LEU:O	50:AJ:71:HIS:HA	2.15	0.47
51:AL:80:GLU:HG2	51:AL:110:LEU:HD12	1.97	0.47
1:A2:2436:G:OP1	53:AN:65:ARG:NH2	2.48	0.46
1:A2:2587:G:H2'	1:A2:2588:G:H8	1.79	0.46
1:A2:4168:C:O2'	1:A2:4297:C:O2'	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B1:527:C:H2'	5:B1:528:A:C4	2.50	0.46
5:B1:1565:C:OP2	14:BT:101:ARG:NH1	2.48	0.46
29:BL:124:ASP:HB3	29:BL:149:ALA:HB2	1.97	0.46
39:A3:53:G:OP1	77:A1:19:GLN:NE2	2.45	0.46
51:AL:168:VAL:HA	66:Aa:97:ALA:HA	1.96	0.46
53:AN:114:ARG:NH1	53:AN:151:ILE:O	2.48	0.46
1:A2:942:G:O2'	1:A2:944:G:N2	2.48	0.46
1:A2:1621:U:H3	1:A2:1625:A:HO2'	1.62	0.46
1:A2:2562:C:H2'	1:A2:2563:G:H8	1.81	0.46
1:A2:4556:U:H2'	1:A2:4557:G:H8	1.79	0.46
5:B1:629:A:O2'	5:B1:631:U:OP2	2.33	0.46
5:B1:1137:U:O2'	21:BA:155:ARG:NH2	2.48	0.46
5:B1:1203:G:H8	5:B1:1699:A:H2	1.62	0.46
33:BW:11:LEU:HD12	33:BW:74:VAL:HG23	1.96	0.46
41:AA:206:PRO:HG3	41:AA:213:GLY:HA3	1.98	0.46
46:AF:236:ARG:HD3	46:AF:239:GLN:HB2	1.97	0.46
52:AM:12:VAL:O	52:AM:58:THR:OG1	2.33	0.46
64:AY:55:VAL:HG13	64:AY:104:VAL:HG13	1.97	0.46
84:Aq:16:ARG:HD2	84:Aq:29:ALA:HB2	1.97	0.46
1:A2:2030:G:H2'	1:A2:2031:G:C8	2.50	0.46
1:A2:2254:G:H2'	1:A2:2255:A:C8	2.50	0.46
1:A2:3826:C:H2'	1:A2:3827:A:H8	1.79	0.46
1:A2:4727:G:H22	1:A2:4825:G:H1	1.62	0.46
5:B1:172:U:OP1	5:B1:314:U:O2'	2.31	0.46
5:B1:1138:C:N3	32:BV:61:ARG:NH1	2.64	0.46
12:BR:122:PRO:HB2	12:BR:124:VAL:HG23	1.97	0.46
17:Bc:15:THR:HG22	17:Bc:16:LYS:HG3	1.98	0.46
22:BB:144:LYS:HB2	22:BB:208:HIS:HB2	1.97	0.46
24:BE:70:ILE:HG13	24:BE:92:ILE:HG12	1.97	0.46
34:BX:124:LYS:HA	34:BX:129:SER:HA	1.97	0.46
44:AD:187:SER:OG	44:AD:189:GLU:OE1	2.32	0.46
54:AO:22:ILE:HG23	58:AS:166:ARG:HH21	1.79	0.46
84:Aq:102:GLY:HA3	84:Aq:139:VAL:HG12	1.97	0.46
1:A2:32:G:H21	1:A2:51:A:H62	1.61	0.46
1:A2:1480:G:OP1	56:AQ:150:ARG:NH1	2.38	0.46
1:A2:1886:U:O2	46:AF:215:SER:OG	2.32	0.46
1:A2:2621:A:N6	1:A2:2622:G:O6	2.48	0.46
1:A2:4069:G:N2	1:A2:4080:U:O2	2.38	0.46
1:A2:4251:U:H4'	1:A2:4282:G:H4'	1.98	0.46
1:A2:4839:U:O2	45:AE:161:ARG:NH2	2.48	0.46
5:B1:71:G:H1'	5:B1:79:A:H61	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BD:110:LEU:HA	6:BD:177:LEU:HD21	1.96	0.46
10:BP:34:MET:HG3	10:BP:45:LEU:HD22	1.97	0.46
1:A2:1261:C:H2'	1:A2:1262:A:H8	1.81	0.46
1:A2:1826:U:H2'	1:A2:1827:G:H8	1.79	0.46
1:A2:2631:G:H22	81:Ap:59:SER:HA	1.79	0.46
1:A2:3688:A:H2'	1:A2:3689:A:H8	1.81	0.46
1:A2:5009:C:H4'	42:AB:324:GLY:HA2	1.97	0.46
5:B1:149:A:N6	5:B1:169:U:C2	2.84	0.46
5:B1:406:U:H2'	5:B1:408:A:H8	1.81	0.46
9:BM:19:GLN:HB3	9:BM:88:TRP:HZ3	1.81	0.46
9:BM:36:ARG:HH21	19:Bf:103:LEU:HD22	1.79	0.46
10:BP:30:TYR:HA	10:BP:33:LEU:HG	1.97	0.46
21:BA:105:PRO:HG3	21:BA:132:GLN:HG2	1.96	0.46
24:BE:125:LYS:H	24:BE:142:HIS:CE1	2.34	0.46
53:AN:84:PRO:HA	53:AN:87:HIS:CD2	2.50	0.46
71:Af:58:VAL:HG11	71:Af:65:ASN:HB2	1.98	0.46
83:Au:160:LYS:HD3	83:Au:162:VAL:HG12	1.98	0.46
86:Ct:26:ALA:HB2	86:Ct:128:VAL:HG13	1.96	0.46
86:Ct:375:GLY:HA2	86:Ct:492:HIS:HD2	1.81	0.46
5:B1:1397:U:O2	20:Bg:63:SER:OG	2.33	0.46
7:BF:49:LEU:HD12	11:BQ:50:LYS:HB2	1.97	0.46
20:Bg:282:GLU:HB3	20:Bg:284:PRO:HD2	1.96	0.46
39:A3:70:G:H22	39:A3:87:G:H1'	1.81	0.46
48:AH:102:ASN:HB3	48:AH:115:ARG:HB2	1.97	0.46
63:AX:123:LYS:NZ	63:AX:125:ASN:OD1	2.48	0.46
1:A2:226:G:OP1	64:AY:15:ARG:NH1	2.49	0.46
1:A2:1663:G:O2'	66:Aa:41:HIS:NE2	2.40	0.46
1:A2:1887:U:H2'	1:A2:1888:A:H8	1.80	0.46
1:A2:4484:G:O2'	1:A2:4487:C:OP2	2.32	0.46
5:B1:482:G:N2	5:B1:485:A:OP2	2.49	0.46
5:B1:1083:A:N7	5:B1:1841:C:O2'	2.44	0.46
31:BO:145:GLY:O	36:Ba:22:ARG:NH1	2.48	0.46
47:AG:67:ARG:NH2	47:AG:162:ASP:OD1	2.49	0.46
49:AI:34:PHE:HD1	49:AI:89:VAL:HB	1.80	0.46
56:AQ:36:ALA:O	56:AQ:45:GLN:NE2	2.48	0.46
75:Aj:25:LYS:HE3	77:Al:51:LEU:HD12	1.97	0.46
76:Ak:26:LYS:HB2	76:Ak:69:LEU:HD12	1.96	0.46
83:Au:38:LEU:HD13	83:Au:41:TYR:HE2	1.80	0.46
1:A2:23:C:OP2	75:Aj:46:LYS:NZ	2.44	0.46
1:A2:239:U:O2'	43:AC:222:ARG:NH2	2.43	0.46
1:A2:4545:C:O2'	1:A2:4680:G:N2	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B1:1337:C:H2'	5:B1:1338:G:H8	1.81	0.46
22:BB:89:GLU:HG2	22:BB:228:LEU:HD22	1.97	0.46
22:BB:228:LEU:O	22:BB:232:HIS:ND1	2.45	0.46
30:BN:86:GLU:HA	30:BN:89:TYR:HB3	1.98	0.46
45:AE:195:ILE:HG23	71:Af:110:ILE:HG21	1.97	0.46
53:AN:84:PRO:HA	53:AN:87:HIS:HD2	1.81	0.46
57:AR:99:MET:HE3	57:AR:103:ARG:HH11	1.81	0.46
85:AK:53:VAL:HG22	85:AK:89:VAL:HG22	1.97	0.46
86:Ct:752:PRO:HD2	86:Ct:807:GLN:HG2	1.98	0.46
1:A2:2689:C:OP2	57:AR:39:GLN:NE2	2.40	0.46
1:A2:4503:G:N2	1:A2:4506:A:OP2	2.41	0.46
1:A2:4974:A:O2'	27:BI:92:ARG:NH2	2.49	0.46
5:B1:1554:C:H42	6:BD:77:PHE:HD1	1.64	0.46
21:BA:145:ILE:HG12	21:BA:159:ILE:HB	1.97	0.46
41:AA:135:THR:HB	41:AA:149:LYS:HB3	1.98	0.46
44:AD:205:ALA:HB1	44:AD:233:PRO:HB3	1.98	0.46
51:AL:161:TYR:HA	66:Aa:105:ARG:HH12	1.80	0.46
66:Aa:123:ILE:HG12	66:Aa:143:ALA:HB3	1.98	0.46
86:Ct:38:SER:OG	86:Ct:346:ALA:O	2.33	0.46
86:Ct:232:TYR:OH	86:Ct:292:LEU:O	2.30	0.46
1:A2:439:U:O2	1:A2:2292:A:O2'	2.34	0.46
1:A2:455:G:N1	1:A2:687:A:C2	2.66	0.46
1:A2:2022:A:N7	1:A2:4396:C:O2'	2.47	0.46
5:B1:5:U:H2'	5:B1:6:G:C8	2.51	0.46
5:B1:993:G:OP1	5:B1:1131:G:N2	2.41	0.46
25:BG:69:THR:HG22	25:BG:71:GLY:H	1.80	0.46
58:AS:7:LEU:HD23	58:AS:107:THR:HA	1.98	0.46
65:AZ:36:ARG:HD3	65:AZ:38:TYR:CZ	2.51	0.46
78:Am:104:HIS:CD2	78:Am:106:ARG:H	2.34	0.46
1:A2:312:A:H2'	1:A2:313:A:H8	1.80	0.45
1:A2:3767:U:HO2'	5:B1:1720:U:HO2'	1.53	0.45
1:A2:4597:A:O2'	1:A2:4599:G:OP1	2.34	0.45
1:A2:4650:C:O2'	48:AH:155:SER:OG	2.25	0.45
1:A2:4925:A:H2'	1:A2:4926:A:H8	1.81	0.45
20:Bg:101:PHE:HE1	20:Bg:136:GLY:HA2	1.81	0.45
21:BA:149:ASN:ND2	21:BA:163:CYS:O	2.49	0.45
46:AF:228:VAL:HA	58:AS:39:VAL:HG22	1.98	0.45
61:AV:83:ARG:HB2	61:AV:102:ALA:HB3	1.98	0.45
1:A2:1628:A:O2'	75:Aj:49:TRP:O	2.29	0.45
1:A2:2500:G:H5'	1:A2:2619:G:H1'	1.97	0.45
5:B1:346:C:H5''	24:BE:38:LEU:HG	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B1:436:G:OP2	5:B1:471:G:O2'	2.33	0.45
5:B1:525:A:N7	5:B1:589:G:N2	2.61	0.45
8:BK:80:ARG:HA	8:BK:83:LEU:HB2	1.98	0.45
26:BH:148:LEU:HD23	33:BW:42:MET:HE2	1.96	0.45
31:BO:34:PHE:HD1	31:BO:98:ARG:HG3	1.81	0.45
35:BY:12:PHE:HZ	35:BY:21:LYS:HD2	1.82	0.45
37:Bb:49:HIS:ND1	37:Bb:69:GLY:O	2.40	0.45
39:A3:106:G:H4'	39:A3:137:A:H5'	1.96	0.45
41:AA:58:LEU:HD21	41:AA:75:LEU:HB3	1.97	0.45
70:Ae:108:ARG:NH2	70:Ae:124:ASN:O	2.49	0.45
72:Ag:60:ARG:HB3	72:Ag:63:VAL:HG23	1.97	0.45
86:Ct:172:GLU:OE2	86:Ct:287:ARG:NE	2.49	0.45
86:Ct:669:VAL:HG11	86:Ct:707:VAL:HB	1.98	0.45
86:Ct:740:LEU:HB2	86:Ct:820:LEU:HD12	1.97	0.45
1:A2:1966:G:O2'	1:A2:1984:G:OP2	2.27	0.45
5:B1:454:U:H2'	5:B1:455:A:H8	1.80	0.45
5:B1:1033:G:N1	5:B1:1080:A:O2'	2.41	0.45
5:B1:1742:C:OP2	27:BI:42:ARG:NH1	2.40	0.45
41:AA:24:LYS:HG3	41:AA:49:ILE:HD12	1.97	0.45
71:Af:59:THR:HG23	71:Af:61:GLY:H	1.82	0.45
74:Ai:65:LYS:HG3	74:Ai:67:LYS:H	1.80	0.45
77:Al:12:PHE:HE2	77:Al:49:LEU:HD13	1.81	0.45
83:Au:38:LEU:HB2	83:Au:163:LEU:HB3	1.99	0.45
84:Aq:82:ILE:HD13	84:Aq:137:GLN:HG2	1.98	0.45
86:Ct:396:MET:HG2	86:Ct:416:VAL:HA	1.97	0.45
1:A2:894:C:H2'	1:A2:895:G:H8	1.80	0.45
1:A2:1833:U:OP1	66:Aa:23:GLY:N	2.47	0.45
1:A2:2297:G:N2	1:A2:2300:G:OP2	2.38	0.45
1:A2:2384:G:H5''	75:Aj:14:LYS:HE3	1.97	0.45
1:A2:2437:C:H5''	53:AN:67:ARG:HE	1.81	0.45
1:A2:2738:G:OP2	1:A2:2738:G:N2	2.49	0.45
1:A2:4964:U:H3	1:A2:4999:G:H5'	1.80	0.45
5:B1:987:A:H4'	36:Ba:70:LYS:HG3	1.98	0.45
5:B1:1227:G:N2	5:B1:1635:C:O2'	2.50	0.45
12:BR:14:ARG:HA	12:BR:17:ILE:HG22	1.98	0.45
20:Bg:23:THR:HG22	20:Bg:31:ILE:HD12	1.98	0.45
38:Be:12:VAL:O	38:Be:16:THR:OG1	2.30	0.45
43:AC:40:VAL:HG13	43:AC:115:VAL:HG11	1.98	0.45
47:AG:104:PRO:HG2	47:AG:194:VAL:HG23	1.99	0.45
84:Aq:30:PRO:O	84:Aq:33:GLY:N	2.49	0.45
1:A2:79:C:OP2	53:AN:194:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:272:G:OP1	53:AN:12:ARG:NH2	2.50	0.45
1:A2:344:C:OP2	43:AC:197:ARG:NH1	2.49	0.45
1:A2:1311:G:O2'	1:A2:2328:A:OP1	2.34	0.45
1:A2:1474:G:O2'	67:Ab:41:ARG:NH1	2.49	0.45
1:A2:2577:A:N3	72:Ag:61:PRO:HG2	2.31	0.45
1:A2:2630:C:O2'	1:A2:2632:C:OP1	2.29	0.45
1:A2:4144:G:H5'	41:AA:226:ARG:HH22	1.82	0.45
1:A2:4678:C:OP1	42:AB:276:HIS:ND1	2.49	0.45
1:A2:4911:G:H2'	1:A2:4912:G:H8	1.81	0.45
5:B1:1652:G:O6	5:B1:1672:U:O4	2.35	0.45
16:BZ:101:SER:OG	16:BZ:103:HIS:NE2	2.48	0.45
22:BB:73:ASP:OD1	22:BB:73:ASP:N	2.49	0.45
24:BE:63:LYS:NZ	35:BY:85:ASN:O	2.50	0.45
43:AC:239:LYS:O	43:AC:248:ARG:NH1	2.43	0.45
44:AD:166:ALA:HB1	44:AD:171:LEU:HD12	1.97	0.45
47:AG:166:LEU:HD21	53:AN:45:PRO:HG2	1.98	0.45
1:A2:1674:C:H41	56:AQ:13:VAL:HG21	1.81	0.45
1:A2:4832:A:H1'	1:A2:4834:U:C2	2.52	0.45
5:B1:1122:A:H1'	22:BB:146:ARG:HH21	1.82	0.45
8:BK:10:ALA:HB1	8:BK:38:LYS:HE2	1.99	0.45
26:BH:145:ARG:HB3	26:BH:153:LEU:HB2	1.98	0.45
32:BV:22:ARG:HH22	32:BV:58:ALA:H	1.63	0.45
54:AO:34:VAL:HG22	54:AO:103:LYS:HB2	1.99	0.45
57:AR:8:LYS:HD3	57:AR:23:TRP:HE1	1.80	0.45
57:AR:32:ILE:HD13	57:AR:44:LEU:HD13	1.98	0.45
1:A2:273:A:OP2	53:AN:8:GLN:NE2	2.50	0.45
1:A2:1073:G:OP1	59:AT:142:ARG:NH2	2.50	0.45
1:A2:1316:A:H2'	1:A2:1317:A:H8	1.82	0.45
1:A2:2702:U:H2'	1:A2:2703:G:C8	2.52	0.45
1:A2:4254:A:O2'	80:Ao:8:ARG:NH2	2.46	0.45
1:A2:4896:A:HO2'	45:AE:240:TYR:HH	1.62	0.45
5:B1:805:U:O3'	33:BW:120:HIS:NE2	2.49	0.45
5:B1:885:U:H2'	5:B1:886:A:C8	2.52	0.45
5:B1:1146:C:O2'	5:B1:1150:A:N1	2.44	0.45
5:B1:1487:A:H1'	23:BC:117:ARG:HH12	1.81	0.45
5:B1:1653:U:H2'	5:B1:1654:G:C8	2.52	0.45
18:Bd:47:ALA:HA	18:Bd:50:ILE:HG12	1.97	0.45
26:BH:27:LEU:HD12	26:BH:45:ILE:HD11	1.98	0.45
41:AA:133:TYR:HB3	41:AA:168:VAL:HG12	1.99	0.45
53:AN:143:ARG:O	53:AN:149:GLN:NE2	2.50	0.45
55:AP:122:ALA:H	55:AP:144:CYS:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:AQ:144:LYS:HA	56:AQ:149:TYR:HD2	1.82	0.45
59:AT:67:VAL:HG22	59:AT:72:VAL:HG23	1.99	0.45
1:A2:54:G:O2'	53:AN:161:MET:SD	2.67	0.45
1:A2:2030:G:HO2'	1:A2:3855:U:HO2'	1.63	0.45
5:B1:370:G:H4'	5:B1:371:A:H5'	1.97	0.45
24:BE:45:ILE:O	24:BE:49:ARG:HB3	2.17	0.45
26:BH:52:GLU:HG3	26:BH:58:LYS:HB3	1.98	0.45
29:BL:101:ARG:HH21	34:BX:13:LEU:HD11	1.81	0.45
43:AC:207:PRO:HB3	43:AC:249:PHE:HD2	1.82	0.45
53:AN:54:LYS:H	53:AN:59:TYR:HD2	1.63	0.45
1:A2:4234:G:C6	1:A2:4298:A:N1	2.85	0.45
1:A2:4435:A:O2'	78:Am:122:ARG:NH2	2.48	0.45
1:A2:4988:U:H2'	1:A2:4989:G:H8	1.82	0.45
3:Bx:27:U:H1'	86:Ct:715:DDE:HAC2	1.77	0.45
5:B1:604:A:N3	5:B1:639:C:O2'	2.46	0.45
5:B1:656:G:H1	5:B1:1156:U:H5	1.65	0.45
5:B1:1407:U:O2'	11:BQ:11:GLN:NE2	2.38	0.45
15:BU:80:PHE:HB3	18:Bd:52:PHE:HB3	1.99	0.45
25:BG:74:ARG:HA	25:BG:96:SER:HA	1.98	0.45
58:AS:95:ARG:NE	58:AS:97:TYR:OH	2.41	0.45
86:Ct:300:VAL:HG11	86:Ct:340:MET:HE3	1.98	0.45
1:A2:1810:C:H2'	1:A2:1811:G:H8	1.81	0.45
1:A2:1893:G:H21	54:AO:87:MET:HE3	1.81	0.45
1:A2:1944:C:HO2'	1:A2:2008:U:HO2'	1.63	0.45
1:A2:2465:G:H2'	1:A2:2466:G:H8	1.82	0.45
1:A2:2727:C:O2'	72:Ag:61:PRO:O	2.33	0.45
1:A2:3695:A:H4'	83:Au:40:ASN:HD21	1.81	0.45
1:A2:4098:G:O6	1:A2:4118:G:N2	2.51	0.45
5:B1:798:G:O6	26:BH:107:LYS:NZ	2.44	0.45
19:Bf:121:CYS:HB3	19:Bf:127:GLY:HA3	1.99	0.45
27:BI:80:ASP:HB3	27:BI:103:LEU:HD13	1.99	0.45
43:AC:79:VAL:HG11	43:AC:86:ARG:HH12	1.82	0.45
44:AD:36:LEU:HD13	44:AD:50:ARG:HH21	1.82	0.45
45:AE:178:PRO:HG2	45:AE:181:LEU:HB2	1.98	0.45
47:AG:75:LYS:HG2	47:AG:240:ASN:HB2	1.99	0.45
58:AS:85:ASP:H	58:AS:123:SER:HB3	1.82	0.45
70:Ae:4:LEU:HD12	70:Ae:121:ARG:HB2	1.98	0.45
72:Ag:49:CYS:HA	81:Ap:61:MET:HG3	1.99	0.45
1:A2:1080:C:H2'	1:A2:1081:G:H8	1.82	0.44
1:A2:1677:U:O2'	1:A2:1701:A:N1	2.45	0.44
5:B1:1513:C:H2'	5:B1:1514:G:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BS:8:LYS:HD2	13:BS:58:GLU:HA	1.99	0.44
13:BS:84:LEU:HD22	13:BS:97:GLN:HB2	1.98	0.44
22:BB:197:ILE:O	22:BB:201:CYS:CB	2.64	0.44
43:AC:24:LEU:HD12	43:AC:25:PRO:HD2	1.99	0.44
46:AF:166:ARG:HH12	46:AF:212:LYS:HD2	1.82	0.44
58:AS:95:ARG:NH2	58:AS:112:ASP:OD2	2.50	0.44
86:Ct:510:GLU:HB3	86:Ct:571:LYS:HB3	1.99	0.44
1:A2:394:A:H5''	55:AP:16:LYS:HG3	1.99	0.44
1:A2:503:A:H2	66:Aa:102:ASP:H	1.65	0.44
1:A2:1865:C:H2'	1:A2:1866:G:H8	1.82	0.44
1:A2:4853:C:OP1	52:AM:132:LYS:NZ	2.44	0.44
1:A2:4953:U:O3'	69:Ad:32:ARG:NH2	2.48	0.44
1:A2:5021:G:H2'	1:A2:5022:G:H8	1.82	0.44
5:B1:525:A:H5''	38:Be:26:LYS:HZ2	1.81	0.44
5:B1:1287:A:N6	19:Bf:100:LEU:O	2.40	0.44
20:Bg:138:CYS:SG	20:Bg:139:LYS:N	2.91	0.44
21:BA:113:GLN:HG3	21:BA:115:ALA:H	1.82	0.44
24:BE:194:VAL:N	24:BE:211:LYS:O	2.50	0.44
34:BX:99:GLU:HB2	34:BX:126:ALA:HA	1.99	0.44
36:Ba:88:SER:H	36:Ba:91:ALA:HB3	1.83	0.44
60:AU:28:PRO:HB2	60:AU:34:MET:HB2	1.98	0.44
65:AZ:91:LEU:HD21	65:AZ:96:VAL:HG21	1.99	0.44
86:Ct:89:ILE:HD11	86:Ct:93:LYS:HB2	1.98	0.44
1:A2:2390:C:H2'	1:A2:2391:A:C8	2.53	0.44
1:A2:3778:A:HO2'	5:B1:1816:G:HO2'	1.62	0.44
1:A2:4724:A:H61	58:AS:171:ARG:HD3	1.83	0.44
5:B1:982:G:H2'	5:B1:983:A:C8	2.52	0.44
12:BR:31:ASN:HD22	12:BR:55:THR:HG22	1.82	0.44
16:BZ:74:SER:HA	16:BZ:79:ILE:HB	1.99	0.44
25:BG:186:GLN:HB3	25:BG:189:ARG:HH21	1.81	0.44
30:BN:102:LEU:HD12	30:BN:115:LEU:HD13	1.98	0.44
31:BO:147:ARG:HA	36:Ba:28:ARG:HG3	2.00	0.44
39:A3:9:A:H2'	39:A3:10:G:H8	1.82	0.44
54:AO:21:ALA:HA	54:AO:87:MET:HE1	1.98	0.44
61:AV:104:VAL:HB	61:AV:112:MET:HE1	1.98	0.44
1:A2:27:C:O2'	1:A2:60:A:N3	2.47	0.44
1:A2:722:G:H22	1:A2:925:C:H5''	1.82	0.44
1:A2:1288:C:OP1	39:A3:7:U:O2'	2.35	0.44
1:A2:1674:C:H41	56:AQ:13:VAL:HG11	1.82	0.44
1:A2:2056:G:H2'	1:A2:2057:G:H8	1.80	0.44
1:A2:2465:G:H2'	1:A2:2466:G:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B1:851:C:O2'	5:B1:852:G:N2	2.51	0.44
25:BG:64:LYS:HB2	25:BG:97:VAL:HG11	1.98	0.44
29:BL:86:ILE:HG12	29:BL:113:LEU:HB2	2.00	0.44
44:AD:53:VAL:HB	44:AD:159:VAL:HG23	1.99	0.44
58:AS:13:VAL:HG23	58:AS:62:VAL:HB	1.99	0.44
65:AZ:64:LYS:HA	65:AZ:67:LYS:HG2	2.00	0.44
86:Ct:42:LYS:NZ	86:Ct:348:ASP:OD1	2.34	0.44
1:A2:161:G:O6	1:A2:266:U:O4	2.36	0.44
1:A2:743:G:O6	1:A2:898:U:C2	2.71	0.44
1:A2:2651:C:OP1	81:Ap:44:LYS:NZ	2.36	0.44
1:A2:4666:C:H2'	1:A2:4667:A:H8	1.82	0.44
1:A2:4856:G:H3'	1:A2:4857:G:H8	1.82	0.44
5:B1:1402:A:OP1	15:BU:52:GLY:N	2.50	0.44
6:BD:168:VAL:HA	6:BD:188:ILE:O	2.18	0.44
16:BZ:88:LEU:HB3	16:BZ:109:TYR:HE2	1.83	0.44
62:AW:68:GLN:HG3	62:AW:69:LYS:HG2	1.98	0.44
65:AZ:59:LYS:HG2	65:AZ:60:LYS:H	1.83	0.44
86:Ct:824:PRO:HB3	86:Ct:835:VAL:HG21	2.00	0.44
1:A2:85:G:O2'	1:A2:97:G:O6	2.35	0.44
1:A2:86:U:H2'	1:A2:87:A:H8	1.82	0.44
1:A2:1627:C:H2'	1:A2:1628:A:C8	2.52	0.44
1:A2:2062:C:H2'	1:A2:2063:G:C8	2.53	0.44
1:A2:3658:A:O2'	41:AA:236:GLY:N	2.49	0.44
1:A2:4486:G:C2	42:AB:252:ALA:HB1	2.53	0.44
5:B1:490:C:O2'	5:B1:574:A:N1	2.49	0.44
5:B1:1395:C:H2'	5:B1:1396:A:C8	2.52	0.44
9:BM:120:ALA:HB1	9:BM:123:VAL:HB	2.00	0.44
17:Bc:12:ALA:O	17:Bc:56:LEU:N	2.47	0.44
23:BC:253:PRO:HG3	33:BW:68:ARG:HH21	1.81	0.44
26:BH:122:LEU:O	26:BH:126:HIS:ND1	2.44	0.44
39:A3:60:G:OP1	63:AX:68:ARG:NH2	2.40	0.44
52:AM:25:VAL:HB	52:AM:38:VAL:HB	1.98	0.44
52:AM:56:GLN:OE1	58:AS:157:ARG:NH2	2.50	0.44
81:Ap:50:ARG:HG3	81:Ap:51:ALA:H	1.82	0.44
82:At:19:LYS:HG2	82:At:24:THR:HG22	1.99	0.44
86:Ct:330:LYS:HB3	86:Ct:334:PRO:HG2	2.00	0.44
1:A2:732:C:H2'	1:A2:733:G:C8	2.53	0.44
1:A2:1190:C:O2'	46:AF:77:LYS:NZ	2.51	0.44
1:A2:1346:C:OP2	51:AL:39:ARG:NH2	2.50	0.44
1:A2:1835:G:N2	1:A2:4356:A:O4'	2.51	0.44
1:A2:1886:U:O2'	46:AF:216:PRO:O	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:2049:C:OP1	71:Af:85:ARG:NH2	2.50	0.44
5:B1:337:C:H2'	5:B1:338:G:C4	2.53	0.44
5:B1:1098:C:H2'	5:B1:1099:G:C8	2.53	0.44
23:BC:108:LYS:HE2	23:BC:110:MET:HB3	1.99	0.44
45:AE:113:PRO:HG2	45:AE:116:TYR:HE1	1.82	0.44
48:AH:159:ALA:HA	48:AH:162:GLN:HG2	1.99	0.44
86:Ct:45:ILE:HD12	86:Ct:46:ILE:HG12	2.00	0.44
86:Ct:224:THR:HG23	86:Ct:226:LYS:H	1.82	0.44
1:A2:356:A:N6	77:Al:37:TYR:O	2.47	0.44
1:A2:686:C:H2'	1:A2:687:A:H8	1.82	0.44
1:A2:1161:G:N2	1:A2:1164:C:OP1	2.43	0.44
1:A2:2722:A:H2'	1:A2:2723:A:C8	2.53	0.44
5:B1:388:U:H2'	5:B1:389:A:C8	2.53	0.44
5:B1:637:U:OP1	38:Be:24:LYS:NZ	2.44	0.44
5:B1:1228:A:H2'	5:B1:1229:G:C8	2.53	0.44
24:BE:11:ARG:HE	24:BE:28:ALA:HA	1.83	0.44
27:BI:172:LEU:HB3	27:BI:190:LEU:HD12	1.99	0.44
29:BL:154:GLN:OE1	29:BL:156:GLN:NE2	2.50	0.44
39:A3:153:C:H2'	39:A3:154:G:C8	2.52	0.44
74:Ai:41:ARG:HA	74:Ai:44:ILE:HG22	2.00	0.44
78:Am:97:ARG:NH1	78:Am:121:LEU:O	2.50	0.44
86:Ct:349:ALA:O	86:Ct:353:MET:HB2	2.17	0.44
86:Ct:592:LEU:HD21	86:Ct:601:ARG:HG3	1.99	0.44
1:A2:2500:G:H5''	72:Ag:25:THR:HG22	1.99	0.44
5:B1:945:U:O2	5:B1:1045:U:O2'	2.35	0.44
5:B1:948:C:H2'	5:B1:949:G:H8	1.82	0.44
5:B1:1232:U:OP2	13:BS:135:HIS:ND1	2.51	0.44
5:B1:1299:A:H4'	10:BP:51:ARG:HH12	1.83	0.44
5:B1:1593:C:H2'	5:B1:1594:A:H8	1.82	0.44
45:AE:213:THR:H	45:AE:216:TYR:HB3	1.83	0.44
51:AL:32:LYS:HE2	51:AL:36:ARG:HH21	1.83	0.44
61:AV:31:ASN:ND2	61:AV:115:SER:OG	2.44	0.44
76:Ak:52:LYS:HA	76:Ak:55:LYS:HG2	1.99	0.44
86:Ct:290:CYS:HA	86:Ct:294:LEU:HB2	2.00	0.44
86:Ct:738:PRO:HD2	86:Ct:825:PHE:HE2	1.83	0.44
1:A2:4950:G:H2'	1:A2:4951:G:C8	2.52	0.43
5:B1:57:U:OP1	5:B1:504:G:O2'	2.36	0.43
5:B1:231:A:OP2	5:B1:889:U:O2'	2.34	0.43
5:B1:1128:C:O2'	37:Bb:19:HIS:ND1	2.33	0.43
5:B1:1190:A:N3	5:B1:1714:U:O2'	2.49	0.43
5:B1:1617:G:N2	5:B1:1620:A:OP2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:AB:220:ILE:HG12	42:AB:278:THR:HG22	2.00	0.43
43:AC:316:LYS:HB3	43:AC:321:ASN:HD21	1.82	0.43
45:AE:152:ILE:O	45:AE:159:GLY:N	2.51	0.43
46:AF:103:PRO:HA	46:AF:106:ARG:HB3	1.99	0.43
82:At:61:VAL:HG12	82:At:81:THR:HG22	2.00	0.43
83:Au:159:MET:HG3	83:Au:165:LEU:HB2	2.00	0.43
1:A2:220:G:O3'	43:AC:222:ARG:NH2	2.52	0.43
1:A2:376:G:N1	1:A2:379:A:OP2	2.43	0.43
1:A2:1485:A:H4'	1:A2:1486:G:H5'	1.98	0.43
1:A2:2576:G:H1	1:A2:2727:C:H5	1.65	0.43
5:B1:873:G:H2'	29:BL:153:LYS:HE3	2.00	0.43
5:B1:1017:U:H5'	30:BN:55:ARG:HD3	1.98	0.43
28:BJ:107:GLU:HA	28:BJ:112:THR:HG21	1.99	0.43
34:BX:107:ARG:HG3	34:BX:109:GLY:H	1.82	0.43
41:AA:27:ALA:O	41:AA:128:ARG:NH2	2.51	0.43
74:Ai:44:ILE:HA	74:Ai:47:VAL:HB	2.00	0.43
86:Ct:129:VAL:HG12	86:Ct:155:LEU:HD11	2.00	0.43
1:A2:4435:A:H4'	78:Am:95:ILE:HG21	2.00	0.43
1:A2:4547:U:OP1	54:AO:74:ARG:N	2.48	0.43
5:B1:149:A:N6	5:B1:169:U:O2	2.51	0.43
5:B1:1016:U:OP2	37:Bb:20:LYS:NZ	2.51	0.43
5:B1:1036:A:H4'	5:B1:1855:G:H21	1.83	0.43
20:Bg:40:ILE:HB	20:Bg:59:LEU:HB2	1.99	0.43
20:Bg:278:SER:HB2	20:Bg:281:ALA:HB3	1.99	0.43
23:BC:191:VAL:HG11	23:BC:236:PHE:HA	2.01	0.43
23:BC:201:GLY:N	23:BC:221:ASP:OD2	2.49	0.43
24:BE:52:LEU:HD21	24:BE:111:VAL:HG11	1.99	0.43
34:BX:100:VAL:HG13	34:BX:122:VAL:HG13	2.00	0.43
40:A4:62:U:O2'	40:A4:64:G:O4'	2.36	0.43
41:AA:129:ALA:HB3	41:AA:132:ASN:HD22	1.83	0.43
43:AC:323:ARG:HA	43:AC:326:LEU:HB2	1.99	0.43
45:AE:206:VAL:HG13	45:AE:256:GLN:HG3	1.99	0.43
45:AE:286:LEU:HD21	52:AM:109:ARG:HH22	1.83	0.43
52:AM:6:PHE:H	52:AM:11:ARG:NH1	2.16	0.43
86:Ct:527:LEU:HD21	86:Ct:557:CYS:HB3	1.99	0.43
1:A2:704:C:H2'	1:A2:705:G:C8	2.53	0.43
1:A2:704:C:H2'	1:A2:705:G:H8	1.81	0.43
1:A2:1439:G:H5'	56:AQ:72:LEU:HD13	2.00	0.43
1:A2:2054:C:O3'	46:AF:157:ARG:NH2	2.39	0.43
1:A2:4285:A:H4'	44:AD:176:SER:HB3	1.99	0.43
5:B1:1084:A:OP1	5:B1:1858:G:O2'	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B1:1605:G:OP1	14:BT:84:ARG:NH2	2.51	0.43
24:BE:180:LEU:HB3	24:BE:229:GLY:HA3	2.01	0.43
26:BH:117:PRO:HD2	26:BH:120:ARG:HG3	2.00	0.43
30:BN:46:THR:HG22	30:BN:48:SER:H	1.84	0.43
42:AB:26:ARG:HD3	42:AB:179:HIS:HB3	2.00	0.43
42:AB:371:THR:HB	42:AB:377:GLY:HA3	1.99	0.43
43:AC:12:SER:OG	43:AC:18:SER:OG	2.36	0.43
46:AF:97:GLY:HA2	46:AF:117:ILE:HD12	1.98	0.43
57:AR:10:LEU:HD11	57:AR:38:ARG:HG2	2.00	0.43
58:AS:5:GLY:O	58:AS:111:ARG:NH2	2.51	0.43
75:Aj:8:PHE:HA	75:Aj:11:ARG:HH11	1.83	0.43
1:A2:2547:C:H2'	1:A2:2548:G:H8	1.84	0.43
1:A2:2678:C:H2'	1:A2:2679:G:H8	1.82	0.43
5:B1:1102:G:H22	5:B1:1130:G:H1	1.67	0.43
5:B1:1299:A:O2'	10:BP:51:ARG:NH2	2.52	0.43
5:B1:1453:C:OP2	12:BR:45:LYS:NZ	2.48	0.43
5:B1:1650:A:H5''	11:BQ:139:ALA:HB2	2.00	0.43
41:AA:27:ALA:HB3	41:AA:128:ARG:HH21	1.84	0.43
46:AF:160:GLY:O	46:AF:166:ARG:HA	2.18	0.43
50:AJ:18:ARG:HG2	50:AJ:75:ARG:HH12	1.83	0.43
64:AY:50:ARG:HD3	64:AY:110:LYS:HB3	2.01	0.43
1:A2:71:C:H5'	51:AL:64:VAL:HG12	1.99	0.43
1:A2:85:G:N2	1:A2:98:A:OP2	2.42	0.43
1:A2:294:A:O2'	53:AN:93:LYS:O	2.27	0.43
1:A2:504:U:H5'	66:Aa:86:THR:HB	2.00	0.43
1:A2:3840:C:O2'	42:AB:261:ARG:NH1	2.52	0.43
1:A2:4652:G:H21	1:A2:4662:A:H62	1.67	0.43
1:A2:4819:G:H2'	1:A2:4820:G:C8	2.54	0.43
5:B1:21:U:O2'	28:BJ:17:ARG:O	2.36	0.43
5:B1:1172:U:H2'	5:B1:1173:A:H8	1.82	0.43
6:BD:25:LEU:O	6:BD:29:LEU:HB2	2.19	0.43
11:BQ:16:LYS:HG3	11:BQ:17:LYS:H	1.84	0.43
55:AP:60:PHE:HD2	55:AP:67:VAL:HG21	1.83	0.43
62:AW:23:ARG:HE	62:AW:25:ASP:HB2	1.83	0.43
1:A2:152:C:N4	1:A2:153:G:O6	2.51	0.43
1:A2:459:G:H22	1:A2:683:U:H3	1.67	0.43
1:A2:1051:G:H2'	1:A2:1052:G:C8	2.54	0.43
1:A2:1072:G:H2'	1:A2:1073:G:C8	2.54	0.43
1:A2:1980:A:H5'	1:A2:2000:C:H4'	2.00	0.43
1:A2:2341:U:H2'	1:A2:2342:A:H8	1.84	0.43
1:A2:3703:A:H2'	1:A2:3704:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:4296:U:O2'	59:AT:7:LYS:O	2.31	0.43
3:Bx:23:U:H5'	31:BO:151:LEU:HD21	2.00	0.43
5:B1:1228:A:H2'	5:B1:1229:G:H8	1.82	0.43
5:B1:1851:A:OP2	79:An:9:ARG:NH2	2.52	0.43
6:BD:33:GLY:HA3	6:BD:53:THR:HB	2.01	0.43
18:Bd:17:GLY:O	18:Bd:27:ARG:NH1	2.52	0.43
42:AB:219:VAL:HG11	42:AB:337:VAL:HG13	1.99	0.43
46:AF:157:ARG:NE	46:AF:212:LYS:O	2.52	0.43
49:AI:51:HIS:CD2	49:AI:168:SER:HB2	2.54	0.43
63:AX:78:LYS:HE3	63:AX:101:ASP:HB2	2.01	0.43
65:AZ:14:LEU:HD23	72:Ag:88:ARG:HB2	2.00	0.43
81:Ap:30:GLU:HA	81:Ap:33:GLN:HG2	1.99	0.43
84:Aq:123:ARG:HB2	84:Aq:129:ILE:HD11	2.00	0.43
1:A2:227:G:N2	1:A2:231:G:N7	2.58	0.43
1:A2:490:G:H2'	1:A2:491:G:C8	2.54	0.43
1:A2:642:G:HO2'	1:A2:643:A:H8	1.66	0.43
1:A2:1226:C:N4	1:A2:1243:G:OP1	2.51	0.43
1:A2:2474:U:H2'	1:A2:2475:G:C8	2.53	0.43
1:A2:2757:G:H22	39:A3:112:G:H5''	1.83	0.43
5:B1:107:A:H2'	5:B1:108:G:C8	2.54	0.43
5:B1:118:C:H1'	5:B1:445:A:C5	2.53	0.43
5:B1:527:C:H4'	28:BJ:125:HIS:HB2	2.00	0.43
5:B1:575:A:OP1	35:BY:93:ARG:NH1	2.51	0.43
12:BR:99:ASP:HB2	12:BR:102:THR:HG22	1.99	0.43
14:BT:41:LYS:HG3	14:BT:42:HIS:H	1.84	0.43
24:BE:121:TYR:HB3	24:BE:161:GLN:HE21	1.83	0.43
27:BI:84:ASN:H	27:BI:91:VAL:HG22	1.83	0.43
39:A3:79:G:H2'	39:A3:80:A:C4	2.53	0.43
42:AB:54:THR:HG22	42:AB:373:LYS:HZ1	1.84	0.43
44:AD:12:TYR:O	44:AD:16:TYR:HB2	2.18	0.43
47:AG:63:LEU:HD23	47:AG:63:LEU:HA	1.88	0.43
47:AG:81:ASN:ND2	47:AG:236:HIS:O	2.39	0.43
47:AG:106:THR:O	47:AG:110:LYS:HB2	2.19	0.43
55:AP:72:GLN:O	55:AP:75:GLN:NE2	2.51	0.43
84:Aq:64:ILE:HB	84:Aq:71:ILE:HB	1.99	0.43
86:Ct:246:PRO:HA	86:Ct:249:ARG:HB3	2.00	0.43
1:A2:150:G:OP2	53:AN:49:ARG:NH2	2.51	0.43
1:A2:1442:C:H5''	56:AQ:144:LYS:HB3	2.00	0.43
1:A2:3671:C:O2'	1:A2:3745:A:N3	2.45	0.43
1:A2:4715:U:C4	1:A2:4837:C:N4	2.87	0.43
1:A2:4722:G:H2'	1:A2:4723:G:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B1:396:U:OP2	29:BL:79:LYS:NZ	2.50	0.43
5:B1:1171:G:O2'	5:B1:1187:G:O6	2.36	0.43
5:B1:1221:G:O2'	5:B1:1676:U:O2	2.34	0.43
5:B1:1268:C:O2	10:BP:97:TYR:OH	2.33	0.43
20:Bg:15:ASN:H	20:Bg:37:ASP:HB3	1.84	0.43
48:AH:137:SER:HB3	48:AH:143:GLU:HB3	2.00	0.43
49:AI:10:ARG:HH21	49:AI:11:TYR:HE2	1.67	0.43
56:AQ:155:ALA:O	56:AQ:161:SER:OG	2.30	0.43
85:AK:34:ASN:HB2	85:AK:185:PHE:HD2	1.83	0.43
86:Ct:22:MET:HG3	86:Ct:354:ILE:HD12	2.00	0.43
1:A2:491:G:H3'	1:A2:492:C:H5''	2.00	0.43
1:A2:963:G:OP2	1:A2:1220:C:N4	2.51	0.43
22:BB:97:LEU:HD12	22:BB:228:LEU:HD21	2.00	0.43
31:BO:149:ARG:HB3	36:Ba:26:CYS:HA	2.00	0.43
44:AD:51:MET:HA	44:AD:63:GLN:O	2.19	0.43
47:AG:137:ARG:HG3	47:AG:146:LEU:HD11	2.01	0.43
56:AQ:176:ARG:HB2	66:Aa:56:VAL:HG11	2.01	0.43
63:AX:76:ILE:HD13	63:AX:108:GLN:HB3	2.01	0.43
63:AX:110:LYS:HG2	63:AX:114:LYS:HE3	2.00	0.43
1:A2:1963:G:O6	1:A2:1968:C:N4	2.52	0.42
1:A2:2381:G:H2'	1:A2:2382:A:H8	1.84	0.42
1:A2:4202:G:H5''	50:AJ:145:LYS:HE3	2.01	0.42
1:A2:4485:A:O2'	42:AB:246:ARG:NH1	2.46	0.42
1:A2:4912:G:H2'	1:A2:4913:A:C8	2.54	0.42
5:B1:941:C:H2'	5:B1:942:G:C8	2.54	0.42
5:B1:1144:A:H2'	5:B1:1145:A:C8	2.53	0.42
7:BF:120:GLY:HA3	7:BF:121:PRO:HD3	1.83	0.42
23:BC:263:LYS:HG2	32:BV:50:PHE:HZ	1.84	0.42
43:AC:28:PHE:HD1	43:AC:132:ALA:HB2	1.84	0.42
43:AC:192:GLY:O	43:AC:195:LYS:NZ	2.52	0.42
47:AG:159:HIS:HB2	47:AG:184:ILE:O	2.19	0.42
86:Ct:82:SER:HA	86:Ct:86:LEU:HD12	2.00	0.42
86:Ct:697:MET:HE2	86:Ct:700:VAL:HG11	2.00	0.42
1:A2:216:G:H1	1:A2:233:G:H22	1.67	0.42
1:A2:2374:A:O2'	1:A2:2786:A:OP2	2.36	0.42
1:A2:2464:U:H3	1:A2:2472:G:H1	1.67	0.42
1:A2:3898:U:H2'	1:A2:3899:A:H8	1.85	0.42
1:A2:4422:U:H3	1:A2:4478:G:H1	1.67	0.42
5:B1:331:C:H3'	5:B1:332:G:H5''	2.00	0.42
5:B1:1260:A:H61	5:B1:1617:G:H1'	1.83	0.42
5:B1:1787:G:H2'	5:B1:1788:A:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BD:72:VAL:HA	8:BK:20:VAL:HG11	2.00	0.42
10:BP:75:VAL:HG21	10:BP:104:GLN:HG2	2.01	0.42
11:BQ:12:VAL:HG21	11:BQ:91:ALA:HA	2.00	0.42
14:BT:140:ALA:HA	14:BT:143:LYS:HE3	2.01	0.42
26:BH:123:THR:HA	26:BH:126:HIS:CE1	2.54	0.42
27:BI:139:LYS:HB3	27:BI:144:LYS:HB2	2.00	0.42
30:BN:34:LYS:HA	30:BN:37:ILE:HG22	2.01	0.42
31:BO:116:LEU:HD13	36:Ba:45:VAL:HG22	2.01	0.42
40:A4:8:G:OP2	44:AD:30:TYR:OH	2.36	0.42
42:AB:55:HIS:ND1	42:AB:369:ASP:OD2	2.38	0.42
54:AO:188:LYS:HA	54:AO:191:LYS:HB2	2.00	0.42
69:Ad:26:THR:HG23	69:Ad:85:ARG:HH11	1.84	0.42
86:Ct:742:GLU:OE2	86:Ct:767:ARG:NH2	2.51	0.42
1:A2:1975:C:H2'	1:A2:1976:G:C8	2.54	0.42
1:A2:4232:C:H5''	1:A2:4233:A:H5''	2.02	0.42
1:A2:4429:A:O2'	1:A2:4472:A:N3	2.43	0.42
5:B1:1521:C:H41	13:BS:137:LYS:HG2	1.84	0.42
5:B1:1610:G:N2	13:BS:85:ASN:OD1	2.52	0.42
12:BR:103:LYS:HD3	12:BR:117:LEU:HD12	2.01	0.42
21:BA:172:GLY:HA3	21:BA:203:PHE:HD1	1.85	0.42
27:BI:159:SER:OG	27:BI:160:SER:N	2.51	0.42
42:AB:80:GLU:OE2	42:AB:328:ASN:ND2	2.52	0.42
46:AF:226:HIS:ND1	46:AF:233:ALA:O	2.52	0.42
52:AM:24:LEU:O	52:AM:43:THR:OG1	2.31	0.42
62:AW:88:ALA:HA	62:AW:91:MET:HB2	2.00	0.42
65:AZ:36:ARG:NH1	65:AZ:38:TYR:OH	2.52	0.42
75:Aj:19:CYS:HB3	75:Aj:27:TYR:HB2	2.00	0.42
1:A2:930:A:H3'	46:AF:148:LYS:HG2	2.02	0.42
7:BF:103:LEU:HD22	7:BF:178:ILE:HD13	2.02	0.42
8:BK:72:THR:HB	8:BK:75:GLY:H	1.83	0.42
24:BE:127:ARG:HE	24:BE:142:HIS:HA	1.83	0.42
30:BN:100:LYS:O	30:BN:104:ARG:HD3	2.20	0.42
40:A4:66:G:O2'	44:AD:13:PHE:O	2.36	0.42
70:Ae:119:ALA:HB3	82:At:119:ARG:HH22	1.85	0.42
86:Ct:315:LEU:O	86:Ct:319:LEU:CB	2.60	0.42
1:A2:37:U:H4'	66:Aa:32:ARG:HD2	2.00	0.42
1:A2:455:G:C6	1:A2:687:A:N1	2.88	0.42
1:A2:700:C:H2'	1:A2:701:G:H8	1.84	0.42
1:A2:735:G:H2'	1:A2:736:G:C8	2.54	0.42
1:A2:1071:C:H2'	1:A2:1072:G:H8	1.84	0.42
1:A2:2547:C:H2'	1:A2:2548:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:2869:C:H42	1:A2:3582:A:H61	1.66	0.42
5:B1:1250:A:H4'	15:BU:73:GLY:HA2	2.01	0.42
13:BS:13:LEU:HB2	13:BS:21:ASP:HB2	2.01	0.42
40:A4:15:C:H2'	40:A4:16:A:C8	2.54	0.42
42:AB:245:HIS:CD2	42:AB:246:ARG:HG3	2.55	0.42
43:AC:292:ILE:HG21	56:AQ:31:LEU:HD11	2.01	0.42
1:A2:52:G:OP2	75:Aj:48:ASN:ND2	2.44	0.42
1:A2:486:U:H2'	1:A2:487:G:C8	2.55	0.42
1:A2:1310:C:H2'	1:A2:1311:G:C8	2.54	0.42
5:B1:53:C:H5'	35:BY:112:ASN:HD21	1.85	0.42
5:B1:980:A:H2'	5:B1:981:A:C8	2.55	0.42
22:BB:139:CYS:HB2	22:BB:172:MET:HE1	2.02	0.42
24:BE:128:LYS:HA	24:BE:156:VAL:HG13	2.00	0.42
39:A3:76:C:H2'	39:A3:77:A:C8	2.54	0.42
42:AB:372:SER:HB2	42:AB:377:GLY:HA2	2.02	0.42
47:AG:173:LEU:HD12	74:Ai:43:MET:HE1	2.01	0.42
52:AM:52:PHE:HA	52:AM:55:MET:HG2	2.01	0.42
59:AT:49:GLN:HA	59:AT:52:MET:HE3	2.01	0.42
63:AX:141:ALA:HB3	63:AX:144:TYR:HD2	1.84	0.42
83:Au:126:PRO:HA	83:Au:130:LYS:HD3	2.01	0.42
1:A2:499:G:N2	1:A2:647:U:O2	2.50	0.42
1:A2:1171:C:H2'	1:A2:1172:G:C8	2.55	0.42
1:A2:4721:C:OP1	54:AO:117:ARG:NH2	2.53	0.42
1:A2:4971:C:HO2'	1:A2:4985:C:H42	1.66	0.42
2:Bv:10:G:C5	2:Bv:45:G:N2	2.87	0.42
2:Bv:60:A:OP1	2:Bv:62:C:N4	2.47	0.42
5:B1:178:C:H2'	5:B1:179:C:H6	1.85	0.42
5:B1:1101:U:H2'	5:B1:1102:G:C8	2.55	0.42
5:B1:1474:A:H2'	5:B1:1475:G:C8	2.54	0.42
41:AA:204:MET:HE2	41:AA:209:HIS:HB2	2.01	0.42
50:AJ:93:GLU:HG2	50:AJ:173:ILE:HD12	2.02	0.42
51:AL:152:GLY:HA2	51:AL:153:PRO:HD3	1.93	0.42
53:AN:193:ARG:O	53:AN:197:THR:OG1	2.28	0.42
55:AP:129:THR:HG23	55:AP:139:TYR:HB2	2.01	0.42
1:A2:149:U:O2	1:A2:150:G:N2	2.52	0.42
1:A2:1496:U:H2'	1:A2:1497:A:C8	2.55	0.42
1:A2:1595:A:H5''	41:AA:183:GLY:HA2	2.01	0.42
1:A2:4244:A:N6	59:AT:47:THR:O	2.53	0.42
5:B1:987:A:OP1	36:Ba:37:LYS:NZ	2.41	0.42
12:BR:35:CYS:HA	12:BR:38:ILE:HG12	2.02	0.42
46:AF:80:ASN:HD21	59:AT:142:ARG:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:AL:50:PRO:HA	51:AL:148:THR:HG23	2.01	0.42
86:Ct:692:LEU:HD13	86:Ct:835:VAL:HG22	2.02	0.42
86:Ct:748:GLU:HA	86:Ct:784:VAL:O	2.20	0.42
1:A2:202:C:O2'	1:A2:205:A:N6	2.53	0.42
1:A2:1573:U:OP2	42:AB:243:LYS:NZ	2.44	0.42
1:A2:2066:G:H2'	1:A2:2067:G:H8	1.85	0.42
1:A2:2304:C:OP1	70:Ae:101:HIS:ND1	2.53	0.42
1:A2:3651:U:OP1	41:AA:54:ARG:NH2	2.50	0.42
1:A2:3888:A:H2'	1:A2:3889:G:H8	1.85	0.42
1:A2:4284:G:N2	1:A2:4287:A:OP2	2.41	0.42
5:B1:991:G:H1	36:Ba:95:ARG:HH22	1.68	0.42
5:B1:1470:C:H2'	5:B1:1471:C:C6	2.55	0.42
31:BO:95:ILE:HB	31:BO:129:ILE:HG12	2.01	0.42
35:BY:26:ASP:HA	35:BY:69:THR:O	2.19	0.42
48:AH:3:THR:HB	48:AH:67:LEU:HD11	2.01	0.42
86:Ct:131:CYS:HA	86:Ct:181:ILE:HD11	2.01	0.42
86:Ct:319:LEU:HD21	86:Ct:339:VAL:HG13	2.02	0.42
1:A2:1854:A:OP2	67:Ab:5:LYS:NZ	2.49	0.42
1:A2:2728:C:H2'	1:A2:2729:G:C8	2.55	0.42
1:A2:4308:U:O2'	80:Ao:80:LYS:O	2.32	0.42
1:A2:4435:A:OP1	78:Am:102:ARG:NH2	2.52	0.42
1:A2:4535:G:N2	1:A2:4684:G:OP2	2.53	0.42
1:A2:4721:C:H5''	54:AO:37:ARG:HH22	1.85	0.42
5:B1:499:G:N1	5:B1:501:C:O2	2.53	0.42
5:B1:1004:U:H2'	5:B1:1005:G:C8	2.55	0.42
5:B1:1609:C:OP1	13:BS:131:VAL:N	2.51	0.42
26:BH:39:GLN:O	26:BH:43:LEU:HB2	2.20	0.42
27:BI:56:ARG:NH1	27:BI:180:GLY:O	2.53	0.42
28:BJ:33:GLY:HA3	38:Be:38:TYR:CG	2.55	0.42
34:BX:68:LYS:HD3	34:BX:91:LEU:HD22	2.01	0.42
34:BX:90:CYS:HA	34:BX:93:PHE:HB2	2.01	0.42
46:AF:134:ARG:HA	46:AF:137:GLU:HG3	2.01	0.42
61:AV:96:LEU:HA	62:AW:20:ARG:O	2.20	0.42
65:AZ:11:VAL:HG11	65:AZ:80:LEU:HD13	2.02	0.42
1:A2:74:G:H5'	51:AL:59:VAL:HG13	2.01	0.41
1:A2:171:C:H2'	1:A2:172:C:C6	2.55	0.41
1:A2:732:C:H2'	1:A2:733:G:H8	1.85	0.41
1:A2:1255:C:OP2	1:A2:1256:G:N1	2.53	0.41
1:A2:1882:C:H2'	1:A2:1883:G:H8	1.85	0.41
1:A2:2038:A:N7	54:AO:18:ARG:NH1	2.68	0.41
1:A2:4139:C:OP2	53:AN:91:GLN:NE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:4547:U:H2'	1:A2:4548:G:C8	2.55	0.41
5:B1:145:G:H2'	5:B1:146:G:C8	2.55	0.41
5:B1:1593:C:H5'	11:BQ:45:ARG:HG3	2.02	0.41
41:AA:180:LEU:HD12	81:Ap:26:VAL:HG21	2.02	0.41
45:AE:213:THR:HG23	45:AE:215:ALA:H	1.84	0.41
49:AI:93:PRO:HA	49:AI:127:ALA:HB2	2.01	0.41
55:AP:42:ARG:NH1	55:AP:110:ASP:O	2.51	0.41
59:AT:8:ARG:HA	59:AT:55:LYS:HD3	2.00	0.41
66:Aa:75:LEU:HD12	66:Aa:114:LYS:H	1.84	0.41
71:Af:56:ASN:HD21	71:Af:64:PRO:HB2	1.85	0.41
83:Au:111:LEU:HD13	83:Au:138:LEU:HD11	2.01	0.41
86:Ct:18:ASN:O	86:Ct:20:ARG:NH1	2.53	0.41
86:Ct:27:HIS:HB3	86:Ct:30:HIS:HE1	1.86	0.41
86:Ct:614:ALA:O	86:Ct:698:ARG:NH2	2.52	0.41
1:A2:363:G:N2	1:A2:366:A:OP2	2.40	0.41
1:A2:730:G:H2'	1:A2:731:G:H8	1.85	0.41
1:A2:920:G:H2'	1:A2:927:C:H41	1.85	0.41
1:A2:1187:C:H2'	1:A2:1188:G:H8	1.85	0.41
1:A2:1297:C:OP1	1:A2:3852:G:N2	2.52	0.41
1:A2:1365:G:OP1	51:AL:66:TYR:OH	2.36	0.41
1:A2:1784:A:O2'	1:A2:1818:A:OP1	2.36	0.41
1:A2:1871:G:N2	1:A2:1920:A:N1	2.56	0.41
1:A2:3868:G:H4'	42:AB:254:ILE:HD13	2.02	0.41
1:A2:4058:C:H2'	1:A2:4059:G:C8	2.55	0.41
1:A2:4376:A:O2'	1:A2:4389:G:N2	2.45	0.41
1:A2:4434:G:O2'	78:Am:100:TYR:O	2.37	0.41
1:A2:4578:A:H4'	42:AB:65:SER:HB3	2.01	0.41
5:B1:1179:G:N2	5:B1:1182:A:OP2	2.52	0.41
23:BC:251:LEU:HD21	32:BV:22:ARG:HA	2.02	0.41
70:Ae:104:SER:O	70:Ae:108:ARG:HB2	2.20	0.41
72:Ag:41:ALA:HB3	72:Ag:52:ARG:HB3	2.00	0.41
79:An:15:ARG:HG2	79:An:19:LYS:HE3	2.02	0.41
1:A2:68:U:OP1	53:AN:178:HIS:ND1	2.37	0.41
1:A2:178:C:H2'	1:A2:179:G:C8	2.55	0.41
1:A2:719:U:OP1	58:AS:63:TYR:OH	2.37	0.41
1:A2:4281:C:H2'	1:A2:4282:G:H8	1.86	0.41
1:A2:4925:A:H5''	42:AB:119:TYR:HE1	1.86	0.41
5:B1:1097:G:H4'	21:BA:32:PHE:HB3	2.02	0.41
5:B1:1337:C:H2'	5:B1:1338:G:C8	2.54	0.41
5:B1:1540:G:H2'	5:B1:1541:G:C8	2.55	0.41
7:BF:30:ILE:HG23	7:BF:117:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BK:63:ALA:HB3	8:BK:68:TYR:HE2	1.86	0.41
9:BM:40:LYS:HG3	19:Bf:129:GLY:HA3	2.03	0.41
28:BJ:109:ARG:HH12	28:BJ:111:GLN:HE21	1.66	0.41
39:A3:133:G:H2'	39:A3:134:G:H8	1.86	0.41
42:AB:226:LYS:HE3	42:AB:272:LYS:HE2	2.02	0.41
51:AL:28:GLN:HG3	53:AN:201:HIS:HE1	1.86	0.41
61:AV:28:CYS:HB2	61:AV:37:LEU:HG	2.02	0.41
75:Aj:28:HIS:N	75:Aj:33:THR:O	2.50	0.41
1:A2:430:C:H2'	1:A2:431:G:C8	2.53	0.41
1:A2:465:A:N6	1:A2:677:G:N2	2.49	0.41
1:A2:1379:G:O2'	1:A2:1450:C:O2'	2.32	0.41
1:A2:1397:C:H2'	1:A2:1398:G:H8	1.86	0.41
1:A2:4221:C:O2'	50:AJ:21:CYS:SG	2.67	0.41
1:A2:4248:C:H2'	1:A2:4249:G:C8	2.56	0.41
1:A2:4597:A:OP1	1:A2:4625:G:N2	2.40	0.41
5:B1:14:C:H2'	5:B1:15:U:C6	2.55	0.41
5:B1:923:G:H2'	5:B1:924:G:H8	1.85	0.41
15:BU:86:LYS:HE2	15:BU:88:LEU:HD11	2.03	0.41
16:BZ:101:SER:HG	16:BZ:103:HIS:CD2	2.38	0.41
30:BN:84:LEU:HD12	30:BN:85:PRO:HD2	2.03	0.41
32:BV:41:LYS:H	32:BV:41:LYS:HD2	1.85	0.41
40:A4:13:A:H1'	40:A4:110:G:N7	2.36	0.41
40:A4:57:C:H2'	40:A4:58:A:H8	1.84	0.41
41:AA:117:GLU:O	41:AA:162:ASN:ND2	2.54	0.41
47:AG:154:LEU:HB3	47:AG:204:PHE:HB2	2.01	0.41
48:AH:117:PHE:HE1	48:AH:165:THR:HA	1.85	0.41
49:AI:156:LYS:NZ	49:AI:163:GLN:O	2.40	0.41
49:AI:169:LYS:NZ	49:AI:177:ASN:OD1	2.53	0.41
52:AM:5:ARG:NH2	58:AS:175:PHE:O	2.52	0.41
54:AO:194:GLU:HG3	54:AO:199:HIS:HA	2.01	0.41
76:Ak:24:LYS:HA	76:Ak:67:LYS:O	2.21	0.41
85:AK:29:ILE:HG23	85:AK:86:VAL:HG13	2.03	0.41
86:Ct:428:ARG:N	86:Ct:486:THR:O	2.47	0.41
1:A2:1679:G:N2	1:A2:2064:C:O3'	2.48	0.41
1:A2:1978:U:O2'	1:A2:1980:A:N7	2.43	0.41
1:A2:2495:G:O2'	72:Ag:62:LYS:NZ	2.53	0.41
1:A2:2586:C:H2'	1:A2:2587:G:C8	2.56	0.41
1:A2:4058:C:H2'	1:A2:4059:G:H8	1.84	0.41
1:A2:4902:C:N3	71:Af:59:THR:N	2.67	0.41
5:B1:654:A:OP2	5:B1:655:A:O2'	2.33	0.41
5:B1:1466:G:H5''	12:BR:3:ARG:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B1:1593:C:H2'	5:B1:1594:A:C8	2.56	0.41
6:BD:106:ARG:HH21	6:BD:173:ARG:HB3	1.84	0.41
25:BG:153:VAL:HG23	25:BG:156:TYR:HB2	2.02	0.41
38:Be:41:ARG:HA	38:Be:45:VAL:HG21	2.03	0.41
39:A3:148:A:H2'	39:A3:149:G:C8	2.55	0.41
47:AG:106:THR:HG22	47:AG:109:GLU:HG2	2.02	0.41
51:AL:61:CYS:HA	51:AL:62:PRO:HD3	1.95	0.41
53:AN:9:GLU:OE1	53:AN:12:ARG:NH1	2.54	0.41
65:AZ:53:VAL:HA	65:AZ:62:ILE:HD11	2.01	0.41
65:AZ:96:VAL:HG22	65:AZ:110:ALA:HB1	2.02	0.41
73:Ah:47:ILE:HD12	73:Ah:47:ILE:HA	1.89	0.41
84:Aq:142:ASN:OD1	84:Aq:143:VAL:N	2.53	0.41
1:A2:705:G:OP1	43:AC:321:ASN:ND2	2.53	0.41
1:A2:2870:U:H1'	1:A2:4974:A:C8	2.55	0.41
1:A2:4148:A:H2'	1:A2:4149:G:C8	2.56	0.41
13:BS:39:ARG:HH21	14:BT:37:VAL:HG12	1.84	0.41
21:BA:208:GLU:HA	21:BA:211:GLU:HB3	2.03	0.41
37:Bb:53:VAL:HG12	37:Bb:66:PRO:HD3	2.03	0.41
39:A3:71:A:H4'	39:A3:72:A:H5'	2.03	0.41
42:AB:47:LEU:HD12	42:AB:84:MET:HE1	2.02	0.41
54:AO:61:ARG:HA	54:AO:70:PRO:HG2	2.03	0.41
81:Ap:3:LYS:HE3	81:Ap:6:LYS:HA	2.02	0.41
84:Aq:149:HIS:HA	84:Aq:152:ILE:HD12	2.03	0.41
1:A2:20:U:OP2	39:A3:36:G:N2	2.47	0.41
1:A2:162:A:H61	1:A2:265:C:H42	1.68	0.41
1:A2:1286:A:H8	70:Ae:33:ARG:HD2	1.86	0.41
1:A2:1654:U:H5''	67:Ab:7:HIS:CE1	2.56	0.41
1:A2:2818:U:O4	1:A2:2819:A:N6	2.54	0.41
1:A2:4714:U:OP2	71:Af:100:ARG:NE	2.54	0.41
5:B1:928:G:H1	5:B1:1013:U:H3	1.68	0.41
5:B1:1013:U:H2'	5:B1:1014:G:C8	2.56	0.41
5:B1:1382:A:H2'	5:B1:1383:A:H8	1.85	0.41
5:B1:1540:G:H2'	5:B1:1541:G:H8	1.85	0.41
25:BG:186:GLN:HA	25:BG:189:ARG:HE	1.86	0.41
30:BN:88:LEU:HD11	30:BN:122:ILE:HG23	2.01	0.41
32:BV:14:PRO:HB2	32:BV:23:ILE:HG23	2.03	0.41
33:BW:24:GLN:NE2	37:Bb:7:LEU:H	2.18	0.41
51:AL:117:LEU:HD23	51:AL:117:LEU:HA	1.92	0.41
53:AN:47:LYS:HA	53:AN:50:ARG:HG2	2.03	0.41
1:A2:172:C:H2'	1:A2:173:G:C8	2.56	0.41
1:A2:511:C:H2'	1:A2:512:G:H8	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:1171:C:H2'	1:A2:1172:G:H8	1.86	0.41
1:A2:1261:C:H2'	1:A2:1262:A:C8	2.54	0.41
1:A2:1336:G:O6	56:AQ:104:ARG:NH2	2.53	0.41
1:A2:1598:U:H2'	1:A2:1599:G:H8	1.86	0.41
1:A2:1731:A:H2'	1:A2:1732:G:C8	2.55	0.41
1:A2:2351:U:H2'	1:A2:2352:C:C6	2.56	0.41
1:A2:2423:U:HO2'	39:A3:112:G:HO2'	1.60	0.41
1:A2:3632:G:H4'	1:A2:3633:A:H5'	2.02	0.41
1:A2:3694:A:H2'	1:A2:3695:A:H8	1.86	0.41
1:A2:4480:A:N7	42:AB:257:TRP:NE1	2.69	0.41
1:A2:4828:G:O5'	52:AM:94:LYS:NZ	2.52	0.41
5:B1:186:C:H2'	5:B1:187:G:C8	2.55	0.41
5:B1:524:U:OP1	5:B1:525:A:O2'	2.38	0.41
5:B1:849:A:O2'	28:BJ:69:ARG:NH1	2.54	0.41
13:BS:27:ALA:HB2	13:BS:45:LEU:HG	2.03	0.41
16:BZ:41:ARG:HH11	16:BZ:42:ASP:HB2	1.84	0.41
35:BY:89:HIS:CE1	35:BY:90:ARG:HG3	2.56	0.41
51:AL:76:PHE:CD2	51:AL:96:ILE:HG23	2.56	0.41
52:AM:7:VAL:HG12	52:AM:57:LEU:HD21	2.03	0.41
66:Aa:83:SER:HB2	66:Aa:86:THR:HG23	2.02	0.41
73:Ah:31:LEU:HB2	73:Ah:47:ILE:HD13	2.03	0.41
73:Ah:70:ARG:O	73:Ah:74:LYS:HB2	2.21	0.41
84:Aq:16:ARG:HH12	84:Aq:28:LEU:HD22	1.84	0.41
84:Aq:154:ASP:HB3	84:Aq:155:ILE:H	1.74	0.41
86:Ct:28:VAL:HG21	86:Ct:108:HIS:CE1	2.55	0.41
1:A2:91:G:OP1	80:Ao:44:LYS:NZ	2.39	0.41
1:A2:708:U:O4	1:A2:938:G:O6	2.39	0.41
1:A2:1499:G:H1	43:AC:104:PRO:HD2	1.86	0.41
1:A2:1545:A:H2'	1:A2:1546:A:C8	2.56	0.41
1:A2:1592:C:H5'	1:A2:1593:C:H5'	2.02	0.41
1:A2:1735:G:H21	44:AD:4:VAL:HG23	1.86	0.41
1:A2:1756:C:H2'	1:A2:1757:A:H8	1.85	0.41
1:A2:2062:C:H2'	1:A2:2063:G:H8	1.86	0.41
1:A2:2814:A:O2'	42:AB:228:TYR:O	2.33	0.41
1:A2:4047:A:N1	1:A2:4133:C:N4	2.66	0.41
1:A2:4499:C:N4	1:A2:4500:G:O6	2.54	0.41
5:B1:409:C:H2'	5:B1:410:G:H8	1.86	0.41
5:B1:582:U:H1'	35:BY:33:ALA:HB2	2.02	0.41
5:B1:929:G:H21	5:B1:1104:G:H4'	1.85	0.41
5:B1:1219:C:O2'	17:Bc:26:GLN:OE1	2.37	0.41
5:B1:1335:G:O6	5:B1:1492:U:O4	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B1:1447:G:H2'	5:B1:1448:A:C8	2.56	0.41
5:B1:1692:U:OP1	36:Ba:89:ARG:NH1	2.53	0.41
10:BP:64:LYS:NZ	10:BP:90:VAL:O	2.49	0.41
11:BQ:11:GLN:HE21	11:BQ:24:HIS:HD2	1.68	0.41
20:Bg:124:SER:OG	20:Bg:125:ARG:N	2.54	0.41
22:BB:36:PRO:HG2	22:BB:39:PHE:HE2	1.86	0.41
22:BB:81:PHE:CD2	22:BB:82:ARG:HG3	2.55	0.41
22:BB:186:ASN:HA	22:BB:189:ILE:HD12	2.03	0.41
25:BG:85:ARG:NH1	25:BG:86:PRO:O	2.54	0.41
32:BV:40:ASP:HB3	32:BV:41:LYS:H	1.70	0.41
36:Ba:36:ILE:HG13	36:Ba:84:VAL:HG21	2.03	0.41
45:AE:141:ARG:HB2	45:AE:144:ILE:HG12	2.03	0.41
46:AF:153:LEU:HD21	46:AF:244:ILE:HD11	2.02	0.41
51:AL:170:THR:OG1	51:AL:171:GLU:N	2.52	0.41
52:AM:25:VAL:HG12	52:AM:45:VAL:HG11	2.03	0.41
54:AO:7:LEU:HD21	54:AO:31:ARG:HH21	1.86	0.41
62:AW:86:SER:HA	62:AW:87:LEU:HA	1.88	0.41
70:Ae:75:ARG:HD2	70:Ae:95:TYR:HE1	1.86	0.41
82:At:32:LEU:HD22	82:At:110:ALA:HA	2.03	0.41
84:Aq:92:ARG:HG2	84:Aq:93:LYS:H	1.86	0.41
86:Ct:581:GLU:OE1	86:Ct:691:ALA:N	2.46	0.41
86:Ct:591:CYS:O	86:Ct:603:TYR:HA	2.20	0.41
86:Ct:766:LYS:HG3	86:Ct:796:PHE:HD1	1.85	0.41
1:A2:56:A:H2'	1:A2:57:G:C8	2.55	0.41
1:A2:708:U:O2	1:A2:938:G:N2	2.38	0.41
1:A2:1352:C:H2'	1:A2:1353:G:H21	1.86	0.41
1:A2:1437:G:H2'	1:A2:1438:G:C8	2.56	0.41
1:A2:2499:C:H2'	1:A2:2500:G:C8	2.55	0.41
1:A2:2517:U:H2'	1:A2:2518:C:H6	1.86	0.41
1:A2:3629:C:H2'	1:A2:3630:G:H8	1.86	0.41
1:A2:4285:A:C6	44:AD:153:THR:HG21	2.56	0.41
1:A2:4642:G:H2'	1:A2:4643:A:C8	2.56	0.41
5:B1:525:A:H2'	5:B1:526:A:C8	2.54	0.41
5:B1:1705:C:H2'	5:B1:1706:G:C8	2.56	0.41
8:BK:59:LYS:HB2	8:BK:70:TYR:HB3	2.02	0.41
20:Bg:236:ILE:HG12	20:Bg:252:THR:HG22	2.03	0.41
22:BB:205:TYR:HA	22:BB:206:PRO:HD3	1.93	0.41
37:Bb:67:THR:OG1	37:Bb:72:ARG:NH1	2.54	0.41
41:AA:115:CYS:HB3	41:AA:165:VAL:HG12	2.02	0.41
43:AC:289:LEU:HB3	82:At:4:HIS:CD2	2.56	0.41
61:AV:107:ASN:HD21	61:AV:111:GLU:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:AX:124:VAL:HG22	63:AX:138:VAL:HG22	2.03	0.41
86:Ct:127:VAL:O	86:Ct:155:LEU:HA	2.21	0.41
86:Ct:428:ARG:HD3	86:Ct:487:THR:HA	2.03	0.41
1:A2:312:A:H2'	1:A2:313:A:C8	2.55	0.40
1:A2:425:G:C8	1:A2:3859:G:H2'	2.56	0.40
1:A2:2575:G:H2'	1:A2:2576:G:C8	2.56	0.40
1:A2:4115:C:H2'	1:A2:4116:G:C8	2.56	0.40
1:A2:4539:U:H2'	1:A2:4540:G:C8	2.56	0.40
1:A2:4666:C:H2'	1:A2:4667:A:C8	2.56	0.40
5:B1:951:C:H2'	5:B1:952:G:H8	1.86	0.40
22:BB:205:TYR:HD2	22:BB:207:LEU:HD12	1.86	0.40
39:A3:90:C:H2'	39:A3:91:A:C8	2.56	0.40
44:AD:180:PHE:HB3	44:AD:195:HIS:CD2	2.57	0.40
56:AQ:100:VAL:HG21	56:AQ:113:ILE:HD13	2.03	0.40
84:Aq:28:LEU:HD12	84:Aq:30:PRO:HG3	2.03	0.40
86:Ct:501:VAL:HG23	86:Ct:533:MET:HE3	2.03	0.40
86:Ct:617:ILE:HG12	86:Ct:652:PHE:HZ	1.86	0.40
1:A2:630:G:H2'	1:A2:631:G:C8	2.55	0.40
1:A2:1074:C:H2'	1:A2:1075:G:C8	2.56	0.40
1:A2:2344:C:H5'	1:A2:2345:A:H5''	2.04	0.40
1:A2:3849:C:O2	1:A2:4362:G:O2'	2.39	0.40
5:B1:337:C:H2'	5:B1:338:G:C5	2.56	0.40
5:B1:940:U:H3	5:B1:1002:U:H3	1.69	0.40
5:B1:1838:U:H1'	31:BO:150:ARG:HD3	2.03	0.40
6:BD:137:VAL:HB	6:BD:185:LYS:HB2	2.03	0.40
8:BK:16:PHE:HZ	8:BK:89:ILE:HB	1.86	0.40
10:BP:24:GLN:O	10:BP:28:MET:CB	2.64	0.40
13:BS:5:ILE:HG23	13:BS:8:LYS:HE3	2.04	0.40
56:AQ:61:LEU:N	56:AQ:85:THR:O	2.54	0.40
1:A2:1806:G:H2'	1:A2:1807:A:C8	2.56	0.40
1:A2:2010:A:H2'	1:A2:2011:A:C8	2.56	0.40
1:A2:2868:G:H21	1:A2:4992:A:H1'	1.87	0.40
1:A2:3578:U:H2'	1:A2:3579:A:C8	2.56	0.40
1:A2:3624:A:H4'	41:AA:179:ILE:HB	2.03	0.40
1:A2:3688:A:N7	1:A2:3707:A:N6	2.68	0.40
1:A2:3767:U:O2'	5:B1:1720:U:O2'	2.29	0.40
1:A2:4525:U:H2'	1:A2:4526:A:H8	1.86	0.40
1:A2:4719:C:H4'	54:AO:116:LYS:HD3	2.04	0.40
5:B1:596:U:O2'	5:B1:645:C:O2	2.36	0.40
5:B1:805:U:H5''	33:BW:83:LEU:HD12	2.03	0.40
5:B1:1050:A:N6	5:B1:1068:G:H21	2.05	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B1:1262:C:O2'	18:Bd:12:ARG:NH1	2.54	0.40
5:B1:1353:A:H2'	5:B1:1354:G:C8	2.56	0.40
10:BP:38:SER:OG	10:BP:39:ALA:N	2.54	0.40
24:BE:79:ASP:HB3	24:BE:82:TYR:HB2	2.03	0.40
29:BL:82:MET:HG2	29:BL:85:THR:HG23	2.03	0.40
34:BX:84:PHE:HB2	34:BX:118:VAL:HG11	2.03	0.40
40:A4:63:C:H5'	40:A4:64:G:H5''	2.02	0.40
44:AD:17:GLN:HG3	59:AT:20:ARG:HA	2.03	0.40
45:AE:168:LEU:HD11	45:AE:174:LEU:HD12	2.02	0.40
49:AI:135:ILE:HG22	49:AI:136:MET:HG3	2.02	0.40
55:AP:64:ASN:HD22	55:AP:78:TRP:HZ2	1.68	0.40
64:AY:86:GLN:HE22	64:AY:96:HIS:CE1	2.39	0.40
70:Ae:21:ILE:HD11	70:Ae:33:ARG:HH11	1.85	0.40
70:Ae:90:MET:HE2	82:At:33:LYS:HE2	2.03	0.40
84:Aq:126:SER:HA	84:Aq:129:ILE:HD12	2.02	0.40
85:AK:126:GLN:NE2	85:AK:127:ASN:OD1	2.48	0.40
86:Ct:55:ARG:NH1	89:Ct:901:GNP:O1A	2.43	0.40
86:Ct:111:PHE:HZ	86:Ct:556:ILE:HG13	1.86	0.40
1:A2:4139:C:H2'	1:A2:4140:A:C8	2.57	0.40
5:B1:307:G:N7	27:BI:44:HIS:ND1	2.52	0.40
5:B1:1377:U:N3	5:B1:1379:A:O3'	2.54	0.40
11:BQ:39:LEU:HD21	11:BQ:55:VAL:HG21	2.04	0.40
20:Bg:65:PHE:HB2	20:Bg:83:TRP:CD1	2.56	0.40
25:BG:213:LEU:HD23	25:BG:217:MET:HE2	2.02	0.40
42:AB:50:LYS:HB2	42:AB:345:LEU:HD11	2.03	0.40
1:A2:175:C:H2'	1:A2:176:G:C8	2.56	0.40
1:A2:435:G:H2'	1:A2:436:G:H8	1.86	0.40
1:A2:1365:G:H2'	1:A2:1366:G:H8	1.85	0.40
1:A2:1923:A:H2'	1:A2:1924:A:H8	1.86	0.40
1:A2:2633:C:H2'	1:A2:2634:C:H6	1.86	0.40
1:A2:3624:A:N6	1:A2:3662:G:O2'	2.49	0.40
1:A2:3676:G:H21	41:AA:224:THR:HG21	1.86	0.40
1:A2:3939:U:H2'	1:A2:3940:G:C8	2.57	0.40
1:A2:4199:C:O2	1:A2:4283:U:O2'	2.37	0.40
1:A2:4201:A:H2'	1:A2:4202:G:H8	1.86	0.40
1:A2:4236:A:H2'	1:A2:4237:G:H8	1.86	0.40
5:B1:24:C:OP1	28:BJ:11:LYS:NZ	2.42	0.40
5:B1:92:A:H61	5:B1:444:G:H1'	1.86	0.40
5:B1:204:G:H2'	5:B1:205:G:H8	1.87	0.40
5:B1:219:U:O2'	27:BI:186:ASP:OD2	2.34	0.40
5:B1:844:U:H2'	5:B1:845:G:H8	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BD:157:MET:HE3	6:BD:187:LYS:HG3	2.04	0.40
11:BQ:15:ARG:HD3	11:BQ:15:ARG:HA	1.92	0.40
14:BT:64:LEU:HB3	14:BT:121:ARG:HD2	2.04	0.40
37:Bb:37:CYS:HA	37:Bb:38:PRO:HD3	1.90	0.40
39:A3:65:A:O2'	73:Ah:10:ARG:NH2	2.48	0.40
43:AC:210:ILE:HG12	43:AC:230:LEU:HD12	2.03	0.40
48:AH:41:ILE:HG22	48:AH:43:VAL:HG23	2.02	0.40
48:AH:86:LEU:HB3	48:AH:186:THR:HB	2.04	0.40
49:AI:46:PHE:HB2	49:AI:139:ARG:CZ	2.52	0.40
59:AT:5:LYS:HA	59:AT:9:ARG:HD3	2.04	0.40
86:Ct:376:PRO:HA	86:Ct:377:PRO:HD3	1.99	0.40
86:Ct:687:THR:HG23	86:Ct:697:MET:HB2	2.03	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	
6	BD	218/220 (99%)	209 (96%)	9 (4%)	0	100	100
7	BF	188/190 (99%)	173 (92%)	15 (8%)	0	100	100
8	BK	96/98 (98%)	82 (85%)	13 (14%)	1 (1%)	12	45
9	BM	118/120 (98%)	110 (93%)	8 (7%)	0	100	100
10	BP	118/120 (98%)	105 (89%)	12 (10%)	1 (1%)	16	49
11	BQ	137/139 (99%)	128 (93%)	9 (7%)	0	100	100
12	BR	123/125 (98%)	109 (89%)	14 (11%)	0	100	100
13	BS	137/139 (99%)	125 (91%)	12 (9%)	0	100	100
14	BT	141/143 (99%)	130 (92%)	10 (7%)	1 (1%)	18	51
15	BU	95/97 (98%)	91 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	BZ	84/86 (98%)	74 (88%)	10 (12%)	0	100	100
17	Bc	60/62 (97%)	55 (92%)	3 (5%)	2 (3%)	3	24
18	Bd	49/51 (96%)	46 (94%)	3 (6%)	0	100	100
19	Bf	71/73 (97%)	63 (89%)	8 (11%)	0	100	100
20	Bg	312/314 (99%)	283 (91%)	29 (9%)	0	100	100
21	BA	213/215 (99%)	199 (93%)	14 (7%)	0	100	100
22	BB	210/212 (99%)	180 (86%)	30 (14%)	0	100	100
23	BC	220/222 (99%)	206 (94%)	14 (6%)	0	100	100
24	BE	255/257 (99%)	236 (92%)	17 (7%)	2 (1%)	16	49
25	BG	230/232 (99%)	216 (94%)	14 (6%)	0	100	100
26	BH	181/183 (99%)	166 (92%)	15 (8%)	0	100	100
27	BI	205/207 (99%)	177 (86%)	27 (13%)	1 (0%)	24	57
28	BJ	177/179 (99%)	157 (89%)	18 (10%)	2 (1%)	11	43
29	BL	151/153 (99%)	138 (91%)	12 (8%)	1 (1%)	18	51
30	BN	147/149 (99%)	131 (89%)	16 (11%)	0	100	100
31	BO	134/136 (98%)	122 (91%)	12 (9%)	0	100	100
32	BV	79/81 (98%)	76 (96%)	3 (4%)	0	100	100
33	BW	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
34	BX	139/141 (99%)	122 (88%)	17 (12%)	0	100	100
35	BY	123/125 (98%)	111 (90%)	12 (10%)	0	100	100
36	Ba	95/97 (98%)	87 (92%)	8 (8%)	0	100	100
37	Bb	78/80 (98%)	71 (91%)	7 (9%)	0	100	100
38	Be	53/55 (96%)	49 (92%)	4 (8%)	0	100	100
41	AA	250/252 (99%)	235 (94%)	15 (6%)	0	100	100
42	AB	392/394 (100%)	361 (92%)	31 (8%)	0	100	100
43	AC	361/363 (99%)	335 (93%)	22 (6%)	4 (1%)	11	43
44	AD	292/294 (99%)	269 (92%)	23 (8%)	0	100	100
45	AE	192/194 (99%)	161 (84%)	30 (16%)	1 (0%)	24	57
46	AF	232/234 (99%)	214 (92%)	18 (8%)	0	100	100
47	AG	232/234 (99%)	218 (94%)	14 (6%)	0	100	100
48	AH	189/191 (99%)	175 (93%)	14 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	AI	204/211 (97%)	181 (89%)	23 (11%)	0	100	100
50	AJ	167/169 (99%)	152 (91%)	14 (8%)	1 (1%)	21	54
51	AL	203/205 (99%)	171 (84%)	31 (15%)	1 (0%)	24	57
52	AM	137/139 (99%)	127 (93%)	10 (7%)	0	100	100
53	AN	201/203 (99%)	185 (92%)	16 (8%)	0	100	100
54	AO	193/195 (99%)	186 (96%)	7 (4%)	0	100	100
55	AP	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
56	AQ	185/187 (99%)	163 (88%)	21 (11%)	1 (0%)	24	57
57	AR	179/181 (99%)	168 (94%)	11 (6%)	0	100	100
58	AS	173/175 (99%)	163 (94%)	10 (6%)	0	100	100
59	AT	155/157 (99%)	138 (89%)	15 (10%)	2 (1%)	9	39
60	AU	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
61	AV	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
62	AW	119/121 (98%)	108 (91%)	11 (9%)	0	100	100
63	AX	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
64	AY	125/127 (98%)	119 (95%)	6 (5%)	0	100	100
65	AZ	132/134 (98%)	115 (87%)	17 (13%)	0	100	100
66	Aa	145/147 (99%)	131 (90%)	14 (10%)	0	100	100
67	Ab	66/68 (97%)	56 (85%)	10 (15%)	0	100	100
68	Ac	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
69	Ad	104/106 (98%)	101 (97%)	3 (3%)	0	100	100
70	Ae	127/129 (98%)	116 (91%)	11 (9%)	0	100	100
71	Af	107/109 (98%)	95 (89%)	10 (9%)	2 (2%)	6	33
72	Ag	112/114 (98%)	100 (89%)	12 (11%)	0	100	100
73	Ah	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
74	Ai	95/97 (98%)	85 (90%)	10 (10%)	0	100	100
75	Aj	82/84 (98%)	73 (89%)	9 (11%)	0	100	100
76	Ak	67/69 (97%)	64 (96%)	3 (4%)	0	100	100
77	Al	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
78	Am	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
79	An	23/25 (92%)	23 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
80	Ao	103/105 (98%)	96 (93%)	7 (7%)	0	100	100
81	Ap	89/91 (98%)	83 (93%)	6 (7%)	0	100	100
82	At	120/122 (98%)	105 (88%)	15 (12%)	0	100	100
83	Au	215/217 (99%)	197 (92%)	18 (8%)	0	100	100
84	Aq	149/151 (99%)	112 (75%)	37 (25%)	0	100	100
85	AK	200/202 (99%)	179 (90%)	20 (10%)	1 (0%)	24	57
86	Ct	850/853 (100%)	768 (90%)	79 (9%)	3 (0%)	30	61
All	All	12538/12702 (99%)	11449 (91%)	1062 (8%)	27 (0%)	44	72

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	BP	51	ARG
28	BJ	138	ARG
71	Af	107	PRO
24	BE	93	GLU
51	AL	78	LEU
71	Af	106	TYR
85	AK	150	GLY
86	Ct	159	LYS
8	BK	41	PRO
14	BT	31	PRO
43	AC	51	PRO
50	AJ	53	ALA
17	Bc	33	GLU
45	AE	136	HIS
56	AQ	161	SER
86	Ct	649	ILE
24	BE	150	PRO
27	BI	160	SER
29	BL	14	PRO
43	AC	52	TYR
86	Ct	464	VAL
43	AC	72	ALA
59	AT	53	PRO
28	BJ	123	ILE
43	AC	151	PRO
17	Bc	32	VAL
59	AT	18	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	
6	BD	183/183 (100%)	183 (100%)	0	100	100
7	BF	160/160 (100%)	160 (100%)	0	100	100
8	BK	89/89 (100%)	89 (100%)	0	100	100
9	BM	102/102 (100%)	102 (100%)	0	100	100
10	BP	109/109 (100%)	108 (99%)	1 (1%)	70	76
11	BQ	115/115 (100%)	115 (100%)	0	100	100
12	BR	113/113 (100%)	113 (100%)	0	100	100
13	BS	121/121 (100%)	121 (100%)	0	100	100
14	BT	113/113 (100%)	112 (99%)	1 (1%)	70	76
15	BU	90/90 (100%)	90 (100%)	0	100	100
16	BZ	75/75 (100%)	75 (100%)	0	100	100
17	Bc	55/55 (100%)	55 (100%)	0	100	100
18	Bd	45/45 (100%)	45 (100%)	0	100	100
19	Bf	66/66 (100%)	66 (100%)	0	100	100
20	Bg	272/272 (100%)	271 (100%)	1 (0%)	84	81
21	BA	180/180 (100%)	180 (100%)	0	100	100
22	BB	193/193 (100%)	193 (100%)	0	100	100
23	BC	188/188 (100%)	188 (100%)	0	100	100
24	BE	220/220 (100%)	220 (100%)	0	100	100
25	BG	202/202 (100%)	202 (100%)	0	100	100
26	BH	164/164 (100%)	164 (100%)	0	100	100
27	BI	179/179 (100%)	179 (100%)	0	100	100
28	BJ	160/160 (100%)	160 (100%)	0	100	100
29	BL	138/138 (100%)	138 (100%)	0	100	100
30	BN	130/130 (100%)	129 (99%)	1 (1%)	73	77
31	BO	106/106 (100%)	106 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	BV	65/65 (100%)	65 (100%)	0	100	100
33	BW	112/112 (100%)	112 (100%)	0	100	100
34	BX	113/113 (100%)	113 (100%)	0	100	100
35	BY	107/107 (100%)	107 (100%)	0	100	100
36	Ba	84/84 (100%)	84 (100%)	0	100	100
37	Bb	72/72 (100%)	72 (100%)	0	100	100
38	Be	44/44 (100%)	44 (100%)	0	100	100
41	AA	194/194 (100%)	194 (100%)	0	100	100
42	AB	343/343 (100%)	343 (100%)	0	100	100
43	AC	302/302 (100%)	301 (100%)	1 (0%)	86	83
44	AD	248/248 (100%)	248 (100%)	0	100	100
45	AE	174/174 (100%)	174 (100%)	0	100	100
46	AF	203/203 (100%)	203 (100%)	0	100	100
47	AG	199/199 (100%)	198 (100%)	1 (0%)	81	80
48	AH	170/170 (100%)	170 (100%)	0	100	100
49	AI	178/179 (99%)	178 (100%)	0	100	100
50	AJ	142/142 (100%)	142 (100%)	0	100	100
51	AL	171/171 (100%)	170 (99%)	1 (1%)	78	79
52	AM	118/118 (100%)	117 (99%)	1 (1%)	73	77
53	AN	171/171 (100%)	171 (100%)	0	100	100
54	AO	168/168 (100%)	167 (99%)	1 (1%)	78	79
55	AP	134/134 (100%)	134 (100%)	0	100	100
56	AQ	164/164 (100%)	164 (100%)	0	100	100
57	AR	160/160 (100%)	160 (100%)	0	100	100
58	AS	156/156 (100%)	156 (100%)	0	100	100
59	AT	138/138 (100%)	138 (100%)	0	100	100
60	AU	89/89 (100%)	89 (100%)	0	100	100
61	AV	100/100 (100%)	100 (100%)	0	100	100
62	AW	100/100 (100%)	100 (100%)	0	100	100
63	AX	105/105 (100%)	105 (100%)	0	100	100
64	AY	119/119 (100%)	119 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
65	AZ	117/117 (100%)	117 (100%)	0	100	100
66	Aa	120/120 (100%)	120 (100%)	0	100	100
67	Ab	58/58 (100%)	58 (100%)	0	100	100
68	Ac	88/88 (100%)	88 (100%)	0	100	100
69	Ad	97/97 (100%)	97 (100%)	0	100	100
70	Ae	115/115 (100%)	115 (100%)	0	100	100
71	Af	88/88 (100%)	88 (100%)	0	100	100
72	Ag	98/98 (100%)	98 (100%)	0	100	100
73	Ah	109/109 (100%)	109 (100%)	0	100	100
74	Ai	83/83 (100%)	83 (100%)	0	100	100
75	Aj	71/71 (100%)	70 (99%)	1 (1%)	59	71
76	Ak	64/64 (100%)	64 (100%)	0	100	100
77	Al	47/47 (100%)	47 (100%)	0	100	100
78	Am	46/46 (100%)	46 (100%)	0	100	100
79	An	24/24 (100%)	24 (100%)	0	100	100
80	Ao	93/93 (100%)	93 (100%)	0	100	100
81	Ap	74/74 (100%)	74 (100%)	0	100	100
82	At	106/106 (100%)	106 (100%)	0	100	100
83	Au	196/196 (100%)	195 (100%)	1 (0%)	81	80
84	Aq	124/124 (100%)	123 (99%)	1 (1%)	73	77
85	AK	170/170 (100%)	170 (100%)	0	100	100
86	Ct	725/725 (100%)	724 (100%)	1 (0%)	88	87
All	All	10924/10925 (100%)	10911 (100%)	13 (0%)	87	87

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	BP	60	LEU
14	BT	37	VAL
20	Bg	133	ASN
30	BN	104	ARG
43	AC	230	LEU
47	AG	84	THR
51	AL	154	VAL

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Mol	Chain	Res	Type
52	AM	95	ILE
54	AO	184	ASN
75	Aj	67	LEU
83	Au	197	ASN
84	Aq	28	LEU
86	Ct	692	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (208) such sidechains are listed below:

Mol	Chain	Res	Type
7	BF	82	ASN
7	BF	95	HIS
7	BF	101	HIS
7	BF	110	GLN
7	BF	165	ASN
7	BF	203	ASN
8	BK	32	HIS
9	BM	55	ASN
10	BP	41	GLN
10	BP	54	HIS
10	BP	103	ASN
11	BQ	11	GLN
11	BQ	80	GLN
12	BR	62	GLN
13	BS	10	GLN
13	BS	17	ASN
13	BS	76	GLN
13	BS	87	GLN
13	BS	97	GLN
14	BT	11	GLN
14	BT	91	HIS
16	BZ	89	GLN
16	BZ	106	GLN
16	BZ	112	ASN
17	Bc	24	GLN
17	Bc	29	GLN
18	Bd	5	GLN
19	Bf	139	HIS
20	Bg	133	ASN
20	Bg	226	HIS
20	Bg	305	ASN
21	BA	36	GLN

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Mol	Chain	Res	Type
21	BA	149	ASN
22	BB	76	ASN
22	BB	157	GLN
22	BB	177	GLN
22	BB	202	GLN
23	BC	134	ASN
23	BC	136	HIS
23	BC	272	HIS
24	BE	67	GLN
24	BE	161	GLN
24	BE	197	ASN
25	BG	56	ASN
25	BG	70	HIS
25	BG	186	GLN
25	BG	187	HIS
25	BG	202	ASN
26	BH	39	GLN
26	BH	97	GLN
26	BH	193	GLN
27	BI	165	GLN
27	BI	168	GLN
28	BJ	140	GLN
28	BJ	156	HIS
29	BL	108	ASN
30	BN	5	HIS
30	BN	58	HIS
30	BN	62	GLN
30	BN	90	HIS
31	BO	32	HIS
33	BW	5	ASN
33	BW	15	ASN
33	BW	16	ASN
33	BW	92	ASN
33	BW	98	GLN
34	BX	16	HIS
34	BX	39	ASN
34	BX	61	GLN
34	BX	97	ASN
34	BX	127	ASN
35	BY	15	ASN
35	BY	29	HIS
35	BY	89	HIS

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Mol	Chain	Res	Type
35	BY	112	ASN
36	Ba	86	ASN
37	Bb	9	HIS
37	Bb	51	GLN
41	AA	83	HIS
41	AA	97	ASN
41	AA	132	ASN
41	AA	162	ASN
41	AA	205	ASN
42	AB	167	GLN
42	AB	179	HIS
42	AB	380	GLN
43	AC	38	ASN
43	AC	41	HIS
43	AC	48	ASN
43	AC	60	HIS
43	AC	94	ASN
43	AC	198	ASN
43	AC	215	ASN
43	AC	278	ASN
43	AC	310	HIS
43	AC	321	ASN
44	AD	9	ASN
44	AD	111	ASN
44	AD	122	GLN
44	AD	191	ASN
44	AD	195	HIS
44	AD	222	GLN
45	AE	167	GLN
45	AE	191	GLN
45	AE	279	ASN
46	AF	24	ASN
46	AF	146	ASN
47	AG	43	GLN
47	AG	149	ASN
47	AG	206	GLN
48	AH	98	HIS
48	AH	140	GLN
49	AI	14	ASN
49	AI	51	HIS
49	AI	130	HIS
49	AI	147	HIS

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Mol	Chain	Res	Type
49	AI	166	HIS
50	AJ	71	HIS
50	AJ	112	HIS
50	AJ	155	HIS
51	AL	149	GLN
51	AL	159	ASN
51	AL	175	ASN
52	AM	70	GLN
52	AM	125	ASN
53	AN	8	GLN
53	AN	15	GLN
53	AN	37	HIS
53	AN	86	HIS
53	AN	87	HIS
53	AN	199	GLN
54	AO	65	ASN
54	AO	143	HIS
54	AO	180	GLN
54	AO	184	ASN
55	AP	40	HIS
55	AP	75	GLN
55	AP	97	ASN
55	AP	133	HIS
56	AQ	7	HIS
57	AR	178	GLN
58	AS	66	GLN
58	AS	77	ASN
58	AS	91	HIS
59	AT	22	HIS
59	AT	98	HIS
59	AT	139	HIS
60	AU	50	ASN
61	AV	101	ASN
62	AW	17	HIS
62	AW	45	ASN
62	AW	48	GLN
63	AX	107	HIS
63	AX	108	GLN
64	AY	4	ASN
64	AY	18	HIS
64	AY	20	ASN
64	AY	61	HIS

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Mol	Chain	Res	Type
64	AY	96	HIS
66	Aa	39	HIS
66	Aa	40	HIS
66	Aa	60	HIS
66	Aa	89	ASN
67	Ab	61	ASN
69	Ad	28	ASN
70	Ae	52	GLN
70	Ae	107	ASN
72	Ag	3	GLN
72	Ag	73	HIS
73	Ah	107	GLN
75	Aj	13	ASN
75	Aj	57	ASN
75	Aj	76	HIS
77	Al	20	ASN
77	Al	43	HIS
78	Am	120	ASN
80	Ao	3	ASN
80	Ao	19	GLN
80	Ao	36	GLN
82	At	36	ASN
82	At	41	ASN
83	Au	21	ASN
83	Au	40	ASN
83	Au	73	HIS
83	Au	143	ASN
83	Au	171	HIS
83	Au	188	ASN
83	Au	197	ASN
84	Aq	111	ASN
85	AK	39	GLN
85	AK	72	ASN
86	Ct	101	ASN
86	Ct	138	GLN
86	Ct	145	GLN
86	Ct	158	ASN
86	Ct	179	GLN
86	Ct	306	ASN
86	Ct	352	GLN
86	Ct	433	ASN
86	Ct	448	GLN

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Mol	Chain	Res	Type
86	Ct	492	HIS
86	Ct	544	HIS
86	Ct	565	HIS
86	Ct	588	ASN
86	Ct	599	HIS
86	Ct	803	ASN
86	Ct	807	GLN
86	Ct	811	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A2	3600/3612 (99%)	706 (19%)	9 (0%)
2	Bv	75/76 (98%)	12 (16%)	0
3	Bx	11/12 (91%)	6 (54%)	0
39	A3	156/157 (99%)	35 (22%)	0
4	Bw	75/76 (98%)	13 (17%)	0
40	A4	118/119 (99%)	21 (17%)	0
5	B1	1701/1708 (99%)	336 (19%)	4 (0%)
All	All	5736/5760 (99%)	1129 (19%)	13 (0%)

All (1129) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A2	8	U
1	A2	9	C
1	A2	10	A
1	A2	12	A
1	A2	14	C
1	A2	25	A
1	A2	32	G
1	A2	39	A
1	A2	40	G
1	A2	42	A
1	A2	48	G
1	A2	49	U
1	A2	59	A
1	A2	65	A
1	A2	71	C
1	A2	72	C
1	A2	74	G

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Mol	Chain	Res	Type
1	A2	76	A
1	A2	84	A
1	A2	91	G
1	A2	101	A
1	A2	108	A
1	A2	110	C
1	A2	116	G
1	A2	119	G
1	A2	120	A
1	A2	131	C
1	A2	132	G
1	A2	133	C
1	A2	134	G
1	A2	135	G
1	A2	143	G
1	A2	149	U
1	A2	155	A
1	A2	157	G
1	A2	167	C
1	A2	169	C
1	A2	176	G
1	A2	181	U
1	A2	182	C
1	A2	183	G
1	A2	184	U
1	A2	185	G
1	A2	196	G
1	A2	198	C
1	A2	201	U
1	A2	206	U
1	A2	212	C
1	A2	213	C
1	A2	214	C
1	A2	215	A
1	A2	228	U
1	A2	229	G
1	A2	230	U
1	A2	233	G
1	A2	234	G
1	A2	236	C
1	A2	241	G
1	A2	253	G

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Mol	Chain	Res	Type
1	A2	258	C
1	A2	260	C
1	A2	275	U
1	A2	282	G
1	A2	286	G
1	A2	289	A
1	A2	291	U
1	A2	300	A
1	A2	309	G
1	A2	310	U
1	A2	311	A
1	A2	323	A
1	A2	330	A
1	A2	334	C
1	A2	338	A
1	A2	351	U
1	A2	357	A
1	A2	367	G
1	A2	370	A
1	A2	375	U
1	A2	380	A
1	A2	381	G
1	A2	390	A
1	A2	425	G
1	A2	426	U
1	A2	434	U
1	A2	446	A
1	A2	447	G
1	A2	448	U
1	A2	449	C
1	A2	450	C
1	A2	460	A
1	A2	463	C
1	A2	479	C
1	A2	482	G
1	A2	487	G
1	A2	489	C
1	A2	492	C
1	A2	494	G
1	A2	496	C
1	A2	497	C
1	A2	498	G

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Mol	Chain	Res	Type
1	A2	499	G
1	A2	504	U
1	A2	505	C
1	A2	507	U
1	A2	509	C
1	A2	513	C
1	A2	634	C
1	A2	635	G
1	A2	643	A
1	A2	647	U
1	A2	649	C
1	A2	658	G
1	A2	661	G
1	A2	676	G
1	A2	677	G
1	A2	678	C
1	A2	680	C
1	A2	691	G
1	A2	692	G
1	A2	695	C
1	A2	698	C
1	A2	714	A
1	A2	719	U
1	A2	720	G
1	A2	721	G
1	A2	737	A
1	A2	738	A
1	A2	739	G
1	A2	902	A
1	A2	905	G
1	A2	906	C
1	A2	907	C
1	A2	909	C
1	A2	914	G
1	A2	917	G
1	A2	918	C
1	A2	919	A
1	A2	923	C
1	A2	924	U
1	A2	925	C
1	A2	927	C
1	A2	929	G

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Mol	Chain	Res	Type
1	A2	931	A
1	A2	932	U
1	A2	933	C
1	A2	934	C
1	A2	944	G
1	A2	947	A
1	A2	948	G
1	A2	949	C
1	A2	950	G
1	A2	951	A
1	A2	953	A
1	A2	955	C
1	A2	956	C
1	A2	960	G
1	A2	961	C
1	A2	962	C
1	A2	968	C
1	A2	969	U
1	A2	1055	C
1	A2	1067	C
1	A2	1087	C
1	A2	1147	G
1	A2	1149	G
1	A2	1150	C
1	A2	1152	G
1	A2	1156	G
1	A2	1161	G
1	A2	1162	U
1	A2	1165	C
1	A2	1167	A
1	A2	1190	C
1	A2	1192	U
1	A2	1193	C
1	A2	1196	G
1	A2	1201	G
1	A2	1220	C
1	A2	1221	A
1	A2	1222	C
1	A2	1223	G
1	A2	1225	G
1	A2	1226	C
1	A2	1229	G

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Mol	Chain	Res	Type
1	A2	1250	C
1	A2	1251	G
1	A2	1255	C
1	A2	1256	G
1	A2	1259	C
1	A2	1263	C
1	A2	1264	G
1	A2	1265	G
1	A2	1268	U
1	A2	1271	G
1	A2	1277	A
1	A2	1278	C
1	A2	1284	C
1	A2	1309	A
1	A2	1336	G
1	A2	1337	A
1	A2	1341	G
1	A2	1343	G
1	A2	1348	C
1	A2	1349	G
1	A2	1351	A
1	A2	1353	G
1	A2	1364	U
1	A2	1370	A
1	A2	1373	G
1	A2	1380	A
1	A2	1381	A
1	A2	1391	G
1	A2	1392	C
1	A2	1403	A
1	A2	1421	U
1	A2	1424	C
1	A2	1426	A
1	A2	1428	U
1	A2	1430	C
1	A2	1432	C
1	A2	1439	G
1	A2	1463	C
1	A2	1464	G
1	A2	1465	C
1	A2	1466	G
1	A2	1468	C

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Mol	Chain	Res	Type
1	A2	1479	A
1	A2	1480	G
1	A2	1483	C
1	A2	1485	A
1	A2	1499	G
1	A2	1500	A
1	A2	1501	C
1	A2	1505	A
1	A2	1516	A
1	A2	1521	G
1	A2	1525	G
1	A2	1548	C
1	A2	1556	G
1	A2	1559	G
1	A2	1560	U
1	A2	1573	U
1	A2	1576	C
1	A2	1578	U
1	A2	1583	A
1	A2	1589	C
1	A2	1593	C
1	A2	1594	G
1	A2	1595	A
1	A2	1606	G
1	A2	1607	G
1	A2	1613	A
1	A2	1615	G
1	A2	1616	A
1	A2	1623	G
1	A2	1631	U
1	A2	1632	A
1	A2	1636	G
1	A2	1643	C
1	A2	1676	C
1	A2	1678	C
1	A2	1679	G
1	A2	1701	A
1	A2	1706	G
1	A2	1713	C
1	A2	1723	G
1	A2	1728	A
1	A2	1736	U

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Mol	Chain	Res	Type
1	A2	1739	U
1	A2	1747	A
1	A2	1748	A
1	A2	1751	G
1	A2	1763	U
1	A2	1769	A
1	A2	1776	A
1	A2	1785	G
1	A2	1786	A
1	A2	1788	G
1	A2	1794	C
1	A2	1797	G
1	A2	1804	U
1	A2	1807	A
1	A2	1814	G
1	A2	1815	U
1	A2	1816	G
1	A2	1818	A
1	A2	1823	G
1	A2	1835	G
1	A2	1836	G
1	A2	1844	U
1	A2	1850	G
1	A2	1862	C
1	A2	1869	A
1	A2	1872	A
1	A2	1873	A
1	A2	1896	C
1	A2	1897	G
1	A2	1898	A
1	A2	1902	C
1	A2	1903	G
1	A2	1911	U
1	A2	1912	C
1	A2	1913	A
1	A2	1916	C
1	A2	1920	A
1	A2	1928	U
1	A2	1929	G
1	A2	1932	G
1	A2	1936	G
1	A2	1940	U

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Mol	Chain	Res	Type
1	A2	1941	A
1	A2	1942	G
1	A2	1943	A
1	A2	1945	A
1	A2	1955	U
1	A2	1956	G
1	A2	1959	C
1	A2	1961	U
1	A2	1963	G
1	A2	1964	A
1	A2	1967	U
1	A2	1968	C
1	A2	1973	U
1	A2	1978	U
1	A2	1983	A
1	A2	1984	G
1	A2	1985	U
1	A2	1988	G
1	A2	1989	U
1	A2	1990	A
1	A2	1991	A
1	A2	2007	A
1	A2	2015	G
1	A2	2026	G
1	A2	2027	G
1	A2	2029	U
1	A2	2033	G
1	A2	2035	U
1	A2	2037	G
1	A2	2043	C
1	A2	2050	A
1	A2	2246	U
1	A2	2258	A
1	A2	2268	C
1	A2	2279	A
1	A2	2280	G
1	A2	2282	C
1	A2	2283	U
1	A2	2285	G
1	A2	2292	A
1	A2	2299	G
1	A2	2301	G

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Mol	Chain	Res	Type
1	A2	2308	U
1	A2	2310	G
1	A2	2327	G
1	A2	2330	C
1	A2	2339	A
1	A2	2340	G
1	A2	2363	U
1	A2	2373	G
1	A2	2374	A
1	A2	2389	C
1	A2	2400	G
1	A2	2401	C
1	A2	2404	U
1	A2	2426	U
1	A2	2442	G
1	A2	2447	U
1	A2	2450	G
1	A2	2467	C
1	A2	2468	C
1	A2	2469	U
1	A2	2482	G
1	A2	2484	C
1	A2	2485	G
1	A2	2492	A
1	A2	2524	U
1	A2	2525	G
1	A2	2526	G
1	A2	2532	A
1	A2	2561	A
1	A2	2565	G
1	A2	2566	A
1	A2	2567	C
1	A2	2568	C
1	A2	2570	A
1	A2	2579	A
1	A2	2580	A
1	A2	2584	G
1	A2	2585	G
1	A2	2606	C
1	A2	2617	G
1	A2	2632	C
1	A2	2637	G

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Mol	Chain	Res	Type
1	A2	2638	A
1	A2	2648	C
1	A2	2665	G
1	A2	2666	U
1	A2	2673	G
1	A2	2675	A
1	A2	2676	A
1	A2	2684	G
1	A2	2690	G
1	A2	2691	G
1	A2	2698	C
1	A2	2700	G
1	A2	2704	A
1	A2	2705	G
1	A2	2706	C
1	A2	2718	C
1	A2	2719	U
1	A2	2720	U
1	A2	2726	U
1	A2	2732	G
1	A2	2733	G
1	A2	2739	G
1	A2	2741	G
1	A2	2742	U
1	A2	2745	A
1	A2	2748	U
1	A2	2751	C
1	A2	2766	A
1	A2	2767	U
1	A2	2769	U
1	A2	2773	C
1	A2	2776	C
1	A2	2785	A
1	A2	2786	A
1	A2	2793	C
1	A2	2804	A
1	A2	2805	U
1	A2	2806	G
1	A2	2814	A
1	A2	2822	U
1	A2	2839	C
1	A2	2858	A

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Mol	Chain	Res	Type
1	A2	2860	A
1	A2	2871	C
1	A2	2879	U
1	A2	3572	C
1	A2	3586	G
1	A2	3588	G
1	A2	3589	C
1	A2	3591	G
1	A2	3596	G
1	A2	3597	G
1	A2	3601	A
1	A2	3606	A
1	A2	3612	U
1	A2	3614	A
1	A2	3615	U
1	A2	3616	U
1	A2	3627	A
1	A2	3633	A
1	A2	3643	G
1	A2	3649	G
1	A2	3651	U
1	A2	3663	A
1	A2	3669	G
1	A2	3682	A
1	A2	3683	A
1	A2	3707	A
1	A2	3719	A
1	A2	3724	G
1	A2	3730	A
1	A2	3732	C
1	A2	3738	C
1	A2	3747	G
1	A2	3748	G
1	A2	3751	G
1	A2	3754	A
1	A2	3781	C
1	A2	3782	G
1	A2	3785	U
1	A2	3788	A
1	A2	3789	U
1	A2	3790	G
1	A2	3795	A

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Mol	Chain	Res	Type
1	A2	3798	G
1	A2	3799	A
1	A2	3809	U
1	A2	3810	G
1	A2	3811	U
1	A2	3814	C
1	A2	3831	A
1	A2	3847	A
1	A2	3848	A
1	A2	3850	G
1	A2	3851	G
1	A2	3852	G
1	A2	3860	G
1	A2	3863	U
1	A2	3866	G
1	A2	3872	A
1	A2	3876	A
1	A2	3878	G
1	A2	3879	A
1	A2	3886	U
1	A2	3889	G
1	A2	3890	C
1	A2	3907	A
1	A2	3909	G
1	A2	3927	G
1	A2	3929	G
1	A2	3935	U
1	A2	3936	A
1	A2	3943	A
1	A2	3944	G
1	A2	4019	U
1	A2	4020	A
1	A2	4027	C
1	A2	4029	C
1	A2	4035	G
1	A2	4046	G
1	A2	4051	G
1	A2	4054	G
1	A2	4058	C
1	A2	4062	G
1	A2	4065	G
1	A2	4066	C

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Mol	Chain	Res	Type
1	A2	4067	G
1	A2	4068	A
1	A2	4069	G
1	A2	4074	A
1	A2	4079	C
1	A2	4084	G
1	A2	4088	C
1	A2	4106	C
1	A2	4109	G
1	A2	4110	C
1	A2	4126	C
1	A2	4132	A
1	A2	4135	G
1	A2	4145	G
1	A2	4146	G
1	A2	4153	G
1	A2	4165	A
1	A2	4174	A
1	A2	4175	A
1	A2	4176	A
1	A2	4191	U
1	A2	4195	A
1	A2	4196	A
1	A2	4211	G
1	A2	4215	A
1	A2	4216	G
1	A2	4228	G
1	A2	4230	A
1	A2	4235	A
1	A2	4243	A
1	A2	4250	C
1	A2	4251	U
1	A2	4252	U
1	A2	4266	A
1	A2	4267	G
1	A2	4268	U
1	A2	4276	C
1	A2	4281	C
1	A2	4285	A
1	A2	4291	G
1	A2	4292	G
1	A2	4294	C

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Mol	Chain	Res	Type
1	A2	4311	C
1	A2	4316	U
1	A2	4330	G
1	A2	4333	G
1	A2	4338	A
1	A2	4339	G
1	A2	4340	A
1	A2	4342	A
1	A2	4349	C
1	A2	4355	G
1	A2	4356	A
1	A2	4358	A
1	A2	4360	C
1	A2	4367	G
1	A2	4384	A
1	A2	4386	A
1	A2	4388	C
1	A2	4406	C
1	A2	4414	U
1	A2	4426	A
1	A2	4428	C
1	A2	4437	G
1	A2	4446	G
1	A2	4455	U
1	A2	4457	G
1	A2	4459	U
1	A2	4474	U
1	A2	4475	A
1	A2	4480	A
1	A2	4482	G
1	A2	4485	A
1	A2	4486	G
1	A2	4510	A
1	A2	4519	U
1	A2	4522	C
1	A2	4537	G
1	A2	4546	A
1	A2	4551	A
1	A2	4552	A
1	A2	4559	U
1	A2	4561	A
1	A2	4570	G

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Mol	Chain	Res	Type
1	A2	4579	G
1	A2	4586	A
1	A2	4593	G
1	A2	4597	A
1	A2	4598	U
1	A2	4599	G
1	A2	4611	G
1	A2	4614	G
1	A2	4618	A
1	A2	4620	G
1	A2	4621	G
1	A2	4624	C
1	A2	4629	C
1	A2	4632	C
1	A2	4640	G
1	A2	4641	G
1	A2	4662	A
1	A2	4665	U
1	A2	4671	U
1	A2	4681	G
1	A2	4693	G
1	A2	4694	G
1	A2	4695	C
1	A2	4696	A
1	A2	4700	C
1	A2	4703	C
1	A2	4704	G
1	A2	4714	U
1	A2	4715	U
1	A2	4718	C
1	A2	4719	C
1	A2	4726	A
1	A2	4732	U
1	A2	4824	C
1	A2	4827	U
1	A2	4828	G
1	A2	4831	G
1	A2	4832	A
1	A2	4833	G
1	A2	4834	U
1	A2	4837	C
1	A2	4838	C

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Mol	Chain	Res	Type
1	A2	4839	U
1	A2	4840	U
1	A2	4847	G
1	A2	4849	G
1	A2	4852	A
1	A2	4853	C
1	A2	4854	G
1	A2	4855	G
1	A2	4858	C
1	A2	4859	G
1	A2	4864	C
1	A2	4865	G
1	A2	4866	G
1	A2	4867	A
1	A2	4868	A
1	A2	4869	A
1	A2	4870	G
1	A2	4871	G
1	A2	4872	C
1	A2	4880	C
1	A2	4883	U
1	A2	4886	C
1	A2	4895	C
1	A2	4896	A
1	A2	4898	C
1	A2	4903	G
1	A2	4906	C
1	A2	4907	G
1	A2	4908	U
1	A2	4909	G
1	A2	4923	U
1	A2	4924	A
1	A2	4934	U
1	A2	4937	A
1	A2	4943	U
1	A2	4947	U
1	A2	4950	G
1	A2	4957	G
1	A2	4964	U
1	A2	4971	C
1	A2	4975	G
1	A2	4981	C

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Mol	Chain	Res	Type
1	A2	4982	C
1	A2	4984	U
1	A2	4985	C
1	A2	4986	G
1	A2	4998	U
1	A2	4999	G
1	A2	5005	C
1	A2	5007	G
1	A2	5008	C
1	A2	5011	U
1	A2	5012	C
1	A2	5013	G
1	A2	5015	C
1	A2	5016	A
1	A2	5019	A
1	A2	5020	G
1	A2	5027	U
2	Bv	16	U
2	Bv	17	G
2	Bv	19	U
2	Bv	20	U
2	Bv	21	A
2	Bv	22	U
2	Bv	34	A
2	Bv	35	A
2	Bv	47	U
2	Bv	59	A
2	Bv	61	C
2	Bv	76	A
3	Bx	23	U
3	Bx	26	G
3	Bx	29	A
3	Bx	31	A
3	Bx	32	G
3	Bx	33	A
4	Bw	10	G
4	Bw	16	U
4	Bw	17	U
4	Bw	18	G
4	Bw	19	G
4	Bw	21	A
4	Bw	26	G

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Mol	Chain	Res	Type
4	Bw	35	A
4	Bw	36	A
4	Bw	47	U
4	Bw	48	C
4	Bw	56	C
4	Bw	71	G
5	B1	4	C
5	B1	33	G
5	B1	37	C
5	B1	41	G
5	B1	42	A
5	B1	46	A
5	B1	67	C
5	B1	68	A
5	B1	71	G
5	B1	72	C
5	B1	73	C
5	B1	74	G
5	B1	76	U
5	B1	77	A
5	B1	79	A
5	B1	85	A
5	B1	103	A
5	B1	112	U
5	B1	113	G
5	B1	114	G
5	B1	115	U
5	B1	125	C
5	B1	126	G
5	B1	142	C
5	B1	143	U
5	B1	155	G
5	B1	158	A
5	B1	161	U
5	B1	162	C
5	B1	163	U
5	B1	170	A
5	B1	171	A
5	B1	172	U
5	B1	174	C
5	B1	183	G
5	B1	217	A

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Mol	Chain	Res	Type
5	B1	220	U
5	B1	226	A
5	B1	228	C
5	B1	230	A
5	B1	238	C
5	B1	284	C
5	B1	286	U
5	B1	288	G
5	B1	292	A
5	B1	293	C
5	B1	306	C
5	B1	312	G
5	B1	313	A
5	B1	314	U
5	B1	319	C
5	B1	320	G
5	B1	327	G
5	B1	328	U
5	B1	329	G
5	B1	332	G
5	B1	333	G
5	B1	338	G
5	B1	339	A
5	B1	351	G
5	B1	364	A
5	B1	368	U
5	B1	370	G
5	B1	371	A
5	B1	385	G
5	B1	386	C
5	B1	400	C
5	B1	407	G
5	B1	408	A
5	B1	409	C
5	B1	426	A
5	B1	428	U
5	B1	448	A
5	B1	450	C
5	B1	463	C
5	B1	464	A
5	B1	465	A
5	B1	472	C

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Mol	Chain	Res	Type
5	B1	474	G
5	B1	476	A
5	B1	487	U
5	B1	489	A
5	B1	492	C
5	B1	493	A
5	B1	496	C
5	B1	501	C
5	B1	502	C
5	B1	508	A
5	B1	522	A
5	B1	523	A
5	B1	524	U
5	B1	525	A
5	B1	533	A
5	B1	534	G
5	B1	535	G
5	B1	536	A
5	B1	541	U
5	B1	542	U
5	B1	544	G
5	B1	545	A
5	B1	546	G
5	B1	547	G
5	B1	548	C
5	B1	549	C
5	B1	553	U
5	B1	554	A
5	B1	555	A
5	B1	560	A
5	B1	565	G
5	B1	567	C
5	B1	570	C
5	B1	576	A
5	B1	585	C
5	B1	588	G
5	B1	590	A
5	B1	591	U
5	B1	592	C
5	B1	594	A
5	B1	608	C
5	B1	614	C

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Mol	Chain	Res	Type
5	B1	617	G
5	B1	620	G
5	B1	626	G
5	B1	628	A
5	B1	629	A
5	B1	643	A
5	B1	644	G
5	B1	645	C
5	B1	655	A
5	B1	660	C
5	B1	662	G
5	B1	668	A
5	B1	669	A
5	B1	673	G
5	B1	684	G
5	B1	687	C
5	B1	688	U
5	B1	689	U
5	B1	690	G
5	B1	695	C
5	B1	738	C
5	B1	742	U
5	B1	743	U
5	B1	744	G
5	B1	746	C
5	B1	748	C
5	B1	751	G
5	B1	791	C
5	B1	797	C
5	B1	798	G
5	B1	799	U
5	B1	800	U
5	B1	801	U
5	B1	811	A
5	B1	827	A
5	B1	833	C
5	B1	836	G
5	B1	837	A
5	B1	839	C
5	B1	841	G
5	B1	847	A
5	B1	859	G

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Mol	Chain	Res	Type
5	B1	861	A
5	B1	862	A
5	B1	865	A
5	B1	868	G
5	B1	870	A
5	B1	874	G
5	B1	888	U
5	B1	890	U
5	B1	913	A
5	B1	914	U
5	B1	917	U
5	B1	918	U
5	B1	919	A
5	B1	920	A
5	B1	928	G
5	B1	929	G
5	B1	930	C
5	B1	934	G
5	B1	950	C
5	B1	956	G
5	B1	959	G
5	B1	975	G
5	B1	990	A
5	B1	992	A
5	B1	1002	U
5	B1	1008	A
5	B1	1015	U
5	B1	1021	U
5	B1	1023	A
5	B1	1044	G
5	B1	1045	U
5	B1	1053	C
5	B1	1060	A
5	B1	1061	U
5	B1	1085	C
5	B1	1089	G
5	B1	1100	A
5	B1	1109	C
5	B1	1110	G
5	B1	1114	U
5	B1	1115	U
5	B1	1119	A

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Mol	Chain	Res	Type
5	B1	1120	U
5	B1	1121	G
5	B1	1133	A
5	B1	1139	C
5	B1	1140	G
5	B1	1146	C
5	B1	1149	A
5	B1	1150	A
5	B1	1170	A
5	B1	1188	A
5	B1	1195	A
5	B1	1199	A
5	B1	1207	G
5	B1	1215	C
5	B1	1216	C
5	B1	1224	G
5	B1	1242	U
5	B1	1243	U
5	B1	1251	A
5	B1	1253	A
5	B1	1256	G
5	B1	1257	G
5	B1	1258	A
5	B1	1259	A
5	B1	1261	C
5	B1	1278	A
5	B1	1285	G
5	B1	1286	G
5	B1	1287	A
5	B1	1288	U
5	B1	1289	U
5	B1	1290	G
5	B1	1301	A
5	B1	1302	G
5	B1	1303	C
5	B1	1313	A
5	B1	1314	U
5	B1	1330	G
5	B1	1333	U
5	B1	1352	G
5	B1	1353	A
5	B1	1363	C

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Mol	Chain	Res	Type
5	B1	1371	U
5	B1	1372	U
5	B1	1375	G
5	B1	1378	A
5	B1	1381	G
5	B1	1395	C
5	B1	1418	C
5	B1	1420	G
5	B1	1421	A
5	B1	1442	U
5	B1	1452	A
5	B1	1454	A
5	B1	1467	C
5	B1	1474	A
5	B1	1476	A
5	B1	1477	U
5	B1	1478	U
5	B1	1487	A
5	B1	1489	A
5	B1	1494	U
5	B1	1497	G
5	B1	1498	A
5	B1	1505	U
5	B1	1507	G
5	B1	1508	A
5	B1	1521	C
5	B1	1522	A
5	B1	1533	A
5	B1	1535	U
5	B1	1537	A
5	B1	1544	C
5	B1	1546	G
5	B1	1553	C
5	B1	1554	C
5	B1	1555	U
5	B1	1558	C
5	B1	1580	A
5	B1	1585	U
5	B1	1586	U
5	B1	1588	A
5	B1	1601	A
5	B1	1604	G

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Mol	Chain	Res	Type
5	B1	1606	G
5	B1	1614	A
5	B1	1620	A
5	B1	1621	U
5	B1	1622	U
5	B1	1623	A
5	B1	1624	U
5	B1	1625	U
5	B1	1639	G
5	B1	1660	C
5	B1	1661	A
5	B1	1662	U
5	B1	1663	A
5	B1	1671	G
5	B1	1677	U
5	B1	1683	C
5	B1	1690	U
5	B1	1695	A
5	B1	1700	C
5	B1	1710	C
5	B1	1721	U
5	B1	1726	G
5	B1	1750	C
5	B1	1756	C
5	B1	1757	G
5	B1	1777	G
5	B1	1780	G
5	B1	1781	A
5	B1	1783	C
5	B1	1784	G
5	B1	1824	A
5	B1	1829	G
5	B1	1831	A
5	B1	1834	A
5	B1	1835	A
5	B1	1837	G
5	B1	1838	U
5	B1	1849	G
5	B1	1852	C
5	B1	1856	C
5	B1	1860	A
5	B1	1861	G

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Mol	Chain	Res	Type
5	B1	1862	G
5	B1	1863	A
5	B1	1864	U
5	B1	1865	C
5	B1	1866	A
5	B1	1869	A
39	A3	16	G
39	A3	34	U
39	A3	35	C
39	A3	37	A
39	A3	38	U
39	A3	39	G
39	A3	51	U
39	A3	59	A
39	A3	63	U
39	A3	71	A
39	A3	72	A
39	A3	77	A
39	A3	80	A
39	A3	81	C
39	A3	87	G
39	A3	94	G
39	A3	96	C
39	A3	103	A
39	A3	105	C
39	A3	107	C
39	A3	109	C
39	A3	110	U
39	A3	111	U
39	A3	112	G
39	A3	114	G
39	A3	121	G
39	A3	123	U
39	A3	124	U
39	A3	125	C
39	A3	126	C
39	A3	128	C
39	A3	129	C
39	A3	130	C
39	A3	148	A
39	A3	151	G
40	A4	7	G

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Mol	Chain	Res	Type
40	A4	10	C
40	A4	11	A
40	A4	14	C
40	A4	22	A
40	A4	27	G
40	A4	33	U
40	A4	45	U
40	A4	47	G
40	A4	48	G
40	A4	50	A
40	A4	51	G
40	A4	53	U
40	A4	63	C
40	A4	64	G
40	A4	74	A
40	A4	76	U
40	A4	91	C
40	A4	97	G
40	A4	110	G
40	A4	119	U

All (13) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A2	31	U
1	A2	71	C
1	A2	901	U
1	A2	959	C
1	A2	1500	A
1	A2	4661	U
1	A2	4865	G
1	A2	4870	G
1	A2	4946	U
5	B1	227	U
5	B1	369	C
5	B1	797	C
5	B1	1554	C

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	$\# Z > 2$
86	DDE	Ct	715	86	18,20,21	1.09	1 (5%)	17,28,30	0.85	1 (5%)

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
86	DDE	Ct	715	86	-	10/20/21/23	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	Ct	715	DDE	CD2-CG	2.62	1.41	1.36

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	Ct	715	DDE	CAC-NCB-CBW	2.18	115.73	110.52

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	Ct	715	DDE	NAD-CBI-CBW-NCB
86	Ct	715	DDE	CBI-CBW-NCB-CAB
86	Ct	715	DDE	CE1-CAT-CAU-CBW
86	Ct	715	DDE	CA-CB-CG-CD2
86	Ct	715	DDE	CA-CB-CG-ND1
86	Ct	715	DDE	OAG-CBI-CBW-CAU
86	Ct	715	DDE	CAT-CAU-CBW-CBI
86	Ct	715	DDE	CBI-CBW-NCB-CAC
86	Ct	715	DDE	CAU-CBW-NCB-CAB

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Mol	Chain	Res	Type	Atoms
86	Ct	715	DDE	NAD-CBI-CBW-CAU

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	Ct	715	DDE	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 333 ligands modelled in this entry, 332 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
89	GNP	Ct	901	-	34,34,34	1.27	5 (14%)	47,54,54	0.68	1 (2%)

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
89	GNP	Ct	901	-	-	6/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	Ct	901	GNP	PB-O3A	4.41	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	Ct	901	GNP	PB-O1B	2.90	1.50	1.46
89	Ct	901	GNP	PG-N3B	2.81	1.70	1.63
89	Ct	901	GNP	PG-O1G	2.79	1.50	1.46
89	Ct	901	GNP	PB-O2B	-2.35	1.50	1.56

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	Ct	901	GNP	O1B-PB-N3B	-2.09	108.70	111.77

There are no chirality outliers.

All (6) torsion outliers are listed below:

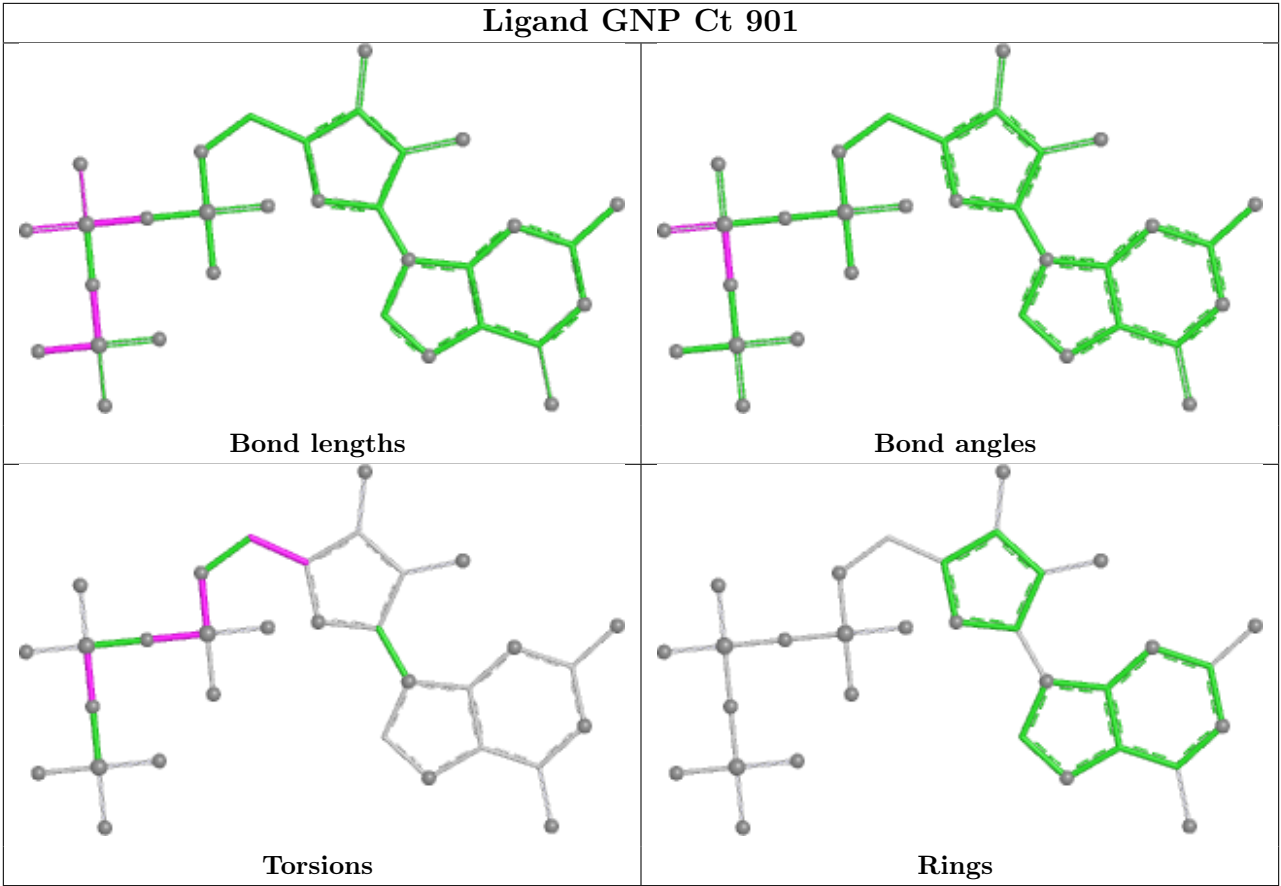
Mol	Chain	Res	Type	Atoms
89	Ct	901	GNP	PG-N3B-PB-O1B
89	Ct	901	GNP	C5'-O5'-PA-O1A
89	Ct	901	GNP	C3'-C4'-C5'-O5'
89	Ct	901	GNP	O4'-C4'-C5'-O5'
89	Ct	901	GNP	C5'-O5'-PA-O3A
89	Ct	901	GNP	PB-O3A-PA-O1A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	Ct	901	GNP	1	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A2	11
5	B1	6

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B1	126:G	O3'	141:A	P	20.66
1	B1	751:G	O3'	790:C	P	20.56
1	A2	517:C	O3'	629:G	P	18.02
1	A2	3948:C	O3'	4004:G	P	17.82
1	B1	1757:G	O3'	1775:U	P	17.75

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A2	1233:C	O3'	1243:G	P	17.73
1	B1	240:G	O3'	282:G	P	17.66
1	A2	4734:C	O3'	4818:G	P	17.59
1	B1	696:G	O3'	737:G	P	17.05
1	A2	750:G	O3'	890:C	P	16.93
1	A2	976:U	O3'	1047:G	P	16.84
1	A2	2881:G	O3'	3569:C	P	16.75
1	B1	1426:U	O3'	1438:A	P	16.52
1	A2	1089:A	O3'	1145:G	P	16.07
1	A2	1680:C	O3'	1699:C	P	15.11
1	A2	1202:G	O3'	1216:G	P	14.53
1	A2	2068:C	O3'	2245:C	P	14.01

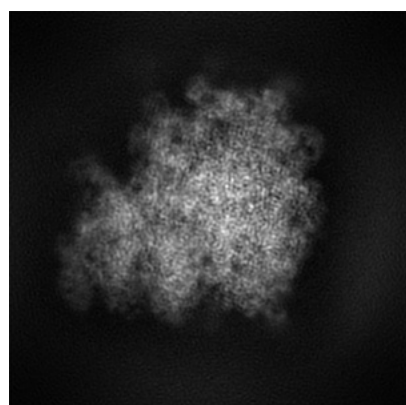
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0098. These allow visual inspection of the internal detail of the map and identification of artifacts.

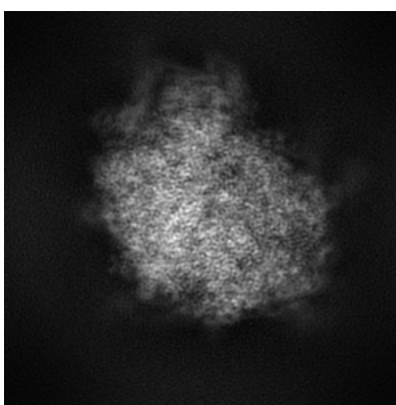
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

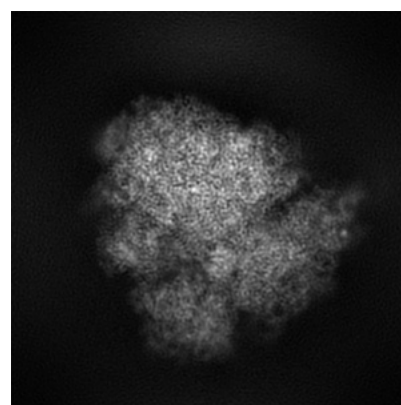
6.1.1 Primary map



X



Y

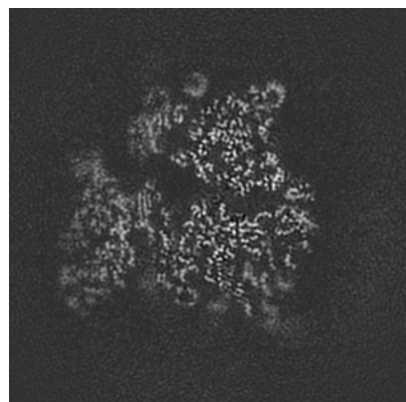


Z

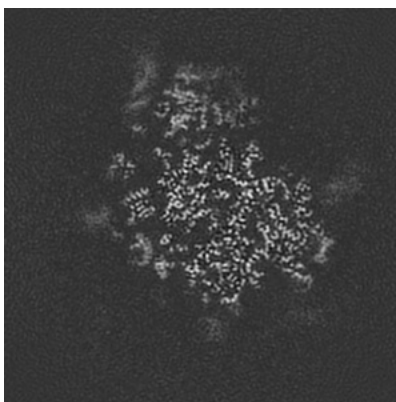
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

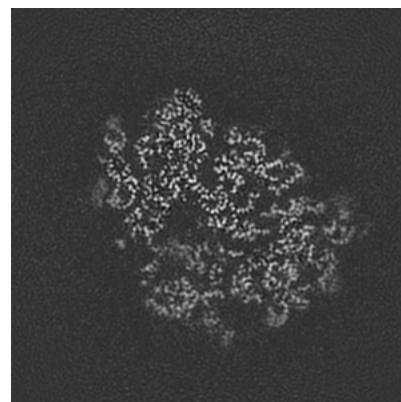
6.2.1 Primary map



X Index: 202



Y Index: 202

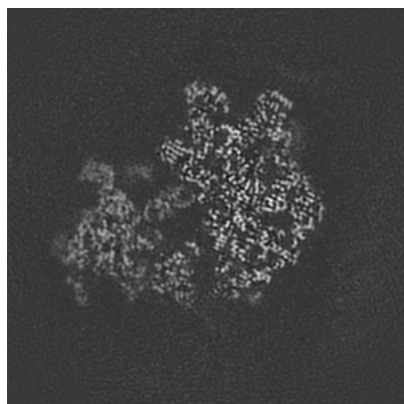


Z Index: 202

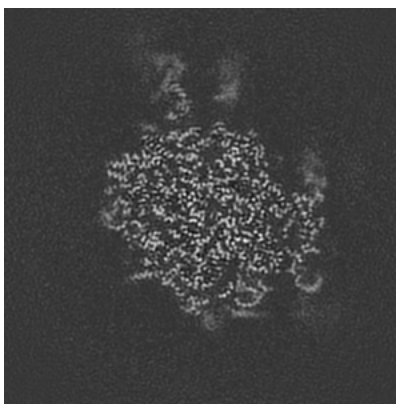
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

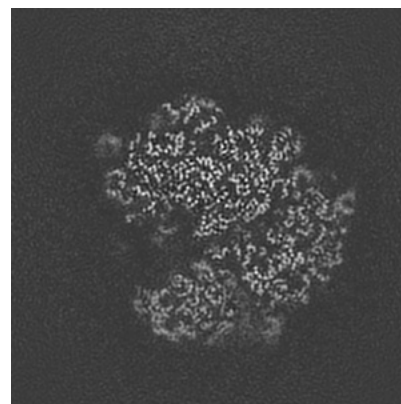
6.3.1 Primary map



X Index: 179



Y Index: 220

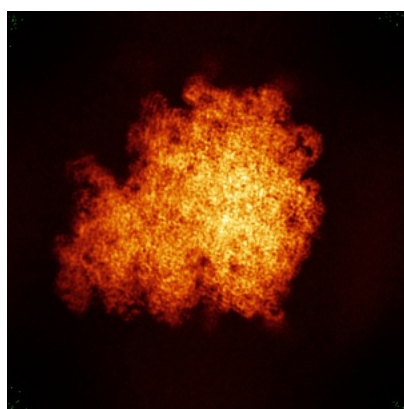


Z Index: 185

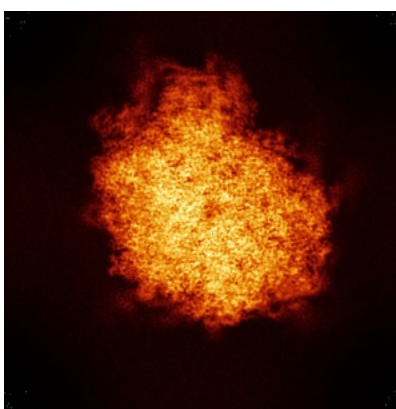
The images above show the largest variance slices of the map in three orthogonal directions.

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

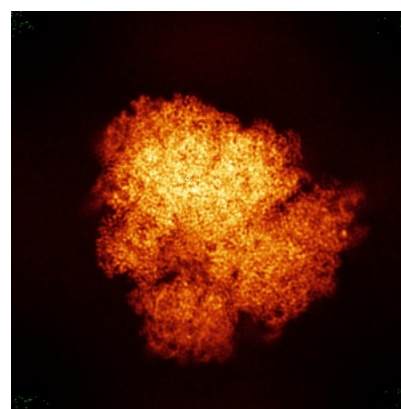
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

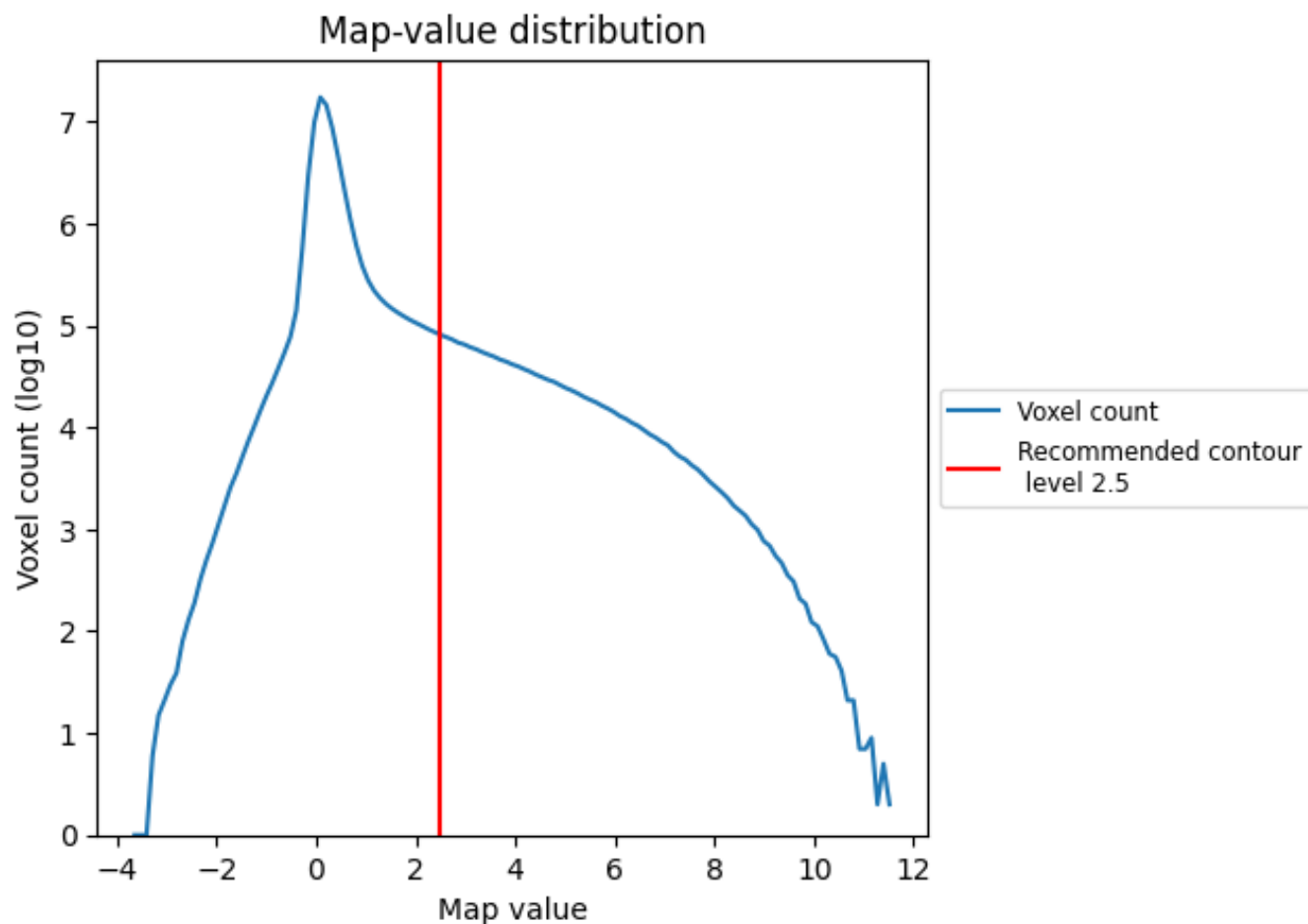
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

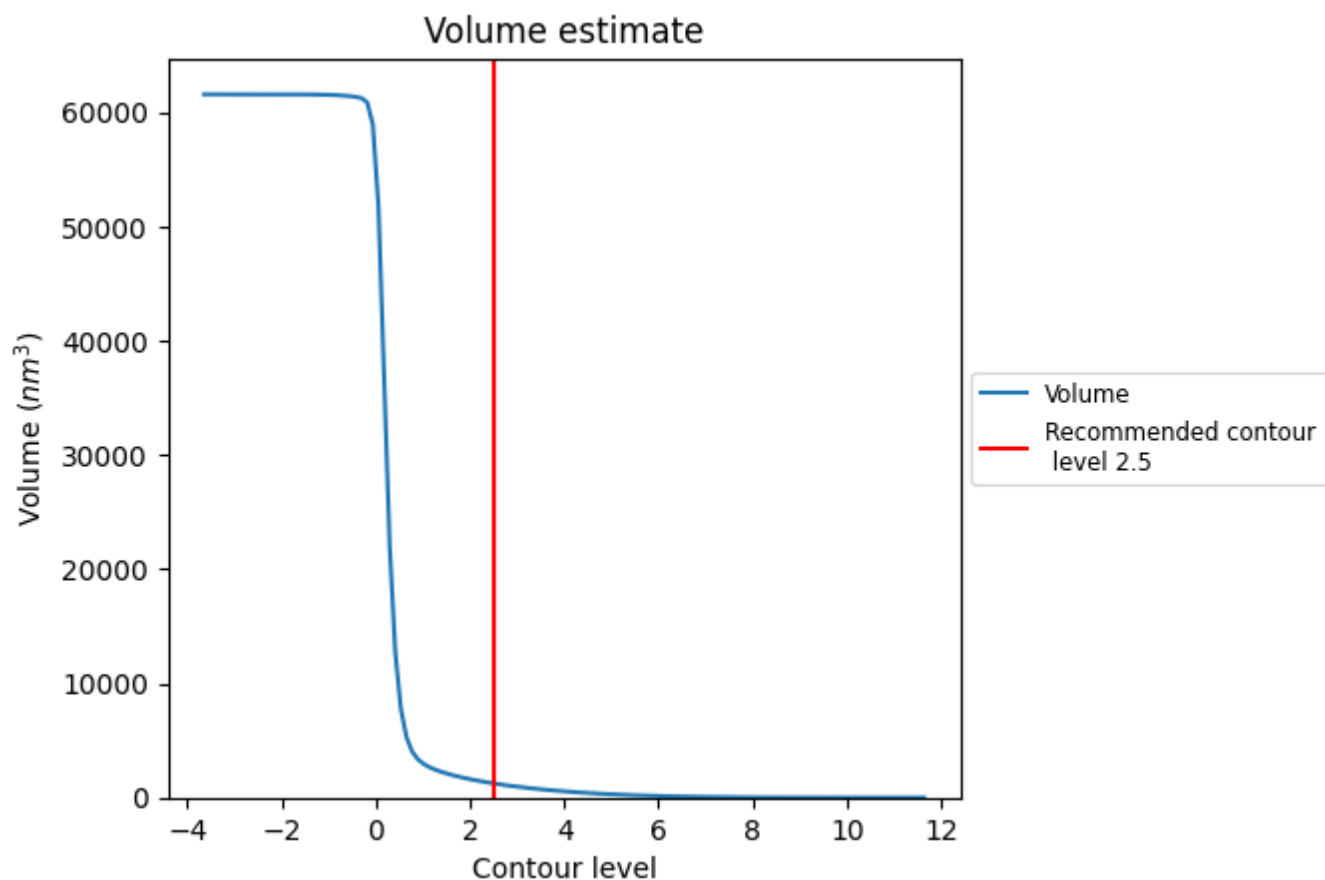
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

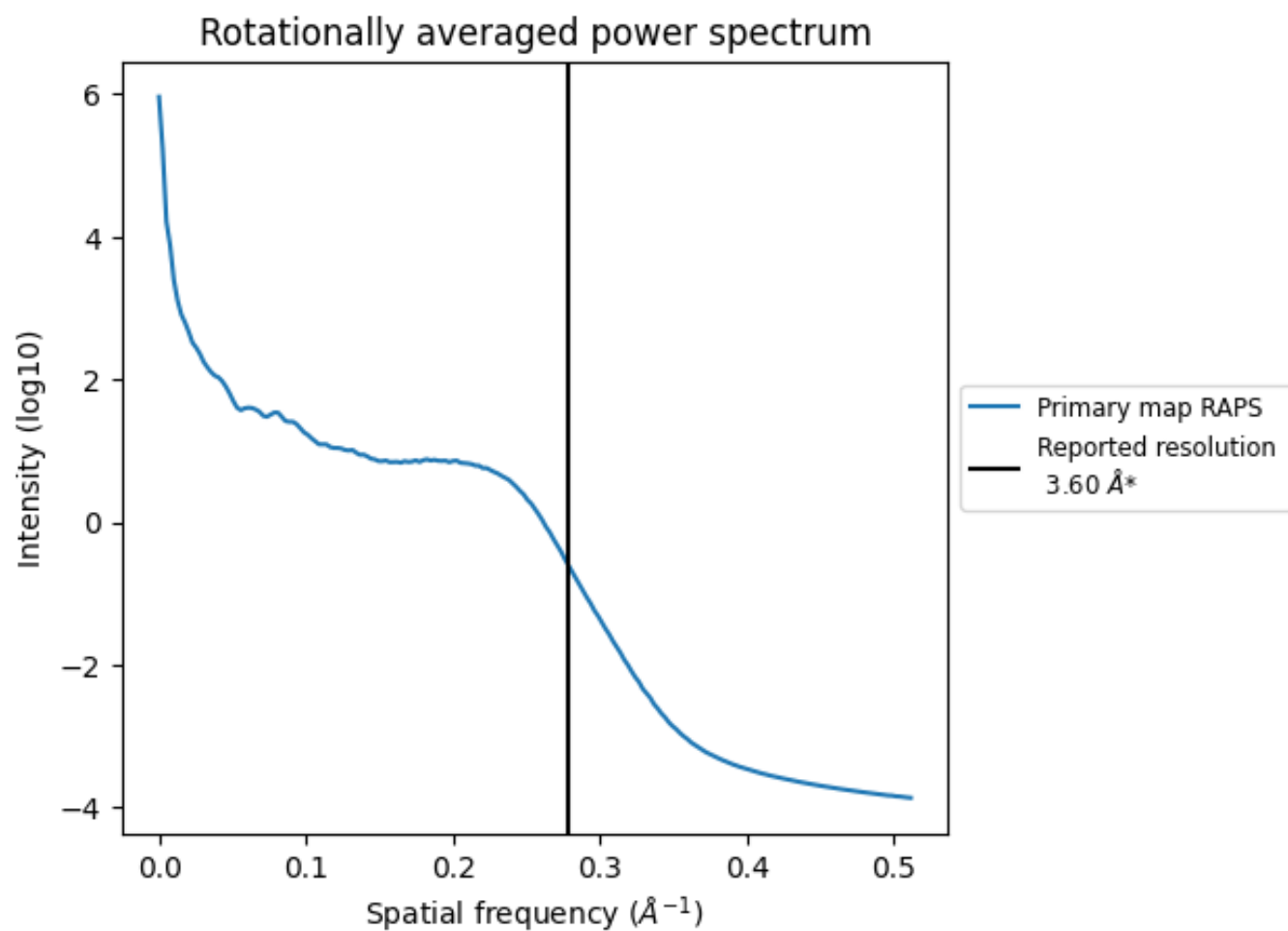
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1237 nm³; this corresponds to an approximate mass of 1118 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 0.278 Å⁻¹

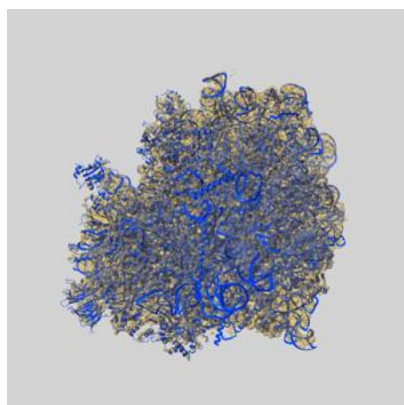
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

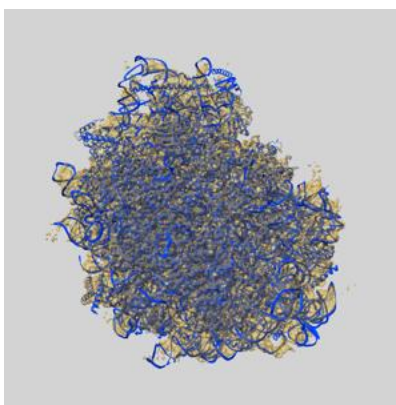
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0098 and PDB model 6GZ3. Per-residue inclusion information can be found in section [3](#) on page [22](#).

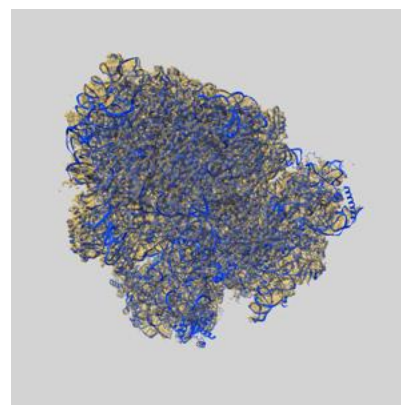
9.1 Map-model overlay [i](#)



X



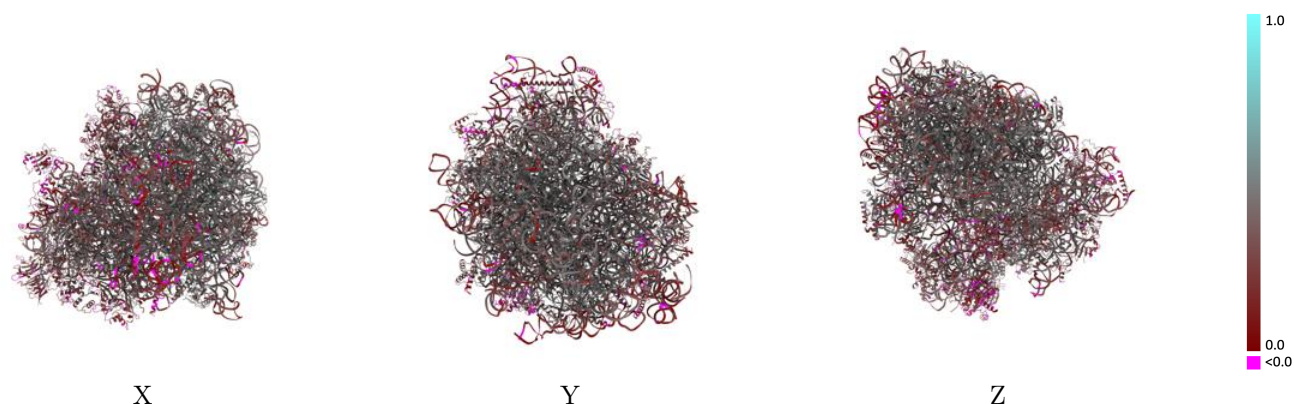
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

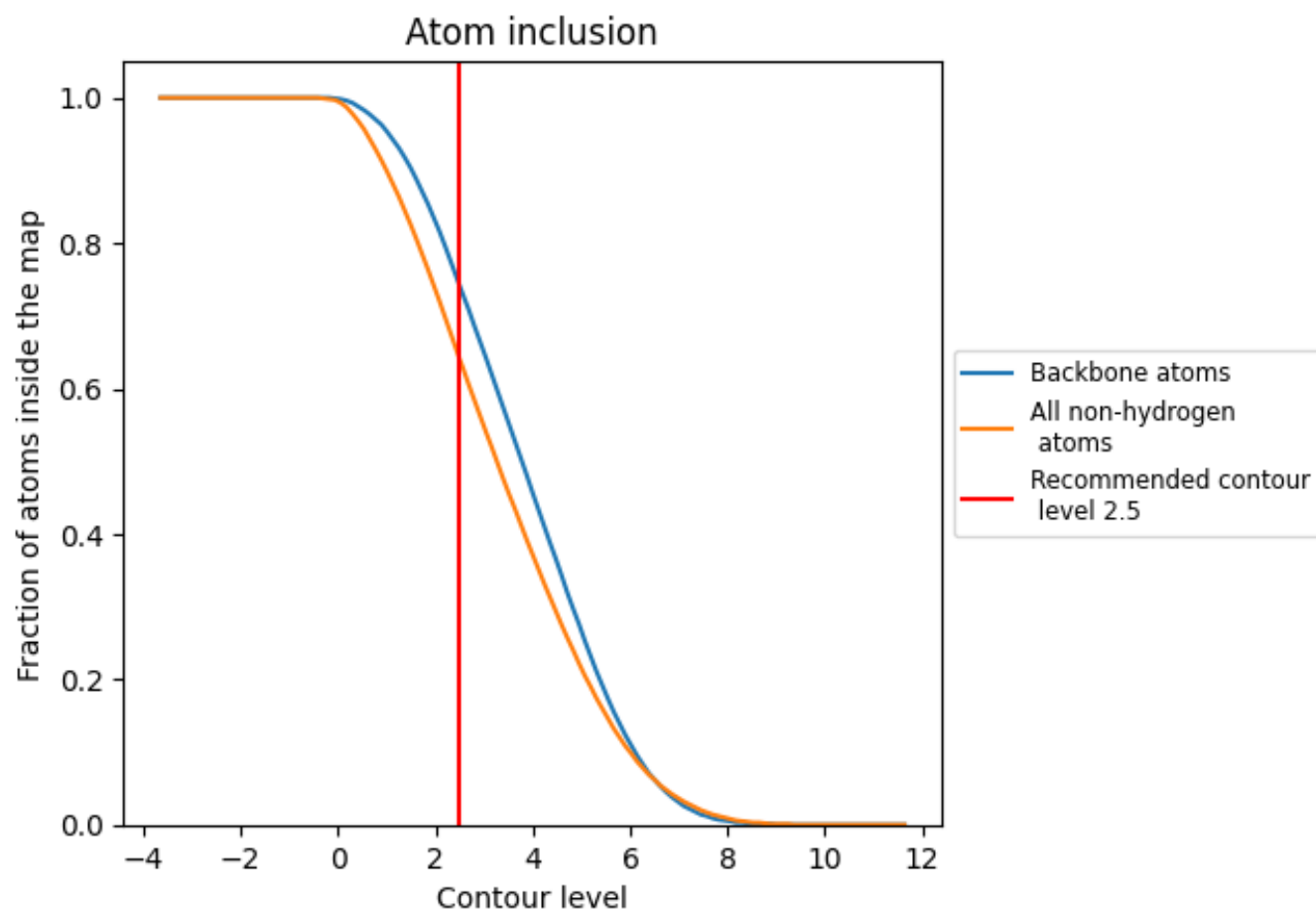


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 64% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6400	 0.3650
A2	 0.7650	 0.3920
A3	 0.7730	 0.3970
A4	 0.8500	 0.4350
AA	 0.6620	 0.4460
AB	 0.6400	 0.4200
AC	 0.6500	 0.4150
AD	 0.6160	 0.3670
AE	 0.5060	 0.3230
AF	 0.6180	 0.3860
AG	 0.5590	 0.3630
AH	 0.5850	 0.4080
AI	 0.6320	 0.4130
AJ	 0.5900	 0.3710
AK	 0.2460	 0.2090
AL	 0.5900	 0.3630
AM	 0.6120	 0.3790
AN	 0.7070	 0.4320
AO	 0.6430	 0.4030
AP	 0.6720	 0.4380
AQ	 0.6450	 0.4010
AR	 0.5690	 0.3590
AS	 0.6590	 0.4180
AT	 0.6250	 0.4120
AU	 0.5210	 0.3620
AV	 0.6400	 0.4570
AW	 0.3250	 0.2310
AX	 0.6220	 0.4310
AY	 0.6420	 0.4130
AZ	 0.6090	 0.3860
Aa	 0.6720	 0.4210
Ab	 0.5470	 0.3440
Ac	 0.5710	 0.3640
Ad	 0.6320	 0.4270
Ae	 0.6600	 0.4260



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Chain	Atom inclusion	Q-score
Af	 0.6730	 0.4220
Ag	 0.6080	 0.3990
Ah	 0.5740	 0.3710
Ai	 0.6180	 0.3750
Aj	 0.7250	 0.4400
Ak	 0.5010	 0.3570
Al	 0.6390	 0.4160
Am	 0.6420	 0.3990
An	 0.2640	 0.3050
Ao	 0.6340	 0.4200
Ap	 0.6470	 0.4240
Aq	 0.1340	 0.1360
At	 0.6540	 0.3970
Au	 0.0200	 0.0060
B1	 0.7140	 0.3680
BA	 0.4250	 0.3060
BB	 0.4750	 0.3290
BC	 0.5400	 0.3640
BD	 0.4470	 0.3190
BE	 0.5130	 0.3390
BF	 0.3860	 0.2870
BG	 0.3770	 0.2420
BH	 0.2990	 0.2680
BI	 0.4770	 0.3280
BJ	 0.5420	 0.3200
BK	 0.3040	 0.1640
BL	 0.4880	 0.3470
BM	 0.0640	 0.1290
BN	 0.5190	 0.3600
BO	 0.5240	 0.3840
BP	 0.3830	 0.2500
BQ	 0.4160	 0.3100
BR	 0.3360	 0.2710
BS	 0.4090	 0.2540
BT	 0.3850	 0.2450
BU	 0.3410	 0.2890
BV	 0.4910	 0.3430
BW	 0.5650	 0.3820
BX	 0.5640	 0.4040
BY	 0.4280	 0.2680
BZ	 0.2310	 0.2110
Ba	 0.5730	 0.3720

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Chain	Atom inclusion	Q-score
Bb	 0.4410	 0.3290
Bc	 0.3430	 0.3010
Bd	 0.5010	 0.2970
Be	 0.4480	 0.3590
Bf	 0.0630	 0.1410
Bg	 0.2020	 0.2380
Bv	 0.5300	 0.3010
Bw	 0.6590	 0.3310
Bx	 0.5040	 0.2800
Ct	 0.4610	 0.3260