



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 08:39 PM UTC

PDB ID : 6GZ5 / pdb_00006gz5
EMDB ID : EMD-0100
Title : tRNA translocation by the eukaryotic 80S ribosome and the impact of GTP hydrolysis, Translocation-intermediate-POST-3 (TI-POST-3)
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 : 3.50 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:

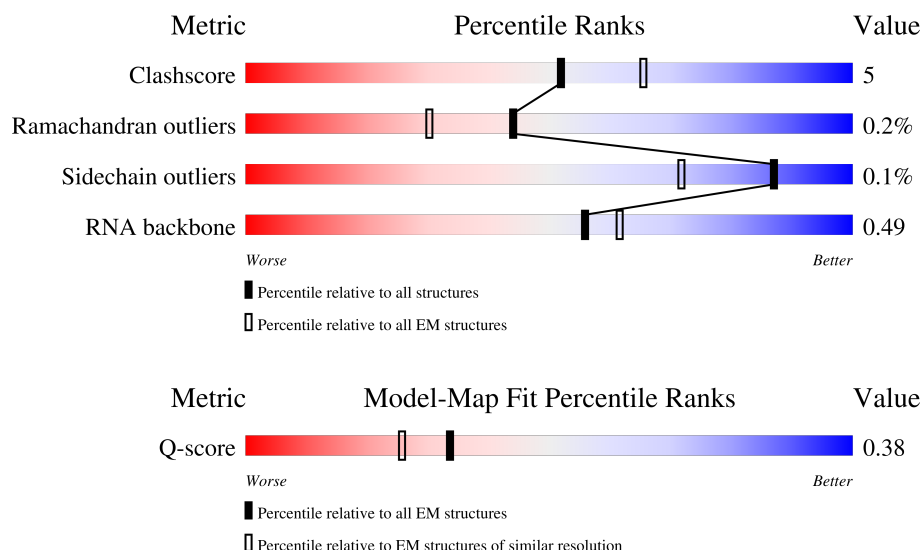
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.50 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	13950 (3.00 - 4.00)

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	
2	Bv	76	
3	Bx	11	

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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	
30	BN	149	
31	BO	136	
32	BV	81	
33	BW	129	
34	BX	141	
35	BY	125	
36	Ba	97	
37	Bb	80	
38	Be	55	
39	A3	157	
40	A4	119	
41	AA	252	
42	AB	394	
43	AC	363	
44	AD	294	
45	AE	194	
46	AF	234	
47	AG	234	
48	AH	191	
49	AI	208	
50	AJ	169	
51	AL	205	
52	AM	139	
53	AN	203	

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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% 80% 20%
80	Ao	105	7% 85% 15%
81	Ap	91	5% 89% 11%
82	At	122	7% 80% 20%
83	Au	217	100% 77% 23%
84	Aq	151	87% 76% 23%
85	AK	202	79% 78% 22%
86	Ct	853	43% 83% 16%

2 Entry composition [i](#)

There are 89 unique types of molecules in this entry. The entry contains 225601 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 P/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	11	Total	C	N	O	P	0	0
			234	105	41	77	11		

- Molecule 4 is a RNA chain called E/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 uS7.

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 ribosomal protein eS12.

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 eS28.

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 eS31.

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 ribosomal protein eS1.

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 ribosomal protein eS6.

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 ribosomal protein eS7.

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 uS4.

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 uS17.

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 uS8.

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 uS12.

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 uL2.

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 uL16.

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

- Molecule 50 is a protein called ribosomal protein uL5.

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 eL15.

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 uL14.

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 uL24.

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 ribosomal protein eL27.

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 eL37.

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 uL1.

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 uL11.

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	229	Total	Mg	0
			229	229	
87	Bx	1	Total	Mg	0
			1	1	
87	B1	73	Total	Mg	0
			73	73	
87	BD	1	Total	Mg	0
			1	1	
87	Ba	1	Total	Mg	0
			1	1	
87	A3	7	Total	Mg	0
			7	7	
87	A4	8	Total	Mg	0
			8	8	
87	AA	1	Total	Mg	0
			1	1	
87	AC	1	Total	Mg	0
			1	1	
87	AL	1	Total	Mg	0
			1	1	
87	AO	1	Total	Mg	0
			1	1	
87	AP	1	Total	Mg	0
			1	1	

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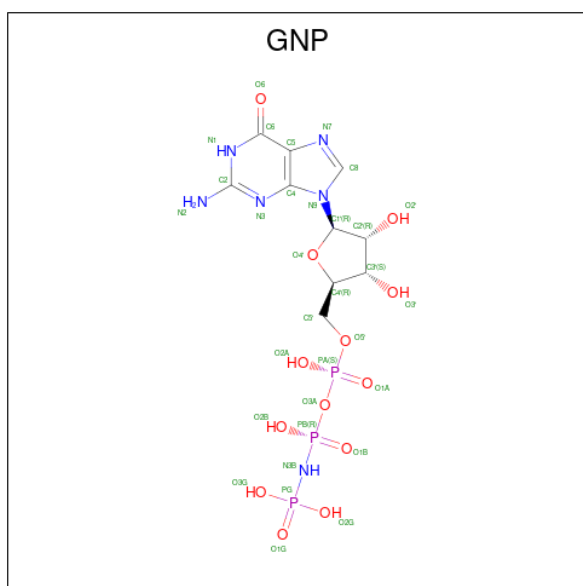
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
87	AY	1	Total	Mg	0
			1	1	
87	An	1	Total	Mg	0
			1	1	

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

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

- Molecule 89 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).

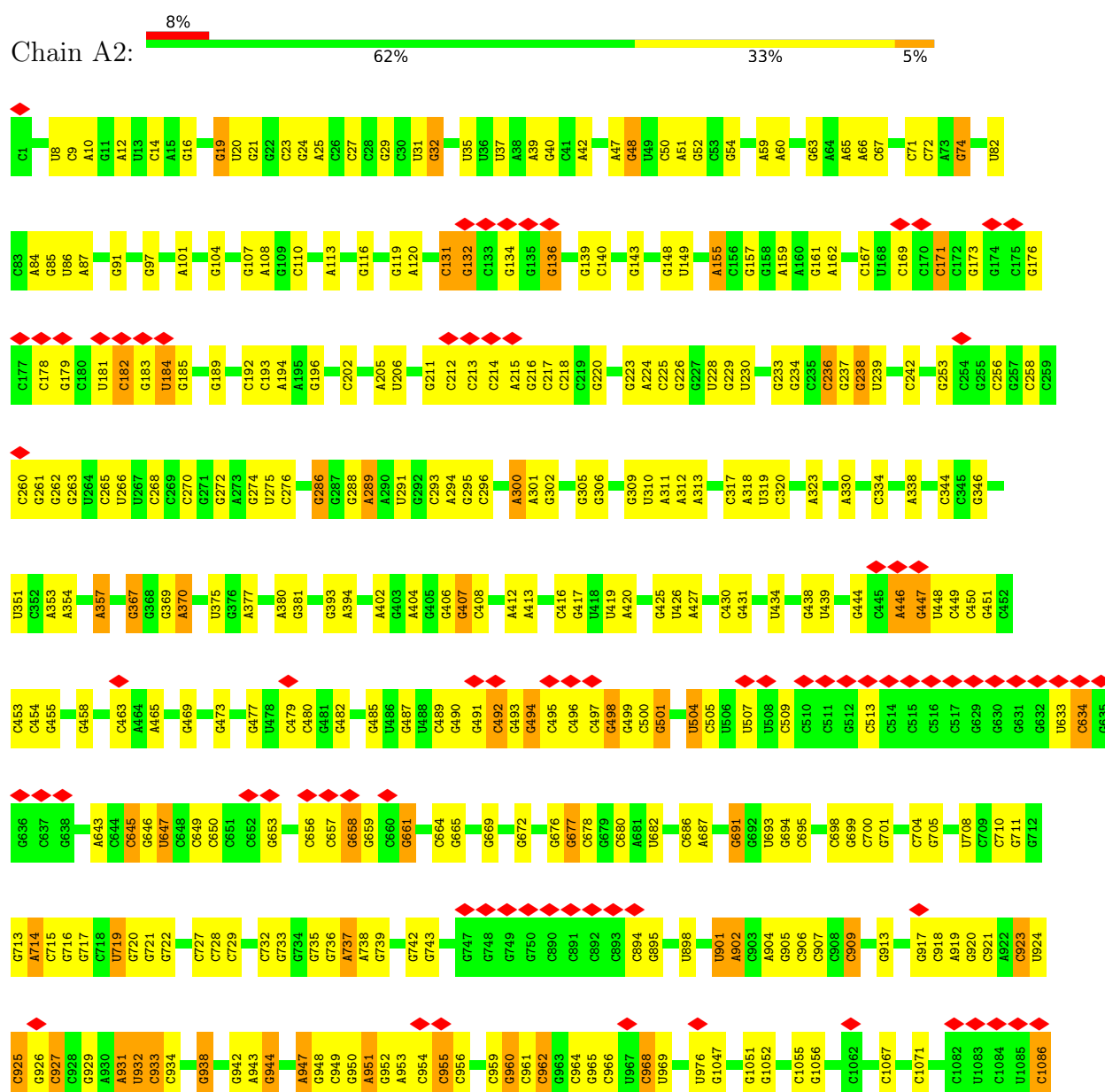


Mol	Chain	Residues	Atoms					AltConf
89	Ct	1	Total	C	N	O	P	0
			32	10	6	13	3	

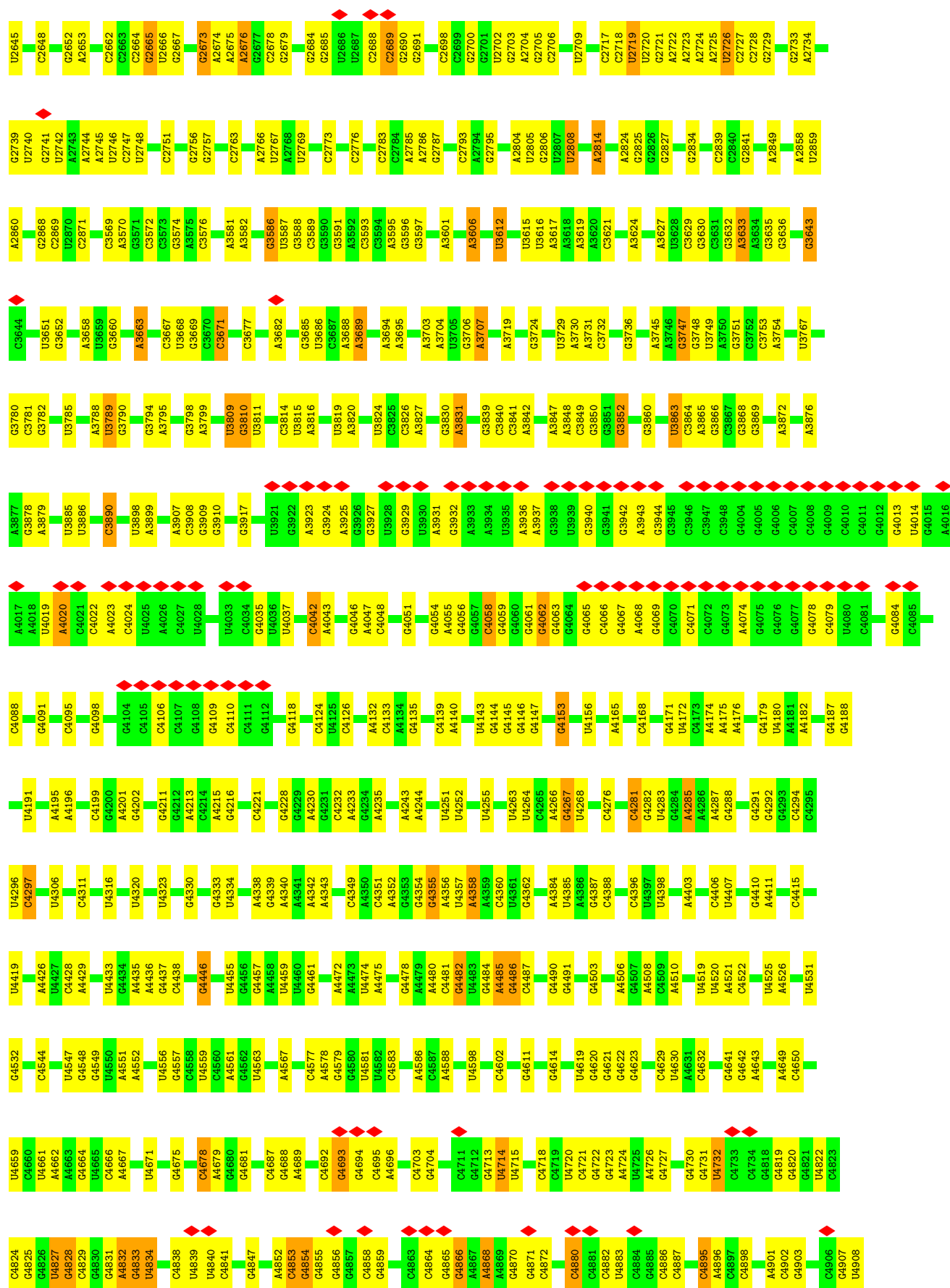
3 Residue-property plots

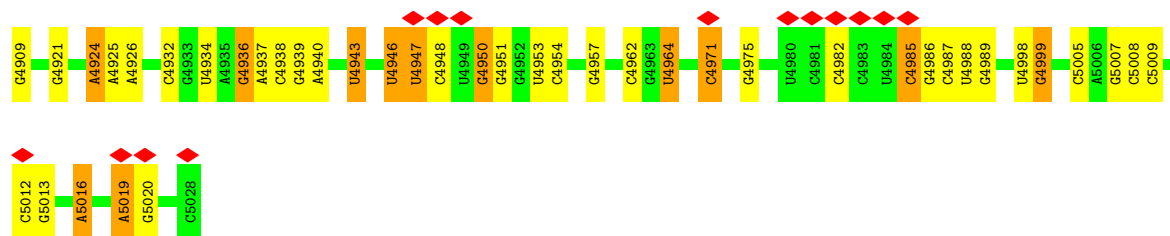
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

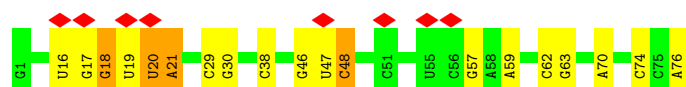
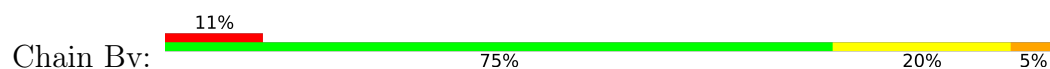


C2536	U2426	A2311	G2036	C1952	C1862	A1752	A1651	G1556	U1423	G1334	C1249	C1087
C2537	C2312	C2313	G2037	G1953	U1862	U1753	C1658	G1560	C1425	A1337	C1250	C1088
C2538	C2314	G2315	G2043	U1955	G1964	C1754	U1659	U1560	A1426	C1338	G1251	A1089
C2540	C2322	G2323	C2043	G1957	A1869	U1756	C1660	U1564	G1427	G1341	G1252	G1145
C2541	U2323	C2324	A2050	C1958	U1870	A1757	G1663	U1564	U1428	G1342	G1253	G1146
C2542	G2324	C2325	U2051	C1959	U1871	C1760	A1664	U1565	C1429	G1343	G1254	G1147
C2543	C2325	C2326	C2054	A1960	A1872	U1761	U1665	U1573	C1430	G1344	C1255	G1148
A2544	U2447	A2326	G2055	U1961	A1873	U1762	A1666	U1578	G1431	G1345	G1256	G1149
U2549	G2450	A2328	G2057	G1963	G1876	A1763	U1669	A1435	C1432	U1347	C1259	C1150
A2552	G2455	U2329	C2062	G1964	C1879	A1768	G1670	A1583	A1435	C1348	C1262	G1155
G2553	A2456	C2330	G2063	A1965	U1879	A1769	G1673	C1589	C1440	C1349	C1263	G1156
A2561	G2462	U2331	C2064	G1966	C1882	U1770	C1674	U1589	A1441	G1350	G1264	
C2562	U2463	C2332	G2065	U1967	G1883	C1771	U1675	C1592	G1450	A1351	G1265	
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G2564	U2465	G2340	G2067	U1973	U1887	A1777	C1678	C1594	C1464	C1358	G1267	G1161
G2565	A2466	U2341	C2068	C1974	A1888	G1785	G1679	G1595	C1465	U1268	U1162	
G2566	G2467	A2342	C2245	C1975	U1887	A1786	C1680	G1599	C1466	C1269	G1163	
C2567	U2467	C2343	U2246	C1976	A1888	U1787	C1689	G1600	C1467	G1270	C1164	
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C2569	C2468	A2345	A2247	U1978	C1895	G1788	C1700	U1602	C1468	G1276	C1176	
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A2577	U2472	C2366	C2268	A1983	A1904	U1712	U1712	G1607	G1480		A1286	
G2578	U2473	G2366	C2268	G1984	C1905	A1807					C1287	
A2579	U2474	C2372	C2274	U1985	U1910	G1810	A1718	C1610	C1483	G1377	C1288	
A2580	G2482	G2373	G2278	G1988	U1911	G1811		G1611	C1483	U1378	C1291	C1190
G2585	C2483	A2374	A2279	A1991	C1912	G1814	G1721	A1612	C1484	G1379	C1292	G1191
C2586	C2484	C2380	G2280	C1992	A1913	U1815	C1722	A1613	A1485	A1380	C1293	U1192
G2587	G2485	G2381	C2281	A1993	G1914	U1815	G1723	A1614	C1486	A1381	C1294	G1193
C2588	A2485	A2382	C2281	A1994	A1915	G1816	A1724	A1616	A1490		C1295	G1195
G2589	C2485	C2383	U2283	C1916	C1916	G1817	A1725	A1619	C1491		C1296	G1196
A2590	G2489	A2384	U2284	C1917	C1917	A1818	A1725	A1620	G1492		C1297	C1197
C2591	C2492	C2385	G2285	C1997	A1920	G1823	A1728	U1621	U1493		C1298	C1198
C2592	G2497	G2386	G2285	A1998	G1921	G1823		C1622	A1497		C1299	G1200
C2606	U2498	C2389	C2288	U2001	C1921	U1826	A1731	A1624	G1498		C1300	G1201
U2609	C2499	C2390	C2289	G2002	A1922	G1827	G1732	C1626	G1499		C1301	C1220
G2617	G2501	A2391	U2291	A2006	A1923	A1831	U1736	C1627	C1503		C1302	C1221
U2618	C2505	C2399	C2293	A2007	U1928	G1832	C1737	A1628	G1504		C1303	C1222
G2619	G2514	G2400	G2294	G2015	G1929	U1833	U1738	U1631	A1505		C1304	G1223
A2620	C2401	A2402	C2294	A2021	U1930	G1834	U1739	A1507	C1392		C1309	C1224
A2621	G2403	G2403	G2298	G2015	G1933	G1836	G1740	A1632	G1395		C1310	G1225
G2622	U2404	U2404	C2299	A2021	G1936	G1836	G1741	C1637	G1311		C1311	C1226
A2626	A2410	G2410	G2300	G2026	G1936	G1845	G1742	C1637	C1315		C1315	G1227
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G2637	U2419	G2419	U2308	A2028	U1940	G1850	C1744	A1410	A1317		A1320	G1229
U2644	G2523	G2418	G2309	G2029	A1941	G1850	C1745	A1540	A1320		U1331	U1230
	G2525	U2419	G2309	G2030	G1942	A1854	G1746	G1541	A1320		C1332	C1231
	G2526	C2420	G2310	C2032	A1943	U1857	A1747	C1548	A1333		C1333	C1232
	G2531						A1748					C1233
	A2532						A1749					G1243
							C1750					G1244
							G1751					G1245
												A1246
												G1247
												C1248

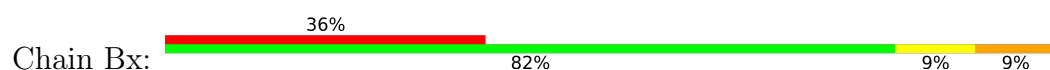




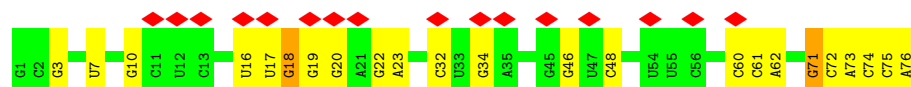
• Molecule 2: P/P-site-tRNA



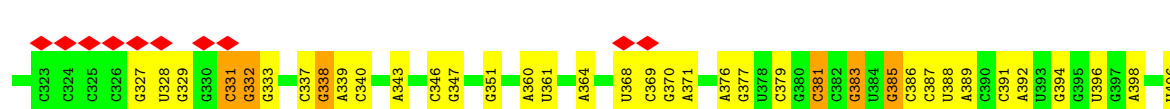
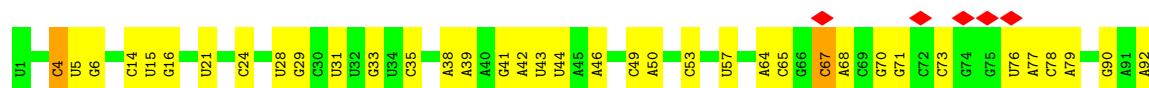
• Molecule 3: mRNA



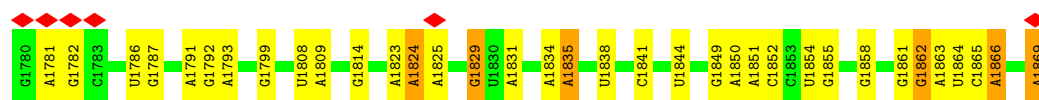
• Molecule 4: E/E-site-tRNA



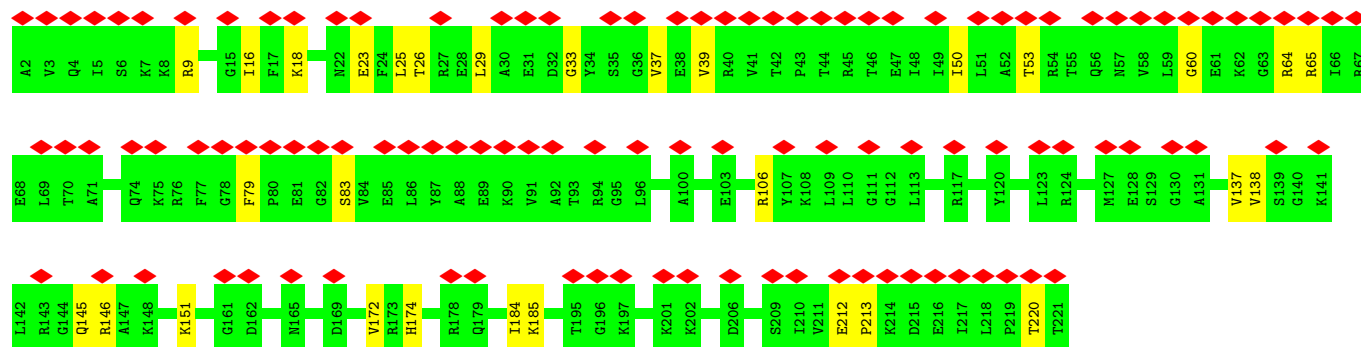
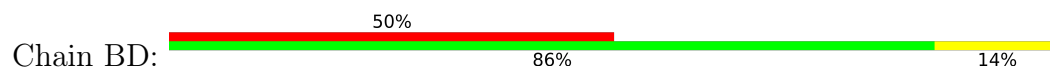
• Molecule 5: 18S ribosomal RNA



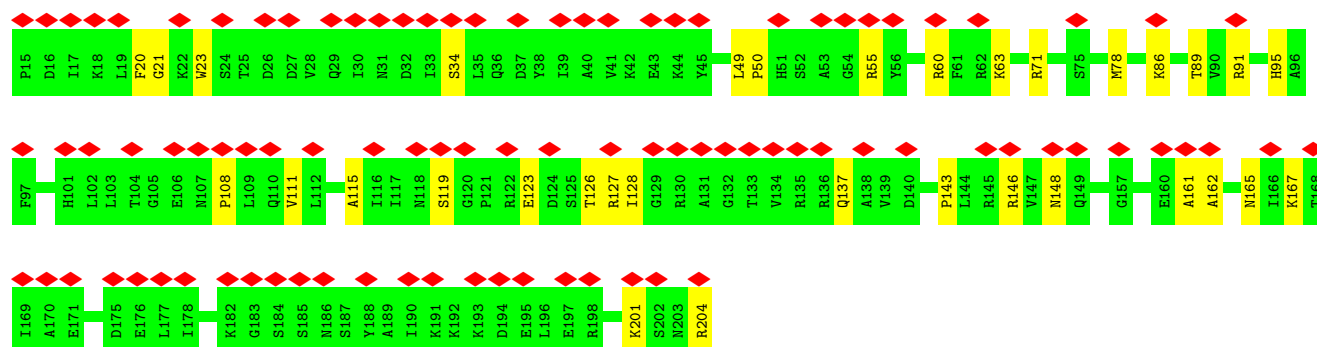
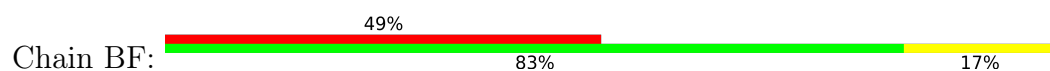




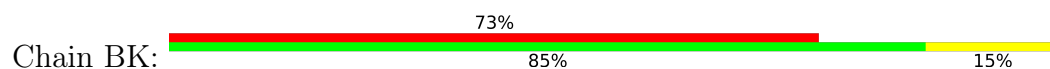
• Molecule 6: ribosomal protein uS3



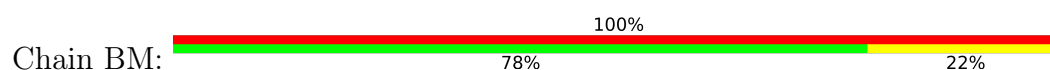
• Molecule 7: ribosomal protein uS7

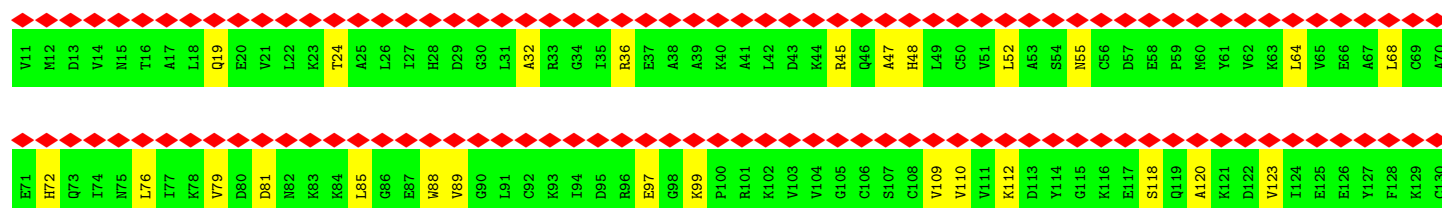


• Molecule 8: ribosomal protein eS10

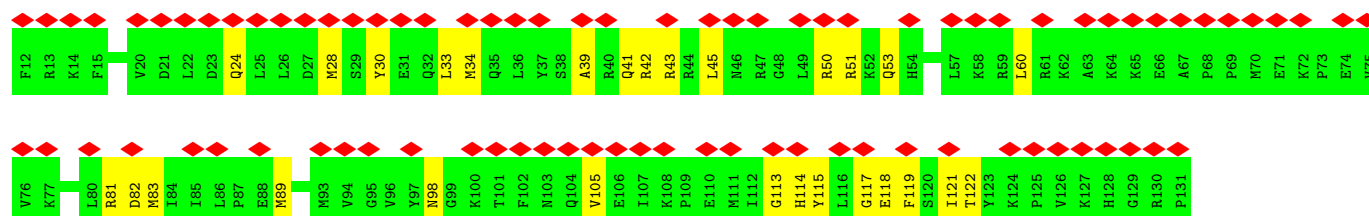
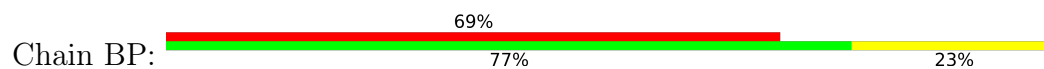


• Molecule 9: ribosomal protein eS12

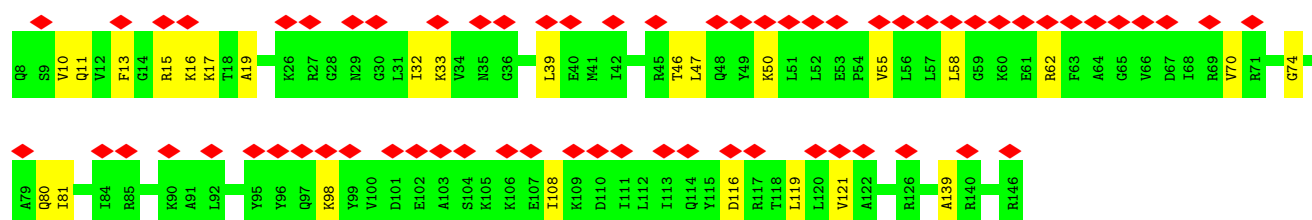
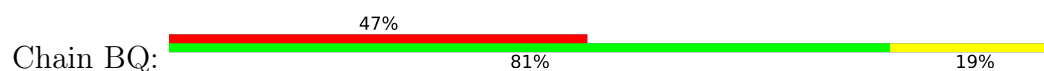




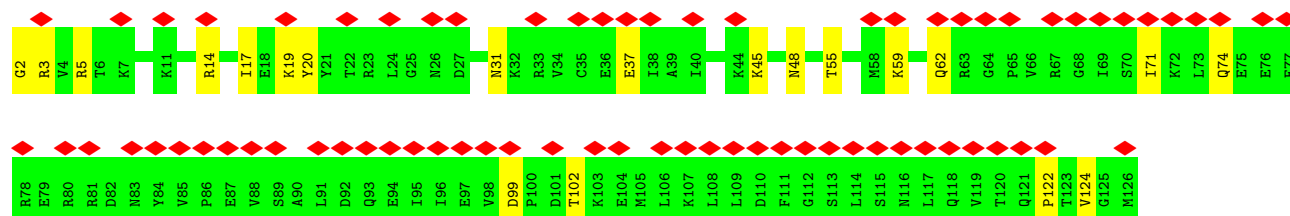
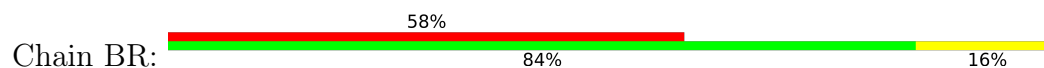
• Molecule 10: ribosomal protein uS19



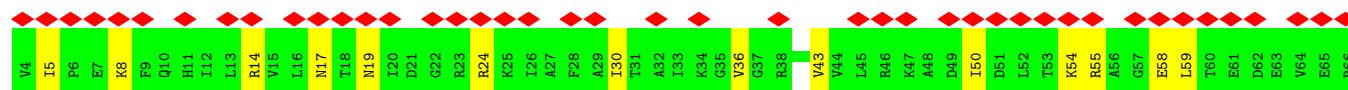
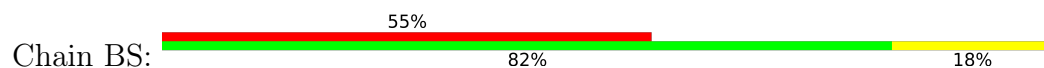
• Molecule 11: ribosomal protein uS9

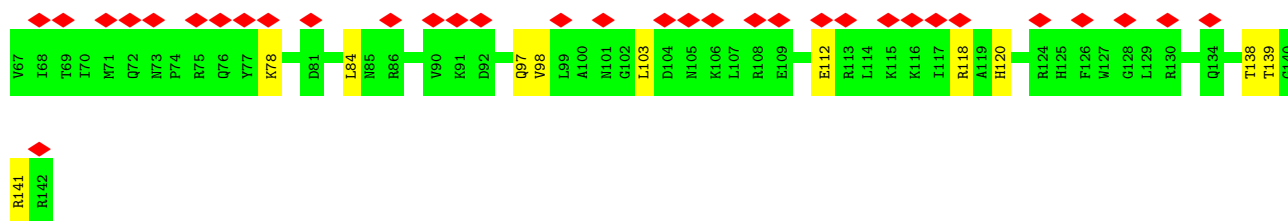


• Molecule 12: ribosomal protein eS17

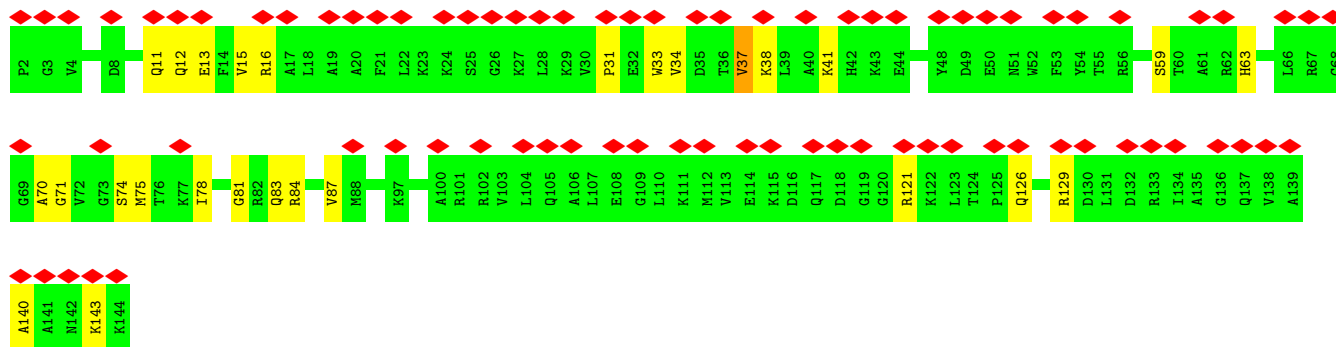
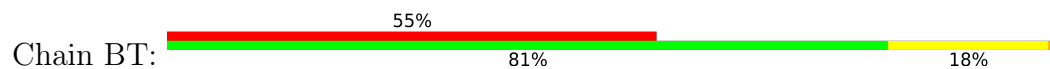


• Molecule 13: ribosomal protein uS13

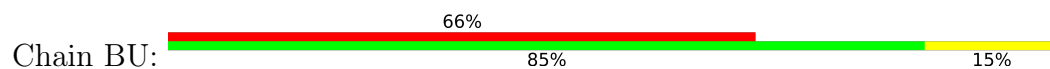




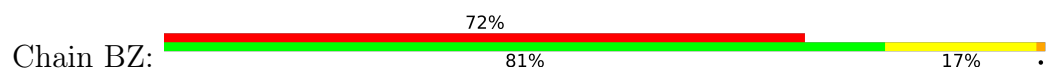
• Molecule 14: ribosomal protein eS19



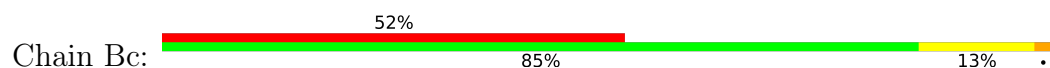
• Molecule 15: ribosomal protein uS10



• Molecule 16: ribosomal protein eS25

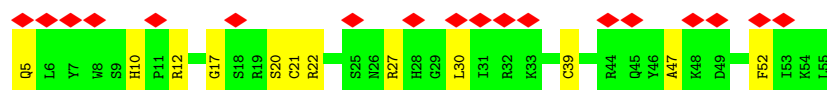
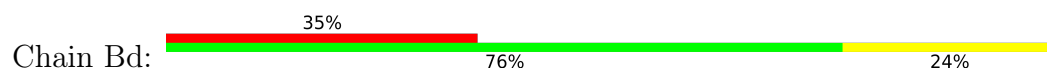


• Molecule 17: ribosomal protein eS28

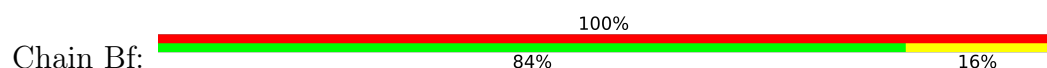




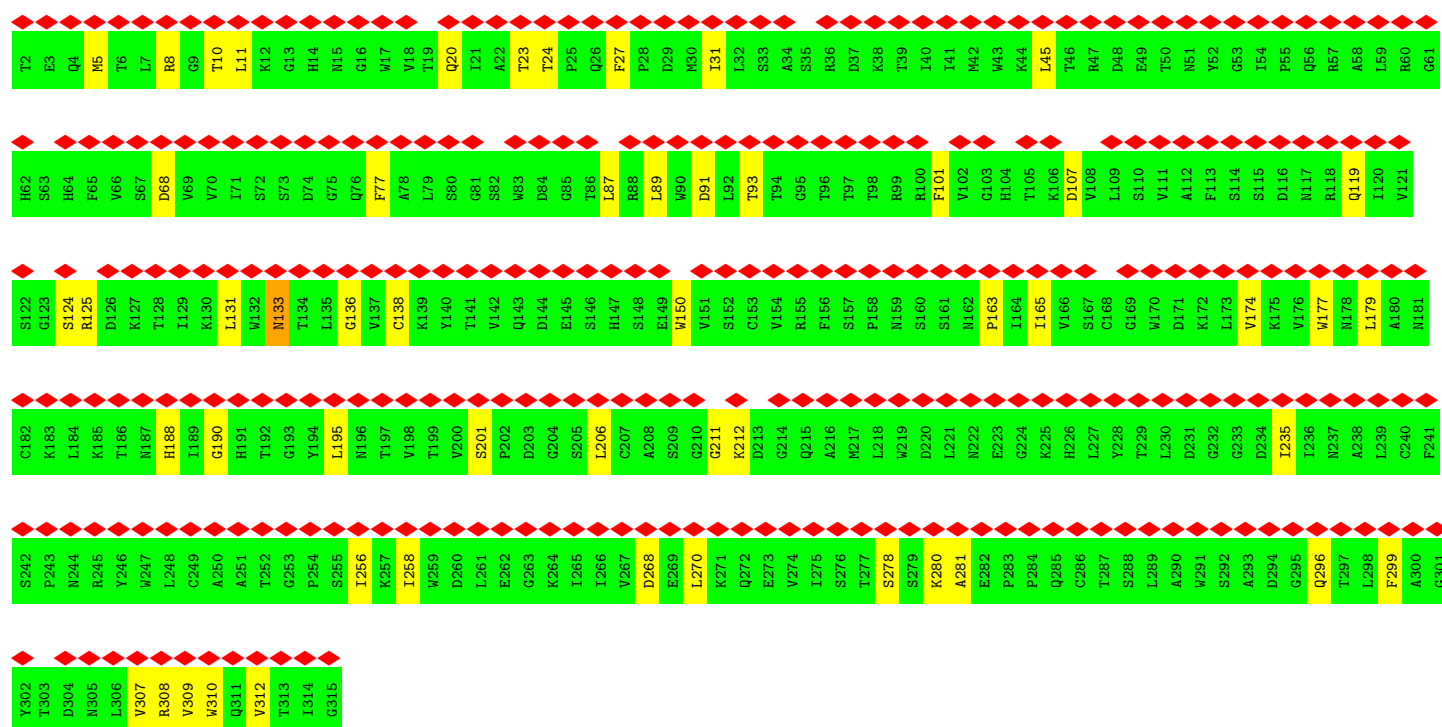
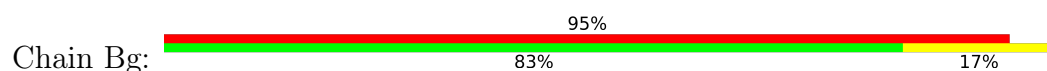
- Molecule 18: ribosomal protein uS14



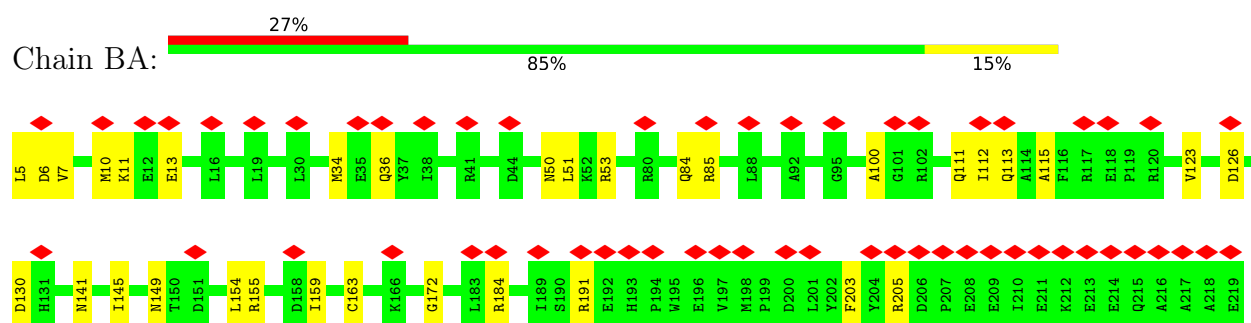
- Molecule 19: ribosomal protein eS31



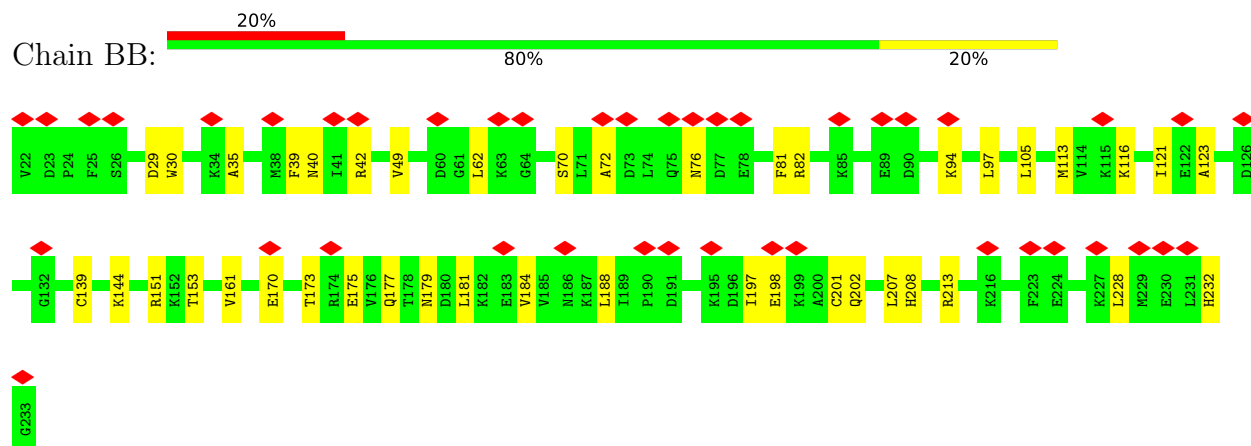
- Molecule 20: ribosomal protein RACK 1



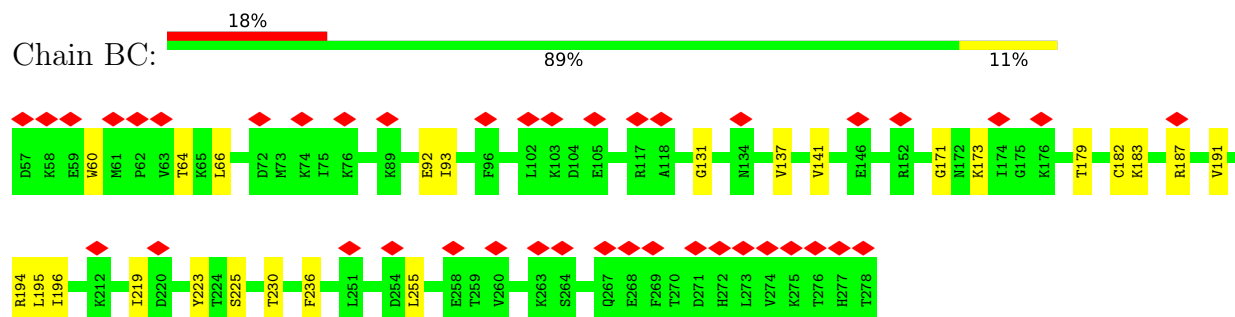
- Molecule 21: ribosomal protein uS2



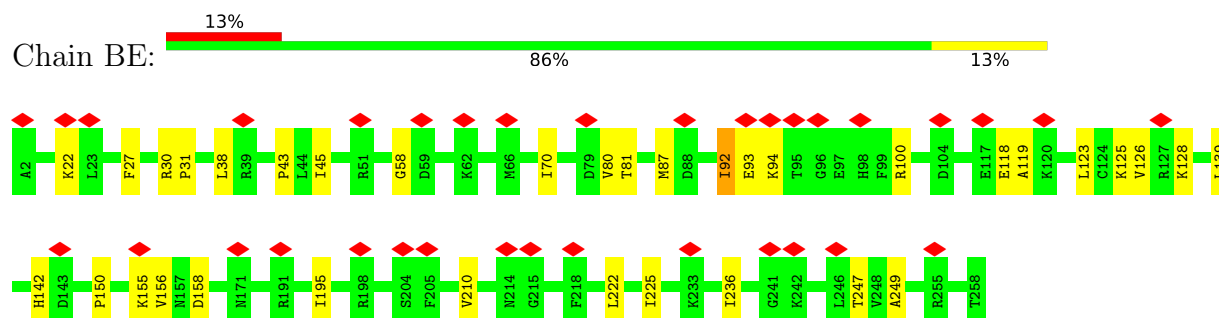
- Molecule 22: ribosomal protein eS1



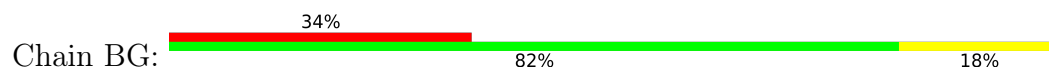
- Molecule 23: ribosomal protein uS5

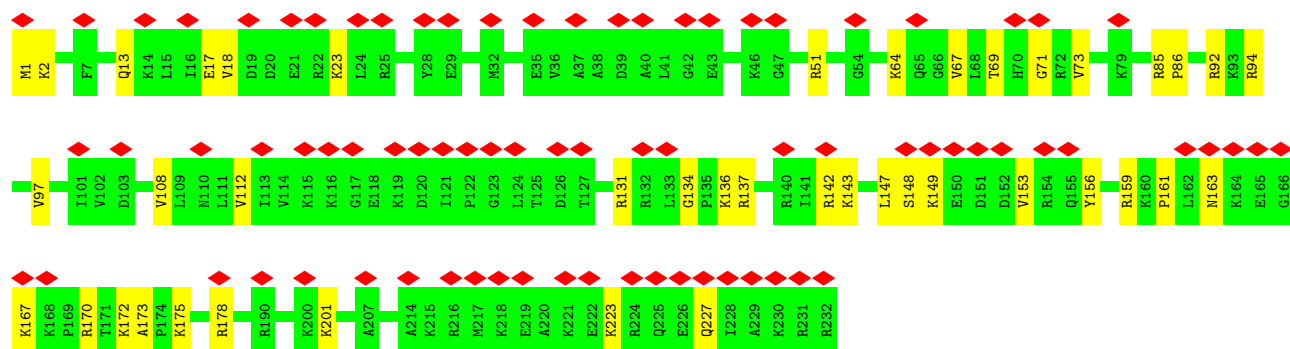


- Molecule 24: ribosomal protein eS4

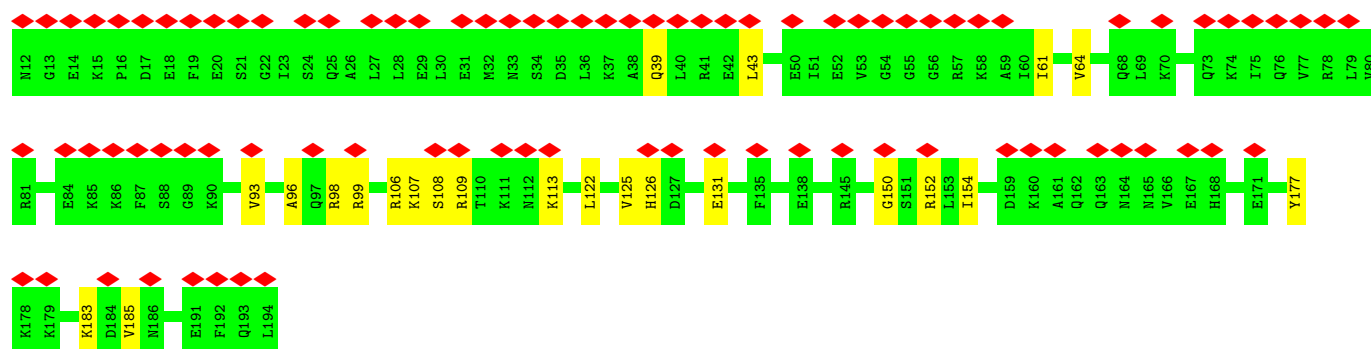


- Molecule 25: ribosomal protein eS6

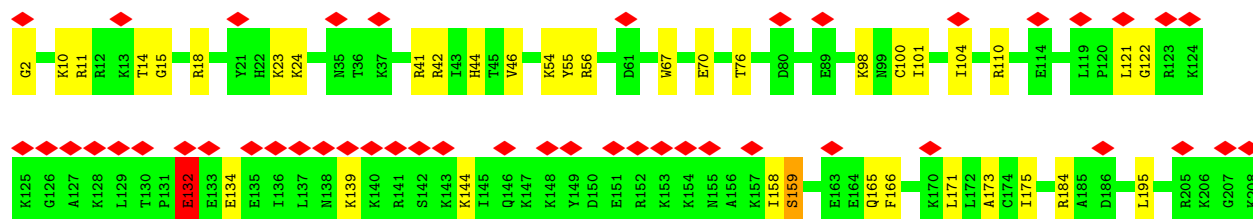
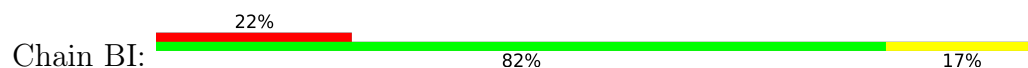




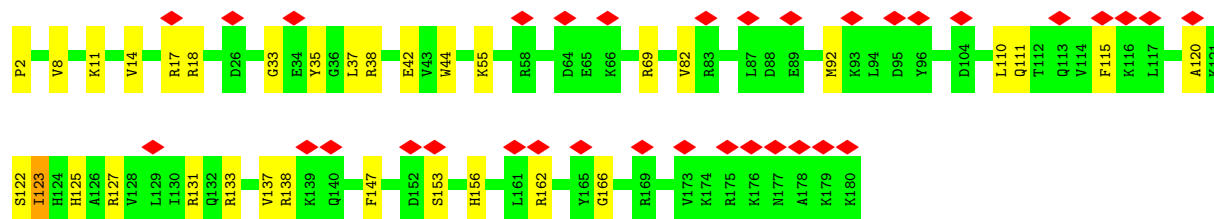
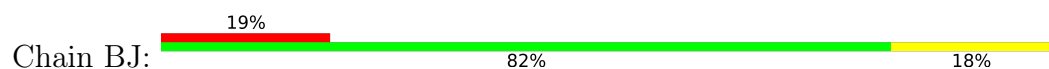
- Molecule 26: ribosomal protein eS7



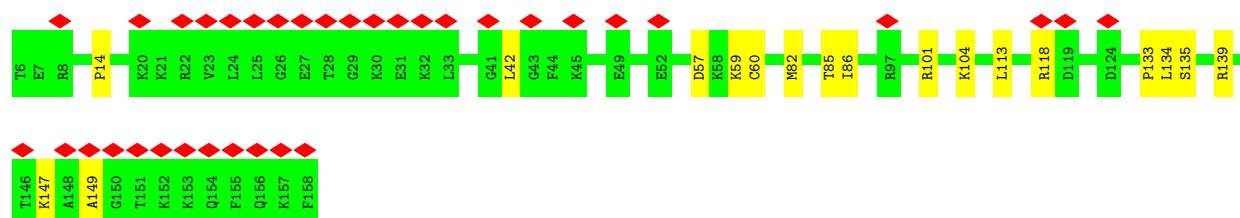
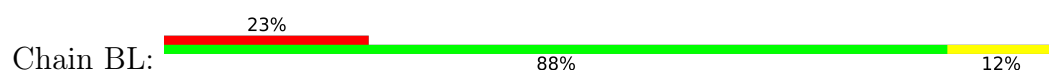
- Molecule 27: ribosomal protein eS8



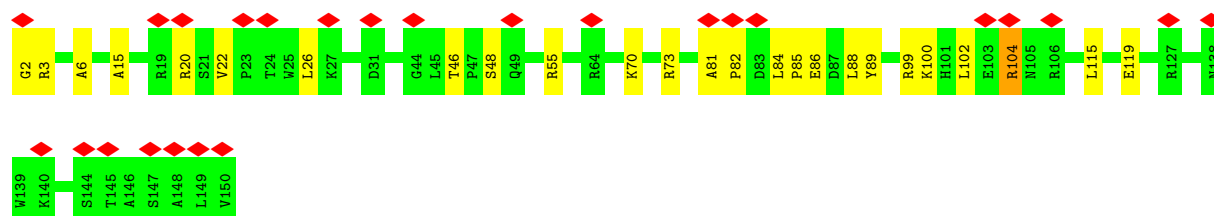
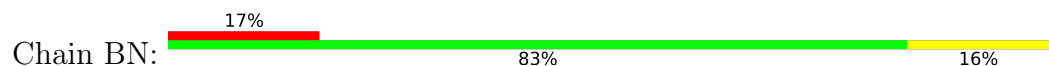
- Molecule 28: ribosomal protein uS4



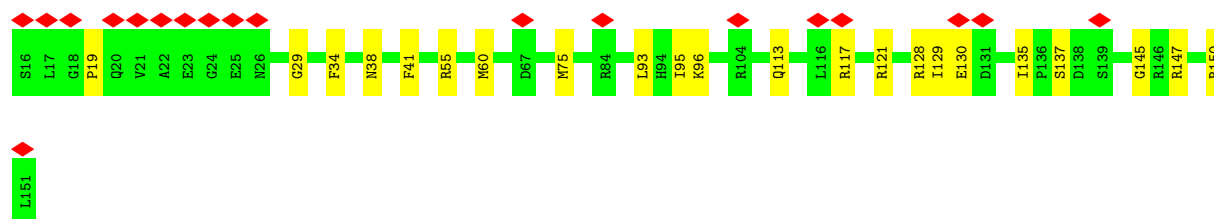
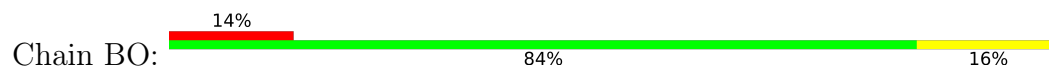
- Molecule 29: ribosomal protein uS17



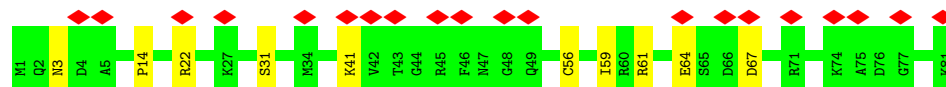
- Molecule 30: ribosomal protein uS15



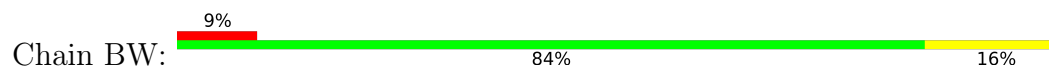
- Molecule 31: ribosomal protein uS11



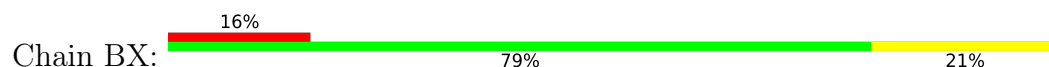
- Molecule 32: ribosomal protein eS21

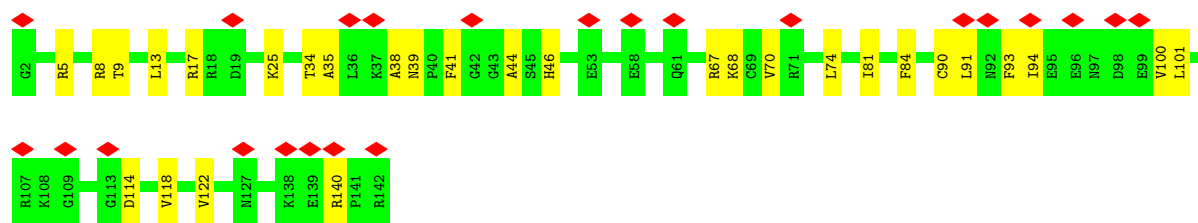


- Molecule 33: ribosomal protein uS8

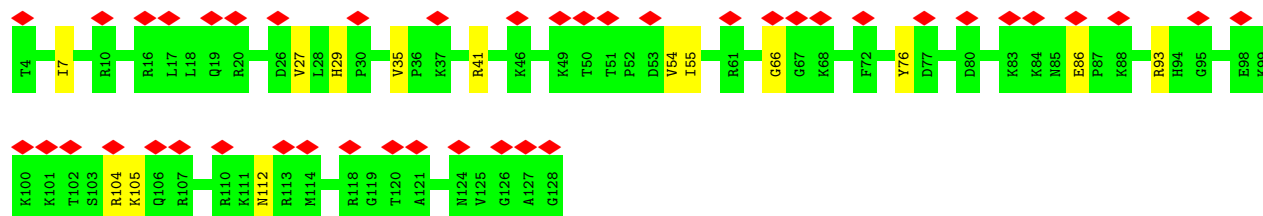
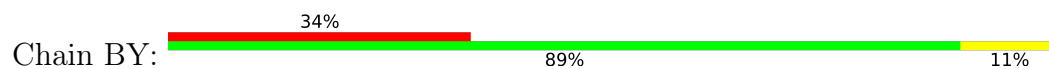


- Molecule 34: ribosomal protein uS12

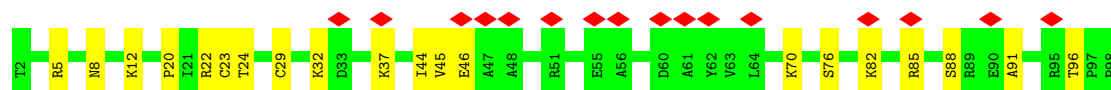
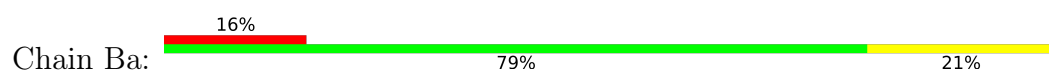




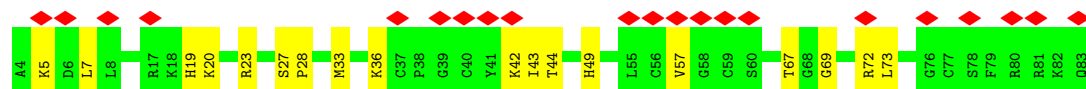
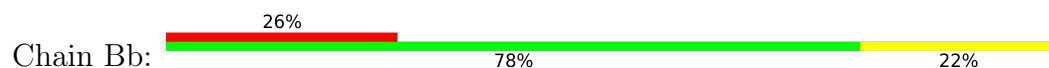
• Molecule 35: ribosomal protein eS24



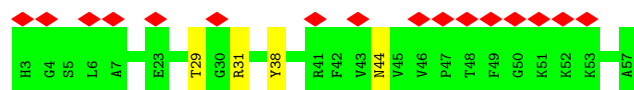
• Molecule 36: ribosomal protein eS26



• Molecule 37: ribosomal protein eS27



• Molecule 38: ribosomal protein eS30



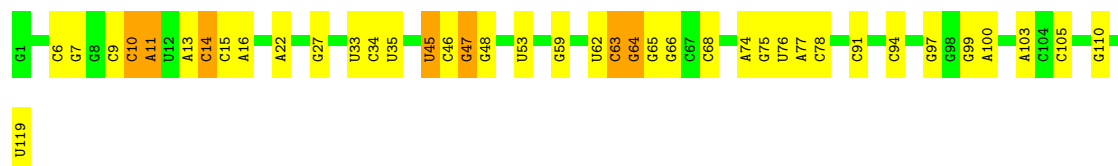
• Molecule 39: 5.8S ribosomal RNA





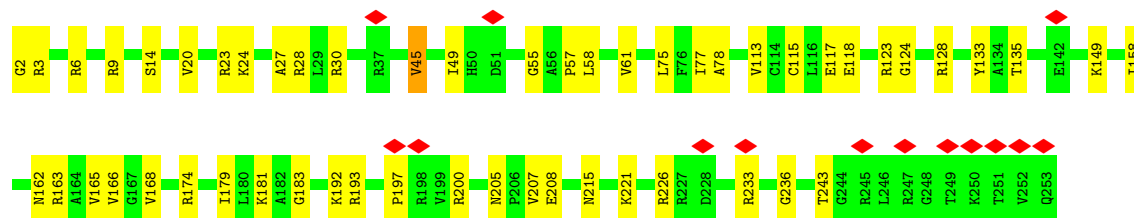
• Molecule 40: 5S ribosomal RNA

Chain A4: 66% 28% 6%



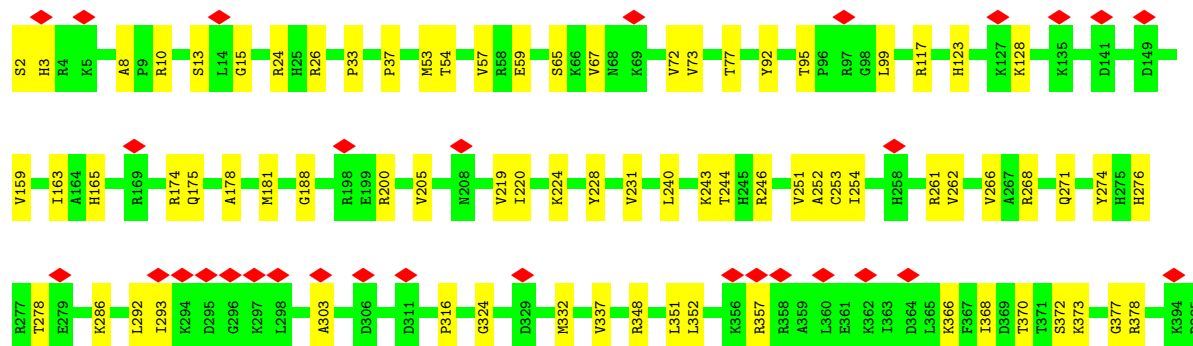
• Molecule 41: ribosomal protein uL2

Chain AA: 6% 79% 21%



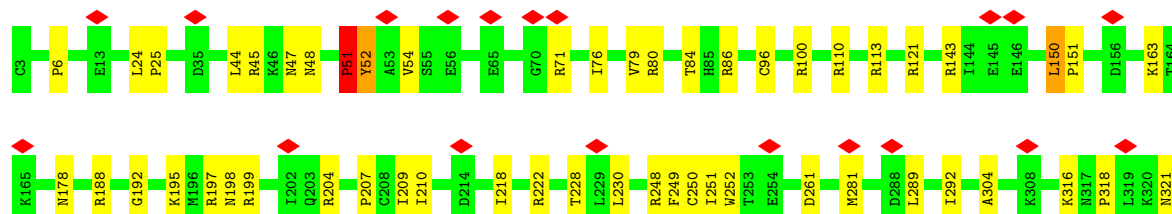
• Molecule 42: ribosomal protein uL3

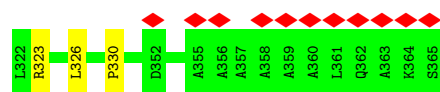
Chain AB: 8% 81% 19%



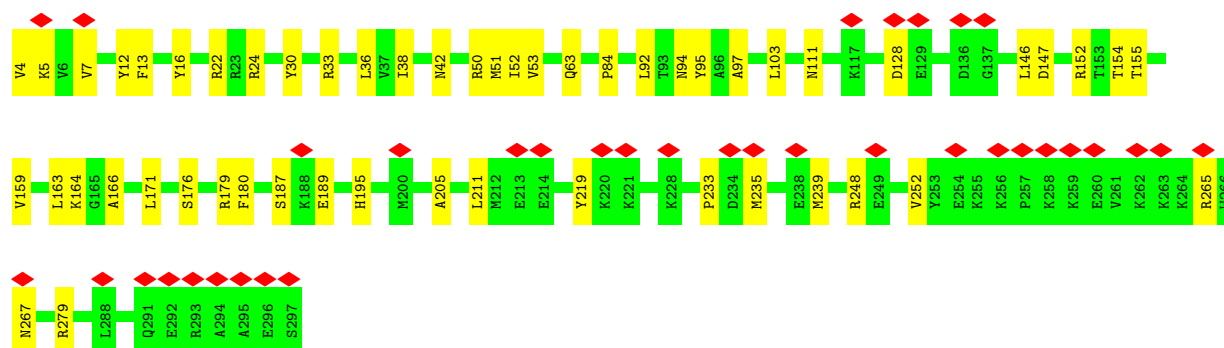
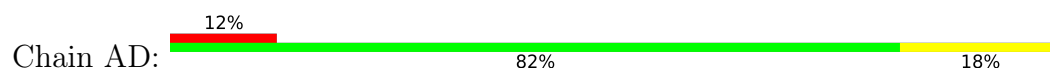
• Molecule 43: ribosomal protein uL4

Chain AC: 8% 85% 15%

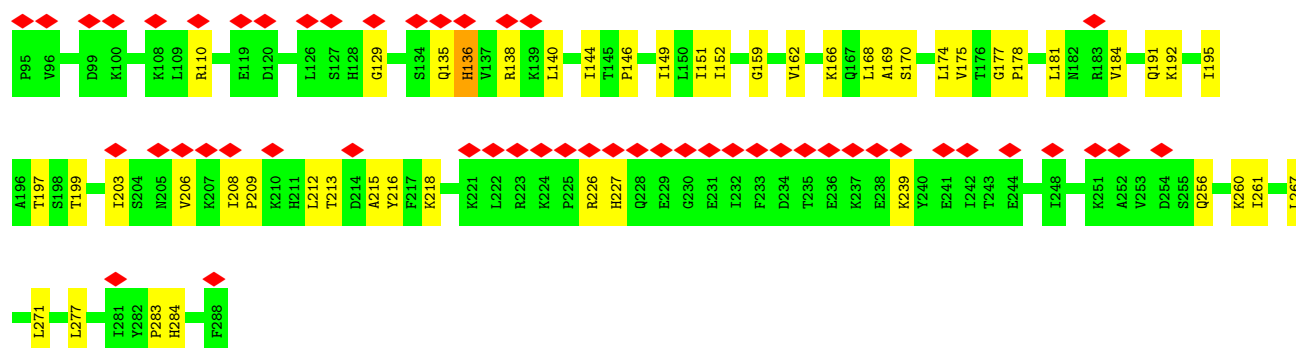
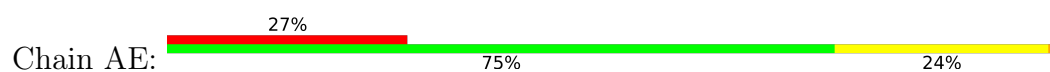




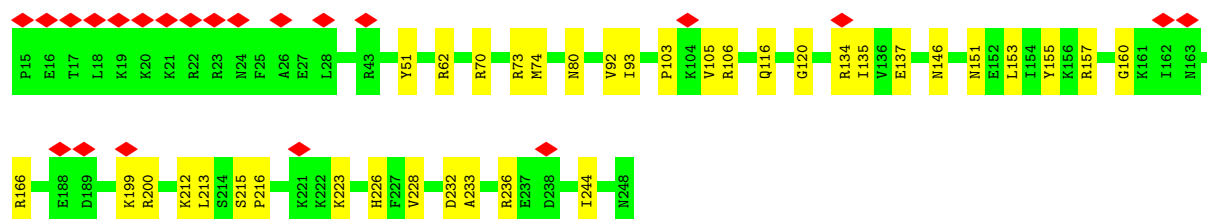
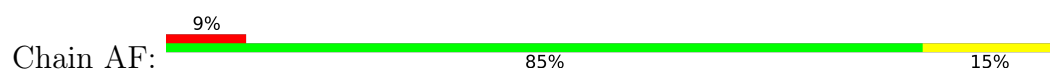
- Molecule 44: ribosomal protein uL18



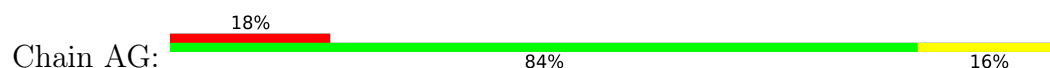
- Molecule 45: ribosomal protein eL6

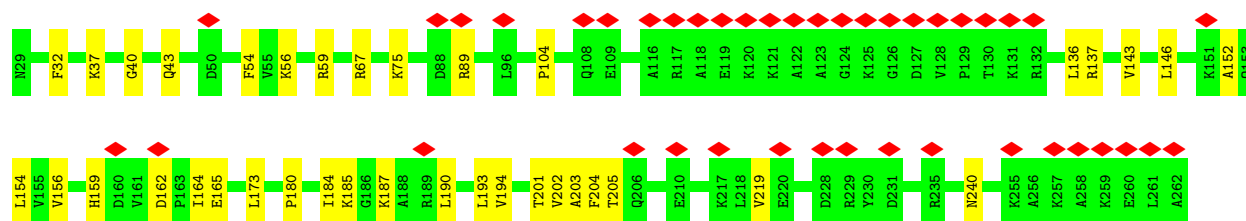


- Molecule 46: ribosomal protein uL30

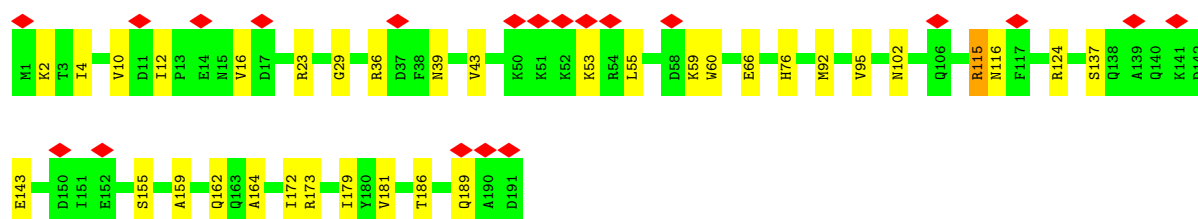
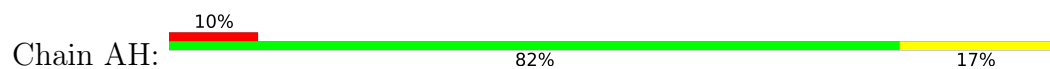


- Molecule 47: ribosomal protein eL8

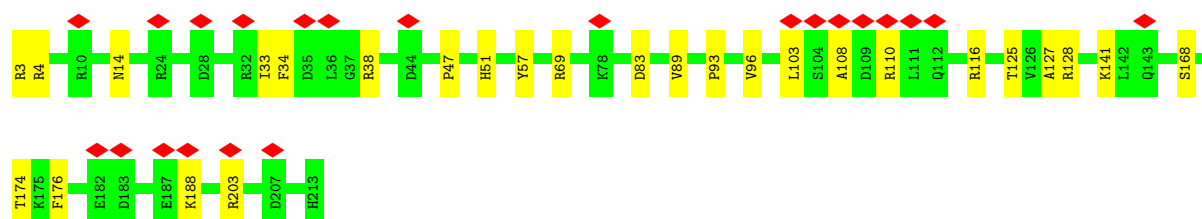
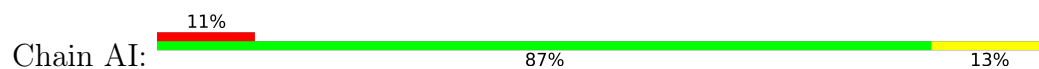




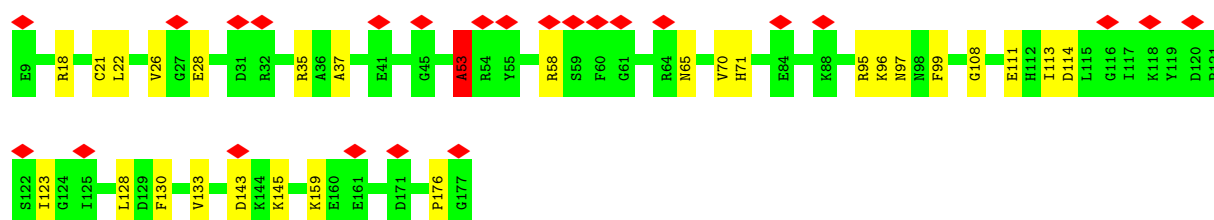
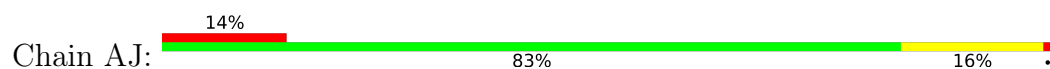
- Molecule 48: ribosomal protein uL6



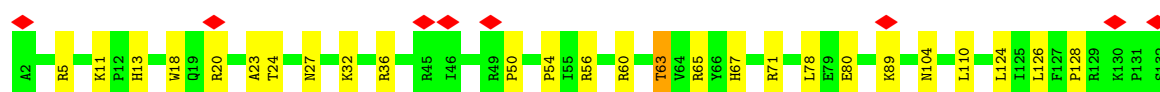
- Molecule 49: ribosomal protein uL16

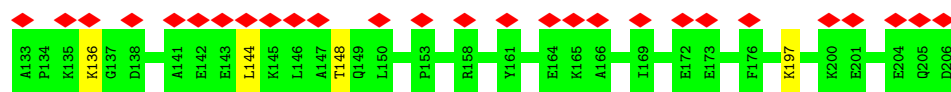


- Molecule 50: ribosomal protein uL5

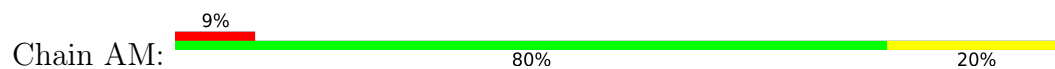


- Molecule 51: ribosomal protein eL13

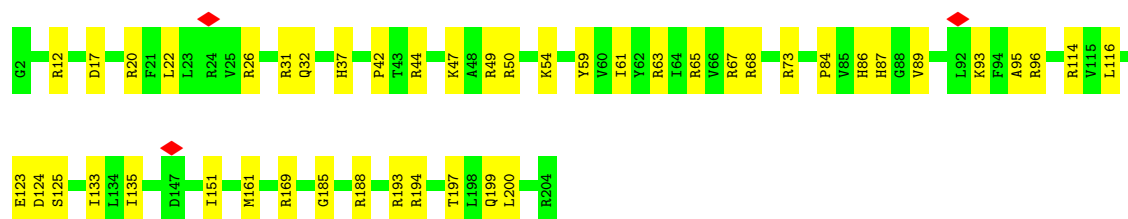
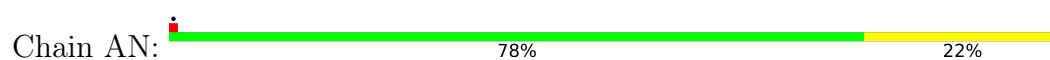




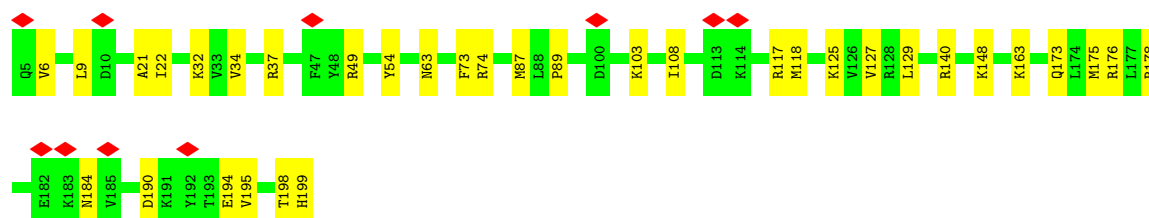
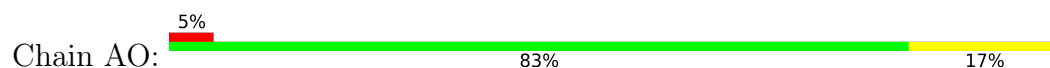
- Molecule 52: ribosomal protein eL14



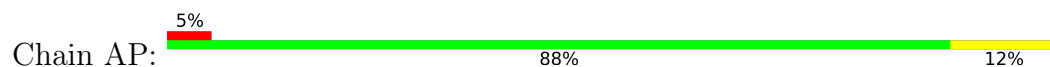
- Molecule 53: ribosomal protein eL15



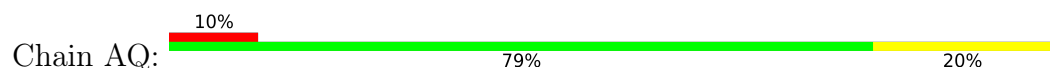
- Molecule 54: ribosomal protein uL13

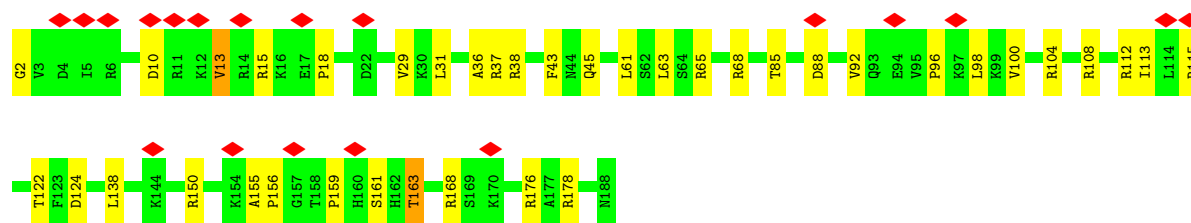


- Molecule 55: ribosomal protein uL22

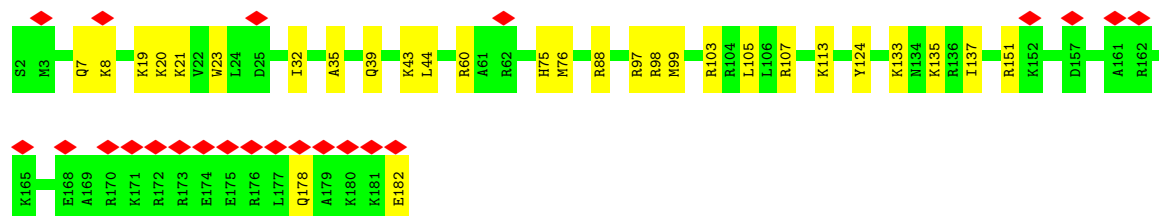
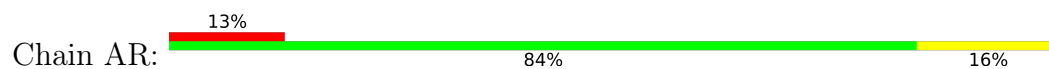


- Molecule 56: ribosomal protein eL18

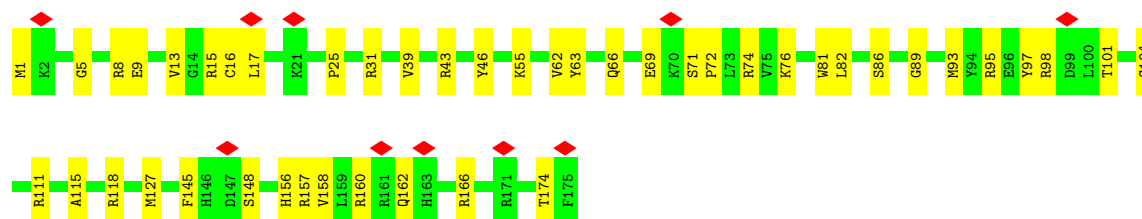
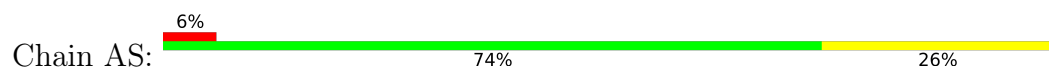




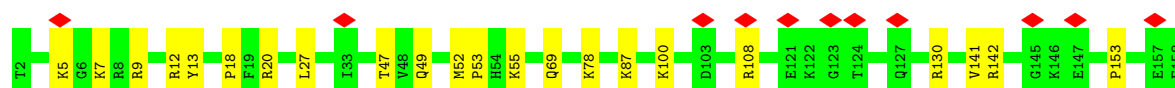
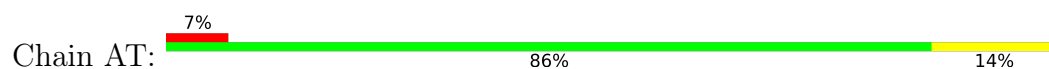
• Molecule 57: ribosomal protein eL19



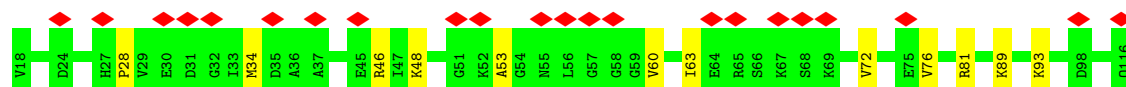
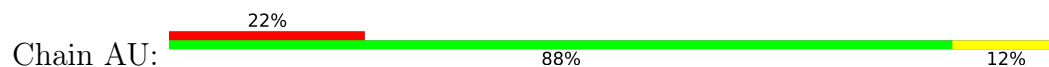
• Molecule 58: ribosomal protein eL20



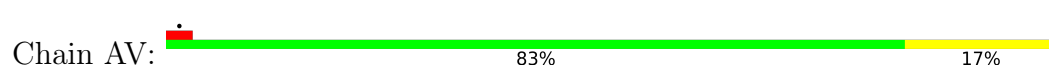
• Molecule 59: ribosomal protein eL21



• Molecule 60: ribosomal protein eL22

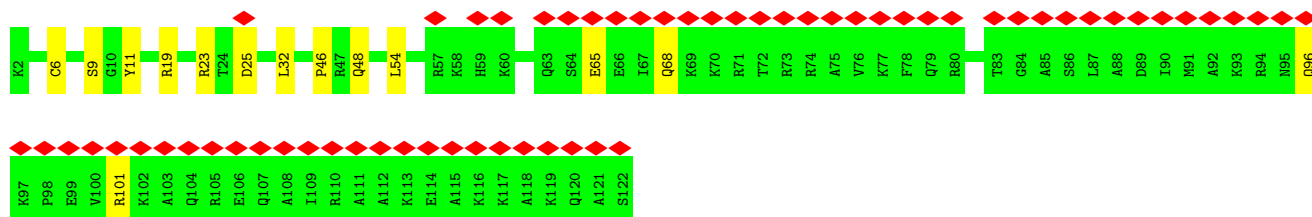
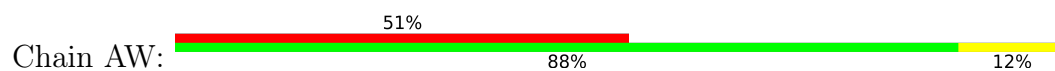


• Molecule 61: ribosomal protein uL14

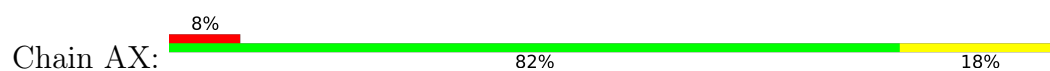




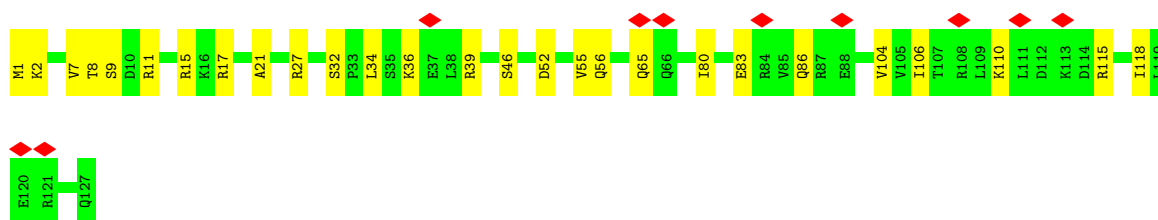
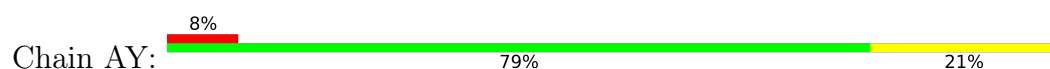
- Molecule 62: ribosomal protein eL24



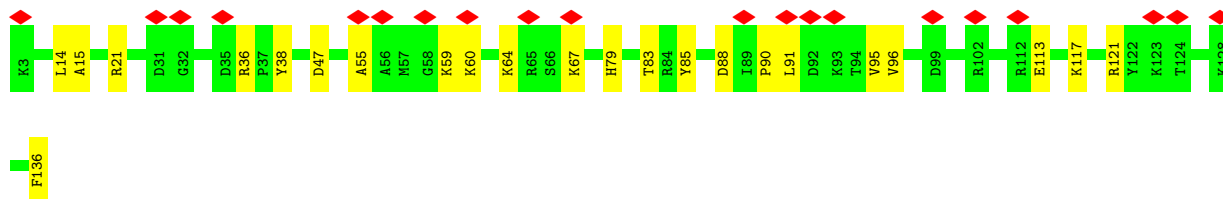
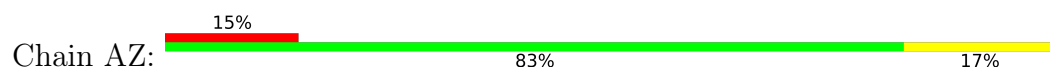
- Molecule 63: ribosomal protein uL23



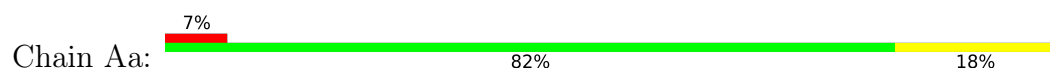
- Molecule 64: ribosomal protein uL24

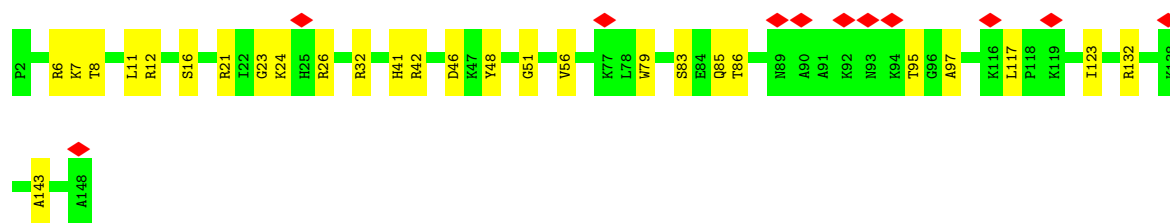


- Molecule 65: ribosomal protein eL27

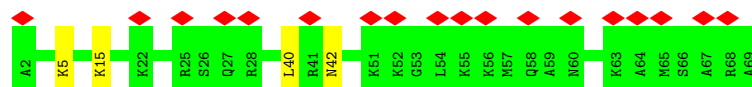


- Molecule 66: ribosomal protein uL15

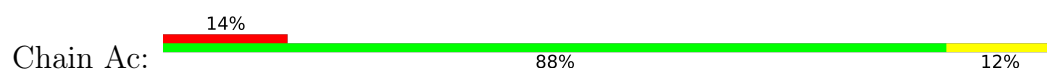




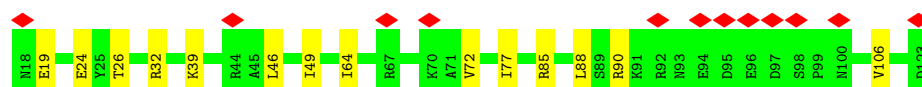
- Molecule 67: ribosomal protein eL29



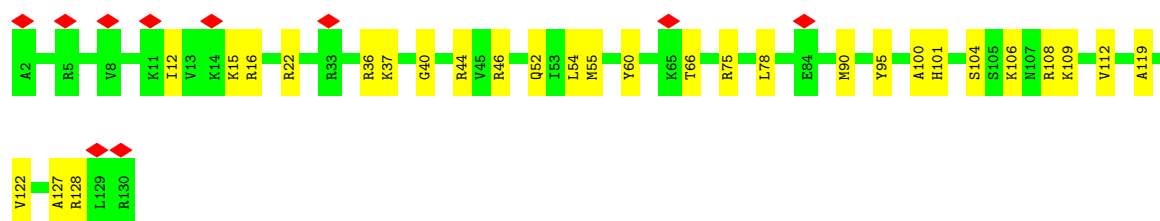
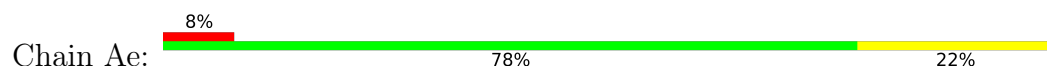
- Molecule 68: ribosomal protein eL30



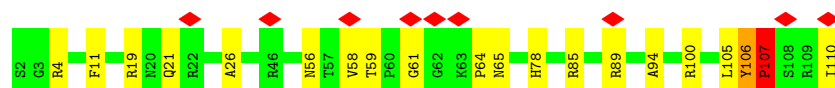
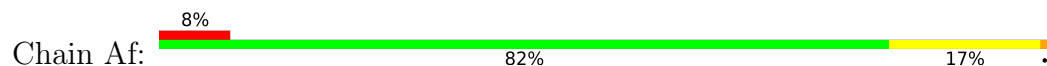
- Molecule 69: ribosomal protein eL31



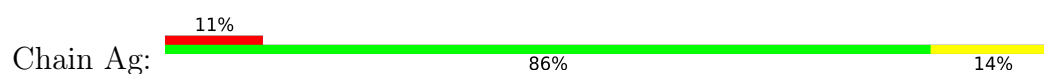
- Molecule 70: ribosomal protein eL32



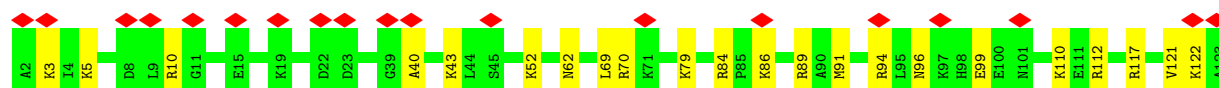
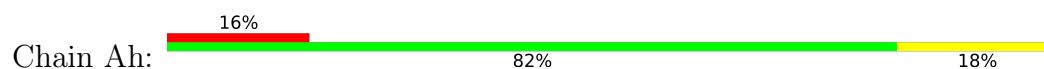
- Molecule 71: ribosomal protein eL33



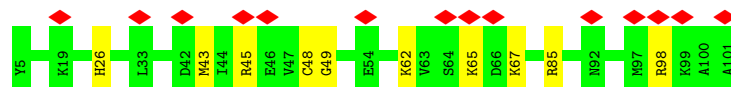
- Molecule 72: ribosomal protein eL34



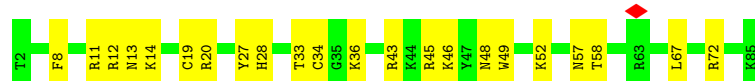
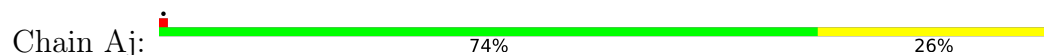
- Molecule 73: ribosomal protein uL29



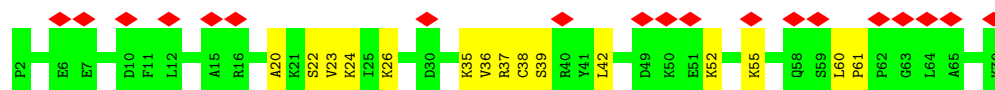
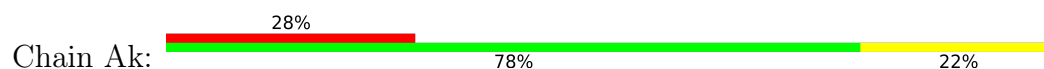
- Molecule 74: ribosomal protein eL36



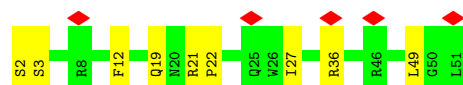
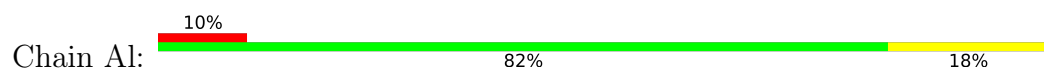
- Molecule 75: ribosomal protein eL37



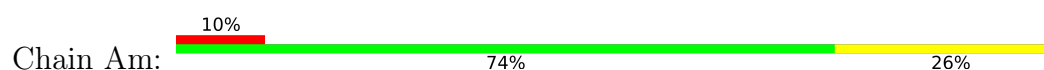
- Molecule 76: ribosomal protein eL38

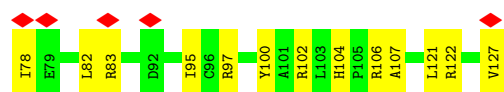


- Molecule 77: ribosomal protein eL39

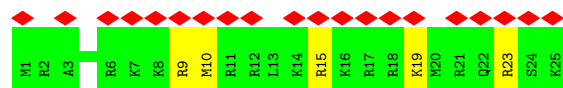
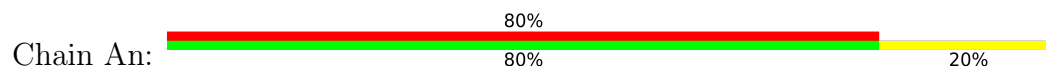


- Molecule 78: ribosomal protein eL40

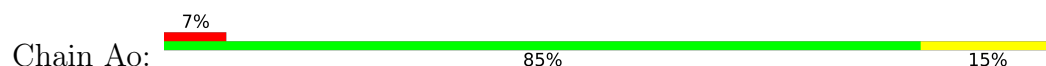




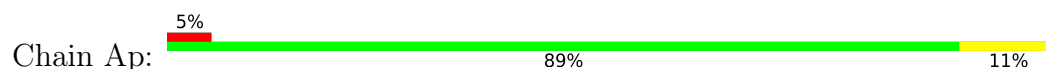
- Molecule 79: ribosomal protein eL41



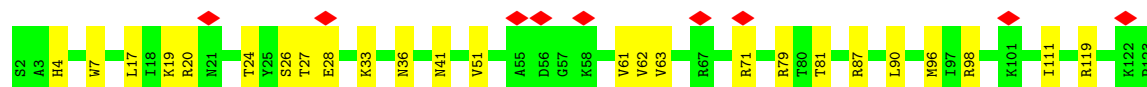
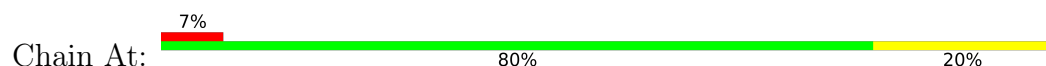
- Molecule 80: ribosomal protein eL42



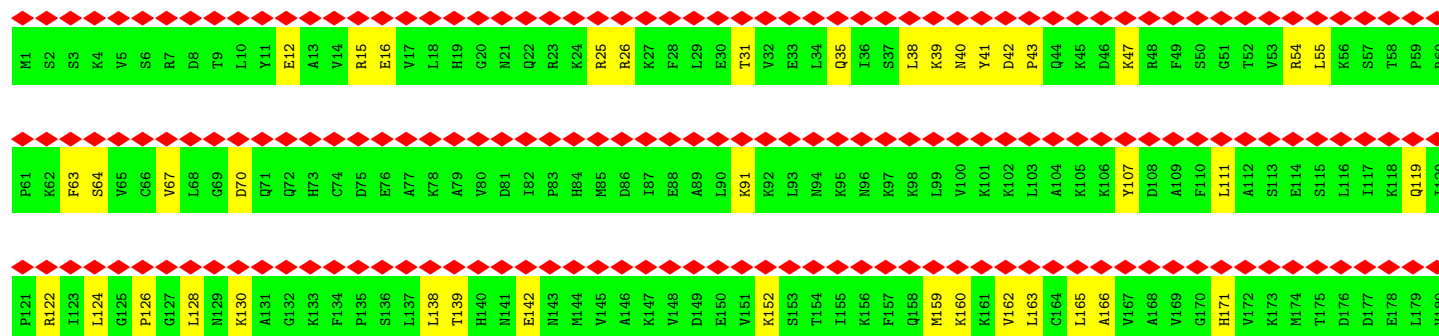
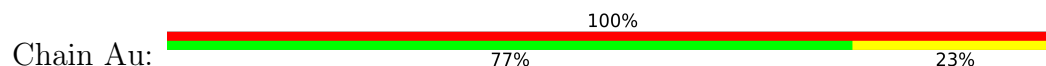
- Molecule 81: ribosomal protein eL43



- Molecule 82: ribosomal protein eL28

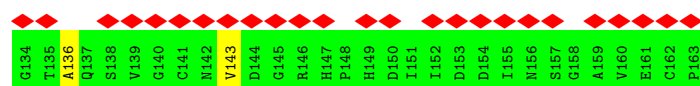
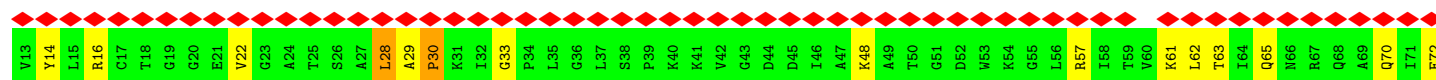
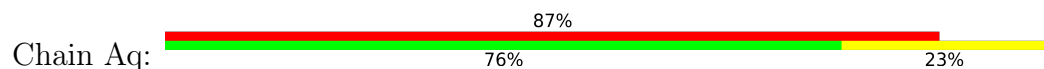


- Molecule 83: ribosomal protein uL1

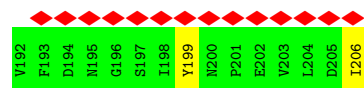
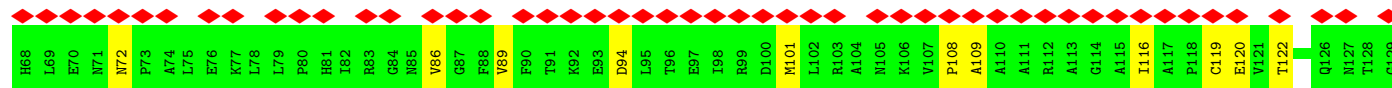
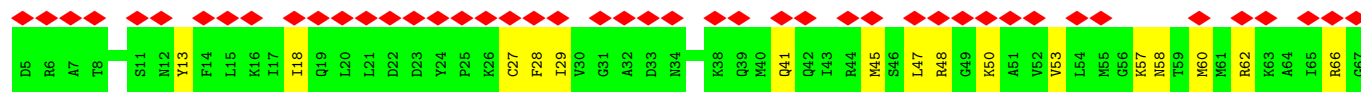
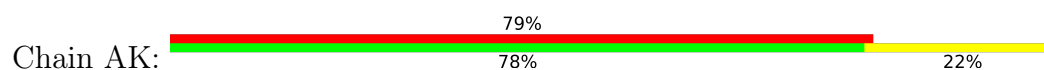




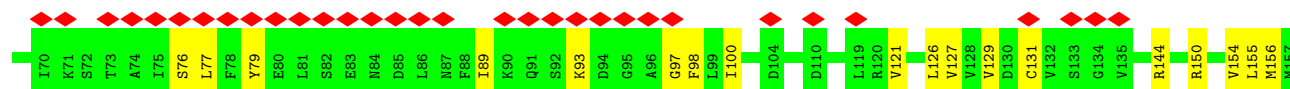
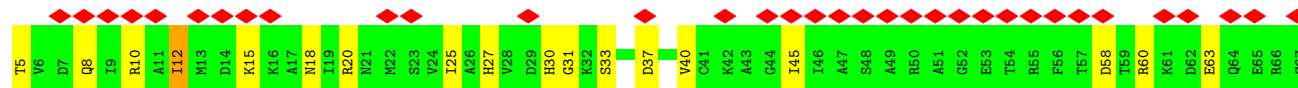
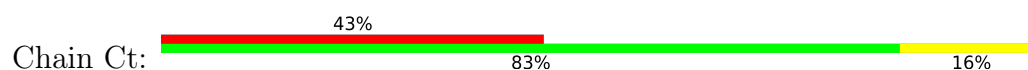
• Molecule 84: ribosomal protein uL11

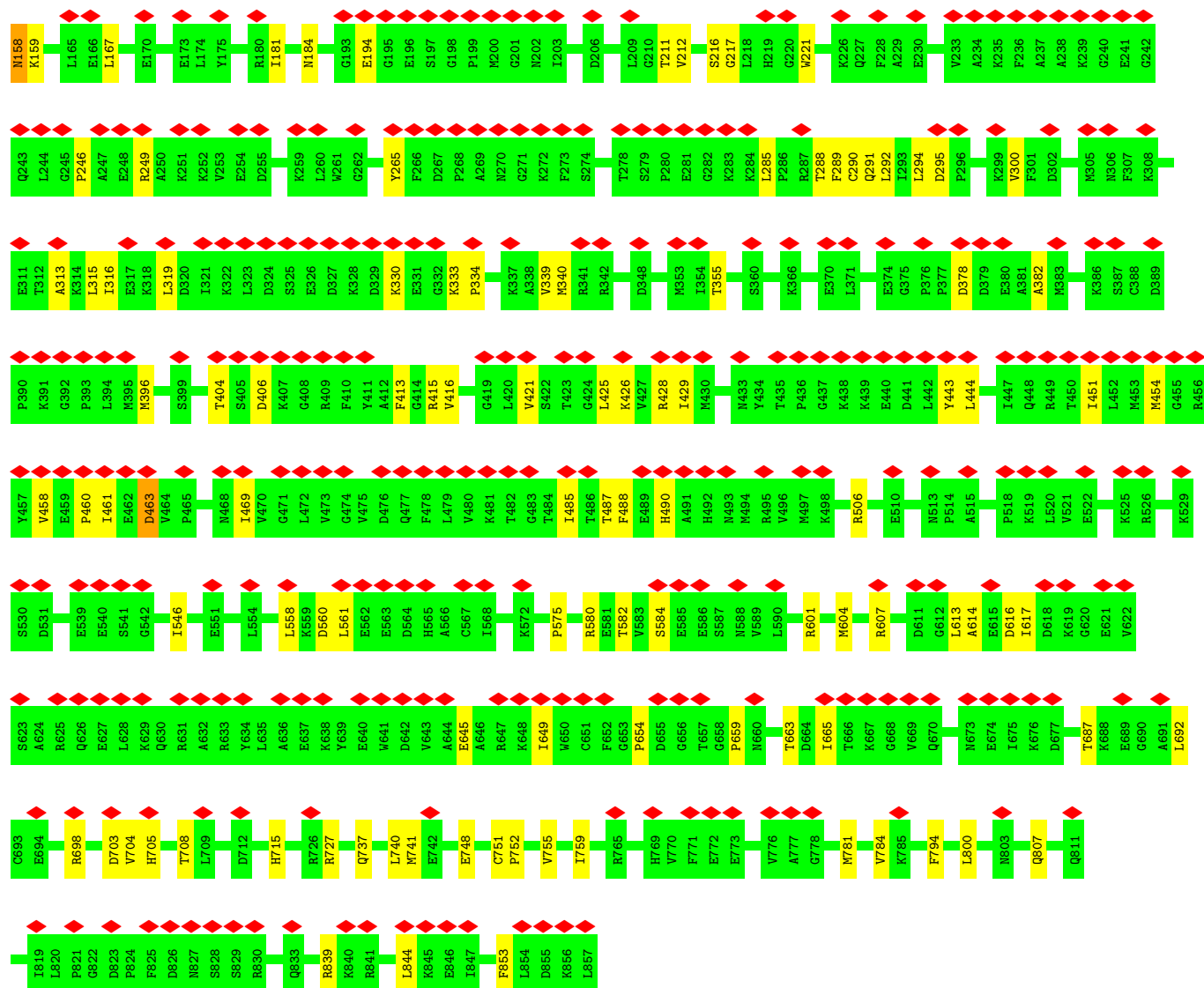


• Molecule 85: ribosomal protein uL10



• Molecule 86: eukaryotic elongation factor 2 (eEF2)





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	44522	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	13.064	Depositor
Minimum map value	-4.149	Depositor
Average map value	0.343	Depositor
Map value standard deviation	0.691	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: GNP, ZN, DDE, MG

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	0/135108
2	Bv	0.13	0/1810	0.26	0/2817
3	Bx	0.11	0/261	0.28	0/404
4	Bw	0.14	0/1819	0.28	0/2833
5	B1	0.16	0/40767	0.33	2/63536 (0.0%)
6	BD	0.17	0/1736	0.47	0/2338
7	BF	0.20	0/1524	0.56	0/2048
8	BK	0.21	0/851	0.55	0/1147
9	BM	0.17	0/941	0.50	0/1264
10	BP	0.23	0/1019	0.63	3/1361 (0.2%)
11	BQ	0.18	0/1126	0.51	0/1506
12	BR	0.18	0/1023	0.50	0/1373
13	BS	0.19	0/1172	0.52	0/1570
14	BT	0.18	0/1131	0.51	0/1515
15	BU	0.17	0/778	0.49	0/1045
16	BZ	0.20	0/696	0.56	0/929
17	Bc	0.18	0/490	0.55	2/656 (0.3%)
18	Bd	0.20	0/437	0.64	2/580 (0.3%)
19	Bf	0.14	0/613	0.44	0/811
20	Bg	0.16	0/2497	0.41	0/3399
21	BA	0.19	0/1741	0.50	0/2366
22	BB	0.21	0/1749	0.64	0/2340
23	BC	0.19	0/1761	0.49	0/2379
24	BE	0.18	0/2072	0.53	0/2793
25	BG	0.17	0/1907	0.47	0/2538
26	BH	0.17	0/1501	0.46	0/2009
27	BI	0.21	0/1725	0.61	2/2298 (0.1%)
28	BJ	0.20	0/1520	0.56	0/2030
29	BL	0.19	0/1281	0.51	0/1710
30	BN	0.19	0/1226	0.50	0/1649
31	BO	0.16	0/1029	0.46	0/1380
32	BV	0.17	0/623	0.51	0/833

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BW	0.19	0/1051	0.51	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	0.50	0/1053
37	Bb	0.16	0/637	0.43	0/854
38	Be	0.20	0/443	0.52	0/583
39	A3	0.16	0/3726	0.33	0/5804
40	A4	0.16	0/2839	0.32	0/4425
41	AA	0.19	0/1968	0.48	0/2639
42	AB	0.20	0/3246	0.50	0/4345
43	AC	0.19	0/2942	0.53	2/3951 (0.1%)
44	AD	0.19	0/2437	0.51	0/3262
45	AE	0.22	0/1603	0.62	0/2153
46	AF	0.20	0/1986	0.52	0/2644
47	AG	0.21	0/1913	0.55	0/2576
48	AH	0.20	0/1545	0.60	2/2077 (0.1%)
49	AI	0.17	0/1730	0.50	0/2311
50	AJ	0.19	0/1376	0.56	2/1841 (0.1%)
51	AL	0.21	0/1688	0.61	0/2260
52	AM	0.20	0/1161	0.49	0/1554
53	AN	0.19	0/1746	0.51	0/2338
54	AO	0.20	0/1638	0.48	0/2191
55	AP	0.18	0/1268	0.46	0/1701
56	AQ	0.20	0/1537	0.60	2/2052 (0.1%)
57	AR	0.18	0/1533	0.51	0/2025
58	AS	0.18	0/1488	0.48	0/1997
59	AT	0.16	0/1312	0.42	0/1753
60	AU	0.16	0/822	0.44	0/1103
61	AV	0.14	0/983	0.39	0/1319
62	AW	0.16	0/1004	0.45	0/1332
63	AX	0.16	0/975	0.44	0/1312
64	AY	0.17	0/1081	0.44	0/1439
65	AZ	0.18	0/1126	0.52	0/1502
66	Aa	0.18	0/1191	0.46	0/1591
67	Ab	0.22	0/569	0.67	0/750
68	Ac	0.17	0/812	0.46	0/1089
69	Ad	0.18	0/894	0.47	0/1204
70	Ae	0.19	0/1082	0.59	2/1443 (0.1%)
71	Af	0.19	0/895	0.58	1/1198 (0.1%)
72	Ag	0.20	0/916	0.56	0/1220
73	Ah	0.19	0/1023	0.53	0/1351
74	Ai	0.17	0/805	0.48	0/1065
75	Aj	0.21	0/703	0.56	0/929

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	Ak	0.17	0/575	0.45	0/761
77	Al	0.20	0/454	0.53	0/599
78	Am	0.19	0/417	0.47	0/553
79	An	0.16	0/241	0.50	0/305
80	Ao	0.18	0/877	0.51	0/1156
81	Ap	0.20	0/718	0.55	0/953
82	At	0.25	0/995	0.69	2/1334 (0.1%)
83	Au	0.20	0/1772	0.52	0/2375
84	Aq	0.27	0/1155	0.75	0/1558
85	AK	0.22	0/1580	0.64	4/2133 (0.2%)
86	Ct	0.21	0/6767	0.58	9/9139 (0.1%)
All	All	0.17	0/241618	0.42	37/353934 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
11	BQ	0	1
16	BZ	0	1
22	BB	0	1
24	BE	0	1
27	BI	0	2
28	BJ	0	1
43	AC	0	3
45	AE	0	2
48	AH	0	3
49	AI	0	1
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	2
All	All	0	27

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	AK	94	ASP	CA-C-N	6.79	133.93	121.70
85	AK	94	ASP	C-N-CA	6.79	133.93	121.70
86	Ct	158	ASN	CA-C-N	6.23	133.44	121.54
86	Ct	158	ASN	C-N-CA	6.23	133.44	121.54
86	Ct	12	ILE	N-CA-C	-6.11	105.41	111.77
27	BI	132	GLU	CA-C-N	6.00	132.99	121.54
27	BI	132	GLU	C-N-CA	6.00	132.99	121.54
86	Ct	463	ASP	CA-C-N	5.82	132.89	122.13
86	Ct	463	ASP	C-N-CA	5.82	132.89	122.13
85	AK	108	PRO	CA-C-N	5.60	131.78	121.70
85	AK	108	PRO	C-N-CA	5.60	131.78	121.70
86	Ct	461	ILE	CA-C-N	5.55	129.14	120.82
86	Ct	461	ILE	C-N-CA	5.55	129.14	120.82
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
48	AH	115	ARG	CA-C-N	5.52	132.08	121.54
48	AH	115	ARG	C-N-CA	5.52	132.08	121.54
71	Af	107	PRO	N-CA-C	5.46	123.72	112.47
56	AQ	159	PRO	CA-C-N	5.40	131.86	121.54
56	AQ	159	PRO	C-N-CA	5.40	131.86	121.54
5	B1	797	C	P-O3'-C3'	5.39	128.29	120.20
18	Bd	39	CYS	CA-C-N	5.37	131.81	121.54
18	Bd	39	CYS	C-N-CA	5.37	131.81	121.54
5	B1	227	U	P-O3'-C3'	5.35	128.22	120.20
50	AJ	53	ALA	CA-C-N	5.26	135.48	126.32
50	AJ	53	ALA	C-N-CA	5.26	135.48	126.32
10	BP	50	ARG	CA-C-N	5.17	131.41	121.54
10	BP	50	ARG	C-N-CA	5.17	131.41	121.54
82	At	26	SER	CA-C-N	5.17	131.40	121.54
82	At	26	SER	C-N-CA	5.17	131.40	121.54
86	Ct	288	THR	CA-C-N	5.10	131.27	121.54
86	Ct	288	THR	C-N-CA	5.10	131.27	121.54
10	BP	50	ARG	CA-CB-CG	5.09	124.29	114.10
70	Ae	15	LYS	CA-C-N	5.06	131.21	121.54
70	Ae	15	LYS	C-N-CA	5.06	131.21	121.54
43	AC	51	PRO	CA-C-N	5.01	131.10	121.54
43	AC	51	PRO	C-N-CA	5.01	131.10	121.54

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
43	AC	150	LEU	Peptide

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Mol	Chain	Res	Type	Group
43	AC	51	PRO	Peptide
43	AC	71	ARG	Peptide
45	AE	129	GLY	Peptide
45	AE	135	GLN	Peptide
48	AH	116	ASN	Peptide
48	AH	4	ILE	Peptide
48	AH	60	TRP	Peptide
49	AI	188	LYS	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
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
11	BQ	13	PHE	Peptide
16	BZ	41	ARG	Peptide
86	Ct	333	LYS	Peptide
86	Ct	463	ASP	Peptide

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A2	77427	0	39115	675	0
2	Bv	1620	0	821	8	0
3	Bx	234	0	118	1	0
4	Bw	1627	0	821	10	0
5	B1	36456	0	18412	307	0
6	BD	1709	0	1803	20	0
7	BF	1502	0	1557	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	BK	827	0	854	11	0
9	BM	931	0	961	15	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	17	0
14	BT	1112	0	1146	18	0
15	BU	769	0	837	9	0
16	BZ	688	0	766	10	0
17	Bc	488	0	514	7	0
18	Bd	427	0	427	12	0
19	Bf	601	0	622	9	0
20	Bg	2440	0	2396	31	0
21	BA	1704	0	1704	23	0
22	BB	1722	0	1794	28	0
23	BC	1724	0	1808	16	0
24	BE	2031	0	2138	23	0
25	BG	1884	0	2044	30	0
26	BH	1479	0	1564	15	0
27	BI	1696	0	1785	28	0
28	BJ	1495	0	1615	23	0
29	BL	1258	0	1334	13	0
30	BN	1202	0	1289	17	0
31	BO	1016	0	1039	19	0
32	BV	617	0	622	8	0
33	BW	1034	0	1080	16	0
34	BX	1098	0	1167	18	0
35	BY	1015	0	1086	9	0
36	Ba	774	0	822	16	0
37	Bb	625	0	646	13	0
38	Be	437	0	483	4	0
39	A3	3337	0	1692	33	0
40	A4	2541	0	1285	23	0
41	AA	1930	0	2030	41	0
42	AB	3178	0	3314	54	0
43	AC	2888	0	3064	46	0
44	AD	2392	0	2425	34	0
45	AE	1571	0	1701	29	0
46	AF	1950	0	2093	29	0
47	AG	1880	0	2018	26	0
48	AH	1526	0	1605	21	0
49	AI	1692	0	1744	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	AJ	1353	0	1386	19	0
51	AL	1657	0	1764	25	0
52	AM	1138	0	1204	23	0
53	AN	1701	0	1749	37	0
54	AO	1606	0	1745	25	0
55	AP	1242	0	1269	11	0
56	AQ	1513	0	1628	29	0
57	AR	1517	0	1670	22	0
58	AS	1449	0	1493	34	0
59	AT	1284	0	1352	18	0
60	AU	808	0	831	7	0
61	AV	969	0	1031	15	0
62	AW	989	0	1041	9	0
63	AX	958	0	1029	15	0
64	AY	1064	0	1145	19	0
65	AZ	1103	0	1179	14	0
66	Aa	1162	0	1213	23	0
67	Ab	559	0	590	4	0
68	Ac	801	0	845	6	0
69	Ad	879	0	924	10	0
70	Ae	1064	0	1160	18	0
71	Af	876	0	912	15	0
72	Ag	906	0	1002	13	0
73	Ah	1015	0	1148	19	0
74	Ai	794	0	870	7	0
75	Aj	689	0	717	18	0
76	Ak	569	0	637	11	0
77	Al	444	0	483	9	0
78	Am	411	0	443	13	0
79	An	240	0	289	4	0
80	Ao	863	0	931	11	0
81	Ap	708	0	757	6	0
82	At	980	0	1041	17	0
83	Au	1744	0	1859	29	0
84	Aq	1140	0	1191	23	0
85	AK	1556	0	1612	22	0
86	Ct	6659	0	6746	82	0
87	A2	229	0	0	0	0
87	A3	7	0	0	0	0
87	A4	8	0	0	0	0
87	AA	1	0	0	0	0
87	AC	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	AL	1	0	0	0	0
87	AO	1	0	0	0	0
87	AP	1	0	0	0	0
87	AY	1	0	0	0	0
87	An	1	0	0	0	0
87	B1	73	0	0	0	0
87	BD	1	0	0	0	0
87	Ba	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	0	0
All	All	225601	0	169553	2040	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 (2040) 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)
1:A2:161:G:H1	1:A2:266:U:H3	1.06	0.99
1:A2:465:A:H62	1:A2:677:G:H21	1.12	0.98
1:A2:3663:A:H62	1:A2:3794:G:N2	1.60	0.98
5:B1:1656:G:H1	5:B1:1668:U:H3	1.03	0.98
1:A2:3663:A:N6	1:A2:3794:G:H21	1.61	0.98
1:A2:1871:G:H1	1:A2:1920:A:N6	1.62	0.97
1:A2:1871:G:H1	1:A2:1920:A:H61	0.98	0.96
5:B1:1396:A:H2	5:B1:1449:G:H1	1.12	0.95
5:B1:442:C:N4	5:B1:449:A:H62	1.64	0.94
1:A2:708:U:H3	1:A2:938:G:H1	0.97	0.93
1:A2:3917:G:H1	1:A2:4037:U:H3	1.16	0.92
5:B1:442:C:H42	5:B1:449:A:N6	1.69	0.91
1:A2:2462:G:H1	1:A2:2474:U:H3	0.92	0.91
5:B1:1652:G:H1	5:B1:1672:U:H3	0.93	0.89
5:B1:1050:A:H62	5:B1:1068:G:H21	1.21	0.85
5:B1:442:C:H42	5:B1:449:A:H62	0.88	0.85
1:A2:499:G:H1	1:A2:647:U:H3	1.22	0.84
86:Ct:645:GLU:O	86:Ct:649:ILE:HB	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B1:677:G:H21	5:B1:1028:A:H62	1.27	0.81
1:A2:465:A:H62	1:A2:677:G:N2	1.79	0.80
1:A2:2356:C:H42	1:A2:2360:A:H62	1.30	0.79
1:A2:1977:C:N4	1:A2:1981:G:H22	1.79	0.79
43:AC:218:ILE:O	43:AC:222:ARG:HB2	1.83	0.79
86:Ct:315:LEU:O	86:Ct:319:LEU:HB2	1.83	0.78
1:A2:346:G:H21	1:A2:354:A:N6	1.82	0.78
71:Af:58:VAL:HG11	71:Af:65:ASN:H	1.50	0.77
1:A2:3942:G:H21	1:A2:4020:A:H62	1.34	0.76
5:B1:1128:C:HO2'	37:Bb:19:HIS:HD1	1.31	0.76
1:A2:1977:C:H42	1:A2:1981:G:N2	1.86	0.74
19:Bf:141:CYS:HB3	19:Bf:146:LEU:H	1.53	0.74
5:B1:1743:G:H21	5:B1:1791:A:H62	1.32	0.73
85:AK:66:ARG:HG3	85:AK:72:ASN:HD21	1.53	0.73
1:A2:455:G:H1	1:A2:687:A:H2	1.37	0.72
50:AJ:53:ALA:HB2	50:AJ:65:ASN:H	1.52	0.72
5:B1:16:G:H21	5:B1:1195:A:H62	1.38	0.71
1:A2:2274:C:H5''	43:AC:199:ARG:HH12	1.56	0.71
10:BP:24:GLN:O	10:BP:28:MET:HB2	1.92	0.70
1:A2:4433:U:H3	1:A2:4446:G:H1	1.39	0.69
5:B1:383:G:H21	29:BL:133:PRO:HG2	1.58	0.69
20:Bg:87:LEU:HB2	20:Bg:101:PHE:HB2	1.73	0.69
1:A2:2617:G:H21	1:A2:2676:A:H62	1.41	0.68
1:A2:1089:A:N6	1:A2:1146:G:H1	1.92	0.67
1:A2:465:A:N6	1:A2:677:G:H21	1.88	0.67
1:A2:1089:A:N6	1:A2:1146:G:N1	2.42	0.67
5:B1:1869:A:H61	22:BB:113:MET:H	1.43	0.67
5:B1:377:G:H5''	27:BI:98:LYS:HB3	1.77	0.66
70:Ae:22:ARG:HE	70:Ae:36:ARG:HB3	1.61	0.66
57:AR:133:LYS:H	57:AR:137:ILE:HD11	1.60	0.66
1:A2:2464:U:H3	1:A2:2472:G:H1	1.41	0.66
1:A2:2356:C:N4	1:A2:2360:A:H62	1.93	0.66
1:A2:159:A:H61	1:A2:268:C:H42	1.44	0.66
1:A2:722:G:H21	58:AS:72:PRO:HG2	1.60	0.66
22:BB:197:ILE:O	22:BB:201:CYS:HB2	1.95	0.66
29:BL:101:ARG:HH21	34:BX:13:LEU:HD11	1.60	0.65
1:A2:289:A:H5'	80:Ao:39:ARG:HD2	1.79	0.65
48:AH:172:ILE:HD11	78:Am:102:ARG:HH22	1.61	0.65
20:Bg:174:VAL:HB	20:Bg:188:HIS:HB2	1.79	0.65
37:Bb:20:LYS:HE3	37:Bb:28:PRO:HA	1.79	0.65
1:A2:1379:G:HO2'	1:A2:1450:C:HO2'	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B1:1396:A:H2	5:B1:1449:G:N1	1.90	0.65
28:BJ:37:LEU:HD23	28:BJ:42:GLU:HG3	1.79	0.65
66:Aa:24:LYS:HD3	66:Aa:26:ARG:HH21	1.62	0.65
71:Af:59:THR:HG23	71:Af:61:GLY:H	1.61	0.65
13:BS:43:VAL:HG22	14:BT:37:VAL:HG21	1.78	0.65
1:A2:686:C:H5''	45:AE:226:ARG:HH22	1.61	0.64
5:B1:659:G:H21	34:BX:17:ARG:HH12	1.44	0.64
26:BH:61:ILE:HG22	26:BH:93:VAL:HB	1.80	0.64
7:BF:21:GLY:H	7:BF:23:TRP:HD1	1.46	0.64
27:BI:132:GLU:HB3	27:BI:134:GLU:HG2	1.80	0.64
64:AY:52:ASP:HB2	64:AY:110:LYS:HD2	1.80	0.64
51:AL:63:THR:HB	51:AL:65:ARG:H	1.62	0.64
5:B1:525:A:H2'	5:B1:526:A:H8	1.62	0.64
42:AB:163:ILE:HA	42:AB:181:MET:O	1.98	0.64
29:BL:101:ARG:HH22	34:BX:5:ARG:HA	1.61	0.63
49:AI:47:PRO:HD2	49:AI:141:LYS:HA	1.80	0.63
56:AQ:18:PRO:HG3	56:AQ:29:VAL:HG21	1.79	0.63
42:AB:26:ARG:NH1	42:AB:181:MET:SD	2.71	0.63
70:Ae:78:LEU:HB3	82:At:20:ARG:HH12	1.62	0.63
86:Ct:429:ILE:HB	86:Ct:443:TYR:HB2	1.81	0.63
1:A2:1353:G:OP1	43:AC:48:ASN:ND2	2.31	0.63
1:A2:2825:G:H5''	61:AV:85:ARG:HE	1.62	0.63
58:AS:101:THR:HG23	58:AS:104:GLY:H	1.64	0.63
83:Au:139:THR:HB	83:Au:142:GLU:HB2	1.80	0.63
1:A2:2645:U:OP2	57:AR:107:ARG:NH2	2.31	0.63
86:Ct:291:GLN:HA	86:Ct:295:ASP:HB2	1.81	0.63
41:AA:117:GLU:HB2	41:AA:162:ASN:HB2	1.81	0.63
1:A2:742:G:N2	1:A2:743:G:N7	2.47	0.62
1:A2:2444:C:H1'	1:A2:3643:G:H1	1.63	0.62
1:A2:2662:C:O2	72:Ag:54:ARG:NH2	2.28	0.62
16:BZ:58:LEU:O	16:BZ:62:VAL:HB	1.99	0.62
66:Aa:42:ARG:O	66:Aa:46:ASP:HB2	1.98	0.62
86:Ct:76:SER:H	86:Ct:454:MET:HB3	1.64	0.62
9:BM:55:ASN:HD22	9:BM:81:ASP:HB3	1.62	0.62
33:BW:52:ILE:HG12	33:BW:61:ILE:HG12	1.81	0.62
27:BI:165:GLN:HE22	27:BI:195:LEU:HD11	1.62	0.62
1:A2:346:G:N2	1:A2:354:A:C6	2.68	0.62
1:A2:2756:G:H5''	1:A2:2757:G:H5'	1.81	0.62
82:At:90:LEU:HD11	82:At:111:ILE:HG23	1.81	0.62
39:A3:153:C:H2'	39:A3:154:G:H8	1.65	0.62
1:A2:477:G:H1	1:A2:665:G:H22	1.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BF:34:SER:HB3	7:BF:146:ARG:HH22	1.65	0.62
35:BY:104:ARG:HG3	35:BY:105:LYS:HG2	1.80	0.62
42:AB:10:ARG:HH22	42:AB:13:SER:HA	1.64	0.62
49:AI:33:ILE:O	49:AI:69:ARG:NH1	2.32	0.62
74:AI:48:CYS:SG	74:AI:49:GLY:N	2.72	0.62
40:A4:105:C:OP2	49:AI:203:ARG:NH1	2.32	0.61
27:BI:104:ILE:HB	27:BI:171:LEU:HB3	1.81	0.61
31:BO:34:PHE:HB3	31:BO:41:PHE:HB2	1.80	0.61
84:Aq:119:ARG:H	84:Aq:123:ARG:HH12	1.47	0.61
5:B1:1270:G:O2'	5:B1:1301:A:N7	2.34	0.61
29:BL:104:LYS:HZ1	34:BX:8:ARG:HH11	1.49	0.61
1:A2:737:A:N1	58:AS:98:ARG:NH2	2.48	0.61
5:B1:1050:A:H62	5:B1:1068:G:N2	1.95	0.61
80:Ao:71:GLU:HG2	80:Ao:80:LYS:HG2	1.82	0.61
5:B1:1172:U:H4'	79:An:10:MET:HE2	1.82	0.61
24:BE:100:ARG:HH12	24:BE:236:ILE:HD12	1.66	0.61
1:A2:412:A:H4'	1:A2:2290:C:H5'	1.82	0.61
1:A2:2536:G:H1	1:A2:2549:U:H3	1.47	0.61
1:A2:1933:G:H4'	58:AS:93:MET:HG3	1.83	0.61
5:B1:186:C:H2'	5:B1:187:G:H8	1.66	0.61
5:B1:1455:A:OP1	12:BR:5:ARG:NH2	2.32	0.61
23:BC:131:GLY:HA3	23:BC:137:VAL:HG12	1.81	0.61
58:AS:81:TRP:HB3	58:AS:127:MET:HE3	1.82	0.61
1:A2:3908:C:H1'	53:AN:125:SER:HB3	1.82	0.61
1:A2:4895:C:N3	45:AE:239:LYS:NZ	2.49	0.61
1:A2:4180:U:OP2	59:AT:9:ARG:NH2	2.33	0.61
1:A2:1712:U:H4'	59:AT:100:LYS:HB2	1.82	0.60
70:Ae:16:ARG:HH12	70:Ae:54:LEU:HG	1.66	0.60
1:A2:1721:G:N3	1:A2:1724:A:N6	2.49	0.60
1:A2:2279:A:N7	43:AC:143:ARG:NH1	2.48	0.60
1:A2:2279:A:N6	43:AC:178:ASN:OD1	2.35	0.60
1:A2:2569:G:N2	1:A2:2734:A:H62	1.98	0.60
1:A2:3606:A:H61	81:Ap:17:ARG:HB2	1.65	0.60
53:AN:68:ARG:NH2	53:AN:123:GLU:OE1	2.34	0.60
1:A2:2365:U:H2'	1:A2:2366:G:H8	1.65	0.60
1:A2:5019:A:OP1	42:AB:123:HIS:NE2	2.35	0.60
14:BT:71:GLY:H	14:BT:74:SER:HB2	1.66	0.60
86:Ct:649:ILE:HG13	86:Ct:663:THR:HG22	1.83	0.60
1:A2:272:G:OP1	53:AN:12:ARG:NH2	2.35	0.60
82:At:63:VAL:HG22	82:At:79:ARG:HG2	1.83	0.60
5:B1:1123:C:OP1	22:BB:151:ARG:NH2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:1483:C:H2'	56:AQ:68:ARG:HH22	1.65	0.60
1:A2:4508:A:N7	41:AA:215:ASN:ND2	2.50	0.60
5:B1:391:C:H2'	5:B1:392:A:H8	1.66	0.60
84:Aq:57:ARG:HH11	84:Aq:83:LYS:HB3	1.66	0.60
24:BE:31:PRO:HG3	24:BE:43:PRO:HG3	1.84	0.60
43:AC:209:ILE:HG13	43:AC:251:ILE:HB	1.82	0.60
57:AR:76:MET:SD	57:AR:88:ARG:NH2	2.74	0.60
57:AR:99:MET:HE3	57:AR:103:ARG:HH11	1.67	0.60
1:A2:1952:C:O2	85:AK:41:GLN:NE2	2.35	0.60
7:BF:71:ARG:NH2	7:BF:148:ASN:OD1	2.35	0.60
58:AS:1:MET:HG3	58:AS:43:ARG:HH21	1.67	0.60
1:A2:4602:C:N3	1:A2:4622:G:N2	2.50	0.59
5:B1:677:G:N2	5:B1:1028:A:H62	1.98	0.59
17:Bc:40:ARG:HH22	31:BO:121:ARG:HH12	1.48	0.59
1:A2:346:G:N2	1:A2:354:A:N6	2.50	0.59
5:B1:104:A:O2'	27:BI:18:ARG:NH2	2.35	0.59
14:BT:75:MET:SD	14:BT:121:ARG:NH1	2.75	0.59
83:Au:64:SER:HB3	83:Au:107:TYR:HD1	1.68	0.59
1:A2:1320:A:H62	1:A2:2325:C:H5	1.49	0.59
34:BX:93:PHE:O	34:BX:140:ARG:NH1	2.35	0.59
52:AM:101:LYS:HB2	54:AO:198:THR:HG21	1.84	0.59
4:Bw:22:G:H2'	4:Bw:23:A:H8	1.67	0.59
34:BX:68:LYS:HD3	34:BX:91:LEU:HD22	1.83	0.59
42:AB:200:ARG:HH22	42:AB:205:VAL:HG22	1.68	0.59
86:Ct:289:PHE:HA	86:Ct:292:LEU:HB2	1.83	0.59
10:BP:98:ASN:ND2	10:BP:121:ILE:O	2.36	0.59
31:BO:145:GLY:O	36:Ba:22:ARG:NH1	2.34	0.59
51:AL:54:PRO:HB2	51:AL:56:ARG:HH12	1.67	0.59
82:At:28:GLU:OE2	82:At:41:ASN:ND2	2.36	0.59
1:A2:4854:G:N7	1:A2:4882:C:N4	2.49	0.59
32:BV:59:ILE:HG23	32:BV:64:GLU:HB3	1.83	0.59
37:Bb:36:LYS:HG2	37:Bb:43:ILE:HG12	1.83	0.59
86:Ct:396:MET:HB2	86:Ct:485:ILE:HB	1.85	0.59
1:A2:1303:U:O2'	1:A2:1872:A:N1	2.35	0.59
5:B1:35:C:H5''	5:B1:579:C:H5''	1.84	0.59
20:Bg:256:ILE:HB	20:Bg:270:LEU:HB2	1.85	0.59
22:BB:82:ARG:NH2	22:BB:188:LEU:O	2.34	0.59
39:A3:29:G:H5''	51:AL:27:ASN:HB3	1.85	0.59
1:A2:5009:C:H4'	42:AB:324:GLY:HA2	1.84	0.59
56:AQ:96:PRO:HG2	56:AQ:98:LEU:HD22	1.85	0.59
57:AR:8:LYS:HE3	57:AR:19:LYS:HG2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:1977:C:N4	1:A2:1981:G:N2	2.46	0.58
5:B1:1648:G:N2	5:B1:1675:A:OP2	2.36	0.58
9:BM:32:ALA:HB3	9:BM:110:VAL:HB	1.85	0.58
85:AK:18:ILE:HD12	85:AK:62:ARG:HH22	1.68	0.58
1:A2:4730:G:H1	1:A2:4822:U:H3	1.51	0.58
40:A4:75:G:N2	40:A4:100:A:OP2	2.36	0.58
42:AB:240:LEU:HB3	42:AB:244:THR:HG21	1.86	0.58
1:A2:50:C:H5''	51:AL:20:ARG:HH12	1.68	0.58
1:A2:2664:C:OP1	72:Ag:57:ARG:NH1	2.36	0.58
86:Ct:40:VAL:HG23	86:Ct:77:LEU:HD21	1.85	0.58
1:A2:24:G:N7	75:Aj:46:LYS:NZ	2.49	0.58
40:A4:14:C:OP1	44:AD:24:ARG:NH1	2.37	0.58
1:A2:1722:C:O2	1:A2:1768:A:N6	2.37	0.58
1:A2:4721:C:OP1	54:AO:117:ARG:NH2	2.36	0.58
75:Aj:36:LYS:HA	75:Aj:45:ARG:HH21	1.69	0.58
1:A2:1086:C:H5''	1:A2:1087:C:H5	1.68	0.58
5:B1:1597:C:OP2	16:BZ:85:ARG:NH2	2.37	0.58
69:Ad:39:LYS:HA	69:Ad:77:ILE:HD12	1.86	0.58
86:Ct:601:ARG:HB3	86:Ct:708:THR:HB	1.85	0.58
1:A2:3863:U:O2'	55:AP:80:GLN:NE2	2.35	0.58
5:B1:1748:G:H1	5:B1:1786:U:H3	1.52	0.58
29:BL:147:LYS:HG2	29:BL:149:ALA:H	1.68	0.58
39:A3:69:U:O2'	64:AY:27:ARG:NH2	2.36	0.58
58:AS:15:ARG:HB2	58:AS:25:PRO:HB2	1.86	0.58
82:At:51:VAL:HG12	82:At:62:VAL:HG22	1.86	0.58
83:Au:54:ARG:NH1	83:Au:55:LEU:O	2.37	0.58
1:A2:1959:C:H4'	84:Aq:99:LYS:HD2	1.84	0.58
1:A2:2372:C:OP2	1:A2:2373:G:N2	2.37	0.58
1:A2:2704:A:H5'	57:AR:97:ARG:HH21	1.68	0.58
1:A2:4567:A:HO2'	86:Ct:27:HIS:HE2	1.51	0.58
18:Bd:47:ALA:HB1	18:Bd:52:PHE:HB2	1.85	0.58
68:Ac:21:VAL:HG11	68:Ac:96:ILE:HD12	1.86	0.58
1:A2:1503:C:OP1	43:AC:100:ARG:NH2	2.36	0.58
5:B1:28:U:H2'	5:B1:29:G:H8	1.69	0.58
5:B1:70:G:H21	5:B1:79:A:H62	1.50	0.58
1:A2:317:C:H2'	1:A2:318:A:H8	1.69	0.58
1:A2:1441:A:OP1	56:AQ:65:ARG:NH2	2.36	0.58
28:BJ:153:SER:HB2	28:BJ:156:HIS:HD2	1.69	0.58
44:AD:52:ILE:HA	44:AD:147:ASP:HB3	1.85	0.58
48:AH:59:LYS:HE2	48:AH:66:GLU:HB3	1.85	0.58
48:AH:124:ARG:HD3	48:AH:164:ALA:HB1	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:Au:38:LEU:HB2	83:Au:163:LEU:HB3	1.85	0.58
5:B1:43:U:OP2	5:B1:485:A:N6	2.36	0.57
5:B1:1143:A:O3'	5:B1:1355:C:N4	2.37	0.57
1:A2:2569:G:H21	1:A2:2734:A:H62	1.51	0.57
8:BK:65:ARG:NH2	18:Bd:21:CYS:O	2.37	0.57
1:A2:296:C:OP1	53:AN:68:ARG:NH1	2.35	0.57
1:A2:454:C:H2'	1:A2:455:G:H8	1.69	0.57
1:A2:3686:U:O2'	4:Bw:71:G:N3	2.37	0.57
7:BF:143:PRO:HB3	7:BF:146:ARG:HH21	1.67	0.57
39:A3:122:G:N2	39:A3:129:C:O2'	2.38	0.57
1:A2:1977:C:H42	1:A2:1981:G:H22	1.43	0.57
1:A2:2580:A:N6	1:A2:2723:A:OP2	2.37	0.57
5:B1:575:A:OP1	35:BY:93:ARG:NH1	2.35	0.57
22:BB:173:THR:O	22:BB:177:GLN:HB2	2.04	0.57
1:A2:453:C:OP1	82:At:87:ARG:NH2	2.38	0.57
1:A2:943:A:H5''	1:A2:944:G:H5'	1.86	0.57
57:AR:7:GLN:NE2	57:AR:35:ALA:O	2.37	0.57
1:A2:2552:A:H62	1:A2:2740:U:H3	1.51	0.57
2:Bv:18:G:O2'	2:Bv:57:G:N2	2.38	0.57
5:B1:886:A:N6	5:B1:901:G:C2	2.72	0.57
45:AE:166:LYS:HD2	45:AE:208:ILE:HD11	1.86	0.57
1:A2:216:G:H1	1:A2:233:G:H22	1.49	0.57
1:A2:920:G:N2	1:A2:925:C:O2'	2.38	0.57
58:AS:82:LEU:HB2	58:AS:93:MET:HB3	1.85	0.57
1:A2:223:G:N2	64:AY:8:THR:O	2.38	0.57
1:A2:451:G:H1	1:A2:691:G:H1	1.52	0.57
43:AC:281:MET:HG2	56:AQ:104:ARG:HA	1.87	0.57
83:Au:63:PHE:HB2	83:Au:152:LYS:HA	1.86	0.57
85:AK:122:THR:HG22	85:AK:159:GLN:HG2	1.87	0.57
1:A2:944:G:N2	1:A2:2056:G:O2'	2.37	0.57
1:A2:4643:A:H4'	54:AO:140:ARG:HH22	1.70	0.57
6:BD:18:LYS:HE2	6:BD:39:VAL:HB	1.86	0.57
21:BA:11:LYS:HE3	21:BA:13:GLU:HB3	1.86	0.57
47:AG:152:ALA:HA	47:AG:205:THR:HG22	1.87	0.57
58:AS:71:SER:O	58:AS:76:LYS:NZ	2.38	0.57
5:B1:973:C:O2	31:BO:55:ARG:NH2	2.38	0.57
11:BQ:16:LYS:HB3	11:BQ:19:ALA:HB3	1.87	0.57
68:Ac:51:ASN:ND2	68:Ac:77:ASN:OD1	2.38	0.57
1:A2:1295:A:O2'	70:Ae:52:GLN:NE2	2.38	0.56
1:A2:1607:G:N2	1:A2:3890:C:OP2	2.38	0.56
31:BO:113:GLN:HE21	36:Ba:46:GLU:HB2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:AK:141:LEU:HD21	85:AK:171:GLU:HG3	1.86	0.56
1:A2:447:G:O6	1:A2:1277:A:N6	2.38	0.56
5:B1:4:C:O2'	28:BJ:18:ARG:NH2	2.38	0.56
5:B1:1743:G:N2	5:B1:1791:A:H62	2.00	0.56
28:BJ:14:VAL:H	28:BJ:44:TRP:HB3	1.71	0.56
33:BW:75:ILE:HD11	33:BW:93:LEU:HD11	1.87	0.56
49:AI:3:ARG:NH1	49:AI:4:ARG:O	2.38	0.56
1:A2:1954:G:H21	84:Aq:132:ILE:HG23	1.70	0.56
1:A2:2685:G:H1	57:AR:43:LYS:HZ2	1.52	0.56
5:B1:39:A:H62	5:B1:515:G:H21	1.51	0.56
5:B1:90:G:OP1	5:B1:445:A:N6	2.38	0.56
5:B1:649:U:H2'	5:B1:650:A:H8	1.71	0.56
9:BM:97:GLU:OE1	9:BM:99:LYS:NZ	2.38	0.56
14:BT:11:GLN:HE21	14:BT:15:VAL:HB	1.70	0.56
20:Bg:11:LEU:HB2	20:Bg:307:VAL:HB	1.88	0.56
42:AB:231:VAL:HG11	42:AB:251:VAL:HG23	1.88	0.56
60:AU:60:VAL:HG21	60:AU:76:VAL:H	1.71	0.56
1:A2:1498:G:O2'	51:AL:18:TRP:NE1	2.39	0.56
1:A2:3731:A:H61	5:B1:1824:A:H2'	1.71	0.56
1:A2:4692:C:H1'	1:A2:4693:G:H2'	1.87	0.56
5:B1:1627:C:OP1	14:BT:83:GLN:NE2	2.38	0.56
20:Bg:163:PRO:HB2	20:Bg:179:LEU:HB2	1.86	0.56
26:BH:122:LEU:O	26:BH:126:HIS:ND1	2.36	0.56
35:BY:7:ILE:HG12	35:BY:27:VAL:HG22	1.85	0.56
42:AB:351:LEU:HD12	42:AB:352:LEU:HG	1.87	0.56
45:AE:151:ILE:HB	45:AE:195:ILE:HB	1.87	0.56
1:A2:2645:U:OP2	57:AR:103:ARG:NH2	2.38	0.56
1:A2:4943:U:OP1	42:AB:117:ARG:NH1	2.39	0.56
5:B1:65:C:N4	25:BG:134:GLY:O	2.38	0.56
5:B1:948:C:H2'	5:B1:949:G:H8	1.70	0.56
5:B1:986:G:OP2	5:B1:988:C:N4	2.39	0.56
22:BB:72:ALA:HB3	31:BO:128:ARG:HH22	1.69	0.56
40:A4:13:A:OP2	40:A4:66:G:N2	2.35	0.56
41:AA:30:ARG:O	41:AA:163:ARG:NH2	2.39	0.56
20:Bg:212:LYS:HA	20:Bg:235:ILE:HG13	1.87	0.56
15:BU:94:PRO:HD2	15:BU:97:ILE:HD12	1.88	0.56
19:Bf:121:CYS:HA	19:Bf:132:MET:HE3	1.86	0.56
46:AF:93:ILE:HD13	46:AF:213:LEU:HD12	1.87	0.56
57:AR:20:LYS:HG3	57:AR:21:LYS:HG3	1.86	0.56
58:AS:69:GLU:HB3	58:AS:72:PRO:HG3	1.88	0.56
86:Ct:580:ARG:HB2	86:Ct:741:MET:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:294:A:H2'	1:A2:295:G:H8	1.71	0.56
9:BM:45:ARG:HE	9:BM:72:HIS:HD2	1.52	0.56
45:AE:195:ILE:HG23	71:Af:110:ILE:HG21	1.87	0.56
1:A2:446:A:O2'	1:A2:1276:G:N2	2.38	0.56
1:A2:4482:G:N2	42:AB:253:CYS:SG	2.79	0.56
27:BI:110:ARG:HH12	27:BI:122:GLY:HA3	1.70	0.56
76:Ak:24:LYS:HB2	76:Ak:35:LYS:HB2	1.88	0.56
1:A2:37:U:H4'	66:Aa:32:ARG:HD2	1.87	0.56
1:A2:1600:G:OP1	75:Aj:13:ASN:ND2	2.38	0.56
5:B1:1231:C:O2'	5:B1:1253:A:N6	2.39	0.56
6:BD:16:ILE:HG21	18:Bd:22:ARG:HH11	1.70	0.56
22:BB:151:ARG:NH1	22:BB:153:THR:OG1	2.39	0.56
46:AF:232:ASP:OD1	46:AF:236:ARG:NH2	2.39	0.56
1:A2:727:C:OP2	52:AM:71:LYS:NZ	2.39	0.55
1:A2:1651:A:H5''	67:Ab:15:LYS:HD3	1.88	0.55
73:Ah:79:LYS:HE3	73:Ah:84:ARG:HA	1.87	0.55
86:Ct:31:GLY:O	86:Ct:158:ASN:ND2	2.39	0.55
1:A2:369:G:OP2	75:Aj:52:LYS:NZ	2.39	0.55
1:A2:4832:A:N3	1:A2:4834:U:N3	2.54	0.55
19:Bf:141:CYS:SG	19:Bf:144:CYS:N	2.78	0.55
42:AB:224:LYS:O	42:AB:274:TYR:N	2.40	0.55
1:A2:455:G:O6	1:A2:687:A:N1	2.39	0.55
1:A2:1191:G:O2'	46:AF:70:ARG:NH1	2.39	0.55
30:BN:15:ALA:HB3	37:Bb:20:LYS:HE2	1.88	0.55
44:AD:42:ASN:ND2	59:AT:69:GLN:OE1	2.39	0.55
64:AY:83:GLU:O	64:AY:86:GLN:NE2	2.39	0.55
66:Aa:6:ARG:HG3	66:Aa:8:THR:H	1.70	0.55
83:Au:111:LEU:HD13	83:Au:138:LEU:HD11	1.86	0.55
1:A2:67:C:N4	1:A2:319:U:O2'	2.36	0.55
1:A2:224:A:H61	1:A2:238:G:H21	1.53	0.55
1:A2:1615:G:H5'	41:AA:205:ASN:HD21	1.72	0.55
1:A2:2245:C:O2	1:A2:2247:A:N6	2.39	0.55
62:AW:96:GLN:O	62:AW:101:ARG:NH1	2.39	0.55
1:A2:192:C:H42	1:A2:242:C:H42	1.54	0.55
1:A2:1195:G:O6	1:A2:1197:C:N4	2.40	0.55
1:A2:4567:A:O2'	86:Ct:27:HIS:NE2	2.34	0.55
20:Bg:5:MET:HB3	20:Bg:310:TRP:HB3	1.89	0.55
39:A3:52:A:OP1	77:Al:21:ARG:NH1	2.39	0.55
69:Ad:88:LEU:HG	69:Ad:106:VAL:HG22	1.88	0.55
1:A2:920:G:H21	1:A2:926:G:H5''	1.70	0.55
1:A2:2618:U:HO2'	1:A2:2673:G:H1	1.49	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:4263:U:OP1	59:AT:78:LYS:NZ	2.38	0.55
1:A2:4650:C:HO2'	48:AH:155:SER:HG	1.48	0.55
5:B1:154:U:O2	5:B1:165:G:N2	2.40	0.55
5:B1:1658:G:OP2	5:B1:1660:C:N4	2.40	0.55
41:AA:221:LYS:HE2	41:AA:233:ARG:HH12	1.70	0.55
48:AH:173:ARG:HH22	78:Am:127:VAL:HG13	1.71	0.55
69:Ad:24:GLU:OE1	69:Ad:85:ARG:NH2	2.40	0.55
1:A2:63:G:OP2	53:AN:169:ARG:NH1	2.40	0.55
21:BA:113:GLN:HG3	21:BA:115:ALA:H	1.71	0.55
21:BA:184:ARG:HD3	21:BA:191:ARG:HD2	1.89	0.55
25:BG:51:ARG:HB2	25:BG:112:VAL:HB	1.89	0.55
86:Ct:614:ALA:O	86:Ct:698:ARG:NH2	2.39	0.55
1:A2:2689:C:OP2	57:AR:39:GLN:NE2	2.39	0.55
1:A2:4047:A:N1	1:A2:4133:C:N4	2.54	0.55
5:B1:1139:C:O2'	5:B1:1140:G:O4'	2.24	0.55
47:AG:143:VAL:HG22	47:AG:203:ALA:HB2	1.89	0.55
68:Ac:47:ILE:HB	68:Ac:94:LEU:HB2	1.88	0.55
1:A2:2553:G:OP2	65:AZ:67:LYS:NZ	2.40	0.55
1:A2:2674:A:H5''	76:Ak:26:LYS:HE3	1.89	0.55
5:B1:4:C:H5'	23:BC:230:THR:HG21	1.88	0.55
8:BK:50:GLN:HA	8:BK:53:LYS:HG2	1.89	0.55
13:BS:30:ILE:HG22	13:BS:36:VAL:HG11	1.88	0.55
22:BB:70:SER:OG	31:BO:128:ARG:NH1	2.39	0.55
29:BL:85:THR:HA	29:BL:113:LEU:H	1.71	0.55
48:AH:10:VAL:HB	48:AH:55:LEU:HB3	1.88	0.55
83:Au:35:GLN:HB2	83:Au:205:TYR:HB2	1.87	0.55
8:BK:30:PRO:HB3	18:Bd:12:ARG:HD2	1.89	0.55
22:BB:49:VAL:HG22	22:BB:62:LEU:HD21	1.89	0.55
22:BB:105:LEU:HD13	22:BB:213:ARG:HA	1.89	0.55
26:BH:154:ILE:HB	26:BH:185:VAL:HG12	1.89	0.55
42:AB:53:MET:HG2	42:AB:77:THR:HG22	1.88	0.55
44:AD:38:ILE:HD11	59:AT:27:LEU:HD22	1.88	0.55
65:AZ:88:ASP:O	65:AZ:121:ARG:NH2	2.40	0.55
1:A2:407:G:H5'	77:Al:36:ARG:HH12	1.72	0.54
1:A2:4971:C:O2'	1:A2:4985:C:N4	2.40	0.54
13:BS:24:ARG:O	13:BS:55:ARG:NH1	2.40	0.54
59:AT:49:GLN:HA	59:AT:52:MET:HE3	1.89	0.54
85:AK:101:MET:HG3	85:AK:206:ILE:HG21	1.88	0.54
1:A2:19:G:OP1	73:Ah:89:ARG:NH2	2.39	0.54
1:A2:1284:C:N4	1:A2:2294:G:OP1	2.40	0.54
1:A2:2278:G:O6	43:AC:188:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B1:1396:A:OP2	11:BQ:15:ARG:NH1	2.40	0.54
10:BP:114:HIS:ND1	10:BP:118:GLU:OE1	2.40	0.54
30:BN:46:THR:HG23	30:BN:86:GLU:HG2	1.90	0.54
41:AA:6:ARG:HD2	41:AA:197:PRO:HG2	1.88	0.54
45:AE:215:ALA:HA	45:AE:218:LYS:HE3	1.87	0.54
1:A2:1879:C:OP1	56:AQ:2:GLY:N	2.40	0.54
1:A2:4520:U:OP2	42:AB:246:ARG:NH2	2.39	0.54
7:BF:204:ARG:O	17:Bc:63:ARG:NH2	2.39	0.54
9:BM:89:VAL:HG21	9:BM:109:VAL:HG21	1.89	0.54
12:BR:62:GLN:HE21	20:Bg:280:LYS:HD3	1.72	0.54
1:A2:1599:G:O3'	75:Aj:12:ARG:NH2	2.40	0.54
1:A2:4828:G:OP1	52:AM:91:TRP:NE1	2.40	0.54
39:A3:86:U:O2'	73:Ah:5:LYS:NZ	2.40	0.54
44:AD:235:MET:O	44:AD:239:MET:HB2	2.08	0.54
49:AI:96:VAL:HG22	49:AI:125:THR:HG22	1.88	0.54
51:AL:89:LYS:HZ3	73:Ah:110:LYS:HG2	1.70	0.54
1:A2:682:U:OP1	82:At:87:ARG:NH1	2.41	0.54
1:A2:3819:U:H2'	1:A2:3820:A:H8	1.72	0.54
1:A2:4503:G:N2	1:A2:4506:A:OP2	2.38	0.54
23:BC:66:LEU:HD12	23:BC:93:ILE:HD13	1.88	0.54
29:BL:59:LYS:HD3	29:BL:134:LEU:HD23	1.88	0.54
84:Aq:107:ASP:O	84:Aq:111:ASN:ND2	2.41	0.54
86:Ct:607:ARG:NH2	86:Ct:703:ASP:OD2	2.40	0.54
1:A2:1628:A:O2'	75:Aj:49:TRP:O	2.26	0.54
6:BD:172:VAL:HG22	6:BD:185:LYS:HG2	1.89	0.54
16:BZ:68:ILE:HG13	16:BZ:97:ILE:HD13	1.89	0.54
86:Ct:404:THR:HG23	86:Ct:406:ASP:H	1.73	0.54
1:A2:1666:A:OP2	51:AL:5:ARG:NH1	2.40	0.54
13:BS:50:ILE:HD13	13:BS:59:LEU:HD11	1.89	0.54
15:BU:59:LYS:HB2	15:BU:84:ILE:HB	1.89	0.54
15:BU:66:ARG:HH12	15:BU:75:LYS:HG2	1.73	0.54
20:Bg:133:ASN:HB2	20:Bg:138:CYS:HB2	1.90	0.54
44:AD:30:TYR:HA	44:AD:33:ARG:HB3	1.89	0.54
48:AH:92:MET:HG2	48:AH:181:VAL:HA	1.90	0.54
73:Ah:96:ASN:HB3	73:Ah:99:GLU:H	1.72	0.54
1:A2:226:G:OP1	64:AY:15:ARG:NH1	2.40	0.54
1:A2:1185:C:H2'	1:A2:1186:G:H8	1.72	0.54
5:B1:53:C:OP1	35:BY:112:ASN:ND2	2.40	0.54
5:B1:156:G:OP1	25:BG:2:LYS:NZ	2.41	0.54
5:B1:538:U:O4	5:B1:546:G:N2	2.41	0.54
21:BA:34:MET:HE2	21:BA:154:LEU:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AH:12:ILE:HB	48:AH:53:LYS:HB3	1.89	0.54
5:B1:962:A:N1	5:B1:1055:A:O2'	2.40	0.54
7:BF:201:LYS:HD2	7:BF:204:ARG:HE	1.73	0.54
10:BP:98:ASN:HB2	10:BP:122:THR:HG22	1.89	0.54
35:BY:29:HIS:HE1	35:BY:35:VAL:HG23	1.72	0.54
50:AJ:18:ARG:NH2	50:AJ:143:ASP:OD2	2.41	0.54
60:AU:28:PRO:HB2	60:AU:34:MET:HB2	1.90	0.54
82:At:17:LEU:HD13	82:At:36:ASN:HD22	1.72	0.54
1:A2:2590:A:H5'	1:A2:2667:G:H4'	1.90	0.54
43:AC:228:THR:OG1	43:AC:248:ARG:NH2	2.40	0.54
1:A2:1888:A:H4'	46:AF:223:LYS:HD2	1.90	0.53
1:A2:1905:C:OP1	52:AM:34:ASN:ND2	2.41	0.53
1:A2:1939:A:O2'	1:A2:2006:A:N1	2.37	0.53
1:A2:4932:C:O2'	42:AB:174:ARG:NH2	2.41	0.53
2:Bv:20:U:OP2	50:AJ:58:ARG:NH2	2.41	0.53
2:Bv:62:C:H2'	2:Bv:63:G:H8	1.73	0.53
10:BP:81:ARG:NH2	10:BP:117:GLY:O	2.41	0.53
56:AQ:88:ASP:OD1	56:AQ:112:ARG:NH2	2.40	0.53
83:Au:126:PRO:HA	83:Au:130:LYS:HD3	1.89	0.53
86:Ct:752:PRO:HA	86:Ct:781:MET:HA	1.90	0.53
1:A2:97:G:N7	51:AL:13:HIS:NE2	2.56	0.53
1:A2:3663:A:H62	1:A2:3794:G:H21	0.78	0.53
6:BD:220:THR:OG1	20:Bg:190:GLY:O	2.25	0.53
45:AE:138:ARG:HH22	45:AE:169:ALA:HA	1.73	0.53
1:A2:909:C:OP1	58:AS:74:ARG:NH2	2.41	0.53
1:A2:2313:C:OP2	43:AC:195:LYS:NZ	2.40	0.53
1:A2:4461:G:N2	1:A2:4491:G:N3	2.47	0.53
5:B1:1396:A:C2	5:B1:1449:G:N1	2.56	0.53
25:BG:2:LYS:HB2	25:BG:108:VAL:HG22	1.90	0.53
31:BO:113:GLN:NE2	36:Ba:46:GLU:OE1	2.42	0.53
1:A2:743:G:O6	1:A2:898:U:O2	2.27	0.53
1:A2:2065:C:H2'	1:A2:2066:G:H8	1.72	0.53
1:A2:4147:G:OP1	41:AA:2:GLY:N	2.41	0.53
5:B1:849:A:O2'	28:BJ:69:ARG:NH1	2.41	0.53
5:B1:1101:U:H2'	5:B1:1102:G:H8	1.74	0.53
63:AX:104:ALA:O	63:AX:134:LYS:NZ	2.40	0.53
86:Ct:150:ARG:NH2	86:Ct:194:GLU:OE2	2.41	0.53
1:A2:2484:C:O2'	1:A2:2485:G:N2	2.42	0.53
42:AB:53:MET:O	42:AB:373:LYS:NZ	2.42	0.53
84:Aq:91:ASP:O	84:Aq:95:GLN:NE2	2.41	0.53
1:A2:289:A:N6	1:A2:4323:U:O2'	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:2561:A:HO2'	1:A2:2632:C:HO2'	1.56	0.53
1:A2:3890:C:H4'	41:AA:207:VAL:HG12	1.89	0.53
5:B1:441:C:OP1	27:BI:2:GLY:N	2.42	0.53
53:AN:84:PRO:HA	53:AN:87:HIS:HD2	1.74	0.53
1:A2:2410:A:H5''	77:AI:22:PRO:HG3	1.91	0.53
1:A2:4721:C:H5''	54:AO:37:ARG:HH22	1.74	0.53
85:AK:119:CYS:SG	85:AK:120:GLU:N	2.74	0.53
1:A2:27:C:O2'	1:A2:60:A:N3	2.42	0.53
1:A2:66:A:H61	1:A2:276:C:HO2'	1.57	0.53
1:A2:1315:C:H2'	1:A2:1316:A:H8	1.74	0.53
1:A2:1619:A:H1'	75:Aj:11:ARG:HH21	1.73	0.53
1:A2:2001:U:H2'	1:A2:2002:G:H8	1.72	0.53
1:A2:2644:U:H5''	57:AR:107:ARG:HH21	1.74	0.53
1:A2:2763:C:N4	77:AI:3:SER:OG	2.42	0.53
5:B1:16:G:N2	5:B1:1195:A:H62	2.07	0.53
40:A4:77:A:H62	40:A4:99:G:H21	1.57	0.53
51:AL:11:LYS:H	56:AQ:168:ARG:HH22	1.57	0.53
63:AX:110:LYS:NZ	63:AX:121:VAL:O	2.42	0.53
86:Ct:20:ARG:HB2	86:Ct:100:ILE:HG12	1.90	0.53
5:B1:417:C:O2	28:BJ:55:LYS:NZ	2.42	0.53
5:B1:827:A:H4'	28:BJ:8:VAL:HG11	1.91	0.53
5:B1:1156:U:O4	23:BC:194:ARG:NH1	2.41	0.53
10:BP:53:GLN:HG3	10:BP:83:MET:HE1	1.91	0.53
20:Bg:77:PHE:HB3	20:Bg:89:LEU:HD11	1.91	0.53
27:BI:110:ARG:NH2	27:BI:166:PHE:O	2.42	0.53
1:A2:4320:U:H4'	51:AL:197:LYS:HD3	1.89	0.53
1:A2:4354:G:N2	1:A2:4357:U:O2	2.39	0.53
5:B1:550:C:O2'	38:Be:44:ASN:ND2	2.41	0.53
13:BS:84:LEU:HD22	13:BS:97:GLN:HB2	1.91	0.53
30:BN:22:VAL:HG21	30:BN:26:LEU:HB3	1.90	0.53
44:AD:4:VAL:HG13	44:AD:5:LYS:HG3	1.90	0.53
1:A2:1627:C:OP1	43:AC:80:ARG:NH1	2.42	0.52
5:B1:346:C:O2'	24:BE:30:ARG:NH2	2.43	0.52
5:B1:913:A:OP2	26:BH:99:ARG:NH1	2.42	0.52
5:B1:959:G:OP2	31:BO:38:ASN:ND2	2.42	0.52
15:BU:80:PHE:HB3	18:Bd:52:PHE:HB3	1.91	0.52
24:BE:247:THR:HG22	24:BE:249:ALA:H	1.74	0.52
83:Au:16:GLU:OE1	83:Au:214:GLN:NE2	2.42	0.52
1:A2:2056:G:H2'	1:A2:2057:G:H8	1.74	0.52
1:A2:3724:G:OP2	1:A2:3747:G:O2'	2.26	0.52
1:A2:4410:G:H5''	1:A2:4411:A:H5''	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B1:385:G:N2	5:B1:388:U:OP2	2.41	0.52
5:B1:1546:G:N2	5:B1:1670:C:O2	2.42	0.52
28:BJ:35:TYR:O	28:BJ:111:GLN:NE2	2.42	0.52
70:Ae:101:HIS:O	70:Ae:128:ARG:NH1	2.42	0.52
1:A2:344:C:OP2	43:AC:197:ARG:NH1	2.42	0.52
1:A2:633:U:H4'	1:A2:634:C:H5'	1.92	0.52
1:A2:1997:C:H2'	1:A2:1998:A:H8	1.75	0.52
5:B1:1137:U:O2'	21:BA:155:ARG:NH2	2.42	0.52
5:B1:1453:C:OP1	12:BR:48:ASN:ND2	2.40	0.52
14:BT:126:GLN:OE1	14:BT:129:ARG:NH2	2.43	0.52
34:BX:35:ALA:O	34:BX:39:ASN:ND2	2.42	0.52
86:Ct:396:MET:HG2	86:Ct:416:VAL:HA	1.91	0.52
1:A2:171:C:O2	73:Ah:112:ARG:NH1	2.42	0.52
1:A2:1160:U:H4'	44:AD:279:ARG:HE	1.75	0.52
1:A2:1298:C:N4	1:A2:1299:G:O6	2.42	0.52
1:A2:1414:C:H42	1:A2:1435:A:H61	1.56	0.52
4:Bw:75:C:H4'	80:Ao:55:ILE:HG22	1.91	0.52
6:BD:79:PHE:HB3	6:BD:83:SER:HB2	1.90	0.52
22:BB:228:LEU:O	22:BB:232:HIS:ND1	2.42	0.52
36:Ba:82:LYS:HD3	36:Ba:85:ARG:HD2	1.90	0.52
44:AD:128:ASP:O	44:AD:164:LYS:NZ	2.42	0.52
1:A2:1573:U:OP2	42:AB:243:LYS:NZ	2.40	0.52
1:A2:2026:G:OP1	54:AO:63:ASN:ND2	2.42	0.52
39:A3:52:A:H62	77:Al:27:ILE:HD13	1.74	0.52
50:AJ:18:ARG:HB3	50:AJ:133:VAL:HG23	1.91	0.52
1:A2:960:G:O6	1:A2:1265:G:N2	2.43	0.52
5:B1:1261:C:O2	18:Bd:10:HIS:NE2	2.40	0.52
13:BS:138:THR:HA	13:BS:141:ARG:HE	1.75	0.52
14:BT:13:GLU:OE1	14:BT:16:ARG:NH2	2.42	0.52
31:BO:147:ARG:HD2	31:BO:150:ARG:HH21	1.75	0.52
43:AC:84:THR:HG22	43:AC:86:ARG:H	1.73	0.52
1:A2:148:G:O6	47:AG:187:LYS:NZ	2.43	0.52
1:A2:2824:A:H61	1:A2:3814:C:H42	1.57	0.52
1:A2:4866:G:H5''	54:AO:163:LYS:HE2	1.92	0.52
4:Bw:32:C:O2'	7:BF:127:ARG:NH2	2.41	0.52
5:B1:1349:G:H21	21:BA:112:ILE:HG21	1.75	0.52
33:BW:60:LYS:NZ	37:Bb:23:ARG:O	2.43	0.52
39:A3:26:C:O2'	43:AC:54:VAL:O	2.27	0.52
40:A4:47:G:OP1	44:AD:95:TYR:N	2.42	0.52
54:AO:54:TYR:OH	54:AO:73:PHE:O	2.27	0.52
57:AR:32:ILE:HD13	57:AR:44:LEU:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:82:U:HO2'	1:A2:1365:G:HO2'	1.58	0.52
1:A2:225:C:N3	1:A2:237:G:N2	2.58	0.52
1:A2:2288:G:O2'	39:A3:18:U:O2	2.28	0.52
1:A2:2314:C:H2'	1:A2:2315:G:H8	1.74	0.52
1:A2:2436:G:OP1	53:AN:65:ARG:NH2	2.42	0.52
5:B1:639:C:H2'	5:B1:640:A:H8	1.75	0.52
5:B1:692:G:H2'	5:B1:693:A:H8	1.74	0.52
6:BD:106:ARG:HH21	6:BD:174:HIS:H	1.57	0.52
8:BK:65:ARG:NH2	18:Bd:20:SER:OG	2.41	0.52
23:BC:173:LYS:HB3	32:BV:3:ASN:HA	1.91	0.52
43:AC:318:PRO:HB2	46:AF:155:TYR:HB3	1.91	0.52
78:Am:97:ARG:NH1	78:Am:121:LEU:O	2.43	0.52
1:A2:48:G:O6	53:AN:188:ARG:NH1	2.43	0.52
1:A2:1706:G:N2	1:A2:1857:U:OP1	2.43	0.52
1:A2:2493:G:O2'	1:A2:2722:A:N6	2.43	0.52
5:B1:486:A:O2'	5:B1:487:U:O2	2.26	0.52
25:BG:223:LYS:O	25:BG:227:GLN:NE2	2.43	0.52
41:AA:3:ARG:HD2	41:AA:208:GLU:HG2	1.92	0.52
64:AY:2:LYS:HD2	64:AY:7:VAL:HG13	1.92	0.52
86:Ct:20:ARG:NH2	86:Ct:79:TYR:OH	2.43	0.52
1:A2:494:G:O2'	1:A2:498:G:OP1	2.28	0.52
1:A2:1674:C:H41	56:AQ:13:VAL:HG21	1.75	0.52
5:B1:124:U:OP1	25:BG:201:LYS:NZ	2.43	0.52
5:B1:681:U:H4'	34:BX:9:THR:HG22	1.91	0.52
7:BF:123:GLU:OE2	7:BF:204:ARG:NH2	2.43	0.52
24:BE:80:VAL:HG13	24:BE:81:THR:HG23	1.92	0.52
30:BN:99:ARG:NH2	30:BN:119:GLU:OE2	2.43	0.52
48:AH:23:ARG:HE	48:AH:39:ASN:HA	1.75	0.52
83:Au:39:LYS:HD2	83:Au:40:ASN:HB2	1.91	0.52
83:Au:207:LYS:HG2	83:Au:213:PRO:HA	1.91	0.52
1:A2:1309:A:OP2	1:A2:4407:U:O2'	2.27	0.51
1:A2:3688:A:OP2	1:A2:3706:G:N2	2.43	0.51
1:A2:4525:U:H2'	1:A2:4526:A:H8	1.75	0.51
1:A2:4936:G:OP1	42:AB:271:GLN:NE2	2.43	0.51
1:A2:4946:U:H1'	1:A2:4947:U:H4'	1.91	0.51
5:B1:1013:U:OP1	5:B1:1129:G:O2'	2.28	0.51
9:BM:64:LEU:HD11	19:Bf:104:LYS:HE3	1.90	0.51
63:AX:91:GLU:HG3	63:AX:147:LEU:HD21	1.91	0.51
1:A2:29:G:O2'	53:AN:96:ARG:NH1	2.44	0.51
1:A2:4403:A:OP2	49:AI:110:ARG:NH1	2.44	0.51
7:BF:143:PRO:HA	7:BF:146:ARG:HE	1.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:BC:182:CYS:HB2	33:BW:95:PRO:HB2	1.93	0.51
26:BH:131:GLU:OE1	30:BN:20:ARG:NH1	2.43	0.51
33:BW:11:LEU:HD12	33:BW:74:VAL:HG23	1.92	0.51
41:AA:57:PRO:HG2	41:AA:78:ALA:HB3	1.90	0.51
48:AH:92:MET:HE2	48:AH:179:ILE:HG22	1.91	0.51
63:AX:123:LYS:NZ	63:AX:125:ASN:OD1	2.43	0.51
76:Ak:38:CYS:SG	76:Ak:39:SER:N	2.83	0.51
83:Au:159:MET:HG3	83:Au:165:LEU:HB2	1.92	0.51
1:A2:23:C:H5''	75:Aj:58:THR:HG22	1.92	0.51
1:A2:1887:U:H2'	1:A2:1888:A:H8	1.74	0.51
1:A2:3652:G:N1	41:AA:118:GLU:OE2	2.43	0.51
7:BF:167:LYS:NZ	16:BZ:75:GLU:OE1	2.40	0.51
13:BS:98:VAL:HG21	13:BS:103:LEU:HD13	1.93	0.51
21:BA:50:ASN:HD21	21:BA:53:ARG:HD2	1.75	0.51
21:BA:141:ASN:ND2	32:BV:31:SER:O	2.38	0.51
24:BE:70:ILE:HG13	24:BE:92:ILE:HG12	1.93	0.51
55:AP:40:HIS:HE1	55:AP:111:SER:HA	1.74	0.51
60:AU:63:ILE:HG12	60:AU:72:VAL:HG12	1.92	0.51
85:AK:47:LEU:HD22	85:AK:50:LYS:HD2	1.91	0.51
1:A2:1227:G:H21	1:A2:1228:C:H41	1.58	0.51
1:A2:2576:G:H1	1:A2:2727:C:H5	1.56	0.51
21:BA:36:GLN:NE2	32:BV:67:ASP:OD1	2.42	0.51
27:BI:121:LEU:HD21	27:BI:158:ILE:HD11	1.91	0.51
43:AC:198:ASN:ND2	64:AY:9:SER:O	2.44	0.51
47:AG:173:LEU:HD12	74:Ai:43:MET:HE1	1.92	0.51
76:Ak:60:LEU:HD22	76:Ak:61:PRO:HD2	1.92	0.51
1:A2:736:G:O6	1:A2:904:A:N6	2.43	0.51
1:A2:1831:A:N3	1:A2:2262:G:O2'	2.43	0.51
5:B1:677:G:H21	5:B1:1028:A:N6	2.03	0.51
27:BI:100:CYS:HB3	27:BI:175:ILE:HD12	1.91	0.51
45:AE:149:ILE:HD12	45:AE:271:LEU:HD21	1.92	0.51
46:AF:80:ASN:ND2	59:AT:141:VAL:O	2.41	0.51
48:AH:186:THR:O	48:AH:189:GLN:NE2	2.43	0.51
63:AX:89:LYS:O	63:AX:93:ASN:HB3	2.10	0.51
84:Aq:22:VAL:HG21	84:Aq:48:LYS:HG3	1.93	0.51
86:Ct:221:TRP:HB3	86:Ct:340:MET:HB3	1.91	0.51
1:A2:2499:C:H2'	1:A2:2500:G:H8	1.75	0.51
1:A2:3621:C:OP1	41:AA:200:ARG:NH2	2.43	0.51
1:A2:4415:C:O2	1:A2:4491:G:N2	2.44	0.51
5:B1:406:U:O2'	5:B1:408:A:OP1	2.29	0.51
7:BF:115:ALA:O	7:BF:119:SER:OG	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Bg:24:THR:OG1	20:Bg:27:PHE:O	2.28	0.51
50:AJ:35:ARG:HD3	50:AJ:123:ILE:HA	1.93	0.51
63:AX:79:PHE:HB2	63:AX:99:ILE:HB	1.93	0.51
85:AK:29:ILE:HG23	85:AK:86:VAL:HG13	1.93	0.51
1:A2:2688:C:OP1	57:AR:39:GLN:NE2	2.43	0.51
1:A2:4731:G:N2	1:A2:4732:U:O4	2.43	0.51
1:A2:4943:U:H4'	42:AB:175:GLN:HG3	1.91	0.51
5:B1:1648:G:O6	7:BF:55:ARG:NH2	2.43	0.51
20:Bg:278:SER:HB2	20:Bg:281:ALA:HB3	1.93	0.51
31:BO:95:ILE:HB	31:BO:129:ILE:HG12	1.93	0.51
57:AR:103:ARG:NH2	57:AR:124:TYR:OH	2.44	0.51
86:Ct:27:HIS:HB3	86:Ct:30:HIS:CE1	2.46	0.51
1:A2:4179:G:OP1	59:AT:55:LYS:NZ	2.40	0.51
36:Ba:44:ILE:HG13	36:Ba:45:VAL:HG23	1.91	0.51
45:AE:283:PRO:O	45:AE:284:HIS:ND1	2.43	0.51
46:AF:92:VAL:O	46:AF:120:GLY:HA2	2.10	0.51
56:AQ:155:ALA:O	56:AQ:163:THR:OG1	2.29	0.51
65:AZ:21:ARG:NH1	65:AZ:47:ASP:O	2.43	0.51
80:Ao:22:LYS:HG3	80:Ao:73:VAL:HG22	1.92	0.51
1:A2:20:U:H3'	1:A2:21:G:H8	1.76	0.51
1:A2:658:G:N2	1:A2:659:G:O6	2.44	0.51
5:B1:1553:C:O2	6:BD:9:ARG:NH2	2.38	0.51
21:BA:149:ASN:ND2	21:BA:163:CYS:O	2.43	0.51
34:BX:67:ARG:NH2	34:BX:114:ASP:OD2	2.37	0.51
55:AP:116:HIS:HB3	55:AP:149:ILE:HB	1.91	0.51
1:A2:413:A:N3	1:A2:1315:C:O2'	2.41	0.51
5:B1:116:U:H3	5:B1:347:G:H1	1.59	0.51
11:BQ:39:LEU:HD21	11:BQ:55:VAL:HG21	1.93	0.51
25:BG:159:ARG:HG2	25:BG:173:ALA:HB2	1.93	0.51
43:AC:192:GLY:O	43:AC:195:LYS:NZ	2.42	0.51
58:AS:115:ALA:O	58:AS:118:ARG:NH1	2.44	0.51
75:Aj:8:PHE:HA	75:Aj:11:ARG:HH11	1.76	0.51
1:A2:430:C:H2'	1:A2:431:G:H8	1.76	0.50
1:A2:2386:G:N2	1:A2:2386:G:OP2	2.42	0.50
1:A2:4478:G:OP2	42:AB:3:HIS:ND1	2.36	0.50
5:B1:851:C:O2'	5:B1:852:G:N2	2.40	0.50
5:B1:941:C:H2'	5:B1:942:G:H8	1.75	0.50
27:BI:100:CYS:SG	27:BI:101:ILE:N	2.84	0.50
32:BV:22:ARG:NH2	32:BV:56:CYS:SG	2.84	0.50
52:AM:11:ARG:HE	52:AM:61:ILE:HG22	1.76	0.50
1:A2:54:G:OP1	75:Aj:43:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:193:C:O2	1:A2:218:C:O2'	2.27	0.50
5:B1:562:U:H2'	5:B1:563:G:H8	1.77	0.50
5:B1:1655:C:H2'	5:B1:1656:G:H8	1.76	0.50
5:B1:1808:U:H2'	5:B1:1809:A:H8	1.76	0.50
26:BH:64:VAL:HB	26:BH:96:ALA:HA	1.92	0.50
39:A3:13:G:O2'	55:AP:121:LYS:O	2.28	0.50
1:A2:113:A:H62	1:A2:155:A:H2	1.60	0.50
1:A2:447:G:N2	45:AE:227:HIS:O	2.44	0.50
1:A2:2331:U:H1'	43:AC:96:CYS:HA	1.92	0.50
1:A2:2709:U:H5''	72:Ag:19:LYS:HD2	1.92	0.50
83:Au:194:LEU:HD13	83:Au:196:LYS:H	1.76	0.50
84:Aq:114:ARG:HH22	84:Aq:130:LYS:HA	1.76	0.50
1:A2:54:G:O2'	53:AN:161:MET:SD	2.69	0.50
1:A2:3942:G:N2	1:A2:4020:A:H62	2.05	0.50
9:BM:19:GLN:HB3	9:BM:88:TRP:HZ3	1.76	0.50
62:AW:46:PRO:HB2	62:AW:54:LEU:HD23	1.93	0.50
83:Au:160:LYS:HB3	83:Au:162:VAL:HG12	1.93	0.50
1:A2:1893:G:H21	54:AO:87:MET:HE3	1.76	0.50
29:BL:135:SER:O	29:BL:139:ARG:NH1	2.44	0.50
64:AY:80:ILE:HD11	64:AY:104:VAL:HG21	1.93	0.50
78:Am:78:ILE:HG12	78:Am:83:ARG:HD2	1.92	0.50
86:Ct:12:ILE:HA	86:Ct:15:LYS:HD3	1.93	0.50
1:A2:3660:G:O2'	1:A2:3789:U:OP2	2.29	0.50
1:A2:4482:G:OP2	42:AB:2:SER:N	2.45	0.50
1:A2:4549:G:N2	42:AB:15:GLY:O	2.41	0.50
5:B1:594:A:O4'	5:B1:643:A:N6	2.45	0.50
5:B1:641:A:O2'	5:B1:645:C:OP1	2.24	0.50
5:B1:1227:G:N2	5:B1:1635:C:O2'	2.45	0.50
27:BI:101:ILE:HA	27:BI:173:ALA:O	2.11	0.50
28:BJ:122:SER:O	28:BJ:125:HIS:N	2.40	0.50
29:BL:57:ASP:HB3	29:BL:60:CYS:HB2	1.94	0.50
58:AS:5:GLY:O	58:AS:111:ARG:NH2	2.45	0.50
63:AX:110:LYS:HG2	63:AX:114:LYS:HE3	1.93	0.50
86:Ct:60:ARG:NH2	86:Ct:560:ASP:OD1	2.44	0.50
1:A2:717:G:OP1	46:AF:73:ARG:NH2	2.43	0.50
1:A2:4829:C:OP2	52:AM:94:LYS:NZ	2.39	0.50
1:A2:4938:C:OP2	1:A2:4939:G:N2	2.45	0.50
5:B1:495:U:O2'	24:BE:27:PHE:O	2.28	0.50
5:B1:1218:C:O2'	17:Bc:24:GLN:NE2	2.44	0.50
5:B1:1488:C:H3'	5:B1:1489:A:H4'	1.94	0.50
5:B1:1656:G:O6	5:B1:1668:U:O4	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BX:34:THR:O	34:BX:38:ALA:HB3	2.11	0.50
39:A3:60:G:O6	73:Ah:62:ASN:ND2	2.44	0.50
55:AP:37:LYS:HD2	55:AP:117:ILE:HG22	1.94	0.50
68:Ac:26:LYS:HB3	68:Ac:98:ASP:HB3	1.94	0.50
71:Af:56:ASN:HD21	71:Af:64:PRO:HB2	1.76	0.50
85:AK:13:TYR:OH	85:AK:60:MET:SD	2.68	0.50
1:A2:1679:G:N2	1:A2:2064:C:O3'	2.45	0.50
1:A2:2500:G:H4'	72:Ag:26:PRO:HD2	1.94	0.50
20:Bg:165:ILE:HG13	20:Bg:177:TRP:HB2	1.94	0.50
47:AG:143:VAL:HG21	47:AG:201:THR:HB	1.94	0.50
86:Ct:79:TYR:OH	86:Ct:355:THR:OG1	2.30	0.50
1:A2:274:G:N2	1:A2:300:A:OP2	2.45	0.50
1:A2:1089:A:N6	1:A2:1146:G:C6	2.80	0.50
1:A2:4387:G:OP1	78:Am:100:TYR:OH	2.30	0.50
1:A2:4732:U:H3	1:A2:4820:G:H22	1.58	0.50
20:Bg:20:GLN:HG3	20:Bg:68:ASP:HA	1.92	0.50
24:BE:100:ARG:HH21	24:BE:119:ALA:HA	1.77	0.50
44:AD:155:THR:HG22	44:AD:179:ARG:HA	1.93	0.50
57:AR:8:LYS:HD3	57:AR:23:TRP:HE1	1.77	0.50
71:Af:11:PHE:HE1	71:Af:26:ALA:HB1	1.77	0.50
84:Aq:63:THR:HG22	84:Aq:72:GLU:HG3	1.94	0.50
1:A2:162:A:H61	1:A2:265:C:H42	1.58	0.49
1:A2:1071:C:O2'	46:AF:74:MET:SD	2.70	0.49
1:A2:1226:C:N4	1:A2:1243:G:OP1	2.44	0.49
1:A2:3753:C:OP2	79:An:23:ARG:NH2	2.42	0.49
1:A2:4623:G:N2	1:A2:4962:C:O3'	2.45	0.49
10:BP:41:GLN:HE22	10:BP:113:GLY:HA2	1.76	0.49
13:BS:54:LYS:NZ	13:BS:58:GLU:O	2.44	0.49
25:BG:69:THR:HG22	25:BG:71:GLY:H	1.77	0.49
39:A3:87:G:OP2	73:Ah:3:LYS:NZ	2.43	0.49
39:A3:116:C:O2'	63:AX:55:ARG:NH1	2.45	0.49
58:AS:9:GLU:OE2	58:AS:31:ARG:NE	2.45	0.49
58:AS:127:MET:HA	59:AT:153:PRO:HG2	1.93	0.49
70:Ae:12:ILE:HG23	70:Ae:66:THR:HB	1.92	0.49
1:A2:1864:G:N2	1:A2:2051:U:O2'	2.45	0.49
1:A2:1923:A:OP2	1:A2:2021:A:N6	2.43	0.49
1:A2:2340:G:O2'	1:A2:3830:G:O6	2.30	0.49
5:B1:989:C:O2	36:Ba:32:LYS:NZ	2.44	0.49
24:BE:126:VAL:HG22	24:BE:139:LEU:HD21	1.94	0.49
42:AB:316:PRO:HA	42:AB:370:THR:HB	1.94	0.49
47:AG:136:LEU:HD13	47:AG:202:VAL:HG13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:AN:193:ARG:NH1	53:AN:197:THR:OG1	2.45	0.49
83:Au:25:ARG:NH1	83:Au:26:ARG:O	2.45	0.49
86:Ct:654:PRO:HG3	86:Ct:687:THR:HG21	1.94	0.49
1:A2:2030:G:H2'	1:A2:2031:G:C8	2.48	0.49
5:B1:146:G:OP1	25:BG:143:LYS:NZ	2.44	0.49
5:B1:744:G:H1'	26:BH:108:SER:HA	1.95	0.49
5:B1:745:C:H1'	26:BH:109:ARG:HD2	1.94	0.49
5:B1:1020:A:OP2	30:BN:70:LYS:NZ	2.34	0.49
5:B1:1652:G:O6	5:B1:1672:U:O4	2.29	0.49
7:BF:115:ALA:O	7:BF:119:SER:CB	2.60	0.49
40:A4:6:C:OP2	44:AD:22:ARG:NH2	2.46	0.49
61:AV:16:ILE:HD11	61:AV:57:VAL:H	1.77	0.49
61:AV:87:SER:HB3	62:AW:19:ARG:HH21	1.78	0.49
70:Ae:37:LYS:NZ	70:Ae:55:MET:SD	2.78	0.49
83:Au:201:VAL:HG11	83:Au:204:LEU:HD23	1.94	0.49
1:A2:1480:G:OP1	56:AQ:150:ARG:NH1	2.38	0.49
1:A2:1958:C:H5'	84:Aq:83:LYS:HD3	1.94	0.49
1:A2:4679:A:OP2	42:AB:24:ARG:NH2	2.42	0.49
5:B1:1719:A:N6	5:B1:1814:G:O2'	2.45	0.49
20:Bg:195:LEU:HA	20:Bg:211:GLY:HA3	1.95	0.49
45:AE:140:LEU:HB3	45:AE:144:ILE:HD11	1.94	0.49
76:Ak:20:ALA:HA	76:Ak:38:CYS:HA	1.95	0.49
78:Am:104:HIS:HB3	78:Am:107:ALA:HB2	1.93	0.49
1:A2:220:G:O3'	43:AC:222:ARG:NH2	2.45	0.49
1:A2:708:U:O4	1:A2:938:G:O6	2.31	0.49
1:A2:1298:C:OP1	70:Ae:44:ARG:NH2	2.45	0.49
1:A2:2382:A:OP1	72:Ag:10:ARG:NH1	2.45	0.49
1:A2:3840:C:O2'	42:AB:261:ARG:NH1	2.45	0.49
1:A2:4581:U:OP1	61:AV:15:ARG:NH1	2.44	0.49
1:A2:4724:A:HO2'	58:AS:174:THR:HG1	1.61	0.49
5:B1:740:C:H2'	5:B1:741:C:H2'	1.95	0.49
5:B1:1092:G:OP1	30:BN:2:GLY:N	2.45	0.49
5:B1:1407:U:O2'	11:BQ:11:GLN:NE2	2.45	0.49
5:B1:1786:U:H2'	5:B1:1787:G:H8	1.78	0.49
16:BZ:92:LEU:HD11	16:BZ:99:LEU:HD23	1.94	0.49
28:BJ:127:ARG:HG3	38:Be:31:ARG:HH22	1.77	0.49
40:A4:59:G:O2'	44:AD:267:ASN:OD1	2.28	0.49
40:A4:99:G:OP2	58:AS:55:LYS:NZ	2.45	0.49
49:AI:57:TYR:OH	49:AI:128:ARG:NH2	2.44	0.49
55:AP:30:ARG:HA	55:AP:119:VAL:HG11	1.94	0.49
1:A2:294:A:O2'	53:AN:93:LYS:O	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:2609:U:OP2	60:AU:46:ARG:NH2	2.46	0.49
1:A2:2618:U:O2'	1:A2:2673:G:N1	2.37	0.49
5:B1:1204:A:O2'	5:B1:1700:C:OP2	2.30	0.49
7:BF:126:THR:OG1	17:Bc:26:GLN:NE2	2.46	0.49
13:BS:14:ARG:NH2	50:AJ:111:GLU:OE1	2.46	0.49
20:Bg:8:ARG:HB3	20:Bg:309:VAL:HG23	1.94	0.49
41:AA:192:LYS:HB3	41:AA:193:ARG:HE	1.76	0.49
42:AB:37:PRO:HA	42:AB:188:GLY:HA2	1.94	0.49
53:AN:42:PRO:HG3	53:AN:61:ILE:HG13	1.93	0.49
61:AV:83:ARG:HB2	61:AV:102:ALA:HB3	1.95	0.49
86:Ct:319:LEU:HD21	86:Ct:339:VAL:HG13	1.94	0.49
86:Ct:582:THR:HB	86:Ct:741:MET:HE2	1.94	0.49
1:A2:1636:G:N2	1:A2:1660:C:OP1	2.45	0.49
1:A2:1723:G:O6	40:A4:103:A:O2'	2.27	0.49
1:A2:1769:A:N3	1:A2:4172:U:O2'	2.46	0.49
1:A2:4583:C:OP1	61:AV:48:ARG:NH1	2.45	0.49
9:BM:47:ALA:HA	9:BM:112:LYS:HA	1.93	0.49
20:Bg:258:ILE:HD12	20:Bg:268:ASP:HB3	1.95	0.49
52:AM:7:VAL:HG12	52:AM:57:LEU:HD21	1.94	0.49
71:Af:78:HIS:HB2	71:Af:85:ARG:HG3	1.95	0.49
84:Aq:28:LEU:HD12	84:Aq:30:PRO:HG3	1.94	0.49
1:A2:161:G:O6	1:A2:266:U:O4	2.31	0.49
1:A2:286:G:H21	1:A2:288:G:H22	1.61	0.49
1:A2:1491:C:H2'	1:A2:1492:G:H8	1.78	0.49
1:A2:1725:A:N1	1:A2:1771:C:O2'	2.40	0.49
1:A2:1895:C:H4'	54:AO:89:PRO:HD3	1.93	0.49
1:A2:4419:U:OP1	61:AV:50:ASN:ND2	2.46	0.49
1:A2:4578:A:H4'	42:AB:65:SER:HB3	1.95	0.49
1:A2:4988:U:H2'	1:A2:4989:G:H8	1.78	0.49
5:B1:1138:C:N3	32:BV:61:ARG:NH1	2.61	0.49
24:BE:100:ARG:NH2	24:BE:118:GLU:O	2.45	0.49
58:AS:86:SER:OG	58:AS:89:GLY:O	2.28	0.49
1:A2:1505:A:N3	1:A2:4351:C:O2'	2.41	0.49
1:A2:2390:C:H2'	1:A2:2391:A:H8	1.77	0.49
5:B1:305:U:O2'	27:BI:41:ARG:NH1	2.46	0.49
5:B1:1152:U:H1'	33:BW:16:ASN:HD21	1.78	0.49
8:BK:29:MET:HG3	8:BK:30:PRO:HD3	1.94	0.49
52:AM:33:GLN:HB2	58:AS:145:PHE:HZ	1.78	0.49
65:AZ:15:ALA:HB3	65:AZ:79:HIS:HD2	1.76	0.49
69:Ad:19:GLU:HB2	69:Ad:90:ARG:HH21	1.77	0.49
86:Ct:315:LEU:O	86:Ct:319:LEU:CB	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:Ct:413:PHE:HZ	86:Ct:469:ILE:HD12	1.78	0.49
86:Ct:506:ARG:HA	86:Ct:546:ILE:O	2.13	0.49
86:Ct:751:CYS:HB3	86:Ct:755:VAL:HG23	1.95	0.49
1:A2:719:U:OP1	58:AS:63:TYR:OH	2.30	0.49
1:A2:1826:U:H2'	1:A2:1827:G:H8	1.77	0.49
5:B1:1087:A:OP1	36:Ba:8:ASN:ND2	2.45	0.49
5:B1:1401:A:H4'	15:BU:52:GLY:HA3	1.95	0.49
25:BG:18:VAL:HA	25:BG:23:LYS:HD3	1.95	0.49
34:BX:100:VAL:HG13	34:BX:122:VAL:HG13	1.95	0.49
39:A3:154:G:OP1	47:AG:89:ARG:NE	2.40	0.49
52:AM:111:LYS:HA	52:AM:114:LYS:HE3	1.95	0.49
54:AO:173:GLN:OE1	54:AO:176:ARG:NH2	2.43	0.49
56:AQ:36:ALA:O	56:AQ:45:GLN:NE2	2.46	0.49
1:A2:1610:C:OP1	41:AA:14:SER:OG	2.30	0.48
1:A2:2418:G:H1	1:A2:2517:U:H3	1.60	0.48
5:B1:144:U:H2'	5:B1:145:G:H8	1.78	0.48
5:B1:1231:C:OP2	13:BS:139:THR:OG1	2.31	0.48
20:Bg:119:GLN:HB3	20:Bg:131:LEU:HD21	1.95	0.48
35:BY:54:VAL:HG22	35:BY:76:TYR:HB2	1.94	0.48
39:A3:110:U:OP2	75:Aj:20:ARG:NH2	2.42	0.48
40:A4:6:C:H4'	44:AD:52:ILE:HD13	1.94	0.48
41:AA:133:TYR:HB3	41:AA:168:VAL:HG12	1.94	0.48
44:AD:205:ALA:HB1	44:AD:233:PRO:HB3	1.95	0.48
83:Au:12:GLU:OE1	83:Au:15:ARG:NH2	2.46	0.48
1:A2:2054:C:O3'	46:AF:157:ARG:NH2	2.40	0.48
5:B1:495:U:OP1	24:BE:58:GLY:N	2.43	0.48
6:BD:25:LEU:O	6:BD:29:LEU:HB2	2.12	0.48
8:BK:59:LYS:HB2	8:BK:70:TYR:HB3	1.94	0.48
20:Bg:201:SER:HB3	20:Bg:206:LEU:HB2	1.95	0.48
20:Bg:296:GLN:NE2	20:Bg:312:VAL:O	2.41	0.48
33:BW:24:GLN:NE2	37:Bb:5:LYS:O	2.38	0.48
39:A3:60:G:OP1	63:AX:68:ARG:NH2	2.39	0.48
51:AL:144:LEU:HD21	73:Ah:122:LYS:H	1.78	0.48
56:AQ:63:LEU:HD12	56:AQ:92:VAL:HG21	1.95	0.48
82:At:61:VAL:HG12	82:At:81:THR:HG22	1.95	0.48
1:A2:931:A:H5''	1:A2:933:C:H5'	1.96	0.48
1:A2:964:C:H2'	1:A2:965:G:C8	2.48	0.48
1:A2:2531:G:N2	1:A2:2746:U:O4	2.47	0.48
1:A2:2621:A:N6	1:A2:2622:G:O6	2.46	0.48
1:A2:2787:G:O2'	57:AR:60:ARG:NH1	2.46	0.48
5:B1:885:U:H3	5:B1:901:G:H1	1.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BD:137:VAL:HG22	6:BD:151:LYS:HG2	1.94	0.48
21:BA:84:GLN:HG2	21:BA:100:ALA:HB1	1.95	0.48
41:AA:117:GLU:O	41:AA:162:ASN:ND2	2.46	0.48
46:AF:157:ARG:NE	46:AF:212:LYS:O	2.46	0.48
50:AJ:22:LEU:O	50:AJ:71:HIS:HA	2.14	0.48
52:AM:115:ALA:HB1	54:AO:190:ASP:HB3	1.95	0.48
54:AO:125:LYS:HG3	54:AO:129:LEU:HD12	1.94	0.48
69:Ad:46:LEU:HD21	69:Ad:72:VAL:HG21	1.96	0.48
84:Aq:65:GLN:HG2	84:Aq:70:GLN:HG3	1.95	0.48
1:A2:485:G:H1'	1:A2:659:G:H1	1.79	0.48
1:A2:931:A:N1	46:AF:151:ASN:ND2	2.62	0.48
1:A2:1965:A:H2'	1:A2:1992:C:H5''	1.95	0.48
1:A2:2500:G:H5'	1:A2:2619:G:H1'	1.94	0.48
34:BX:46:HIS:HB3	34:BX:101:LEU:HD11	1.94	0.48
40:A4:34:C:N4	40:A4:46:C:O2	2.45	0.48
43:AC:150:LEU:HB2	82:At:71:ARG:HB3	1.95	0.48
66:Aa:95:THR:HG23	66:Aa:97:ALA:H	1.78	0.48
1:A2:3719:A:OP1	41:AA:243:THR:OG1	2.31	0.48
1:A2:3841:C:H2'	1:A2:3842:A:H8	1.79	0.48
1:A2:4048:C:OP1	53:AN:32:GLN:NE2	2.46	0.48
7:BF:161:ALA:O	7:BF:165:ASN:ND2	2.47	0.48
41:AA:58:LEU:HD21	41:AA:75:LEU:HB3	1.95	0.48
48:AH:16:VAL:HG12	48:AH:29:GLY:HA3	1.95	0.48
72:Ag:49:CYS:HA	81:Ap:61:MET:HG3	1.96	0.48
5:B1:379:C:OP1	27:BI:56:ARG:NH1	2.45	0.48
14:BT:59:SER:O	14:BT:63:HIS:ND1	2.41	0.48
24:BE:125:LYS:H	24:BE:142:HIS:CE1	2.31	0.48
28:BJ:162:ARG:H	28:BJ:166:GLY:HA3	1.78	0.48
47:AG:156:VAL:HB	47:AG:202:VAL:HB	1.96	0.48
58:AS:156:HIS:HD2	58:AS:174:THR:HG21	1.78	0.48
1:A2:1297:C:OP1	1:A2:3852:G:N2	2.47	0.48
1:A2:3753:C:H2'	1:A2:3780:G:H1	1.79	0.48
4:Bw:18:G:O2'	4:Bw:60:C:N3	2.44	0.48
5:B1:1403:C:OP2	5:B1:1405:A:N6	2.46	0.48
5:B1:1593:C:H1'	14:BT:12:GLN:HE22	1.79	0.48
37:Bb:67:THR:OG1	37:Bb:72:ARG:NH1	2.46	0.48
41:AA:207:VAL:HG23	41:AA:208:GLU:HG3	1.96	0.48
61:AV:13:LYS:HB2	61:AV:128:LEU:HD21	1.96	0.48
83:Au:38:LEU:HD13	83:Au:41:TYR:HE2	1.77	0.48
85:AK:57:LYS:HG2	85:AK:58:ASN:H	1.78	0.48
85:AK:109:ALA:HB2	85:AK:184:SER:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:AK:139:GLN:NE2	86:Ct:184:ASN:OD1	2.41	0.48
1:A2:211:G:OP2	1:A2:211:G:N2	2.47	0.48
1:A2:942:G:O2'	1:A2:944:G:N2	2.47	0.48
1:A2:1913:A:H61	1:A2:2037:G:H22	1.61	0.48
1:A2:3612:U:OP2	1:A2:3617:A:N6	2.45	0.48
1:A2:4199:C:H1'	1:A2:4283:U:H1'	1.95	0.48
1:A2:4263:U:OP2	1:A2:4267:G:N1	2.44	0.48
5:B1:1201:U:HO2'	5:B1:1358:U:HO2'	1.62	0.48
22:BB:170:GLU:O	22:BB:173:THR:OG1	2.31	0.48
48:AH:36:ARG:HH12	48:AH:76:HIS:CD2	2.32	0.48
54:AO:34:VAL:HG22	54:AO:103:LYS:HB2	1.95	0.48
1:A2:664:C:H2'	1:A2:665:G:H8	1.78	0.48
1:A2:976:U:H3	1:A2:1047:G:H1	1.61	0.48
1:A2:1292:C:O2'	71:Af:21:GLN:NE2	2.37	0.48
1:A2:4964:U:H3	1:A2:4999:G:H5'	1.78	0.48
5:B1:172:U:OP1	5:B1:314:U:O2'	2.32	0.48
5:B1:1084:A:OP1	5:B1:1858:G:O2'	2.29	0.48
22:BB:121:ILE:HD12	22:BB:207:LEU:HD21	1.95	0.48
30:BN:3:ARG:HB2	30:BN:6:ALA:HB3	1.95	0.48
35:BY:41:ARG:NE	35:BY:55:ILE:O	2.46	0.48
56:AQ:100:VAL:HG21	56:AQ:113:ILE:HD13	1.96	0.48
86:Ct:126:LEU:HD11	86:Ct:156:MET:HE3	1.96	0.48
86:Ct:575:PRO:HD2	86:Ct:794:PHE:HE1	1.78	0.48
5:B1:490:C:O2'	5:B1:574:A:N1	2.46	0.48
5:B1:525:A:N7	5:B1:589:G:N2	2.59	0.48
5:B1:1010:G:H2'	5:B1:1011:A:H8	1.78	0.48
5:B1:1064:C:H2'	5:B1:1065:G:H8	1.78	0.48
5:B1:1605:G:OP1	14:BT:84:ARG:NH2	2.46	0.48
15:BU:86:LYS:HE2	15:BU:88:LEU:HD11	1.95	0.48
42:AB:254:ILE:HG23	42:AB:266:VAL:HG11	1.96	0.48
45:AE:261:ILE:HA	45:AE:267:LEU:HD23	1.95	0.48
47:AG:67:ARG:NH2	47:AG:162:ASP:OD1	2.47	0.48
53:AN:185:GLY:O	53:AN:194:ARG:NH2	2.47	0.48
69:Ad:46:LEU:HD23	69:Ad:49:ILE:HD12	1.95	0.48
80:Ao:44:LYS:HE2	80:Ao:52:THR:HB	1.96	0.48
86:Ct:839:ARG:HH21	86:Ct:844:LEU:HB2	1.79	0.48
1:A2:1300:U:OP1	66:Aa:21:ARG:NH2	2.47	0.47
1:A2:4714:U:H3'	71:Af:4:ARG:HD3	1.95	0.47
2:Bv:21:A:N6	2:Bv:48:C:OP2	2.46	0.47
5:B1:67:C:OP2	25:BG:172:LYS:NZ	2.40	0.47
5:B1:1396:A:N1	5:B1:1449:G:O6	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B1:1866:A:H8	36:Ba:96:THR:HA	1.79	0.47
45:AE:177:GLY:HA3	45:AE:184:VAL:HB	1.95	0.47
54:AO:9:LEU:HD23	54:AO:118:MET:HB2	1.94	0.47
65:AZ:14:LEU:HD23	72:Ag:88:ARG:HB2	1.94	0.47
76:Ak:22:SER:HB3	76:Ak:37:ARG:HB3	1.96	0.47
1:A2:67:C:OP2	1:A2:306:G:N2	2.47	0.47
1:A2:715:C:H2'	1:A2:716:G:H8	1.78	0.47
1:A2:920:G:N2	1:A2:925:C:HO2'	2.12	0.47
1:A2:1315:C:H2'	1:A2:1316:A:C8	2.48	0.47
3:Bx:33:A:H4'	6:BD:146:ARG:HH12	1.79	0.47
5:B1:78:C:H1'	25:BG:175:LYS:HG2	1.96	0.47
5:B1:886:A:C6	5:B1:901:G:C2	3.02	0.47
5:B1:916:A:O2'	30:BN:73:ARG:NH1	2.45	0.47
5:B1:925:G:H1	5:B1:1017:U:H3	1.60	0.47
5:B1:1086:G:OP2	36:Ba:12:LYS:NZ	2.47	0.47
5:B1:1324:G:O2'	5:B1:1510:G:O2'	2.32	0.47
15:BU:62:ARG:HG2	15:BU:81:GLN:HG2	1.95	0.47
16:BZ:41:ARG:HH11	16:BZ:42:ASP:HB2	1.79	0.47
34:BX:41:PHE:HB3	34:BX:44:ALA:HB3	1.96	0.47
46:AF:153:LEU:HD21	46:AF:244:ILE:HD11	1.96	0.47
47:AG:104:PRO:HG2	47:AG:194:VAL:HG23	1.95	0.47
85:AK:45:MET:HA	85:AK:48:ARG:HG2	1.96	0.47
1:A2:407:G:OP2	77:Al:36:ARG:NH1	2.47	0.47
1:A2:4285:A:H4'	44:AD:176:SER:HB3	1.95	0.47
5:B1:64:A:O5'	25:BG:136:LYS:NZ	2.46	0.47
41:AA:113:VAL:HG12	41:AA:166:VAL:HA	1.96	0.47
44:AD:51:MET:HA	44:AD:63:GLN:O	2.14	0.47
52:AM:6:PHE:H	52:AM:11:ARG:NH1	2.13	0.47
56:AQ:156:PRO:HG3	66:Aa:48:TYR:HA	1.96	0.47
70:Ae:40:GLY:O	70:Ae:46:ARG:NE	2.45	0.47
1:A2:4047:A:O3'	53:AN:31:ARG:NH2	2.47	0.47
5:B1:106:C:O2'	5:B1:410:G:N3	2.48	0.47
5:B1:600:G:H2'	5:B1:601:G:H8	1.78	0.47
5:B1:1203:G:H8	5:B1:1699:A:H2	1.61	0.47
7:BF:20:PHE:HE1	7:BF:50:PRO:HD3	1.79	0.47
20:Bg:107:ASP:OD2	20:Bg:125:ARG:NH1	2.47	0.47
41:AA:135:THR:HB	41:AA:149:LYS:HB3	1.96	0.47
47:AG:89:ARG:HH22	47:AG:185:LYS:HD3	1.79	0.47
47:AG:190:LEU:HD13	47:AG:193:LEU:HD21	1.95	0.47
52:AM:23:LYS:HE2	52:AM:45:VAL:HB	1.96	0.47
86:Ct:378:ASP:H	86:Ct:382:ALA:HB3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B1:92:A:H61	5:B1:444:G:H1'	1.80	0.47
5:B1:886:A:C5	5:B1:901:G:N2	2.81	0.47
9:BM:36:ARG:HH21	19:Bf:103:LEU:HD22	1.78	0.47
14:BT:70:ALA:HB3	14:BT:121:ARG:HE	1.80	0.47
34:BX:84:PHE:HB2	34:BX:118:VAL:HG11	1.96	0.47
46:AF:166:ARG:HH12	46:AF:212:LYS:HD2	1.80	0.47
65:AZ:91:LEU:HD21	65:AZ:96:VAL:HG21	1.95	0.47
70:Ae:75:ARG:HD2	70:Ae:95:TYR:HE1	1.79	0.47
84:Aq:14:TYR:O	84:Aq:62:LEU:HA	2.15	0.47
1:A2:1255:C:OP2	1:A2:1256:G:N1	2.47	0.47
5:B1:1146:C:O2'	5:B1:1150:A:N1	2.44	0.47
6:BD:23:GLU:HA	6:BD:26:THR:HG22	1.97	0.47
11:BQ:19:ALA:HA	11:BQ:74:GLY:HA2	1.97	0.47
49:AI:103:LEU:HD22	49:AI:108:ALA:HA	1.96	0.47
51:AL:50:PRO:HA	51:AL:148:THR:HG23	1.96	0.47
53:AN:73:ARG:HB3	53:AN:89:VAL:HG13	1.97	0.47
64:AY:55:VAL:HG13	64:AY:104:VAL:HG13	1.96	0.47
77:Al:12:PHE:HE2	77:Al:49:LEU:HD13	1.79	0.47
1:A2:85:G:O2'	1:A2:97:G:O6	2.32	0.47
1:A2:113:A:H4'	53:AN:49:ARG:HG2	1.97	0.47
1:A2:346:G:N2	1:A2:354:A:N1	2.62	0.47
1:A2:1475:G:H5''	67:Ab:40:LEU:HD23	1.96	0.47
1:A2:1564:U:H2'	1:A2:1565:A:H8	1.80	0.47
1:A2:1756:C:H2'	1:A2:1757:A:H8	1.79	0.47
1:A2:2462:G:O6	1:A2:2474:U:O4	2.32	0.47
1:A2:2532:A:N6	1:A2:2744:A:OP2	2.43	0.47
1:A2:3624:A:H4'	41:AA:179:ILE:HB	1.97	0.47
1:A2:3686:U:OP1	4:Bw:3:G:O2'	2.32	0.47
1:A2:4143:U:O2'	41:AA:226:ARG:NH2	2.47	0.47
1:A2:4156:U:O3'	49:AI:116:ARG:NH1	2.48	0.47
1:A2:4334:U:OP2	80:Ao:61:LYS:NZ	2.38	0.47
5:B1:1452:A:H61	5:B1:1473:G:H8	1.63	0.47
13:BS:14:ARG:HH21	50:AJ:113:ILE:HD11	1.79	0.47
22:BB:123:ALA:HB3	22:BB:139:CYS:HB3	1.95	0.47
22:BB:144:LYS:HB2	22:BB:208:HIS:HB2	1.97	0.47
23:BC:255:LEU:HD21	32:BV:14:PRO:HD2	1.97	0.47
42:AB:220:ILE:HD11	42:AB:348:ARG:HE	1.79	0.47
43:AC:210:ILE:HG12	43:AC:230:LEU:HD12	1.96	0.47
46:AF:226:HIS:ND1	46:AF:233:ALA:O	2.48	0.47
48:AH:23:ARG:NH2	48:AH:39:ASN:OD1	2.39	0.47
55:AP:60:PHE:HD2	55:AP:67:VAL:HG21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:Ad:64:ILE:HG22	69:Ad:106:VAL:HB	1.95	0.47
86:Ct:663:THR:OG1	86:Ct:703:ASP:OD1	2.28	0.47
1:A2:66:A:O2'	1:A2:320:C:O2	2.31	0.47
1:A2:270:C:O2	74:Ai:26:HIS:NE2	2.40	0.47
1:A2:1978:U:O2'	1:A2:1980:A:N7	2.36	0.47
5:B1:387:C:OP1	27:Bi:10:LYS:NZ	2.39	0.47
5:B1:942:G:H21	31:BO:137:SER:HB2	1.79	0.47
54:AO:127:VAL:HA	58:AS:158:VAL:HG21	1.96	0.47
56:AQ:122:THR:OG1	56:AQ:124:ASP:OD1	2.26	0.47
68:Ac:48:LEU:HD13	68:Ac:57:LYS:HG3	1.97	0.47
73:Ah:40:ALA:HB1	73:Ah:43:LYS:HD2	1.96	0.47
86:Ct:665:ILE:HB	86:Ct:705:HIS:HA	1.95	0.47
1:A2:220:G:O2'	1:A2:239:U:O2	2.32	0.47
1:A2:1871:G:N2	1:A2:1920:A:N1	2.50	0.47
1:A2:2027:G:H4'	1:A2:2028:A:H5'	1.96	0.47
1:A2:2374:A:O2'	1:A2:2786:A:OP2	2.32	0.47
1:A2:3569:C:H2'	1:A2:3570:A:H8	1.79	0.47
1:A2:4022:C:H2'	1:A2:4023:A:C8	2.50	0.47
4:Bw:61:C:H2'	4:Bw:62:A:H8	1.79	0.47
22:BB:97:LEU:HD12	22:BB:228:LEU:HD21	1.97	0.47
49:AI:174:THR:HG23	49:AI:176:PHE:H	1.79	0.47
52:AM:56:GLN:OE1	58:AS:157:ARG:NH2	2.48	0.47
72:Ag:82:MET:HB3	72:Ag:86:CYS:HB2	1.96	0.47
86:Ct:613:LEU:HD12	86:Ct:616:ASP:HB3	1.97	0.47
1:A2:932:U:OP2	46:AF:62:ARG:NH1	2.48	0.47
1:A2:4436:A:OP2	1:A2:4438:C:N4	2.48	0.47
1:A2:4547:U:OP1	54:AO:74:ARG:N	2.46	0.47
5:B1:28:U:H2'	5:B1:29:G:C8	2.50	0.47
5:B1:1288:U:O2	5:B1:1312:G:N2	2.48	0.47
25:BG:142:ARG:NH2	25:BG:148:SER:O	2.48	0.47
39:A3:63:U:O2'	73:Ah:52:LYS:NZ	2.48	0.47
47:AG:159:HIS:HB2	47:AG:184:ILE:O	2.14	0.47
47:AG:165:GLU:OE1	53:AN:26:ARG:NH2	2.47	0.47
51:AL:60:ARG:NH2	51:AL:67:HIS:O	2.48	0.47
53:AN:31:ARG:NH1	53:AN:124:ASP:OD2	2.47	0.47
82:At:62:VAL:HG11	82:At:96:MET:HE1	1.96	0.47
86:Ct:144:ARG:NH1	86:Ct:781:MET:SD	2.89	0.47
1:A2:2401:C:N4	1:A2:2808:U:O2'	2.48	0.46
1:A2:4435:A:H4'	78:Am:95:ILE:HG21	1.95	0.46
1:A2:4924:A:H5'	42:AB:128:LYS:HG3	1.96	0.46
5:B1:148:U:H2'	5:B1:149:A:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B1:982:G:H2'	5:B1:983:A:C8	2.50	0.46
16:BZ:50:PHE:HB3	16:BZ:83:LEU:HD11	1.96	0.46
37:Bb:23:ARG:NH2	37:Bb:27:SER:O	2.48	0.46
43:AC:323:ARG:HA	43:AC:326:LEU:HB2	1.97	0.46
50:AJ:95:ARG:HH12	50:AJ:97:ASN:HD21	1.63	0.46
54:AO:194:GLU:HG3	54:AO:199:HIS:HA	1.97	0.46
57:AR:178:GLN:NE2	57:AR:182:GLU:OE1	2.48	0.46
1:A2:894:C:H2'	1:A2:895:G:H8	1.79	0.46
1:A2:1761:U:H2'	1:A2:1762:A:C8	2.50	0.46
1:A2:4061:G:H2'	1:A2:4062:G:H8	1.81	0.46
1:A2:4954:C:OP1	69:Ad:32:ARG:NH1	2.49	0.46
5:B1:987:A:OP1	36:Ba:37:LYS:NZ	2.43	0.46
5:B1:1753:C:H2'	5:B1:1754:G:H8	1.80	0.46
24:BE:195:ILE:HA	24:BE:210:VAL:HG12	1.97	0.46
36:Ba:23:CYS:SG	36:Ba:24:THR:N	2.88	0.46
39:A3:53:G:OP1	77:Al:19:GLN:NE2	2.41	0.46
46:AF:228:VAL:HA	58:AS:39:VAL:HG22	1.95	0.46
54:AO:22:ILE:HG23	58:AS:166:ARG:HH21	1.80	0.46
81:Ap:42:CYS:SG	81:Ap:59:SER:OG	2.74	0.46
1:A2:305:G:OP1	74:Ai:85:ARG:NH1	2.49	0.46
1:A2:4139:C:H2'	1:A2:4140:A:H8	1.80	0.46
5:B1:524:U:H3'	38:Be:29:THR:HG22	1.98	0.46
5:B1:1050:A:N6	5:B1:1068:G:H21	2.00	0.46
11:BQ:58:LEU:HD22	11:BQ:108:ILE:HD11	1.97	0.46
22:BB:198:GLU:OE2	22:BB:202:GLN:NE2	2.48	0.46
25:BG:142:ARG:HH22	25:BG:149:LYS:HA	1.81	0.46
26:BH:150:GLY:O	26:BH:152:ARG:NH1	2.47	0.46
39:A3:14:U:H4'	55:AP:123:PRO:HB3	1.98	0.46
53:AN:73:ARG:NH1	53:AN:86:HIS:O	2.49	0.46
76:Ak:52:LYS:HA	76:Ak:55:LYS:HG2	1.97	0.46
81:Ap:50:ARG:HG3	81:Ap:51:ALA:H	1.80	0.46
1:A2:8:U:O2	39:A3:149:G:N2	2.47	0.46
1:A2:1988:G:H21	1:A2:1993:A:H62	1.64	0.46
1:A2:2274:C:O2'	43:AC:45:ARG:NH2	2.48	0.46
1:A2:2390:C:H2'	1:A2:2391:A:C8	2.51	0.46
4:Bw:72:C:H2'	4:Bw:73:A:C5	2.50	0.46
10:BP:34:MET:HG3	10:BP:45:LEU:HD22	1.97	0.46
21:BA:10:MET:HE1	21:BA:51:LEU:HB3	1.96	0.46
40:A4:35:U:O2	40:A4:45:U:O2'	2.33	0.46
42:AB:262:VAL:HG11	42:AB:268:ARG:HE	1.80	0.46
86:Ct:604:MET:HG2	86:Ct:704:VAL:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:223:G:H21	64:AY:9:SER:HA	1.81	0.46
1:A2:274:G:OP2	53:AN:44:ARG:NH2	2.48	0.46
1:A2:2356:C:H42	1:A2:2360:A:N6	2.07	0.46
1:A2:2450:G:H5''	47:AG:59:ARG:HH21	1.81	0.46
1:A2:3767:U:HO2'	5:B1:1720:U:HO2'	1.49	0.46
1:A2:3815:U:H2'	1:A2:3816:A:H8	1.80	0.46
1:A2:4547:U:H2'	1:A2:4548:G:H8	1.79	0.46
5:B1:1144:A:H5'	5:B1:1355:C:H41	1.79	0.46
5:B1:1650:A:H5''	11:BQ:139:ALA:HB2	1.98	0.46
7:BF:86:LYS:HA	7:BF:89:THR:HG22	1.97	0.46
49:AI:34:PHE:HD1	49:AI:89:VAL:HB	1.80	0.46
54:AO:6:VAL:HA	54:AO:32:LYS:O	2.16	0.46
1:A2:473:G:H1	1:A2:669:G:H22	1.62	0.46
1:A2:4055:A:H5''	47:AG:56:LYS:HB2	1.98	0.46
1:A2:4144:G:H5'	41:AA:226:ARG:HH22	1.81	0.46
1:A2:4713:G:H5'	71:Af:100:ARG:HE	1.80	0.46
5:B1:1394:G:N2	5:B1:1475:G:N3	2.63	0.46
5:B1:1492:U:O2'	5:B1:1495:G:OP1	2.33	0.46
5:B1:1606:G:H5''	14:BT:87:VAL:HG23	1.97	0.46
9:BM:120:ALA:HB1	9:BM:123:VAL:HB	1.98	0.46
42:AB:378:ARG:HG3	62:AW:32:LEU:HD21	1.98	0.46
70:Ae:106:LYS:HD2	70:Ae:109:LYS:HE2	1.98	0.46
86:Ct:18:ASN:ND2	86:Ct:97:GLY:O	2.49	0.46
86:Ct:617:ILE:HD13	86:Ct:659:PRO:HA	1.98	0.46
1:A2:182:C:O2'	1:A2:184:U:O2'	2.32	0.46
1:A2:419:U:H2'	1:A2:420:A:H8	1.81	0.46
1:A2:1611:G:N7	41:AA:9:ARG:NH1	2.48	0.46
1:A2:1975:C:H2'	1:A2:1976:G:C8	2.51	0.46
1:A2:2054:C:H5''	46:AF:212:LYS:HB3	1.97	0.46
5:B1:527:C:H4'	28:BJ:125:HIS:HB2	1.98	0.46
11:BQ:10:VAL:HG21	11:BQ:98:LYS:HG3	1.97	0.46
20:Bg:10:THR:HG22	20:Bg:308:ARG:HG2	1.98	0.46
23:BC:171:GLY:O	33:BW:98:GLN:NE2	2.48	0.46
24:BE:45:ILE:HB	24:BE:80:VAL:HG22	1.97	0.46
44:AD:146:LEU:HD11	44:AD:163:LEU:HG	1.97	0.46
53:AN:116:LEU:HB3	53:AN:133:ILE:HG23	1.98	0.46
59:AT:108:ARG:HD3	59:AT:130:ARG:HD3	1.96	0.46
65:AZ:64:LYS:HA	65:AZ:67:LYS:HG2	1.97	0.46
86:Ct:121:VAL:O	86:Ct:415:ARG:NH2	2.46	0.46
1:A2:52:G:OP2	75:Aj:48:ASN:ND2	2.44	0.46
1:A2:353:A:N3	1:A2:357:A:O2'	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:1316:A:H2'	1:A2:1317:A:H8	1.81	0.46
1:A2:2587:G:H2'	1:A2:2588:G:H8	1.80	0.46
1:A2:3826:C:H2'	1:A2:3827:A:H8	1.80	0.46
1:A2:4827:U:H3'	52:AM:91:TRP:HE1	1.81	0.46
5:B1:801:U:O4	26:BH:106:ARG:NH2	2.49	0.46
12:BR:31:ASN:HD22	12:BR:55:THR:HG22	1.80	0.46
12:BR:71:ILE:HG13	12:BR:74:GLN:H	1.80	0.46
22:BB:197:ILE:O	22:BB:201:CYS:CB	2.62	0.46
33:BW:14:ILE:HD11	33:BW:27:ILE:HD11	1.97	0.46
51:AL:80:GLU:HG2	51:AL:110:LEU:HD12	1.96	0.46
86:Ct:692:LEU:HD11	86:Ct:740:LEU:HD21	1.98	0.46
1:A2:3581:A:H2'	1:A2:3582:A:H8	1.81	0.46
1:A2:3824:U:O2'	1:A2:4937:A:N3	2.48	0.46
5:B1:309:G:H21	5:B1:340:C:H1'	1.81	0.46
5:B1:1094:C:OP1	33:BW:28:ARG:NH2	2.49	0.46
46:AF:137:GLU:HB3	46:AF:226:HIS:HE1	1.81	0.46
85:AK:53:VAL:HG22	85:AK:89:VAL:HG22	1.98	0.46
86:Ct:421:VAL:HG23	86:Ct:425:LEU:HD23	1.97	0.46
86:Ct:580:ARG:HB3	86:Ct:698:ARG:HB3	1.97	0.46
1:A2:645:C:O2	66:Aa:85:GLN:NE2	2.40	0.46
1:A2:743:G:O6	1:A2:898:U:C2	2.69	0.46
1:A2:1845:G:OP2	49:AI:14:ASN:ND2	2.48	0.46
1:A2:2562:C:H2'	1:A2:2563:G:H8	1.81	0.46
5:B1:804:U:O2'	33:BW:121:THR:O	2.27	0.46
7:BF:91:ARG:NH2	11:BQ:46:THR:OG1	2.49	0.46
9:BM:79:VAL:HG21	9:BM:85:LEU:HD21	1.98	0.46
12:BR:14:ARG:HA	12:BR:17:ILE:HG22	1.97	0.46
44:AD:211:LEU:HB3	44:AD:219:TYR:HB2	1.97	0.46
45:AE:146:PRO:HB2	45:AE:203:ILE:HG21	1.98	0.46
58:AS:16:CYS:SG	58:AS:17:LEU:N	2.89	0.46
70:Ae:119:ALA:HB3	82:At:119:ARG:HH22	1.81	0.46
84:Aq:108:GLU:HA	84:Aq:111:ASN:HD22	1.81	0.46
86:Ct:58:ASP:HB2	86:Ct:63:GLU:HB3	1.97	0.46
1:A2:947:A:N6	1:A2:1266:G:O6	2.49	0.45
1:A2:1410:A:H2	56:AQ:138:LEU:HD23	1.82	0.45
1:A2:1637:C:O2	1:A2:4352:A:O2'	2.33	0.45
1:A2:1983:A:H61	84:Aq:136:ALA:HA	1.81	0.45
1:A2:2390:C:O2'	1:A2:2505:C:O2	2.31	0.45
1:A2:4833:G:H1	58:AS:160:ARG:HH12	1.64	0.45
1:A2:4925:A:H2'	1:A2:4926:A:H8	1.81	0.45
5:B1:955:A:H4'	31:BO:60:MET:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B1:1216:C:N4	5:B1:1342:U:OP1	2.49	0.45
5:B1:1263:U:H5''	18:Bd:27:ARG:HD3	1.97	0.45
5:B1:1862:G:H22	36:Ba:76:SER:HG	1.63	0.45
7:BF:63:LYS:HG2	7:BF:71:ARG:HH12	1.81	0.45
14:BT:41:LYS:HD3	14:BT:81:GLY:HA3	1.97	0.45
26:BH:39:GLN:HE22	26:BH:43:LEU:HD22	1.81	0.45
29:BL:86:ILE:HG12	29:BL:113:LEU:HB2	1.98	0.45
39:A3:153:C:H2'	39:A3:154:G:C8	2.50	0.45
41:AA:55:GLY:HA3	41:AA:174:ARG:HH11	1.81	0.45
42:AB:8:ALA:HB2	61:AV:49:LEU:HD22	1.98	0.45
86:Ct:558:LEU:HD23	86:Ct:561:LEU:HD12	1.97	0.45
1:A2:16:G:H5''	63:AX:60:TYR:HE1	1.81	0.45
1:A2:951:A:H5''	82:At:98:ARG:HH11	1.81	0.45
1:A2:2066:G:H2'	1:A2:2067:G:H8	1.81	0.45
1:A2:2340:G:N2	1:A2:3831:A:OP2	2.41	0.45
1:A2:4171:G:H4'	59:AT:12:ARG:HD2	1.98	0.45
11:BQ:58:LEU:O	11:BQ:62:ARG:NH1	2.49	0.45
12:BR:122:PRO:HB2	12:BR:124:VAL:HG23	1.97	0.45
17:Bc:64:GLU:OE1	31:BO:117:ARG:NH2	2.48	0.45
73:Ah:91:MET:HA	73:Ah:94:ARG:HG3	1.98	0.45
74:Ai:62:LYS:HZ1	74:Ai:98:ARG:HD3	1.80	0.45
86:Ct:5:THR:HB	86:Ct:8:GLN:HB3	1.97	0.45
86:Ct:131:CYS:HA	86:Ct:181:ILE:HD11	1.97	0.45
1:A2:1347:U:O4	51:AL:36:ARG:NH2	2.50	0.45
5:B1:524:U:O4	28:BJ:38:ARG:NH2	2.49	0.45
5:B1:1416:C:N4	5:B1:1422:G:O6	2.49	0.45
22:BB:40:ASN:HD22	22:BB:76:ASN:HB2	1.80	0.45
23:BC:60:TRP:HE1	23:BC:92:GLU:HB2	1.82	0.45
43:AC:47:ASN:OD1	43:AC:113:ARG:N	2.50	0.45
51:AL:32:LYS:HE2	51:AL:36:ARG:HH21	1.80	0.45
57:AR:98:ARG:HH21	57:AR:133:LYS:HA	1.81	0.45
1:A2:705:G:OP1	43:AC:321:ASN:ND2	2.49	0.45
1:A2:1224:C:N4	1:A2:1253:A:OP1	2.49	0.45
1:A2:3658:A:O2'	41:AA:236:GLY:N	2.50	0.45
1:A2:4951:G:H22	1:A2:5016:A:H2	1.64	0.45
5:B1:1380:C:O2'	21:BA:113:GLN:OE1	2.34	0.45
46:AF:80:ASN:HD21	59:AT:142:ARG:HA	1.81	0.45
48:AH:159:ALA:HA	48:AH:162:GLN:HG2	1.98	0.45
56:AQ:178:ARG:H	66:Aa:51:GLY:HA2	1.81	0.45
65:AZ:90:PRO:HB2	65:AZ:117:LYS:HD2	1.99	0.45
1:A2:1747:A:O2'	13:BS:118:ARG:NH2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:3923:A:H2'	1:A2:3924:G:H8	1.82	0.45
1:A2:4544:C:H4'	42:AB:99:LEU:HB2	1.98	0.45
1:A2:4856:G:H1	1:A2:4880:C:H41	1.63	0.45
5:B1:987:A:H4'	36:Ba:70:LYS:HG3	1.97	0.45
37:Bb:42:LYS:NZ	37:Bb:44:THR:OG1	2.46	0.45
39:A3:70:G:H22	39:A3:87:G:H1'	1.81	0.45
40:A4:94:C:OP1	58:AS:46:TYR:OH	2.29	0.45
45:AE:209:PRO:HB2	45:AE:212:LEU:HD22	1.99	0.45
47:AG:32:PHE:HE1	65:AZ:55:ALA:HA	1.82	0.45
47:AG:154:LEU:HB3	47:AG:204:PHE:HB2	1.97	0.45
47:AG:184:ILE:HD13	47:AG:190:LEU:HD21	1.99	0.45
58:AS:95:ARG:NE	58:AS:97:TYR:OH	2.40	0.45
83:Au:42:ASP:H	83:Au:47:LYS:HD2	1.81	0.45
1:A2:1365:G:H2'	1:A2:1366:G:H8	1.80	0.45
1:A2:2324:G:OP2	66:Aa:12:ARG:NH1	2.50	0.45
1:A2:2437:C:H5''	53:AN:67:ARG:HE	1.82	0.45
1:A2:2702:U:H2'	1:A2:2703:G:C8	2.52	0.45
1:A2:4306:U:O2'	80:Ao:28:LYS:O	2.31	0.45
5:B1:57:U:O2	5:B1:499:G:O2'	2.35	0.45
72:Ag:40:LYS:HD2	72:Ag:52:ARG:HH21	1.81	0.45
1:A2:404:A:O2'	1:A2:408:C:O2'	2.33	0.45
1:A2:1833:U:OP1	66:Aa:23:GLY:N	2.49	0.45
1:A2:2569:G:H21	1:A2:2734:A:N6	2.14	0.45
1:A2:4675:G:OP1	54:AO:148:LYS:NZ	2.43	0.45
5:B1:562:U:H2'	5:B1:563:G:C8	2.51	0.45
5:B1:814:U:OP1	24:BE:22:LYS:NZ	2.49	0.45
21:BA:123:VAL:HG22	21:BA:145:ILE:HB	1.98	0.45
22:BB:30:TRP:CD2	31:BO:19:PRO:HB3	2.52	0.45
42:AB:59:GLU:HB2	42:AB:366:LYS:HE3	1.98	0.45
42:AB:165:HIS:HB2	42:AB:178:ALA:HB1	1.98	0.45
43:AC:250:CYS:SG	43:AC:252:TRP:NE1	2.89	0.45
44:AD:12:TYR:O	44:AD:16:TYR:HB2	2.17	0.45
60:AU:89:LYS:HG2	60:AU:93:LYS:HE2	1.98	0.45
76:Ak:23:VAL:HA	76:Ak:35:LYS:O	2.16	0.45
86:Ct:25:ILE:O	86:Ct:127:VAL:HA	2.17	0.45
86:Ct:155:LEU:HB3	86:Ct:212:VAL:HG12	1.99	0.45
86:Ct:752:PRO:HD2	86:Ct:807:GLN:HG2	1.99	0.45
1:A2:1331:U:H2'	1:A2:1332:G:H8	1.82	0.45
1:A2:4727:G:H22	1:A2:4825:G:H1	1.63	0.45
5:B1:602:G:H3'	5:B1:603:C:H2'	1.98	0.45
5:B1:1544:C:O2'	11:BQ:80:GLN:NE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:AE:162:VAL:HG12	45:AE:175:VAL:HG12	1.99	0.45
53:AN:114:ARG:NH1	53:AN:151:ILE:O	2.50	0.45
62:AW:6:CYS:SG	62:AW:9:SER:OG	2.70	0.45
62:AW:23:ARG:HE	62:AW:25:ASP:HB2	1.82	0.45
79:An:15:ARG:HG2	79:An:19:LYS:HE3	1.98	0.45
1:A2:132:G:H1	1:A2:136:G:H22	1.64	0.45
1:A2:493:G:OP2	1:A2:495:C:N4	2.49	0.45
1:A2:704:C:H2'	1:A2:705:G:H8	1.81	0.45
1:A2:2827:G:O2'	1:A2:3809:U:O4	2.31	0.45
1:A2:4202:G:H5''	50:AJ:145:LYS:HE3	1.99	0.45
5:B1:861:A:H62	26:BH:107:LYS:HE2	1.81	0.45
63:AX:89:LYS:HD2	63:AX:93:ASN:HD22	1.82	0.45
80:Ao:9:ARG:HG2	80:Ao:18:HIS:HB3	1.98	0.45
84:Aq:61:LYS:HD2	84:Aq:72:GLU:HB3	1.98	0.45
1:A2:1288:C:OP1	39:A3:7:U:O2'	2.35	0.45
1:A2:1975:C:H2'	1:A2:1976:G:H8	1.82	0.45
1:A2:2869:C:H42	1:A2:3582:A:H61	1.65	0.45
1:A2:4556:U:H2'	1:A2:4557:G:H8	1.81	0.45
5:B1:652:U:H2'	5:B1:653:A:H8	1.82	0.45
5:B1:864:A:H2'	5:B1:865:A:C8	2.52	0.45
5:B1:1036:A:N3	5:B1:1844:U:O2'	2.45	0.45
5:B1:1228:A:O2'	5:B1:1634:A:N3	2.43	0.45
5:B1:1615:U:OP2	10:BP:43:ARG:NH2	2.44	0.45
25:BG:153:VAL:HG23	25:BG:156:TYR:HB2	1.98	0.45
55:AP:29:THR:HA	55:AP:32:THR:HG22	1.98	0.45
61:AV:43:LYS:HD3	61:AV:62:MET:HE2	1.97	0.45
80:Ao:21:HIS:HA	80:Ao:71:GLU:O	2.17	0.45
86:Ct:89:ILE:HD11	86:Ct:93:LYS:HB2	1.99	0.45
86:Ct:584:SER:HB3	86:Ct:737:GLN:HB2	1.99	0.45
1:A2:1647:C:O2'	56:AQ:10:ASP:OD2	2.35	0.44
1:A2:2036:G:O6	58:AS:156:HIS:ND1	2.50	0.44
1:A2:2062:C:H2'	1:A2:2063:G:C8	2.52	0.44
1:A2:2719:U:O2'	1:A2:2721:G:N2	2.50	0.44
1:A2:4267:G:O6	59:AT:87:LYS:NZ	2.46	0.44
1:A2:4287:A:H1'	44:AD:36:LEU:HD23	1.99	0.44
1:A2:4722:G:H2'	1:A2:4723:G:C8	2.52	0.44
76:Ak:23:VAL:HG22	76:Ak:36:VAL:HG22	1.99	0.44
81:Ap:15:GLY:O	81:Ap:23:ARG:NH1	2.50	0.44
86:Ct:290:CYS:HA	86:Ct:294:LEU:HB2	1.99	0.44
1:A2:131:C:H2'	1:A2:132:G:C2	2.52	0.44
1:A2:4577:C:H5''	42:AB:357:ARG:HE	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:4666:C:H2'	1:A2:4667:A:H8	1.82	0.44
5:B1:591:U:OP1	5:B1:593:C:N4	2.51	0.44
36:Ba:88:SER:H	36:Ba:91:ALA:HB3	1.82	0.44
42:AB:54:THR:HG22	42:AB:373:LYS:HZ1	1.82	0.44
44:AD:94:ASN:OD1	44:AD:97:ALA:N	2.45	0.44
57:AR:105:LEU:HD22	57:AR:135:LYS:HG3	2.00	0.44
80:Ao:67:VAL:HG12	80:Ao:84:ALA:HA	1.99	0.44
1:A2:1338:G:OP1	56:AQ:108:ARG:NH1	2.45	0.44
1:A2:1772:U:OP2	59:AT:13:TYR:OH	2.26	0.44
6:BD:106:ARG:NE	6:BD:174:HIS:O	2.50	0.44
9:BM:68:LEU:HD11	19:Bf:106:TYR:HE2	1.82	0.44
17:Bc:63:ARG:HD3	31:BO:75:MET:HE1	2.00	0.44
19:Bf:105:TYR:O	19:Bf:116:ARG:NH2	2.50	0.44
20:Bg:23:THR:HG22	20:Bg:31:ILE:HD12	1.99	0.44
25:BG:85:ARG:NH1	25:BG:86:PRO:O	2.50	0.44
25:BG:163:ASN:HD21	25:BG:167:LYS:HA	1.82	0.44
27:BI:11:ARG:NH1	27:BI:15:GLY:O	2.46	0.44
31:BO:29:GLY:O	31:BO:93:LEU:HA	2.17	0.44
39:A3:106:G:H4'	39:A3:137:A:H5'	1.98	0.44
41:AA:117:GLU:HG2	41:AA:124:GLY:H	1.82	0.44
44:AD:152:ARG:NH1	44:AD:154:THR:OG1	2.51	0.44
45:AE:136:HIS:CE1	45:AE:170:SER:HA	2.52	0.44
82:At:19:LYS:HG2	82:At:24:THR:HG22	1.99	0.44
1:A2:220:G:OP1	43:AC:163:LYS:NZ	2.50	0.44
1:A2:1921:G:H22	1:A2:4396:C:H5''	1.82	0.44
1:A2:4531:U:OP1	1:A2:4940:A:O2'	2.34	0.44
5:B1:5:U:H2'	5:B1:6:G:C8	2.52	0.44
5:B1:57:U:OP1	5:B1:504:G:O2'	2.36	0.44
5:B1:153:G:H21	25:BG:13:GLN:HG3	1.82	0.44
5:B1:1228:A:H2'	5:B1:1229:G:H8	1.81	0.44
5:B1:1546:G:N3	5:B1:1670:C:O2'	2.40	0.44
9:BM:24:THR:HG21	9:BM:118:SER:HB3	1.99	0.44
13:BS:14:ARG:NH1	13:BS:19:ASN:O	2.50	0.44
16:BZ:74:SER:HA	16:BZ:79:ILE:HB	2.00	0.44
23:BC:191:VAL:HG11	23:BC:236:PHE:HA	1.99	0.44
41:AA:24:LYS:HG3	41:AA:49:ILE:HD12	1.98	0.44
41:AA:28:ARG:HB3	41:AA:123:ARG:HB3	2.00	0.44
56:AQ:37:ARG:HG3	56:AQ:38:ARG:HG2	2.00	0.44
1:A2:661:G:H5'	43:AC:6:PRO:HB3	1.98	0.44
1:A2:2278:G:OP2	43:AC:204:ARG:NH1	2.50	0.44
1:A2:2497:G:O2'	1:A2:2517:U:O2	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:3671:C:O2'	1:A2:3745:A:N3	2.45	0.44
1:A2:4485:A:O2'	42:AB:246:ARG:NH1	2.49	0.44
40:A4:68:C:OP1	59:AT:20:ARG:NH2	2.50	0.44
41:AA:45:VAL:HB	41:AA:61:VAL:HG22	1.99	0.44
42:AB:240:LEU:HD21	42:AB:252:ALA:HB2	2.00	0.44
43:AC:304:ALA:O	56:AQ:38:ARG:NH1	2.37	0.44
58:AS:162:GLN:OE1	58:AS:166:ARG:NH1	2.50	0.44
83:Au:119:GLN:OE1	83:Au:122:ARG:NE	2.43	0.44
85:AK:161:ILE:HD13	85:AK:167:VAL:HG22	1.99	0.44
1:A2:67:C:H41	1:A2:319:U:HO2'	1.65	0.44
1:A2:2341:U:H2'	1:A2:2342:A:H8	1.82	0.44
5:B1:381:C:OP2	27:BI:54:LYS:NZ	2.51	0.44
5:B1:526:A:H2	5:B1:559:G:H22	1.65	0.44
5:B1:1165:G:OP2	5:B1:1165:G:N2	2.46	0.44
5:B1:1284:A:OP2	5:B1:1285:G:O2'	2.30	0.44
10:BP:24:GLN:O	10:BP:28:MET:CB	2.63	0.44
30:BN:102:LEU:HD12	30:BN:115:LEU:HD13	1.99	0.44
44:AD:36:LEU:HB3	44:AD:50:ARG:HE	1.83	0.44
44:AD:53:VAL:HB	44:AD:159:VAL:HG23	1.99	0.44
83:Au:43:PRO:HA	83:Au:47:LYS:HB2	1.99	0.44
85:AK:191:GLN:NE2	85:AK:199:TYR:O	2.40	0.44
1:A2:32:G:H21	1:A2:51:A:H62	1.66	0.44
1:A2:40:G:N3	1:A2:3885:U:N3	2.64	0.44
1:A2:370:A:H4'	43:AC:86:ARG:HD2	1.98	0.44
1:A2:737:A:H1'	58:AS:148:SER:HB2	1.99	0.44
1:A2:955:C:OP2	45:AE:110:ARG:NH1	2.43	0.44
1:A2:1663:G:H2'	1:A2:1664:A:H8	1.83	0.44
1:A2:2322:G:OP1	43:AC:52:TYR:OH	2.28	0.44
1:A2:3931:A:N3	1:A2:4014:U:O2'	2.44	0.44
1:A2:4484:G:O2'	1:A2:4487:C:OP2	2.32	0.44
1:A2:4548:G:O6	1:A2:4679:A:N6	2.50	0.44
20:Bg:101:PHE:HE1	20:Bg:136:GLY:HA2	1.82	0.44
23:BC:179:THR:HA	23:BC:219:ILE:HG23	2.00	0.44
30:BN:86:GLU:HA	30:BN:89:TYR:HB3	1.98	0.44
46:AF:199:LYS:HG3	46:AF:200:ARG:HG2	1.99	0.44
69:Ad:26:THR:HG23	69:Ad:85:ARG:HH11	1.83	0.44
1:A2:1886:U:O2'	46:AF:216:PRO:O	2.36	0.44
1:A2:2652:G:H5''	1:A2:2653:A:H3'	1.99	0.44
1:A2:2757:G:H22	39:A3:112:G:H5''	1.83	0.44
1:A2:3810:G:N2	1:A2:3814:C:O2'	2.50	0.44
1:A2:4687:C:H2'	1:A2:4688:G:H8	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B1:190:G:O2'	5:B1:209:A:N6	2.51	0.44
27:BI:46:VAL:HB	27:BI:54:LYS:HB3	2.00	0.44
48:AH:2:LYS:HG3	52:AM:33:GLN:HE22	1.83	0.44
54:AO:21:ALA:HA	54:AO:87:MET:HE1	1.99	0.44
61:AV:48:ARG:HG2	61:AV:51:ARG:HE	1.83	0.44
63:AX:78:LYS:HE3	63:AX:101:ASP:HB2	1.99	0.44
64:AY:17:ARG:O	64:AY:21:ALA:HB2	2.18	0.44
68:Ac:42:LYS:HG3	68:Ac:97:ILE:HB	1.99	0.44
86:Ct:216:SER:OG	86:Ct:217:GLY:N	2.50	0.44
86:Ct:692:LEU:O	86:Ct:839:ARG:NH1	2.41	0.44
1:A2:728:C:O2'	1:A2:729:C:O4'	2.33	0.44
1:A2:2365:U:H2'	1:A2:2366:G:C8	2.49	0.44
1:A2:4281:C:H2'	1:A2:4282:G:H8	1.82	0.44
1:A2:4486:G:OP1	1:A2:4521:A:N6	2.48	0.44
5:B1:1467:C:H5	12:BR:3:ARG:HH22	1.65	0.44
5:B1:1471:C:H2'	5:B1:1472:C:C2	2.52	0.44
5:B1:1567:G:O2'	14:BT:38:LYS:NZ	2.51	0.44
8:BK:24:LYS:O	8:BK:42:ASN:ND2	2.44	0.44
21:BA:36:GLN:O	21:BA:53:ARG:NH1	2.44	0.44
21:BA:145:ILE:HG12	21:BA:159:ILE:HB	2.00	0.44
25:BG:161:PRO:HA	25:BG:170:ARG:O	2.18	0.44
47:AG:75:LYS:HG2	47:AG:240:ASN:HB2	1.99	0.44
1:A2:1267:G:N2	1:A2:1267:G:OP2	2.48	0.43
1:A2:1351:A:H1'	64:AY:1:MET:HE2	2.00	0.43
1:A2:1485:A:H4'	1:A2:1486:G:H5'	1.99	0.43
1:A2:2541:G:N2	1:A2:2544:A:OP2	2.38	0.43
1:A2:4953:U:O3'	69:Ad:32:ARG:NH2	2.51	0.43
5:B1:1349:G:H21	21:BA:112:ILE:HD13	1.82	0.43
11:BQ:58:LEU:HB3	11:BQ:62:ARG:HH11	1.83	0.43
22:BB:228:LEU:HG	22:BB:232:HIS:HE1	1.83	0.43
25:BG:2:LYS:O	25:BG:108:VAL:HA	2.18	0.43
30:BN:84:LEU:HD11	30:BN:88:LEU:HD23	2.00	0.43
41:AA:77:ILE:HD11	41:AA:128:ARG:HE	1.81	0.43
41:AA:158:ILE:HD12	41:AA:162:ASN:HD21	1.83	0.43
42:AB:92:TYR:HB2	42:AB:159:VAL:HB	1.99	0.43
48:AH:137:SER:HB3	48:AH:143:GLU:HB3	1.98	0.43
53:AN:193:ARG:O	53:AN:197:THR:OG1	2.27	0.43
1:A2:1914:G:H2'	1:A2:1915:A:C8	2.53	0.43
1:A2:4232:C:H5''	1:A2:4233:A:H5''	1.99	0.43
1:A2:4355:G:N2	1:A2:4358:A:OP2	2.45	0.43
5:B1:168:C:H4'	25:BG:131:ARG:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B1:307:G:N7	27:BI:44:HIS:ND1	2.55	0.43
14:BT:75:MET:HA	14:BT:78:ILE:HD12	2.00	0.43
20:Bg:124:SER:OG	20:Bg:125:ARG:N	2.52	0.43
45:AE:168:LEU:HD11	45:AE:174:LEU:HD12	2.00	0.43
45:AE:178:PRO:HG2	45:AE:181:LEU:HB2	1.99	0.43
83:Au:31:THR:HA	83:Au:171:HIS:HA	1.99	0.43
86:Ct:313:ALA:HA	86:Ct:316:ILE:HD12	1.98	0.43
1:A2:66:A:N6	1:A2:276:C:O2'	2.42	0.43
1:A2:86:U:H2'	1:A2:87:A:H8	1.83	0.43
1:A2:202:C:O2'	1:A2:205:A:N6	2.52	0.43
1:A2:920:G:H2'	1:A2:927:C:H41	1.83	0.43
1:A2:1051:G:H2'	1:A2:1052:G:H8	1.83	0.43
1:A2:1450:C:OP1	66:Aa:132:ARG:NH2	2.47	0.43
1:A2:3703:A:H2'	1:A2:3704:A:C8	2.53	0.43
1:A2:4058:C:H2'	1:A2:4059:G:C8	2.54	0.43
1:A2:4264:U:H5''	59:AT:5:LYS:HE2	2.00	0.43
1:A2:4678:C:OP1	42:AB:276:HIS:ND1	2.42	0.43
4:Bw:18:G:H21	4:Bw:60:C:H41	1.65	0.43
5:B1:303:C:O2	27:BI:184:ARG:NH1	2.52	0.43
5:B1:396:U:H1'	27:BI:14:THR:HG23	1.99	0.43
24:BE:222:LEU:HA	24:BE:225:ILE:HD12	2.00	0.43
50:AJ:22:LEU:HB3	50:AJ:128:LEU:HD11	2.00	0.43
66:Aa:79:TRP:HE1	66:Aa:117:LEU:HD12	1.83	0.43
1:A2:1876:G:O2'	1:A2:1888:A:N3	2.46	0.43
1:A2:3586:G:OP2	62:AW:48:GLN:NE2	2.52	0.43
5:B1:31:U:O2'	5:B1:643:A:N1	2.46	0.43
5:B1:951:C:H2'	5:B1:952:G:H8	1.83	0.43
5:B1:1244:U:H5''	19:Bf:79:LYS:HE3	1.98	0.43
5:B1:1560:U:H2'	5:B1:1561:A:H8	1.82	0.43
6:BD:33:GLY:HA3	6:BD:53:THR:HB	2.01	0.43
6:BD:37:VAL:HG12	6:BD:50:ILE:HG12	2.01	0.43
6:BD:138:VAL:HG22	6:BD:184:ILE:HG22	2.01	0.43
20:Bg:5:MET:HG2	20:Bg:312:VAL:HG22	2.00	0.43
30:BN:84:LEU:HD12	30:BN:85:PRO:HD2	2.01	0.43
39:A3:65:A:O2'	73:Ah:10:ARG:NH2	2.47	0.43
52:AM:14:TYR:O	52:AM:56:GLN:N	2.49	0.43
53:AN:84:PRO:HA	53:AN:87:HIS:CD2	2.52	0.43
61:AV:21:PRO:HA	61:AV:54:ALA:HA	2.01	0.43
65:AZ:95:VAL:HG11	65:AZ:113:GLU:HG3	1.99	0.43
75:Aj:19:CYS:HB3	75:Aj:27:TYR:HB2	1.99	0.43
84:Aq:63:THR:HB	84:Aq:70:GLN:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:704:C:H2'	1:A2:705:G:C8	2.53	0.43
1:A2:1291:C:O2'	71:Af:94:ALA:O	2.35	0.43
1:A2:1611:G:O6	41:AA:9:ARG:NH2	2.52	0.43
1:A2:2500:G:H5''	72:Ag:25:THR:HG22	2.00	0.43
1:A2:3730:A:H5'	1:A2:3736:G:H22	1.83	0.43
1:A2:4221:C:O2'	50:Aj:21:CYS:SG	2.62	0.43
1:A2:4435:A:O2'	78:Am:122:ARG:NH2	2.52	0.43
2:Bv:38:C:O2'	5:B1:1058:A:OP1	2.37	0.43
5:B1:941:C:H2'	5:B1:942:G:C8	2.53	0.43
5:B1:1332:A:O2'	6:BD:145:GLN:O	2.31	0.43
8:BK:24:LYS:HA	8:BK:66:HIS:HA	2.01	0.43
37:Bb:42:LYS:HE3	37:Bb:57:VAL:HG22	1.99	0.43
40:A4:15:C:H2'	40:A4:16:A:H8	1.84	0.43
45:AE:152:ILE:O	45:AE:159:GLY:N	2.52	0.43
75:Aj:27:TYR:HA	75:Aj:34:CYS:HA	2.01	0.43
86:Ct:33:SER:O	86:Ct:37:ASP:HB2	2.18	0.43
1:A2:393:G:H2'	1:A2:394:A:H8	1.83	0.43
1:A2:1304:G:H21	1:A2:3847:A:H5'	1.82	0.43
1:A2:1521:G:O6	1:A2:1602:U:O2	2.36	0.43
1:A2:4071:C:N3	1:A2:4078:G:N2	2.63	0.43
1:A2:4168:C:HO2'	1:A2:4297:C:HO2'	1.62	0.43
1:A2:4868:A:H5''	42:AB:95:THR:HG22	2.00	0.43
5:B1:523:A:P	28:BJ:131:ARG:HH12	2.42	0.43
5:B1:1456:G:OP1	12:BR:59:LYS:NZ	2.42	0.43
5:B1:1799:G:OP1	27:BI:24:LYS:NZ	2.51	0.43
15:BU:32:LEU:HD22	15:BU:85:HIS:HB3	2.00	0.43
33:BW:2:VAL:HG12	33:BW:3:ARG:HG2	2.01	0.43
40:A4:11:A:N6	44:AD:13:PHE:O	2.50	0.43
46:AF:134:ARG:HA	46:AF:137:GLU:HG3	2.01	0.43
51:AL:80:GLU:OE2	51:AL:104:ASN:ND2	2.51	0.43
52:AM:101:LYS:HA	52:AM:104:MET:HG3	2.01	0.43
53:AN:59:TYR:HB3	53:AN:133:ILE:HD11	2.00	0.43
64:AY:34:LEU:HD23	64:AY:106:ILE:HB	2.01	0.43
83:Au:124:LEU:HB3	83:Au:128:LEU:HD12	2.01	0.43
85:AK:116:ILE:HB	85:AK:164:GLY:HA2	2.01	0.43
86:Ct:246:PRO:HA	86:Ct:249:ARG:HB3	2.00	0.43
86:Ct:759:ILE:HG22	86:Ct:800:LEU:HD22	2.01	0.43
5:B1:1453:C:OP2	12:BR:45:LYS:NZ	2.44	0.43
40:A4:64:G:H2'	40:A4:65:G:H8	1.84	0.43
42:AB:286:LYS:H	42:AB:332:MET:HB3	1.84	0.43
44:AD:103:LEU:HD11	44:AD:248:ARG:HH11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:Ae:78:LEU:HD21	70:Ae:100:ALA:HB2	2.00	0.43
86:Ct:451:ILE:HG23	86:Ct:458:VAL:HG13	2.01	0.43
1:A2:301:A:OP1	74:Ai:45:ARG:NH2	2.52	0.43
1:A2:1199:C:H4'	1:A2:1233:C:H4'	2.01	0.43
1:A2:1658:C:O2	1:A2:4153:G:O2'	2.32	0.43
1:A2:1718:A:N3	40:A4:78:C:O2'	2.51	0.43
1:A2:2592:C:OP1	72:Ag:24:ARG:NH2	2.47	0.43
1:A2:4689:A:HO2'	1:A2:4924:A:HO2'	1.63	0.43
5:B1:388:U:H2'	5:B1:389:A:C8	2.53	0.43
5:B1:1474:A:H5''	11:BQ:121:VAL:HG13	2.01	0.43
10:BP:30:TYR:HA	10:BP:33:LEU:HG	2.00	0.43
24:BE:155:LYS:N	24:BE:158:ASP:OD2	2.51	0.43
42:AB:220:ILE:HG23	42:AB:278:THR:HG22	2.01	0.43
44:AD:84:PRO:HD3	44:AD:92:LEU:HD21	2.01	0.43
45:AE:206:VAL:HG22	45:AE:260:LYS:HE3	2.00	0.43
47:AG:40:GLY:H	47:AG:43:GLN:HE21	1.67	0.43
52:AM:24:LEU:HB2	52:AM:43:THR:HG21	2.00	0.43
65:AZ:59:LYS:HG2	65:AZ:60:LYS:H	1.84	0.43
1:A2:35:U:H4'	1:A2:1507:A:H2	1.83	0.43
1:A2:312:A:H2'	1:A2:313:A:H8	1.83	0.43
1:A2:2575:G:H2'	1:A2:2576:G:H8	1.83	0.43
1:A2:4095:C:OP1	47:AG:37:LYS:NZ	2.52	0.43
1:A2:4936:G:HO2'	1:A2:4939:G:H1	1.61	0.43
5:B1:1143:A:OP2	23:BC:187:ARG:NH2	2.47	0.43
5:B1:1742:C:OP2	27:BI:42:ARG:NH1	2.45	0.43
33:BW:24:GLN:NE2	37:Bb:7:LEU:H	2.17	0.43
43:AC:198:ASN:HD21	64:AY:11:ARG:N	2.16	0.43
43:AC:207:PRO:HB3	43:AC:249:PHE:HD2	1.84	0.43
45:AE:140:LEU:HA	45:AE:191:GLN:HE22	1.84	0.43
45:AE:197:THR:HG22	45:AE:199:THR:H	1.84	0.43
46:AF:105:VAL:HG12	46:AF:135:ILE:HG22	2.01	0.43
63:AX:90:ILE:HG22	63:AX:147:LEU:HD22	1.99	0.43
75:Aj:36:LYS:HE2	75:Aj:57:ASN:HD21	1.84	0.43
86:Ct:20:ARG:HH22	86:Ct:98:PHE:HB3	1.84	0.43
1:A2:194:A:O2'	1:A2:217:C:O2	2.32	0.43
1:A2:693:U:H3'	1:A2:694:G:H21	1.83	0.43
1:A2:2062:C:H2'	1:A2:2063:G:H8	1.84	0.43
1:A2:3898:U:H2'	1:A2:3899:A:H8	1.84	0.43
5:B1:1864:U:H3'	36:Ba:5:ARG:HH21	1.84	0.43
7:BF:49:LEU:HD12	11:BQ:50:LYS:HB2	2.01	0.43
12:BR:99:ASP:HB2	12:BR:102:THR:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Bg:107:ASP:O	20:Bg:124:SER:OG	2.28	0.43
25:BG:67:VAL:HG21	25:BG:73:VAL:HG21	2.01	0.43
42:AB:219:VAL:HG11	42:AB:337:VAL:HG13	2.00	0.43
51:AL:128:PRO:HD2	51:AL:136:LYS:HD3	2.01	0.43
65:AZ:36:ARG:HD3	65:AZ:38:TYR:CZ	2.54	0.43
1:A2:104:G:HO2'	1:A2:1344:G:HO2'	1.59	0.42
1:A2:1249:G:N2	1:A2:1251:G:O6	2.43	0.42
1:A2:2577:A:N3	72:Ag:61:PRO:HG2	2.34	0.42
1:A2:2795:G:O2'	1:A2:3593:C:O2'	2.34	0.42
1:A2:3569:C:H2'	1:A2:3570:A:C8	2.54	0.42
1:A2:4056:G:H5'	47:AG:54:PHE:HB3	2.00	0.42
1:A2:4650:C:O2'	48:AH:155:SER:OG	2.26	0.42
2:Bv:21:A:O2'	2:Bv:46:G:O6	2.31	0.42
5:B1:223:C:H2'	5:B1:224:A:C8	2.54	0.42
5:B1:337:C:H2'	5:B1:338:G:C4	2.54	0.42
5:B1:360:A:H4'	5:B1:361:U:H3'	2.01	0.42
5:B1:1467:C:OP1	12:BR:2:GLY:N	2.52	0.42
11:BQ:33:LYS:O	11:BQ:70:VAL:N	2.45	0.42
21:BA:7:VAL:O	21:BA:191:ARG:NH2	2.50	0.42
28:BJ:82:VAL:HG21	28:BJ:92:MET:HE1	2.00	0.42
37:Bb:33:MET:HE1	37:Bb:73:LEU:HD11	2.00	0.42
51:AL:124:LEU:HA	73:Ah:121:VAL:HG12	2.01	0.42
58:AS:8:ARG:HD3	58:AS:66:GLN:HE22	1.84	0.42
1:A2:1358:C:OP1	43:AC:121:ARG:NE	2.49	0.42
1:A2:2868:G:OP1	57:AR:75:HIS:ND1	2.52	0.42
5:B1:24:C:OP1	28:BJ:11:LYS:NZ	2.37	0.42
5:B1:228:C:H42	5:B1:901:G:H1'	1.83	0.42
5:B1:434:G:OP1	27:BI:23:LYS:NZ	2.48	0.42
5:B1:453:C:O2'	25:BG:92:ARG:O	2.36	0.42
5:B1:1291:A:OP2	18:Bd:5:GLN:NE2	2.50	0.42
5:B1:1553:C:H41	5:B1:1556:A:H5'	1.83	0.42
5:B1:1597:C:H4'	5:B1:1603:G:C6	2.54	0.42
24:BE:128:LYS:HA	24:BE:156:VAL:HG13	2.00	0.42
35:BY:76:TYR:OH	35:BY:86:GLU:OE2	2.27	0.42
37:Bb:49:HIS:ND1	37:Bb:69:GLY:O	2.42	0.42
44:AD:166:ALA:HB1	44:AD:171:LEU:HD12	2.00	0.42
51:AL:144:LEU:HG	73:Ah:122:LYS:HB3	2.02	0.42
70:Ae:108:ARG:HH21	70:Ae:127:ALA:HB3	1.84	0.42
84:Aq:16:ARG:HH12	84:Aq:28:LEU:HD22	1.84	0.42
1:A2:710:C:H2'	1:A2:711:G:H8	1.83	0.42
1:A2:1333:C:H2'	1:A2:1334:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:1615:G:H21	41:AA:3:ARG:HH21	1.68	0.42
1:A2:1674:C:H41	56:AQ:13:VAL:HG11	1.84	0.42
1:A2:2626:A:H62	1:A2:2665:G:H8	1.66	0.42
1:A2:2678:C:H2'	1:A2:2679:G:H8	1.84	0.42
2:Bv:29:C:H2'	2:Bv:30:G:H8	1.84	0.42
5:B1:524:U:OP1	5:B1:525:A:O2'	2.35	0.42
5:B1:1083:A:N7	5:B1:1841:C:O2'	2.48	0.42
5:B1:1528:G:O2'	5:B1:1666:C:OP1	2.30	0.42
6:BD:64:ARG:HG2	8:BK:93:THR:HG22	2.01	0.42
10:BP:82:ASP:HA	10:BP:115:TYR:HB3	2.01	0.42
24:BE:31:PRO:HD2	24:BE:38:LEU:HD22	2.00	0.42
39:A3:102:G:OP2	39:A3:104:A:O2'	2.31	0.42
45:AE:213:THR:H	45:AE:216:TYR:HB3	1.85	0.42
50:AJ:96:LYS:HB2	50:AJ:176:PRO:HA	2.01	0.42
52:AM:52:PHE:HA	52:AM:55:MET:HG2	2.01	0.42
61:AV:57:VAL:HG11	61:AV:122:ALA:HB3	2.01	0.42
66:Aa:24:LYS:HB3	66:Aa:26:ARG:HE	1.83	0.42
85:AK:27:CYS:SG	85:AK:28:PHE:N	2.93	0.42
86:Ct:426:LYS:HD3	86:Ct:444:LEU:HD22	2.01	0.42
86:Ct:727:ARG:HE	86:Ct:853:PHE:HA	1.84	0.42
1:A2:713:G:H2'	1:A2:714:A:C8	2.55	0.42
1:A2:3694:A:H2'	1:A2:3695:A:H8	1.83	0.42
1:A2:3816:A:H4'	1:A2:4630:U:H4'	2.01	0.42
1:A2:4199:C:O2	1:A2:4283:U:O2'	2.37	0.42
1:A2:4819:G:H2'	1:A2:4820:G:C8	2.54	0.42
5:B1:454:U:H5''	25:BG:94:ARG:HB2	2.01	0.42
5:B1:1222:G:H5''	7:BF:78:MET:HE3	2.01	0.42
5:B1:1680:G:OP1	7:BF:60:ARG:NH1	2.53	0.42
5:B1:1792:G:H2'	5:B1:1793:A:H8	1.83	0.42
11:BQ:116:ASP:HB3	11:BQ:119:LEU:HG	2.01	0.42
21:BA:111:GLN:NE2	23:BC:64:THR:OG1	2.49	0.42
23:BC:196:ILE:HB	23:BC:223:TYR:HB2	2.00	0.42
31:BO:96:LYS:NZ	31:BO:130:GLU:OE1	2.52	0.42
53:AN:37:HIS:HE1	53:AN:63:ARG:HH11	1.68	0.42
86:Ct:727:ARG:HH11	86:Ct:853:PHE:HA	1.85	0.42
1:A2:469:G:H22	1:A2:672:G:H1	1.66	0.42
1:A2:3677:C:H5''	41:AA:226:ARG:HB3	2.01	0.42
1:A2:3923:A:H2'	1:A2:3924:G:C8	2.55	0.42
5:B1:1854:U:H2'	5:B1:1855:G:H8	1.83	0.42
7:BF:115:ALA:O	7:BF:119:SER:HB2	2.20	0.42
22:BB:121:ILE:HG12	22:BB:161:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BG:142:ARG:HG2	25:BG:147:LEU:HD21	2.02	0.42
27:BI:76:THR:HG21	27:BI:104:ILE:HG12	2.00	0.42
56:AQ:176:ARG:HB2	66:Aa:56:VAL:HG11	2.01	0.42
1:A2:293:C:O2'	53:AN:95:ALA:O	2.37	0.42
1:A2:2516:A:OP2	76:Ak:37:ARG:NH1	2.42	0.42
5:B1:951:C:H2'	5:B1:952:G:C8	2.55	0.42
5:B1:1092:G:H2'	5:B1:1093:A:H8	1.84	0.42
18:Bd:12:ARG:HH11	18:Bd:17:GLY:HA3	1.85	0.42
22:BB:29:ASP:OD2	22:BB:94:LYS:NZ	2.53	0.42
28:BJ:133:ARG:HB3	28:BJ:162:ARG:HE	1.83	0.42
30:BN:81:ALA:HA	30:BN:82:PRO:HD3	1.91	0.42
42:AB:57:VAL:HG22	42:AB:73:VAL:HG22	2.01	0.42
43:AC:79:VAL:HG11	43:AC:86:ARG:HH12	1.85	0.42
47:AG:180:PRO:HG3	47:AG:219:VAL:HG13	2.01	0.42
54:AO:175:MET:HA	54:AO:178:ARG:HG2	2.00	0.42
61:AV:104:VAL:HB	61:AV:112:MET:HE1	2.01	0.42
63:AX:64:SER:HB3	73:Ah:69:LEU:HD13	2.01	0.42
66:Aa:7:LYS:HE2	66:Aa:11:LEU:HD11	2.01	0.42
66:Aa:83:SER:HB2	66:Aa:86:THR:HG23	2.02	0.42
66:Aa:123:ILE:HG12	66:Aa:143:ALA:HB3	2.00	0.42
84:Aq:105:THR:HG22	84:Aq:143:VAL:HG13	2.01	0.42
86:Ct:10:ARG:HH11	86:Ct:460:PRO:HB2	1.84	0.42
86:Ct:506:ARG:HG3	86:Ct:575:PRO:HG2	2.00	0.42
1:A2:86:U:H2'	1:A2:87:A:C8	2.55	0.42
1:A2:1731:A:H2'	1:A2:1732:G:C8	2.54	0.42
1:A2:1854:A:OP2	67:Ab:5:LYS:NZ	2.45	0.42
1:A2:1910:A:H2	54:AO:49:ARG:HH12	1.68	0.42
1:A2:2262:G:OP1	66:Aa:16:SER:OG	2.36	0.42
1:A2:2297:G:O2'	1:A2:2299:G:O6	2.34	0.42
1:A2:2380:A:N1	1:A2:2783:C:N4	2.68	0.42
1:A2:2567:C:OP1	1:A2:2747:C:O2'	2.32	0.42
1:A2:4950:G:H2'	1:A2:4951:G:C8	2.54	0.42
5:B1:21:U:O2'	28:BJ:17:ARG:O	2.36	0.42
5:B1:1278:A:OP1	8:BK:55:ARG:NH2	2.52	0.42
12:BR:37:GLU:HG3	20:Bg:150:TRP:HE1	1.84	0.42
14:BT:33:TRP:CD1	14:BT:34:VAL:HG13	2.54	0.42
20:Bg:45:LEU:HD11	20:Bg:299:PHE:HZ	1.85	0.42
22:BB:181:LEU:HA	22:BB:184:VAL:HG22	2.02	0.42
25:BG:137:ARG:HG3	25:BG:178:ARG:HG3	2.00	0.42
32:BV:41:LYS:H	32:BV:41:LYS:HD2	1.85	0.42
39:A3:94:G:OP2	75:Aj:72:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:AA:20:VAL:HA	41:AA:23:ARG:HH11	1.85	0.42
65:AZ:83:THR:HG23	65:AZ:85:TYR:H	1.84	0.42
85:AK:120:GLU:HG2	85:AK:162:LYS:HA	2.01	0.42
86:Ct:300:VAL:HG11	86:Ct:340:MET:HE3	2.02	0.42
1:A2:262:G:H2'	1:A2:263:G:H8	1.84	0.42
1:A2:1333:C:H2'	1:A2:1334:G:H8	1.85	0.42
1:A2:1621:U:N3	1:A2:1625:A:O2'	2.53	0.42
1:A2:3667:C:N4	1:A2:3668:U:O4	2.53	0.42
1:A2:3868:G:H4'	42:AB:254:ILE:HD13	2.02	0.42
1:A2:4062:G:H3'	1:A2:4063:G:H21	1.85	0.42
5:B1:1208:A:O2'	5:B1:1835:A:N1	2.48	0.42
5:B1:1851:A:OP2	79:An:9:ARG:NH2	2.52	0.42
40:A4:62:U:O2'	40:A4:64:G:O4'	2.37	0.42
43:AC:44:LEU:HD23	43:AC:47:ASN:HD22	1.84	0.42
81:Ap:30:GLU:HA	81:Ap:33:GLN:HG2	2.01	0.42
83:Au:91:LYS:HG2	83:Au:122:ARG:HH22	1.85	0.42
1:A2:500:C:N4	1:A2:501:G:O6	2.53	0.42
1:A2:1747:A:N6	13:BS:112:GLU:OE2	2.53	0.42
1:A2:2331:U:H5'	43:AC:76:ILE:HD12	2.02	0.42
1:A2:4042:C:H2'	1:A2:4043:A:H8	1.84	0.42
1:A2:4091:G:O2'	65:AZ:136:PHE:O	2.36	0.42
1:A2:4659:U:H5'	78:Am:104:HIS:CE1	2.55	0.42
5:B1:331:C:H3'	5:B1:332:G:H5''	2.02	0.42
5:B1:1829:G:H1'	5:B1:1850:A:H2	1.83	0.42
10:BP:105:VAL:HG21	10:BP:119:PHE:HB3	2.01	0.42
20:Bg:91:ASP:OD2	20:Bg:93:THR:OG1	2.36	0.42
26:BH:177:TYR:HE2	26:BH:183:LYS:HB2	1.84	0.42
34:BX:70:VAL:HG21	34:BX:94:ILE:HG21	2.02	0.42
41:AA:115:CYS:HB3	41:AA:165:VAL:HG12	2.01	0.42
1:A2:178:C:H2'	1:A2:179:G:C8	2.55	0.42
1:A2:236:C:OP1	64:AY:46:SER:OG	2.37	0.42
1:A2:367:G:HO2'	1:A2:1627:C:HO2'	1.67	0.42
1:A2:439:U:O2	1:A2:2292:A:O2'	2.37	0.42
1:A2:1559:G:OP2	41:AA:181:LYS:NZ	2.52	0.42
1:A2:2246:U:H4'	82:At:7:TRP:HZ2	1.85	0.42
1:A2:2814:A:O2'	42:AB:228:TYR:O	2.34	0.42
5:B1:454:U:H2'	5:B1:455:A:C8	2.54	0.42
5:B1:1103:C:H2'	5:B1:1104:G:H8	1.85	0.42
5:B1:1738:C:OP1	25:BG:92:ARG:NH1	2.46	0.42
22:BB:81:PHE:CD2	22:BB:82:ARG:HG3	2.54	0.42
36:Ba:20:PRO:HB2	36:Ba:29:CYS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:Ae:104:SER:O	70:Ae:108:ARG:HB2	2.20	0.42
84:Aq:77:ALA:HB3	84:Aq:80:LEU:HD12	2.02	0.42
86:Ct:265:TYR:HB3	86:Ct:285:LEU:HD12	2.01	0.42
1:A2:438:G:H21	1:A2:2292:A:H8	1.67	0.41
1:A2:490:G:H2'	1:A2:491:G:C8	2.54	0.41
1:A2:1741:G:H1	1:A2:1755:U:H3	1.68	0.41
1:A2:1810:C:H2'	1:A2:1811:G:H8	1.85	0.41
1:A2:1912:C:N4	1:A2:2021:A:O3'	2.53	0.41
1:A2:2499:C:H2'	1:A2:2500:G:C8	2.54	0.41
1:A2:3932:G:O2'	1:A2:4013:G:N2	2.44	0.41
1:A2:4999:G:N2	62:AW:11:TYR:OH	2.53	0.41
5:B1:520:A:O2'	5:B1:825:A:N3	2.49	0.41
7:BF:108:PRO:HA	7:BF:111:VAL:HG22	2.02	0.41
9:BM:52:LEU:HD23	9:BM:76:LEU:HD21	2.01	0.41
11:BQ:16:LYS:HG3	11:BQ:17:LYS:H	1.85	0.41
11:BQ:32:ILE:HD12	11:BQ:39:LEU:HD22	2.01	0.41
22:BB:35:ALA:HB3	22:BB:42:ARG:HA	2.02	0.41
34:BX:74:LEU:HD21	34:BX:81:ILE:HD12	2.01	0.41
35:BY:29:HIS:O	35:BY:66:GLY:CA	2.68	0.41
43:AC:330:PRO:HB2	46:AF:51:TYR:HE1	1.85	0.41
49:AI:51:HIS:CD2	49:AI:168:SER:HB2	2.55	0.41
70:Ae:112:VAL:HG23	70:Ae:122:VAL:HG11	2.02	0.41
74:Ai:65:LYS:HG3	74:Ai:67:LYS:H	1.84	0.41
75:Aj:28:HIS:N	75:Aj:33:THR:O	2.51	0.41
78:Am:104:HIS:CD2	78:Am:106:ARG:H	2.37	0.41
84:Aq:30:PRO:O	84:Aq:33:GLY:N	2.47	0.41
84:Aq:76:SER:OG	84:Aq:117:ARG:NH2	2.50	0.41
86:Ct:488:PHE:HB3	86:Ct:490:HIS:CE1	2.55	0.41
1:A2:74:G:O3'	51:AL:71:ARG:NH2	2.52	0.41
1:A2:1490:A:OP1	43:AC:110:ARG:NH1	2.48	0.41
1:A2:1627:C:H2'	1:A2:1628:A:C8	2.54	0.41
1:A2:2841:G:N2	1:A2:3595:A:O2'	2.48	0.41
5:B1:433:A:H2'	5:B1:434:G:C8	2.54	0.41
5:B1:1659:U:H4'	18:Bd:30:LEU:HB2	2.02	0.41
7:BF:95:HIS:HE1	16:BZ:103:HIS:CD2	2.37	0.41
10:BP:39:ALA:HA	10:BP:42:ARG:HE	1.85	0.41
42:AB:303:ALA:HB1	42:AB:368:ILE:HB	2.01	0.41
44:AD:146:LEU:HD21	44:AD:163:LEU:HD23	2.02	0.41
44:AD:187:SER:OG	44:AD:189:GLU:OE1	2.37	0.41
60:AU:81:ARG:HA	60:AU:81:ARG:HD3	1.94	0.41
86:Ct:428:ARG:HD3	86:Ct:487:THR:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:1316:A:H2'	1:A2:1317:A:C8	2.55	0.41
1:A2:2578:G:N2	1:A2:2726:U:O4	2.54	0.41
1:A2:2586:C:H2'	1:A2:2587:G:C8	2.55	0.41
1:A2:2849:A:OP2	1:A2:2858:A:N6	2.53	0.41
1:A2:3849:C:O2	1:A2:4362:G:O2'	2.38	0.41
1:A2:4854:G:N2	1:A2:4883:U:O2	2.53	0.41
5:B1:511:U:H2'	5:B1:512:A:H8	1.85	0.41
5:B1:693:A:H3'	5:B1:694:G:H8	1.84	0.41
5:B1:943:U:O2'	31:BO:135:ILE:O	2.31	0.41
5:B1:1166:G:N7	34:BX:25:LYS:NZ	2.58	0.41
5:B1:1468:C:H2'	5:B1:1469:A:C8	2.55	0.41
13:BS:17:ASN:ND2	50:AJ:114:ASP:OD2	2.54	0.41
43:AC:25:PRO:HB3	43:AC:261:ASP:HB2	2.02	0.41
53:AN:54:LYS:H	53:AN:59:TYR:HD2	1.66	0.41
83:Au:41:TYR:OH	83:Au:200:ASN:ND2	2.40	0.41
1:A2:944:G:N7	1:A2:1267:G:O2'	2.48	0.41
1:A2:1493:U:OP2	66:Aa:6:ARG:NH1	2.54	0.41
1:A2:1595:A:H5''	41:AA:183:GLY:HA2	2.01	0.41
1:A2:1673:G:OP1	56:AQ:15:ARG:NE	2.44	0.41
1:A2:4024:C:H5'	83:Au:205:TYR:HE2	1.85	0.41
5:B1:1310:U:H5'	19:Bf:130:VAL:HG13	2.01	0.41
15:BU:75:LYS:HB3	15:BU:77:TRP:HE1	1.85	0.41
23:BC:183:LYS:HA	23:BC:195:LEU:O	2.20	0.41
43:AC:292:ILE:HG21	56:AQ:31:LEU:HD11	2.03	0.41
45:AE:192:LYS:HE3	71:Af:107:PRO:HB3	2.01	0.41
51:AL:23:ALA:O	53:AN:199:GLN:NE2	2.53	0.41
52:AM:32:ASP:OD1	52:AM:32:ASP:N	2.53	0.41
58:AS:13:VAL:HG23	58:AS:62:VAL:HB	2.01	0.41
62:AW:65:GLU:HA	62:AW:68:GLN:HG3	2.03	0.41
1:A2:923:C:HO2'	52:AM:20:HIS:CE1	2.37	0.41
1:A2:1540:A:H2'	1:A2:1541:G:H8	1.84	0.41
1:A2:2402:A:H2'	1:A2:2403:G:C4	2.55	0.41
1:A2:3629:C:H2'	1:A2:3630:G:H8	1.84	0.41
1:A2:3632:G:H4'	1:A2:3633:A:H5'	2.03	0.41
1:A2:4058:C:H2'	1:A2:4059:G:H8	1.84	0.41
1:A2:4255:U:O2'	80:Ao:81:ARG:NH2	2.53	0.41
1:A2:4296:U:O2'	59:AT:7:LYS:O	2.34	0.41
5:B1:647:U:H2'	5:B1:648:A:H8	1.85	0.41
5:B1:907:G:H2'	5:B1:908:A:C8	2.55	0.41
5:B1:1156:U:OP1	33:BW:71:LYS:NZ	2.45	0.41
21:BA:85:ARG:HH12	21:BA:205:ARG:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:BA:126:ASP:O	21:BA:130:ASP:HB2	2.20	0.41
39:A3:96:C:OP1	73:Ah:70:ARG:NH2	2.54	0.41
45:AE:277:LEU:HD11	71:Af:105:LEU:HD11	2.02	0.41
48:AH:43:VAL:HG22	48:AH:59:LYS:HD2	2.03	0.41
60:AU:48:LYS:HG2	60:AU:53:ALA:HB2	2.03	0.41
1:A2:416:C:H2'	1:A2:417:G:H8	1.85	0.41
1:A2:656:C:H2'	1:A2:657:C:C6	2.56	0.41
1:A2:735:G:H2'	1:A2:736:G:C8	2.55	0.41
1:A2:1293:C:O2'	71:Af:19:ARG:O	2.32	0.41
1:A2:1385:C:H2'	1:A2:1386:G:H8	1.86	0.41
1:A2:2724:A:H2'	1:A2:2725:A:H8	1.86	0.41
1:A2:2728:C:H2'	1:A2:2729:G:C8	2.55	0.41
1:A2:4666:C:H2'	1:A2:4667:A:C8	2.55	0.41
1:A2:4986:G:H2'	1:A2:4987:C:C6	2.55	0.41
5:B1:5:U:H2'	5:B1:6:G:H8	1.85	0.41
5:B1:115:U:H2'	5:B1:116:U:C6	2.55	0.41
5:B1:309:G:OP2	27:BI:55:TYR:OH	2.34	0.41
5:B1:346:C:H5''	24:BE:38:LEU:HG	2.02	0.41
5:B1:1244:U:H2'	5:B1:1245:G:C8	2.56	0.41
22:BB:175:GLU:O	22:BB:179:ASN:ND2	2.51	0.41
23:BC:194:ARG:HB3	23:BC:225:SER:HB2	2.02	0.41
27:BI:139:LYS:HB3	27:BI:144:LYS:HB2	2.02	0.41
28:BJ:115:PHE:HB2	28:BJ:123:ILE:HD11	2.02	0.41
33:BW:90:GLN:HE21	33:BW:113:HIS:CE1	2.38	0.41
34:BX:90:CYS:HA	34:BX:93:PHE:HB2	2.01	0.41
39:A3:99:U:H5''	63:AX:67:ARG:HH22	1.85	0.41
40:A4:15:C:H2'	40:A4:16:A:C8	2.56	0.41
44:AD:111:ASN:HD21	44:AD:252:VAL:HG12	1.86	0.41
64:AY:32:SER:OG	64:AY:104:VAL:O	2.38	0.41
86:Ct:129:VAL:HG12	86:Ct:155:LEU:HD11	2.02	0.41
1:A2:699:G:OP1	71:Af:89:ARG:NH2	2.54	0.41
1:A2:1508:G:N1	1:A2:1631:U:O4	2.54	0.41
1:A2:4098:G:O6	1:A2:4118:G:N2	2.54	0.41
2:Bv:20:U:H5	2:Bv:48:C:H42	1.68	0.41
5:B1:107:A:H2'	5:B1:108:G:C8	2.56	0.41
5:B1:988:C:H5'	22:BB:116:LYS:HA	2.02	0.41
5:B1:1139:C:H42	5:B1:1149:A:N6	2.19	0.41
5:B1:1593:C:OP2	16:BZ:104:ARG:NH2	2.53	0.41
6:BD:60:GLY:HA2	6:BD:65:ARG:HH11	1.86	0.41
13:BS:5:ILE:HG23	13:BS:8:LYS:HE3	2.03	0.41
28:BJ:110:LEU:HB2	28:BJ:147:PHE:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:A3:9:A:H2'	39:A3:10:G:H8	1.85	0.41
43:AC:289:LEU:HB3	82:At:4:HIS:CD2	2.56	0.41
45:AE:213:THR:HG23	45:AE:215:ALA:H	1.85	0.41
46:AF:116:GLN:HE22	46:AF:212:LYS:HG2	1.86	0.41
49:AI:93:PRO:HA	49:AI:127:ALA:HB2	2.03	0.41
51:AL:128:PRO:HB3	73:Ah:117:ARG:HH22	1.86	0.41
54:AO:195:VAL:HA	54:AO:199:HIS:HB2	2.03	0.41
83:Au:67:VAL:HA	83:Au:111:LEU:O	2.21	0.41
1:A2:189:G:O2'	39:A3:68:G:O2'	2.38	0.41
1:A2:491:G:H3'	1:A2:492:C:H5''	2.03	0.41
1:A2:700:C:H2'	1:A2:701:G:H8	1.86	0.41
1:A2:1592:C:H5'	1:A2:1593:C:H5'	2.01	0.41
1:A2:1942:G:N2	1:A2:2006:A:C8	2.89	0.41
1:A2:3864:C:H2'	1:A2:3865:A:H8	1.85	0.41
30:BN:46:THR:HG22	30:BN:48:SER:H	1.86	0.41
42:AB:67:VAL:HG13	42:AB:72:VAL:HG21	2.01	0.41
42:AB:292:LEU:HD22	42:AB:293:ILE:H	1.85	0.41
48:AH:102:ASN:HB3	48:AH:115:ARG:HB2	2.03	0.41
55:AP:122:ALA:HB3	55:AP:143:PRO:HG2	2.02	0.41
70:Ae:16:ARG:HD3	70:Ae:60:TYR:HE1	1.86	0.41
1:A2:224:A:N6	1:A2:238:G:H21	2.18	0.41
1:A2:317:C:H2'	1:A2:318:A:C8	2.53	0.41
1:A2:504:U:H5'	66:Aa:86:THR:HB	2.03	0.41
1:A2:901:U:O2'	1:A2:902:A:O4'	2.37	0.41
1:A2:962:C:H42	1:A2:1262:A:H61	1.68	0.41
1:A2:1195:G:C6	1:A2:1197:C:N3	2.88	0.41
1:A2:1301:C:OP1	66:Aa:24:LYS:NZ	2.50	0.41
1:A2:1677:U:O2'	1:A2:1701:A:N1	2.52	0.41
1:A2:1806:G:H21	67:Ab:42:ASN:HD21	1.69	0.41
1:A2:2385:G:O6	77:Al:2:SER:N	2.54	0.41
1:A2:2499:C:H5	1:A2:2514:G:H1	1.69	0.41
1:A2:2532:A:OP2	1:A2:2553:G:O2'	2.34	0.41
1:A2:3635:G:H2'	1:A2:3636:G:H8	1.85	0.41
1:A2:4385:U:H2'	78:Am:97:ARG:HD3	2.02	0.41
5:B1:38:A:O2'	5:B1:517:C:N4	2.53	0.41
5:B1:291:G:H21	29:BL:42:LEU:HB2	1.86	0.41
5:B1:551:U:H2'	5:B1:552:G:C8	2.56	0.41
5:B1:844:U:H2'	5:B1:845:G:H8	1.86	0.41
5:B1:876:C:H5'	26:BH:113:LYS:NZ	2.36	0.41
5:B1:925:G:H2'	5:B1:926:A:H8	1.86	0.41
5:B1:929:G:H21	5:B1:1104:G:H4'	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BD:212:GLU:O	12:BR:20:TYR:OH	2.35	0.41
7:BF:162:ALA:HA	7:BF:165:ASN:HD21	1.84	0.41
8:BK:80:ARG:HA	8:BK:83:LEU:HB2	2.02	0.41
17:Bc:28:THR:N	17:Bc:46:VAL:O	2.50	0.41
21:BA:172:GLY:HA3	21:BA:203:PHE:HD1	1.86	0.41
24:BE:87:MET:HE2	24:BE:123:LEU:H	1.86	0.41
27:BI:67:TRP:CD1	27:BI:70:GLU:H	2.39	0.41
28:BJ:33:GLY:HA3	38:Be:38:TYR:CG	2.56	0.41
29:BL:118:ARG:HD3	57:AR:151:ARG:HH12	1.86	0.41
41:AA:27:ALA:HB3	41:AA:128:ARG:HH21	1.85	0.41
42:AB:372:SER:HB2	42:AB:377:GLY:HA2	2.03	0.41
43:AC:24:LEU:HD12	43:AC:25:PRO:HD2	2.01	0.41
46:AF:103:PRO:HA	46:AF:106:ARG:HB3	2.02	0.41
47:AG:137:ARG:HG3	47:AG:146:LEU:HD11	2.03	0.41
49:AI:38:ARG:HH21	49:AI:83:ASP:HB3	1.86	0.41
50:AJ:37:ALA:HB2	50:AJ:70:VAL:HG11	2.02	0.41
50:AJ:99:PHE:O	50:AJ:159:LYS:NZ	2.41	0.41
50:AJ:108:GLY:HA2	50:AJ:130:PHE:H	1.85	0.41
52:AM:25:VAL:HG12	52:AM:45:VAL:HG11	2.03	0.41
53:AN:47:LYS:HA	53:AN:50:ARG:HG2	2.03	0.41
70:Ae:90:MET:HE2	82:At:33:LYS:HE2	2.03	0.41
1:A2:2384:G:H5''	75:Aj:14:LYS:HE3	2.03	0.41
1:A2:4201:A:H2'	1:A2:4202:G:H8	1.85	0.41
1:A2:4547:U:H2'	1:A2:4548:G:C8	2.56	0.41
5:B1:406:U:H2'	5:B1:408:A:H8	1.86	0.41
5:B1:928:G:H1	5:B1:1013:U:H3	1.69	0.41
5:B1:982:G:H21	5:B1:1045:U:H1'	1.86	0.41
5:B1:1017:U:H5'	30:BN:55:ARG:HD3	2.02	0.41
5:B1:1144:A:H2'	5:B1:1145:A:C8	2.55	0.41
6:BD:213:PRO:HG3	12:BR:19:LYS:HD2	2.02	0.41
7:BF:128:ILE:HD11	7:BF:137:GLN:HB3	2.03	0.41
28:BJ:115:PHE:HA	28:BJ:120:ALA:HB2	2.03	0.41
40:A4:63:C:H5'	40:A4:64:G:H5''	2.02	0.41
46:AF:160:GLY:O	46:AF:166:ARG:HA	2.21	0.41
48:AH:95:VAL:HG22	78:Am:82:LEU:HD22	2.02	0.41
50:AJ:35:ARG:HB3	50:AJ:123:ILE:HG23	2.04	0.41
56:AQ:61:LEU:N	56:AQ:85:THR:O	2.53	0.41
64:AY:56:GLN:HE21	64:AY:65:GLN:H	1.68	0.41
1:A2:104:G:O2'	1:A2:1344:G:O2'	2.33	0.40
1:A2:732:C:H2'	1:A2:733:G:C8	2.55	0.40
1:A2:2344:C:H5'	1:A2:2345:A:H5''	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:2500:G:H2'	1:A2:2501:G:C8	2.56	0.40
1:A2:2500:G:H2'	1:A2:2501:G:H8	1.86	0.40
1:A2:2515:A:H5''	76:Ak:42:LEU:HD22	2.04	0.40
1:A2:3668:U:H5''	1:A2:3669:G:H5'	2.04	0.40
5:B1:931:C:H2'	5:B1:932:G:C8	2.56	0.40
5:B1:1651:A:H2'	5:B1:1652:G:H8	1.86	0.40
5:B1:1679:A:OP1	7:BF:60:ARG:NH2	2.55	0.40
5:B1:1705:C:H2'	5:B1:1706:G:C8	2.56	0.40
21:BA:5:LEU:HB3	21:BA:6:ASP:H	1.58	0.40
25:BG:1:MET:N	25:BG:17:GLU:OE2	2.50	0.40
50:AJ:26:VAL:HG12	50:AJ:28:GLU:H	1.85	0.40
51:AL:24:THR:HA	53:AN:200:LEU:O	2.20	0.40
51:AL:126:LEU:HD13	73:Ah:117:ARG:HH21	1.86	0.40
71:Af:58:VAL:HG21	71:Af:64:PRO:HA	2.03	0.40
86:Ct:154:VAL:HG12	86:Ct:211:THR:HG23	2.02	0.40
1:A2:966:C:O2'	1:A2:968:C:OP2	2.27	0.40
1:A2:1161:G:N2	1:A2:1164:C:OP1	2.54	0.40
1:A2:1602:U:H2'	1:A2:1603:A:H8	1.86	0.40
1:A2:1669:U:H2'	1:A2:1670:G:C8	2.56	0.40
1:A2:1760:C:H5''	44:AD:7:VAL:HG22	2.03	0.40
1:A2:1882:C:H2'	1:A2:1883:G:H8	1.86	0.40
1:A2:2455:G:H2'	1:A2:2456:A:C8	2.56	0.40
1:A2:4429:A:O2'	1:A2:4472:A:N3	2.45	0.40
1:A2:4435:A:OP1	78:Am:102:ARG:NH2	2.54	0.40
1:A2:4642:G:H2'	1:A2:4643:A:C8	2.56	0.40
5:B1:428:U:H4'	28:BJ:2:PRO:HG2	2.02	0.40
5:B1:656:G:H1	5:B1:1156:U:H5	1.70	0.40
5:B1:1775:U:H2'	5:B1:1776:G:C8	2.57	0.40
10:BP:60:LEU:HD11	10:BP:89:MET:HA	2.03	0.40
10:BP:118:GLU:HG2	13:BS:120:HIS:CE1	2.56	0.40
11:BQ:47:LEU:HD13	11:BQ:81:ILE:HG21	2.03	0.40
24:BE:92:ILE:O	24:BE:94:LYS:N	2.53	0.40
49:AI:51:HIS:HD2	49:AI:168:SER:HB2	1.86	0.40
54:AO:37:ARG:HE	54:AO:108:ILE:HD11	1.85	0.40
56:AQ:43:PHE:HE1	56:AQ:138:LEU:HB2	1.86	0.40
64:AY:36:LYS:HA	64:AY:39:ARG:HG2	2.03	0.40
86:Ct:748:GLU:HA	86:Ct:784:VAL:O	2.21	0.40
1:A2:646:G:O2'	56:AQ:115:ARG:NH2	2.55	0.40
1:A2:705:G:H5''	43:AC:316:LYS:HA	2.04	0.40
1:A2:1311:G:O2'	1:A2:2328:A:OP1	2.38	0.40
1:A2:1886:U:O2	46:AF:215:SER:OG	2.31	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:3688:A:H2'	1:A2:3689:A:H8	1.86	0.40
5:B1:178:C:H2'	5:B1:179:C:H6	1.86	0.40
5:B1:371:A:O2'	5:B1:394:G:N2	2.55	0.40
5:B1:909:G:H2'	5:B1:910:G:C8	2.56	0.40
5:B1:1659:U:H5'	18:Bd:30:LEU:HD13	2.04	0.40
11:BQ:15:ARG:HD3	11:BQ:15:ARG:HA	1.86	0.40
24:BE:222:LEU:HD23	24:BE:225:ILE:HD12	2.04	0.40
26:BH:98:ARG:NH2	26:BH:125:VAL:O	2.53	0.40
47:AG:164:ILE:HD12	53:AN:22:LEU:HD11	2.03	0.40
84:Aq:92:ARG:HG2	84:Aq:93:LYS:H	1.86	0.40
85:AK:132:PRO:HA	85:AK:133:GLU:HA	1.64	0.40
85:AK:147:ILE:HG12	85:AK:152:ILE:HG12	2.02	0.40
1:A2:394:A:H5''	55:AP:16:LYS:HG3	2.04	0.40
1:A2:1806:G:H2'	1:A2:1807:A:C8	2.56	0.40
1:A2:1863:U:OP1	1:A2:2259:G:O2'	2.37	0.40
1:A2:1903:G:H2'	1:A2:1904:A:H8	1.85	0.40
1:A2:2443:C:H2'	1:A2:2444:C:H6	1.87	0.40
1:A2:3940:G:O2'	83:Au:166:ALA:O	2.26	0.40
1:A2:4244:A:N6	59:AT:47:THR:O	2.55	0.40
1:A2:4481:C:H5''	1:A2:4482:G:H5''	2.03	0.40
4:Bw:22:G:N7	4:Bw:46:G:O6	2.54	0.40
5:B1:909:G:H2'	5:B1:910:G:H8	1.86	0.40
5:B1:952:G:H2'	5:B1:953:C:C6	2.56	0.40
5:B1:1228:A:H2'	5:B1:1229:G:C8	2.55	0.40
5:B1:1567:G:H5'	14:BT:33:TRP:CD1	2.56	0.40
25:BG:64:LYS:HB2	25:BG:97:VAL:HG11	2.04	0.40
39:A3:107:C:H2'	39:A3:108:A:C4	2.56	0.40
40:A4:9:C:OP2	40:A4:10:C:N4	2.35	0.40
44:AD:180:PHE:HB3	44:AD:195:HIS:CD2	2.56	0.40
64:AY:115:ARG:HD3	64:AY:118:ILE:HD12	2.04	0.40
83:Au:70:ASP:OD1	83:Au:70:ASP:N	2.55	0.40
86:Ct:330:LYS:HB3	86:Ct:334:PRO:HG2	2.04	0.40
1:A2:1440:C:N4	1:A2:1676:C:OP1	2.51	0.40
1:A2:1663:G:O2'	66:Aa:41:HIS:NE2	2.43	0.40
1:A2:3688:A:N7	1:A2:3707:A:N6	2.69	0.40
1:A2:4853:C:OP1	52:AM:132:LYS:NZ	2.46	0.40
5:B1:14:C:H2'	5:B1:15:U:C6	2.57	0.40
5:B1:50:A:H62	5:B1:477:G:H21	1.69	0.40
5:B1:96:C:H1'	5:B1:474:G:H5'	2.02	0.40
5:B1:215:G:H2'	5:B1:216:C:H6	1.87	0.40
5:B1:475:C:O2'	5:B1:507:G:N3	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B1:805:U:H5''	33:BW:83:LEU:HD12	2.04	0.40
5:B1:981:A:O2'	5:B1:1044:G:OP1	2.32	0.40
9:BM:48:HIS:ND1	9:BM:112:LYS:O	2.38	0.40
14:BT:140:ALA:HA	14:BT:143:LYS:HE3	2.04	0.40
29:BL:82:MET:HG2	29:BL:85:THR:HG23	2.03	0.40
30:BN:100:LYS:O	30:BN:104:ARG:HD3	2.21	0.40
42:AB:33:PRO:HB3	42:AB:351:LEU:HA	2.02	0.40
45:AE:206:VAL:HG13	45:AE:256:GLN:HG3	2.03	0.40
53:AN:17:ASP:HA	53:AN:20:ARG:HG2	2.03	0.40
53:AN:116:LEU:HD22	53:AN:135:ILE:HD11	2.03	0.40
61:AV:24:ALA:HB3	61:AV:39:ILE:HD12	2.03	0.40
72:Ag:64:LEU:HA	72:Ag:67:LEU:HD23	2.03	0.40
86:Ct:45:ILE:H	86:Ct:45:ILE:HG13	1.67	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%)	210 (96%)	8 (4%)	0	100	100
7	BF	188/190 (99%)	173 (92%)	15 (8%)	0	100	100
8	BK	96/98 (98%)	81 (84%)	14 (15%)	1 (1%)	12	44
9	BM	118/120 (98%)	109 (92%)	9 (8%)	0	100	100
10	BP	118/120 (98%)	102 (86%)	15 (13%)	1 (1%)	16	49
11	BQ	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
12	BR	123/125 (98%)	107 (87%)	16 (13%)	0	100	100
13	BS	137/139 (99%)	126 (92%)	11 (8%)	0	100	100
14	BT	141/143 (99%)	129 (92%)	11 (8%)	1 (1%)	18	51
15	BU	95/97 (98%)	92 (97%)	3 (3%)	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%)	54 (90%)	4 (7%)	2 (3%)	3	23
18	Bd	49/51 (96%)	45 (92%)	4 (8%)	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%)	201 (94%)	12 (6%)	0	100	100
22	BB	210/212 (99%)	179 (85%)	31 (15%)	0	100	100
23	BC	220/222 (99%)	208 (94%)	12 (6%)	0	100	100
24	BE	255/257 (99%)	236 (92%)	17 (7%)	2 (1%)	16	49
25	BG	230/232 (99%)	213 (93%)	17 (7%)	0	100	100
26	BH	181/183 (99%)	172 (95%)	9 (5%)	0	100	100
27	BI	205/207 (99%)	176 (86%)	28 (14%)	1 (0%)	24	57
28	BJ	177/179 (99%)	153 (86%)	22 (12%)	2 (1%)	11	43
29	BL	151/153 (99%)	137 (91%)	13 (9%)	1 (1%)	18	51
30	BN	147/149 (99%)	133 (90%)	14 (10%)	0	100	100
31	BO	134/136 (98%)	123 (92%)	11 (8%)	0	100	100
32	BV	79/81 (98%)	76 (96%)	3 (4%)	0	100	100
33	BW	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
34	BX	139/141 (99%)	126 (91%)	13 (9%)	0	100	100
35	BY	123/125 (98%)	108 (88%)	15 (12%)	0	100	100
36	Ba	95/97 (98%)	86 (90%)	9 (10%)	0	100	100
37	Bb	78/80 (98%)	71 (91%)	7 (9%)	0	100	100
38	Be	53/55 (96%)	48 (91%)	5 (9%)	0	100	100
41	AA	250/252 (99%)	233 (93%)	17 (7%)	0	100	100
42	AB	392/394 (100%)	358 (91%)	34 (9%)	0	100	100
43	AC	361/363 (99%)	325 (90%)	33 (9%)	3 (1%)	16	49
44	AD	292/294 (99%)	268 (92%)	24 (8%)	0	100	100
45	AE	192/194 (99%)	161 (84%)	30 (16%)	1 (0%)	24	57
46	AF	232/234 (99%)	215 (93%)	17 (7%)	0	100	100
47	AG	232/234 (99%)	219 (94%)	13 (6%)	0	100	100
48	AH	189/191 (99%)	174 (92%)	15 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	AI	204/208 (98%)	187 (92%)	17 (8%)	0	100	100
50	AJ	167/169 (99%)	151 (90%)	15 (9%)	1 (1%)	21	54
51	AL	203/205 (99%)	171 (84%)	31 (15%)	1 (0%)	24	57
52	AM	137/139 (99%)	126 (92%)	11 (8%)	0	100	100
53	AN	201/203 (99%)	182 (90%)	19 (10%)	0	100	100
54	AO	193/195 (99%)	184 (95%)	9 (5%)	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%)	162 (94%)	11 (6%)	0	100	100
59	AT	155/157 (99%)	138 (89%)	15 (10%)	2 (1%)	9	39
60	AU	97/99 (98%)	93 (96%)	4 (4%)	0	100	100
61	AV	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
62	AW	119/121 (98%)	110 (92%)	9 (8%)	0	100	100
63	AX	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
64	AY	125/127 (98%)	119 (95%)	6 (5%)	0	100	100
65	AZ	132/134 (98%)	117 (89%)	15 (11%)	0	100	100
66	Aa	145/147 (99%)	129 (89%)	16 (11%)	0	100	100
67	Ab	66/68 (97%)	55 (83%)	11 (17%)	0	100	100
68	Ac	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
69	Ad	104/106 (98%)	99 (95%)	5 (5%)	0	100	100
70	Ae	127/129 (98%)	115 (91%)	12 (9%)	0	100	100
71	Af	107/109 (98%)	97 (91%)	8 (8%)	2 (2%)	6	33
72	Ag	112/114 (98%)	101 (90%)	11 (10%)	0	100	100
73	Ah	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
74	Ai	95/97 (98%)	85 (90%)	10 (10%)	0	100	100
75	Aj	82/84 (98%)	75 (92%)	7 (8%)	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%)	45 (94%)	3 (6%)	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%)	98 (95%)	5 (5%)	0	100	100
81	Ap	89/91 (98%)	82 (92%)	7 (8%)	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%)	115 (77%)	34 (23%)	0	100	100
85	AK	200/202 (99%)	179 (90%)	20 (10%)	1 (0%)	24	57
86	Ct	850/853 (100%)	758 (89%)	91 (11%)	1 (0%)	48	79
All	All	12538/12699 (99%)	11430 (91%)	1084 (9%)	24 (0%)	44	74

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
24	BE	93	GLU
28	BJ	138	ARG
71	Af	107	PRO
10	BP	51	ARG
43	AC	51	PRO
51	AL	78	LEU
86	Ct	159	LYS
14	BT	31	PRO
27	BI	159	SER
71	Af	106	TYR
8	BK	41	PRO
17	Bc	33	GLU
45	AE	136	HIS
50	AJ	53	ALA
56	AQ	161	SER
85	AK	150	GLY
24	BE	150	PRO
29	BL	14	PRO
43	AC	52	TYR
28	BJ	123	ILE
59	AT	18	PRO
59	AT	53	PRO
17	Bc	32	VAL
43	AC	151	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%)	109 (100%)	0	100	100
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%)	120 (99%)	1 (1%)	73	77
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%)	187 (100%)	1 (0%)	81	80
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%)	193 (100%)	1 (0%)	81	80
42	AB	343/343 (100%)	343 (100%)	0	100	100
43	AC	302/302 (100%)	302 (100%)	0	100	100
44	AD	248/248 (100%)	247 (100%)	1 (0%)	84	81
45	AE	174/174 (100%)	174 (100%)	0	100	100
46	AF	203/203 (100%)	202 (100%)	1 (0%)	81	80
47	AG	199/199 (100%)	199 (100%)	0	100	100
48	AH	170/170 (100%)	170 (100%)	0	100	100
49	AI	178/178 (100%)	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%)	194 (99%)	2 (1%)	68	75
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	10924/10924 (100%)	10908 (100%)	16 (0%)	87	87

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	BS	78	LYS
14	BT	37	VAL
20	Bg	133	ASN
23	BC	141	VAL
30	BN	104	ARG
41	AA	45	VAL
44	AD	265	ARG

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Mol	Chain	Res	Type
46	AF	146	ASN
51	AL	63	THR
52	AM	95	ILE
54	AO	184	ASN
75	Aj	67	LEU
83	Au	194	LEU
83	Au	197	ASN
84	Aq	28	LEU
86	Ct	167	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (214) such sidechains are listed below:

Mol	Chain	Res	Type
7	BF	95	HIS
7	BF	101	HIS
7	BF	186	ASN
7	BF	203	ASN
9	BM	55	ASN
10	BP	41	GLN
10	BP	98	ASN
11	BQ	11	GLN
11	BQ	80	GLN
11	BQ	86	GLN
11	BQ	142	GLN
12	BR	62	GLN
13	BS	10	GLN
13	BS	17	ASN
13	BS	76	GLN
13	BS	97	GLN
13	BS	134	GLN
14	BT	11	GLN
14	BT	42	HIS
15	BU	92	HIS
16	BZ	112	ASN
17	Bc	24	GLN
17	Bc	26	GLN
18	Bd	41	GLN
20	Bg	20	GLN
20	Bg	133	ASN
20	Bg	191	HIS
20	Bg	226	HIS
20	Bg	305	ASN

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Mol	Chain	Res	Type
21	BA	36	GLN
21	BA	50	ASN
21	BA	149	ASN
21	BA	164	ASN
22	BB	40	ASN
22	BB	76	ASN
22	BB	124	HIS
22	BB	157	GLN
23	BC	113	GLN
23	BC	120	GLN
23	BC	134	ASN
24	BE	36	HIS
24	BE	197	ASN
24	BE	230	ASN
25	BG	13	GLN
25	BG	56	ASN
25	BG	81	HIS
25	BG	202	ASN
25	BG	227	GLN
26	BH	39	GLN
26	BH	91	HIS
26	BH	97	GLN
26	BH	193	GLN
27	BI	165	GLN
28	BJ	111	GLN
28	BJ	132	GLN
28	BJ	134	HIS
28	BJ	140	GLN
28	BJ	156	HIS
29	BL	11	GLN
29	BL	19	ASN
29	BL	108	ASN
30	BN	5	HIS
30	BN	123	HIS
31	BO	32	HIS
31	BO	113	GLN
33	BW	5	ASN
33	BW	15	ASN
33	BW	16	ASN
33	BW	92	ASN
34	BX	16	HIS
34	BX	61	GLN

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Mol	Chain	Res	Type
34	BX	127	ASN
35	BY	29	HIS
35	BY	89	HIS
35	BY	94	HIS
35	BY	112	ASN
36	Ba	86	ASN
37	Bb	51	GLN
37	Bb	83	GLN
38	Be	3	HIS
41	AA	22	HIS
41	AA	97	ASN
41	AA	132	ASN
41	AA	162	ASN
41	AA	205	ASN
41	AA	209	HIS
41	AA	215	ASN
42	AB	109	HIS
42	AB	167	GLN
42	AB	179	HIS
42	AB	302	ASN
42	AB	322	HIS
42	AB	380	GLN
43	AC	38	ASN
43	AC	41	HIS
43	AC	94	ASN
43	AC	198	ASN
43	AC	215	ASN
43	AC	282	HIS
43	AC	310	HIS
44	AD	9	ASN
44	AD	111	ASN
44	AD	122	GLN
44	AD	138	GLN
44	AD	191	ASN
44	AD	195	HIS
45	AE	190	HIS
45	AE	191	GLN
45	AE	279	ASN
46	AF	24	ASN
46	AF	146	ASN
47	AG	43	GLN
47	AG	149	ASN

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Mol	Chain	Res	Type
48	AH	140	GLN
49	AI	14	ASN
49	AI	51	HIS
49	AI	130	HIS
49	AI	147	HIS
50	AJ	46	GLN
50	AJ	71	HIS
50	AJ	112	HIS
51	AL	159	ASN
51	AL	175	ASN
52	AM	33	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	182	HIS
54	AO	42	ASN
54	AO	65	ASN
54	AO	143	HIS
54	AO	180	GLN
54	AO	184	ASN
55	AP	40	HIS
55	AP	64	ASN
55	AP	80	GLN
55	AP	97	ASN
55	AP	133	HIS
57	AR	141	HIS
57	AR	178	GLN
58	AS	50	GLN
58	AS	66	GLN
58	AS	77	ASN
59	AT	22	HIS
59	AT	70	HIS
59	AT	98	HIS
60	AU	50	ASN
61	AV	101	ASN
61	AV	135	ASN
62	AW	17	HIS
62	AW	45	ASN
62	AW	48	GLN

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Mol	Chain	Res	Type
62	AW	63	GLN
63	AX	107	HIS
64	AY	4	ASN
64	AY	20	ASN
64	AY	40	GLN
64	AY	56	GLN
65	AZ	40	HIS
66	Aa	17	HIS
66	Aa	40	HIS
66	Aa	60	HIS
66	Aa	62	HIS
66	Aa	66	ASN
66	Aa	89	ASN
67	Ab	42	ASN
67	Ab	60	ASN
67	Ab	61	ASN
68	Ac	51	ASN
69	Ad	28	ASN
70	Ae	52	GLN
70	Ae	107	ASN
71	Af	56	ASN
71	Af	99	HIS
72	Ag	73	HIS
73	Ah	98	HIS
73	Ah	107	GLN
75	Aj	57	ASN
75	Aj	66	HIS
77	Al	20	ASN
77	Al	43	HIS
78	Am	120	ASN
80	Ao	3	ASN
80	Ao	19	GLN
80	Ao	25	GLN
80	Ao	102	GLN
82	At	36	ASN
82	At	41	ASN
82	At	70	GLN
82	At	100	ASN
83	Au	21	ASN
83	Au	71	GLN
83	Au	73	HIS
83	Au	143	ASN

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Mol	Chain	Res	Type
83	Au	171	HIS
83	Au	184	HIS
83	Au	188	ASN
83	Au	197	ASN
83	Au	214	GLN
84	Aq	111	ASN
85	AK	39	GLN
85	AK	72	ASN
86	Ct	138	GLN
86	Ct	145	GLN
86	Ct	179	GLN
86	Ct	270	ASN
86	Ct	544	HIS
86	Ct	588	ASN
86	Ct	696	ASN
86	Ct	710	HIS
86	Ct	803	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A2	3600/3612 (99%)	701 (19%)	8 (0%)
2	Bv	75/76 (98%)	12 (16%)	0
3	Bx	10/11 (90%)	2 (20%)	0
39	A3	156/157 (99%)	37 (23%)	0
4	Bw	75/76 (98%)	12 (16%)	0
40	A4	118/119 (99%)	19 (16%)	0
5	B1	1701/1708 (99%)	339 (19%)	3 (0%)
All	All	5735/5759 (99%)	1122 (19%)	11 (0%)

All (1122) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A2	9	C
1	A2	10	A
1	A2	12	A
1	A2	14	C
1	A2	19	G
1	A2	25	A
1	A2	32	G
1	A2	39	A

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Mol	Chain	Res	Type
1	A2	42	A
1	A2	47	A
1	A2	48	G
1	A2	59	A
1	A2	65	A
1	A2	71	C
1	A2	72	C
1	A2	74	G
1	A2	84	A
1	A2	91	G
1	A2	101	A
1	A2	107	G
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	134	G
1	A2	136	G
1	A2	139	G
1	A2	140	C
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	171	C
1	A2	173	G
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	206	U
1	A2	212	C
1	A2	213	C
1	A2	214	C

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Mol	Chain	Res	Type
1	A2	215	A
1	A2	228	U
1	A2	229	G
1	A2	230	U
1	A2	234	G
1	A2	236	C
1	A2	238	G
1	A2	253	G
1	A2	256	C
1	A2	258	C
1	A2	260	C
1	A2	261	G
1	A2	275	U
1	A2	286	G
1	A2	289	A
1	A2	291	U
1	A2	300	A
1	A2	302	G
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	377	A
1	A2	380	A
1	A2	381	G
1	A2	402	A
1	A2	406	G
1	A2	407	G
1	A2	425	G
1	A2	426	U
1	A2	427	A
1	A2	434	U
1	A2	444	G
1	A2	446	A

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Mol	Chain	Res	Type
1	A2	447	G
1	A2	448	U
1	A2	449	C
1	A2	450	C
1	A2	458	G
1	A2	463	C
1	A2	479	C
1	A2	480	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
1	A2	501	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	643	A
1	A2	645	C
1	A2	647	U
1	A2	649	C
1	A2	650	C
1	A2	653	G
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	695	C
1	A2	698	C
1	A2	714	A
1	A2	719	U
1	A2	720	G
1	A2	721	G

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Mol	Chain	Res	Type
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	913	G
1	A2	917	G
1	A2	918	C
1	A2	919	A
1	A2	921	C
1	A2	923	C
1	A2	924	U
1	A2	925	C
1	A2	927	C
1	A2	929	G
1	A2	931	A
1	A2	932	U
1	A2	933	C
1	A2	934	C
1	A2	938	G
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	952	G
1	A2	953	A
1	A2	954	C
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	1056	G
1	A2	1067	C

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Mol	Chain	Res	Type
1	A2	1086	C
1	A2	1087	C
1	A2	1149	G
1	A2	1150	C
1	A2	1156	G
1	A2	1161	G
1	A2	1162	U
1	A2	1165	C
1	A2	1180	C
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	1226	C
1	A2	1229	G
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	1267	G
1	A2	1268	U
1	A2	1269	C
1	A2	1271	G
1	A2	1277	A
1	A2	1278	C
1	A2	1284	C
1	A2	1286	A
1	A2	1301	C
1	A2	1309	A
1	A2	1337	A
1	A2	1341	G
1	A2	1343	G
1	A2	1348	C

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Mol	Chain	Res	Type
1	A2	1349	G
1	A2	1351	A
1	A2	1353	G
1	A2	1362	C
1	A2	1364	U
1	A2	1370	A
1	A2	1373	G
1	A2	1377	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	1425	C
1	A2	1426	A
1	A2	1428	U
1	A2	1430	C
1	A2	1432	C
1	A2	1440	C
1	A2	1463	C
1	A2	1464	G
1	A2	1465	C
1	A2	1466	G
1	A2	1468	C
1	A2	1479	A
1	A2	1480	G
1	A2	1483	C
1	A2	1485	A
1	A2	1497	A
1	A2	1499	G
1	A2	1500	A
1	A2	1505	A
1	A2	1507	A
1	A2	1516	A
1	A2	1521	G
1	A2	1548	C
1	A2	1556	G
1	A2	1559	G
1	A2	1560	U
1	A2	1573	U
1	A2	1578	U

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Mol	Chain	Res	Type
1	A2	1583	A
1	A2	1589	C
1	A2	1593	C
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	1632	A
1	A2	1636	G
1	A2	1643	C
1	A2	1676	C
1	A2	1701	A
1	A2	1706	G
1	A2	1723	G
1	A2	1728	A
1	A2	1736	U
1	A2	1737	C
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	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	1850	G
1	A2	1862	C
1	A2	1863	U

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Mol	Chain	Res	Type
1	A2	1869	A
1	A2	1871	G
1	A2	1872	A
1	A2	1873	A
1	A2	1896	C
1	A2	1902	C
1	A2	1903	G
1	A2	1917	C
1	A2	1928	U
1	A2	1929	G
1	A2	1930	U
1	A2	1936	G
1	A2	1940	U
1	A2	1941	A
1	A2	1942	G
1	A2	1943	A
1	A2	1955	U
1	A2	1956	G
1	A2	1958	C
1	A2	1961	U
1	A2	1962	G
1	A2	1964	A
1	A2	1965	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	1991	A
1	A2	1993	A
1	A2	1994	A
1	A2	2007	A
1	A2	2015	G
1	A2	2029	U
1	A2	2033	G
1	A2	2037	G
1	A2	2043	C
1	A2	2050	A
1	A2	2246	U
1	A2	2247	A

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Mol	Chain	Res	Type
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
1	A2	2308	U
1	A2	2310	G
1	A2	2311	A
1	A2	2324	G
1	A2	2327	G
1	A2	2330	C
1	A2	2339	A
1	A2	2340	G
1	A2	2373	G
1	A2	2374	A
1	A2	2381	G
1	A2	2389	C
1	A2	2399	A
1	A2	2400	G
1	A2	2401	C
1	A2	2404	U
1	A2	2420	C
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

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Mol	Chain	Res	Type
1	A2	2565	G
1	A2	2566	A
1	A2	2568	C
1	A2	2570	A
1	A2	2579	A
1	A2	2580	A
1	A2	2585	G
1	A2	2606	C
1	A2	2617	G
1	A2	2632	C
1	A2	2637	G
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	2689	C
1	A2	2690	G
1	A2	2691	G
1	A2	2698	C
1	A2	2700	G
1	A2	2705	G
1	A2	2706	C
1	A2	2717	C
1	A2	2718	C
1	A2	2719	U
1	A2	2720	U
1	A2	2726	U
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

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Mol	Chain	Res	Type
1	A2	2785	A
1	A2	2793	C
1	A2	2804	A
1	A2	2805	U
1	A2	2806	G
1	A2	2808	U
1	A2	2814	A
1	A2	2834	G
1	A2	2839	C
1	A2	2859	U
1	A2	2860	A
1	A2	2871	C
1	A2	3572	C
1	A2	3574	G
1	A2	3576	C
1	A2	3586	G
1	A2	3587	U
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	3615	U
1	A2	3616	U
1	A2	3619	A
1	A2	3627	A
1	A2	3633	A
1	A2	3643	G
1	A2	3651	U
1	A2	3663	A
1	A2	3671	C
1	A2	3682	A
1	A2	3685	G
1	A2	3689	A
1	A2	3707	A
1	A2	3729	U
1	A2	3732	C
1	A2	3747	G
1	A2	3748	G

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Mol	Chain	Res	Type
1	A2	3749	U
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
1	A2	3798	G
1	A2	3799	A
1	A2	3809	U
1	A2	3810	G
1	A2	3811	U
1	A2	3831	A
1	A2	3839	G
1	A2	3848	A
1	A2	3850	G
1	A2	3852	G
1	A2	3860	G
1	A2	3863	U
1	A2	3866	G
1	A2	3869	G
1	A2	3872	A
1	A2	3876	A
1	A2	3878	G
1	A2	3879	A
1	A2	3886	U
1	A2	3890	C
1	A2	3907	A
1	A2	3909	G
1	A2	3910	G
1	A2	3925	A
1	A2	3927	G
1	A2	3929	G
1	A2	3936	A
1	A2	3937	A
1	A2	3943	A
1	A2	3944	G
1	A2	4019	U
1	A2	4020	A

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Mol	Chain	Res	Type
1	A2	4035	G
1	A2	4042	C
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
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	4124	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	4182	A
1	A2	4187	G
1	A2	4188	G
1	A2	4191	U
1	A2	4195	A
1	A2	4196	A
1	A2	4211	G
1	A2	4213	A
1	A2	4215	A
1	A2	4216	G
1	A2	4228	G
1	A2	4230	A

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Mol	Chain	Res	Type
1	A2	4235	A
1	A2	4243	A
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	4288	G
1	A2	4291	G
1	A2	4292	G
1	A2	4294	C
1	A2	4297	C
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	4343	A
1	A2	4349	C
1	A2	4355	G
1	A2	4356	A
1	A2	4358	A
1	A2	4360	C
1	A2	4384	A
1	A2	4388	C
1	A2	4398	U
1	A2	4406	C
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

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Mol	Chain	Res	Type
1	A2	4480	A
1	A2	4482	G
1	A2	4485	A
1	A2	4486	G
1	A2	4490	G
1	A2	4510	A
1	A2	4519	U
1	A2	4522	C
1	A2	4532	G
1	A2	4551	A
1	A2	4552	A
1	A2	4559	U
1	A2	4561	A
1	A2	4563	U
1	A2	4579	G
1	A2	4586	A
1	A2	4588	A
1	A2	4598	U
1	A2	4611	G
1	A2	4614	G
1	A2	4619	U
1	A2	4620	G
1	A2	4621	G
1	A2	4629	C
1	A2	4632	C
1	A2	4641	G
1	A2	4649	A
1	A2	4662	A
1	A2	4664	G
1	A2	4671	U
1	A2	4678	C
1	A2	4681	G
1	A2	4693	G
1	A2	4694	G
1	A2	4695	C
1	A2	4696	A
1	A2	4703	C
1	A2	4704	G
1	A2	4714	U
1	A2	4715	U
1	A2	4718	C
1	A2	4720	U

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Mol	Chain	Res	Type
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	4838	C
1	A2	4839	U
1	A2	4840	U
1	A2	4841	C
1	A2	4847	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	4868	A
1	A2	4870	G
1	A2	4871	G
1	A2	4872	C
1	A2	4880	C
1	A2	4886	C
1	A2	4887	C
1	A2	4895	C
1	A2	4896	A
1	A2	4898	C
1	A2	4901	A
1	A2	4902	C
1	A2	4903	G
1	A2	4907	G
1	A2	4908	U
1	A2	4909	G
1	A2	4921	G
1	A2	4924	A
1	A2	4934	U

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Mol	Chain	Res	Type
1	A2	4936	G
1	A2	4943	U
1	A2	4947	U
1	A2	4948	C
1	A2	4950	G
1	A2	4957	G
1	A2	4964	U
1	A2	4971	C
1	A2	4975	G
1	A2	4982	C
1	A2	4985	C
1	A2	4998	U
1	A2	4999	G
1	A2	5005	C
1	A2	5007	G
1	A2	5008	C
1	A2	5012	C
1	A2	5013	G
1	A2	5016	A
1	A2	5019	A
1	A2	5020	G
2	Bv	16	U
2	Bv	17	G
2	Bv	18	G
2	Bv	19	U
2	Bv	20	U
2	Bv	21	A
2	Bv	47	U
2	Bv	48	C
2	Bv	59	A
2	Bv	70	A
2	Bv	74	C
2	Bv	76	A
3	Bx	31	A
3	Bx	33	A
4	Bw	7	U
4	Bw	10	G
4	Bw	16	U
4	Bw	17	U
4	Bw	18	G
4	Bw	19	G
4	Bw	20	G

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Mol	Chain	Res	Type
4	Bw	34	G
4	Bw	48	C
4	Bw	71	G
4	Bw	74	C
4	Bw	76	A
5	B1	4	C
5	B1	33	G
5	B1	41	G
5	B1	42	A
5	B1	44	U
5	B1	46	A
5	B1	49	C
5	B1	67	C
5	B1	68	A
5	B1	71	G
5	B1	73	C
5	B1	76	U
5	B1	77	A
5	B1	103	A
5	B1	113	G
5	B1	114	G
5	B1	115	U
5	B1	125	C
5	B1	143	U
5	B1	146	G
5	B1	155	G
5	B1	158	A
5	B1	162	C
5	B1	170	A
5	B1	171	A
5	B1	172	U
5	B1	175	A
5	B1	183	G
5	B1	209	A
5	B1	213	G
5	B1	217	A
5	B1	220	U
5	B1	228	C
5	B1	230	A
5	B1	236	A
5	B1	238	C
5	B1	284	C

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Mol	Chain	Res	Type
5	B1	286	U
5	B1	287	U
5	B1	292	A
5	B1	293	C
5	B1	305	U
5	B1	306	C
5	B1	312	G
5	B1	313	A
5	B1	314	U
5	B1	315	C
5	B1	319	C
5	B1	327	G
5	B1	328	U
5	B1	329	G
5	B1	331	C
5	B1	332	G
5	B1	333	G
5	B1	338	G
5	B1	339	A
5	B1	343	A
5	B1	351	G
5	B1	364	A
5	B1	368	U
5	B1	369	C
5	B1	370	G
5	B1	376	A
5	B1	381	C
5	B1	383	G
5	B1	385	G
5	B1	386	C
5	B1	398	A
5	B1	407	G
5	B1	408	A
5	B1	409	C
5	B1	417	C
5	B1	428	U
5	B1	448	A
5	B1	450	C
5	B1	464	A
5	B1	465	A
5	B1	472	C
5	B1	474	G

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Mol	Chain	Res	Type
5	B1	483	C
5	B1	484	A
5	B1	487	U
5	B1	489	A
5	B1	492	C
5	B1	493	A
5	B1	501	C
5	B1	502	C
5	B1	507	G
5	B1	508	A
5	B1	523	A
5	B1	525	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	553	U
5	B1	554	A
5	B1	555	A
5	B1	558	G
5	B1	560	A
5	B1	567	C
5	B1	570	C
5	B1	576	A
5	B1	590	A
5	B1	591	U
5	B1	592	C
5	B1	594	A
5	B1	608	C
5	B1	611	G
5	B1	614	C
5	B1	617	G
5	B1	620	G
5	B1	621	C
5	B1	628	A
5	B1	629	A

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Mol	Chain	Res	Type
5	B1	631	U
5	B1	634	A
5	B1	643	A
5	B1	644	G
5	B1	645	C
5	B1	655	A
5	B1	660	C
5	B1	663	C
5	B1	666	U
5	B1	668	A
5	B1	669	A
5	B1	672	A
5	B1	673	G
5	B1	684	G
5	B1	687	C
5	B1	688	U
5	B1	738	C
5	B1	739	C
5	B1	741	C
5	B1	743	U
5	B1	744	G
5	B1	750	C
5	B1	751	G
5	B1	791	C
5	B1	797	C
5	B1	798	G
5	B1	799	U
5	B1	801	U
5	B1	806	U
5	B1	808	A
5	B1	809	A
5	B1	810	A
5	B1	811	A
5	B1	821	G
5	B1	833	C
5	B1	837	A
5	B1	839	C
5	B1	841	G
5	B1	842	C
5	B1	847	A
5	B1	852	G
5	B1	869	A

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Mol	Chain	Res	Type
5	B1	870	A
5	B1	874	G
5	B1	888	U
5	B1	890	U
5	B1	901	G
5	B1	913	A
5	B1	914	U
5	B1	918	U
5	B1	919	A
5	B1	920	A
5	B1	929	G
5	B1	930	C
5	B1	933	G
5	B1	934	G
5	B1	943	U
5	B1	950	C
5	B1	956	G
5	B1	959	G
5	B1	963	A
5	B1	969	U
5	B1	971	G
5	B1	975	G
5	B1	985	G
5	B1	990	A
5	B1	1002	U
5	B1	1008	A
5	B1	1015	U
5	B1	1016	U
5	B1	1017	U
5	B1	1023	A
5	B1	1027	A
5	B1	1044	G
5	B1	1053	C
5	B1	1061	U
5	B1	1084	A
5	B1	1085	C
5	B1	1087	A
5	B1	1109	C
5	B1	1110	G
5	B1	1114	U
5	B1	1117	C
5	B1	1118	C

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Mol	Chain	Res	Type
5	B1	1119	A
5	B1	1120	U
5	B1	1121	G
5	B1	1133	A
5	B1	1140	G
5	B1	1146	C
5	B1	1149	A
5	B1	1150	A
5	B1	1154	U
5	B1	1157	G
5	B1	1170	A
5	B1	1175	G
5	B1	1195	A
5	B1	1197	G
5	B1	1199	A
5	B1	1208	A
5	B1	1215	C
5	B1	1221	G
5	B1	1224	G
5	B1	1242	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	1262	C
5	B1	1263	U
5	B1	1271	C
5	B1	1278	A
5	B1	1283	C
5	B1	1285	G
5	B1	1286	G
5	B1	1287	A
5	B1	1288	U
5	B1	1290	G
5	B1	1291	A
5	B1	1297	U
5	B1	1301	A
5	B1	1302	G
5	B1	1303	C

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Mol	Chain	Res	Type
5	B1	1313	A
5	B1	1321	G
5	B1	1333	U
5	B1	1342	U
5	B1	1344	A
5	B1	1371	U
5	B1	1372	U
5	B1	1378	A
5	B1	1382	A
5	B1	1395	C
5	B1	1404	U
5	B1	1411	G
5	B1	1419	C
5	B1	1420	G
5	B1	1421	A
5	B1	1439	A
5	B1	1440	C
5	B1	1446	A
5	B1	1452	A
5	B1	1454	A
5	B1	1455	A
5	B1	1462	U
5	B1	1463	U
5	B1	1476	A
5	B1	1477	U
5	B1	1478	U
5	B1	1489	A
5	B1	1494	U
5	B1	1497	G
5	B1	1498	A
5	B1	1505	U
5	B1	1506	A
5	B1	1507	G
5	B1	1508	A
5	B1	1512	C
5	B1	1519	U
5	B1	1521	C
5	B1	1522	A
5	B1	1535	U
5	B1	1544	C
5	B1	1545	A
5	B1	1553	C

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Mol	Chain	Res	Type
5	B1	1554	C
5	B1	1555	U
5	B1	1558	C
5	B1	1560	U
5	B1	1580	A
5	B1	1584	G
5	B1	1587	G
5	B1	1588	A
5	B1	1593	C
5	B1	1601	A
5	B1	1604	G
5	B1	1606	G
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	1661	A
5	B1	1662	U
5	B1	1663	A
5	B1	1664	A
5	B1	1671	G
5	B1	1695	A
5	B1	1698	C
5	B1	1710	C
5	B1	1721	U
5	B1	1726	G
5	B1	1744	G
5	B1	1746	U
5	B1	1756	C
5	B1	1757	G
5	B1	1781	A
5	B1	1782	G
5	B1	1823	A
5	B1	1824	A
5	B1	1825	A
5	B1	1829	G
5	B1	1831	A
5	B1	1834	A
5	B1	1835	A
5	B1	1838	U

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Mol	Chain	Res	Type
5	B1	1849	G
5	B1	1852	C
5	B1	1861	G
5	B1	1862	G
5	B1	1863	A
5	B1	1865	C
5	B1	1866	A
5	B1	1869	A
39	A3	14	U
39	A3	15	G
39	A3	16	G
39	A3	23	C
39	A3	34	U
39	A3	35	C
39	A3	37	A
39	A3	38	U
39	A3	39	G
39	A3	49	G
39	A3	58	G
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	95	A
39	A3	96	C
39	A3	103	A
39	A3	105	C
39	A3	107	C
39	A3	109	C
39	A3	120	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

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Mol	Chain	Res	Type
39	A3	130	C
39	A3	148	A
39	A3	151	G
40	A4	7	G
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	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 (11) 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	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

5.4 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	1.04	1 (5%)	17,28,30	0.87	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	-	8/20/21/23	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	2.54	1.41	1.36

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	Ct	715	DDE	CAU-CBW-CBI	-2.50	106.32	111.22

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	0.71	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	-	-	4/18/38/38	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	4.49	1.64	1.59
89	Ct	901	GNP	PG-N3B	2.89	1.70	1.63
89	Ct	901	GNP	PB-O1B	2.82	1.50	1.46
89	Ct	901	GNP	PG-O1G	2.77	1.50	1.46
89	Ct	901	GNP	PB-O2B	-2.26	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	-2.32	108.35	111.77

There are no chirality outliers.

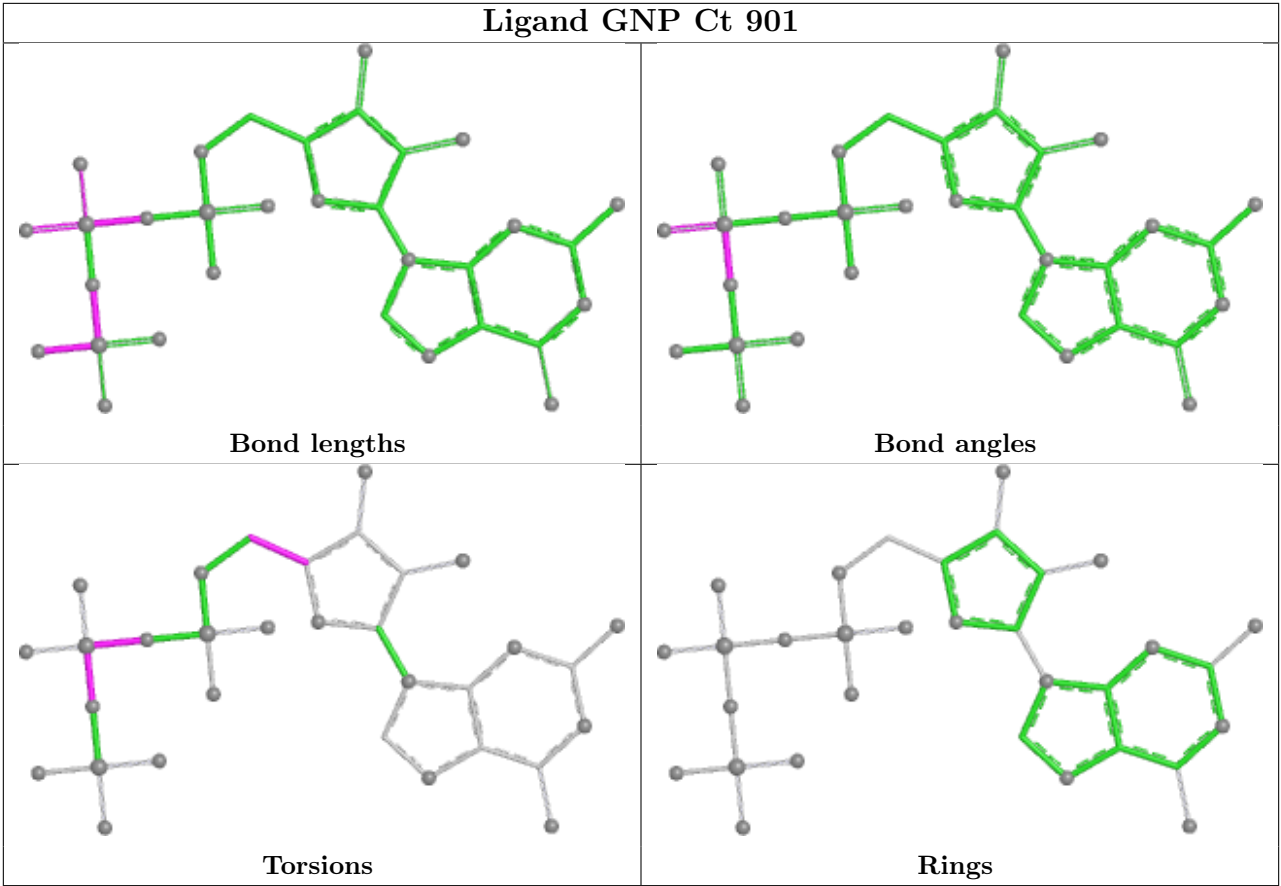
All (4) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

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
49	AI	1

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	20.96
1	B1	751:G	O3'	790:C	P	20.10
1	A2	517:C	O3'	629:G	P	18.31
1	B1	1757:G	O3'	1775:U	P	18.01

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A2	3948:C	O3'	4004:G	P	17.65
1	A2	4734:C	O3'	4818:G	P	17.53
1	A2	1233:C	O3'	1243:G	P	17.52
1	A2	750:G	O3'	890:C	P	17.33
1	B1	696:G	O3'	737:G	P	16.94
1	B1	1426:U	O3'	1438:A	P	16.88
1	A2	976:U	O3'	1047:G	P	16.86
1	B1	240:G	O3'	282:G	P	16.12
1	A2	2881:G	O3'	3569:C	P	15.91
1	A2	1089:A	O3'	1145:G	P	15.22
1	A2	1202:G	O3'	1216:G	P	14.61
1	A2	1680:C	O3'	1699:C	P	14.55
1	A2	2068:C	O3'	2245:C	P	13.67
1	AI	104:SER	C	108:ALA	N	6.64

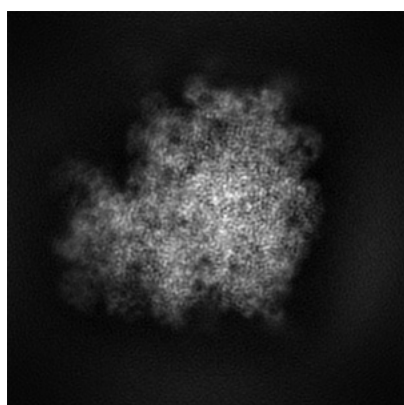
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0100. These allow visual inspection of the internal detail of the map and identification of artifacts.

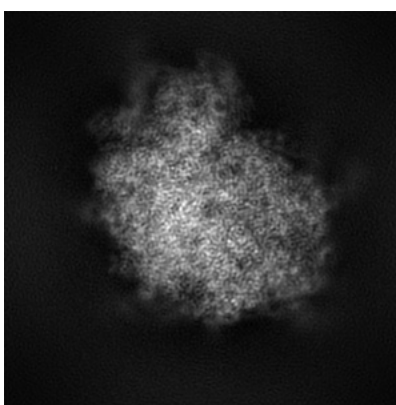
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

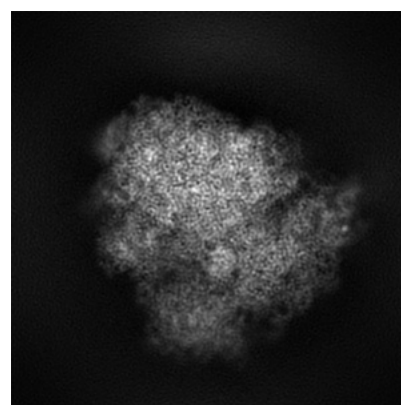
6.1.1 Primary map



X



Y

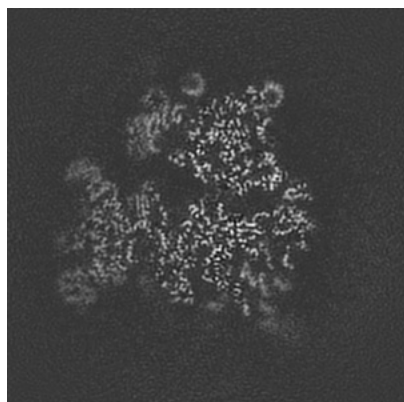


Z

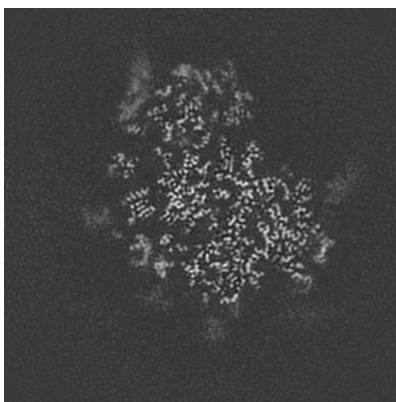
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

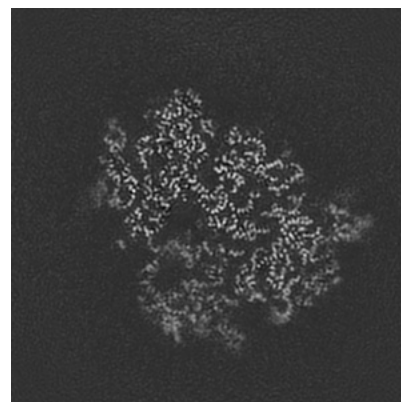
6.2.1 Primary map



X Index: 202



Y Index: 202

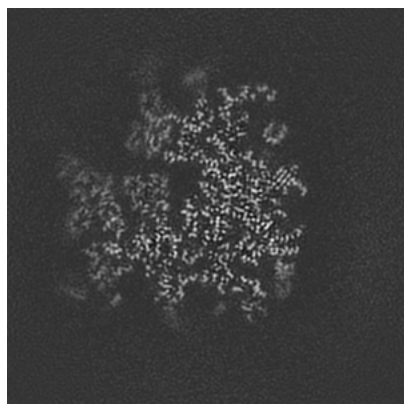


Z Index: 202

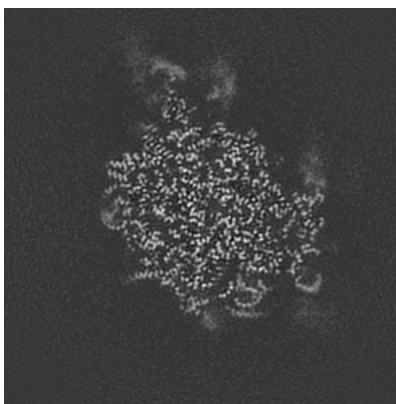
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

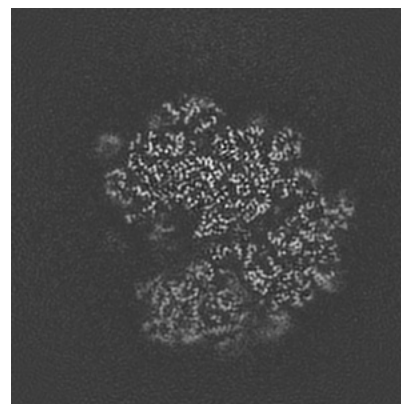
6.3.1 Primary map



X Index: 214



Y Index: 220

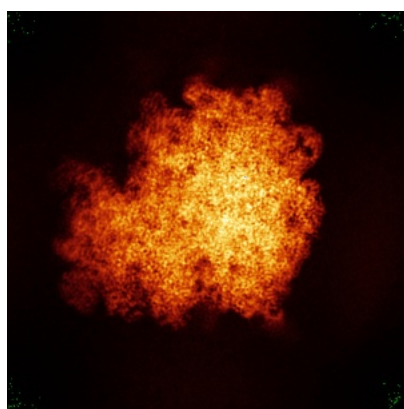


Z Index: 185

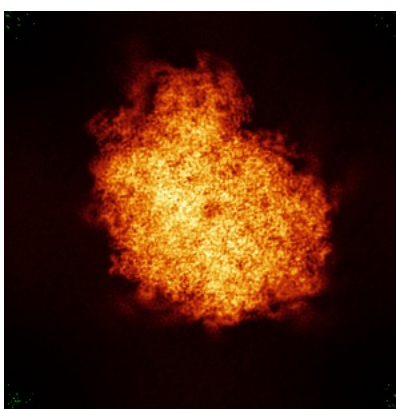
The images above show the largest variance slices of the map in three orthogonal directions.

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

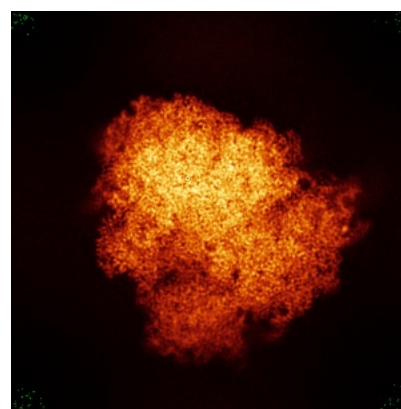
6.4.1 Primary map



X



Y

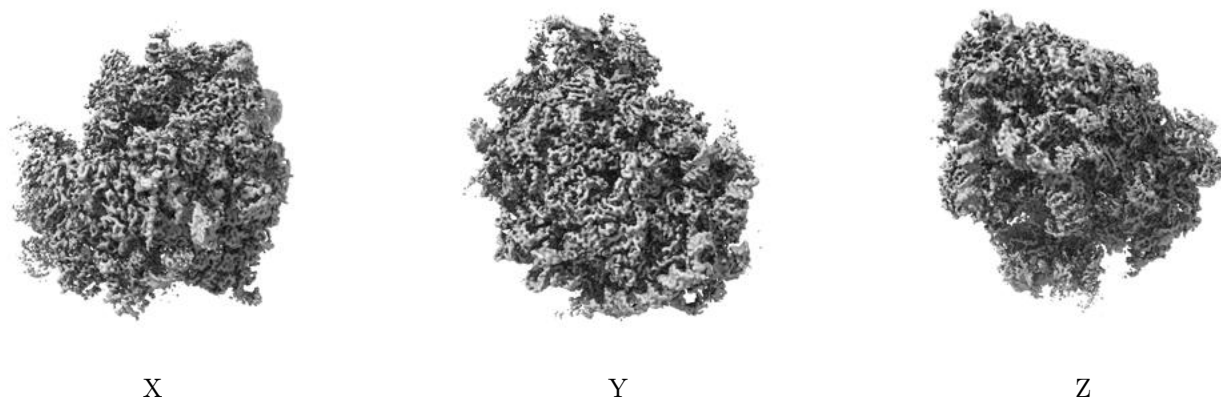


Z

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.

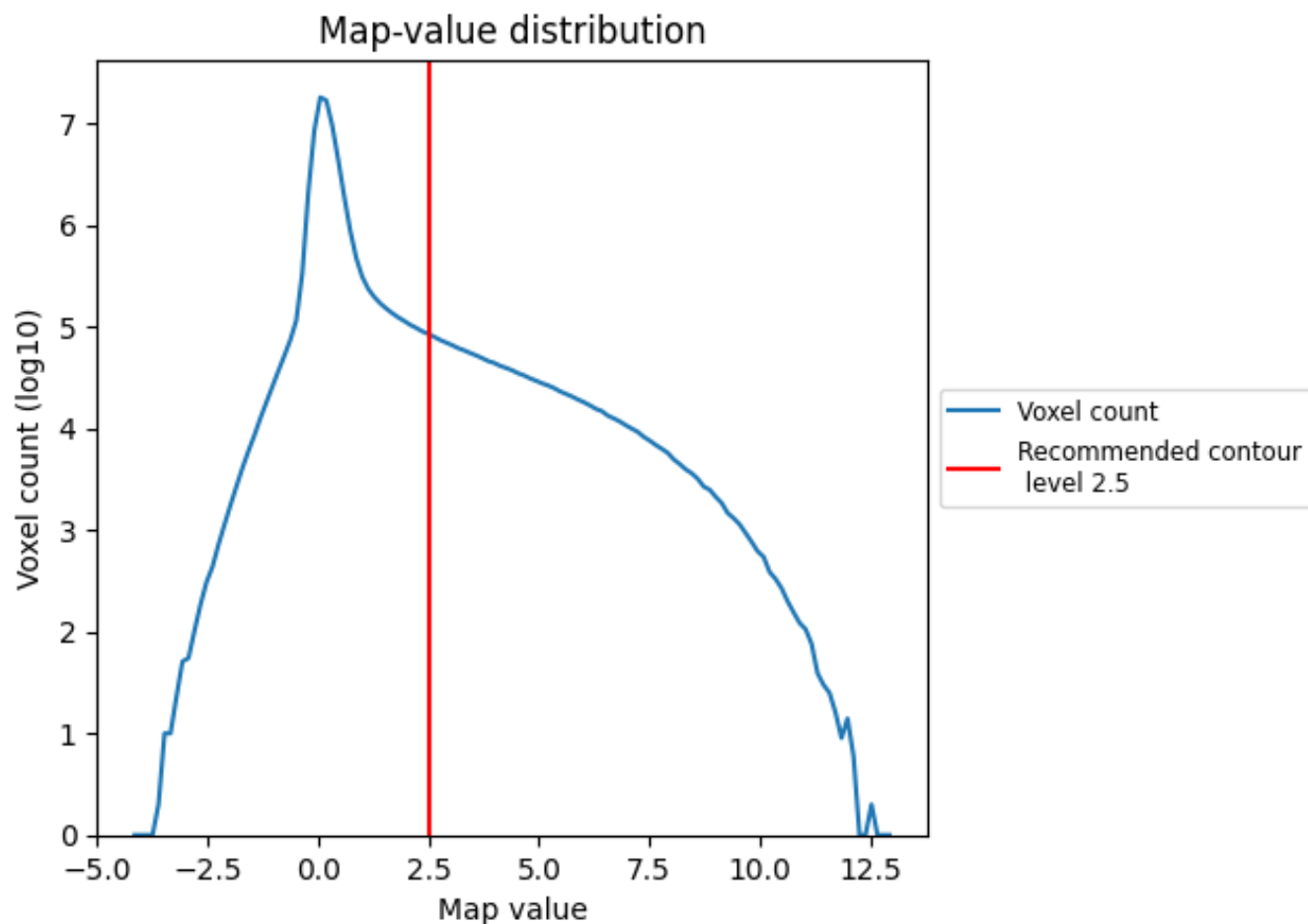
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

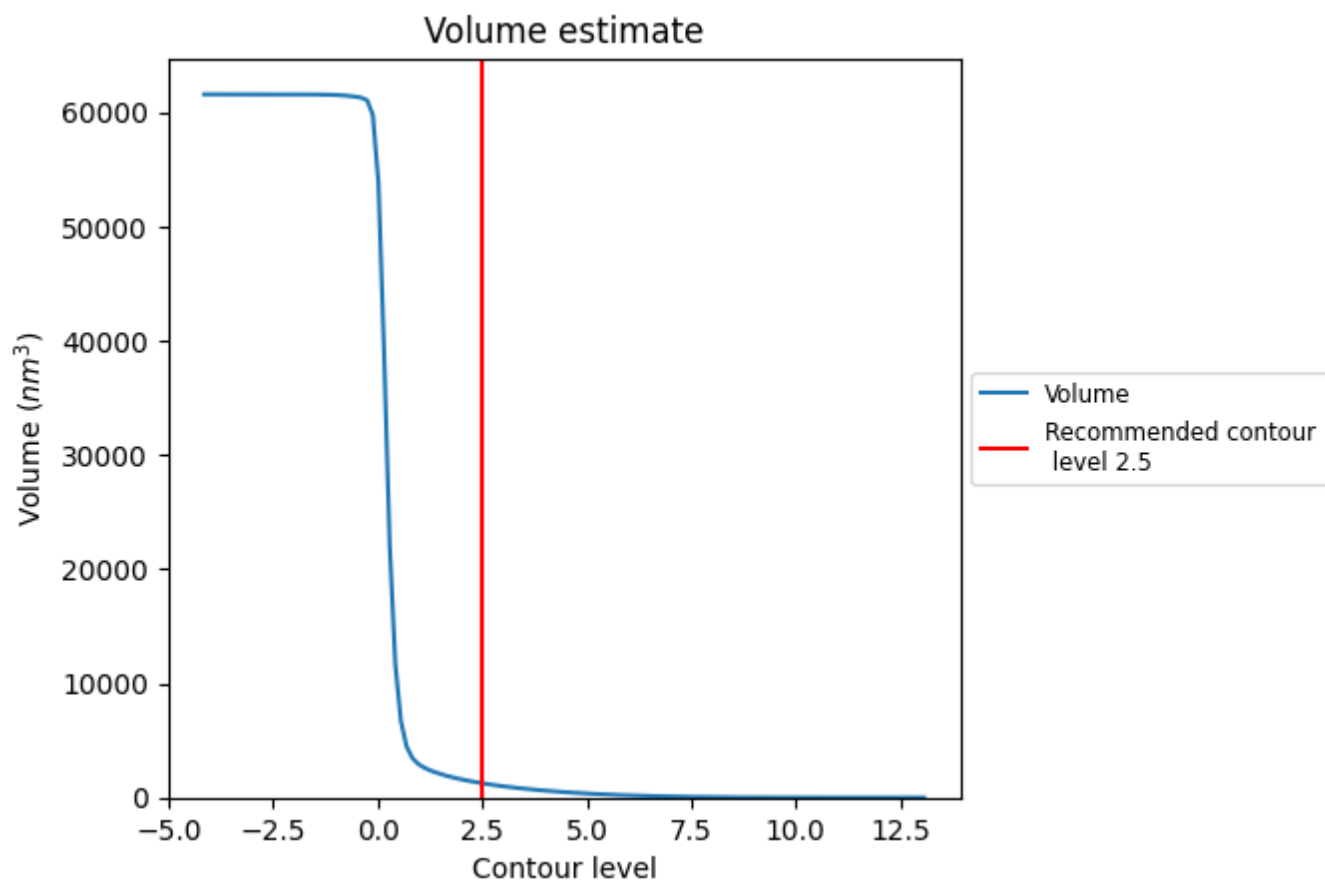
This section contains the results of statistical analysis of the map.

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.

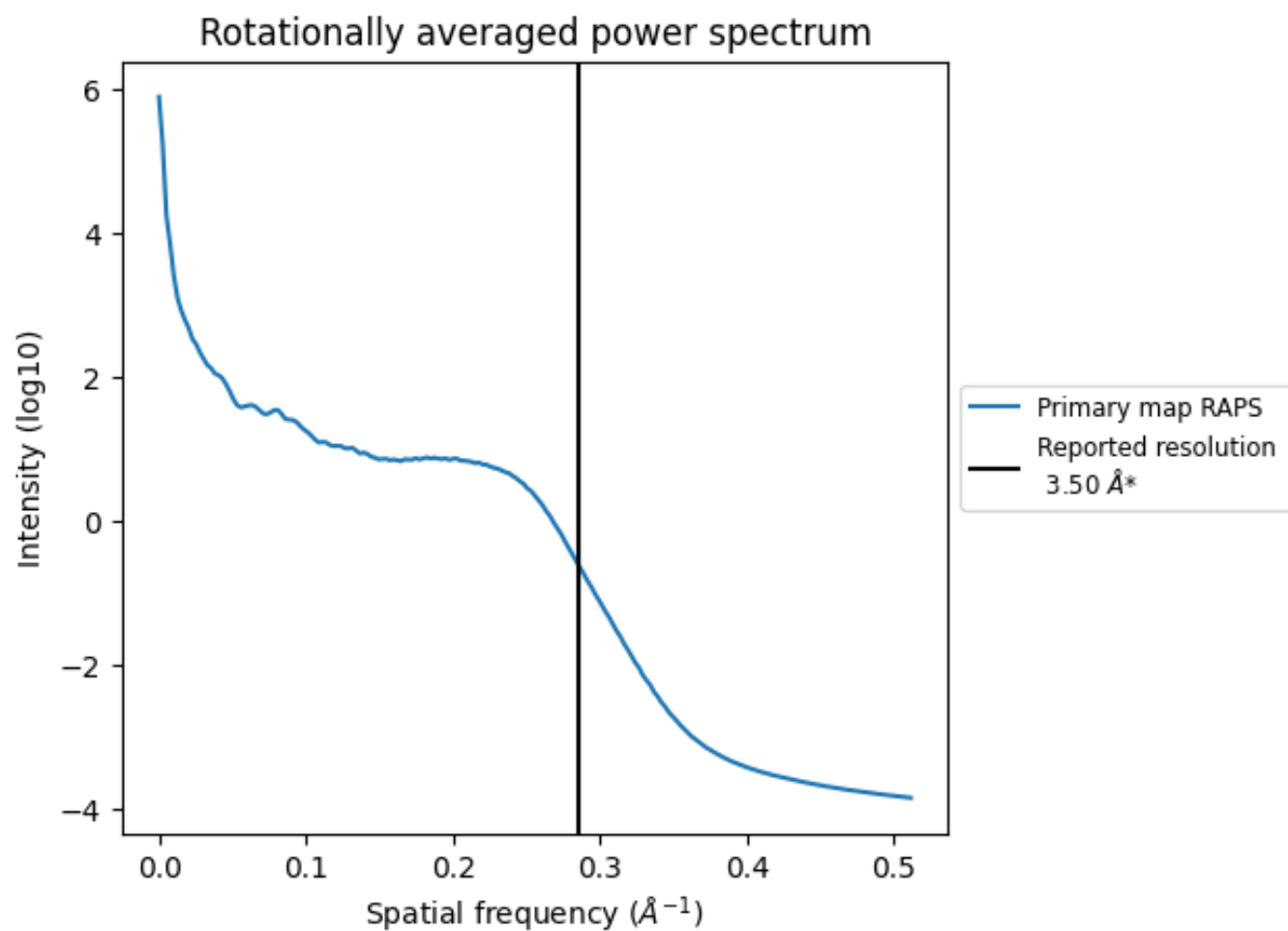
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1254 nm³; this corresponds to an approximate mass of 1133 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

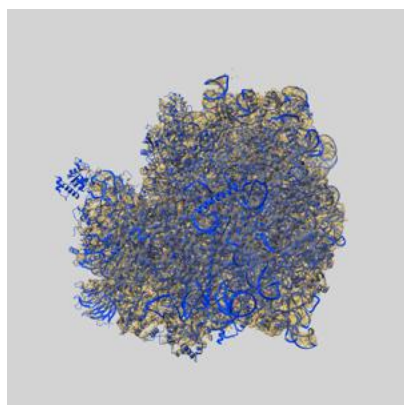
8 Fourier-Shell correlation ⓘ

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

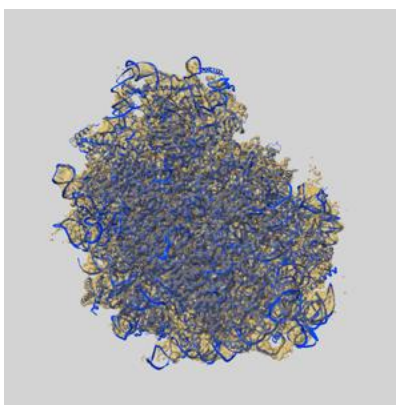
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0100 and PDB model 6GZ5. Per-residue inclusion information can be found in section [3](#) on page [21](#).

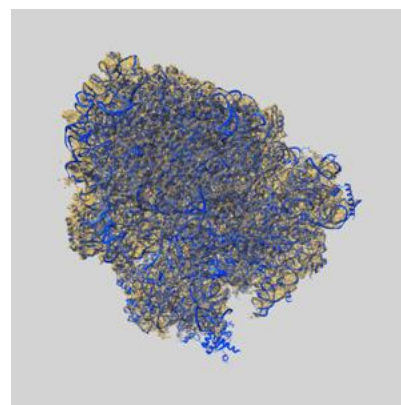
9.1 Map-model overlay [i](#)



X



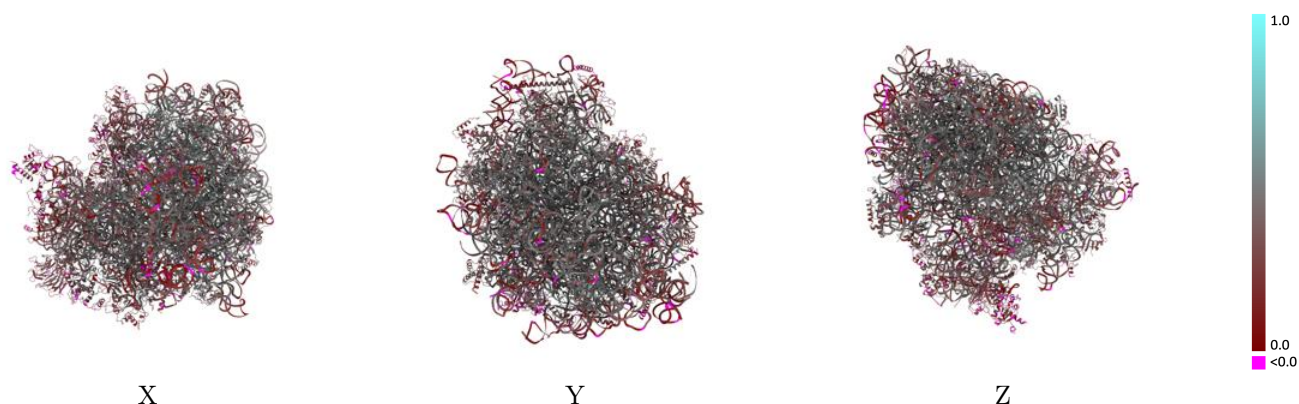
Y



Z

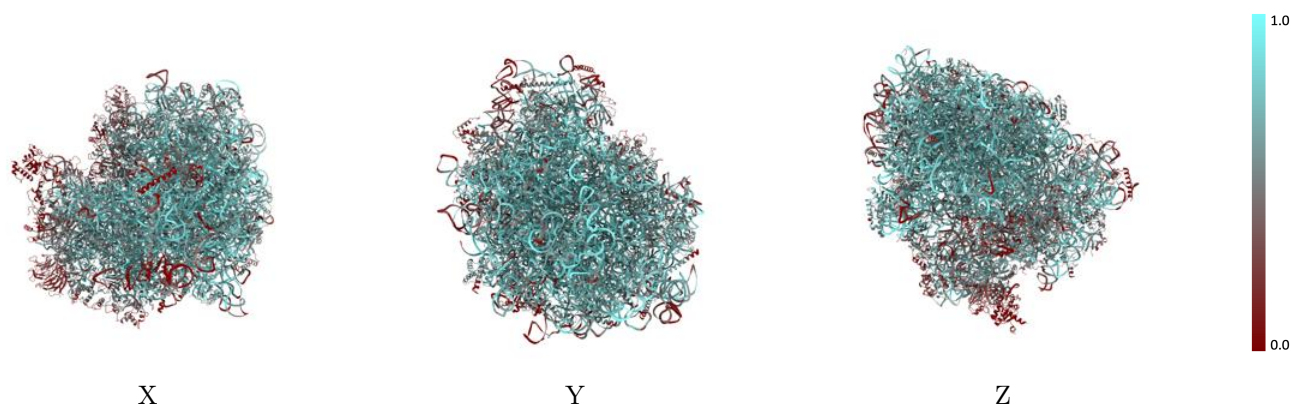
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



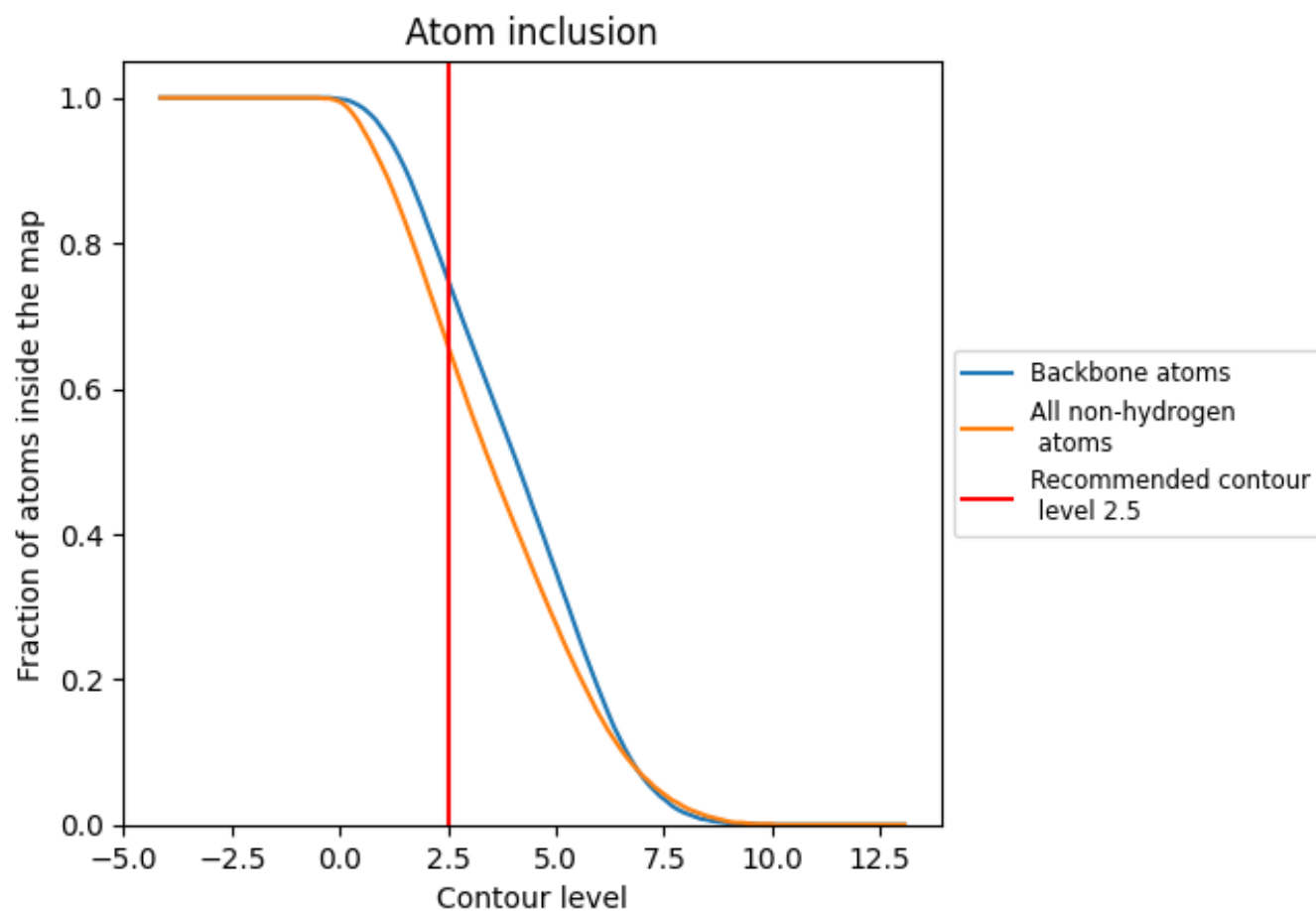
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 66% 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	 0.6590	 0.3800
A2	 0.7810	 0.4050
A3	 0.7840	 0.4080
A4	 0.8680	 0.4500
AA	 0.6950	 0.4590
AB	 0.6600	 0.4290
AC	 0.6770	 0.4270
AD	 0.6400	 0.3830
AE	 0.5300	 0.3270
AF	 0.6480	 0.3960
AG	 0.5850	 0.3840
AH	 0.6140	 0.4210
AI	 0.6430	 0.4220
AJ	 0.6010	 0.3840
AK	 0.2400	 0.2380
AL	 0.6070	 0.3680
AM	 0.6290	 0.3990
AN	 0.7330	 0.4440
AO	 0.6590	 0.4090
AP	 0.7060	 0.4470
AQ	 0.6730	 0.4200
AR	 0.6220	 0.4020
AS	 0.6740	 0.4360
AT	 0.6720	 0.4260
AU	 0.5530	 0.3730
AV	 0.6760	 0.4690
AW	 0.3640	 0.2890
AX	 0.6540	 0.4360
AY	 0.6670	 0.4220
AZ	 0.6440	 0.3990
Aa	 0.7040	 0.4350
Ab	 0.5910	 0.3520
Ac	 0.6110	 0.4040
Ad	 0.6660	 0.4400
Ae	 0.6600	 0.4370



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Chain	Atom inclusion	Q-score
Af	 0.6860	 0.4210
Ag	 0.6320	 0.4160
Ah	 0.6120	 0.3860
Ai	 0.6180	 0.3730
Aj	 0.7590	 0.4580
Ak	 0.5220	 0.3650
Al	 0.6760	 0.4360
Am	 0.6830	 0.4150
An	 0.3820	 0.3300
Ao	 0.6710	 0.4430
Ap	 0.6590	 0.4310
Aq	 0.1380	 0.1370
At	 0.6880	 0.4000
Au	 0.0160	 0.0650
B1	 0.7340	 0.3890
BA	 0.5090	 0.3400
BB	 0.5630	 0.3700
BC	 0.5690	 0.3920
BD	 0.3710	 0.3110
BE	 0.5770	 0.3810
BF	 0.4170	 0.3130
BG	 0.4770	 0.2990
BH	 0.3900	 0.2870
BI	 0.5550	 0.3640
BJ	 0.5660	 0.3220
BK	 0.2410	 0.1910
BL	 0.5630	 0.3700
BM	 0.0130	 0.1000
BN	 0.5970	 0.3960
BO	 0.5930	 0.4050
BP	 0.3250	 0.2610
BQ	 0.3910	 0.3010
BR	 0.3500	 0.2690
BS	 0.3680	 0.2680
BT	 0.3670	 0.2370
BU	 0.2810	 0.2680
BV	 0.5390	 0.3690
BW	 0.6160	 0.3980
BX	 0.5990	 0.4060
BY	 0.4990	 0.3120
BZ	 0.2410	 0.2450
Ba	 0.6200	 0.3960

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Chain	Atom inclusion	Q-score
Bb	 0.5220	 0.3620
Bc	 0.3640	 0.3350
Bd	 0.4800	 0.2810
Be	 0.4980	 0.3380
Bf	 0.0220	 0.1160
Bg	 0.1180	 0.2480
Bv	 0.6440	 0.3670
Bw	 0.5330	 0.2810
Bx	 0.5400	 0.3780
Ct	 0.4280	 0.3080