



Full wwPDB EM Validation Report ⓘ

Sep 21, 2026 – 01:27 PM EDT

PDB ID : 9YDD / pdb_00009ydd
EMDB ID : EMD-72801
Title : Eukaryotic 80S ribosome with A/A, P/P tRNAs from uL16 P-site loop mutants
in bypass condition
Authors : Guan, K.; Taylor, D.W.
Deposited on : 2025-09-22
Resolution : 2.66 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:

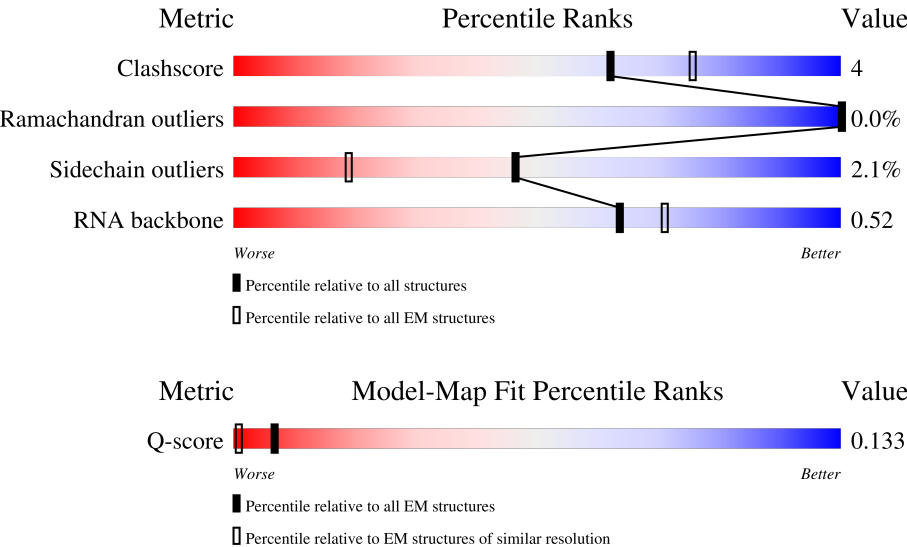
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.66 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	9119 (2.16 - 3.16)

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	A	3396	16% 65% 23% 10%
2	B	121	27% 78% 20%
3	C	158	7% 77% 20%

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Mol	Chain	Length	Quality of chain
4	D	10	
5	E	1800	
6	LD	254	
7	LE	387	
8	LF	362	
9	LG	297	
10	LH	176	
11	LI	244	
12	LJ	256	
13	LK	191	
14	LL	210	
15	LM	174	
16	LN	199	
17	LO	138	
18	LP	204	
19	LQ	199	
20	LR	184	
21	LS	186	
22	LT	189	
23	LU	172	
24	LV	160	
25	LW	121	
26	LX	137	
27	LY	155	
28	LZ	142	

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Mol	Chain	Length	Quality of chain
29	La	127	
30	Lb	136	
31	Lc	149	
32	Ld	59	
33	Le	105	
34	Lf	113	
35	Lg	130	
36	Lh	107	
37	Li	121	
38	Lj	120	
39	Lk	100	
40	Ll	88	
41	Lm	78	
42	Ln	51	
43	Lo	128	
44	Lp	25	
45	Lq	106	
46	Lr	92	
47	SA	240	
48	SB	225	
49	SC	105	
50	SD	143	
51	SE	142	
52	SF	143	
53	SG	136	

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Mol	Chain	Length	Quality of chain
54	SH	146	
55	SI	144	
56	SJ	121	
57	SK	108	
58	SL	67	
59	SM	56	
60	SN	152	
61	SO	319	
62	SP	252	
63	SQ	255	
64	SR	254	
65	SS	261	
66	ST	236	
67	SU	190	
68	SV	200	
69	SW	197	
70	SX	156	
71	SY	151	
72	SZ	138	
73	Sa	87	
74	Sb	130	
75	Sc	145	
76	Sd	135	
77	Se	119	
78	Sf	82	

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Mol	Chain	Length	Quality of chain
79	Sg	63	43% 68% 17% 13%
80	m	76	25% 59% 33% 8%
81	n	75	48% 40% 41% 8% 11%

2 Entry composition [i](#)

There are 82 unique types of molecules in this entry. The entry contains 194356 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 25S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3041	Total	C	N	O	P	0	0
			65056	29059	11741	21215	3041		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	493	U	G	conflict	GB 831416132

- Molecule 2 is a RNA chain called 5S RNA.

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

- Molecule 3 is a RNA chain called 8S RNA.

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

- Molecule 4 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	10	Total	C	N	O	P	0	0
			218	98	44	66	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	1583	Total	C	N	O	P	0	0
			33767	15095	6008	11081	1583		

- Molecule 6 is a protein called 60S ribosomal protein L2-A.

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

- Molecule 7 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LE	386	Total	C	N	O	S	0	0
			3079	1954	584	533	8		

- Molecule 8 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LF	361	Total	C	N	O	S	0	0
			2749	1730	522	494	3		

- Molecule 9 is a protein called 60S ribosomal protein L5.

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

- Molecule 10 is a protein called Large ribosomal subunit protein eL6B.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	LH	156	Total	C	N	O	0	0
			1243	803	222	218		

- Molecule 11 is a protein called 60S ribosomal protein L7-A.

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

- Molecule 12 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LJ	233	Total	C	N	O	S	0	0
			1804	1151	323	327	3		

- Molecule 13 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LK	188	Total	C	N	O	S	0	0
			1493	948	271	270	4		

- Molecule 14 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LL	207	Total	C	N	O	S	0	0
			1686	1071	319	291	5		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LL	?	-	MET	deletion	UNP P41805
LL	?	-	LEU	deletion	UNP P41805
LL	?	-	SER	deletion	UNP P41805
LL	?	-	CYS	deletion	UNP P41805
LL	?	-	ALA	deletion	UNP P41805
LL	?	-	GLY	deletion	UNP P41805
LL	?	-	ALA	deletion	UNP P41805
LL	?	-	ASP	deletion	UNP P41805
LL	?	-	ARG	deletion	UNP P41805
LL	?	-	LEU	deletion	UNP P41805
LL	?	-	GLN	deletion	UNP P41805

- Molecule 15 is a protein called Large ribosomal subunit protein uL5B.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LM	169	Total	C	N	O	S	0	0
			1346	843	252	247	4		

- Molecule 16 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LN	193	Total	C	N	O	S	0	0
			1543	962	315	266			

- Molecule 17 is a protein called 60S ribosomal protein L14-A.

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

- Molecule 18 is a protein called 60S ribosomal protein L15-A.

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

- Molecule 19 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 20 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LR	172	Total	C	N	O	S	0	0
			1361	846	273	242			

- Molecule 21 is a protein called 60S ribosomal protein L18-A.

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

- Molecule 22 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LT	183	Total	C	N	O	S	0	0
			1482	911	320	251			

- Molecule 23 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LU	171	Total	C	N	O	S	0	0
			1437	925	266	243	3		

- Molecule 24 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LV	159	Total	C	N	O	S	0	0
			1272	802	245	221	4		

- Molecule 25 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	LW	100	Total	C	N	O	0	0
			796	516	131	149		

- Molecule 26 is a protein called 60S ribosomal protein L23-A.

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

- Molecule 27 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LY	62	Total	C	N	O	S	0	0
			513	330	101	81	1		

- Molecule 28 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LZ	120	Total	C	N	O	S	0	0
			959	617	168	172	2		

- Molecule 29 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	La	125	Total	C	N	O	0	0
			984	620	191	173		

- Molecule 30 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	Lb	133	Total	C	N	O	0	0
			1066	692	196	178		

- Molecule 31 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Lc	148	Total	C	N	O	S	0	0
			1169	747	231	188	3		

- Molecule 32 is a protein called 60S ribosomal protein L29.

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

- Molecule 33 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Le	96	Total	C	N	O	S	0	0
			737	476	123	137	1		

- Molecule 34 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Lf	105	Total	C	N	O	S	0	0
			856	544	163	148	1		

- Molecule 35 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Lg	126	Total	C	N	O	S	0	0
			1008	638	203	166	1		

- Molecule 36 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 37 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Li	110	Total	C	N	O	S	0	0
			866	536	176	150	4		

- Molecule 38 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 39 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Lk	98	Total	C	N	O	S	0	0
			761	475	153	131	2		

- Molecule 40 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Ll	81	Total	C	N	O	S	0	0
			645	393	141	106	5		

- Molecule 41 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lm	77	Total	C	N	O	S	0	0
			608	388	114	106			

- Molecule 42 is a protein called 60S ribosomal protein L39.

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

- Molecule 43 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lo	51	Total	C	N	O	S	0	0
			409	253	85	66	5		

- Molecule 44 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Lp	24	Total	C	N	O	S	0	0
			224	136	61	26	1		

- Molecule 45 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lq	100	Total	C	N	O	S	0	0
			805	506	163	131	5		

- Molecule 46 is a protein called 60S ribosomal protein L43-A.

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

- Molecule 47 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SA	222	Total	C	N	O	S	0	0
			1729	1098	312	313	6		

- Molecule 48 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SB	206	Total	C	N	O	S	0	0
			1605	1005	299	298	3		

- Molecule 49 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SC	83	Total	C	N	O	S	0	0
			708	461	113	132	2		

- Molecule 50 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SD	97	Total	C	N	O	S	0	0
			736	466	127	141	2		

- Molecule 51 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SE	116	Total	C	N	O	S	0	0
			905	577	167	154	7		

- Molecule 52 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SF	141	Total	C	N	O		0	0
			1095	702	199	194			

- Molecule 53 is a protein called 40S ribosomal protein S17-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SG	114	Total	C	N	O	S	0	0
			908	573	169	164	2		

- Molecule 54 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SH	145	Total	C	N	O	S	0	0
			1188	741	237	208	2		

- Molecule 55 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SI	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 56 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SJ	100	Total	C	N	O	S	0	0
			797	506	144	146	1		

- Molecule 57 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	SK	84	Total	C	N	O	0	0
			650	415	121	114		

- Molecule 58 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SL	62	Total	C	N	O	S	0	0
			486	300	95	90	1		

- Molecule 59 is a protein called 40S ribosomal protein S29-A.

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

- Molecule 60 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SN	56	Total	C	N	O	S	0	0
			429	271	84	70	4		

- Molecule 61 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SO	311	Total	C	N	O	S	0	0
			2375	1509	408	451	7		

- Molecule 62 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SP	205	Total	C	N	O	S	0	0
			1596	1025	283	286	2		

- Molecule 63 is a protein called Small ribosomal subunit protein eS1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SQ	225	Total	C	N	O	S	0	0
			1787	1131	328	324	4		

- Molecule 64 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SR	216	Total	C	N	O	S	0	0
			1626	1042	287	295	2		

- Molecule 65 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SS	258	Total	C	N	O	S	0	0
			2056	1308	387	358	3		

- Molecule 66 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	ST	218	Total	C	N	O	S	0	0
			1755	1102	337	313	3		

- Molecule 67 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
67	SU	180	Total	C	N	O		
			1451	932	259	260	0	0

- Molecule 68 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SV	186	Total	C	N	O	S		
			1471	913	294	262	2	0	0

- Molecule 69 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SW	184	Total	C	N	O	S		
			1479	935	285	258	1	0	0

- Molecule 70 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SX	141	Total	C	N	O	S		
			1137	730	216	188	3	0	0

- Molecule 71 is a protein called 40S ribosomal protein S13.

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

- Molecule 72 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SZ	127	Total	C	N	O	S		
			923	568	185	167	3	0	0

- Molecule 73 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Sa	87	Total	C	N	O	S		
			673	415	125	131	2	0	0

- Molecule 74 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 75 is a protein called 40S ribosomal protein S23-A.

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

- Molecule 76 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Sd	131	Total	C	N	O	S	0	0
			1016	642	192	182			

- Molecule 77 is a protein called Small ribosomal subunit protein eS26B.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Se	97	Total	C	N	O	S	0	0
			765	473	160	127	5		

- Molecule 78 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Sf	74	Total	C	N	O	S	0	0
			562	353	101	105	3		

- Molecule 79 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Sg	55	Total	C	N	O	S	0	0
			437	276	89	71	1		

- Molecule 80 is a RNA chain called A site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	m	76	Total	C	N	O	P	0	0
			1611	721	281	534	75		

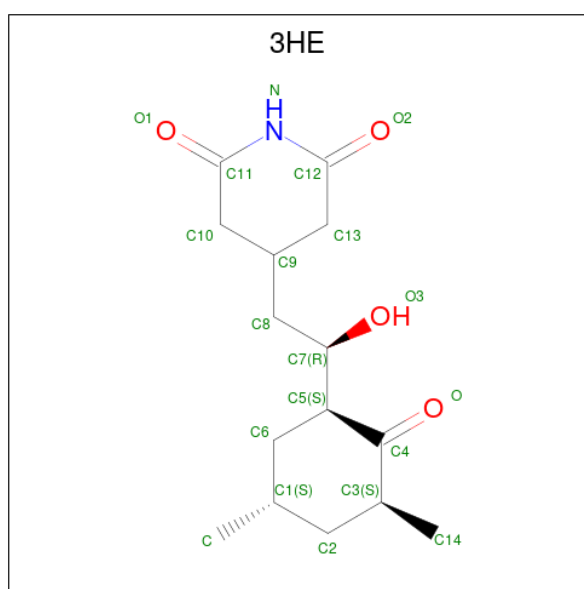
- Molecule 81 is a RNA chain called P site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	n	67	Total	C	N	O	P	0	0
			1431	638	262	464	67		

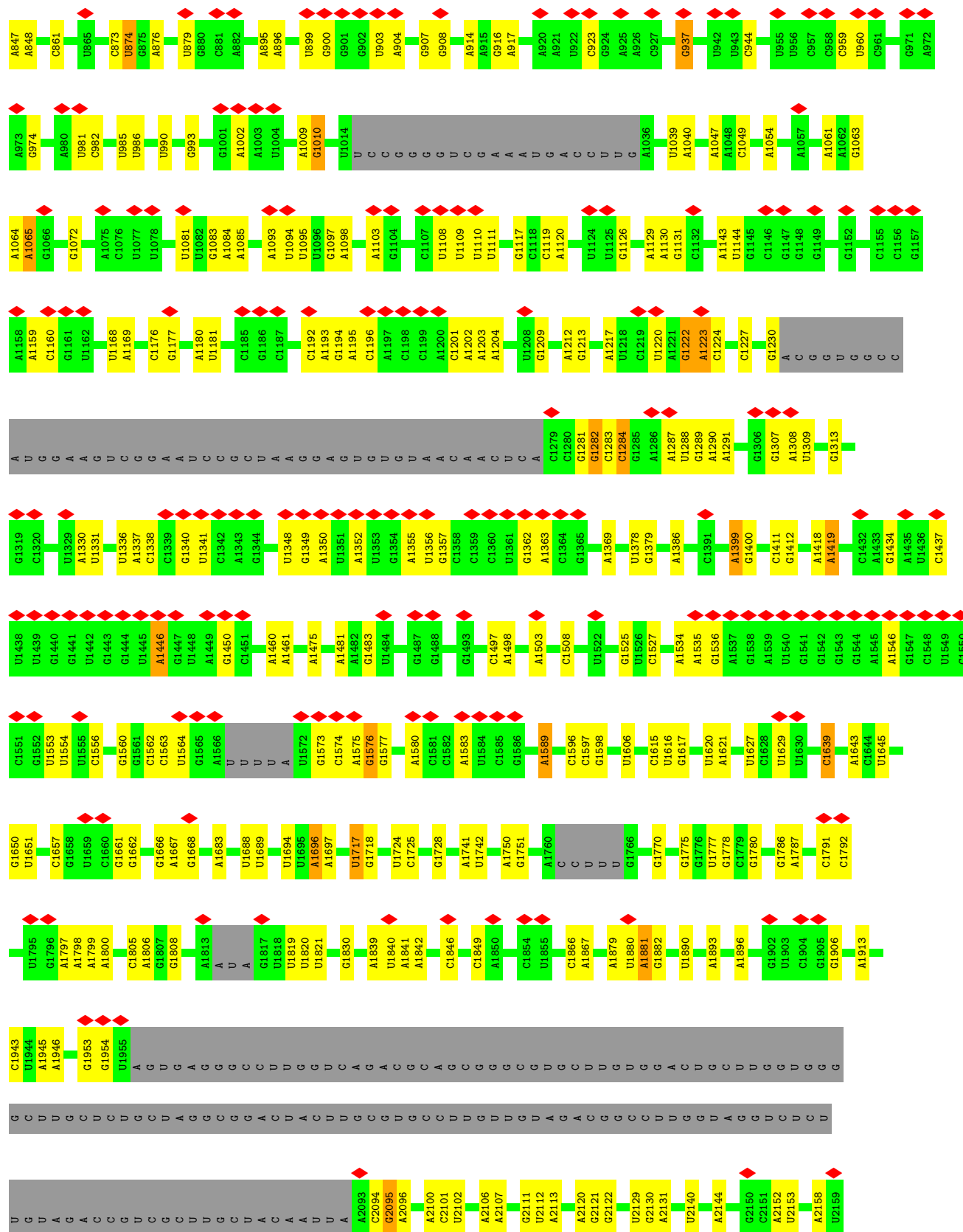
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	10	A	G	conflict	GB 176433

- Molecule 82 is 4-{(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl}piperidine-2,6-dione (CCD ID: 3HE) (formula: C₁₅H₂₃NO₄) (labeled as "Ligand of Interest" by depositor).

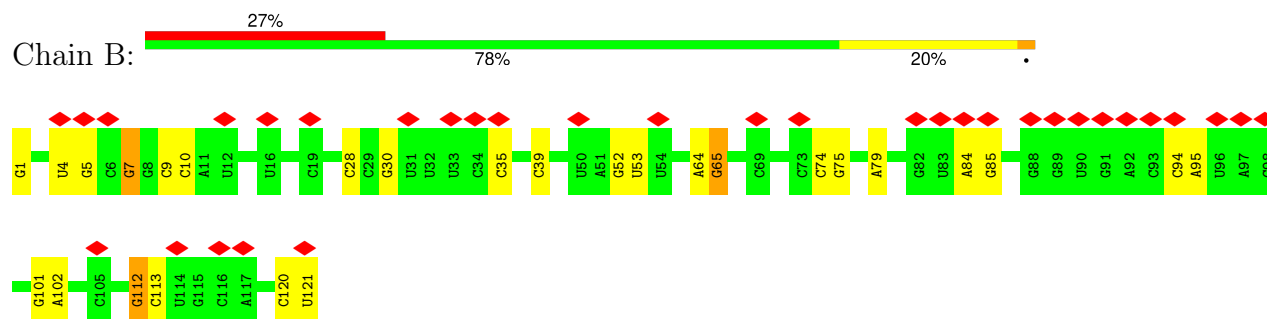


Mol	Chain	Residues	Atoms				AltConf
82	A	1	Total	C	N	O	0
			20	15	1	4	

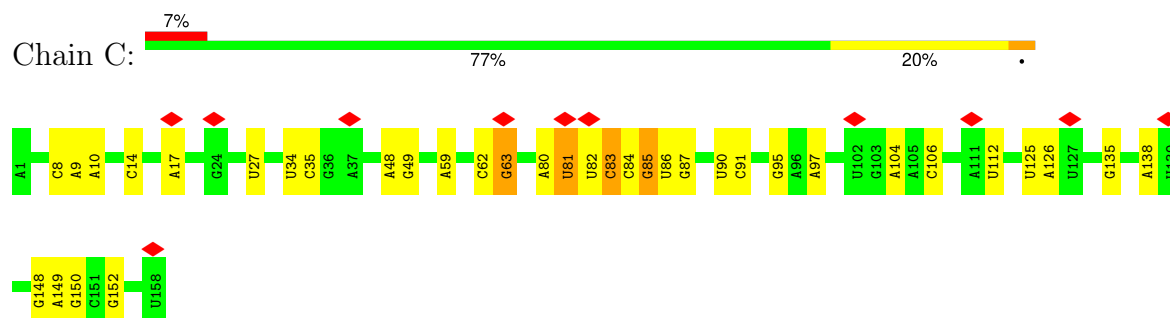




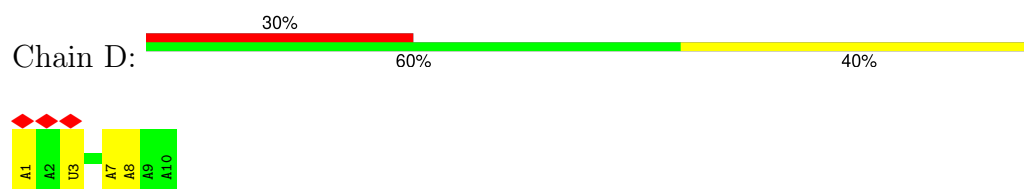
- Molecule 2: 5S RNA



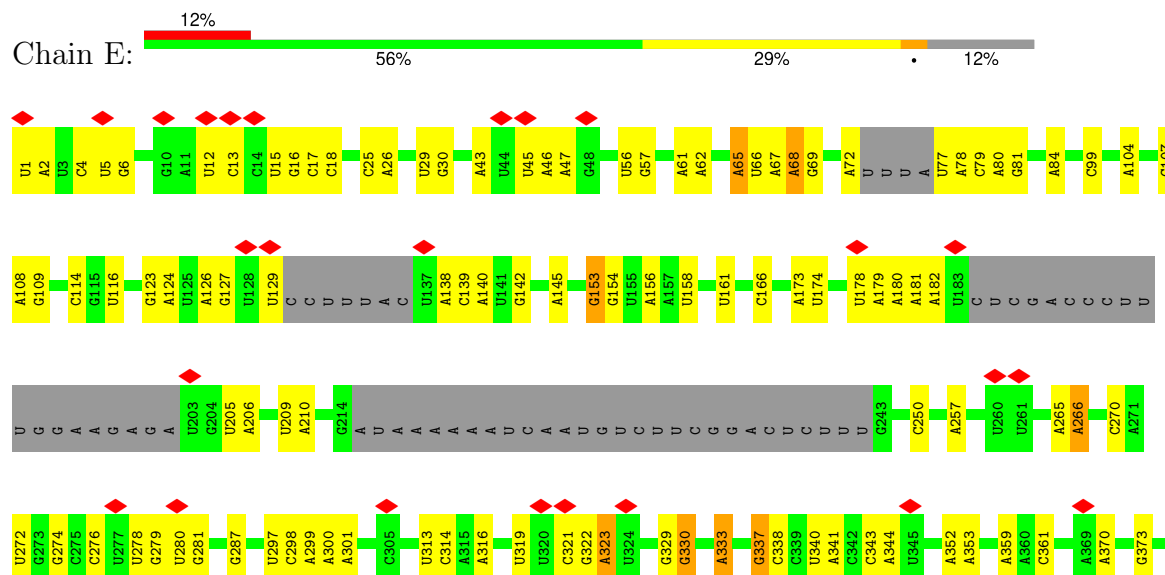
- Molecule 3: 8S RNA

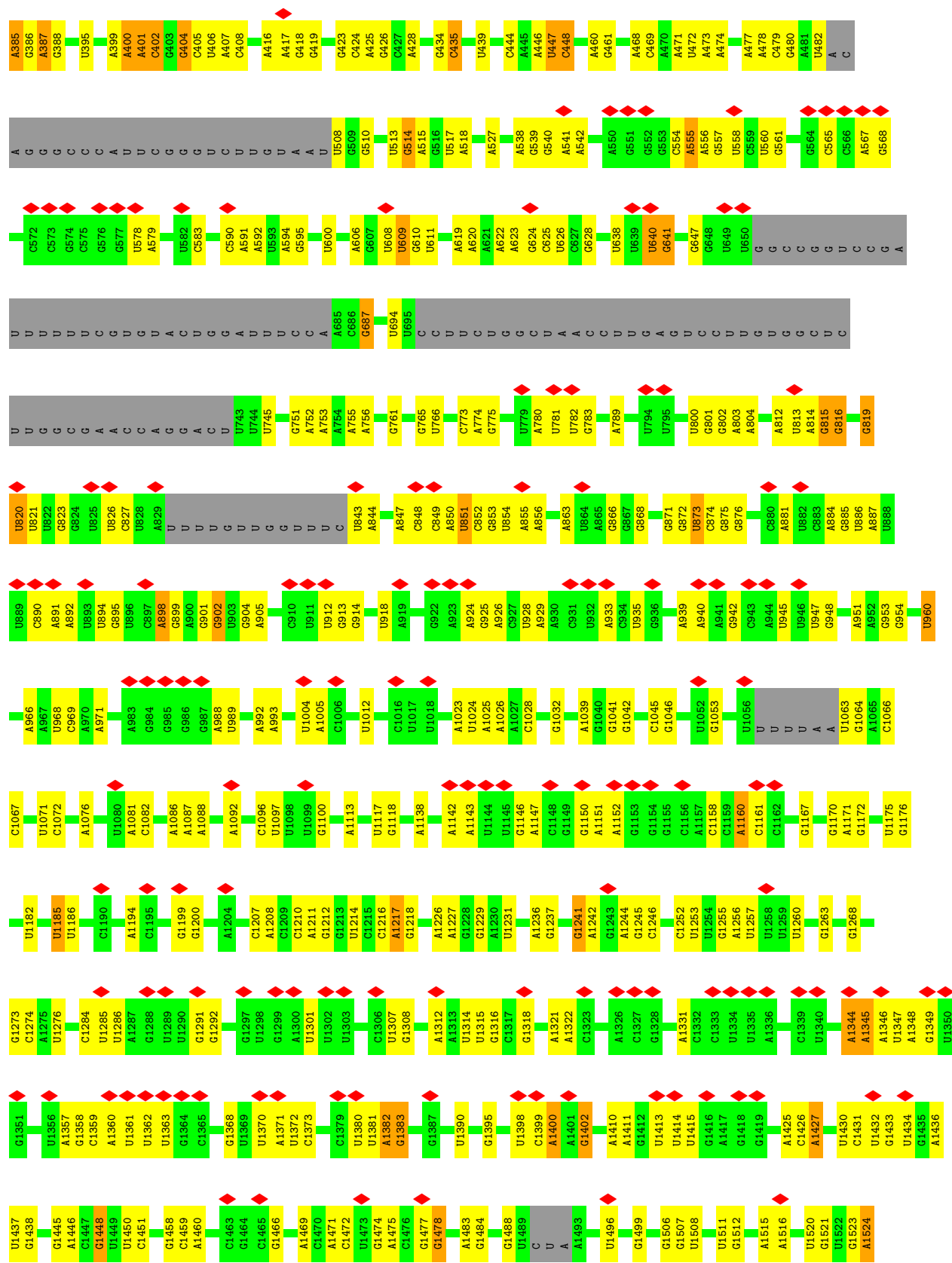


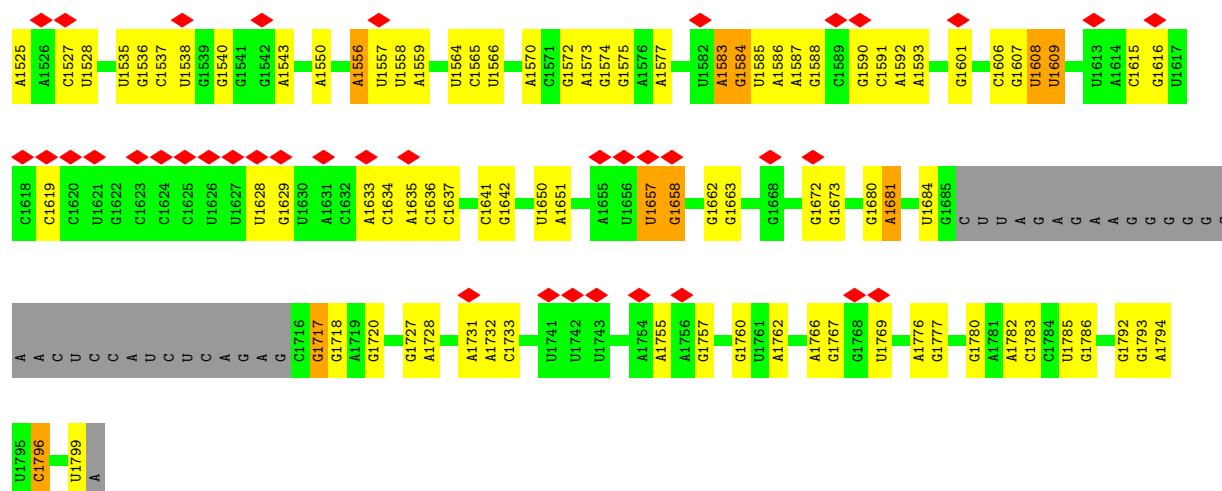
- Molecule 4: messenger RNA



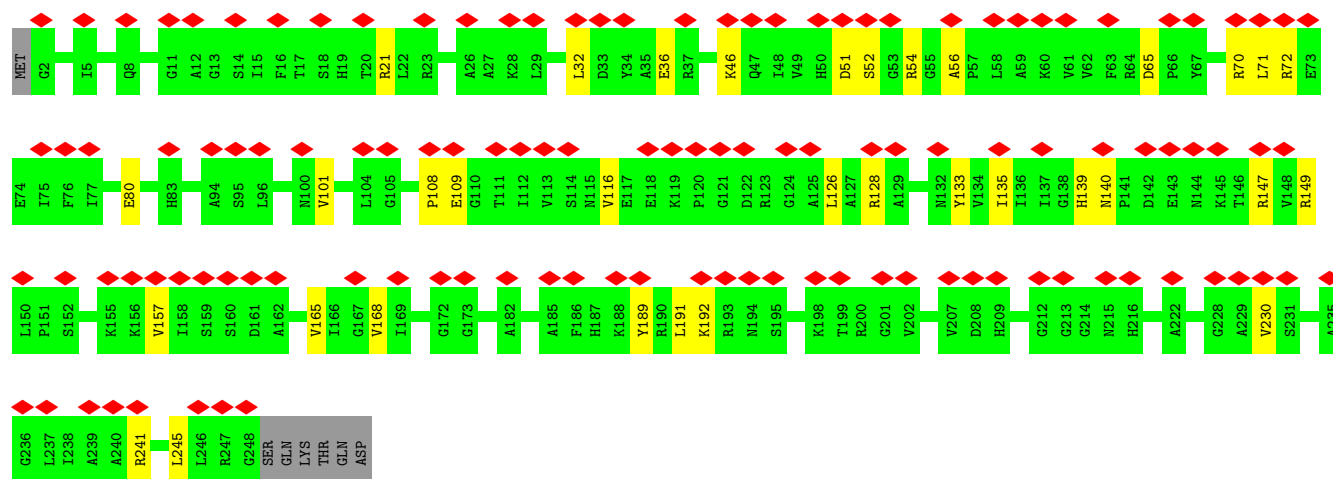
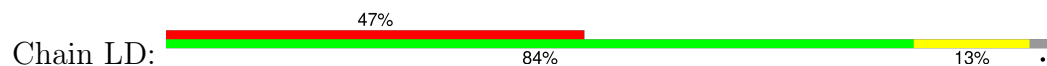
- Molecule 5: 18S rRNA



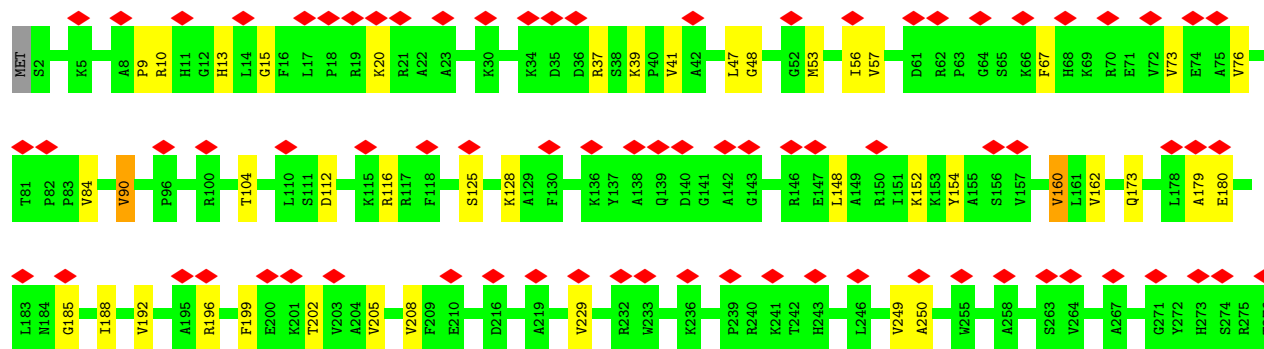
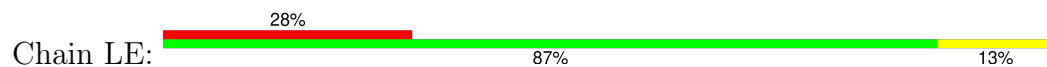


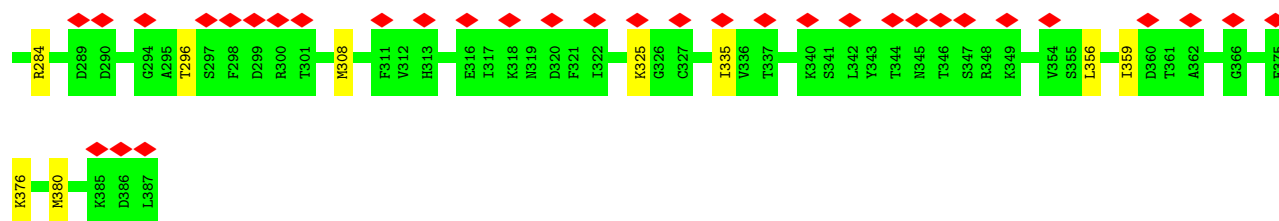


• Molecule 6: 60S ribosomal protein L2-A

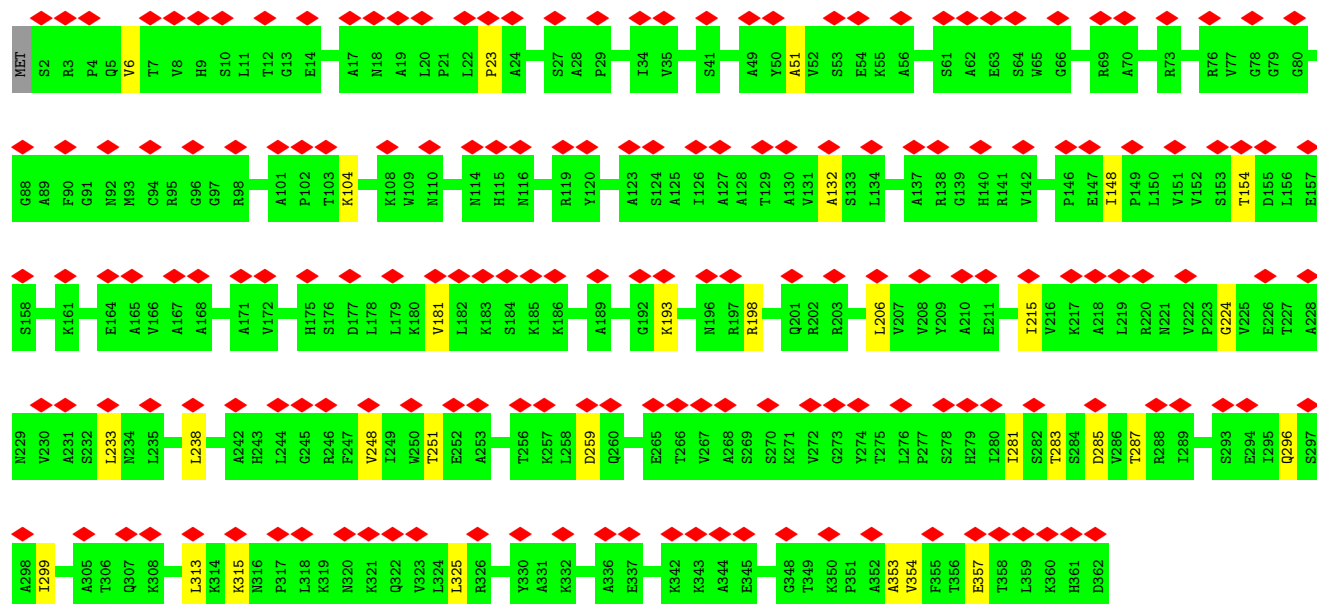


• Molecule 7: 60S ribosomal protein L3

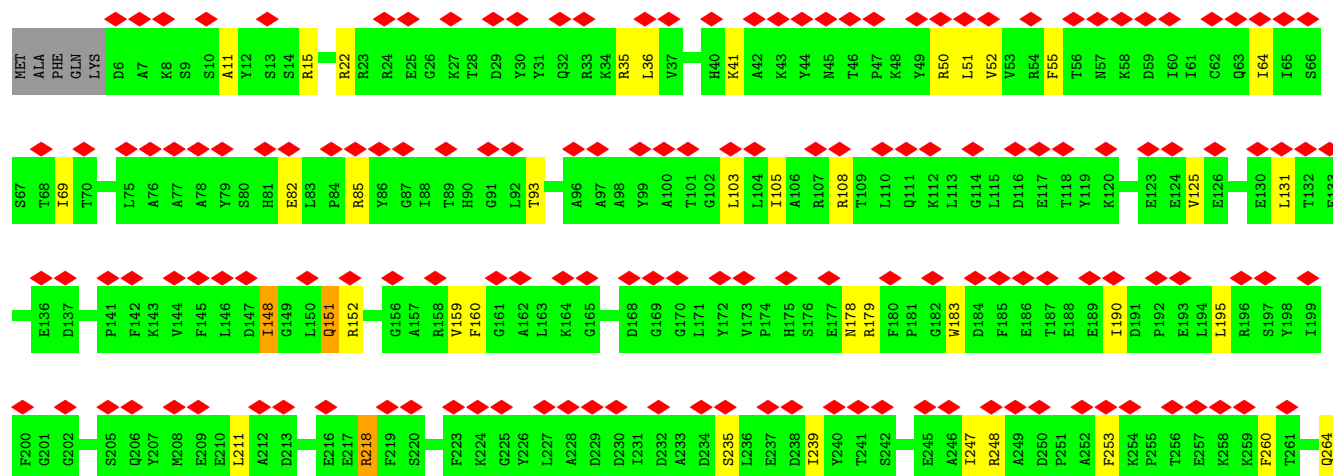
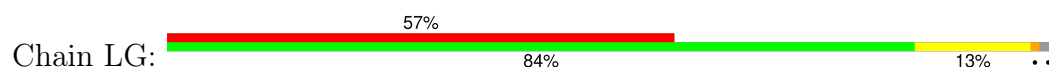


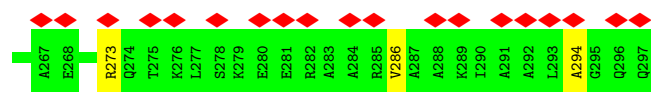


• Molecule 8: 60S ribosomal protein L4-A

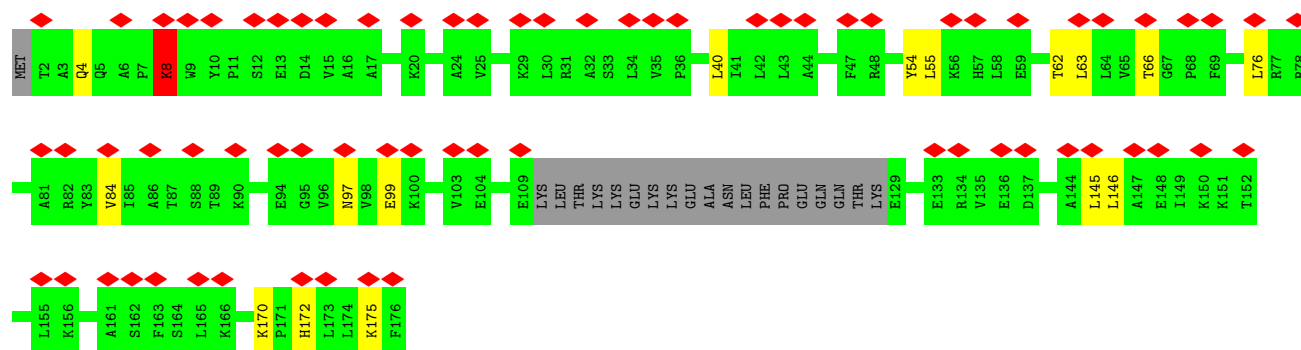
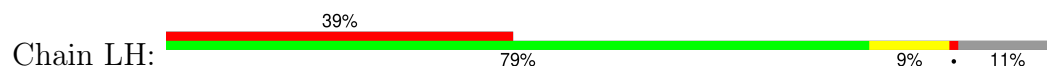


• Molecule 9: 60S ribosomal protein L5

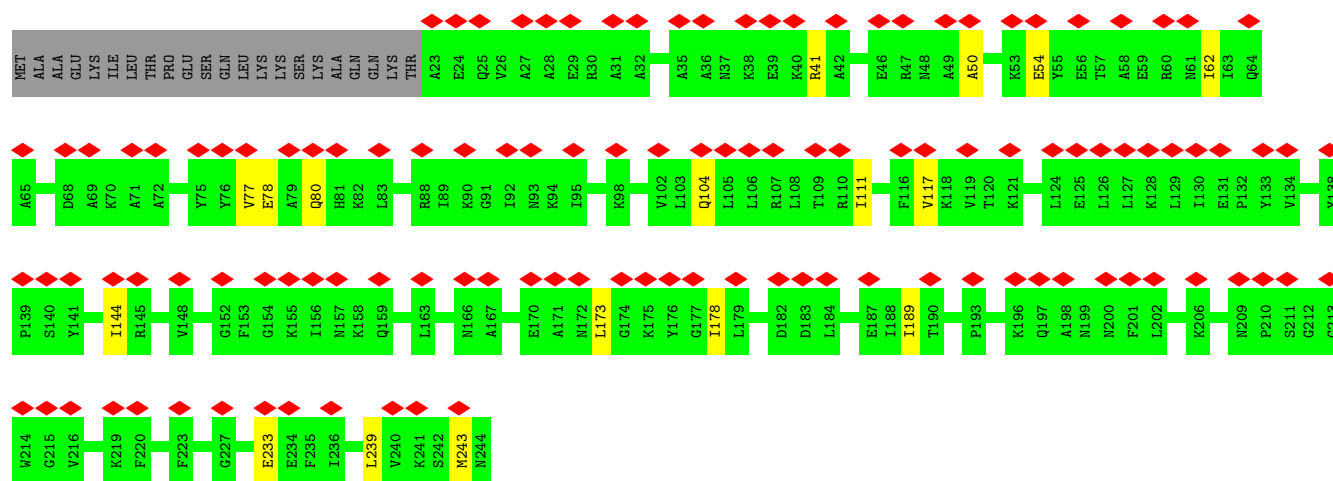
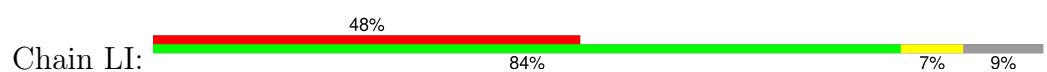




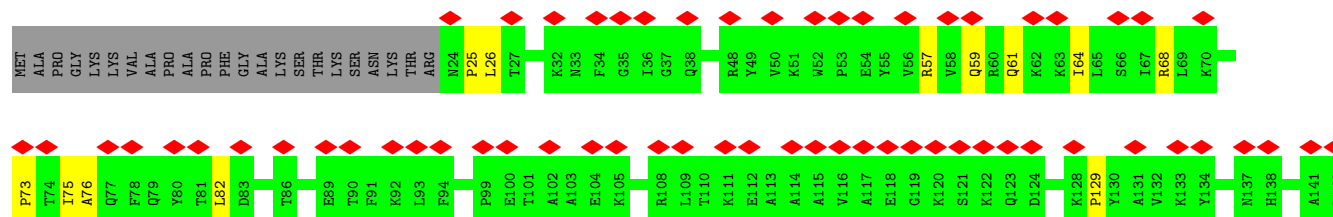
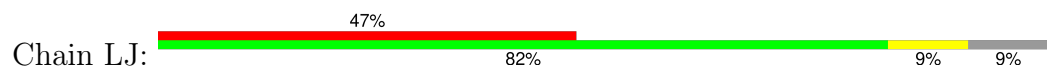
- Molecule 10: Large ribosomal subunit protein eL6B

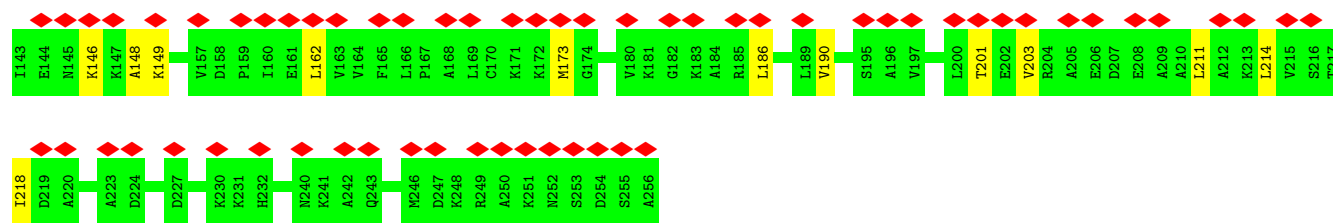


- Molecule 11: 60S ribosomal protein L7-A

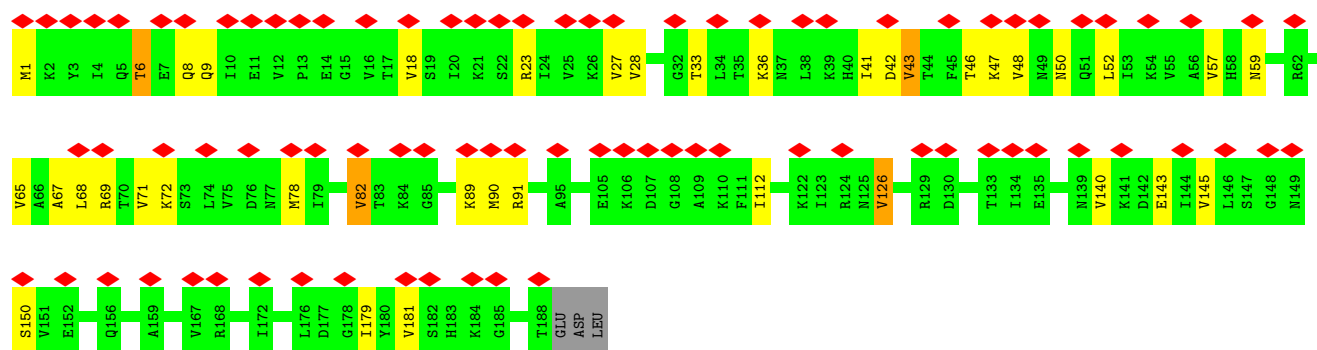
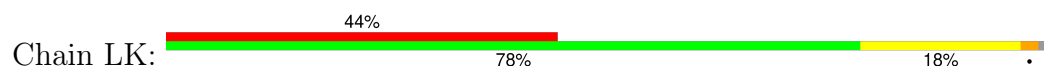


- Molecule 12: 60S ribosomal protein L8-A

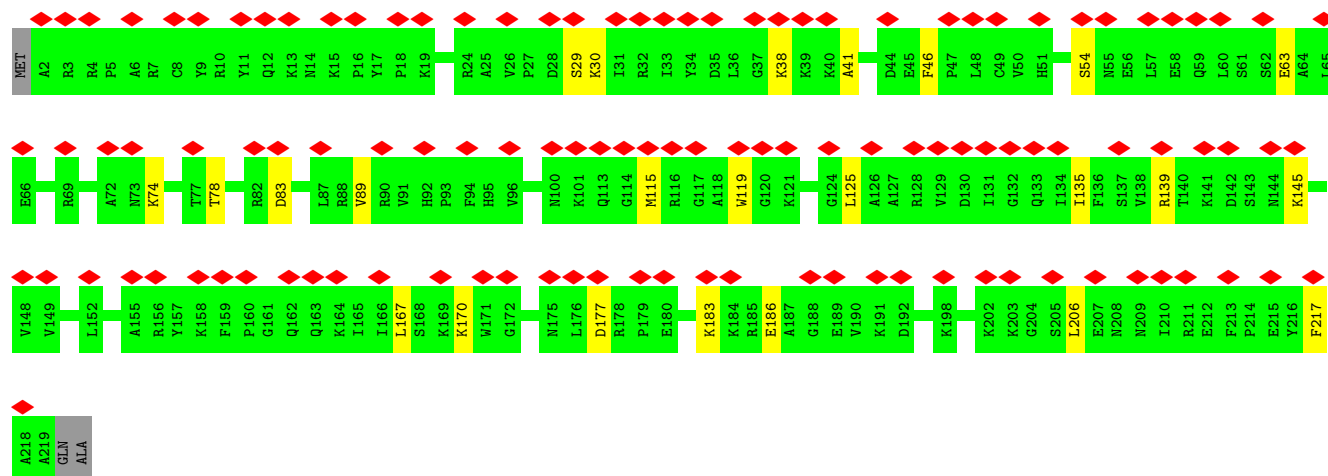
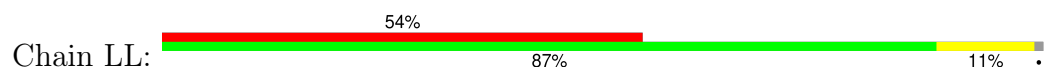




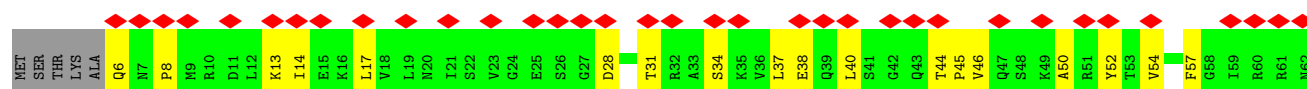
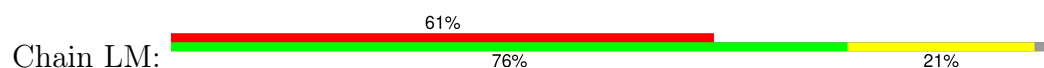
• Molecule 13: 60S ribosomal protein L9-A

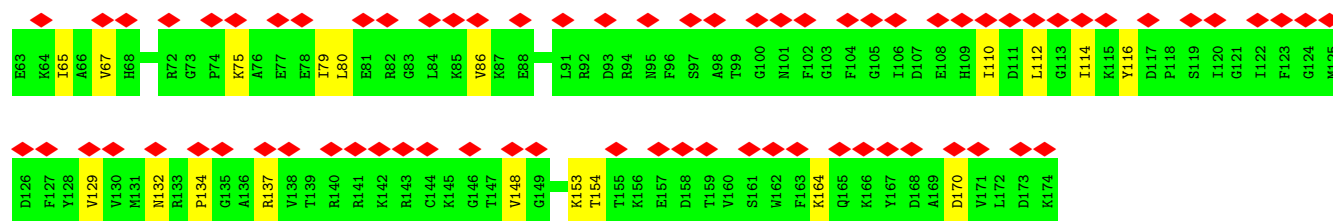


• Molecule 14: Large ribosomal subunit protein uL16

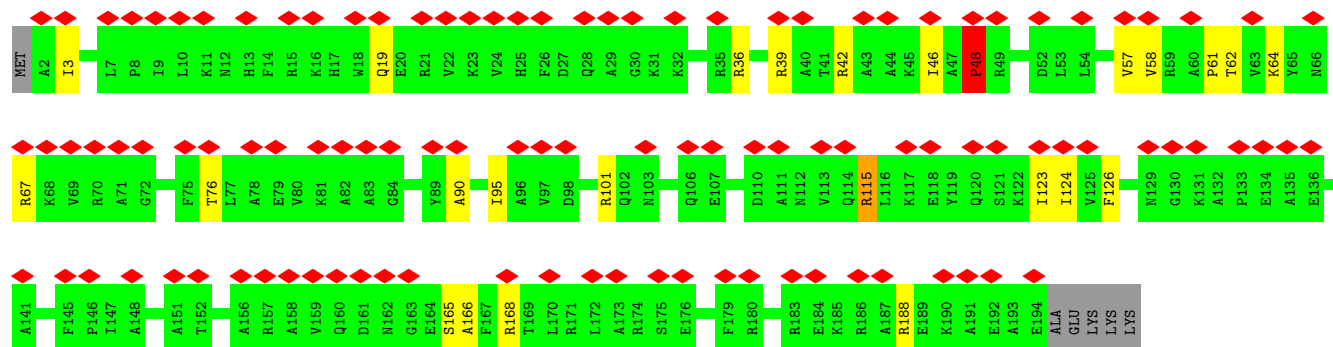
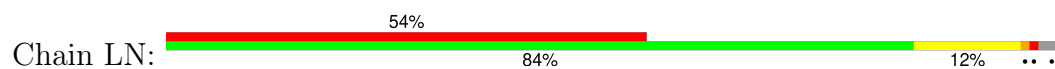


• Molecule 15: Large ribosomal subunit protein uL5B

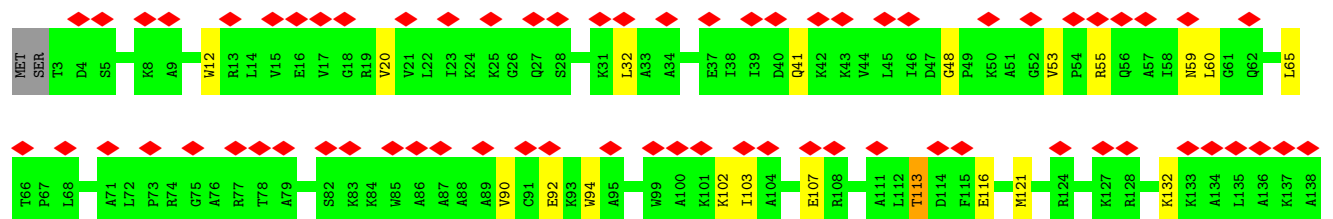
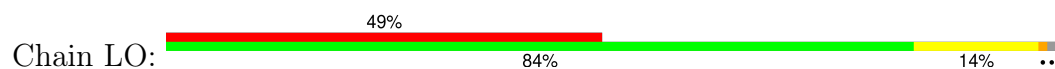




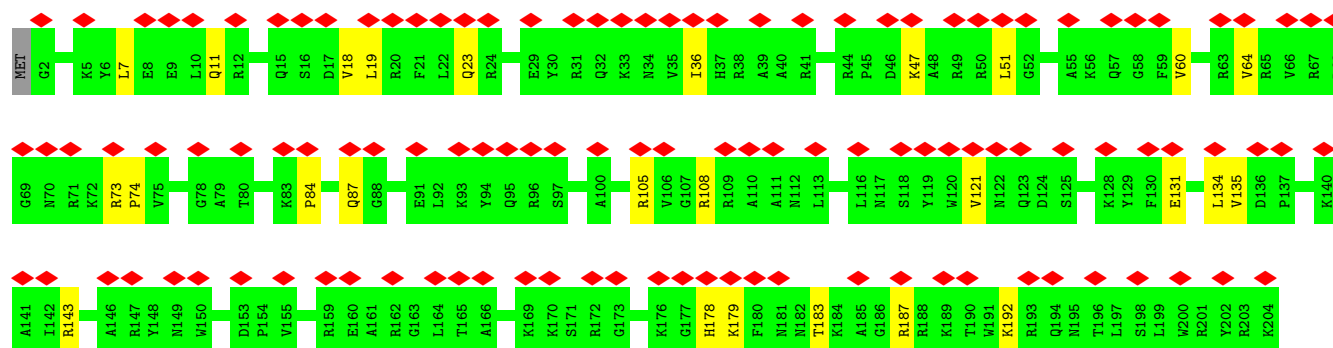
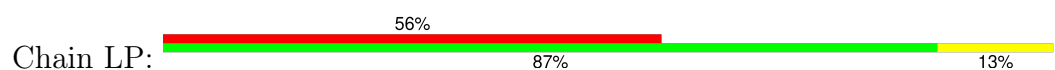
• Molecule 16: 60S ribosomal protein L13-A



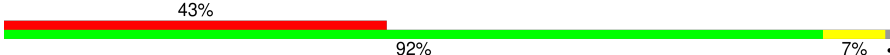
• Molecule 17: 60S ribosomal protein L14-A

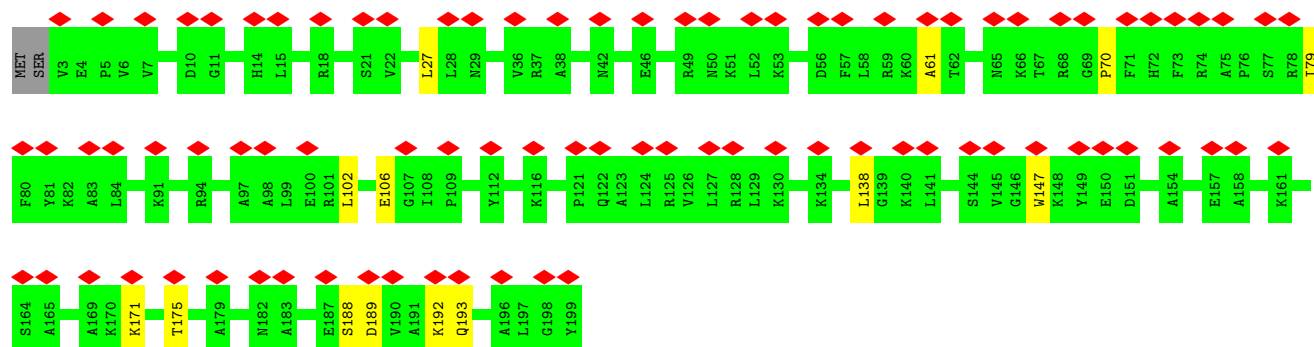


• Molecule 18: 60S ribosomal protein L15-A



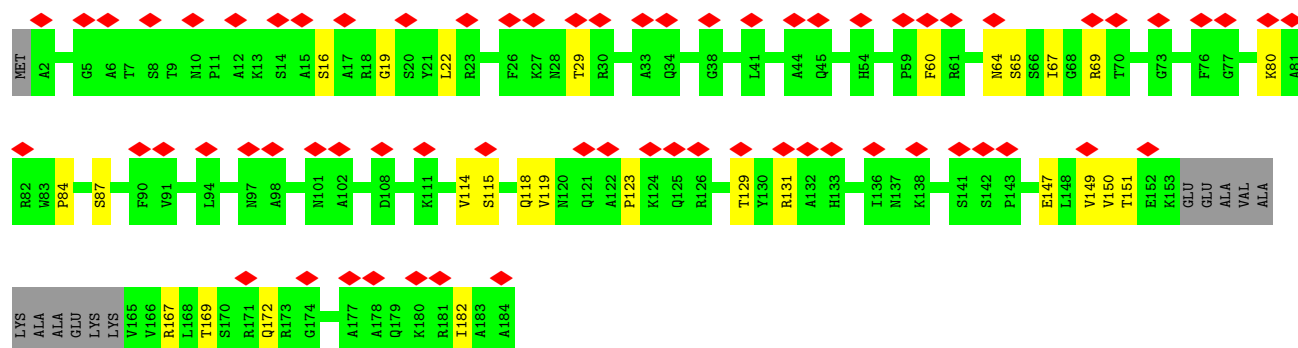
• Molecule 19: 60S ribosomal protein L16-A

Chain LQ: 



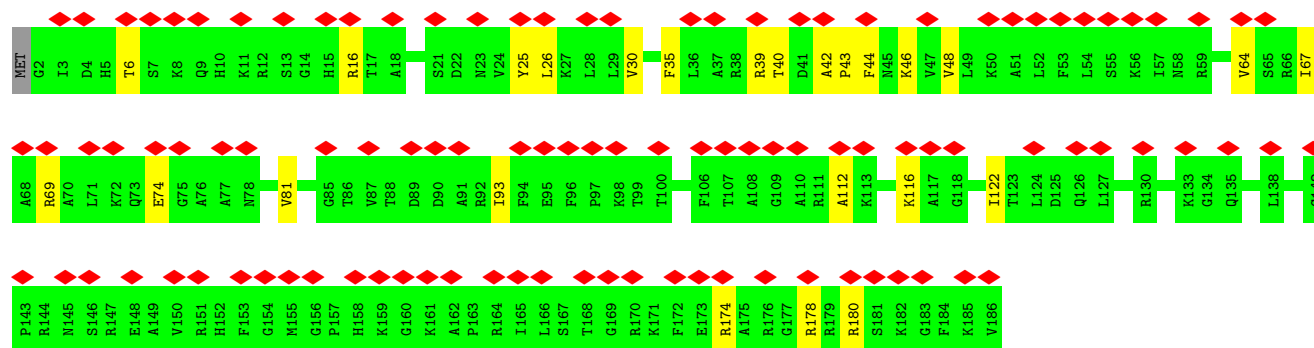
- Molecule 20: 60S ribosomal protein L17-A

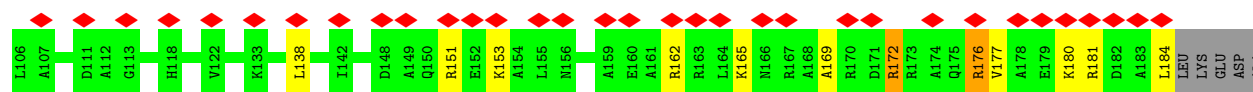
Chain LR: 



- Molecule 21: 60S ribosomal protein L18-A

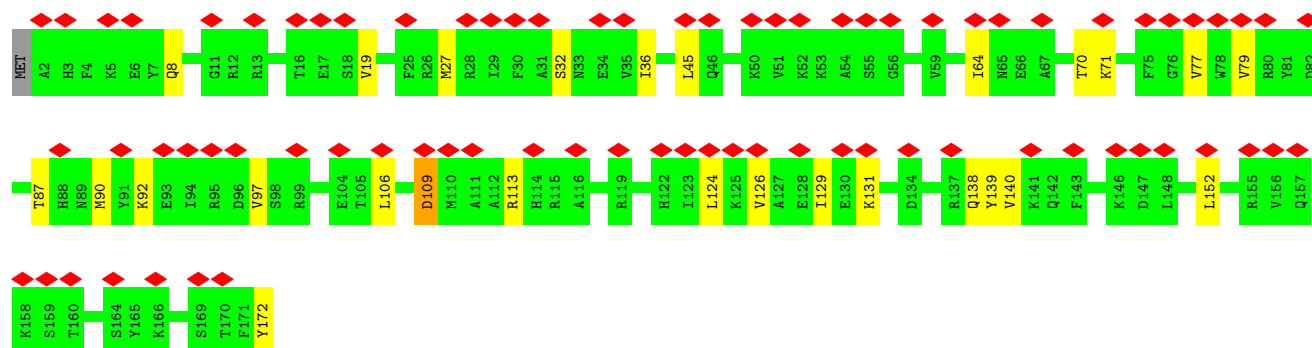
Chain LS: 





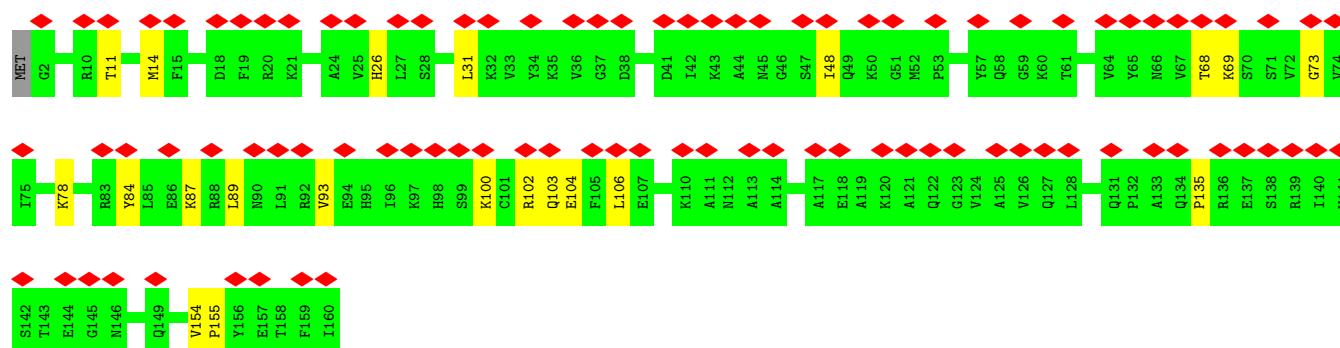
• Molecule 23: 60S ribosomal protein L20-A

Chain LU: 45% 84% 15% ..



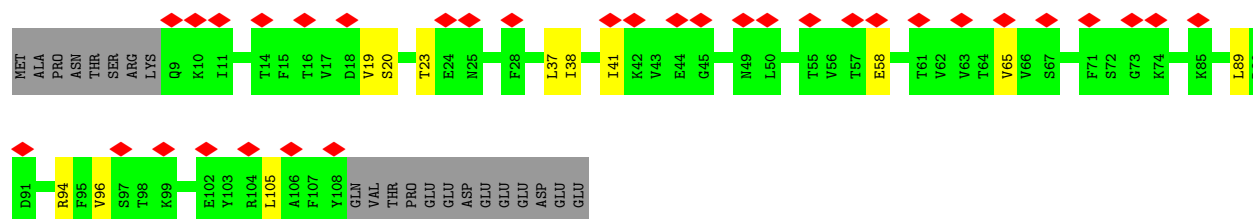
• Molecule 24: 60S ribosomal protein L21-A

Chain LV: 58% 86% 13% .



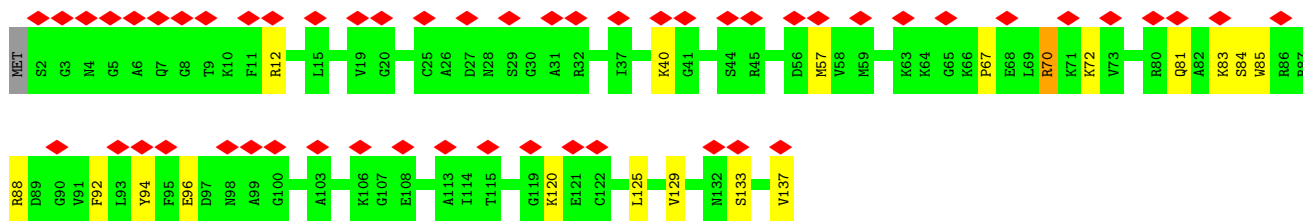
• Molecule 25: 60S ribosomal protein L22-A

Chain LW: 27% 73% 10% 17%

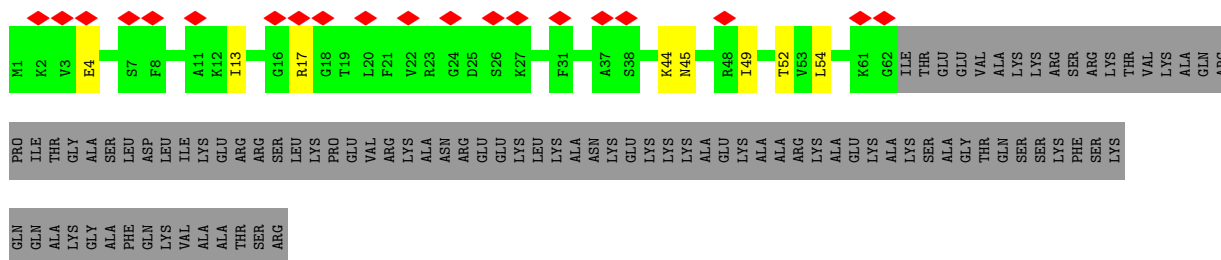
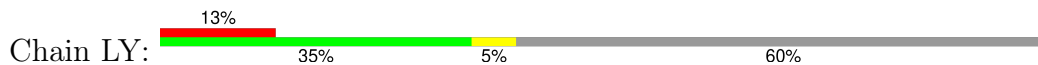


• Molecule 26: 60S ribosomal protein L23-A

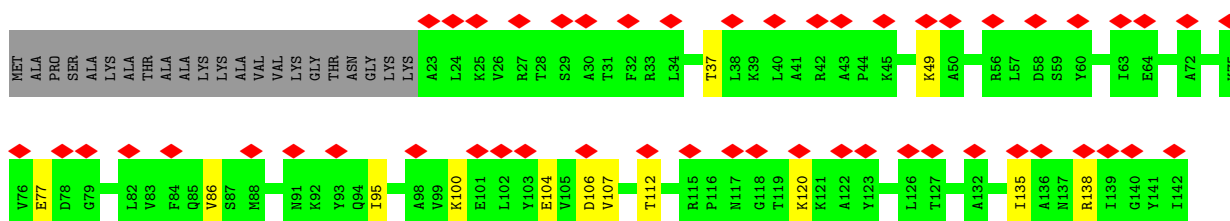
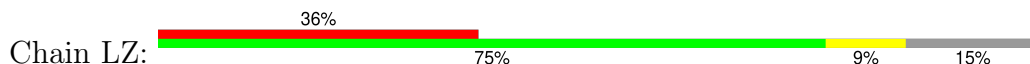
Chain LX: 39% 85% 13% ..



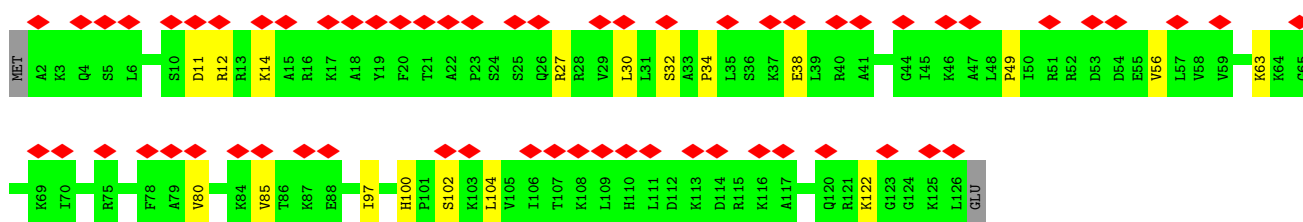
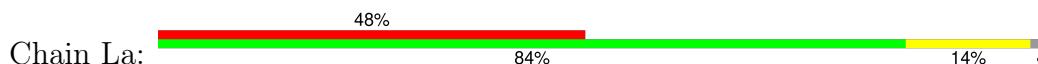
• Molecule 27: 60S ribosomal protein L24-A



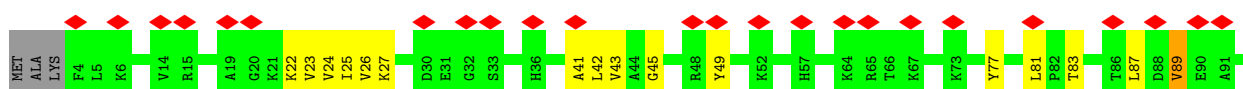
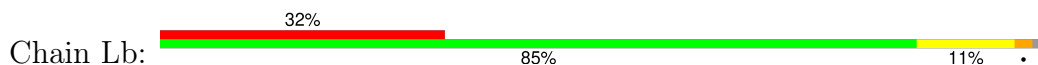
• Molecule 28: 60S ribosomal protein L25

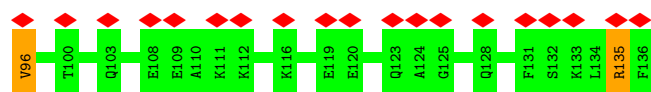


• Molecule 29: 60S ribosomal protein L26-A

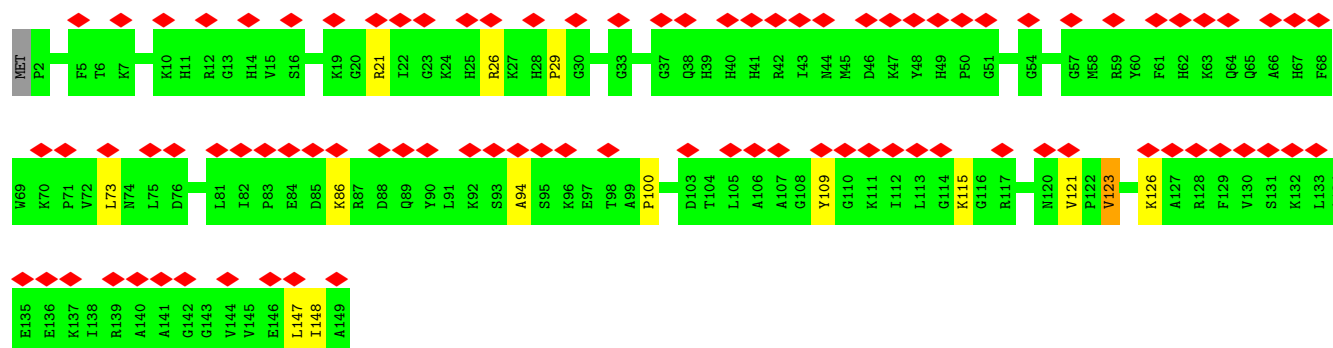
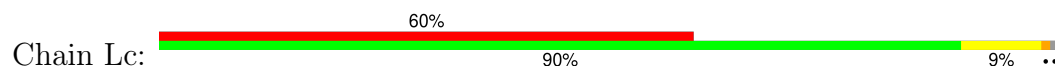


• Molecule 30: 60S ribosomal protein L27-A

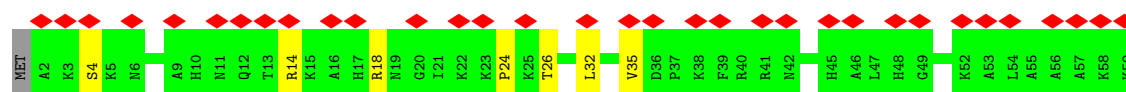
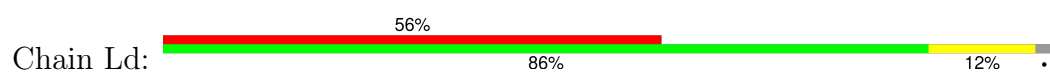




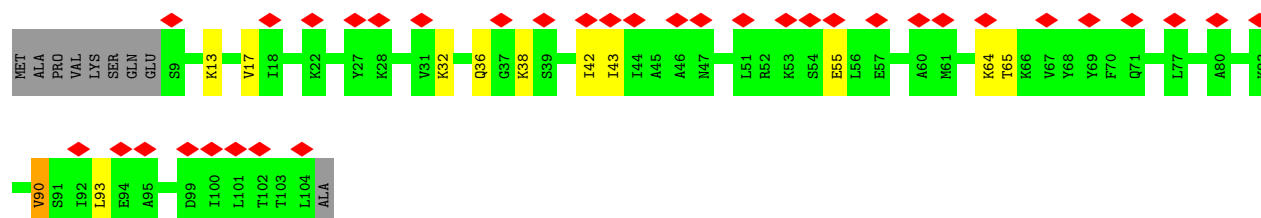
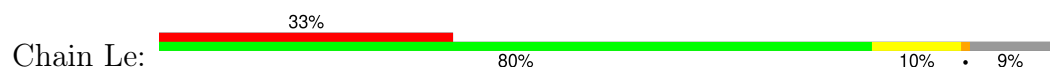
- Molecule 31: 60S ribosomal protein L28



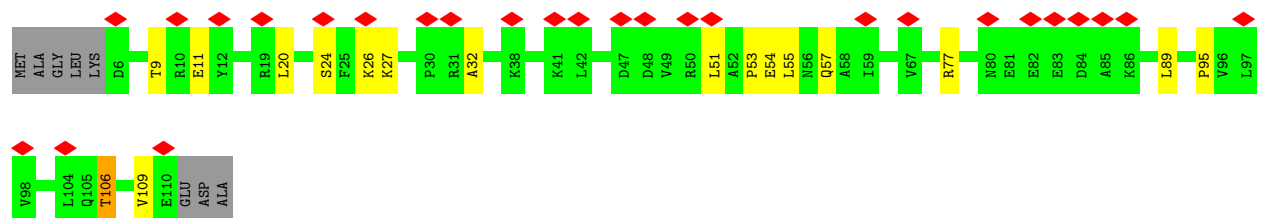
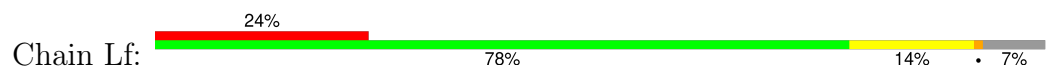
- Molecule 32: 60S ribosomal protein L29



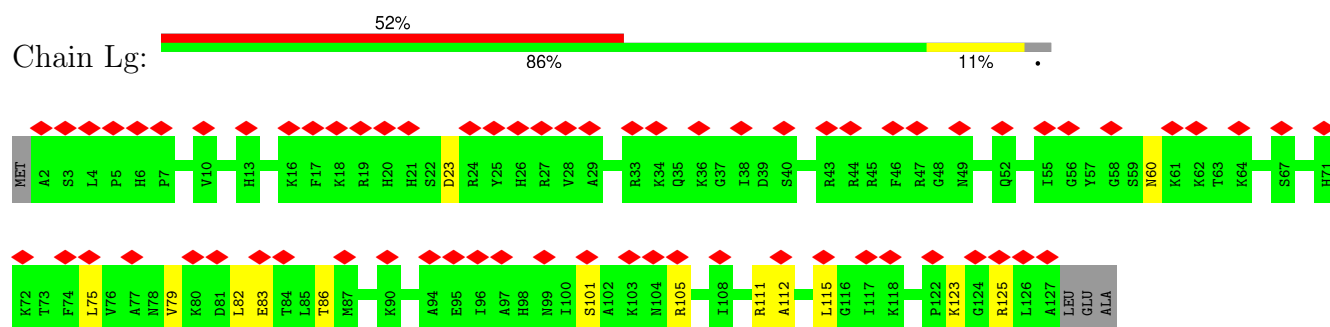
- Molecule 33: 60S ribosomal protein L30



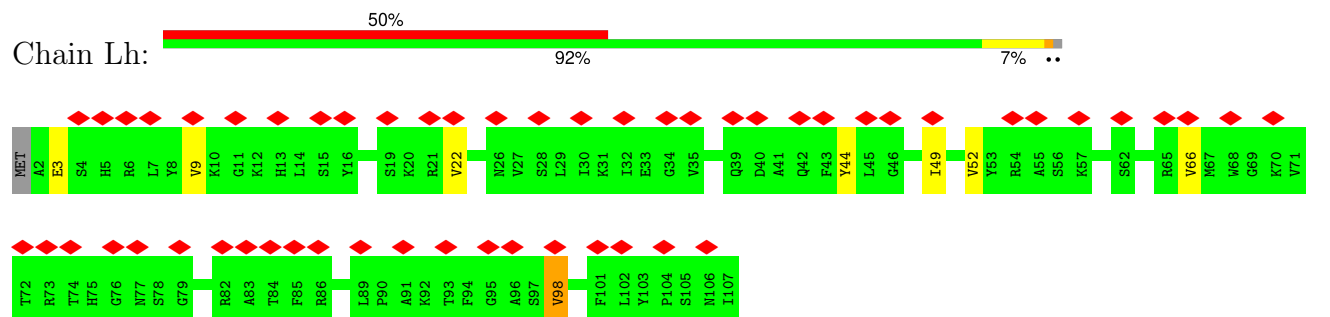
- Molecule 34: 60S ribosomal protein L31-A



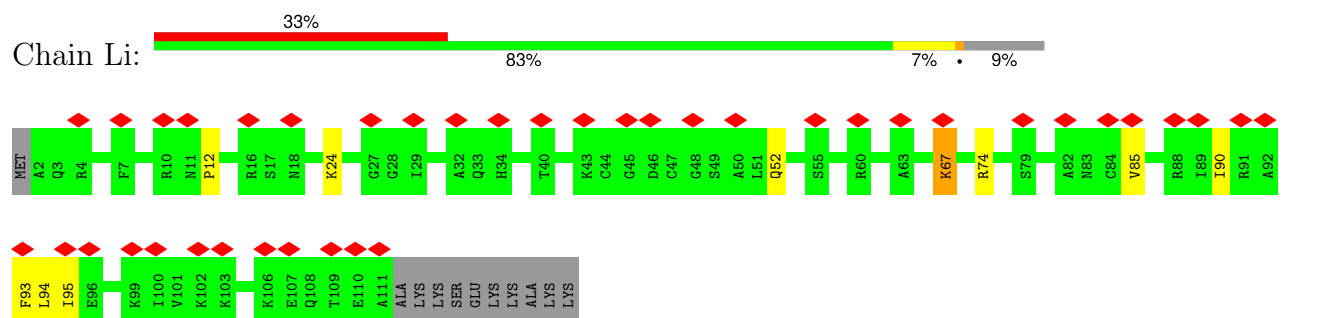
- Molecule 35: 60S ribosomal protein L32



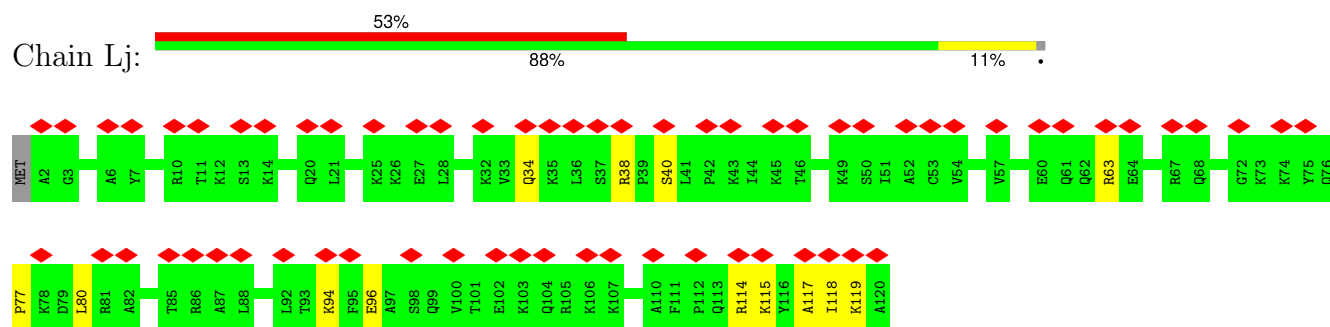
• Molecule 36: 60S ribosomal protein L33-A



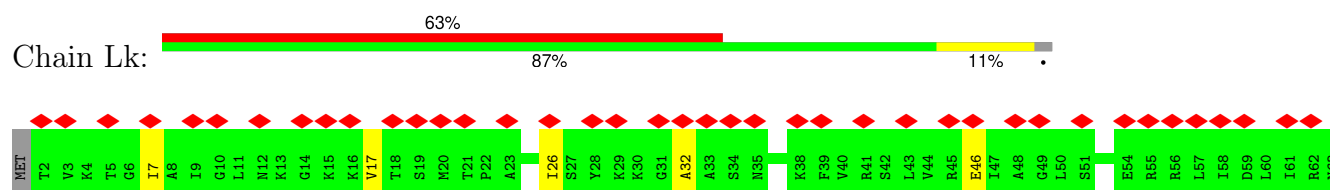
• Molecule 37: 60S ribosomal protein L34-A

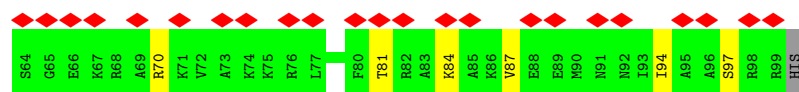


• Molecule 38: 60S ribosomal protein L35-A

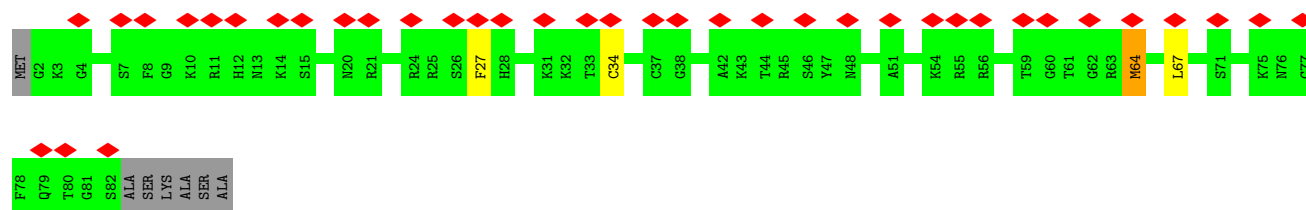
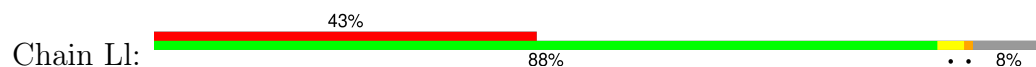


• Molecule 39: 60S ribosomal protein L36-A

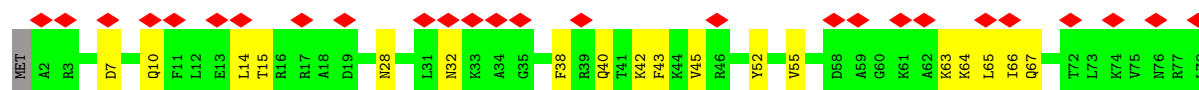
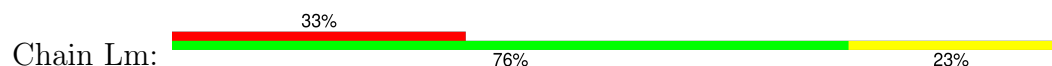




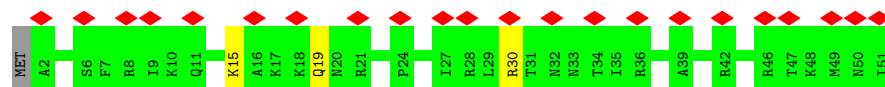
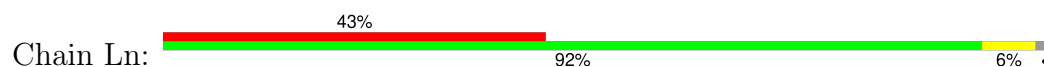
- Molecule 40: 60S ribosomal protein L37-A



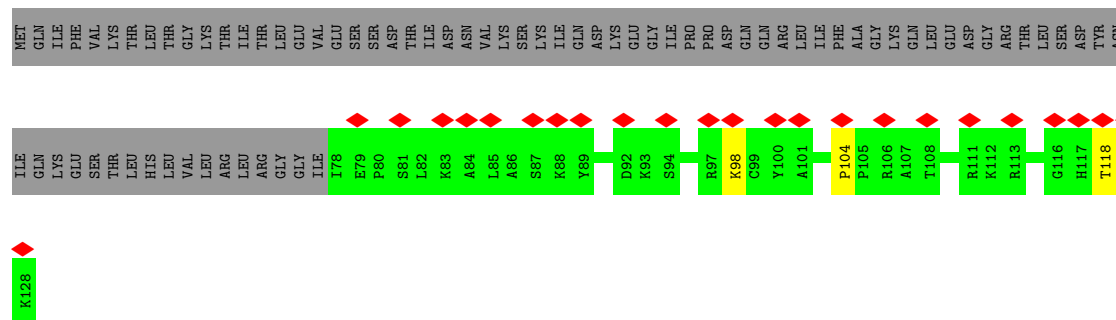
- Molecule 41: 60S ribosomal protein L38



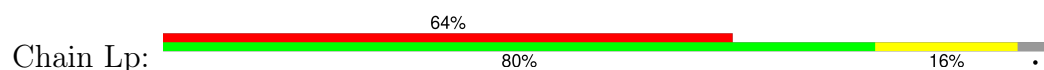
- Molecule 42: 60S ribosomal protein L39



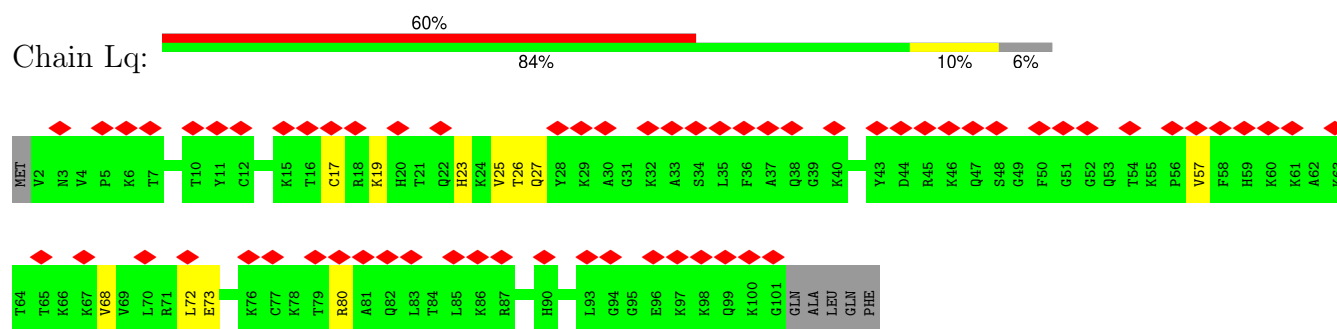
- Molecule 43: Ubiquitin-60S ribosomal protein L40



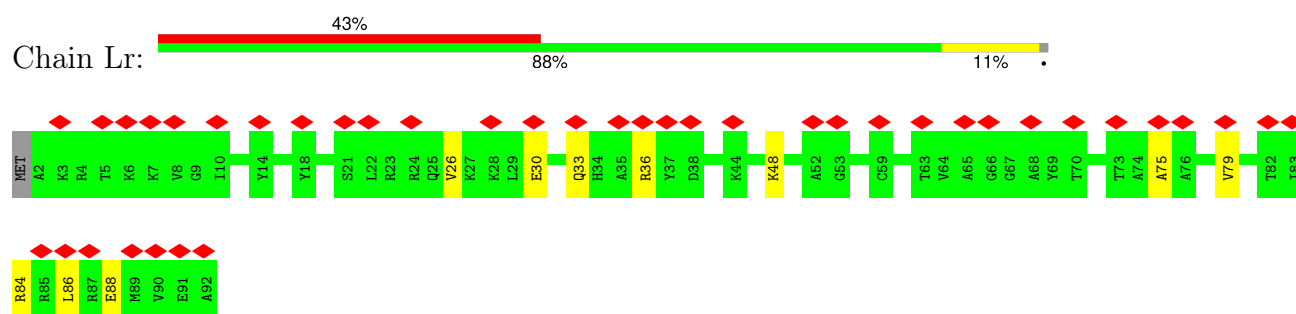
- Molecule 44: 60S ribosomal protein L41-A



- Molecule 45: 60S ribosomal protein L42-A



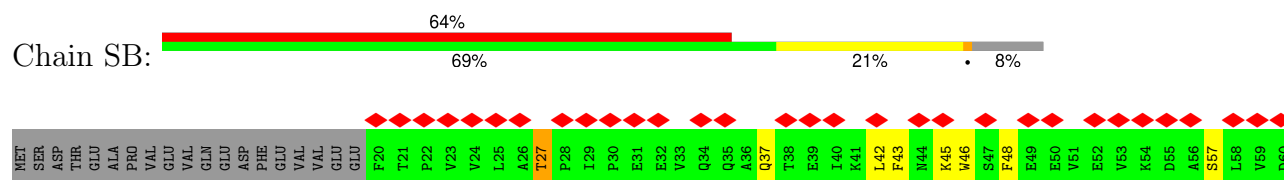
- Molecule 46: 60S ribosomal protein L43-A

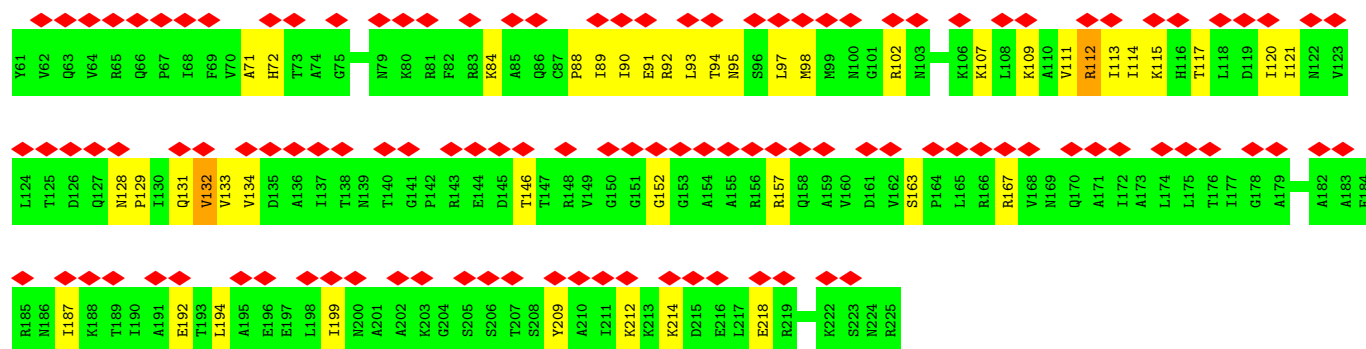


- Molecule 47: 40S ribosomal protein S3

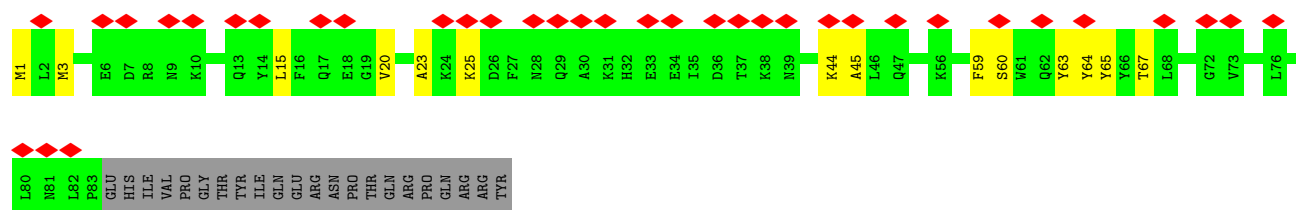


- Molecule 48: 40S ribosomal protein S5

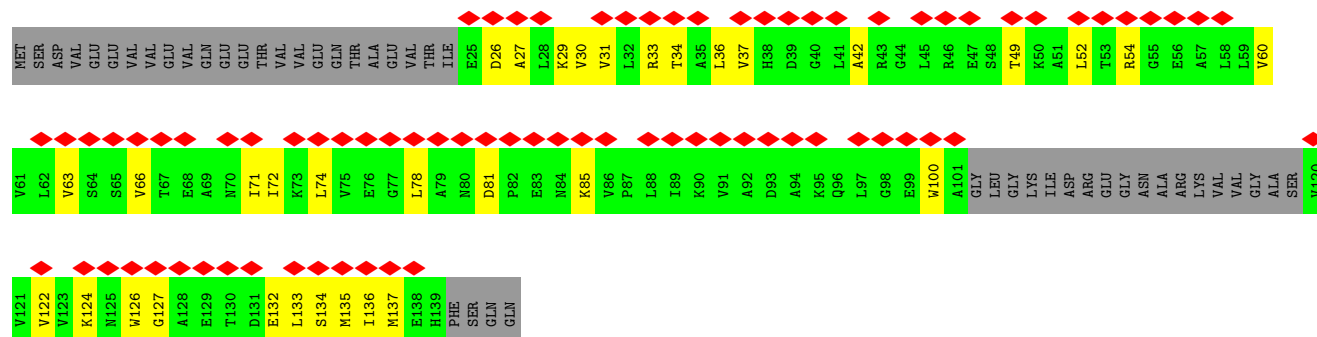




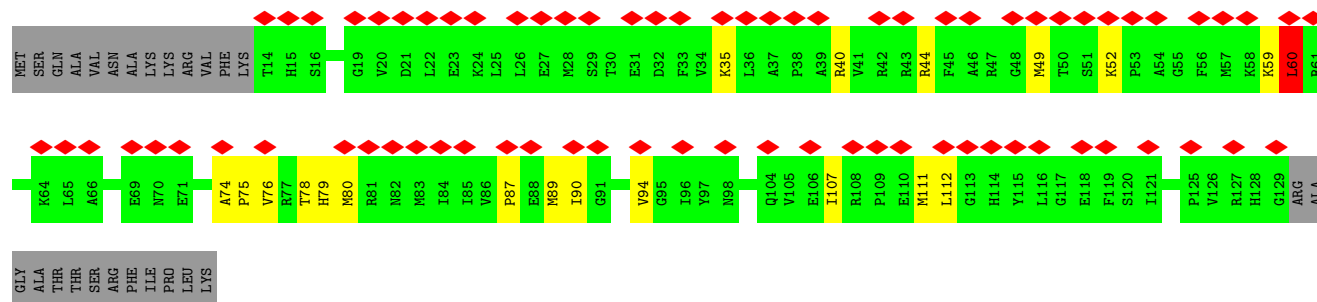
• Molecule 49: 40S ribosomal protein S10-A



• Molecule 50: 40S ribosomal protein S12

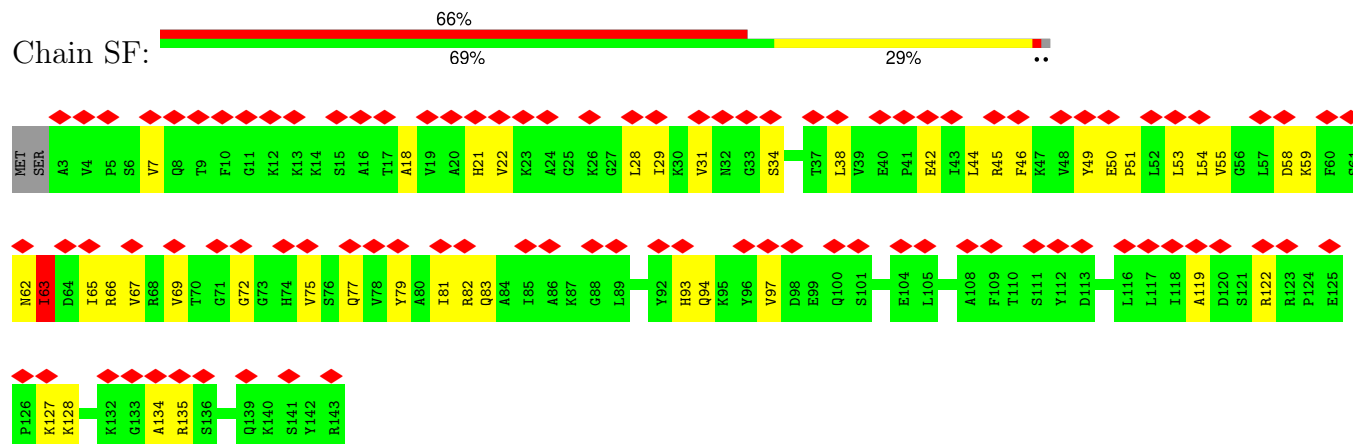


• Molecule 51: 40S ribosomal protein S15



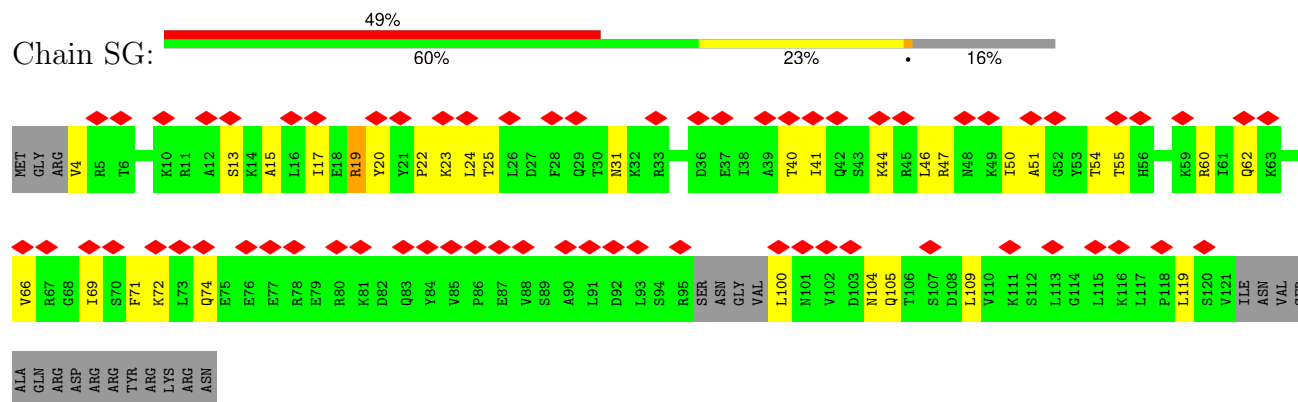
- Molecule 52: 40S ribosomal protein S16-A

Chain SF:



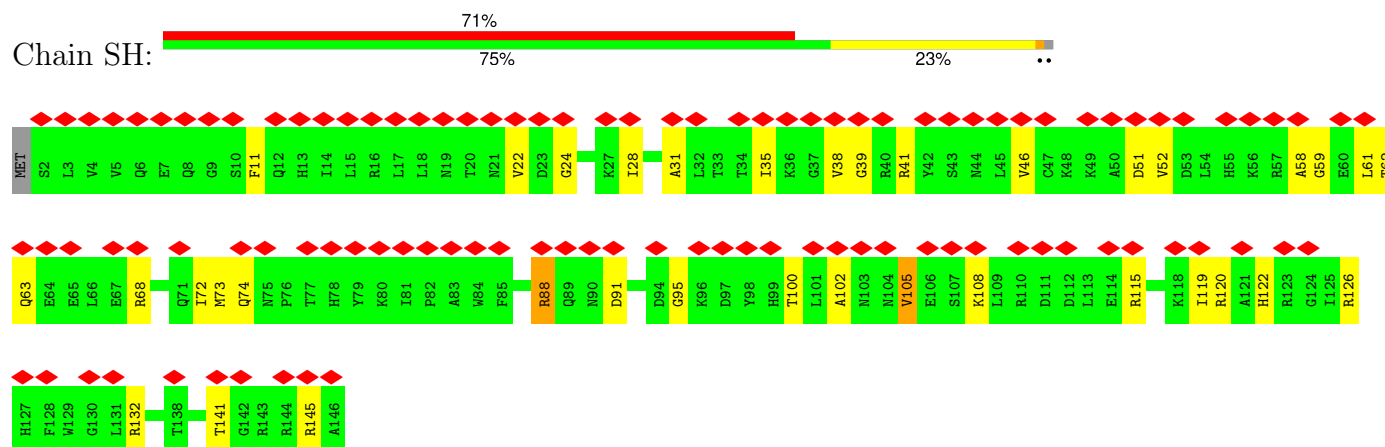
- Molecule 53: 40S ribosomal protein S17-B

Chain SG:



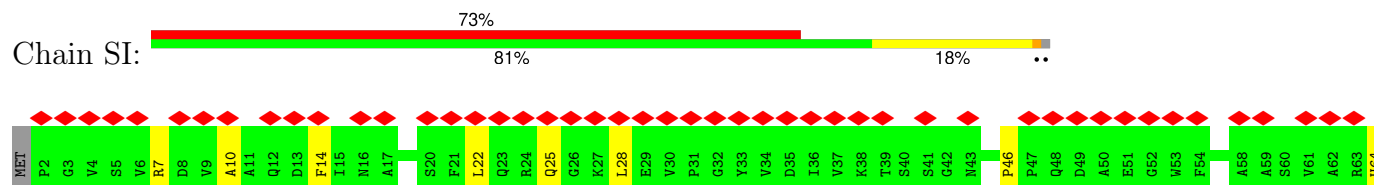
- Molecule 54: 40S ribosomal protein S18-A

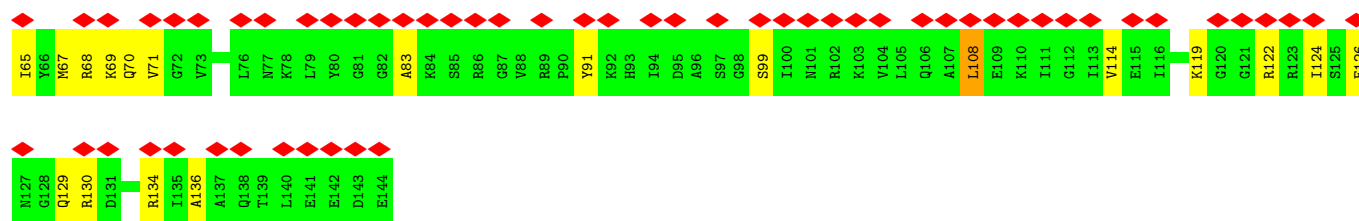
Chain SH:



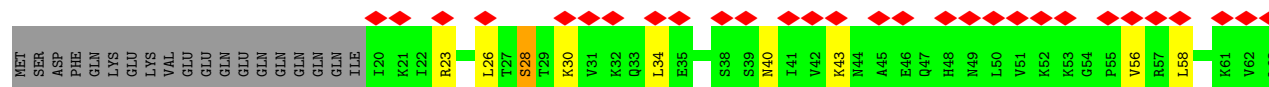
- Molecule 55: 40S ribosomal protein S19-A

Chain SI:

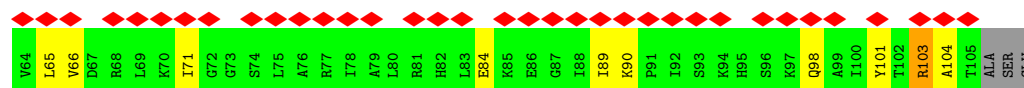
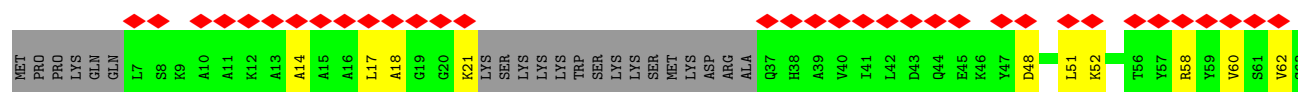




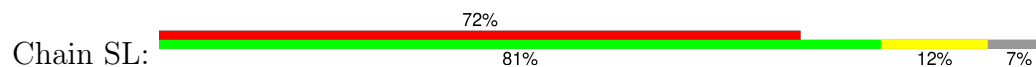
• Molecule 56: 40S ribosomal protein S20



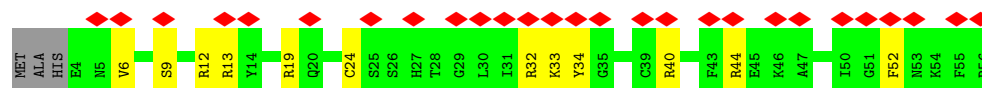
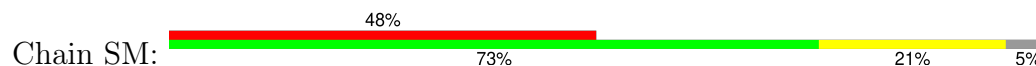
• Molecule 57: 40S ribosomal protein S25-A



• Molecule 58: 40S ribosomal protein S28-A



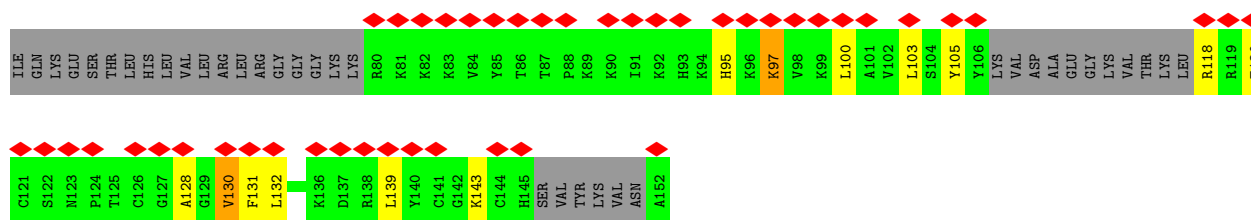
• Molecule 59: 40S ribosomal protein S29-A



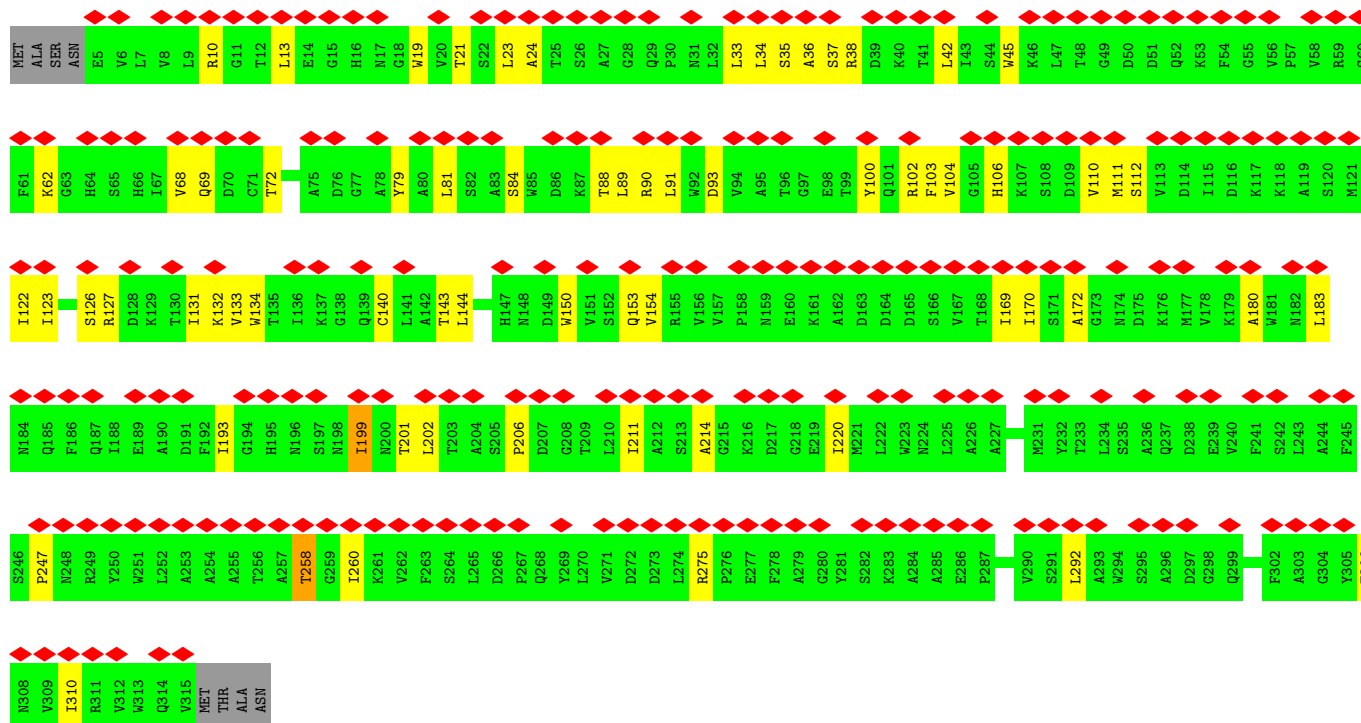
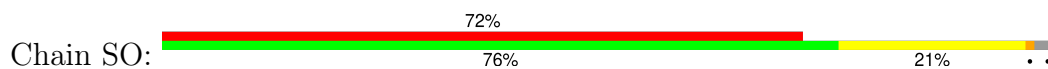
• Molecule 60: Ubiquitin-40S ribosomal protein S31



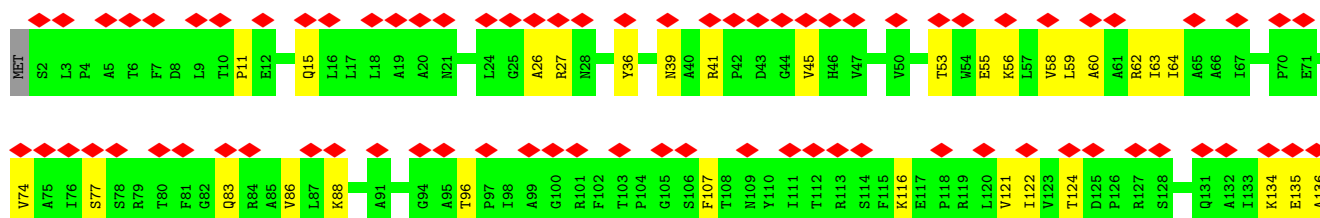
MET GLN ILE PHE VAL THR THR GLY THR LYS THR ILE THR GLY VAL GLY SER SER ASP THR ILE ASP ASN VAL LYS SER LYS ILE GLN ASP LYS GLY ILE PRO PRO ASP GLN ARG LYS LEU ILE PHE ALA GLY LYS GLN LEU GLU ASP GLY ARG THR LEU SER ASP ASN



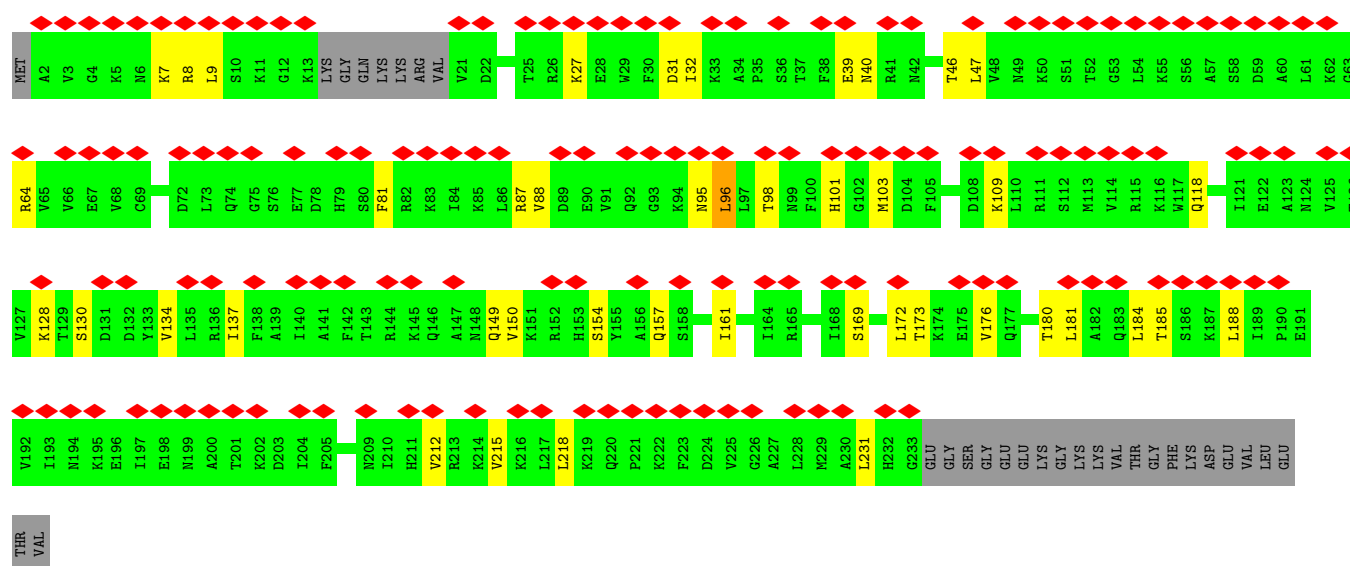
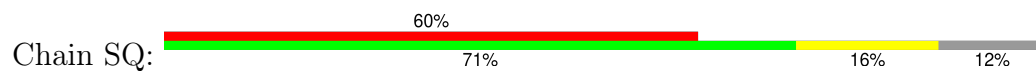
• Molecule 61: Guanine nucleotide-binding protein subunit beta-like protein



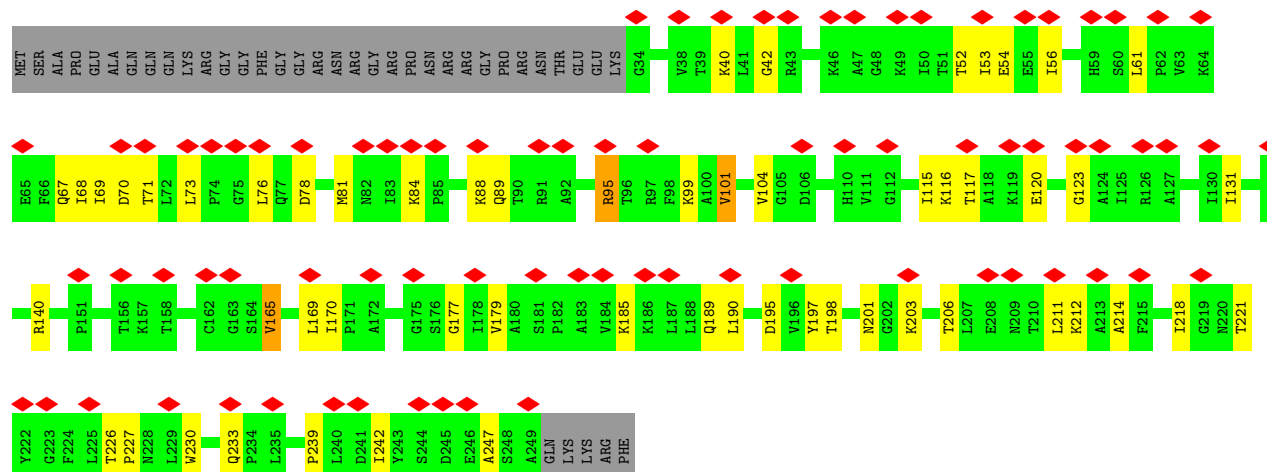
• Molecule 62: 40S ribosomal protein S0-A



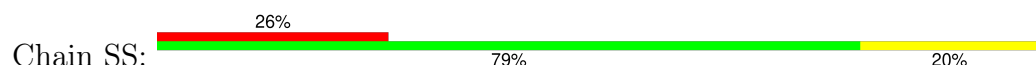
- Molecule 63: Small ribosomal subunit protein eS1A

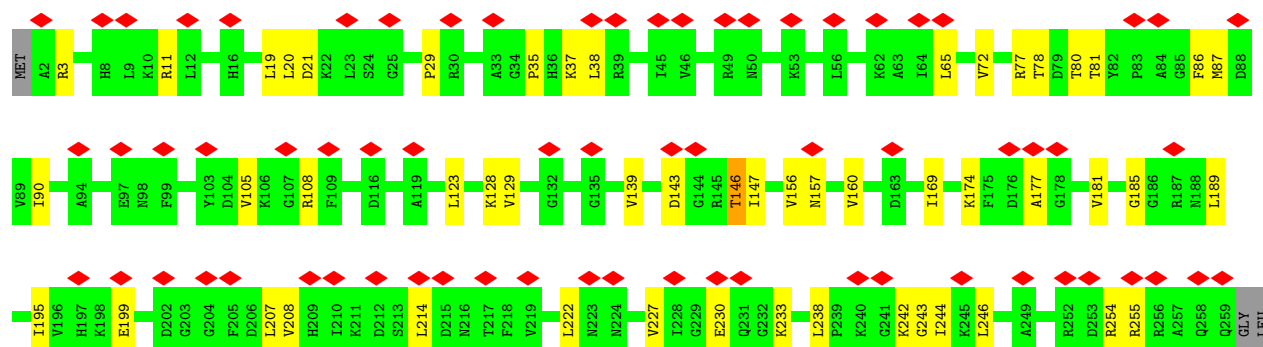


- Molecule 64: 40S ribosomal protein S2

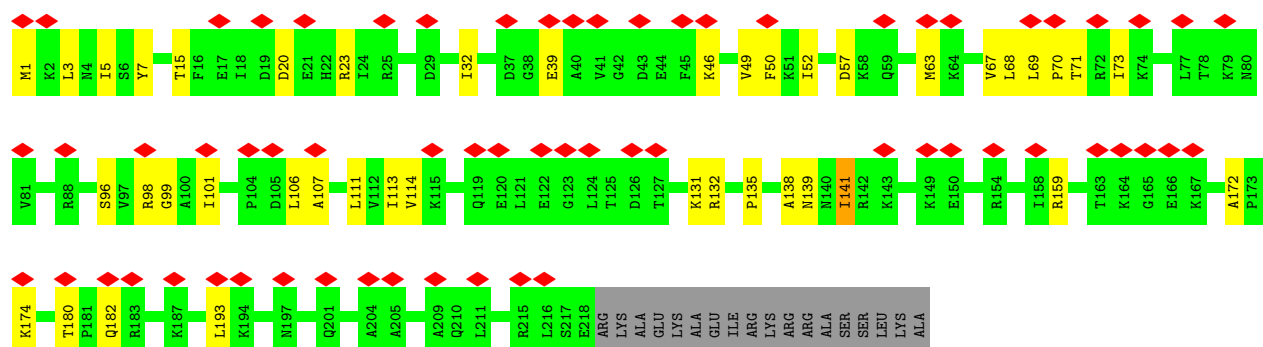
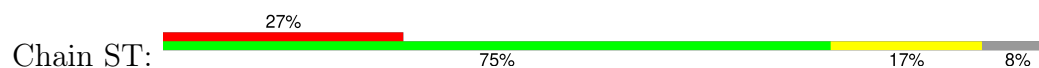


- Molecule 65: 40S ribosomal protein S4-A

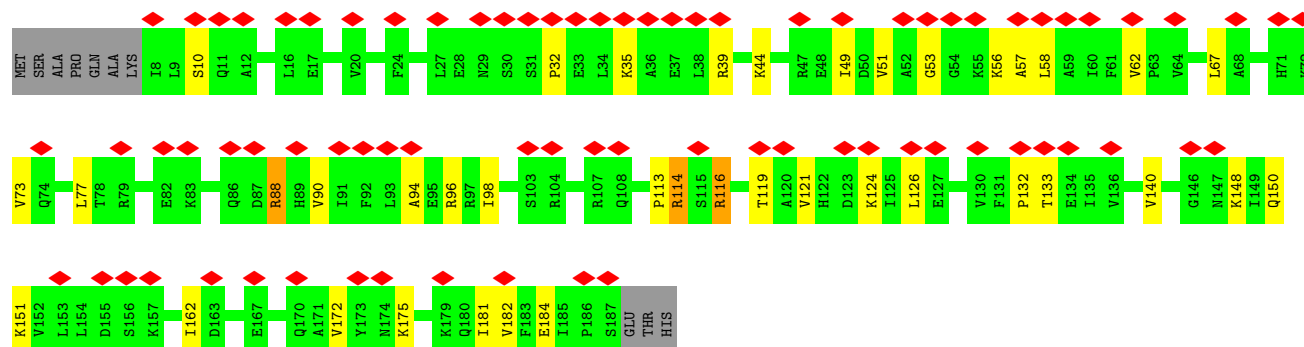
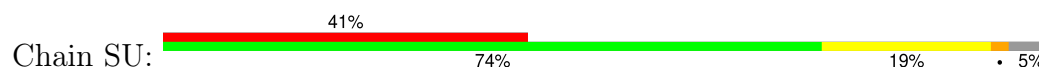




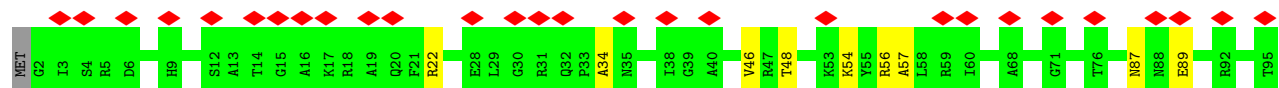
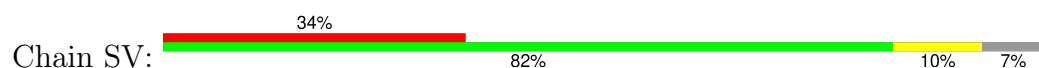
• Molecule 66: 40S ribosomal protein S6-A

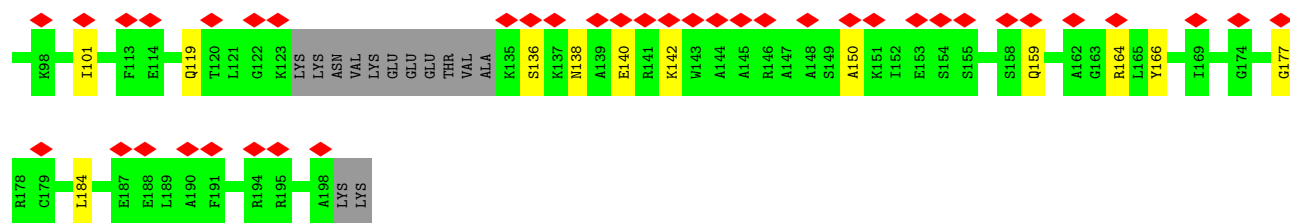


• Molecule 67: 40S ribosomal protein S7-A



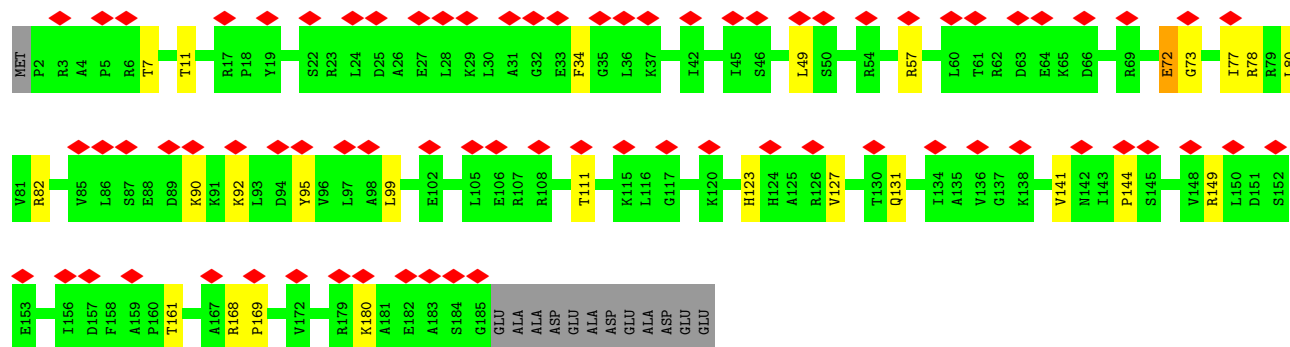
• Molecule 68: 40S ribosomal protein S8-A





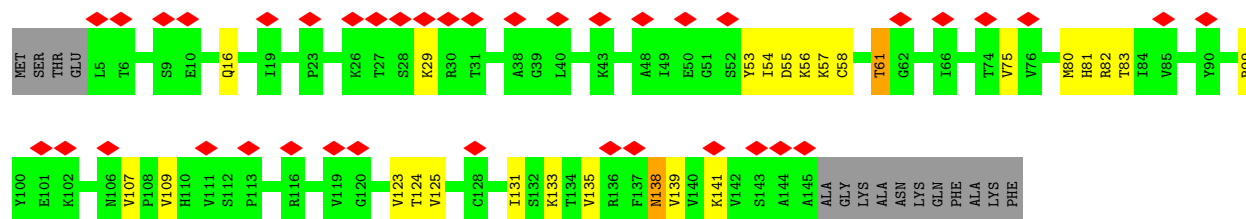
• Molecule 69: 40S ribosomal protein S9-A

Chain SW: 38% 80% 13% 7%



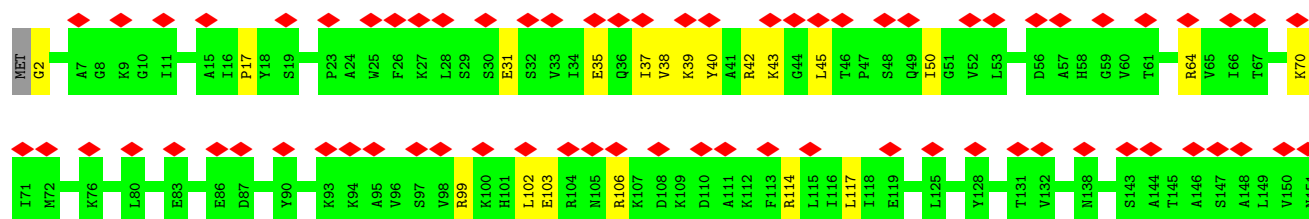
• Molecule 70: 40S ribosomal protein S11-A

Chain SX: 25% 74% 15% 10%



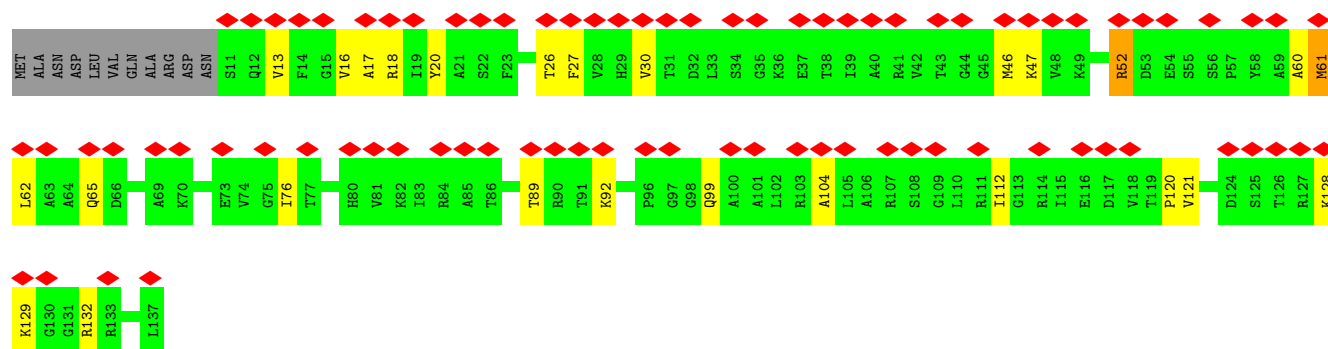
• Molecule 71: 40S ribosomal protein S13

Chain SY: 46% 86% 13% 5%

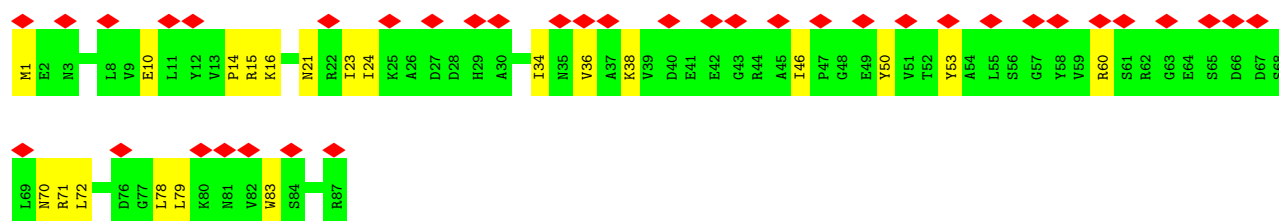
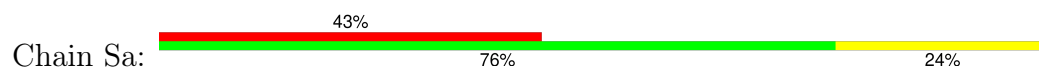


• Molecule 72: 40S ribosomal protein S14-B

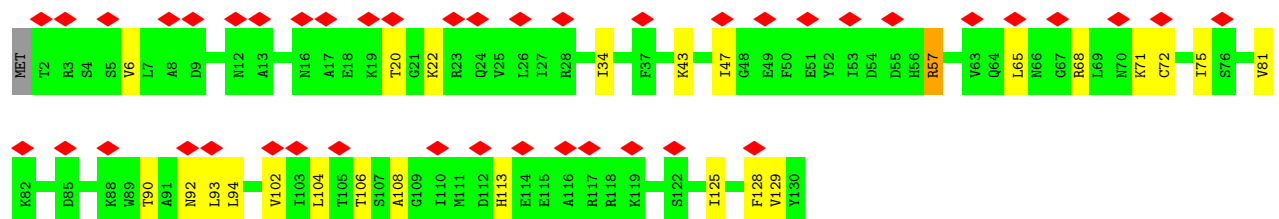
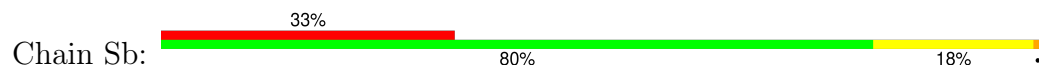
Chain SZ: 59% 73% 17% 8%



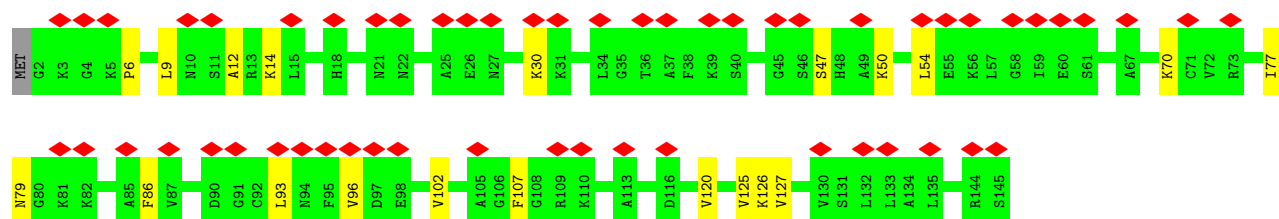
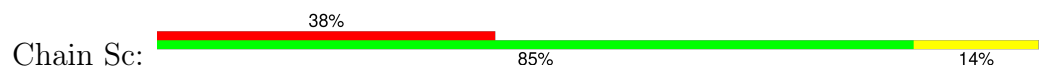
• Molecule 73: 40S ribosomal protein S21-A



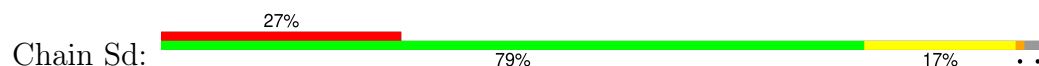
• Molecule 74: 40S ribosomal protein S22-A

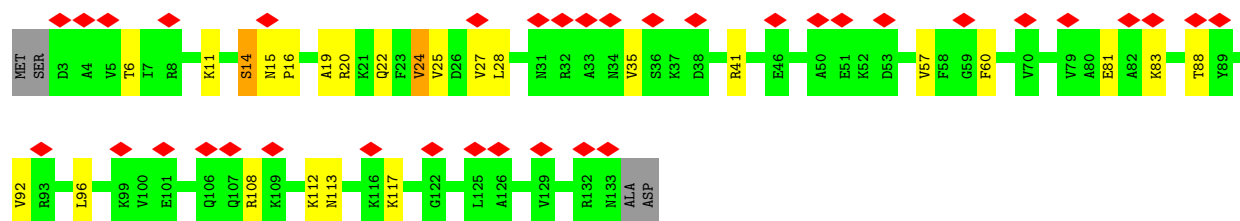


• Molecule 75: 40S ribosomal protein S23-A

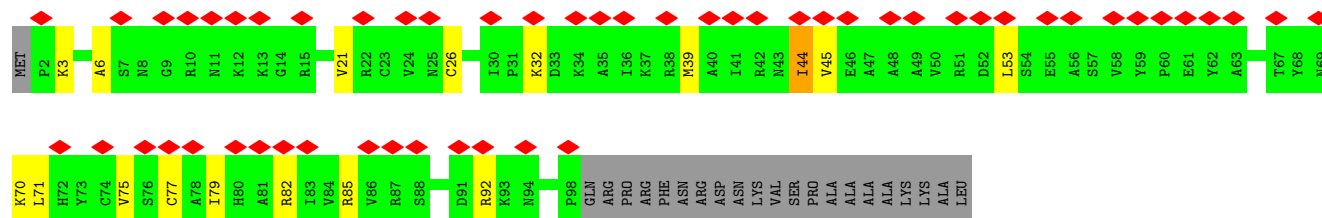


• Molecule 76: 40S ribosomal protein S24-A

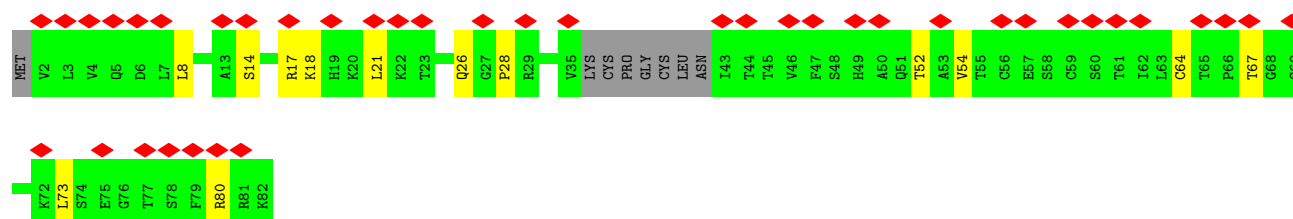
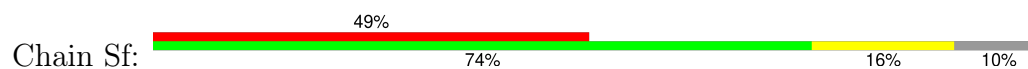




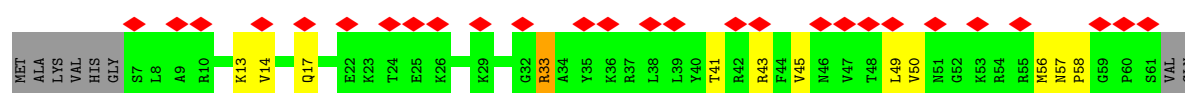
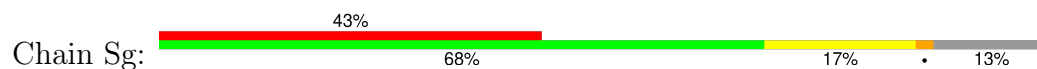
- Molecule 77: Small ribosomal subunit protein eS26B



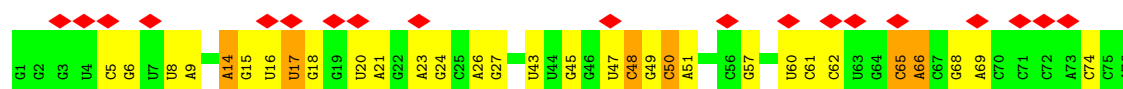
- Molecule 78: 40S ribosomal protein S27-A



- Molecule 79: 40S ribosomal protein S30-A

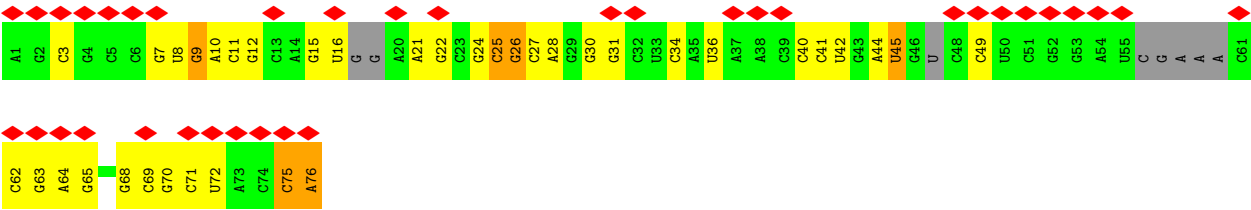


- Molecule 80: A site tRNA



- Molecule 81: P site tRNA





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	79307	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.833	Depositor
Minimum map value	-0.316	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	498.0, 498.0, 498.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3HE

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	A	0.27	0/72816	0.38	0/113508
2	B	0.22	0/2883	0.36	0/4491
3	C	0.27	0/3746	0.37	0/5832
4	D	0.33	0/245	0.61	0/378
5	E	0.25	0/37769	0.44	0/58836
6	LD	0.29	0/1912	0.59	0/2569
7	LE	0.27	0/3150	0.51	0/4236
8	LF	0.27	0/2801	0.54	0/3792
9	LG	0.27	0/2390	0.64	0/3225
10	LH	0.30	0/1265	0.72	1/1706 (0.1%)
11	LI	0.30	0/1821	0.57	0/2451
12	LJ	0.27	0/1836	0.60	0/2481
13	LK	0.26	0/1514	0.59	0/2039
14	LL	0.28	0/1723	0.62	0/2312
15	LM	0.33	0/1367	0.79	0/1834
16	LN	0.28	0/1568	0.59	1/2106 (0.0%)
17	LO	0.27	0/1068	0.55	0/1438
18	LP	0.30	0/1757	0.58	0/2354
19	LQ	0.29	0/1585	0.50	0/2128
20	LR	0.30	0/1383	0.53	0/1858
21	LS	0.28	0/1465	0.59	0/1965
22	LT	0.28	0/1499	0.54	0/1998
23	LU	0.28	0/1473	0.54	0/1980
24	LV	0.29	0/1296	0.63	0/1739
25	LW	0.29	0/812	0.67	0/1099
26	LX	0.27	0/1018	0.57	0/1369
27	LY	0.30	0/525	0.61	0/696
28	LZ	0.27	0/974	0.57	0/1314
29	La	0.25	0/995	0.53	0/1329
30	Lb	0.27	0/1092	0.60	1/1467 (0.1%)
31	Lc	0.29	0/1200	0.56	0/1607
32	Ld	0.23	0/473	0.50	0/629

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Le	0.30	0/745	0.64	0/1001
34	Lf	0.26	0/870	0.53	0/1168
35	Lg	0.26	0/1029	0.51	0/1379
36	Lh	0.28	0/868	0.57	0/1168
37	Li	0.30	0/876	0.58	0/1171
38	Lj	0.27	0/978	0.60	0/1301
39	Lk	0.27	0/767	0.67	0/1019
40	Ll	0.27	0/660	0.53	0/875
41	Lm	0.27	0/614	0.58	0/822
42	Ln	0.28	0/443	0.53	0/588
43	Lo	0.25	0/415	0.54	0/551
44	Lp	0.26	0/225	0.52	0/289
45	Lq	0.26	0/817	0.58	0/1078
46	Lr	0.26	0/701	0.56	0/934
47	SA	0.30	0/1754	0.71	0/2361
48	SB	0.29	0/1625	0.73	0/2197
49	SC	0.33	0/725	0.77	0/978
50	SD	0.36	0/742	0.81	0/1005
51	SE	0.32	0/925	0.75	1/1245 (0.1%)
52	SF	0.31	0/1115	0.76	1/1499 (0.1%)
53	SG	0.29	0/917	0.70	0/1229
54	SH	0.33	0/1207	0.80	1/1623 (0.1%)
55	SI	0.31	0/1130	0.74	0/1517
56	SJ	0.31	0/807	0.79	0/1091
57	SK	0.30	0/657	0.78	0/880
58	SL	0.29	0/488	0.73	0/656
59	SM	0.30	0/453	0.69	0/602
60	SN	0.60	0/437	0.91	0/585
61	SO	0.27	0/2428	0.71	0/3308
62	SP	0.29	0/1636	0.71	0/2237
63	SQ	0.28	0/1812	0.68	0/2433
64	SR	0.31	0/1656	0.71	0/2251
65	SS	0.29	0/2097	0.70	1/2823 (0.0%)
66	ST	0.29	0/1779	0.68	1/2379 (0.0%)
67	SU	0.29	0/1475	0.72	0/1987
68	SV	0.30	0/1496	0.65	0/1999
69	SW	0.28	0/1504	0.67	0/2016
70	SX	0.29	0/1163	0.68	0/1568
71	SY	0.32	0/1215	0.71	0/1638
72	SZ	0.27	0/934	0.68	0/1257
73	Sa	0.27	0/682	0.64	0/921
74	Sb	0.31	0/1038	0.64	0/1395
75	Sc	0.26	0/1139	0.57	0/1518

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	Sd	0.27	0/1030	0.66	0/1379
77	Se	0.26	0/778	0.61	0/1042
78	Sf	0.27	0/570	0.65	0/769
79	Sg	0.32	0/444	0.81	0/591
80	m	0.22	0/1799	0.51	0/2801
81	n	0.26	0/1596	0.54	0/2479
All	All	0.27	0/208682	0.51	8/306369 (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
6	LD	0	1
7	LE	0	1
9	LG	0	4
13	LK	0	1
16	LN	0	3
18	LP	0	1
21	LS	0	1
22	LT	0	3
26	LX	0	2
38	Lj	0	1
47	SA	0	4
48	SB	0	2
50	SD	0	1
52	SF	0	1
53	SG	0	1
54	SH	0	1
55	SI	0	1
57	SK	0	1
59	SM	0	3
60	SN	0	1
63	SQ	0	1
64	SR	0	1
65	SS	0	2
66	ST	0	1
67	SU	0	3
69	SW	0	2
72	SZ	0	2
74	Sb	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
76	Sd	0	2
79	Sg	0	2
All	All	0	51

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	ST	141	ILE	CA-CB-CG1	6.94	122.20	110.40
10	LH	8	LYS	CA-CB-CG	6.00	126.10	114.10
52	SF	63	ILE	CA-CB-CG1	5.67	120.05	110.40
16	LN	48	PRO	CA-N-CD	-5.49	104.31	112.00
51	SE	60	LEU	CA-CB-CG	5.49	135.52	116.30
54	SH	63	GLN	CA-CB-CG	5.44	124.98	114.10
30	Lb	89	VAL	CA-CB-CG1	5.11	119.08	110.40
65	SS	86	PHE	N-CA-C	5.10	117.24	111.02

There are no chirality outliers.

All (51) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	LD	241	ARG	Sidechain
7	LE	10	ARG	Sidechain
9	LG	152	ARG	Sidechain
9	LG	218	ARG	Sidechain
9	LG	35	ARG	Sidechain
9	LG	85	ARG	Sidechain
13	LK	23	ARG	Sidechain
16	LN	115	ARG	Sidechain
16	LN	188	ARG	Sidechain
16	LN	67	ARG	Sidechain
18	LP	108	ARG	Sidechain
21	LS	16	ARG	Sidechain
22	LT	151	ARG	Sidechain
22	LT	172	ARG	Sidechain
22	LT	176	ARG	Sidechain
26	LX	12	ARG	Sidechain
26	LX	70	ARG	Sidechain
38	Lj	114	ARG	Sidechain
47	SA	116	ARG	Sidechain
47	SA	117	ARG	Sidechain

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Mol	Chain	Res	Type	Group
47	SA	76	ARG	Sidechain
47	SA	90	ARG	Sidechain
48	SB	102	ARG	Sidechain
48	SB	112	ARG	Sidechain
50	SD	54	ARG	Sidechain
52	SF	135	ARG	Sidechain
53	SG	19	ARG	Sidechain
54	SH	88	ARG	Sidechain
55	SI	122	ARG	Sidechain
57	SK	103	ARG	Sidechain
59	SM	12	ARG	Sidechain
59	SM	13	ARG	Sidechain
59	SM	44	ARG	Sidechain
60	SN	118	ARG	Sidechain
63	SQ	64	ARG	Sidechain
64	SR	95	ARG	Sidechain
65	SS	254	ARG	Sidechain
65	SS	255	ARG	Sidechain
66	ST	98	ARG	Sidechain
67	SU	114	ARG	Sidechain
67	SU	116	ARG	Sidechain
67	SU	88	ARG	Sidechain
69	SW	149	ARG	Sidechain
69	SW	57	ARG	Sidechain
72	SZ	132	ARG	Sidechain
72	SZ	52	ARG	Sidechain
74	Sb	57	ARG	Sidechain
76	Sd	108	ARG	Sidechain
76	Sd	41	ARG	Sidechain
79	Sg	33	ARG	Sidechain
79	Sg	43	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	65056	0	32701	286	0
2	B	2579	0	1304	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	3353	0	1695	13	0
4	D	218	0	109	1	0
5	E	33767	0	16988	214	0
6	LD	1878	0	1946	23	0
7	LE	3079	0	3158	31	0
8	LF	2749	0	2863	19	0
9	LG	2341	0	2290	25	0
10	LH	1243	0	1327	11	0
11	LI	1784	0	1862	7	0
12	LJ	1804	0	1877	18	0
13	LK	1493	0	1566	21	0
14	LL	1686	0	1725	14	0
15	LM	1346	0	1370	22	0
16	LN	1543	0	1608	14	0
17	LO	1053	0	1149	14	0
18	LP	1720	0	1779	15	0
19	LQ	1555	0	1659	7	0
20	LR	1361	0	1398	17	0
21	LS	1441	0	1543	15	0
22	LT	1482	0	1578	12	0
23	LU	1437	0	1475	19	0
24	LV	1272	0	1312	15	0
25	LW	796	0	812	6	0
26	LX	1003	0	1048	11	0
27	LY	513	0	540	5	0
28	LZ	959	0	1023	7	0
29	La	984	0	1075	11	0
30	Lb	1066	0	1104	10	0
31	Lc	1169	0	1211	10	0
32	Ld	462	0	491	4	0
33	Le	737	0	792	7	0
34	Lf	856	0	904	9	0
35	Lg	1008	0	1068	9	0
36	Lh	850	0	880	3	0
37	Li	866	0	927	10	0
38	Lj	969	0	1078	10	0
39	Lk	761	0	842	6	0
40	Ll	645	0	649	2	0
41	Lm	608	0	671	10	0
42	Ln	436	0	475	2	0
43	Lo	409	0	448	3	0
44	Lp	224	0	271	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	Lq	805	0	877	6	0
46	Lr	694	0	738	6	0
47	SA	1729	0	1812	33	0
48	SB	1605	0	1669	34	0
49	SC	708	0	701	11	0
50	SD	736	0	771	22	0
51	SE	905	0	928	16	0
52	SF	1095	0	1144	31	0
53	SG	908	0	961	19	0
54	SH	1188	0	1218	22	0
55	SI	1112	0	1124	20	0
56	SJ	797	0	863	12	0
57	SK	650	0	704	12	0
58	SL	486	0	522	4	0
59	SM	443	0	436	4	0
60	SN	429	0	412	9	0
61	SO	2375	0	2323	45	0
62	SP	1596	0	1603	32	0
63	SQ	1787	0	1870	24	0
64	SR	1626	0	1715	33	0
65	SS	2056	0	2140	28	0
66	ST	1755	0	1846	25	0
67	SU	1451	0	1538	24	0
68	SV	1471	0	1499	13	0
69	SW	1479	0	1556	13	0
70	SX	1137	0	1207	15	0
71	SY	1192	0	1255	12	0
72	SZ	923	0	948	18	0
73	Sa	673	0	662	14	0
74	Sb	1021	0	1060	15	0
75	Sc	1121	0	1196	13	0
76	Sd	1016	0	1032	13	0
77	Se	765	0	811	10	0
78	Sf	562	0	582	9	0
79	Sg	437	0	484	7	0
80	m	1611	0	817	11	0
81	n	1431	0	732	15	0
82	A	20	0	23	0	0
All	All	194356	0	144370	1450	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (1450) 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)
81:n:10:A:H61	81:n:25:C:H42	1.14	0.94
5:E:401:A:H3'	5:E:402:C:H4'	1.58	0.85
5:E:868:G:H1	5:E:960:U:H3	1.26	0.83
5:E:851:U:H3'	22:LT:172:ARG:HH22	1.43	0.82
3:C:150:G:H21	12:LJ:59:GLN:HE22	1.27	0.82
62:SP:107:PHE:HB2	62:SP:135:GLU:HG2	1.63	0.79
5:E:819:G:C8	5:E:853:G:N2	2.50	0.79
5:E:819:G:N7	5:E:853:G:C2	2.50	0.79
5:E:819:G:N7	5:E:853:G:N1	2.30	0.78
63:SQ:149:GLN:HE22	63:SQ:154:SER:HB3	1.48	0.77
5:E:647:G:H22	5:E:687:G:H1	1.34	0.76
64:SR:42:GLY:HA2	64:SR:68:ILE:HD11	1.70	0.74
62:SP:139:VAL:HG13	62:SP:141:ILE:HD12	1.71	0.73
48:SB:27:THR:HG23	52:SF:28:LEU:HD12	1.70	0.72
1:A:3165:A:H61	1:A:3285:C:H42	1.35	0.71
7:LE:152:LYS:HG2	7:LE:192:VAL:HG11	1.72	0.71
10:LH:97:ASN:HD21	10:LH:99:GLU:HG3	1.53	0.70
1:A:2193:U:H5'	1:A:2194:G:H5'	1.72	0.70
51:SE:107:ILE:HA	51:SE:111:MET:HE2	1.71	0.70
23:LU:77:VAL:HG13	23:LU:126:VAL:HG12	1.73	0.70
22:LT:169:ALA:HA	22:LT:172:ARG:HH21	1.55	0.70
18:LP:183:THR:HG22	18:LP:187:ARG:HG3	1.74	0.69
50:SD:42:ALA:HB2	50:SD:124:LYS:HE3	1.74	0.69
5:E:298:C:H5''	65:SS:38:LEU:HB2	1.74	0.69
7:LE:229:VAL:HG11	7:LE:249:VAL:HG23	1.74	0.69
64:SR:56:ILE:HG23	64:SR:61:LEU:HB2	1.73	0.69
47:SA:48:VAL:HG22	47:SA:86:LEU:HD22	1.72	0.69
62:SP:63:ILE:HD13	73:Sa:34:ILE:HD11	1.75	0.69
5:E:1499:G:H1	5:E:1508:U:H3	1.41	0.69
67:SU:133:THR:HG22	67:SU:162:ILE:HD11	1.74	0.68
9:LG:103:LEU:HD11	9:LG:248:ARG:HD3	1.74	0.68
66:ST:20:ASP:HB3	66:ST:23:ARG:HB2	1.75	0.68
8:LF:193:LYS:HG2	8:LF:198:ARG:HG3	1.75	0.68
67:SU:32:PRO:HA	67:SU:35:LYS:HG3	1.75	0.68
5:E:123:G:H21	65:SS:146:THR:HG21	1.58	0.68
60:SN:132:LEU:HD12	60:SN:139:LEU:HB3	1.74	0.68
65:SS:19:LEU:HD11	65:SS:108:ARG:HD3	1.77	0.67
13:LK:89:LYS:HG2	13:LK:145:VAL:HG22	1.76	0.67
54:SH:41:ARG:HH21	55:SI:46:PRO:HG3	1.59	0.67
24:LV:11:THR:HG22	24:LV:14:MET:HE3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:SP:148:ASP:HB2	62:SP:164:ASN:HB2	1.76	0.66
13:LK:57:VAL:HG12	13:LK:68:LEU:HD22	1.76	0.66
53:SG:71:PHE:HD1	53:SG:72:LYS:H	1.39	0.66
62:SP:146:LEU:HD11	62:SP:173:ILE:HG21	1.78	0.66
47:SA:220:PRO:HA	61:SO:193:ILE:HD11	1.78	0.66
67:SU:67:LEU:HG	67:SU:94:ALA:HB2	1.78	0.66
57:SK:65:LEU:HB3	57:SK:71:ILE:HD11	1.78	0.65
79:Sg:56:MET:O	79:Sg:58:PRO:HD3	1.97	0.65
71:SY:37:ILE:HA	71:SY:50:ILE:HD11	1.79	0.65
48:SB:187:ILE:HG21	57:SK:66:VAL:HG21	1.77	0.65
48:SB:88:PRO:HG2	48:SB:91:GLU:HG3	1.80	0.64
80:m:27:G:H1	80:m:43:U:H3	1.43	0.64
16:LN:166:ALA:HB1	31:Lc:147:LEU:HD21	1.77	0.64
5:E:1426:C:H3'	5:E:1427:A:H4'	1.79	0.64
5:E:1587:A:H2'	5:E:1588:G:H8	1.61	0.64
68:SV:57:ALA:HB2	68:SV:177:GLY:HA2	1.80	0.64
47:SA:93:ASP:HB3	47:SA:96:LEU:HD23	1.79	0.64
48:SB:57:SER:HA	58:SL:53:ILE:HB	1.79	0.64
45:Lq:25:VAL:HG12	45:Lq:72:LEU:HD23	1.79	0.63
1:A:824:C:H5''	6:LD:21:ARG:HD3	1.80	0.63
1:A:1639:C:H5'	37:Li:52:GLN:HG2	1.79	0.63
57:SK:18:ALA:HA	57:SK:21:LYS:HE2	1.79	0.63
1:A:1650:G:H5'	6:LD:70:ARG:HG2	1.79	0.63
72:SZ:20:TYR:HB3	72:SZ:27:PHE:HB2	1.79	0.63
64:SR:53:ILE:HA	64:SR:56:ILE:HD12	1.79	0.63
67:SU:58:LEU:HB2	67:SU:90:VAL:HG12	1.81	0.63
47:SA:42:THR:HB	47:SA:45:LYS:HB2	1.80	0.63
66:ST:180:THR:HG22	66:ST:182:GLN:H	1.63	0.63
74:Sb:75:ILE:HD11	74:Sb:93:LEU:HD21	1.81	0.63
16:LN:124:ILE:HB	38:Lj:119:LYS:HE3	1.81	0.63
1:A:1213:G:H4'	23:LU:90:MET:HG3	1.81	0.62
47:SA:47:GLU:HB3	47:SA:85:VAL:HG23	1.80	0.62
65:SS:80:THR:HG23	65:SS:81:THR:HG23	1.82	0.62
9:LG:51:LEU:HD23	9:LG:64:ILE:HG12	1.81	0.62
13:LK:1:MET:HE1	23:LU:138:GLN:HG3	1.81	0.62
72:SZ:99:GLN:HE22	77:Se:45:VAL:HA	1.64	0.62
15:LM:164:LYS:HG2	15:LM:170:ASP:HA	1.81	0.62
61:SO:106:HIS:HD1	61:SO:110:VAL:HG12	1.65	0.62
66:ST:39:GLU:HG2	66:ST:46:LYS:HG2	1.81	0.62
29:La:56:VAL:HG21	29:La:104:LEU:HD13	1.81	0.62
61:SO:93:ASP:HB2	61:SO:100:TYR:HE1	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:SR:73:LEU:HD23	64:SR:76:LEU:HD21	1.81	0.62
34:Lf:24:SER:HB2	34:Lf:27:LYS:HD2	1.82	0.62
1:A:2514:U:H5'	12:LJ:68:ARG:HG3	1.83	0.61
74:Sb:6:VAL:HG22	74:Sb:34:ILE:HD11	1.82	0.61
48:SB:117:THR:HG21	48:SB:194:LEU:HD23	1.81	0.61
13:LK:9:GLN:HB3	13:LK:52:LEU:HD21	1.82	0.61
1:A:68:C:H41	1:A:315:C:H5'	1.66	0.61
1:A:3343:G:H21	1:A:3362:A:H2	1.47	0.61
16:LN:48:PRO:HB3	38:Lj:117:ALA:HB2	1.83	0.60
54:SH:24:GLY:HA2	54:SH:58:ALA:HB3	1.83	0.60
55:SI:108:LEU:HD12	55:SI:114:VAL:HG22	1.83	0.60
62:SP:136:ALA:HA	62:SP:139:VAL:HG12	1.83	0.60
70:SX:138:ASN:HD22	70:SX:139:VAL:N	1.99	0.60
1:A:597:G:H2'	1:A:598:A:H8	1.65	0.60
13:LK:90:MET:HE2	13:LK:179:ILE:HG22	1.84	0.60
54:SH:88:ARG:HH21	54:SH:108:LYS:HD3	1.66	0.60
67:SU:150:GLN:HB3	67:SU:181:ILE:HG22	1.82	0.60
5:E:142:G:H22	5:E:173:A:H2	1.49	0.60
63:SQ:32:ILE:HA	63:SQ:96:LEU:HG	1.81	0.60
5:E:1:U:H5'	64:SR:179:VAL:HG13	1.82	0.60
30:Lb:27:LYS:HB3	30:Lb:42:LEU:HD12	1.84	0.60
49:SC:60:SER:O	49:SC:63:TYR:HB2	2.02	0.60
1:A:655:C:H2'	1:A:656:A:H8	1.67	0.59
6:LD:52:SER:HB3	6:LD:191:LEU:HD22	1.82	0.59
12:LJ:148:ALA:HA	12:LJ:201:THR:HG22	1.83	0.59
47:SA:94:ARG:H	47:SA:94:ARG:HE	1.50	0.59
5:E:1171:A:H2'	5:E:1172:G:C8	2.38	0.59
53:SG:25:THR:H	53:SG:31:ASN:HD21	1.48	0.59
56:SJ:28:SER:HB3	56:SJ:112:VAL:HA	1.82	0.59
76:Sd:15:ASN:HB3	76:Sd:20:ARG:HG3	1.84	0.59
5:E:343:C:H2'	5:E:344:A:H8	1.68	0.59
16:LN:165:SER:HB3	16:LN:168:ARG:HB3	1.84	0.59
56:SJ:82:TYR:HB3	59:SM:52:PHE:HB3	1.84	0.59
8:LF:313:LEU:HD23	8:LF:315:LYS:HE2	1.85	0.59
30:Lb:23:VAL:HG12	30:Lb:45:GLY:HA3	1.85	0.59
9:LG:41:LYS:HE3	24:LV:93:VAL:HG11	1.84	0.58
67:SU:151:LYS:HD2	67:SU:184:GLU:HG3	1.83	0.58
79:Sg:41:THR:HA	79:Sg:45:VAL:HB	1.85	0.58
50:SD:52:LEU:HB2	50:SD:85:LYS:HD3	1.85	0.58
5:E:174:U:H3	5:E:266:A:H62	1.51	0.58
46:Lr:30:GLU:HA	46:Lr:33:GLN:HG2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:SA:102:ALA:HB1	47:SA:173:ARG:HG3	1.86	0.58
67:SU:113:PRO:HG2	67:SU:116:ARG:HB2	1.85	0.58
69:SW:123:HIS:HB3	79:Sg:33:ARG:HH11	1.69	0.58
5:E:1483:A:H4'	52:SF:72:GLY:H	1.66	0.58
5:E:1591:C:H2'	5:E:1592:A:H8	1.68	0.58
31:Lc:100:PRO:HG2	31:Lc:123:VAL:HG12	1.85	0.58
49:SC:20:VAL:HG12	49:SC:67:THR:HA	1.85	0.58
70:SX:57:LYS:HD3	70:SX:131:ILE:HG23	1.85	0.58
5:E:29:U:H2'	5:E:30:G:H8	1.68	0.58
5:E:385:A:H5''	68:SV:22:ARG:HG2	1.84	0.58
49:SC:3:MET:HE1	49:SC:45:ALA:HB2	1.85	0.58
64:SR:170:ILE:HB	64:SR:197:TYR:HB2	1.84	0.58
75:Sc:102:VAL:HG12	75:Sc:127:VAL:HG23	1.86	0.58
50:SD:134:SER:HA	50:SD:137:MET:HE3	1.86	0.58
62:SP:58:VAL:HG12	62:SP:180:GLU:HG2	1.84	0.58
61:SO:106:HIS:CD2	61:SO:132:LYS:HD2	2.39	0.58
17:LO:55:ARG:HE	23:LU:70:THR:HB	1.67	0.57
19:LQ:27:LEU:HD11	19:LQ:102:LEU:HB2	1.85	0.57
61:SO:169:ILE:HG23	61:SO:183:LEU:HD11	1.84	0.57
16:LN:76:THR:HG22	16:LN:101:ARG:HB3	1.86	0.57
54:SH:22:VAL:HG13	54:SH:31:ALA:HB1	1.86	0.57
5:E:1171:A:H2'	5:E:1172:G:H8	1.69	0.57
13:LK:18:VAL:HG22	13:LK:27:VAL:HG22	1.87	0.57
3:C:81:U:H1'	3:C:83:C:H5''	1.86	0.57
61:SO:13:LEU:HB2	61:SO:310:ILE:HB	1.86	0.57
80:m:17:U:H2'	80:m:18:G:H3'	1.86	0.57
47:SA:5:ILE:HD11	47:SA:9:ARG:HE	1.69	0.57
52:SF:83:GLN:HE22	52:SF:119:ALA:HA	1.70	0.57
75:Sc:6:PRO:HG3	75:Sc:14:LYS:HG2	1.86	0.57
47:SA:71:LEU:HD22	49:SC:20:VAL:HG23	1.86	0.57
48:SB:71:ALA:HB1	48:SB:91:GLU:HG2	1.87	0.57
54:SH:52:VAL:HG21	54:SH:61:LEU:HD21	1.86	0.57
1:A:1661:G:H2'	1:A:1662:G:C8	2.39	0.57
5:E:142:G:H5''	66:ST:139:ASN:HD21	1.69	0.57
63:SQ:128:LYS:HB2	63:SQ:134:VAL:HG12	1.87	0.57
15:LM:13:LYS:HD2	15:LM:134:PRO:HG3	1.87	0.56
47:SA:71:LEU:HA	47:SA:74:GLN:HE21	1.70	0.56
63:SQ:103:MET:HE1	63:SQ:212:VAL:HG23	1.87	0.56
64:SR:84:LYS:HE2	64:SR:99:LYS:HD2	1.86	0.56
6:LD:189:TYR:HA	6:LD:192:LYS:HB2	1.86	0.56
57:SK:14:ALA:HA	57:SK:17:LEU:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:LM:45:PRO:HB2	15:LM:67:VAL:HG22	1.88	0.56
7:LE:13:HIS:CD2	7:LE:15:GLY:H	2.23	0.56
66:ST:69:LEU:HD12	66:ST:71:THR:H	1.70	0.56
5:E:1402:G:H5'	53:SG:4:VAL:HG22	1.87	0.56
20:LR:169:THR:HG23	20:LR:172:GLN:H	1.70	0.56
32:Ld:14:ARG:HG2	32:Ld:18:ARG:HH21	1.71	0.56
49:SC:25:LYS:HD3	49:SC:59:PHE:HE1	1.69	0.56
1:A:2553:U:C4	37:Li:95:ILE:HG22	2.40	0.56
47:SA:40:ARG:HB3	47:SA:47:GLU:HG2	1.87	0.56
61:SO:90:ARG:HH12	61:SO:102:ARG:HE	1.53	0.56
81:n:25:C:H3'	81:n:26:G:H8	1.71	0.56
1:A:2746:A:N1	9:LG:148:ILE:HG12	2.21	0.56
26:LX:129:VAL:O	26:LX:133:SER:HB3	2.06	0.56
72:SZ:16:VAL:HG12	72:SZ:18:ARG:HG2	1.87	0.56
9:LG:36:LEU:HD22	9:LG:50:ARG:HG2	1.87	0.55
30:Lb:81:LEU:HD22	37:Li:90:ILE:HD12	1.88	0.55
61:SO:69:GLN:HG2	61:SO:111:MET:HG3	1.88	0.55
1:A:2208:A:C2	1:A:2236:G:N1	2.74	0.55
5:E:1587:A:H2'	5:E:1588:G:C8	2.41	0.55
41:Lm:15:THR:HG22	41:Lm:45:VAL:HG21	1.88	0.55
1:A:1651:U:H5''	6:LD:71:LEU:HD12	1.88	0.55
5:E:871:G:H2'	5:E:872:G:C8	2.40	0.55
5:E:1586:A:H3'	5:E:1587:A:H8	1.72	0.55
1:A:3348:G:H1	1:A:3357:U:H3	1.54	0.55
14:LL:54:SER:HB2	14:LL:135:ILE:HD11	1.89	0.55
55:SI:70:GLN:HE22	55:SI:119:LYS:HB2	1.71	0.55
62:SP:53:THR:HG22	62:SP:161:PRO:HG2	1.88	0.55
46:Lr:36:ARG:HG2	46:Lr:48:LYS:HD3	1.89	0.55
79:Sg:13:LYS:O	79:Sg:17:GLN:HG2	2.05	0.55
1:A:990:U:H4'	24:LV:100:LYS:HB3	1.89	0.55
5:E:1344:A:H2'	5:E:1345:A:C8	2.41	0.55
7:LE:160:VAL:O	7:LE:180:GLU:HA	2.07	0.55
69:SW:90:LYS:HB3	69:SW:95:TYR:HD2	1.72	0.55
81:n:10:A:H61	81:n:25:C:N4	1.95	0.55
1:A:571:U:H2'	1:A:572:A:H8	1.70	0.55
2:B:7:G:H5''	9:LG:22:ARG:HD3	1.88	0.55
48:SB:89:ILE:HD11	48:SB:134:VAL:HG12	1.89	0.55
53:SG:41:ILE:HG23	53:SG:46:LEU:HD23	1.88	0.55
70:SX:56:LYS:HG3	70:SX:57:LYS:HG3	1.89	0.55
80:m:65:C:H2'	80:m:66:A:C8	2.41	0.55
62:SP:88:LYS:HE3	62:SP:201:LEU:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2555:G:N7	37:Li:95:ILE:HD11	2.22	0.55
56:SJ:40:ASN:HD21	56:SJ:107:THR:HG21	1.71	0.55
69:SW:168:ARG:HG2	69:SW:169:PRO:HD2	1.89	0.55
72:SZ:13:VAL:HG23	72:SZ:76:ILE:HA	1.88	0.55
5:E:640:U:H2'	5:E:641:G:C8	2.42	0.55
8:LF:296:GLN:HA	8:LF:299:ILE:HG12	1.88	0.55
21:LS:112:ALA:O	21:LS:116:LYS:HB2	2.06	0.55
5:E:1727:G:H2'	5:E:1728:A:C8	2.42	0.54
25:LW:19:VAL:HG12	25:LW:105:LEU:HD22	1.89	0.54
1:A:1717:U:H2'	1:A:1718:G:C8	2.43	0.54
6:LD:108:PRO:HG2	46:Lr:86:LEU:HD13	1.88	0.54
1:A:3057:U:H5'	1:A:3086:A:H61	1.73	0.54
19:LQ:61:ALA:HA	19:LQ:70:PRO:HD2	1.89	0.54
71:SY:40:TYR:HB3	71:SY:45:LEU:HD11	1.88	0.54
72:SZ:61:MET:HG2	72:SZ:104:ALA:HB2	1.88	0.54
1:A:2413:A:H2'	1:A:2414:G:H8	1.73	0.54
1:A:2960:C:H2'	1:A:2961:G:C8	2.43	0.54
5:E:205:U:H2'	5:E:206:A:H8	1.71	0.54
5:E:891:A:H2'	5:E:892:A:H8	1.72	0.54
5:E:924:A:H2'	5:E:925:G:C8	2.43	0.54
50:SD:30:VAL:HG11	50:SD:132:GLU:HG3	1.88	0.54
70:SX:16:GLN:HE21	70:SX:61:THR:HG23	1.72	0.54
70:SX:109:VAL:HG21	70:SX:125:VAL:HG11	1.88	0.54
6:LD:51:ASP:HB3	6:LD:54:ARG:HB3	1.89	0.54
6:LD:101:VAL:HG22	6:LD:165:VAL:HG22	1.90	0.54
30:Lb:25:ILE:HA	30:Lb:43:VAL:HG12	1.90	0.54
1:A:1576:G:H2'	1:A:1577:G:C8	2.43	0.54
7:LE:90:VAL:HB	7:LE:104:THR:HG22	1.89	0.54
13:LK:90:MET:HG2	13:LK:181:VAL:HG22	1.89	0.54
41:Lm:7:ASP:HB3	41:Lm:10:GLN:HB3	1.90	0.54
77:Se:39:MET:HE2	77:Se:70:LYS:HE3	1.89	0.54
1:A:655:C:H2'	1:A:656:A:C8	2.43	0.54
9:LG:286:VAL:HG23	14:LL:206:LEU:HD11	1.89	0.54
49:SC:23:ALA:HB3	49:SC:64:TYR:HB2	1.89	0.54
1:A:2107:A:H2	1:A:3344:A:H8	1.56	0.53
1:A:2737:C:H4'	24:LV:68:THR:HG21	1.90	0.53
3:C:27:U:H4'	8:LF:51:ALA:HB3	1.90	0.53
5:E:513:U:H2'	5:E:514:G:C8	2.43	0.53
26:LX:70:ARG:HB3	26:LX:70:ARG:HH11	1.72	0.53
34:Lf:77:ARG:HD2	34:Lf:89:LEU:HD23	1.89	0.53
50:SD:29:LYS:HE2	50:SD:100:TRP:CE2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1411:C:H2'	1:A:1412:G:H8	1.73	0.53
5:E:819:G:C8	5:E:853:G:C2	2.96	0.53
58:SL:10:ALA:HA	58:SL:32:PHE:HA	1.90	0.53
64:SR:67:GLN:HA	64:SR:70:ASP:HB2	1.89	0.53
25:LW:37:LEU:O	25:LW:41:ILE:HG13	2.07	0.53
1:A:2357:A:H2'	1:A:2358:A:H8	1.74	0.53
5:E:153:G:H2'	5:E:154:G:H8	1.73	0.53
5:E:1524:A:H2'	5:E:1525:A:C8	2.43	0.53
81:n:11:C:H2'	81:n:12:G:C8	2.43	0.53
1:A:1786:G:H2'	1:A:1787:A:C8	2.43	0.53
5:E:1672:G:H2'	5:E:1673:G:C8	2.43	0.53
69:SW:73:GLY:O	69:SW:77:ILE:HG13	2.09	0.53
1:A:3016:A:H2'	1:A:3017:A:H8	1.74	0.53
1:A:3358:U:H2'	1:A:3359:A:H8	1.74	0.53
5:E:513:U:H2'	5:E:514:G:H8	1.72	0.53
54:SH:100:THR:HG21	54:SH:108:LYS:HG3	1.90	0.53
1:A:631:U:H2'	1:A:632:G:C8	2.44	0.53
7:LE:57:VAL:HG22	7:LE:73:VAL:HG22	1.90	0.53
24:LV:84:TYR:HB2	32:Ld:24:PRO:HD3	1.90	0.53
54:SH:91:ASP:HB3	54:SH:95:GLY:H	1.74	0.53
61:SO:21:THR:HG23	61:SO:37:SER:HA	1.91	0.53
23:LU:8:GLN:HB3	23:LU:64:ILE:HD11	1.91	0.53
54:SH:35:ILE:HG23	54:SH:38:VAL:HB	1.91	0.53
70:SX:99:ARG:HG3	75:Sc:12:ALA:HB2	1.89	0.53
5:E:514:G:H2'	5:E:515:A:H8	1.74	0.53
8:LF:353:ALA:O	8:LF:357:GLU:HG3	2.08	0.53
33:Le:55:GLU:HB2	37:Li:94:LEU:HD11	1.89	0.53
66:ST:67:VAL:HG23	66:ST:99:GLY:HA2	1.90	0.53
1:A:1168:U:H2'	1:A:1169:A:H8	1.74	0.53
1:A:3329:U:H5''	7:LE:308:MET:HE3	1.91	0.53
15:LM:54:VAL:HG12	15:LM:57:PHE:H	1.74	0.53
17:LO:60:LEU:HD13	23:LU:152:LEU:HD11	1.89	0.53
39:Lk:81:THR:HA	39:Lk:84:LYS:HE2	1.91	0.53
53:SG:22:PRO:HD3	53:SG:72:LYS:HG3	1.91	0.53
53:SG:44:LYS:HG3	53:SG:47:ARG:HH21	1.73	0.53
67:SU:98:ILE:HG12	67:SU:121:VAL:HG21	1.90	0.53
72:SZ:17:ALA:HA	72:SZ:30:VAL:HG22	1.91	0.53
24:LV:68:THR:HG22	24:LV:69:LYS:H	1.73	0.52
71:SY:38:VAL:O	71:SY:42:ARG:HG2	2.09	0.52
7:LE:13:HIS:HD2	7:LE:15:GLY:H	1.55	0.52
29:La:100:HIS:CD2	29:La:102:SER:HB3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:SI:124:ILE:HD12	55:SI:129:GLN:HB2	1.90	0.52
67:SU:49:ILE:HD12	67:SU:175:LYS:HG2	1.91	0.52
81:n:10:A:N6	81:n:25:C:H42	1.96	0.52
33:Le:43:ILE:HB	33:Le:90:VAL:HG13	1.92	0.52
1:A:1497:C:H2'	1:A:1498:A:H8	1.74	0.52
5:E:472:U:H5''	69:SW:11:THR:HG23	1.92	0.52
5:E:1217:A:H1'	49:SC:44:LYS:HE3	1.91	0.52
71:SY:17:PRO:HG3	78:Sf:28:PRO:HG3	1.92	0.52
1:A:68:C:N4	1:A:315:C:H5'	2.25	0.52
5:E:816:G:H22	5:E:855:A:H2	1.58	0.52
5:E:898:A:H4'	72:SZ:46:MET:HE3	1.91	0.52
72:SZ:47:LYS:HZ3	72:SZ:62:LEU:HB3	1.74	0.52
1:A:2571:U:H1'	1:A:2572:C:H2'	1.91	0.52
5:E:477:A:H2'	5:E:478:A:H8	1.74	0.52
5:E:992:A:H2	5:E:1012:U:H3	1.58	0.52
5:E:1063:U:H2'	5:E:1064:G:H8	1.75	0.52
62:SP:74:VAL:HG12	62:SP:96:THR:HB	1.92	0.52
64:SR:239:PRO:HA	64:SR:242:ILE:HG22	1.91	0.52
1:A:289:A:H2'	1:A:290:G:H8	1.75	0.52
5:E:1785:U:H2'	5:E:1786:G:H8	1.75	0.52
8:LF:132:ALA:HA	8:LF:148:ILE:HD11	1.91	0.52
61:SO:172:ALA:HB1	61:SO:199:ILE:HG21	1.92	0.52
63:SQ:88:VAL:HG22	63:SQ:98:THR:HG22	1.92	0.52
66:ST:5:ILE:HG12	66:ST:111:LEU:HD12	1.91	0.52
6:LD:32:LEU:HD12	6:LD:36:GLU:HG2	1.91	0.52
15:LM:6:GLN:HB2	15:LM:8:PRO:HD3	1.90	0.52
51:SE:94:VAL:HG23	51:SE:107:ILE:HD11	1.91	0.52
53:SG:46:LEU:O	53:SG:50:ILE:HG13	2.10	0.52
62:SP:124:THR:HA	62:SP:146:LEU:HB2	1.91	0.52
62:SP:198:MET:HG3	62:SP:199:PRO:HD2	1.92	0.52
1:A:1203:A:H2'	1:A:1204:A:C8	2.45	0.52
1:A:1553:U:H4'	1:A:1554:U:H5'	1.91	0.52
1:A:2555:G:C5	37:Li:95:ILE:HD11	2.45	0.52
5:E:590:C:H2'	5:E:591:A:H8	1.74	0.52
7:LE:41:VAL:HA	7:LE:185:GLY:HA3	1.92	0.52
35:Lg:101:SER:O	35:Lg:105:ARG:HG3	2.10	0.52
1:A:627:U:H2'	1:A:628:A:C8	2.46	0.51
1:A:728:G:H5''	21:LS:43:PRO:HB2	1.93	0.51
1:A:1694:U:H4'	37:Li:24:LYS:HE3	1.93	0.51
1:A:3231:U:H2'	1:A:3232:G:H8	1.75	0.51
9:LG:294:ALA:HB1	14:LL:217:PHE:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:LT:181:ARG:HH12	22:LT:184:LEU:HD13	1.75	0.51
36:Lh:49:ILE:HG23	36:Lh:98:VAL:HG13	1.91	0.51
71:SY:35:GLU:O	71:SY:39:LYS:HG2	2.10	0.51
73:Sa:1:MET:HB3	73:Sa:10:GLU:HB2	1.92	0.51
1:A:307:A:H2'	1:A:308:A:C8	2.46	0.51
1:A:873:C:H3'	1:A:874:U:H4'	1.92	0.51
9:LG:103:LEU:HG	9:LG:247:ILE:HG21	1.92	0.51
69:SW:78:ARG:O	69:SW:82:ARG:HB2	2.09	0.51
5:E:1606:C:H2'	5:E:1607:G:H8	1.75	0.51
50:SD:33:ARG:HH21	50:SD:36:LEU:HD22	1.75	0.51
67:SU:88:ARG:HG2	67:SU:88:ARG:HH11	1.75	0.51
5:E:270:C:H41	66:ST:182:GLN:HE22	1.59	0.51
5:E:1474:G:H2'	5:E:1475:A:H8	1.76	0.51
8:LF:283:THR:HG22	8:LF:285:ASP:H	1.75	0.51
11:LI:239:LEU:O	11:LI:243:MET:HG3	2.10	0.51
65:SS:87:MET:HE3	65:SS:123:LEU:HB2	1.92	0.51
1:A:821:U:H2'	1:A:822:G:H8	1.75	0.51
1:A:2880:U:H1'	7:LE:250:ALA:HB3	1.93	0.51
5:E:1607:G:H2'	5:E:1608:U:C6	2.46	0.51
9:LG:211:LEU:HD21	9:LG:218:ARG:HG2	1.93	0.51
17:LO:48:GLY:HA3	17:LO:53:VAL:HB	1.91	0.51
62:SP:144:ILE:HG12	62:SP:158:VAL:HB	1.91	0.51
66:ST:135:PRO:HG2	66:ST:141:ILE:HG22	1.92	0.51
67:SU:49:ILE:HB	67:SU:57:ALA:HB3	1.93	0.51
68:SV:159:GLN:HE21	68:SV:166:TYR:H	1.58	0.51
45:Lq:27:GLN:HE22	45:Lq:68:VAL:HG22	1.74	0.51
58:SL:15:VAL:HA	58:SL:28:VAL:HG23	1.92	0.51
63:SQ:169:SER:O	63:SQ:173:THR:HG23	2.10	0.51
68:SV:34:ALA:HB2	68:SV:56:ARG:HD2	1.93	0.51
1:A:597:G:H2'	1:A:598:A:C8	2.46	0.51
30:Lb:26:VAL:HG11	30:Lb:96:VAL:HG13	1.91	0.51
63:SQ:27:LYS:HD3	63:SQ:47:LEU:HB3	1.93	0.51
65:SS:129:VAL:HG22	65:SS:139:VAL:HG12	1.92	0.51
1:A:664:U:H2'	1:A:665:A:C8	2.45	0.51
1:A:2526:C:H2'	1:A:2527:G:H8	1.76	0.51
37:Li:74:ARG:HD2	37:Li:85:VAL:HG11	1.92	0.51
61:SO:106:HIS:HD1	61:SO:126:SER:HB2	1.75	0.51
69:SW:127:VAL:O	69:SW:131:GLN:HG2	2.10	0.51
1:A:1799:A:H2'	1:A:1800:A:C8	2.46	0.51
6:LD:70:ARG:HD2	6:LD:72:ARG:HH22	1.76	0.51
11:LI:173:LEU:HB3	11:LI:178:ILE:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:LJ:57:ARG:O	12:LJ:61:GLN:HG3	2.11	0.51
19:LQ:189:ASP:O	19:LQ:193:GLN:HG3	2.10	0.51
1:A:1378:U:H2'	1:A:1379:G:H8	1.76	0.51
8:LF:154:THR:HA	8:LF:251:THR:HG23	1.92	0.51
56:SJ:23:ARG:HG2	56:SJ:23:ARG:HH11	1.75	0.51
62:SP:77:SER:OG	62:SP:86:VAL:HG21	2.10	0.51
5:E:1358:G:H2'	5:E:1359:C:C6	2.46	0.50
20:LR:118:GLN:HG2	20:LR:147:GLU:HG2	1.92	0.50
53:SG:105:GLN:NE2	62:SP:41:ARG:HA	2.25	0.50
76:Sd:11:LYS:HB2	76:Sd:24:VAL:HG12	1.92	0.50
78:Sf:64:CYS:HB3	78:Sf:73:LEU:HD23	1.92	0.50
1:A:1119:C:H2'	1:A:1120:A:H8	1.76	0.50
2:B:64:A:H5'	2:B:65:G:H5''	1.93	0.50
5:E:1160:A:H2'	5:E:1161:C:C6	2.47	0.50
5:E:1657:U:H5'	5:E:1658:G:H5''	1.92	0.50
1:A:2768:U:H2'	1:A:2769:A:H8	1.76	0.50
8:LF:181:VAL:HG11	8:LF:224:GLY:HA3	1.93	0.50
35:Lg:101:SER:HA	35:Lg:125:ARG:HH21	1.75	0.50
1:A:629:U:H2'	1:A:630:A:H8	1.76	0.50
5:E:953:G:H2'	5:E:954:G:H8	1.77	0.50
50:SD:134:SER:O	50:SD:137:MET:HG2	2.11	0.50
61:SO:36:ALA:HB1	61:SO:68:VAL:HG23	1.93	0.50
1:A:528:U:H2'	1:A:529:A:C8	2.47	0.50
15:LM:17:LEU:HG	15:LM:80:LEU:HG	1.93	0.50
67:SU:10:SER:HB2	67:SU:44:LYS:HA	1.92	0.50
76:Sd:20:ARG:HD2	76:Sd:22:GLN:NE2	2.27	0.50
1:A:2160:G:H2'	1:A:2161:G:H8	1.77	0.50
5:E:1474:G:H2'	5:E:1475:A:C8	2.47	0.50
48:SB:43:PHE:HB3	48:SB:46:TRP:HD1	1.77	0.50
74:Sb:90:THR:O	74:Sb:94:LEU:HB2	2.11	0.50
5:E:1331:A:H61	47:SA:161:GLY:HA2	1.75	0.50
29:La:63:LYS:HG2	29:La:85:VAL:HG13	1.94	0.50
52:SF:55:VAL:HG22	52:SF:59:LYS:HG3	1.93	0.50
64:SR:99:LYS:HB2	64:SR:117:THR:HG22	1.93	0.50
76:Sd:19:ALA:HB3	76:Sd:81:GLU:HG2	1.93	0.50
5:E:1591:C:H2'	5:E:1592:A:C8	2.47	0.50
8:LF:23:PRO:HB3	8:LF:259:ASP:HB3	1.94	0.50
21:LS:180:ARG:HH11	21:LS:180:ARG:HB2	1.77	0.50
52:SF:31:VAL:HG12	52:SF:67:VAL:HB	1.94	0.50
54:SH:28:ILE:HG22	54:SH:58:ALA:HA	1.93	0.50
65:SS:230:GLU:HG3	65:SS:233:LYS:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:8:C:H2'	3:C:9:A:H8	1.77	0.50
5:E:399:A:H4'	65:SS:3:ARG:HB2	1.94	0.50
9:LG:55:PHE:HE1	9:LG:159:VAL:HG23	1.76	0.50
10:LH:8:LYS:HD2	10:LH:8:LYS:C	2.37	0.50
12:LJ:146:LYS:HE2	12:LJ:173:MET:HE3	1.93	0.50
15:LM:28:ASP:HA	15:LM:31:THR:HG22	1.93	0.50
48:SB:94:THR:HG21	48:SB:111:VAL:HG12	1.94	0.50
50:SD:81:ASP:HB2	50:SD:85:LYS:HB2	1.93	0.50
54:SH:68:ARG:O	54:SH:72:ILE:HG12	2.12	0.50
76:Sd:57:VAL:HB	76:Sd:60:PHE:HE1	1.77	0.50
80:m:50:C:H2'	80:m:51:A:H8	1.75	0.50
1:A:1798:A:H2'	1:A:1799:A:C8	2.47	0.49
1:A:2364:G:H22	1:A:2396:G:H1'	1.77	0.49
1:A:2772:C:H4'	1:A:2773:C:H5'	1.93	0.49
74:Sb:20:THR:HG23	74:Sb:22:LYS:HG3	1.93	0.49
1:A:567:G:H2'	1:A:568:G:C8	2.47	0.49
1:A:629:U:H2'	1:A:630:A:C8	2.47	0.49
1:A:2681:U:H2'	1:A:2682:C:H6	1.77	0.49
1:A:3121:U:H1'	1:A:3122:A:H5''	1.94	0.49
5:E:333:A:H5'	68:SV:48:THR:HB	1.95	0.49
5:E:479:C:H2'	5:E:480:G:H8	1.78	0.49
16:LN:57:VAL:HG23	16:LN:115:ARG:HD2	1.94	0.49
47:SA:211:PRO:HG3	53:SG:19:ARG:HG3	1.94	0.49
1:A:417:A:H2'	1:A:418:A:C8	2.47	0.49
1:A:1896:A:H61	1:A:2339:C:H42	1.59	0.49
5:E:800:U:H2'	5:E:801:G:H8	1.77	0.49
6:LD:147:ARG:HG3	6:LD:157:VAL:HG22	1.95	0.49
7:LE:47:LEU:HD22	7:LE:335:ILE:HD11	1.94	0.49
61:SO:19:TRP:HB2	61:SO:38:ARG:HD2	1.94	0.49
61:SO:131:ILE:HG23	61:SO:144:LEU:HB2	1.93	0.49
5:E:29:U:H2'	5:E:30:G:C8	2.48	0.49
5:E:590:C:H2'	5:E:591:A:C8	2.47	0.49
5:E:1357:A:H2'	5:E:1358:G:C8	2.47	0.49
5:E:1606:C:H2'	5:E:1607:G:C8	2.48	0.49
20:LR:19:GLY:HA3	20:LR:22:LEU:HD11	1.94	0.49
51:SE:44:ARG:HE	51:SE:49:MET:HG3	1.78	0.49
68:SV:48:THR:HG21	68:SV:54:LYS:HE3	1.94	0.49
1:A:3016:A:H2'	1:A:3017:A:C8	2.47	0.49
4:D:1:A:C8	48:SB:152:GLY:HA3	2.47	0.49
5:E:1684:U:H3	5:E:1717:G:H1	1.58	0.49
48:SB:37:GLN:HA	52:SF:53:LEU:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:SR:88:LYS:HD2	64:SR:95:ARG:NH2	2.28	0.49
67:SU:62:VAL:O	67:SU:94:ALA:HA	2.12	0.49
73:Sa:34:ILE:HG23	73:Sa:53:TYR:HB2	1.95	0.49
74:Sb:75:ILE:HD12	74:Sb:125:ILE:HG12	1.93	0.49
5:E:12:U:H2'	5:E:13:C:C6	2.48	0.49
5:E:153:G:H2'	5:E:154:G:C8	2.48	0.49
5:E:337:G:H3'	70:SX:133:LYS:HB2	1.93	0.49
22:LT:176:ARG:HH22	22:LT:180:LYS:HD3	1.77	0.49
48:SB:129:PRO:HA	48:SB:132:VAL:HG13	1.94	0.49
66:ST:32:ILE:HD11	66:ST:63:MET:HE2	1.95	0.49
1:A:2960:C:H2'	1:A:2961:G:H8	1.77	0.49
1:A:3306:U:H2'	1:A:3307:A:H5''	1.94	0.49
5:E:918:U:H4'	72:SZ:18:ARG:HD2	1.94	0.49
28:LZ:86:VAL:O	28:LZ:120:LYS:HB3	2.12	0.49
1:A:105:C:H2'	1:A:106:A:H8	1.78	0.49
1:A:700:C:H2'	1:A:701:G:H8	1.77	0.49
1:A:1497:C:H2'	1:A:1498:A:C8	2.47	0.49
5:E:554:C:H1'	5:E:555:A:C2	2.47	0.49
5:E:1583:A:H1'	5:E:1585:U:C2	2.48	0.49
5:E:1588:G:H1	5:E:1608:U:H3	1.60	0.49
15:LM:50:ALA:HB2	15:LM:65:ILE:HG12	1.95	0.49
54:SH:115:ARG:O	54:SH:119:ILE:HG12	2.13	0.49
72:SZ:61:MET:O	72:SZ:65:GLN:HG2	2.13	0.49
81:n:62:C:H2'	81:n:63:G:H8	1.77	0.49
1:A:2812:C:H2'	1:A:2813:A:C8	2.48	0.49
20:LR:129:THR:HG23	20:LR:131:ARG:HD3	1.94	0.49
35:Lg:79:VAL:O	35:Lg:83:GLU:HG2	2.13	0.49
48:SB:93:LEU:HD11	48:SB:133:VAL:HG21	1.95	0.49
62:SP:59:LEU:HB2	73:Sa:79:LEU:HD21	1.95	0.49
1:A:589:A:H1'	1:A:1337:A:H5''	1.95	0.49
1:A:1576:G:H2'	1:A:1577:G:H8	1.76	0.49
5:E:591:A:H2'	5:E:592:A:C8	2.47	0.49
24:LV:100:LYS:O	24:LV:104:GLU:HG2	2.13	0.49
62:SP:27:ARG:HG2	62:SP:45:VAL:HG22	1.95	0.49
64:SR:140:ARG:HH21	64:SR:226:THR:HG21	1.77	0.49
68:SV:87:ASN:HD21	68:SV:89:GLU:HB2	1.78	0.49
1:A:2597:U:H2'	1:A:2598:G:H8	1.77	0.48
5:E:1434:U:H4'	59:SM:24:CYS:HB2	1.95	0.48
50:SD:26:ASP:HA	50:SD:29:LYS:HG2	1.94	0.48
52:SF:42:GLU:HA	52:SF:45:ARG:HB2	1.94	0.48
63:SQ:103:MET:HB3	63:SQ:215:VAL:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:SQ:149:GLN:NE2	63:SQ:154:SER:HB3	2.24	0.48
81:n:75:C:H3'	81:n:76:A:H4'	1.95	0.48
9:LG:178:ASN:HA	9:LG:183:TRP:CE3	2.48	0.48
42:Ln:15:LYS:O	42:Ln:19:GLN:HG2	2.13	0.48
64:SR:140:ARG:HB3	64:SR:221:THR:HB	1.93	0.48
1:A:1799:A:H2'	1:A:1800:A:H8	1.79	0.48
5:E:884:A:H2'	5:E:885:G:C8	2.46	0.48
5:E:891:A:H2'	5:E:892:A:C8	2.47	0.48
11:LI:80:GLN:HB2	24:LV:135:PRO:HB2	1.95	0.48
5:E:1566:U:H5'	54:SH:39:GLY:HA3	1.95	0.48
12:LJ:173:MET:HE3	12:LJ:173:MET:HB3	1.77	0.48
13:LK:59:ASN:HD21	17:LO:41:GLN:HG2	1.79	0.48
29:La:11:ASP:HB3	29:La:14:LYS:HB2	1.94	0.48
48:SB:43:PHE:HD1	48:SB:48:PHE:HZ	1.60	0.48
48:SB:214:LYS:O	48:SB:218:GLU:HG2	2.12	0.48
1:A:411:U:H2'	1:A:412:G:H8	1.79	0.48
1:A:597:G:H5''	11:LI:41:ARG:HD2	1.94	0.48
1:A:3217:C:C2	20:LR:182:ILE:HD12	2.48	0.48
5:E:1210:C:H2'	5:E:1211:A:H8	1.78	0.48
52:SF:18:ALA:HB2	52:SF:69:VAL:HG13	1.96	0.48
64:SR:81:MET:HB2	64:SR:101:VAL:HG13	1.96	0.48
64:SR:120:GLU:HG2	64:SR:123:GLY:H	1.78	0.48
1:A:2357:A:H2'	1:A:2358:A:C8	2.49	0.48
2:B:112:G:H2'	2:B:113:C:C6	2.48	0.48
19:LQ:188:SER:O	19:LQ:192:LYS:HG3	2.13	0.48
35:Lg:86:THR:HG23	35:Lg:115:LEU:HD22	1.95	0.48
50:SD:34:THR:HA	50:SD:37:VAL:HG22	1.95	0.48
55:SI:64:HIS:CD2	55:SI:71:VAL:HG11	2.49	0.48
81:n:62:C:H2'	81:n:63:G:C8	2.48	0.48
81:n:63:G:H2'	81:n:64:A:H8	1.78	0.48
1:A:3015:G:H2'	1:A:3016:A:H8	1.78	0.48
5:E:1041:G:H2'	5:E:1042:G:C8	2.49	0.48
48:SB:84:LYS:HG2	48:SB:92:ARG:HH12	1.79	0.48
5:E:894:U:H2'	5:E:895:G:C8	2.49	0.48
5:E:1641:C:H2'	5:E:1642:G:C8	2.48	0.48
7:LE:84:VAL:O	7:LE:202:THR:HA	2.14	0.48
12:LJ:75:ILE:HD11	18:LP:18:VAL:HG23	1.96	0.48
65:SS:11:ARG:NH1	65:SS:20:LEU:HB3	2.28	0.48
70:SX:81:HIS:CE1	70:SX:82:ARG:HD3	2.49	0.48
78:Sf:14:SER:HA	78:Sf:17:ARG:HD3	1.96	0.48
1:A:937:G:H5''	31:Lc:29:PRO:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1437:U:H2'	5:E:1438:G:H8	1.78	0.48
55:SI:130:ARG:O	55:SI:134:ARG:HG2	2.14	0.48
62:SP:182:LEU:HG	62:SP:187:ALA:HB3	1.96	0.48
63:SQ:87:ARG:HB2	63:SQ:101:HIS:CD2	2.48	0.48
66:ST:50:PHE:HB3	66:ST:111:LEU:HD22	1.96	0.48
1:A:1777:U:H2'	1:A:1778:G:C8	2.48	0.48
1:A:3252:G:H2'	1:A:3253:G:C8	2.48	0.48
13:LK:27:VAL:HG12	13:LK:82:VAL:HG21	1.96	0.48
45:Lq:19:LYS:HB2	45:Lq:19:LYS:HE3	1.63	0.48
66:ST:7:TYR:HD1	66:ST:113:ILE:HB	1.78	0.48
1:A:800:G:H1	8:LF:104:LYS:HZ1	1.62	0.47
1:A:1596:C:H2'	1:A:1597:C:C6	2.49	0.47
1:A:598:A:H4'	8:LF:325:LEU:HD13	1.96	0.47
3:C:9:A:H2'	3:C:10:A:C8	2.48	0.47
5:E:1241:G:H4'	51:SE:78:THR:HA	1.95	0.47
31:Lc:126:LYS:HB3	31:Lc:148:ILE:HD13	1.96	0.47
51:SE:52:LYS:HG2	51:SE:80:MET:HE1	1.96	0.47
52:SF:34:SER:HB2	52:SF:38:LEU:HD21	1.94	0.47
54:SH:41:ARG:HE	55:SI:46:PRO:HD3	1.79	0.47
67:SU:39:ARG:HG2	67:SU:39:ARG:HH11	1.79	0.47
70:SX:55:ASP:HB3	70:SX:58:CYS:HB2	1.96	0.47
5:E:947:U:H2'	5:E:948:G:H8	1.78	0.47
5:E:1216:C:O2'	5:E:1217:A:H3'	2.13	0.47
13:LK:6:THR:HG23	13:LK:57:VAL:HG13	1.97	0.47
18:LP:84:PRO:HA	18:LP:87:GLN:HG3	1.96	0.47
20:LR:114:VAL:HG12	20:LR:150:VAL:HG12	1.95	0.47
31:Lc:147:LEU:HB2	39:Lk:7:ILE:HG22	1.96	0.47
50:SD:132:GLU:O	50:SD:135:MET:HG2	2.14	0.47
53:SG:66:VAL:HG13	53:SG:69:ILE:HB	1.96	0.47
5:E:953:G:H2'	5:E:954:G:C8	2.50	0.47
6:LD:116:VAL:HB	6:LD:126:LEU:HB2	1.96	0.47
14:LL:30:LYS:HG2	14:LL:63:GLU:HG3	1.96	0.47
48:SB:109:LYS:O	48:SB:113:ILE:HG12	2.15	0.47
57:SK:84:GLU:HA	57:SK:89:ILE:HD11	1.97	0.47
61:SO:68:VAL:HG12	61:SO:84:SER:HB2	1.95	0.47
61:SO:172:ALA:HB2	61:SO:202:LEU:HD13	1.96	0.47
66:ST:49:VAL:HG13	66:ST:114:VAL:HG13	1.96	0.47
1:A:1666:G:H2'	1:A:1667:A:H8	1.79	0.47
1:A:2812:C:H2'	1:A:2813:A:H8	1.78	0.47
18:LP:36:ILE:HG12	18:LP:64:VAL:HG23	1.97	0.47
73:Sa:78:LEU:O	73:Sa:79:LEU:HD23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2213:A:H2'	1:A:2214:A:C8	2.50	0.47
1:A:2344:U:H2'	1:A:2345:A:C8	2.50	0.47
3:C:8:C:H2'	3:C:9:A:C8	2.49	0.47
5:E:866:G:H5''	71:SY:2:GLY:HA3	1.96	0.47
5:E:1776:A:H2'	5:E:1777:G:C8	2.50	0.47
13:LK:91:ARG:HD2	13:LK:143:GLU:HB2	1.97	0.47
15:LM:40:LEU:HD23	15:LM:114:ILE:HD11	1.97	0.47
18:LP:47:LYS:HE3	18:LP:51:LEU:HD11	1.97	0.47
27:LY:52:THR:HG22	27:LY:54:LEU:H	1.79	0.47
49:SC:25:LYS:HD3	49:SC:59:PHE:CE1	2.49	0.47
1:A:159:A:H2'	1:A:160:G:H8	1.79	0.47
1:A:584:G:H2'	1:A:585:A:H8	1.78	0.47
1:A:2351:U:H2'	1:A:2352:A:H8	1.79	0.47
5:E:387:A:H2'	5:E:402:C:H5'	1.97	0.47
5:E:1210:C:H2'	5:E:1211:A:C8	2.49	0.47
5:E:1592:A:H2'	5:E:1593:A:H8	1.79	0.47
12:LJ:73:PRO:HA	12:LJ:76:ALA:HB3	1.95	0.47
14:LL:29:SER:HB2	14:LL:125:LEU:HD12	1.95	0.47
15:LM:148:VAL:HG23	15:LM:153:LYS:HD3	1.95	0.47
50:SD:34:THR:HG22	50:SD:127:GLY:HA3	1.96	0.47
63:SQ:134:VAL:HG23	63:SQ:218:LEU:HB2	1.96	0.47
63:SQ:181:LEU:O	63:SQ:185:THR:HG23	2.13	0.47
70:SX:80:MET:HE3	70:SX:83:THR:HB	1.97	0.47
78:Sf:80:ARG:HH11	78:Sf:80:ARG:HB2	1.79	0.47
1:A:312:C:H2'	1:A:313:A:H8	1.79	0.47
1:A:1419:A:H5''	8:LF:193:LYS:HZ2	1.78	0.47
1:A:2344:U:H2'	1:A:2345:A:H8	1.79	0.47
12:LJ:149:LYS:HG2	12:LJ:211:LEU:HD21	1.97	0.47
14:LL:46:PHE:HB2	14:LL:139:ARG:HH11	1.80	0.47
15:LM:34:SER:HB3	15:LM:67:VAL:HG21	1.97	0.47
21:LS:69:ARG:HG2	21:LS:69:ARG:HH11	1.80	0.47
30:Lb:24:VAL:HG21	30:Lb:87:LEU:HB3	1.96	0.47
52:SF:21:HIS:HB2	52:SF:66:ARG:HB2	1.96	0.47
54:SH:100:THR:HB	54:SH:105:VAL:HG12	1.97	0.47
55:SI:14:PHE:HE2	55:SI:136:ALA:HB2	1.79	0.47
55:SI:64:HIS:CE1	55:SI:68:ARG:HE	2.33	0.47
66:ST:57:ASP:HA	66:ST:107:ALA:H	1.79	0.47
74:Sb:106:THR:HG23	74:Sb:108:ALA:H	1.80	0.47
5:E:843:U:H2'	5:E:844:A:H8	1.80	0.47
5:E:947:U:H2'	5:E:948:G:C8	2.50	0.47
5:E:1506:G:H2'	5:E:1507:G:H8	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:LH:66:THR:HB	10:LH:76:LEU:HD23	1.97	0.47
13:LK:8:GLN:HB3	13:LK:72:LYS:HG3	1.96	0.47
13:LK:112:ILE:HB	13:LK:126:VAL:HG13	1.97	0.47
61:SO:122:ILE:HB	61:SO:134:TRP:HB2	1.97	0.47
5:E:406:U:H2'	5:E:407:A:C8	2.50	0.47
5:E:1087:A:H2'	5:E:1088:A:C8	2.50	0.47
53:SG:15:ALA:O	53:SG:19:ARG:HB2	2.15	0.47
54:SH:46:VAL:HG21	54:SH:73:MET:HE1	1.97	0.47
1:A:1083:G:H2'	1:A:1084:A:C8	2.50	0.46
1:A:2526:C:H2'	1:A:2527:G:C8	2.49	0.46
1:A:3309:G:H1'	20:LR:69:ARG:HD3	1.96	0.46
5:E:567:A:H1'	79:Sg:14:VAL:HG23	1.97	0.46
9:LG:260:PHE:HB3	9:LG:264:GLN:HE21	1.80	0.46
74:Sb:43:LYS:HB2	74:Sb:43:LYS:HE2	1.69	0.46
75:Sc:78:LYS:C	75:Sc:79:ASN:HD22	2.23	0.46
1:A:627:U:H2'	1:A:628:A:H8	1.81	0.46
1:A:631:U:H2'	1:A:632:G:H8	1.81	0.46
1:A:985:U:H2'	1:A:986:U:H6	1.80	0.46
1:A:2152:A:H2'	1:A:2153:U:H6	1.80	0.46
5:E:319:U:H4'	5:E:323:A:C8	2.50	0.46
5:E:1511:U:H2'	5:E:1512:G:C8	2.50	0.46
5:E:1556:A:H2'	51:SE:40:ARG:HH11	1.80	0.46
20:LR:115:SER:HB3	20:LR:151:THR:HG22	1.98	0.46
24:LV:78:LYS:HD3	24:LV:87:LYS:HZ2	1.80	0.46
62:SP:11:PRO:O	62:SP:15:GLN:HG3	2.14	0.46
1:A:2228:A:H2'	1:A:2229:A:C8	2.51	0.46
1:A:2697:A:H2'	1:A:2698:G:C8	2.49	0.46
5:E:901:G:H3'	5:E:902:G:H8	1.79	0.46
5:E:939:A:H2'	5:E:940:A:C8	2.51	0.46
10:LH:40:LEU:HD11	10:LH:54:TYR:HB2	1.97	0.46
16:LN:62:THR:HG23	16:LN:64:LYS:H	1.81	0.46
45:Lq:23:HIS:HA	45:Lq:73:GLU:O	2.16	0.46
46:Lr:26:VAL:O	46:Lr:30:GLU:HB2	2.15	0.46
54:SH:61:LEU:HD12	54:SH:61:LEU:HA	1.80	0.46
61:SO:19:TRP:CE2	61:SO:306:THR:HB	2.50	0.46
63:SQ:137:ILE:HD11	63:SQ:172:LEU:HB3	1.97	0.46
64:SR:88:LYS:HG2	64:SR:89:GLN:H	1.80	0.46
71:SY:40:TYR:HD1	71:SY:43:LYS:HD2	1.80	0.46
71:SY:64:ARG:HD2	71:SY:70:LYS:HD3	1.96	0.46
76:Sd:83:LYS:HD3	76:Sd:96:LEU:HD12	1.97	0.46
1:A:1696:A:H2'	1:A:1697:A:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:890:C:H2'	5:E:891:A:H8	1.81	0.46
11:LI:104:GLN:HE21	21:LS:6:THR:HG22	1.80	0.46
13:LK:69:ARG:HE	13:LK:72:LYS:HD2	1.81	0.46
18:LP:121:VAL:HG11	18:LP:131:GLU:HG3	1.98	0.46
20:LR:60:PHE:HB3	20:LR:64:ASN:HB3	1.97	0.46
36:Lh:52:VAL:HG22	36:Lh:66:VAL:HG22	1.98	0.46
53:SG:13:SER:O	53:SG:17:ILE:HG13	2.16	0.46
54:SH:120:ARG:HD3	54:SH:120:ARG:HA	1.78	0.46
63:SQ:31:ASP:O	63:SQ:95:ASN:HA	2.15	0.46
65:SS:147:ILE:HG21	65:SS:169:ILE:HD13	1.98	0.46
66:ST:138:ALA:O	66:ST:141:ILE:HD12	2.16	0.46
74:Sb:57:ARG:CZ	78:Sf:26:GLN:HE21	2.28	0.46
1:A:900:G:H1'	1:A:1589:A:N6	2.30	0.46
1:A:1126:G:H21	14:LL:115:MET:HE2	1.81	0.46
1:A:3255:U:H2'	1:A:3256:G:H8	1.81	0.46
1:A:3294:A:H5'	7:LE:128:LYS:HG3	1.98	0.46
14:LL:38:LYS:HE3	14:LL:41:ALA:HB2	1.97	0.46
20:LR:16:SER:HB3	20:LR:149:VAL:HG22	1.97	0.46
52:SF:29:ILE:HG23	52:SF:65:ILE:HB	1.96	0.46
64:SR:230:TRP:CE2	74:Sb:68:ARG:HB3	2.50	0.46
74:Sb:47:ILE:HG22	74:Sb:65:LEU:HD23	1.97	0.46
1:A:185:C:H5''	29:La:122:LYS:HG2	1.97	0.46
1:A:243:G:H2'	1:A:244:G:O4'	2.16	0.46
7:LE:47:LEU:HD11	7:LE:179:ALA:HB3	1.97	0.46
9:LG:148:ILE:HG23	9:LG:151:GLN:HB3	1.98	0.46
33:Le:38:LYS:HB3	33:Le:93:LEU:HD12	1.98	0.46
52:SF:93:HIS:HA	52:SF:97:VAL:HB	1.97	0.46
57:SK:48:ASP:O	57:SK:52:LYS:HD2	2.16	0.46
61:SO:106:HIS:HD2	61:SO:132:LYS:HD2	1.78	0.46
64:SR:40:LYS:HG3	64:SR:247:ALA:HB1	1.98	0.46
5:E:68:A:N6	66:ST:132:ARG:HG2	2.31	0.46
5:E:209:U:H2'	5:E:210:A:C8	2.51	0.46
19:LQ:171:LYS:O	19:LQ:175:THR:HG23	2.15	0.46
52:SF:67:VAL:HG11	52:SF:81:ILE:HG23	1.98	0.46
55:SI:7:ARG:HG2	55:SI:67:MET:HE1	1.98	0.46
61:SO:24:ALA:HB3	61:SO:34:LEU:HB3	1.98	0.46
62:SP:155:PHE:HA	73:Sa:60:ARG:HE	1.81	0.46
67:SU:151:LYS:HA	67:SU:182:VAL:O	2.16	0.46
73:Sa:53:TYR:CE1	73:Sa:72:LEU:HD22	2.51	0.46
74:Sb:92:ASN:HD22	74:Sb:92:ASN:HA	1.58	0.46
7:LE:112:ASP:O	7:LE:116:ARG:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:LF:193:LYS:HE3	8:LF:193:LYS:HB2	1.79	0.46
67:SU:49:ILE:HG13	67:SU:172:VAL:HG13	1.96	0.46
1:A:129:U:H2'	1:A:130:A:C8	2.51	0.46
1:A:157:A:N7	39:Lk:26:ILE:HG12	2.31	0.46
1:A:314:U:H2'	1:A:315:C:C6	2.51	0.46
1:A:1805:C:H2'	1:A:1806:A:H8	1.81	0.46
5:E:1382:A:H2'	5:E:1383:G:C8	2.51	0.46
6:LD:65:ASP:HB2	6:LD:72:ARG:HG2	1.98	0.46
12:LJ:25:PRO:HG2	12:LJ:26:LEU:HD22	1.98	0.46
1:A:1061:A:H4'	24:LV:102:ARG:HH21	1.81	0.46
5:E:751:G:H2'	5:E:752:A:H8	1.81	0.46
24:LV:73:GLY:HA2	24:LV:89:LEU:O	2.16	0.46
49:SC:63:TYR:HB3	49:SC:65:TYR:HE1	1.81	0.46
50:SD:66:VAL:HG22	50:SD:72:ILE:HG12	1.98	0.46
52:SF:51:PRO:O	52:SF:55:VAL:HG12	2.16	0.46
54:SH:11:PHE:CE1	54:SH:59:GLY:HA3	2.51	0.46
57:SK:90:LYS:HB2	57:SK:104:ALA:HA	1.97	0.46
65:SS:185:GLY:N	65:SS:189:LEU:HD23	2.30	0.46
74:Sb:71:LYS:HD3	74:Sb:128:PHE:HE2	1.80	0.46
1:A:536:U:H2'	1:A:537:A:H8	1.82	0.45
1:A:656:A:H2'	1:A:657:A:C8	2.51	0.45
1:A:1083:G:H2'	1:A:1084:A:H8	1.80	0.45
1:A:1419:A:H5''	8:LF:193:LYS:NZ	2.31	0.45
1:A:2971:A:H2'	81:n:76:A:H3'	1.98	0.45
1:A:3295:A:H2'	1:A:3296:A:C8	2.51	0.45
5:E:108:A:H2'	5:E:109:G:C8	2.51	0.45
16:LN:126:PHE:HD2	38:Lj:115:LYS:HD2	1.81	0.45
26:LX:40:LYS:HG3	26:LX:57:MET:HG2	1.97	0.45
60:SN:130:VAL:HG11	60:SN:143:LYS:HG3	1.97	0.45
60:SN:143:LYS:HE2	60:SN:143:LYS:HB3	1.57	0.45
5:E:1067:C:H5''	63:SQ:150:VAL:HG22	1.99	0.45
5:E:1071:U:H2'	5:E:1072:C:C6	2.51	0.45
10:LH:40:LEU:HD13	10:LH:84:VAL:HG21	1.98	0.45
23:LU:92:LYS:HE2	23:LU:109:ASP:OD2	2.15	0.45
43:Lo:98:LYS:HG3	43:Lo:118:THR:HG21	1.97	0.45
57:SK:89:ILE:HB	57:SK:101:TYR:HB3	1.98	0.45
63:SQ:130:SER:HB2	63:SQ:180:THR:HG22	1.96	0.45
63:SQ:176:VAL:HG22	63:SQ:184:LEU:HD11	1.98	0.45
78:Sf:52:THR:HG23	78:Sf:54:VAL:HG22	1.98	0.45
1:A:1534:A:H2'	1:A:1535:A:C8	2.51	0.45
7:LE:48:GLY:O	7:LE:335:ILE:HA	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:LU:124:LEU:HD21	24:LV:155:PRO:HB3	1.98	0.45
41:Lm:14:LEU:HD21	41:Lm:52:TYR:CG	2.51	0.45
48:SB:95:ASN:HA	48:SB:98:MET:HE2	1.97	0.45
60:SN:105:TYR:HD2	60:SN:131:PHE:HD2	1.63	0.45
63:SQ:32:ILE:HG22	63:SQ:96:LEU:HD11	1.99	0.45
65:SS:72:VAL:HG22	65:SS:90:ILE:HG12	1.98	0.45
74:Sb:72:CYS:HB3	74:Sb:129:VAL:HG23	1.98	0.45
1:A:2882:U:H2'	1:A:2883:U:C6	2.52	0.45
5:E:1477:G:H2'	5:E:1478:G:H8	1.80	0.45
5:E:1564:U:H2'	5:E:1565:C:C6	2.51	0.45
18:LP:60:VAL:HB	18:LP:134:LEU:HB2	1.99	0.45
61:SO:79:TYR:HB3	61:SO:91:LEU:HD11	1.99	0.45
61:SO:112:SER:HB2	61:SO:153:GLN:HA	1.97	0.45
66:ST:3:LEU:O	66:ST:15:THR:HA	2.17	0.45
78:Sf:80:ARG:HB2	78:Sf:80:ARG:NH1	2.31	0.45
1:A:2376:G:H2'	1:A:2377:G:C8	2.51	0.45
1:A:3322:A:H2'	1:A:3323:A:C8	2.51	0.45
5:E:329:G:H2'	5:E:330:G:H8	1.82	0.45
5:E:385:A:H2'	5:E:386:G:C8	2.52	0.45
5:E:868:G:N2	5:E:960:U:O2	2.40	0.45
5:E:1253:U:H5''	60:SN:130:VAL:HG12	1.99	0.45
47:SA:10:LYS:HG2	47:SA:11:LEU:HD23	1.99	0.45
47:SA:207:THR:HG23	53:SG:40:THR:HB	1.98	0.45
51:SE:60:LEU:HB3	51:SE:76:VAL:HG11	1.97	0.45
52:SF:77:GLN:O	52:SF:81:ILE:HG13	2.17	0.45
76:Sd:20:ARG:HH11	76:Sd:22:GLN:NE2	2.15	0.45
1:A:1288:U:H2'	1:A:1289:G:H8	1.82	0.45
1:A:1338:C:H4'	35:Lg:60:ASN:HD22	1.82	0.45
5:E:625:C:H2'	5:E:626:U:C6	2.52	0.45
5:E:800:U:H2'	5:E:801:G:C8	2.51	0.45
28:LZ:86:VAL:HG11	28:LZ:95:ILE:HD11	1.98	0.45
47:SA:76:ARG:HD2	49:SC:65:TYR:OH	2.17	0.45
50:SD:49:THR:HA	50:SD:52:LEU:HG	1.97	0.45
51:SE:49:MET:HE2	51:SE:49:MET:H	1.81	0.45
53:SG:51:ALA:O	53:SG:55:THR:HG23	2.16	0.45
64:SR:169:LEU:HD23	64:SR:198:THR:HG22	1.99	0.45
80:m:14:A:H3'	80:m:15:G:H8	1.81	0.45
1:A:3164:C:O2'	1:A:3165:A:H8	1.99	0.45
5:E:1268:G:H1'	5:E:1448:G:H5''	1.97	0.45
5:E:1291:G:H2'	5:E:1292:G:H8	1.81	0.45
21:LS:43:PRO:HA	21:LS:46:LYS:HD2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:LS:44:PHE:O	21:LS:48:VAL:HG12	2.17	0.45
45:Lq:72:LEU:O	45:Lq:80:ARG:HA	2.16	0.45
47:SA:64:ARG:O	47:SA:68:GLU:HG3	2.17	0.45
50:SD:66:VAL:HG21	50:SD:71:ILE:HB	1.98	0.45
52:SF:22:VAL:HG22	52:SF:65:ILE:HD12	1.99	0.45
65:SS:65:LEU:HB3	65:SS:78:THR:HA	1.99	0.45
67:SU:124:LYS:HD3	67:SU:124:LYS:HA	1.81	0.45
1:A:255:A:H2'	1:A:256:G:H8	1.82	0.45
1:A:3049:A:C8	7:LE:53:MET:HE2	2.51	0.45
5:E:1477:G:H2'	5:E:1478:G:C8	2.51	0.45
7:LE:188:ILE:O	7:LE:192:VAL:HG12	2.17	0.45
7:LE:284:ARG:HH22	7:LE:296:THR:HG22	1.81	0.45
48:SB:209:TYR:HA	48:SB:212:LYS:HD2	1.98	0.45
58:SL:57:MET:HE3	58:SL:57:MET:HB3	1.89	0.45
1:A:620:U:H4'	20:LR:167:ARG:HH22	1.81	0.45
1:A:1290:A:H2'	1:A:1291:A:C8	2.52	0.45
1:A:2611:U:H2'	1:A:2612:U:C6	2.51	0.45
2:B:9:C:OP1	24:LV:26:HIS:HB2	2.17	0.45
5:E:474:A:H5''	69:SW:144:PRO:HD2	1.99	0.45
5:E:925:G:H2'	5:E:926:A:C8	2.51	0.45
15:LM:37:LEU:HD12	15:LM:37:LEU:HA	1.80	0.45
23:LU:79:VAL:HG11	23:LU:106:LEU:HD21	1.99	0.45
47:SA:157:LEU:HD22	47:SA:189:MET:HB2	1.99	0.45
51:SE:111:MET:HB3	54:SH:119:ILE:HG21	1.98	0.45
68:SV:138:ASN:O	68:SV:142:LYS:HG2	2.15	0.45
1:A:541:U:H2'	1:A:542:G:C8	2.52	0.45
1:A:801:A:N6	16:LN:19:GLN:HE22	2.15	0.45
1:A:1336:U:H2'	1:A:1337:A:H8	1.82	0.45
1:A:1689:U:H5''	22:LT:61:SER:HB3	1.99	0.45
5:E:815:G:O4'	22:LT:162:ARG:HD3	2.16	0.45
5:E:1151:A:H2'	5:E:1152:A:H8	1.81	0.45
6:LD:109:GLU:H	6:LD:109:GLU:CD	2.25	0.45
15:LM:54:VAL:HG12	15:LM:57:PHE:HB2	1.99	0.45
48:SB:163:SER:O	48:SB:167:ARG:HG3	2.16	0.45
65:SS:199:GLU:HG3	65:SS:207:LEU:HD22	1.98	0.45
74:Sb:102:VAL:HG13	74:Sb:113:HIS:HB3	1.99	0.45
76:Sd:27:VAL:HG21	76:Sd:35:VAL:HG11	1.97	0.45
80:m:5:C:H2'	80:m:6:G:H8	1.81	0.45
1:A:993:G:N3	1:A:2637:A:H2'	2.32	0.44
1:A:2413:A:H2'	1:A:2414:G:C8	2.52	0.44
1:A:3294:A:H2'	1:A:3295:A:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:79:C:H1'	66:ST:174:LYS:HD2	2.00	0.44
8:LF:233:LEU:HD13	8:LF:238:LEU:HD11	1.99	0.44
26:LX:57:MET:HE3	26:LX:57:MET:HB2	1.90	0.44
32:Ld:32:LEU:HD22	32:Ld:35:VAL:HG21	1.99	0.44
47:SA:120:TYR:HA	47:SA:123:VAL:HG22	1.99	0.44
66:ST:70:PRO:HG3	66:ST:101:ILE:HG21	1.99	0.44
1:A:3119:U:H4'	43:Lo:104:PRO:HG2	1.98	0.44
5:E:107:C:H2'	5:E:108:A:H8	1.82	0.44
5:E:874:C:H2'	5:E:875:G:C8	2.52	0.44
14:LL:74:LYS:O	14:LL:78:THR:HG23	2.16	0.44
33:Le:42:ILE:HD13	33:Le:65:THR:HG21	1.98	0.44
47:SA:208:ILE:HD11	53:SG:20:TYR:HE1	1.82	0.44
48:SB:37:GLN:HA	52:SF:53:LEU:HD23	1.99	0.44
52:SF:128:LYS:HB2	52:SF:128:LYS:HE2	1.74	0.44
55:SI:64:HIS:O	55:SI:68:ARG:HG2	2.17	0.44
61:SO:33:LEU:HB3	61:SO:45:TRP:HB2	1.98	0.44
61:SO:123:ILE:HG22	61:SO:133:VAL:HG12	1.99	0.44
66:ST:69:LEU:HD21	66:ST:73:ILE:HG12	1.99	0.44
69:SW:180:LYS:HE3	69:SW:180:LYS:HB2	1.74	0.44
1:A:3313:U:H4'	7:LE:173:GLN:HG2	2.00	0.44
2:B:79:A:H62	2:B:101:G:H21	1.66	0.44
5:E:447:U:H2'	5:E:448:C:O4'	2.16	0.44
9:LG:11:ALA:O	9:LG:15:ARG:HG3	2.18	0.44
13:LK:28:VAL:HG12	13:LK:33:THR:HG23	1.99	0.44
15:LM:75:LYS:O	15:LM:79:ILE:HD12	2.17	0.44
20:LR:29:THR:HG22	20:LR:119:VAL:HG21	1.99	0.44
72:SZ:16:VAL:O	72:SZ:30:VAL:HA	2.18	0.44
1:A:531:G:H2'	1:A:532:A:C8	2.53	0.44
1:A:710:A:H2'	1:A:711:A:C8	2.53	0.44
1:A:1108:U:H2'	1:A:1109:U:C6	2.53	0.44
1:A:1119:C:H2'	1:A:1120:A:C8	2.52	0.44
1:A:3354:U:H5''	1:A:3355:U:H3'	1.98	0.44
3:C:83:C:H1'	3:C:85:G:H21	1.82	0.44
5:E:925:G:H2'	5:E:926:A:H8	1.81	0.44
14:LL:38:LYS:HB2	14:LL:83:ASP:HA	2.00	0.44
19:LQ:79:ILE:HG21	19:LQ:138:LEU:HD11	2.00	0.44
26:LX:84:SER:HA	26:LX:94:TYR:HB3	1.99	0.44
77:Se:44:ILE:H	77:Se:44:ILE:HG13	1.47	0.44
1:A:1110:U:H2'	1:A:1111:U:C6	2.53	0.44
1:A:1369:A:H4'	31:Lc:21:ARG:HG3	2.00	0.44
1:A:3162:C:H2'	1:A:3163:A:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:LK:41:ILE:HG22	13:LK:43:VAL:HB	1.98	0.44
34:Lf:26:LYS:HD3	34:Lf:26:LYS:HA	1.80	0.44
48:SB:90:ILE:O	48:SB:94:THR:HG23	2.18	0.44
50:SD:60:VAL:HG22	50:SD:122:VAL:HG22	2.00	0.44
60:SN:97:LYS:HA	60:SN:100:LEU:HB2	2.00	0.44
61:SO:127:ARG:HA	61:SO:150:TRP:HB2	2.00	0.44
61:SO:132:LYS:NZ	61:SO:143:THR:HB	2.33	0.44
63:SQ:39:GLU:HG3	63:SQ:40:ASN:HD22	1.83	0.44
72:SZ:92:LYS:HD3	72:SZ:121:VAL:HG12	1.98	0.44
75:Sc:125:VAL:HG12	75:Sc:126:LYS:HG3	1.99	0.44
1:A:19:U:H2'	1:A:20:A:C8	2.52	0.44
1:A:307:A:H2'	1:A:308:A:H8	1.81	0.44
1:A:565:U:H2'	1:A:566:G:H8	1.82	0.44
1:A:786:A:H4'	1:A:787:G:H5'	1.99	0.44
5:E:1776:A:H2'	5:E:1777:G:H8	1.82	0.44
15:LM:14:ILE:HD13	15:LM:80:LEU:HD12	2.00	0.44
33:Le:64:LYS:HE2	33:Le:64:LYS:HB2	1.79	0.44
48:SB:97:LEU:HD21	48:SB:194:LEU:HD22	2.00	0.44
53:SG:71:PHE:HB3	53:SG:74:GLN:HB3	1.99	0.44
1:A:411:U:H2'	1:A:412:G:C8	2.53	0.44
1:A:1666:G:H2'	1:A:1667:A:C8	2.52	0.44
5:E:826:U:H2'	5:E:827:C:C6	2.53	0.44
5:E:1358:G:H2'	5:E:1359:C:H6	1.83	0.44
17:LO:113:THR:H	17:LO:116:GLU:HG3	1.83	0.44
30:Lb:22:LYS:HG2	30:Lb:49:TYR:OH	2.18	0.44
40:Ll:27:PHE:HA	40:Ll:34:CYS:HA	1.99	0.44
47:SA:126:VAL:HG11	47:SA:134:CYS:HB2	2.00	0.44
48:SB:72:HIS:CD2	52:SF:44:LEU:HD11	2.53	0.44
54:SH:35:ILE:HD11	54:SH:102:ALA:HA	1.98	0.44
65:SS:214:LEU:HD11	65:SS:244:ILE:HD12	2.00	0.44
68:SV:119:GLN:HG3	68:SV:150:ALA:HB2	1.98	0.44
1:A:1065:A:N1	32:Ld:26:THR:HG23	2.32	0.44
1:A:1281:G:H2'	1:A:1282:G:H8	1.83	0.44
1:A:2177:G:H2'	6:LD:128:ARG:HD3	2.00	0.44
1:A:2947:G:N3	7:LE:250:ALA:HB1	2.33	0.44
1:A:3107:U:H2'	1:A:3108:G:C8	2.52	0.44
2:B:94:C:H2'	2:B:95:A:C8	2.53	0.44
5:E:1732:A:H2'	5:E:1733:C:C6	2.53	0.44
7:LE:148:LEU:HD11	7:LE:196:ARG:HD3	1.99	0.44
23:LU:45:LEU:HD12	23:LU:45:LEU:HA	1.90	0.44
38:Lj:34:GLN:O	38:Lj:38:ARG:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:SB:94:THR:HG22	48:SB:114:ILE:HG13	2.00	0.44
61:SO:35:SER:O	61:SO:42:LEU:HA	2.18	0.44
5:E:1368:G:H5''	55:SI:69:LYS:HD2	1.99	0.44
21:LS:67:ILE:HG23	21:LS:81:VAL:HG21	1.99	0.44
30:Lb:83:THR:HG22	37:Li:93:PHE:CZ	2.53	0.44
63:SQ:7:LYS:HG3	63:SQ:8:ARG:HG3	1.98	0.44
1:A:662:U:H2'	1:A:663:C:C6	2.53	0.43
1:A:1945:A:H2'	1:A:1946:A:C8	2.53	0.43
1:A:2532:U:H2'	1:A:2533:G:C8	2.52	0.43
5:E:1650:U:H2'	5:E:1651:A:C8	2.52	0.43
10:LH:54:TYR:CE1	10:LH:63:LEU:HG	2.53	0.43
29:La:32:SER:HA	29:La:49:PRO:HA	1.99	0.43
41:Lm:28:ASN:HB2	41:Lm:40:GLN:HB3	2.00	0.43
44:Lp:19:LYS:HE2	44:Lp:19:LYS:HB3	1.67	0.43
48:SB:128:ASN:HB3	48:SB:131:GLN:HB2	1.98	0.43
51:SE:87:PRO:HA	51:SE:90:ILE:HG13	2.00	0.43
67:SU:56:LYS:O	67:SU:88:ARG:HA	2.18	0.43
1:A:215:G:H5''	29:La:12:ARG:HG3	1.99	0.43
1:A:255:A:H2'	1:A:256:G:C8	2.53	0.43
1:A:428:A:H2'	1:A:429:U:C6	2.53	0.43
1:A:650:C:H2'	1:A:651:G:C8	2.53	0.43
1:A:899:U:H2'	1:A:900:G:H8	1.83	0.43
1:A:2129:U:H2'	1:A:2130:G:C8	2.53	0.43
2:B:1:G:H4'	9:LG:273:ARG:NH1	2.33	0.43
5:E:872:G:H2'	5:E:873:U:O4'	2.18	0.43
6:LD:245:LEU:HD23	6:LD:245:LEU:HA	1.85	0.43
41:Lm:63:LYS:O	41:Lm:67:GLN:HG2	2.18	0.43
57:SK:60:VAL:HG13	57:SK:101:TYR:HB2	1.99	0.43
67:SU:96:ARG:HB2	67:SU:121:VAL:HG13	2.00	0.43
71:SY:31:GLU:O	71:SY:35:GLU:HG2	2.18	0.43
1:A:2681:U:H2'	1:A:2682:C:C6	2.54	0.43
1:A:3157:U:H4'	1:A:3158:G:H8	1.84	0.43
5:E:773:C:H5''	65:SS:21:ASP:HB3	2.00	0.43
6:LD:46:LYS:HD2	6:LD:46:LYS:HA	1.84	0.43
26:LX:85:TRP:O	26:LX:92:PHE:HA	2.18	0.43
34:Lf:53:PRO:O	34:Lf:57:GLN:HG3	2.17	0.43
41:Lm:42:LYS:HG2	41:Lm:55:VAL:HG22	2.00	0.43
52:SF:94:GLN:HE21	61:SO:62:LYS:NZ	2.17	0.43
61:SO:131:ILE:HD11	61:SO:154:VAL:HG21	2.00	0.43
61:SO:132:LYS:HZ3	61:SO:143:THR:HB	1.82	0.43
65:SS:105:VAL:HG22	65:SS:243:GLY:HA2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:SY:114:ARG:HE	71:SY:114:ARG:HB2	1.52	0.43
81:n:64:A:H2'	81:n:65:G:H8	1.84	0.43
1:A:3023:U:H2'	1:A:3024:A:H8	1.82	0.43
1:A:3233:C:H2'	1:A:3234:A:C8	2.54	0.43
3:C:49:G:H1'	38:Lj:40:SER:HB2	2.00	0.43
5:E:15:U:H2'	5:E:16:G:O4'	2.18	0.43
5:E:297:U:H5''	65:SS:37:LYS:HD2	1.99	0.43
10:LH:4:GLN:HE21	35:Lg:75:LEU:HB2	1.84	0.43
12:LJ:203:VAL:HG21	12:LJ:211:LEU:HD22	1.99	0.43
15:LM:17:LEU:HD23	15:LM:129:VAL:HG22	2.00	0.43
18:LP:23:GLN:HE21	18:LP:23:GLN:HB3	1.67	0.43
30:Lb:135:ARG:HB3	30:Lb:135:ARG:NH1	2.33	0.43
41:Lm:65:LEU:HA	41:Lm:65:LEU:HD23	1.80	0.43
46:Lr:84:ARG:HH11	46:Lr:88:GLU:HG2	1.82	0.43
56:SJ:58:LEU:HD21	56:SJ:90:TYR:HD2	1.83	0.43
61:SO:93:ASP:HB2	61:SO:100:TYR:CE1	2.49	0.43
77:Se:75:VAL:O	77:Se:79:ILE:HG12	2.19	0.43
1:A:3033:A:H2'	1:A:3034:C:H6	1.83	0.43
5:E:1236:A:H2'	5:E:1237:G:C8	2.54	0.43
6:LD:135:ILE:HB	6:LD:149:ARG:HB3	2.01	0.43
8:LF:215:ILE:HD12	8:LF:215:ILE:HA	1.83	0.43
14:LL:145:LYS:HD2	14:LL:167:LEU:HD11	2.00	0.43
17:LO:132:LYS:HE3	17:LO:132:LYS:HB2	1.81	0.43
28:LZ:100:LYS:HE3	28:LZ:100:LYS:HB3	1.81	0.43
39:Lk:70:ARG:HG2	39:Lk:87:VAL:HG21	2.01	0.43
77:Se:21:VAL:HG13	77:Se:32:LYS:HB2	1.99	0.43
1:A:1667:A:H2'	1:A:1668:G:C8	2.54	0.43
5:E:848:C:H2'	5:E:849:C:C6	2.53	0.43
5:E:1175:U:H2'	5:E:1176:G:H8	1.83	0.43
5:E:1592:A:H2'	5:E:1593:A:C8	2.53	0.43
6:LD:133:TYR:HB3	6:LD:168:VAL:HG12	2.01	0.43
10:LH:55:LEU:HD21	10:LH:145:LEU:HD11	2.01	0.43
21:LS:35:PHE:CE1	21:LS:39:ARG:HD3	2.53	0.43
44:Lp:8:LYS:HE3	44:Lp:8:LYS:HB2	1.86	0.43
52:SF:62:ASN:C	52:SF:63:ILE:HD13	2.44	0.43
55:SI:22:LEU:HD13	55:SI:28:LEU:HD11	2.00	0.43
62:SP:121:VAL:O	62:SP:143:VAL:HA	2.18	0.43
63:SQ:81:PHE:HB2	63:SQ:109:LYS:HB2	2.01	0.43
65:SS:77:ARG:HA	65:SS:77:ARG:HD3	1.82	0.43
66:ST:1:MET:HB3	66:ST:1:MET:HE2	1.87	0.43
67:SU:114:ARG:HA	67:SU:114:ARG:HD3	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1242:A:H5''	51:SE:59:LYS:HE3	2.00	0.43
14:LL:183:LYS:O	14:LL:186:GLU:HG3	2.19	0.43
18:LP:11:GLN:HA	18:LP:19:LEU:HD21	1.99	0.43
18:LP:73:ARG:HA	18:LP:74:PRO:HD3	1.86	0.43
34:Lf:51:LEU:HB3	34:Lf:55:LEU:HD23	2.01	0.43
47:SA:136:VAL:HA	47:SA:185:LYS:O	2.19	0.43
47:SA:159:HIS:C	47:SA:164:VAL:HG11	2.44	0.43
61:SO:88:THR:HG22	61:SO:104:VAL:HG12	2.00	0.43
61:SO:89:LEU:HB2	61:SO:103:PHE:HB2	2.00	0.43
80:m:50:C:H2'	80:m:51:A:C8	2.53	0.43
1:A:3015:G:H2'	1:A:3016:A:C8	2.53	0.43
1:A:3255:U:H2'	1:A:3256:G:C8	2.54	0.43
5:E:107:C:H2'	5:E:108:A:C8	2.54	0.43
5:E:1425:A:H2'	5:E:1426:C:C6	2.54	0.43
11:LI:144:ILE:HD12	11:LI:189:ILE:HD12	2.00	0.43
13:LK:78:MET:HE2	13:LK:78:MET:HB3	1.87	0.43
20:LR:67:ILE:HD11	20:LR:80:LYS:HB3	1.99	0.43
55:SI:65:ILE:HG22	55:SI:124:ILE:HG23	2.00	0.43
61:SO:202:LEU:HD12	61:SO:211:ILE:HD11	2.00	0.43
64:SR:78:ASP:HB3	64:SR:104:VAL:HG23	1.99	0.43
1:A:254:A:H2'	1:A:255:A:C8	2.54	0.43
1:A:528:U:H2'	1:A:529:A:H8	1.81	0.43
5:E:1609:U:H5''	52:SF:75:VAL:HB	2.01	0.43
14:LL:170:LYS:HA	14:LL:177:ASP:HA	2.01	0.43
21:LS:64:VAL:HG12	21:LS:93:ILE:HD11	2.01	0.43
26:LX:72:LYS:HE2	26:LX:72:LYS:HB3	1.79	0.43
50:SD:27:ALA:O	50:SD:31:VAL:HG12	2.19	0.43
65:SS:35:PRO:HB2	65:SS:143:ASP:HB2	2.00	0.43
66:ST:69:LEU:HA	66:ST:70:PRO:HD3	1.79	0.43
68:SV:101:ILE:HD12	68:SV:184:LEU:HD11	2.00	0.43
68:SV:164:ARG:HA	68:SV:164:ARG:HD3	1.71	0.43
73:Sa:71:ARG:HB2	73:Sa:83:TRP:CE2	2.53	0.43
1:A:1194:G:H2'	1:A:1195:A:C8	2.53	0.43
5:E:17:C:H2'	5:E:18:C:C6	2.54	0.43
5:E:448:C:H5'	65:SS:29:PRO:HB3	2.00	0.43
9:LG:160:PHE:CE2	9:LG:179:ARG:HG2	2.54	0.43
17:LO:55:ARG:HH21	23:LU:70:THR:HB	1.84	0.43
17:LO:102:LYS:HD2	17:LO:102:LYS:HA	1.79	0.43
56:SJ:58:LEU:HD23	56:SJ:88:LYS:HG2	2.00	0.43
61:SO:260:ILE:HG22	61:SO:292:LEU:HD23	2.00	0.43
64:SR:165:VAL:HA	64:SR:201:ASN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:SS:238:LEU:HB2	65:SS:242:LYS:HD2	2.01	0.43
72:SZ:129:LYS:HB2	72:SZ:129:LYS:HE2	1.84	0.43
80:m:15:G:N2	80:m:48:C:O2	2.46	0.43
1:A:1039:U:H2'	1:A:1040:A:C8	2.54	0.42
1:A:2106:A:H2'	1:A:2107:A:H8	1.84	0.42
1:A:2222:A:H2'	1:A:2223:A:C8	2.54	0.42
1:A:2423:U:H2'	1:A:2424:A:C8	2.54	0.42
1:A:3110:C:H2'	1:A:3111:U:C6	2.54	0.42
5:E:1357:A:H4'	55:SI:126:GLU:HG3	2.00	0.42
5:E:1450:U:H2'	5:E:1451:C:C6	2.54	0.42
9:LG:235:SER:O	9:LG:239:ILE:HG12	2.19	0.42
18:LP:192:LYS:HB3	18:LP:192:LYS:HE2	1.83	0.42
21:LS:40:THR:HG22	21:LS:42:ALA:H	1.83	0.42
41:Lm:32:ASN:HD22	41:Lm:38:PHE:HB3	1.84	0.42
50:SD:126:TRP:NE1	50:SD:133:LEU:HD21	2.34	0.42
64:SR:190:LEU:HD23	64:SR:190:LEU:HA	1.83	0.42
1:A:2428:U:H2'	1:A:2429:G:H8	1.84	0.42
9:LG:50:ARG:O	9:LG:64:ILE:HA	2.19	0.42
18:LP:178:HIS:CE1	18:LP:179:LYS:HG2	2.54	0.42
21:LS:174:ARG:HA	21:LS:178:ARG:HG3	2.00	0.42
47:SA:69:LEU:O	47:SA:73:VAL:HG12	2.19	0.42
48:SB:146:THR:HB	48:SB:157:ARG:HB3	2.00	0.42
63:SQ:185:THR:HA	63:SQ:188:LEU:HD12	2.01	0.42
79:Sg:56:MET:HB3	79:Sg:57:ASN:H	1.66	0.42
1:A:300:G:H2'	1:A:301:G:H8	1.84	0.42
1:A:1525:G:H5'	1:A:1830:G:OP2	2.19	0.42
1:A:2095:G:H2'	1:A:2096:A:C8	2.55	0.42
1:A:2218:G:H2'	1:A:2219:A:H8	1.84	0.42
2:B:4:U:H2'	2:B:5:G:C8	2.55	0.42
3:C:14:C:H5''	20:LR:123:PRO:HD3	2.02	0.42
5:E:1160:A:H2'	5:E:1161:C:H6	1.84	0.42
13:LK:47:LYS:HE3	13:LK:50:ASN:HA	2.02	0.42
15:LM:38:GLU:HG2	15:LM:44:THR:HA	2.02	0.42
18:LP:143:ARG:HG2	38:Lj:96:GLU:CD	2.44	0.42
29:La:38:GLU:CD	29:La:38:GLU:H	2.28	0.42
52:SF:83:GLN:NE2	52:SF:119:ALA:HA	2.34	0.42
56:SJ:34:LEU:HD12	56:SJ:34:LEU:HA	1.79	0.42
65:SS:157:ASN:HD22	65:SS:222:LEU:HD21	1.83	0.42
65:SS:177:ALA:HA	65:SS:195:ILE:HB	2.01	0.42
71:SY:102:LEU:O	71:SY:106:ARG:HD2	2.20	0.42
1:A:2419:A:H2'	1:A:2420:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2768:U:H2'	1:A:2769:A:C8	2.54	0.42
2:B:4:U:H2'	2:B:5:G:H8	1.84	0.42
5:E:1410:A:H2'	5:E:1411:A:C8	2.53	0.42
8:LF:281:ILE:HG22	21:LS:25:TYR:HB3	2.01	0.42
9:LG:41:LYS:HB2	24:LV:68:THR:O	2.19	0.42
10:LH:175:LYS:HA	10:LH:175:LYS:HD3	1.89	0.42
15:LM:110:ILE:HG23	15:LM:116:TYR:HB2	2.01	0.42
31:Lc:94:ALA:HA	31:Lc:121:VAL:HG13	2.00	0.42
33:Le:13:LYS:O	33:Le:17:VAL:HG23	2.19	0.42
33:Le:32:LYS:O	33:Le:36:GLN:HG3	2.19	0.42
41:Lm:64:LYS:HD2	41:Lm:64:LYS:HA	1.86	0.42
52:SF:79:TYR:HA	52:SF:82:ARG:HG2	2.02	0.42
53:SG:24:LEU:HD22	53:SG:54:THR:HG21	2.00	0.42
59:SM:33:LYS:HE2	59:SM:34:TYR:CZ	2.53	0.42
60:SN:120:GLU:HB3	60:SN:128:ALA:HA	2.02	0.42
64:SR:177:GLY:H	64:SR:195:ASP:HB3	1.84	0.42
75:Sc:86:PHE:HB2	75:Sc:120:VAL:HG11	2.01	0.42
78:Sf:18:LYS:HE3	78:Sf:18:LYS:HB3	1.81	0.42
1:A:138:U:H2'	1:A:139:G:H8	1.85	0.42
1:A:640:U:H2'	1:A:641:C:C6	2.55	0.42
1:A:846:A:H2'	1:A:847:A:C8	2.54	0.42
1:A:2508:U:H2'	1:A:2509:U:C6	2.54	0.42
1:A:2683:U:H2'	1:A:2684:C:C6	2.54	0.42
5:E:819:G:H8	5:E:820:U:C4	2.38	0.42
5:E:1628:U:H2'	5:E:1629:G:C8	2.54	0.42
7:LE:376:LYS:O	7:LE:380:MET:HB2	2.20	0.42
16:LN:36:ARG:HG2	16:LN:39:ARG:HH21	1.84	0.42
34:Lf:20:LEU:HD11	34:Lf:32:ALA:HB2	2.01	0.42
48:SB:42:LEU:HD13	48:SB:45:LYS:HA	2.01	0.42
48:SB:192:GLU:H	48:SB:192:GLU:HG3	1.68	0.42
52:SF:46:PHE:HA	52:SF:49:TYR:CD2	2.55	0.42
66:ST:57:ASP:HB3	66:ST:106:LEU:HD23	2.00	0.42
79:Sg:49:LEU:HD22	79:Sg:58:PRO:HG2	2.01	0.42
80:m:5:C:H2'	80:m:6:G:C8	2.55	0.42
1:A:501:A:H2'	1:A:502:U:C6	2.54	0.42
1:A:2424:A:H61	6:LD:230:VAL:HG11	1.84	0.42
5:E:1358:G:H5''	55:SI:130:ARG:NH2	2.35	0.42
7:LE:37:ARG:HA	7:LE:37:ARG:HD3	1.76	0.42
25:LW:38:ILE:HD13	25:LW:38:ILE:HA	1.84	0.42
25:LW:94:ARG:HG3	25:LW:96:VAL:HG23	2.01	0.42
31:Lc:73:LEU:HB2	31:Lc:109:TYR:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:Lj:63:ARG:HG2	38:Lj:63:ARG:HH11	1.85	0.42
38:Lj:94:LYS:HB2	38:Lj:94:LYS:HE2	1.71	0.42
47:SA:4:LEU:HD23	47:SA:4:LEU:HA	1.88	0.42
62:SP:134:LYS:O	62:SP:138:TYR:HD1	2.03	0.42
65:SS:181:VAL:HG12	65:SS:227:VAL:HG22	2.01	0.42
67:SU:132:PRO:HD2	67:SU:162:ILE:HD13	2.02	0.42
68:SV:101:ILE:HD13	68:SV:101:ILE:HA	1.93	0.42
69:SW:92:LYS:HE2	69:SW:92:LYS:H	1.84	0.42
81:n:9:G:H1'	81:n:45:U:H2'	2.02	0.42
1:A:627:U:H4'	1:A:1399:A:H1'	2.00	0.42
1:A:1176:C:H2'	1:A:1177:G:N2	2.35	0.42
2:B:28:C:H5''	15:LM:137:ARG:HG2	2.00	0.42
5:E:407:A:H2'	5:E:408:C:C6	2.55	0.42
5:E:1117:U:H2'	5:E:1118:G:C8	2.55	0.42
6:LD:140:ASN:ND2	6:LD:147:ARG:HH11	2.18	0.42
12:LJ:186:LEU:O	12:LJ:190:VAL:HG22	2.20	0.42
47:SA:65:ARG:HH11	47:SA:65:ARG:HG3	1.85	0.42
61:SO:23:LEU:HD23	61:SO:35:SER:HB3	2.02	0.42
61:SO:132:LYS:HD3	61:SO:140:CYS:SG	2.60	0.42
64:SR:214:ALA:O	64:SR:218:ILE:HG22	2.18	0.42
66:ST:159:ARG:HD2	66:ST:172:ALA:HB2	2.02	0.42
1:A:54:C:H2'	1:A:55:G:H8	1.84	0.42
1:A:1009:A:H2'	1:A:1010:G:C8	2.54	0.42
1:A:2196:C:H2'	1:A:2242:A:H61	1.85	0.42
5:E:628:G:H21	5:E:971:A:H62	1.67	0.42
5:E:884:A:H2'	5:E:885:G:H8	1.84	0.42
5:E:1253:U:O4	60:SN:95:HIS:NE2	2.50	0.42
5:E:1358:G:O2'	55:SI:130:ARG:HA	2.20	0.42
7:LE:20:LYS:HE3	7:LE:20:LYS:HB2	1.88	0.42
7:LE:76:VAL:HG12	7:LE:325:LYS:HA	2.00	0.42
16:LN:42:ARG:O	16:LN:46:ILE:HG12	2.20	0.42
21:LS:122:ILE:HD13	21:LS:122:ILE:HA	1.81	0.42
22:LT:43:LYS:HB2	22:LT:43:LYS:HE2	1.58	0.42
26:LX:67:PRO:HA	26:LX:70:ARG:HG3	2.02	0.42
29:La:27:ARG:HA	29:La:30:LEU:HB2	2.02	0.42
47:SA:94:ARG:H	47:SA:94:ARG:NE	2.14	0.42
47:SA:109:LEU:HD23	47:SA:109:LEU:HA	1.90	0.42
51:SE:107:ILE:H	51:SE:107:ILE:HD12	1.84	0.42
54:SH:132:ARG:HH22	54:SH:145:ARG:HD3	1.84	0.42
64:SR:211:LEU:HD23	64:SR:211:LEU:HA	1.82	0.42
65:SS:160:VAL:HB	65:SS:169:ILE:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:SY:99:ARG:O	71:SY:103:GLU:HG3	2.20	0.42
81:n:75:C:C4	81:n:76:A:H1'	2.55	0.42
1:A:2544:U:H2'	1:A:2545:C:C6	2.55	0.42
1:A:2696:A:H2'	1:A:2697:A:C8	2.55	0.42
1:A:3107:U:H2'	1:A:3108:G:H8	1.85	0.42
5:E:1142:A:H2'	5:E:1143:A:C8	2.55	0.42
5:E:1380:U:H2'	5:E:1381:U:C6	2.54	0.42
7:LE:39:LYS:H	7:LE:39:LYS:HG2	1.63	0.42
15:LM:86:VAL:HG21	15:LM:112:LEU:HD23	2.02	0.42
17:LO:65:LEU:HB2	23:LU:172:TYR:CZ	2.55	0.42
25:LW:89:LEU:HD23	25:LW:89:LEU:HA	1.85	0.42
39:Lk:94:ILE:HA	39:Lk:97:SER:HB2	2.00	0.42
62:SP:26:ALA:HB3	62:SP:149:LEU:HB2	2.02	0.42
62:SP:60:ALA:O	62:SP:64:ILE:HG13	2.20	0.42
62:SP:62:ARG:HH21	73:Sa:38:LYS:HA	1.85	0.42
64:SR:67:GLN:O	64:SR:71:THR:HG22	2.20	0.42
1:A:50:U:H2'	1:A:51:A:H8	1.84	0.42
1:A:121:A:C6	12:LJ:129:PRO:HG3	2.55	0.42
1:A:129:U:H2'	1:A:130:A:H8	1.85	0.42
1:A:273:A:H2'	1:A:274:G:H8	1.84	0.42
1:A:2897:A:H5''	43:Lo:125:LYS:HD2	2.01	0.42
1:A:3204:C:H2'	1:A:3205:G:C8	2.54	0.42
5:E:850:A:H4'	22:LT:165:LYS:HE3	2.00	0.42
5:E:1590:G:OP1	55:SI:91:TYR:HB2	2.20	0.42
5:E:1684:U:O2	5:E:1717:G:N2	2.44	0.42
7:LE:356:LEU:HD13	7:LE:359:ILE:HD11	2.02	0.42
28:LZ:104:GLU:H	28:LZ:138:ARG:HH22	1.66	0.42
62:SP:147:THR:HB	62:SP:151:SER:OG	2.20	0.42
67:SU:51:VAL:HG22	67:SU:53:GLY:H	1.85	0.42
77:Se:3:LYS:HE2	77:Se:6:ALA:HA	2.02	0.42
1:A:532:A:HO2'	1:A:533:A:H8	1.66	0.41
1:A:1084:A:H2'	1:A:1085:A:C8	2.55	0.41
3:C:149:A:H2'	3:C:150:G:C8	2.55	0.41
5:E:340:U:H2'	5:E:341:A:H8	1.85	0.41
5:E:1182:U:H5	5:E:1185:U:H5''	1.84	0.41
6:LD:139:HIS:C	6:LD:140:ASN:HD22	2.28	0.41
12:LJ:214:LEU:HD23	12:LJ:214:LEU:HA	1.94	0.41
17:LO:103:ILE:O	17:LO:107:GLU:HG3	2.20	0.41
21:LS:26:LEU:O	21:LS:30:VAL:HG23	2.20	0.41
38:Lj:77:PRO:HD2	38:Lj:80:LEU:HD12	2.01	0.41
61:SO:201:THR:HG23	61:SO:214:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:SW:80:LEU:HD23	69:SW:80:LEU:HA	1.88	0.41
72:SZ:89:THR:HG23	72:SZ:128:LYS:HA	2.02	0.41
1:A:298:U:H5'	39:Lk:32:ALA:HA	2.02	0.41
1:A:656:A:H2'	1:A:657:A:H8	1.85	0.41
1:A:2232:A:H2'	1:A:2233:A:C8	2.55	0.41
1:A:2946:A:H5''	1:A:2947:G:H5'	2.02	0.41
1:A:3281:U:H2'	1:A:3282:U:C6	2.55	0.41
5:E:340:U:H2'	5:E:341:A:C8	2.55	0.41
5:E:435:C:H5'	75:Sc:50:LYS:HD2	2.02	0.41
5:E:609:U:H5'	5:E:609:U:C6	2.55	0.41
5:E:1086:A:H2'	5:E:1087:A:C8	2.55	0.41
5:E:1117:U:H2'	5:E:1118:G:H8	1.85	0.41
16:LN:123:ILE:HG22	38:Lj:118:ILE:HG12	2.01	0.41
19:LQ:106:GLU:HG2	19:LQ:147:TRP:CZ2	2.54	0.41
20:LR:84:PRO:HB2	20:LR:87:SER:HB3	2.02	0.41
26:LX:120:LYS:HD2	26:LX:120:LYS:HA	1.87	0.41
28:LZ:112:THR:HB	28:LZ:120:LYS:HD2	2.01	0.41
31:Lc:26:ARG:HA	31:Lc:26:ARG:HD3	1.91	0.41
35:Lg:82:LEU:HD12	35:Lg:111:ARG:HG3	2.02	0.41
48:SB:121:ILE:HG23	48:SB:199:ILE:HD11	2.02	0.41
50:SD:135:MET:HE2	50:SD:135:MET:HB3	1.86	0.41
52:SF:38:LEU:HD12	55:SI:10:ALA:HA	2.02	0.41
64:SR:185:LYS:HE2	64:SR:189:GLN:HE22	1.84	0.41
64:SR:203:LYS:HG2	64:SR:206:THR:HG23	2.02	0.41
76:Sd:6:THR:HG22	76:Sd:28:LEU:HB2	2.02	0.41
1:A:546:C:H4'	1:A:547:G:C4	2.55	0.41
1:A:595:G:H1	1:A:609:G:H5''	1.85	0.41
1:A:2510:U:H2'	1:A:2511:A:H8	1.85	0.41
1:A:3050:U:H4'	27:LY:17:ARG:HD2	2.01	0.41
5:E:5:U:H2'	5:E:6:G:H8	1.86	0.41
5:E:404:G:H2'	5:E:405:C:H6	1.85	0.41
5:E:472:U:H2'	5:E:473:A:C8	2.55	0.41
5:E:1564:U:H2'	5:E:1565:C:H6	1.84	0.41
5:E:1796:C:OP2	77:Se:92:ARG:HD3	2.21	0.41
9:LG:82:GLU:H	9:LG:82:GLU:HG2	1.58	0.41
9:LG:190:ILE:HD11	9:LG:195:LEU:HD22	2.01	0.41
10:LH:170:LYS:HB3	10:LH:172:HIS:CE1	2.55	0.41
12:LJ:64:ILE:O	12:LJ:68:ARG:HG2	2.20	0.41
13:LK:67:ALA:O	13:LK:71:VAL:HG12	2.19	0.41
22:LT:92:GLN:O	22:LT:96:ILE:HG13	2.20	0.41
22:LT:153:LYS:HE3	22:LT:153:LYS:HB3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:SJ:99:ILE:O	56:SJ:103:ILE:HG12	2.20	0.41
59:SM:19:ARG:HD2	59:SM:32:ARG:HD3	2.02	0.41
61:SO:10:ARG:HD2	61:SO:10:ARG:HA	1.79	0.41
64:SR:68:ILE:HG22	64:SR:69:ILE:HD13	2.01	0.41
73:Sa:15:ARG:HH21	73:Sa:24:ILE:HG21	1.85	0.41
74:Sb:104:LEU:HB2	74:Sb:125:ILE:HA	2.03	0.41
75:Sc:50:LYS:HB3	75:Sc:77:ILE:HD12	2.02	0.41
77:Se:82:ARG:HG2	77:Se:85:ARG:HH21	1.86	0.41
1:A:29:C:H4'	1:A:62:A:H4'	2.02	0.41
1:A:72:C:H1'	16:LN:61:PRO:O	2.20	0.41
1:A:876:A:H5''	1:A:1890:U:H5''	2.01	0.41
1:A:2836:C:H5	1:A:2852:C:H42	1.69	0.41
2:B:1:G:H4'	9:LG:273:ARG:HH12	1.86	0.41
5:E:406:U:H2'	5:E:407:A:H8	1.85	0.41
5:E:1359:C:H2'	5:E:1360:A:O4'	2.20	0.41
5:E:1483:A:H2'	5:E:1484:G:C8	2.55	0.41
12:LJ:61:GLN:HA	12:LJ:64:ILE:HB	2.02	0.41
29:La:85:VAL:HG12	29:La:97:ILE:HG12	2.01	0.41
42:Ln:30:ARG:HE	42:Ln:30:ARG:HB2	1.65	0.41
52:SF:127:LYS:HA	52:SF:134:ALA:HA	2.02	0.41
54:SH:122:HIS:CE1	54:SH:126:ARG:HD2	2.55	0.41
62:SP:56:LYS:HE3	73:Sa:70:ASN:HD21	1.85	0.41
67:SU:148:LYS:HE3	67:SU:148:LYS:HB2	1.83	0.41
76:Sd:14:SER:O	76:Sd:16:PRO:HD3	2.20	0.41
80:m:23:A:H2'	80:m:24:G:H8	1.84	0.41
1:A:312:C:H2'	1:A:313:A:C8	2.55	0.41
1:A:792:G:H2'	1:A:793:C:C6	2.56	0.41
1:A:2914:G:H5''	7:LE:9:PRO:HG3	2.03	0.41
5:E:600:U:H1'	75:Sc:47:SER:HB2	2.03	0.41
5:E:1241:G:H1'	51:SE:79:HIS:HB2	2.01	0.41
5:E:1662:G:H2'	5:E:1663:G:H8	1.85	0.41
13:LK:36:LYS:HE3	13:LK:36:LYS:HB3	1.92	0.41
17:LO:32:LEU:HD11	17:LO:94:TRP:CD1	2.56	0.41
23:LU:32:SER:HB3	23:LU:36:ILE:HD12	2.01	0.41
34:Lf:9:THR:HG22	34:Lf:109:VAL:HB	2.02	0.41
47:SA:70:THR:HB	47:SA:86:LEU:HG	2.02	0.41
51:SE:74:ALA:HA	51:SE:75:PRO:HD3	1.92	0.41
56:SJ:23:ARG:HD3	56:SJ:92:ASP:OD1	2.20	0.41
60:SN:95:HIS:HB3	60:SN:97:LYS:HG3	2.01	0.41
62:SP:74:VAL:HG11	62:SP:116:LYS:HG2	2.03	0.41
64:SR:52:THR:HB	64:SR:54:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70: SX:53: TYR:O	70: SX:54: ILE:HD13	2.20	0.41
76: Sd:112: LYS:HE2	76: Sd:112: LYS:HB3	1.95	0.41
1: A:616: G:H2'	1: A:617: G:C8	2.55	0.41
1: A:903: U:H2'	1: A:904: A:H8	1.86	0.41
1: A:2369: G:H2'	1: A:2370: G:C8	2.55	0.41
1: A:2930: A:H2'	1: A:2931: C:C6	2.56	0.41
1: A:3190: C:H2'	1: A:3191: G:H8	1.86	0.41
1: A:3284: G:H2'	1: A:3285: C:C6	2.56	0.41
3: C:63: G:H22	3: C:97: A:H2	1.67	0.41
5: E:300: A:H2'	5: E:301: A:C8	2.56	0.41
5: E:761: G:H4'	69: SW:72: GLU:OE1	2.21	0.41
5: E:1175: U:H2'	5: E:1176: G:C8	2.55	0.41
5: E:1681: A:H2	5: E:1720: G:H21	1.68	0.41
23: LU:27: MET:HE3	23: LU:27: MET:HB2	1.80	0.41
27: LY:44: LYS:HB3	27: LY:49: ILE:HD11	2.03	0.41
41: Lm:43: PHE:HE2	41: Lm:66: ILE:HG12	1.85	0.41
48: SB:120: ILE:HD11	57: SK:98: GLN:HE21	1.85	0.41
57: SK:62: VAL:O	57: SK:66: VAL:HG22	2.20	0.41
62: SP:55: GLU:HA	62: SP:58: VAL:HG22	2.03	0.41
62: SP:59: LEU:HD22	73: Sa:79: LEU:HD11	2.02	0.41
62: SP:122: ILE:HA	62: SP:144: ILE:O	2.21	0.41
63: SQ:157: GLN:O	63: SQ:161: ILE:HG12	2.21	0.41
66: ST:52: ILE:HD13	66: ST:52: ILE:HA	1.94	0.41
70: SX:124: THR:HG23	70: SX:141: LYS:HB3	2.03	0.41
76: Sd:113: ASN:O	76: Sd:117: LYS:HG3	2.21	0.41
1: A:422: A:C2	1: A:2363: A:H4'	2.55	0.41
3: C:135: G:H5''	28: LZ:49: LYS:HD2	2.03	0.41
5: E:751: G:H2'	5: E:752: A:C8	2.56	0.41
5: E:1146: G:H2'	5: E:1147: A:C8	2.56	0.41
13: LK:6: THR:HG21	13: LK:65: VAL:HG12	2.02	0.41
15: LM:80: LEU:HD23	15: LM:80: LEU:HA	1.78	0.41
27: LY:45: ASN:O	27: LY:49: ILE:HG12	2.21	0.41
50: SD:132: GLU:HA	50: SD:135: MET:HG2	2.01	0.41
73: Sa:46: ILE:HD12	73: Sa:46: ILE:H	1.86	0.41
1: A:225: C:H5'	29: La:34: PRO:HD3	2.02	0.41
1: A:1126: G:H5''	14: LL:119: TRP:HZ3	1.85	0.41
5: E:887: A:H5''	72: SZ:120: PRO:HB2	2.03	0.41
5: E:1151: A:H2'	5: E:1152: A:C8	2.55	0.41
5: E:1345: A:H1'	56: SJ:56: VAL:HG13	2.03	0.41
6: LD:54: ARG:HG2	6: LD:56: ALA:H	1.86	0.41
7: LE:67: PHE:CZ	26: LX:88: ARG:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:LJ:82:LEU:HD21	12:LJ:218:ILE:HD13	2.03	0.41
40:LI:64:MET:HG2	40:LI:67:LEU:HB3	2.02	0.41
50:SD:132:GLU:O	50:SD:136:ILE:HG13	2.20	0.41
56:SJ:40:ASN:HA	56:SJ:43:LYS:HE3	2.02	0.41
61:SO:206:PRO:HG3	61:SO:247:PRO:HA	2.03	0.41
75:Sc:70:LYS:HD2	75:Sc:93:LEU:HD22	2.02	0.41
1:A:20:A:H2'	1:A:21:G:C8	2.55	0.41
1:A:407:A:C2	3:C:17:A:H1'	2.55	0.41
1:A:1222:G:H4'	1:A:1223:A:O5'	2.21	0.41
1:A:1283:C:H2'	1:A:1284:C:C6	2.56	0.41
1:A:1340:G:H2'	1:A:1341:U:C6	2.55	0.41
1:A:1616:U:H2'	1:A:1617:G:C8	2.55	0.41
1:A:2609:A:H2'	1:A:2610:G:C8	2.55	0.41
1:A:3283:U:H2'	1:A:3284:G:C8	2.55	0.41
2:B:74:C:H2'	2:B:75:G:C8	2.55	0.41
5:E:647:G:N2	5:E:687:G:H22	2.19	0.41
5:E:1607:G:H2'	5:E:1608:U:H6	1.83	0.41
11:LI:50:ALA:O	11:LI:54:GLU:HG2	2.21	0.41
22:LT:105:LEU:HD23	22:LT:138:LEU:HD23	2.02	0.41
22:LT:177:VAL:O	22:LT:181:ARG:HG2	2.21	0.41
24:LV:69:LYS:HE3	24:LV:69:LYS:HB3	1.81	0.41
30:Lb:41:ALA:HB2	30:Lb:77:TYR:HE1	1.86	0.41
36:Lh:9:VAL:HG21	36:Lh:44:TYR:HE2	1.86	0.41
46:Lr:75:ALA:O	46:Lr:79:VAL:HG23	2.20	0.41
50:SD:74:LEU:HD23	50:SD:78:LEU:HD23	2.02	0.41
52:SF:7:VAL:HG23	52:SF:22:VAL:HB	2.03	0.41
52:SF:50:GLU:O	52:SF:54:LEU:HB2	2.21	0.41
56:SJ:30:LYS:HE2	56:SJ:30:LYS:HB3	1.94	0.41
61:SO:72:THR:HG22	61:SO:81:LEU:HB2	2.02	0.41
61:SO:258:THR:HG22	61:SO:275:ARG:HD3	2.02	0.41
64:SR:116:LYS:HE3	64:SR:131:ILE:HD11	2.03	0.41
69:SW:34:PHE:HD1	69:SW:111:THR:HG21	1.86	0.41
77:Se:53:LEU:HD13	77:Se:53:LEU:HA	1.92	0.41
1:A:1913:A:N3	1:A:2120:A:H2'	2.36	0.41
1:A:2429:G:H2'	1:A:2430:A:C8	2.56	0.41
1:A:2683:U:H2'	1:A:2684:C:H6	1.86	0.41
2:B:94:C:H2'	2:B:95:A:H8	1.86	0.41
5:E:65:A:H2	5:E:84:A:H62	1.69	0.41
5:E:968:U:H2'	5:E:969:C:O4'	2.20	0.41
5:E:1357:A:H2'	5:E:1358:G:H8	1.84	0.41
7:LE:56:ILE:HG22	7:LE:359:ILE:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:LH:97:ASN:ND2	10:LH:99:GLU:HG3	2.27	0.41
15:LM:132:ASN:HA	15:LM:154:THR:HG21	2.03	0.41
23:LU:131:LYS:HA	23:LU:131:LYS:HD3	1.71	0.41
26:LX:81:GLN:HE21	26:LX:83:LYS:HB3	1.85	0.41
49:SC:1:MET:HE3	49:SC:1:MET:HB2	1.80	0.41
65:SS:174:LYS:HE3	65:SS:174:LYS:HB3	1.97	0.41
75:Sc:96:VAL:HG12	75:Sc:127:VAL:HG21	2.02	0.41
1:A:254:A:H2'	1:A:255:A:H8	1.87	0.40
1:A:507:U:H2'	1:A:508:U:C6	2.56	0.40
1:A:1129:A:H2'	1:A:1130:A:C8	2.56	0.40
1:A:1283:C:H2'	1:A:1284:C:C5	2.56	0.40
1:A:1615:C:H2'	1:A:1616:U:C6	2.55	0.40
5:E:849:C:H2'	5:E:850:A:C8	2.56	0.40
8:LF:206:LEU:HB3	8:LF:248:VAL:HG22	2.03	0.40
9:LG:105:ILE:HD12	9:LG:105:ILE:HA	1.92	0.40
12:LJ:162:LEU:HD23	18:LP:7:LEU:HD21	2.02	0.40
16:LN:90:ALA:HB1	16:LN:95:ILE:HB	2.03	0.40
18:LP:36:ILE:HD11	18:LP:105:ARG:HB3	2.03	0.40
47:SA:24:PHE:CE1	47:SA:28:GLU:HG3	2.56	0.40
47:SA:168:ILE:HD12	47:SA:189:MET:HG3	2.03	0.40
48:SB:72:HIS:CD2	48:SB:107:LYS:HG2	2.55	0.40
51:SE:90:ILE:HD11	51:SE:112:LEU:HD21	2.03	0.40
55:SI:83:ALA:HB1	55:SI:91:TYR:HB3	2.04	0.40
61:SO:169:ILE:HG12	61:SO:183:LEU:HD21	2.03	0.40
62:SP:36:TYR:CD1	62:SP:161:PRO:HG3	2.56	0.40
68:SV:136:SER:O	68:SV:140:GLU:HG2	2.21	0.40
70:SX:16:GLN:NE2	70:SX:61:THR:HG23	2.36	0.40
70:SX:99:ARG:HB2	75:Sc:9:LEU:O	2.21	0.40
76:Sd:88:THR:O	76:Sd:92:VAL:HG13	2.21	0.40
81:n:64:A:H2'	81:n:65:G:C8	2.56	0.40
1:A:715:A:C8	31:Lc:115:LYS:HD2	2.56	0.40
1:A:1362:G:H2'	1:A:1363:A:C8	2.57	0.40
1:A:1460:A:H2'	1:A:1461:A:H8	1.86	0.40
1:A:2197:C:H4'	1:A:2198:A:H5'	2.02	0.40
1:A:3162:C:H2'	1:A:3163:A:H8	1.87	0.40
5:E:480:G:N2	5:E:508:U:O2	2.49	0.40
5:E:560:U:H2'	5:E:561:G:H8	1.86	0.40
5:E:905:A:H5''	72:SZ:52:ARG:HG2	2.03	0.40
5:E:1045:C:H2'	5:E:1046:G:H8	1.86	0.40
5:E:1488:G:H3'	5:E:1515:A:H61	1.85	0.40
5:E:1584:G:H5''	52:SF:122:ARG:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:LO:20:VAL:HG21	17:LO:90:VAL:HG21	2.03	0.40
20:LR:182:ILE:HD13	20:LR:182:ILE:HA	1.89	0.40
25:LW:20:SER:HA	25:LW:23:THR:HG22	2.03	0.40
28:LZ:135:ILE:HD12	28:LZ:135:ILE:H	1.86	0.40
47:SA:39:VAL:HG22	47:SA:48:VAL:HG12	2.01	0.40
48:SB:112:ARG:HA	48:SB:112:ARG:HD3	1.92	0.40
48:SB:115:LYS:HD3	48:SB:115:LYS:HA	1.78	0.40
61:SO:170:ILE:HD13	61:SO:180:ALA:HB2	2.01	0.40
65:SS:128:LYS:HA	65:SS:156:VAL:HG22	2.02	0.40
67:SU:73:VAL:HG23	67:SU:77:LEU:HD12	2.03	0.40
73:Sa:14:PRO:HG2	73:Sa:23:ILE:HD12	2.03	0.40
80:m:26:A:H2'	80:m:27:G:H8	1.86	0.40
1:A:562:C:H5''	23:LU:71:LYS:HD3	2.03	0.40
1:A:1597:C:H2'	1:A:1598:G:C8	2.57	0.40
1:A:1662:G:H22	1:A:1787:A:H2	1.70	0.40
1:A:2406:C:H2'	1:A:2407:C:C6	2.56	0.40
1:A:2661:G:H2'	1:A:2662:G:H8	1.85	0.40
2:B:84:A:H2'	2:B:85:G:C8	2.56	0.40
9:LG:108:ARG:CZ	9:LG:253:PHE:HB2	2.52	0.40
27:LY:4:GLU:HB2	27:LY:13:ILE:HB	2.03	0.40
51:SE:60:LEU:HD21	51:SE:89:MET:HG2	2.04	0.40
52:SF:46:PHE:HA	52:SF:49:TYR:HD2	1.86	0.40
57:SK:58:ARG:HA	57:SK:103:ARG:HG2	2.03	0.40
1:A:682:U:H5''	1:A:683:U:H5	1.86	0.40
1:A:1054:A:H5''	1:A:2637:A:H61	1.87	0.40
1:A:1212:A:H5'	23:LU:113:ARG:HE	1.86	0.40
1:A:1446:A:H5''	20:LR:65:SER:HB2	2.04	0.40
1:A:2423:U:H2'	1:A:2424:A:H8	1.87	0.40
1:A:3214:U:C4	17:LO:121:MET:HG3	2.56	0.40
1:A:3217:C:C4	1:A:3220:G:H1'	2.56	0.40
5:E:1063:U:H2'	5:E:1064:G:C8	2.55	0.40
5:E:1400:A:H4'	53:SG:60:ARG:NH1	2.36	0.40
17:LO:65:LEU:HB2	23:LU:172:TYR:CE1	2.56	0.40
34:Lf:55:LEU:HB2	34:Lf:95:PRO:HD3	2.02	0.40
35:Lg:123:LYS:HB2	35:Lg:123:LYS:HE3	1.87	0.40
37:Li:67:LYS:HB2	37:Li:67:LYS:HE3	1.72	0.40
45:Lq:17:CYS:O	45:Lq:19:LYS:HG3	2.22	0.40
47:SA:217:ILE:HG21	61:SO:193:ILE:HD13	2.02	0.40
53:SG:23:LYS:HD2	53:SG:23:LYS:H	1.86	0.40
70:SX:123:VAL:HG13	70:SX:139:VAL:HG13	2.03	0.40
75:Sc:30:LYS:HE2	75:Sc:30:LYS:HB3	1.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:Sf:8:LEU:HD13	78:Sf:8:LEU:HA	1.94	0.40
1:A:584:G:H2'	1:A:585:A:C8	2.56	0.40
1:A:1791:C:H2'	1:A:1792:C:C6	2.57	0.40
1:A:1881:A:H2'	1:A:1882:G:H8	1.86	0.40
1:A:2428:U:H2'	1:A:2429:G:C8	2.57	0.40
5:E:400:A:H4'	5:E:401:A:O5'	2.21	0.40
23:LU:139:TYR:HD1	23:LU:140:VAL:HG23	1.87	0.40
34:Lf:11:GLU:O	34:Lf:106:THR:HA	2.21	0.40
35:Lg:82:LEU:HD11	35:Lg:112:ALA:HA	2.03	0.40
63:SQ:118:GLN:HE21	63:SQ:118:GLN:HB3	1.67	0.40
64:SR:115:ILE:HD13	64:SR:212:LYS:HE3	2.03	0.40
64:SR:227:PRO:HA	64:SR:230:TRP:CG	2.57	0.40
72:SZ:26:THR:HG21	72:SZ:60:ALA:HB2	2.02	0.40
72:SZ:47:LYS:HG3	72:SZ:62:LEU:HB3	2.03	0.40
77:Se:26:CYS:HB3	77:Se:77:CYS:SG	2.62	0.40
81:n:11:C:H2'	81:n:12:G:H8	1.85	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	LD	245/254 (96%)	240 (98%)	5 (2%)	0	100	100
7	LE	384/387 (99%)	372 (97%)	12 (3%)	0	100	100
8	LF	359/362 (99%)	345 (96%)	14 (4%)	0	100	100
9	LG	290/297 (98%)	284 (98%)	6 (2%)	0	100	100
10	LH	152/176 (86%)	142 (93%)	10 (7%)	0	100	100
11	LI	220/244 (90%)	217 (99%)	3 (1%)	0	100	100
12	LJ	231/256 (90%)	225 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	LK	186/191 (97%)	179 (96%)	7 (4%)	0	100	100
14	LL	205/210 (98%)	195 (95%)	10 (5%)	0	100	100
15	LM	167/174 (96%)	165 (99%)	2 (1%)	0	100	100
16	LN	191/199 (96%)	184 (96%)	6 (3%)	1 (0%)	24	39
17	LO	134/138 (97%)	132 (98%)	2 (2%)	0	100	100
18	LP	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
19	LQ	195/199 (98%)	193 (99%)	2 (1%)	0	100	100
20	LR	168/184 (91%)	162 (96%)	6 (4%)	0	100	100
21	LS	183/186 (98%)	177 (97%)	6 (3%)	0	100	100
22	LT	181/189 (96%)	178 (98%)	3 (2%)	0	100	100
23	LU	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
24	LV	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
25	LW	98/121 (81%)	92 (94%)	6 (6%)	0	100	100
26	LX	134/137 (98%)	133 (99%)	1 (1%)	0	100	100
27	LY	60/155 (39%)	59 (98%)	1 (2%)	0	100	100
28	LZ	118/142 (83%)	116 (98%)	2 (2%)	0	100	100
29	La	123/127 (97%)	122 (99%)	1 (1%)	0	100	100
30	Lb	131/136 (96%)	129 (98%)	2 (2%)	0	100	100
31	Lc	146/149 (98%)	138 (94%)	8 (6%)	0	100	100
32	Ld	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
33	Le	94/105 (90%)	93 (99%)	1 (1%)	0	100	100
34	Lf	103/113 (91%)	101 (98%)	2 (2%)	0	100	100
35	Lg	124/130 (95%)	124 (100%)	0	0	100	100
36	Lh	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
37	Li	108/121 (89%)	104 (96%)	3 (3%)	1 (1%)	14	24
38	Lj	117/120 (98%)	116 (99%)	1 (1%)	0	100	100
39	Lk	96/100 (96%)	91 (95%)	5 (5%)	0	100	100
40	Ll	79/88 (90%)	77 (98%)	2 (2%)	0	100	100
41	Lm	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
42	Ln	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
43	Lo	49/128 (38%)	49 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	Lp	22/25 (88%)	22 (100%)	0	0	100	100
45	Lq	98/106 (92%)	95 (97%)	3 (3%)	0	100	100
46	Lr	89/92 (97%)	83 (93%)	6 (7%)	0	100	100
47	SA	220/240 (92%)	214 (97%)	6 (3%)	0	100	100
48	SB	204/225 (91%)	187 (92%)	17 (8%)	0	100	100
49	SC	81/105 (77%)	79 (98%)	2 (2%)	0	100	100
50	SD	93/143 (65%)	86 (92%)	7 (8%)	0	100	100
51	SE	114/142 (80%)	109 (96%)	5 (4%)	0	100	100
52	SF	139/143 (97%)	134 (96%)	5 (4%)	0	100	100
53	SG	110/136 (81%)	105 (96%)	5 (4%)	0	100	100
54	SH	143/146 (98%)	135 (94%)	8 (6%)	0	100	100
55	SI	141/144 (98%)	138 (98%)	3 (2%)	0	100	100
56	SJ	98/121 (81%)	98 (100%)	0	0	100	100
57	SK	80/108 (74%)	76 (95%)	4 (5%)	0	100	100
58	SL	60/67 (90%)	57 (95%)	3 (5%)	0	100	100
59	SM	51/56 (91%)	47 (92%)	4 (8%)	0	100	100
60	SN	51/152 (34%)	48 (94%)	3 (6%)	0	100	100
61	SO	309/319 (97%)	296 (96%)	13 (4%)	0	100	100
62	SP	203/252 (81%)	193 (95%)	10 (5%)	0	100	100
63	SQ	221/255 (87%)	216 (98%)	5 (2%)	0	100	100
64	SR	214/254 (84%)	207 (97%)	7 (3%)	0	100	100
65	SS	256/261 (98%)	245 (96%)	11 (4%)	0	100	100
66	ST	216/236 (92%)	214 (99%)	2 (1%)	0	100	100
67	SU	178/190 (94%)	173 (97%)	5 (3%)	0	100	100
68	SV	182/200 (91%)	175 (96%)	7 (4%)	0	100	100
69	SW	182/197 (92%)	179 (98%)	3 (2%)	0	100	100
70	SX	139/156 (89%)	133 (96%)	6 (4%)	0	100	100
71	SY	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
72	SZ	125/138 (91%)	119 (95%)	6 (5%)	0	100	100
73	Sa	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
74	Sb	127/130 (98%)	123 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
75	Sc	142/145 (98%)	141 (99%)	1 (1%)	0	100	100
76	Sd	129/135 (96%)	125 (97%)	4 (3%)	0	100	100
77	Se	95/119 (80%)	91 (96%)	4 (4%)	0	100	100
78	Sf	70/82 (85%)	66 (94%)	4 (6%)	0	100	100
79	Sg	53/63 (84%)	49 (92%)	4 (8%)	0	100	100
All	All	10749/11870 (91%)	10405 (97%)	342 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	LN	48	PRO
37	Li	12	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	LD	189/196 (96%)	188 (100%)	1 (0%)	81	91
7	LE	321/323 (99%)	313 (98%)	8 (2%)	42	64
8	LF	288/289 (100%)	285 (99%)	3 (1%)	68	81
9	LG	241/245 (98%)	234 (97%)	7 (3%)	37	58
10	LH	136/155 (88%)	133 (98%)	3 (2%)	45	67
11	LI	186/205 (91%)	180 (97%)	6 (3%)	34	55
12	LJ	187/208 (90%)	187 (100%)	0	100	100
13	LK	168/171 (98%)	159 (95%)	9 (5%)	20	35
14	LL	177/179 (99%)	176 (99%)	1 (1%)	78	88
15	LM	145/151 (96%)	143 (99%)	2 (1%)	59	76
16	LN	154/159 (97%)	151 (98%)	3 (2%)	50	71
17	LO	107/109 (98%)	103 (96%)	4 (4%)	30	50
18	LP	175/176 (99%)	174 (99%)	1 (1%)	78	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	LQ	160/162 (99%)	160 (100%)	0	100	100
20	LR	138/146 (94%)	138 (100%)	0	100	100
21	LS	150/151 (99%)	149 (99%)	1 (1%)	76	86
22	LT	149/154 (97%)	148 (99%)	1 (1%)	76	86
23	LU	155/156 (99%)	150 (97%)	5 (3%)	34	55
24	LV	135/137 (98%)	130 (96%)	5 (4%)	30	50
25	LW	87/107 (81%)	85 (98%)	2 (2%)	44	66
26	LX	104/105 (99%)	101 (97%)	3 (3%)	37	58
27	LY	54/129 (42%)	54 (100%)	0	100	100
28	LZ	104/118 (88%)	100 (96%)	4 (4%)	29	49
29	La	108/110 (98%)	107 (99%)	1 (1%)	70	82
30	Lb	111/116 (96%)	108 (97%)	3 (3%)	39	61
31	Lc	117/119 (98%)	115 (98%)	2 (2%)	53	73
32	Ld	46/47 (98%)	45 (98%)	1 (2%)	45	67
33	Le	81/88 (92%)	80 (99%)	1 (1%)	63	79
34	Lf	92/97 (95%)	90 (98%)	2 (2%)	45	67
35	Lg	107/111 (96%)	106 (99%)	1 (1%)	70	82
36	Lh	90/91 (99%)	87 (97%)	3 (3%)	33	55
37	Li	94/103 (91%)	93 (99%)	1 (1%)	65	80
38	Lj	104/105 (99%)	104 (100%)	0	100	100
39	Lk	80/82 (98%)	78 (98%)	2 (2%)	42	64
40	Ll	67/71 (94%)	66 (98%)	1 (2%)	57	75
41	Lm	67/69 (97%)	67 (100%)	0	100	100
42	Ln	45/46 (98%)	45 (100%)	0	100	100
43	Lo	46/116 (40%)	46 (100%)	0	100	100
44	Lp	22/23 (96%)	20 (91%)	2 (9%)	9	14
45	Lq	86/91 (94%)	84 (98%)	2 (2%)	44	66
46	Lr	71/72 (99%)	71 (100%)	0	100	100
47	SA	182/195 (93%)	175 (96%)	7 (4%)	29	49
48	SB	172/191 (90%)	170 (99%)	2 (1%)	63	79
49	SC	77/98 (79%)	76 (99%)	1 (1%)	61	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	SD	80/119 (67%)	79 (99%)	1 (1%)	61	77
51	SE	94/118 (80%)	92 (98%)	2 (2%)	47	69
52	SF	115/119 (97%)	113 (98%)	2 (2%)	53	73
53	SG	100/124 (81%)	95 (95%)	5 (5%)	22	37
54	SH	127/129 (98%)	122 (96%)	5 (4%)	28	48
55	SI	115/116 (99%)	112 (97%)	3 (3%)	40	63
56	SJ	93/114 (82%)	87 (94%)	6 (6%)	15	27
57	SK	67/89 (75%)	66 (98%)	1 (2%)	57	75
58	SL	55/60 (92%)	53 (96%)	2 (4%)	31	51
59	SM	47/49 (96%)	44 (94%)	3 (6%)	16	28
60	SN	42/135 (31%)	39 (93%)	3 (7%)	13	23
61	SO	249/262 (95%)	246 (99%)	3 (1%)	63	79
62	SP	169/210 (80%)	165 (98%)	4 (2%)	43	65
63	SQ	198/224 (88%)	194 (98%)	4 (2%)	48	69
64	SR	175/205 (85%)	172 (98%)	3 (2%)	53	73
65	SS	220/222 (99%)	217 (99%)	3 (1%)	59	76
66	ST	187/201 (93%)	183 (98%)	4 (2%)	47	69
67	SU	162/170 (95%)	159 (98%)	3 (2%)	50	71
68	SV	148/161 (92%)	147 (99%)	1 (1%)	76	86
69	SW	156/166 (94%)	150 (96%)	6 (4%)	29	49
70	SX	126/137 (92%)	120 (95%)	6 (5%)	23	39
71	SY	127/128 (99%)	126 (99%)	1 (1%)	73	85
72	SZ	90/105 (86%)	88 (98%)	2 (2%)	45	67
73	Sa	71/74 (96%)	67 (94%)	4 (6%)	19	32
74	Sb	110/111 (99%)	109 (99%)	1 (1%)	70	82
75	Sc	119/120 (99%)	117 (98%)	2 (2%)	53	73
76	Sd	101/113 (89%)	98 (97%)	3 (3%)	36	57
77	Se	82/100 (82%)	80 (98%)	2 (2%)	43	65
78	Sf	64/71 (90%)	62 (97%)	2 (3%)	35	56
79	Sg	47/54 (87%)	46 (98%)	1 (2%)	47	69
All	All	9111/9978 (91%)	8922 (98%)	189 (2%)	46	69

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	LD	80	GLU
7	LE	90	VAL
7	LE	125	SER
7	LE	154	TYR
7	LE	160	VAL
7	LE	162	VAL
7	LE	199	PHE
7	LE	205	VAL
7	LE	208	VAL
8	LF	6	VAL
8	LF	287	THR
8	LF	354	VAL
9	LG	52	VAL
9	LG	69	ILE
9	LG	93	THR
9	LG	125	VAL
9	LG	131	LEU
9	LG	148	ILE
9	LG	151	GLN
10	LH	8	LYS
10	LH	62	THR
10	LH	146	LEU
11	LI	62	ILE
11	LI	77	VAL
11	LI	78	GLU
11	LI	111	ILE
11	LI	117	VAL
11	LI	233	GLU
13	LK	6	THR
13	LK	42	ASP
13	LK	43	VAL
13	LK	46	THR
13	LK	48	VAL
13	LK	82	VAL
13	LK	126	VAL
13	LK	140	VAL
13	LK	150	SER
14	LL	89	VAL
15	LM	46	VAL
15	LM	52	TYR
16	LN	3	ILE
16	LN	48	PRO

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Mol	Chain	Res	Type
16	LN	58	VAL
17	LO	12	TRP
17	LO	59	ASN
17	LO	92	GLU
17	LO	113	THR
18	LP	135	VAL
21	LS	74	GLU
22	LT	6	THR
23	LU	19	VAL
23	LU	87	THR
23	LU	97	VAL
23	LU	109	ASP
23	LU	129	ILE
24	LV	31	LEU
24	LV	48	ILE
24	LV	103	GLN
24	LV	106	LEU
24	LV	154	VAL
25	LW	58	GLU
25	LW	65	VAL
26	LX	96	GLU
26	LX	125	LEU
26	LX	137	VAL
28	LZ	37	THR
28	LZ	77	GLU
28	LZ	106	ASP
28	LZ	107	VAL
29	La	80	VAL
30	Lb	89	VAL
30	Lb	96	VAL
30	Lb	135	ARG
31	Lc	86	LYS
31	Lc	123	VAL
32	Ld	4	SER
33	Le	90	VAL
34	Lf	54	GLU
34	Lf	106	THR
35	Lg	23	ASP
36	Lh	3	GLU
36	Lh	22	VAL
36	Lh	98	VAL
37	Li	67	LYS

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Mol	Chain	Res	Type
39	Lk	17	VAL
39	Lk	46	GLU
40	Ll	64	MET
44	Lp	13	LEU
44	Lp	20	VAL
45	Lq	26	THR
45	Lq	57	VAL
47	SA	99	VAL
47	SA	170	THR
47	SA	172	THR
47	SA	176	LEU
47	SA	186	VAL
47	SA	206	VAL
47	SA	207	THR
48	SB	27	THR
48	SB	132	VAL
49	SC	15	LEU
50	SD	63	VAL
51	SE	35	LYS
51	SE	60	LEU
52	SF	58	ASP
52	SF	63	ILE
53	SG	62	GLN
53	SG	100	LEU
53	SG	104	ASN
53	SG	109	LEU
53	SG	119	LEU
54	SH	51	ASP
54	SH	62	THR
54	SH	74	GLN
54	SH	105	VAL
54	SH	141	THR
55	SI	25	GLN
55	SI	99	SER
55	SI	108	LEU
56	SJ	26	LEU
56	SJ	28	SER
56	SJ	94	GLU
56	SJ	100	VAL
56	SJ	106	ILE
56	SJ	114	VAL
57	SK	51	LEU

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Mol	Chain	Res	Type
58	SL	12	VAL
58	SL	66	LEU
59	SM	6	VAL
59	SM	9	SER
59	SM	40	ARG
60	SN	97	LYS
60	SN	103	LEU
60	SN	130	VAL
61	SO	199	ILE
61	SO	220	ILE
61	SO	258	THR
62	SP	39	ASN
62	SP	83	GLN
62	SP	198	MET
62	SP	206	ASP
63	SQ	9	LEU
63	SQ	46	THR
63	SQ	96	LEU
63	SQ	231	LEU
64	SR	101	VAL
64	SR	165	VAL
64	SR	233	GLN
65	SS	146	THR
65	SS	208	VAL
65	SS	246	LEU
66	ST	68	LEU
66	ST	96	SER
66	ST	131	LYS
66	ST	193	LEU
67	SU	119	THR
67	SU	126	LEU
67	SU	140	VAL
68	SV	46	VAL
69	SW	7	THR
69	SW	49	LEU
69	SW	72	GLU
69	SW	99	LEU
69	SW	141	VAL
69	SW	161	THR
70	SX	29	LYS
70	SX	61	THR
70	SX	75	VAL

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Mol	Chain	Res	Type
70	SX	107	VAL
70	SX	135	VAL
70	SX	138	ASN
71	SY	117	LEU
72	SZ	61	MET
72	SZ	112	ILE
73	Sa	16	LYS
73	Sa	21	ASN
73	Sa	36	VAL
73	Sa	50	TYR
74	Sb	81	VAL
75	Sc	54	LEU
75	Sc	107	PHE
76	Sd	14	SER
76	Sd	24	VAL
76	Sd	25	VAL
77	Se	44	ILE
77	Se	71	LEU
78	Sf	21	LEU
78	Sf	67	THR
79	Sg	50	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (159) such sidechains are listed below:

Mol	Chain	Res	Type
6	LD	97	ASN
6	LD	140	ASN
7	LE	184	ASN
7	LE	345	ASN
8	LF	140	HIS
8	LF	221	ASN
8	LF	291	ASN
9	LG	178	ASN
9	LG	206	GLN
9	LG	244	HIS
9	LG	264	GLN
10	LH	4	GLN
10	LH	97	ASN
10	LH	138	GLN
10	LH	167	ASN
11	LI	64	GLN
11	LI	104	GLN

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Mol	Chain	Res	Type
11	LI	166	ASN
11	LI	186	HIS
12	LJ	59	GLN
12	LJ	61	GLN
12	LJ	232	HIS
13	LK	8	GLN
13	LK	9	GLN
13	LK	58	HIS
13	LK	59	ASN
13	LK	125	ASN
13	LK	169	ASN
14	LL	123	HIS
17	LO	119	GLN
18	LP	23	GLN
18	LP	32	GLN
18	LP	138	GLN
18	LP	182	ASN
20	LR	45	GLN
20	LR	55	GLN
20	LR	97	ASN
21	LS	73	GLN
22	LT	68	GLN
22	LT	92	GLN
23	LU	46	GLN
23	LU	63	GLN
23	LU	142	GLN
24	LV	134	GLN
24	LV	149	GLN
25	LW	87	ASN
26	LX	81	GLN
27	LY	42	GLN
29	La	26	GLN
29	La	81	GLN
29	La	98	ASN
30	Lb	29	HIS
30	Lb	122	HIS
30	Lb	123	GLN
31	Lc	38	GLN
31	Lc	62	HIS
31	Lc	120	ASN
32	Ld	6	ASN
32	Ld	19	ASN

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Mol	Chain	Res	Type
32	Ld	45	HIS
33	Le	11	ASN
36	Lh	42	GLN
36	Lh	77	ASN
36	Lh	88	ASN
37	Li	3	GLN
37	Li	61	GLN
38	Lj	20	GLN
38	Lj	34	GLN
38	Lj	62	GLN
40	Ll	13	ASN
40	Ll	69	HIS
41	Lm	10	GLN
41	Lm	28	ASN
42	Ln	4	GLN
42	Ln	19	GLN
42	Ln	43	ASN
43	Lo	109	ASN
45	Lq	27	GLN
45	Lq	82	GLN
46	Lr	34	HIS
47	SA	56	GLN
47	SA	74	GLN
47	SA	165	ASN
48	SB	34	GLN
48	SB	131	GLN
50	SD	80	ASN
50	SD	96	GLN
52	SF	8	GLN
52	SF	32	ASN
52	SF	94	GLN
53	SG	29	GLN
53	SG	31	ASN
53	SG	83	GLN
54	SH	12	GLN
54	SH	21	ASN
54	SH	25	ASN
54	SH	74	GLN
54	SH	103	ASN
55	SI	43	ASN
55	SI	70	GLN
55	SI	106	GLN

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Mol	Chain	Res	Type
55	SI	129	GLN
56	SJ	40	ASN
57	SK	82	HIS
58	SL	43	ASN
59	SM	20	GLN
59	SM	53	ASN
62	SP	15	GLN
62	SP	39	ASN
62	SP	109	ASN
62	SP	140	ASN
63	SQ	40	ASN
63	SQ	42	ASN
63	SQ	118	GLN
63	SQ	148	ASN
63	SQ	149	GLN
63	SQ	183	GLN
63	SQ	208	GLN
64	SR	87	GLN
64	SR	108	ASN
64	SR	189	GLN
65	SS	153	ASN
65	SS	157	ASN
65	SS	197	HIS
66	ST	56	ASN
66	ST	59	GLN
66	ST	139	ASN
66	ST	182	GLN
66	ST	190	GLN
66	ST	197	ASN
67	SU	19	GLN
67	SU	29	ASN
68	SV	52	ASN
68	SV	64	ASN
68	SV	94	ASN
69	SW	38	ASN
69	SW	74	ASN
70	SX	81	HIS
70	SX	138	ASN
71	SY	36	GLN
71	SY	62	GLN
71	SY	69	ASN
71	SY	151	ASN

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Mol	Chain	Res	Type
72	SZ	12	GLN
72	SZ	65	GLN
72	SZ	99	GLN
73	Sa	70	ASN
73	Sa	75	ASN
73	Sa	81	ASN
74	Sb	92	ASN
75	Sc	65	ASN
75	Sc	79	ASN
76	Sd	15	ASN
76	Sd	22	GLN
76	Sd	110	GLN
77	Se	17	HIS
77	Se	43	ASN
78	Sf	26	GLN
78	Sf	51	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	3029/3396 (89%)	474 (15%)	25 (0%)
2	B	120/121 (99%)	10 (8%)	2 (1%)
3	C	157/158 (99%)	25 (15%)	1 (0%)
4	D	9/10 (90%)	3 (33%)	1 (11%)
5	E	1572/1800 (87%)	343 (21%)	51 (3%)
80	m	75/76 (98%)	21 (28%)	0
81	n	63/75 (84%)	30 (47%)	0
All	All	5025/5636 (89%)	906 (18%)	80 (1%)

All (906) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	13	A
1	A	14	U
1	A	26	A
1	A	40	A
1	A	43	A
1	A	49	A
1	A	59	G
1	A	60	A
1	A	65	A

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Mol	Chain	Res	Type
1	A	66	A
1	A	74	G
1	A	77	A
1	A	92	G
1	A	110	G
1	A	111	C
1	A	116	A
1	A	117	U
1	A	121	A
1	A	122	A
1	A	135	C
1	A	136	G
1	A	156	G
1	A	157	A
1	A	166	C
1	A	187	A
1	A	190	U
1	A	191	U
1	A	200	C
1	A	206	G
1	A	210	U
1	A	211	A
1	A	213	A
1	A	218	G
1	A	219	A
1	A	234	G
1	A	239	G
1	A	240	U
1	A	241	G
1	A	242	C
1	A	243	G
1	A	257	U
1	A	269	G
1	A	270	U
1	A	286	U
1	A	295	A
1	A	305	U
1	A	329	U
1	A	330	G
1	A	339	C
1	A	350	C
1	A	351	A

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Mol	Chain	Res	Type
1	A	376	G
1	A	395	A
1	A	399	A
1	A	401	U
1	A	402	A
1	A	403	C
1	A	404	G
1	A	420	G
1	A	421	G
1	A	422	A
1	A	438	A
1	A	440	A
1	A	441	U
1	A	494	G
1	A	503	C
1	A	518	G
1	A	520	U
1	A	521	A
1	A	523	A
1	A	533	A
1	A	535	G
1	A	543	C
1	A	544	C
1	A	545	U
1	A	546	C
1	A	548	G
1	A	549	U
1	A	555	U
1	A	557	A
1	A	559	A
1	A	560	G
1	A	579	G
1	A	592	A
1	A	604	G
1	A	609	G
1	A	611	A
1	A	620	U
1	A	621	A
1	A	637	C
1	A	649	A
1	A	677	A
1	A	681	U

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Mol	Chain	Res	Type
1	A	683	U
1	A	691	A
1	A	705	A
1	A	712	G
1	A	715	A
1	A	716	A
1	A	719	U
1	A	720	A
1	A	721	G
1	A	727	G
1	A	742	G
1	A	758	C
1	A	764	U
1	A	765	C
1	A	766	U
1	A	767	U
1	A	776	U
1	A	779	G
1	A	781	G
1	A	785	G
1	A	787	G
1	A	806	A
1	A	808	A
1	A	817	A
1	A	830	A
1	A	848	A
1	A	861	C
1	A	874	U
1	A	879	U
1	A	895	A
1	A	896	A
1	A	907	G
1	A	908	G
1	A	914	A
1	A	916	G
1	A	917	A
1	A	923	C
1	A	937	G
1	A	944	C
1	A	959	C
1	A	960	U
1	A	974	G

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Mol	Chain	Res	Type
1	A	981	U
1	A	982	C
1	A	1002	A
1	A	1010	G
1	A	1047	A
1	A	1049	C
1	A	1063	G
1	A	1064	A
1	A	1065	A
1	A	1072	G
1	A	1081	U
1	A	1093	A
1	A	1094	U
1	A	1095	U
1	A	1097	G
1	A	1098	A
1	A	1103	A
1	A	1117	G
1	A	1131	G
1	A	1143	A
1	A	1144	U
1	A	1159	A
1	A	1160	C
1	A	1180	A
1	A	1181	U
1	A	1192	C
1	A	1193	A
1	A	1196	C
1	A	1201	C
1	A	1202	A
1	A	1209	G
1	A	1217	A
1	A	1220	U
1	A	1222	G
1	A	1223	A
1	A	1224	C
1	A	1227	C
1	A	1230	G
1	A	1282	G
1	A	1284	C
1	A	1287	A
1	A	1307	G

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Mol	Chain	Res	Type
1	A	1308	A
1	A	1309	U
1	A	1313	G
1	A	1330	A
1	A	1331	U
1	A	1349	G
1	A	1350	A
1	A	1352	A
1	A	1355	A
1	A	1356	U
1	A	1357	G
1	A	1386	A
1	A	1399	A
1	A	1400	G
1	A	1418	A
1	A	1419	A
1	A	1434	G
1	A	1437	C
1	A	1446	A
1	A	1450	G
1	A	1475	A
1	A	1481	A
1	A	1483	G
1	A	1503	A
1	A	1508	C
1	A	1527	C
1	A	1536	G
1	A	1546	A
1	A	1556	C
1	A	1560	G
1	A	1563	C
1	A	1564	U
1	A	1573	G
1	A	1574	C
1	A	1575	A
1	A	1576	G
1	A	1580	A
1	A	1583	A
1	A	1589	A
1	A	1606	U
1	A	1620	U
1	A	1621	A

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Mol	Chain	Res	Type
1	A	1627	U
1	A	1629	U
1	A	1639	C
1	A	1643	A
1	A	1645	U
1	A	1657	C
1	A	1683	A
1	A	1688	U
1	A	1696	A
1	A	1717	U
1	A	1724	U
1	A	1725	C
1	A	1728	G
1	A	1741	A
1	A	1742	U
1	A	1750	A
1	A	1751	G
1	A	1770	G
1	A	1775	G
1	A	1780	G
1	A	1797	A
1	A	1808	G
1	A	1819	U
1	A	1820	U
1	A	1821	U
1	A	1839	A
1	A	1840	U
1	A	1841	A
1	A	1842	A
1	A	1846	C
1	A	1849	C
1	A	1866	C
1	A	1867	A
1	A	1879	A
1	A	1880	U
1	A	1881	A
1	A	1893	A
1	A	1906	G
1	A	1943	C
1	A	1953	G
1	A	1954	G
1	A	2094	C

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Mol	Chain	Res	Type
1	A	2095	G
1	A	2100	A
1	A	2101	C
1	A	2102	U
1	A	2111	G
1	A	2112	U
1	A	2113	A
1	A	2121	G
1	A	2122	G
1	A	2131	A
1	A	2140	U
1	A	2144	A
1	A	2158	A
1	A	2166	A
1	A	2169	G
1	A	2170	U
1	A	2206	G
1	A	2207	A
1	A	2209	U
1	A	2210	G
1	A	2223	A
1	A	2249	G
1	A	2256	A
1	A	2272	G
1	A	2273	G
1	A	2281	A
1	A	2282	U
1	A	2307	G
1	A	2310	U
1	A	2313	A
1	A	2314	U
1	A	2315	G
1	A	2318	U
1	A	2325	G
1	A	2334	U
1	A	2335	G
1	A	2336	U
1	A	2372	A
1	A	2373	A
1	A	2374	C
1	A	2375	G
1	A	2385	G

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Mol	Chain	Res	Type
1	A	2388	U
1	A	2393	G
1	A	2394	G
1	A	2397	A
1	A	2402	A
1	A	2403	G
1	A	2404	A
1	A	2411	U
1	A	2418	G
1	A	2419	A
1	A	2435	G
1	A	2437	G
1	A	2440	G
1	A	2514	U
1	A	2515	A
1	A	2522	G
1	A	2525	G
1	A	2526	C
1	A	2531	C
1	A	2532	U
1	A	2544	U
1	A	2549	G
1	A	2552	C
1	A	2559	U
1	A	2561	A
1	A	2569	A
1	A	2570	U
1	A	2572	C
1	A	2573	G
1	A	2585	G
1	A	2593	A
1	A	2594	C
1	A	2595	A
1	A	2606	G
1	A	2607	G
1	A	2614	G
1	A	2619	G
1	A	2629	U
1	A	2635	A
1	A	2652	U
1	A	2656	A
1	A	2664	C

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Mol	Chain	Res	Type
1	A	2674	A
1	A	2677	G
1	A	2681	U
1	A	2689	A
1	A	2691	A
1	A	2694	A
1	A	2696	A
1	A	2700	G
1	A	2706	G
1	A	2714	G
1	A	2719	U
1	A	2728	G
1	A	2729	U
1	A	2737	C
1	A	2749	G
1	A	2753	G
1	A	2762	A
1	A	2772	C
1	A	2777	G
1	A	2778	G
1	A	2780	A
1	A	2796	G
1	A	2800	G
1	A	2801	A
1	A	2802	A
1	A	2803	A
1	A	2810	C
1	A	2814	G
1	A	2816	G
1	A	2817	A
1	A	2818	U
1	A	2842	U
1	A	2845	A
1	A	2847	A
1	A	2849	C
1	A	2856	G
1	A	2867	C
1	A	2871	G
1	A	2872	A
1	A	2875	U
1	A	2876	C
1	A	2887	A

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Mol	Chain	Res	Type
1	A	2889	C
1	A	2923	U
1	A	2929	C
1	A	2935	U
1	A	2936	A
1	A	2947	G
1	A	2955	U
1	A	2957	G
1	A	2964	G
1	A	2983	C
1	A	2990	G
1	A	2996	U
1	A	2997	G
1	A	3003	G
1	A	3012	A
1	A	3056	U
1	A	3057	U
1	A	3059	G
1	A	3078	U
1	A	3079	U
1	A	3086	A
1	A	3092	C
1	A	3093	C
1	A	3101	G
1	A	3104	U
1	A	3116	G
1	A	3117	C
1	A	3119	U
1	A	3122	A
1	A	3129	A
1	A	3130	A
1	A	3131	U
1	A	3142	A
1	A	3143	C
1	A	3153	U
1	A	3154	C
1	A	3155	U
1	A	3156	U
1	A	3157	U
1	A	3165	A
1	A	3170	A
1	A	3173	G

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Mol	Chain	Res	Type
1	A	3174	A
1	A	3176	G
1	A	3179	U
1	A	3181	C
1	A	3187	A
1	A	3196	U
1	A	3197	G
1	A	3207	U
1	A	3210	A
1	A	3217	C
1	A	3218	A
1	A	3219	G
1	A	3239	G
1	A	3243	A
1	A	3245	A
1	A	3247	G
1	A	3249	C
1	A	3259	U
1	A	3270	U
1	A	3273	A
1	A	3276	G
1	A	3281	U
1	A	3287	U
1	A	3288	G
1	A	3289	G
1	A	3294	A
1	A	3295	A
1	A	3304	U
1	A	3316	A
1	A	3318	G
1	A	3320	A
1	A	3331	U
1	A	3334	U
1	A	3345	G
1	A	3351	U
1	A	3352	U
1	A	3354	U
1	A	3355	U
1	A	3363	U
1	A	3369	G
1	A	3378	C
1	A	3382	U

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Mol	Chain	Res	Type
1	A	3386	G
1	A	3389	U
1	A	3390	G
2	B	7	G
2	B	10	C
2	B	30	G
2	B	35	C
2	B	39	C
2	B	53	U
2	B	65	G
2	B	102	A
2	B	112	G
2	B	121	U
3	C	34	U
3	C	35	C
3	C	48	A
3	C	59	A
3	C	62	C
3	C	63	G
3	C	80	A
3	C	81	U
3	C	82	U
3	C	83	C
3	C	84	C
3	C	85	G
3	C	86	U
3	C	87	G
3	C	90	U
3	C	91	C
3	C	95	G
3	C	104	A
3	C	106	C
3	C	112	U
3	C	125	U
3	C	126	A
3	C	138	A
3	C	148	G
3	C	152	G
4	D	3	U
4	D	7	A
4	D	8	A
5	E	2	A

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Mol	Chain	Res	Type
5	E	4	C
5	E	25	C
5	E	26	A
5	E	43	A
5	E	45	U
5	E	46	A
5	E	47	A
5	E	56	U
5	E	57	G
5	E	61	A
5	E	62	A
5	E	65	A
5	E	66	U
5	E	67	A
5	E	68	A
5	E	69	G
5	E	72	A
5	E	78	A
5	E	80	A
5	E	81	G
5	E	104	A
5	E	114	C
5	E	116	U
5	E	124	A
5	E	126	A
5	E	127	G
5	E	129	U
5	E	138	A
5	E	139	C
5	E	140	A
5	E	145	A
5	E	153	G
5	E	156	A
5	E	158	U
5	E	161	U
5	E	166	C
5	E	178	U
5	E	179	A
5	E	181	A
5	E	182	A
5	E	250	C
5	E	257	A

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Mol	Chain	Res	Type
5	E	265	A
5	E	266	A
5	E	272	U
5	E	274	G
5	E	276	C
5	E	278	U
5	E	279	G
5	E	280	U
5	E	281	G
5	E	287	G
5	E	299	A
5	E	313	U
5	E	314	C
5	E	316	A
5	E	321	C
5	E	322	G
5	E	323	A
5	E	330	G
5	E	333	A
5	E	337	G
5	E	338	C
5	E	352	A
5	E	353	A
5	E	359	A
5	E	361	C
5	E	370	A
5	E	373	G
5	E	385	A
5	E	388	G
5	E	395	U
5	E	400	A
5	E	401	A
5	E	402	C
5	E	404	G
5	E	416	A
5	E	417	A
5	E	418	G
5	E	419	G
5	E	423	G
5	E	424	C
5	E	425	A
5	E	426	G

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Mol	Chain	Res	Type
5	E	428	A
5	E	434	G
5	E	435	C
5	E	439	U
5	E	444	C
5	E	446	A
5	E	447	U
5	E	448	C
5	E	460	A
5	E	461	G
5	E	468	A
5	E	469	C
5	E	471	A
5	E	482	U
5	E	510	G
5	E	514	G
5	E	517	U
5	E	518	A
5	E	527	A
5	E	538	A
5	E	540	G
5	E	541	A
5	E	542	A
5	E	555	A
5	E	556	A
5	E	557	G
5	E	558	U
5	E	565	C
5	E	568	G
5	E	578	U
5	E	579	A
5	E	583	C
5	E	594	A
5	E	595	G
5	E	606	A
5	E	608	U
5	E	609	U
5	E	610	G
5	E	611	U
5	E	619	A
5	E	620	A
5	E	622	A

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Mol	Chain	Res	Type
5	E	623	A
5	E	624	G
5	E	638	U
5	E	641	G
5	E	687	G
5	E	694	U
5	E	745	U
5	E	753	A
5	E	756	A
5	E	765	G
5	E	766	U
5	E	774	A
5	E	775	G
5	E	780	A
5	E	781	U
5	E	782	U
5	E	783	G
5	E	789	A
5	E	804	A
5	E	812	A
5	E	813	U
5	E	814	A
5	E	815	G
5	E	816	G
5	E	820	U
5	E	821	U
5	E	823	G
5	E	847	A
5	E	851	U
5	E	852	C
5	E	854	U
5	E	856	A
5	E	863	A
5	E	873	U
5	E	876	G
5	E	881	A
5	E	886	U
5	E	898	A
5	E	899	G
5	E	902	G
5	E	904	G
5	E	912	U

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Mol	Chain	Res	Type
5	E	913	G
5	E	914	G
5	E	929	A
5	E	933	A
5	E	935	U
5	E	942	G
5	E	945	U
5	E	951	A
5	E	960	U
5	E	966	A
5	E	988	A
5	E	989	U
5	E	993	A
5	E	1004	U
5	E	1005	A
5	E	1023	A
5	E	1024	U
5	E	1025	A
5	E	1026	A
5	E	1028	C
5	E	1032	G
5	E	1039	A
5	E	1053	G
5	E	1066	C
5	E	1076	A
5	E	1081	A
5	E	1082	C
5	E	1092	A
5	E	1096	C
5	E	1097	U
5	E	1100	G
5	E	1113	A
5	E	1138	A
5	E	1150	G
5	E	1158	C
5	E	1160	A
5	E	1167	G
5	E	1170	G
5	E	1185	U
5	E	1186	U
5	E	1194	A
5	E	1199	G

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Mol	Chain	Res	Type
5	E	1200	G
5	E	1208	A
5	E	1212	G
5	E	1214	U
5	E	1217	A
5	E	1218	G
5	E	1227	A
5	E	1229	G
5	E	1231	U
5	E	1241	G
5	E	1244	A
5	E	1245	G
5	E	1246	C
5	E	1252	C
5	E	1255	G
5	E	1256	A
5	E	1257	U
5	E	1260	U
5	E	1263	G
5	E	1274	C
5	E	1276	U
5	E	1284	C
5	E	1285	U
5	E	1286	U
5	E	1301	U
5	E	1307	U
5	E	1308	G
5	E	1312	A
5	E	1314	U
5	E	1315	U
5	E	1316	G
5	E	1318	G
5	E	1321	A
5	E	1322	A
5	E	1344	A
5	E	1345	A
5	E	1346	A
5	E	1347	U
5	E	1348	A
5	E	1349	G
5	E	1361	U
5	E	1362	U

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Mol	Chain	Res	Type
5	E	1363	U
5	E	1370	U
5	E	1371	A
5	E	1372	U
5	E	1373	C
5	E	1382	A
5	E	1383	G
5	E	1390	U
5	E	1395	G
5	E	1398	U
5	E	1399	C
5	E	1400	A
5	E	1402	G
5	E	1413	U
5	E	1414	U
5	E	1415	U
5	E	1427	A
5	E	1431	C
5	E	1432	U
5	E	1433	G
5	E	1436	A
5	E	1445	G
5	E	1446	A
5	E	1448	G
5	E	1458	G
5	E	1459	C
5	E	1460	A
5	E	1466	G
5	E	1469	A
5	E	1471	A
5	E	1472	C
5	E	1478	G
5	E	1496	U
5	E	1516	A
5	E	1520	U
5	E	1521	G
5	E	1523	G
5	E	1524	A
5	E	1527	C
5	E	1528	U
5	E	1535	U
5	E	1536	G

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Mol	Chain	Res	Type
5	E	1537	C
5	E	1538	U
5	E	1540	G
5	E	1543	A
5	E	1550	A
5	E	1557	U
5	E	1558	U
5	E	1559	A
5	E	1570	A
5	E	1572	G
5	E	1573	A
5	E	1574	G
5	E	1575	G
5	E	1577	A
5	E	1583	A
5	E	1584	G
5	E	1601	G
5	E	1608	U
5	E	1609	U
5	E	1615	C
5	E	1616	G
5	E	1619	C
5	E	1633	A
5	E	1634	C
5	E	1635	A
5	E	1637	C
5	E	1657	U
5	E	1658	G
5	E	1680	G
5	E	1681	A
5	E	1717	G
5	E	1718	G
5	E	1731	A
5	E	1755	A
5	E	1757	G
5	E	1760	G
5	E	1762	A
5	E	1766	A
5	E	1767	G
5	E	1769	U
5	E	1780	G
5	E	1782	A

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Mol	Chain	Res	Type
5	E	1783	C
5	E	1792	G
5	E	1793	G
5	E	1794	A
5	E	1796	C
5	E	1799	U
80	m	8	U
80	m	9	A
80	m	14	A
80	m	16	U
80	m	17	U
80	m	20	U
80	m	21	A
80	m	45	G
80	m	47	U
80	m	48	C
80	m	49	G
80	m	50	C
80	m	57	G
80	m	60	U
80	m	61	C
80	m	62	C
80	m	65	C
80	m	66	A
80	m	68	G
80	m	69	A
80	m	74	C
81	n	3	C
81	n	7	G
81	n	8	U
81	n	9	G
81	n	15	G
81	n	16	U
81	n	21	A
81	n	22	G
81	n	24	G
81	n	25	C
81	n	26	G
81	n	27	C
81	n	28	A
81	n	30	G
81	n	31	G

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Mol	Chain	Res	Type
81	n	34	C
81	n	36	U
81	n	40	C
81	n	41	C
81	n	42	U
81	n	44	A
81	n	45	U
81	n	49	C
81	n	68	G
81	n	69	C
81	n	70	G
81	n	71	C
81	n	72	U
81	n	75	C
81	n	76	A

All (80) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	13	A
1	A	73	C
1	A	186	U
1	A	636	C
1	A	763	G
1	A	916	G
1	A	1064	A
1	A	1097	G
1	A	1222	G
1	A	1348	U
1	A	1355	A
1	A	1562	C
1	A	1820	U
1	A	1821	U
1	A	2112	U
1	A	2255	A
1	A	2513	U
1	A	2525	G
1	A	2689	A
1	A	3078	U
1	A	3121	U
1	A	3218	A
1	A	3269	U

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Mol	Chain	Res	Type
1	A	3350	C
1	A	3352	U
2	B	52	G
2	B	120	C
3	C	85	G
4	D	7	A
5	E	65	A
5	E	68	A
5	E	77	U
5	E	80	A
5	E	99	C
5	E	139	C
5	E	178	U
5	E	180	A
5	E	279	G
5	E	313	U
5	E	321	C
5	E	322	G
5	E	352	A
5	E	387	A
5	E	539	G
5	E	541	A
5	E	609	U
5	E	640	U
5	E	755	A
5	E	802	G
5	E	803	A
5	E	814	A
5	E	819	G
5	E	912	U
5	E	913	G
5	E	928	U
5	E	1023	A
5	E	1207	C
5	E	1217	A
5	E	1226	A
5	E	1255	G
5	E	1256	A
5	E	1273	G
5	E	1344	A
5	E	1346	A
5	E	1347	U

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Mol	Chain	Res	Type
5	E	1362	U
5	E	1382	A
5	E	1430	U
5	E	1471	A
5	E	1535	U
5	E	1536	G
5	E	1556	A
5	E	1557	U
5	E	1572	G
5	E	1573	A
5	E	1574	G
5	E	1615	C
5	E	1633	A
5	E	1634	C
5	E	1636	C

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand 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	$\# Z > 2$
82	3HE	A	3401	-	21,21,21	0.56	0	23,30,30	0.91	2 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	3HE	A	3401	-	-	2/8/36/36	0/2/2/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	A	3401	3HE	O3-C7-C8	2.42	114.00	109.15
82	A	3401	3HE	C9-C10-C11	-2.13	110.87	114.46

There are no chirality outliers.

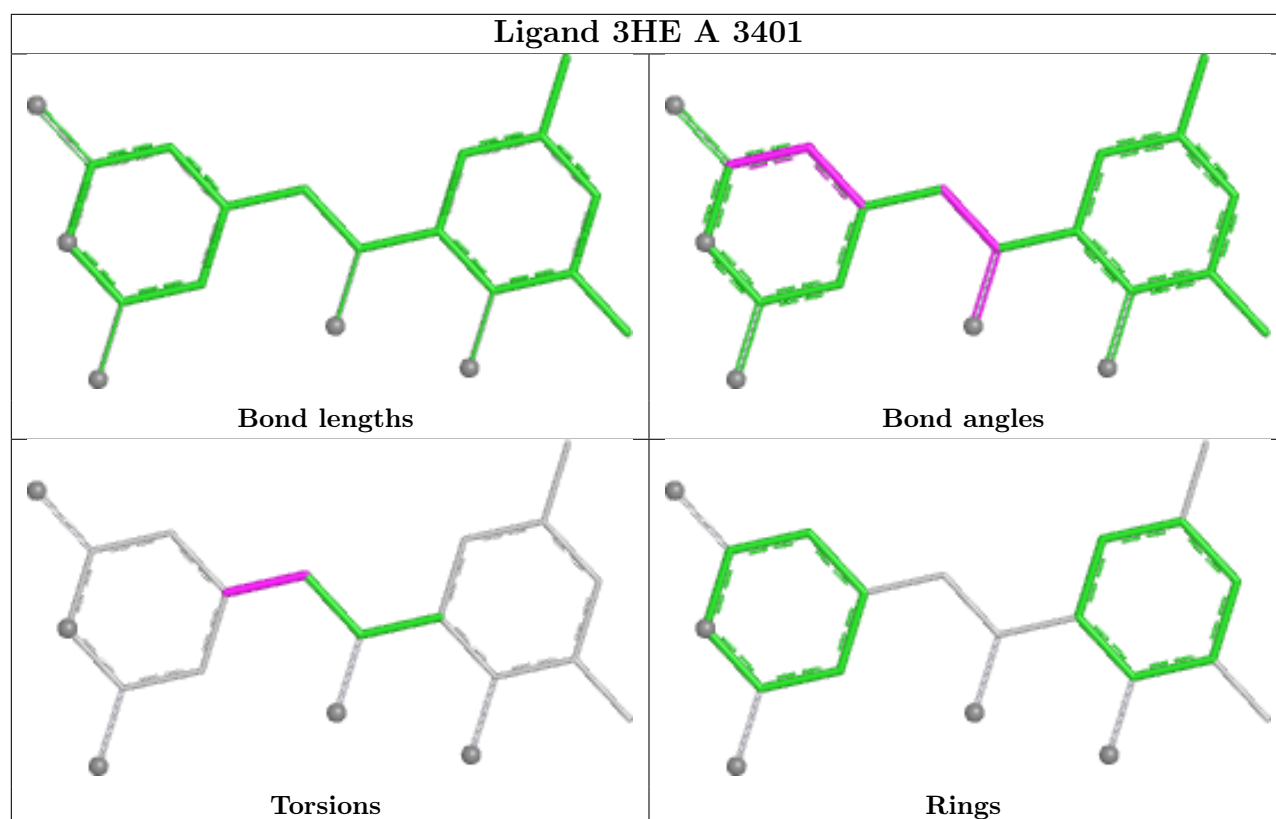
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
82	A	3401	3HE	C7-C8-C9-C10
82	A	3401	3HE	C7-C8-C9-C13

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

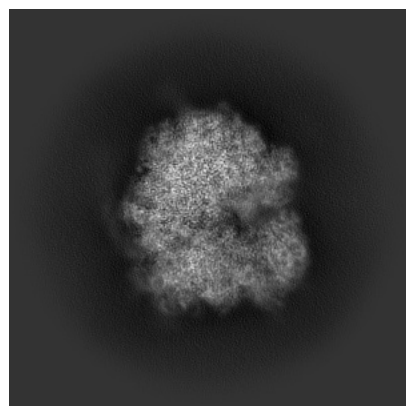
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72801. These allow visual inspection of the internal detail of the map and identification of artifacts.

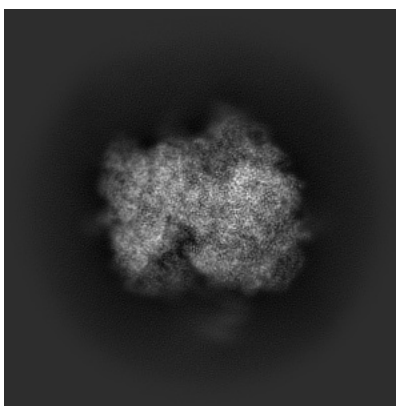
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

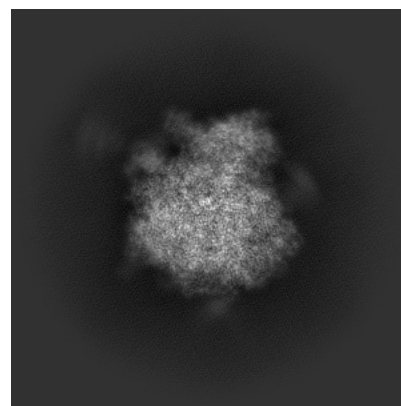
6.1.1 Primary map



X

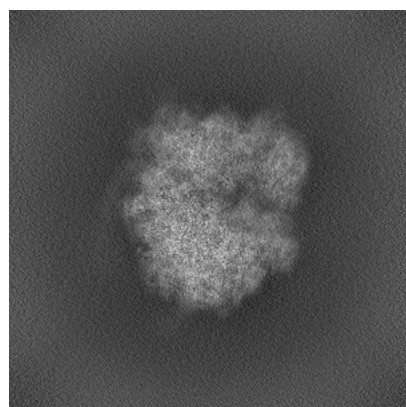


Y

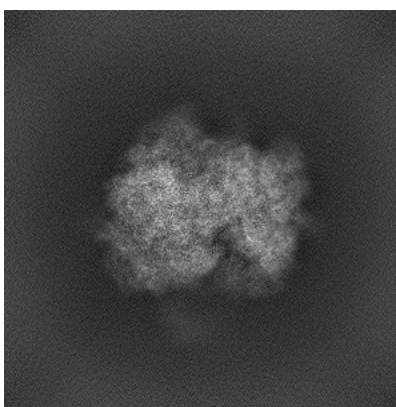


Z

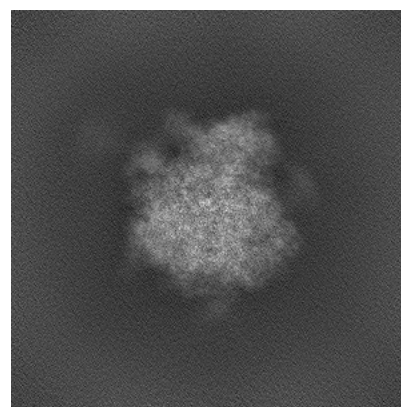
6.1.2 Raw map



X



Y

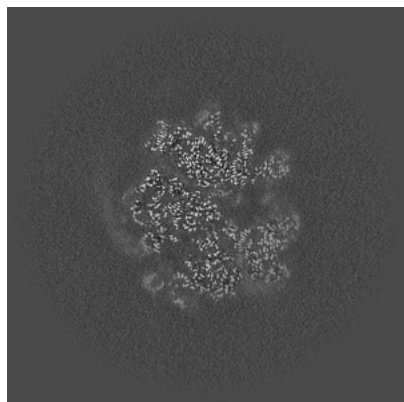


Z

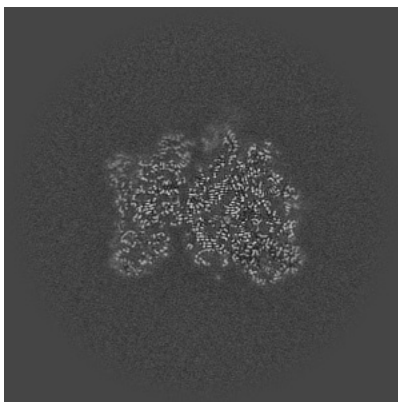
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

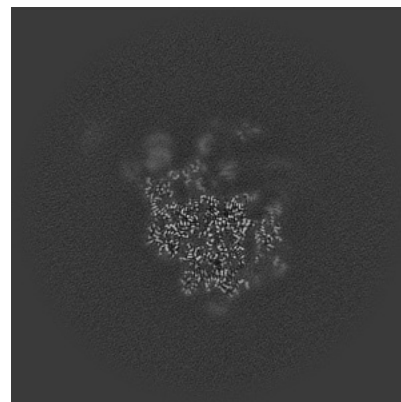
6.2.1 Primary map



X Index: 300

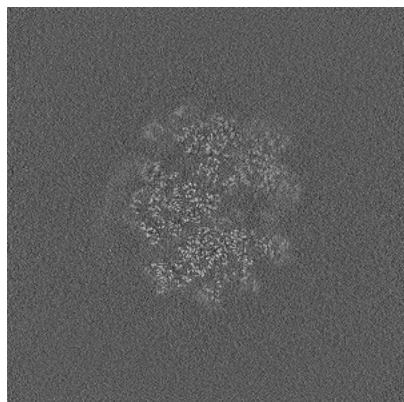


Y Index: 300

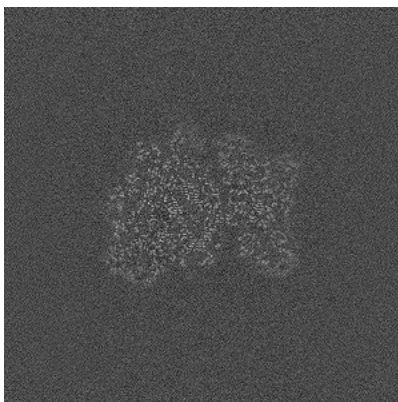


Z Index: 300

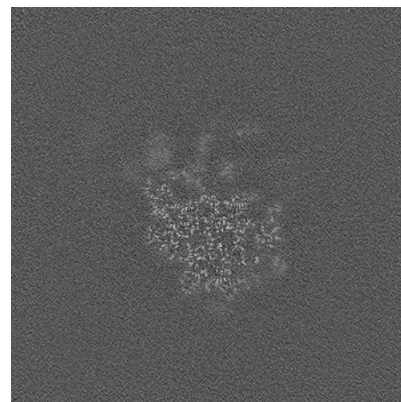
6.2.2 Raw map



X Index: 300



Y Index: 300

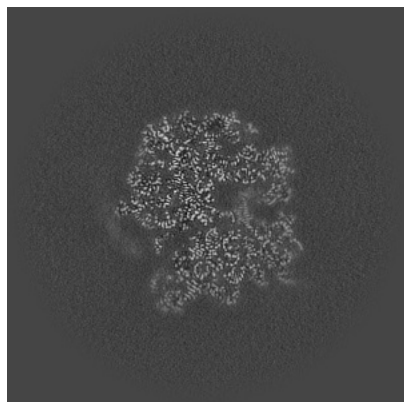


Z Index: 300

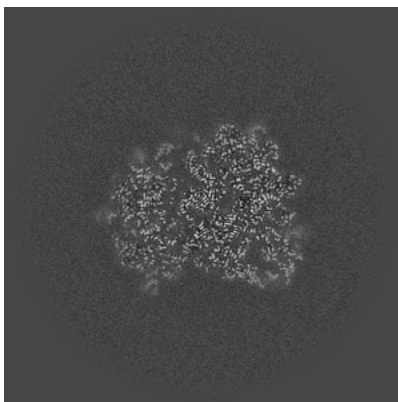
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

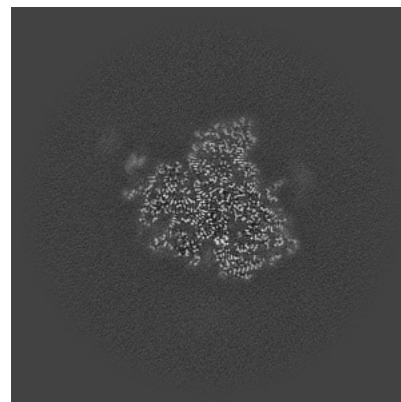
6.3.1 Primary map



X Index: 323

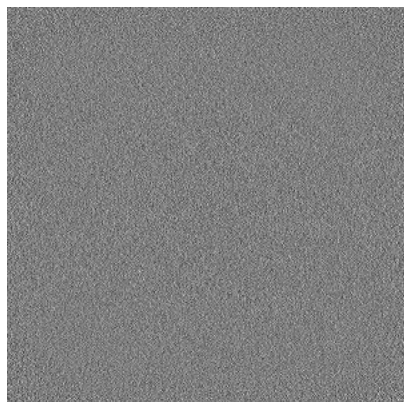


Y Index: 276

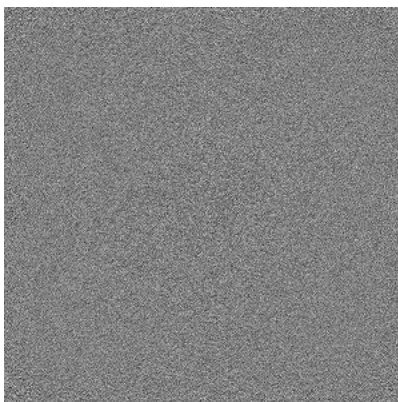


Z Index: 364

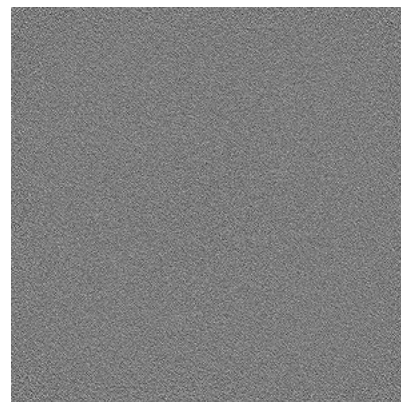
6.3.2 Raw map



X Index: 0



Y Index: 0

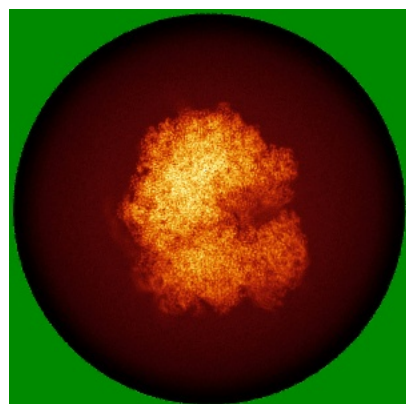


Z Index: 0

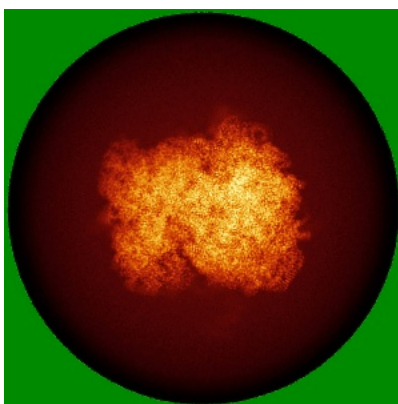
The images above show the largest variance slices of the map in three orthogonal directions.

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

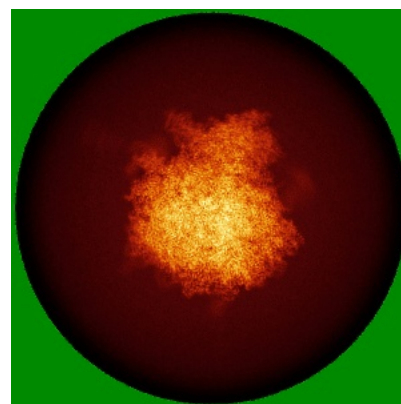
6.4.1 Primary map



X

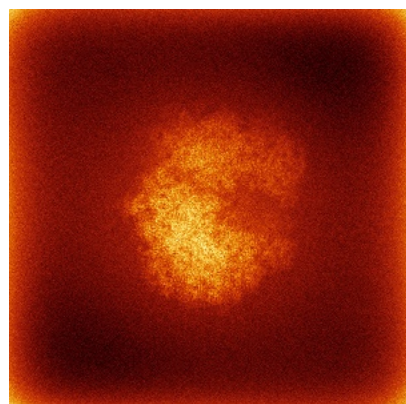


Y

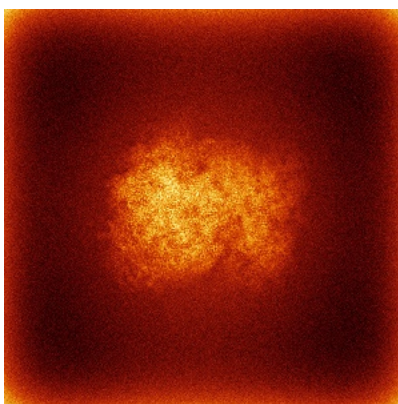


Z

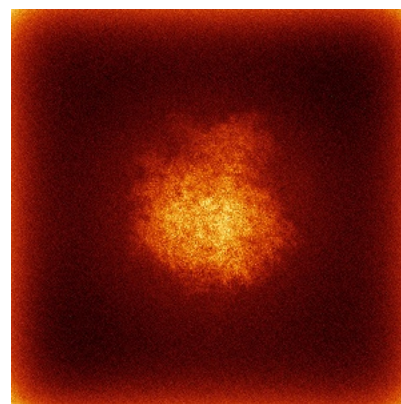
6.4.2 Raw map



X



Y

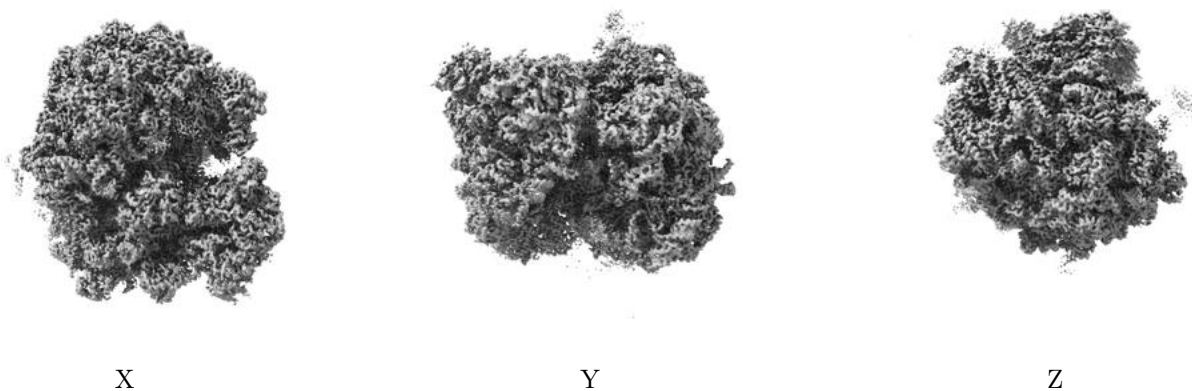


Z

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

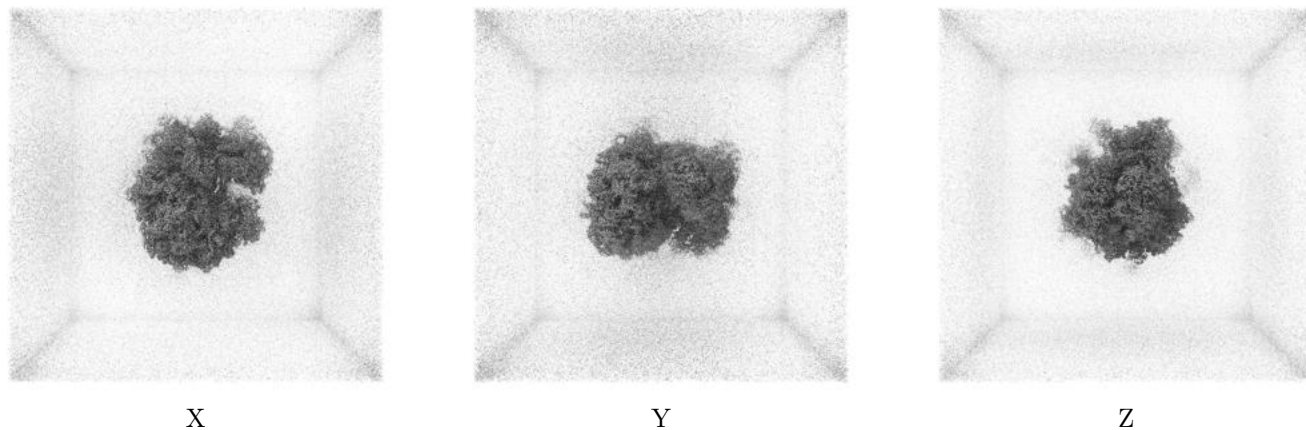
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

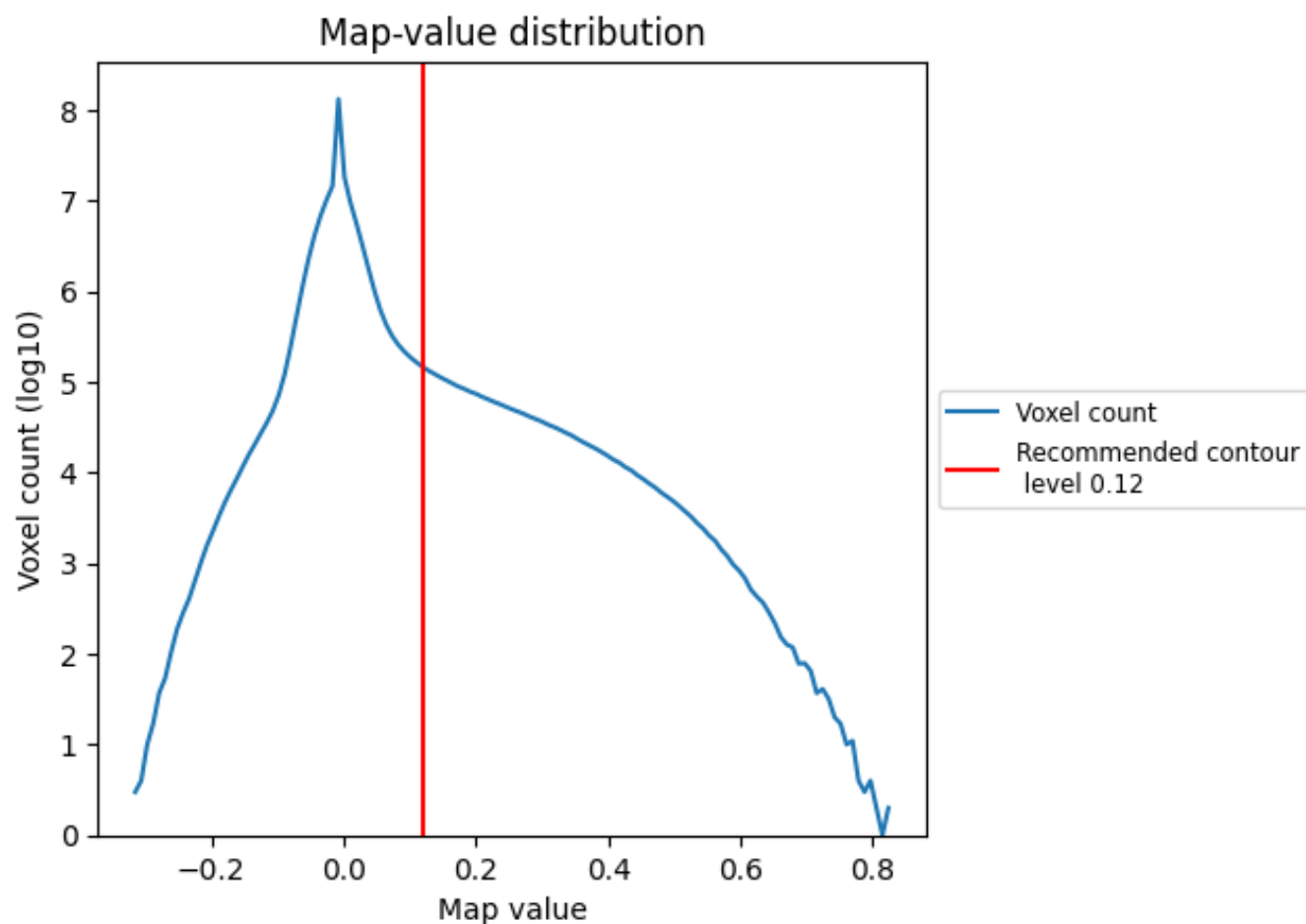
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

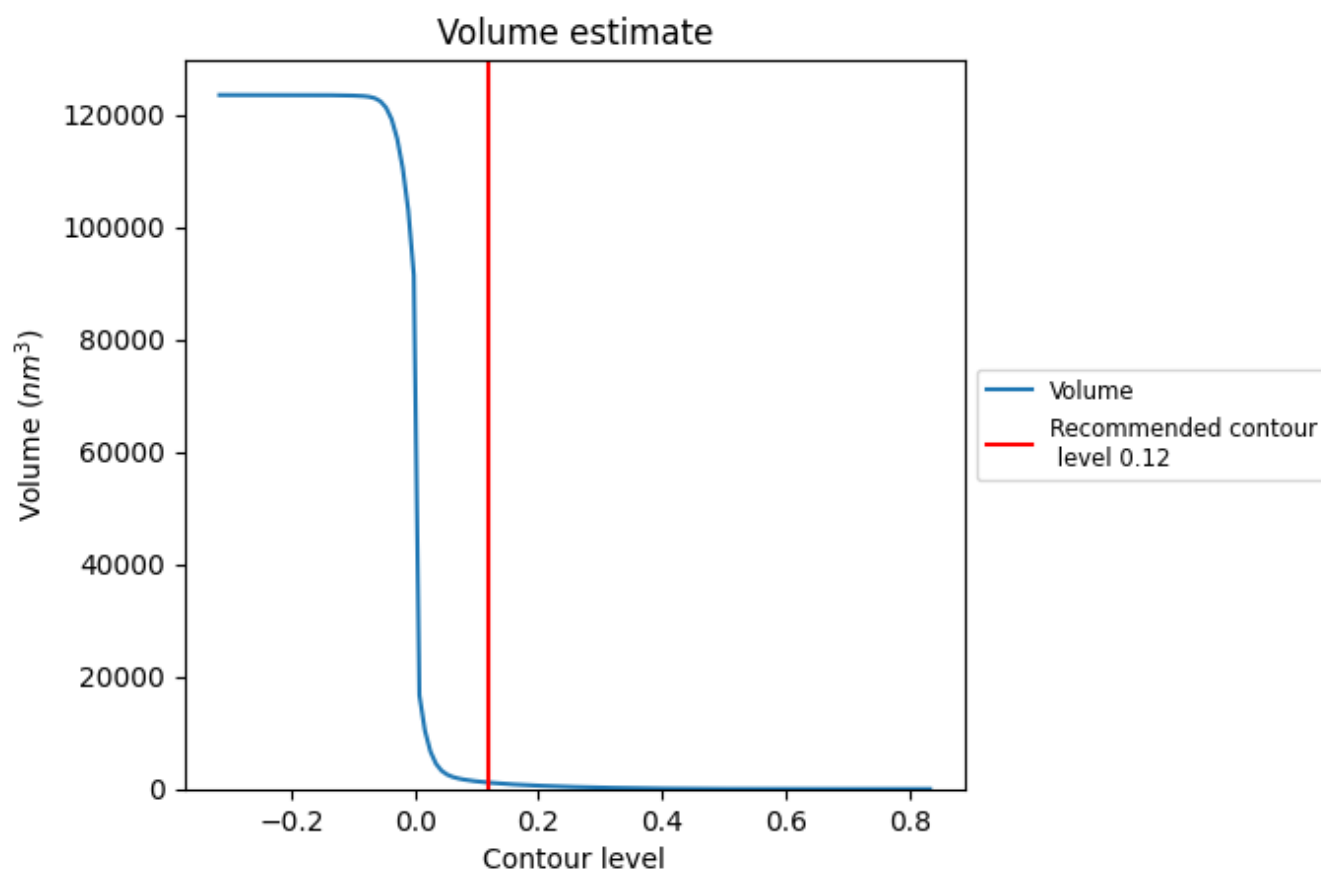
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

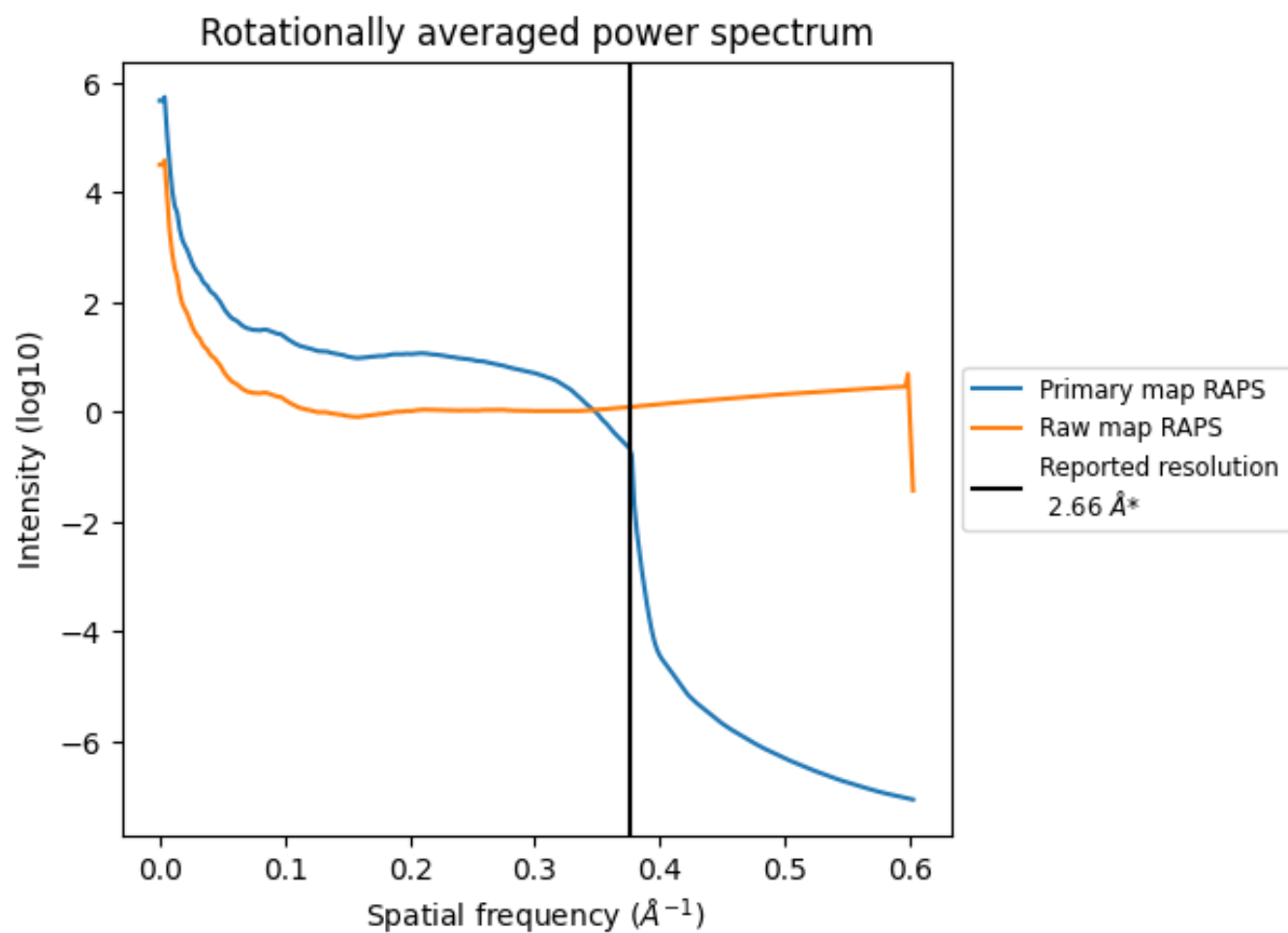
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1131 nm³; this corresponds to an approximate mass of 1021 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 ⓘ

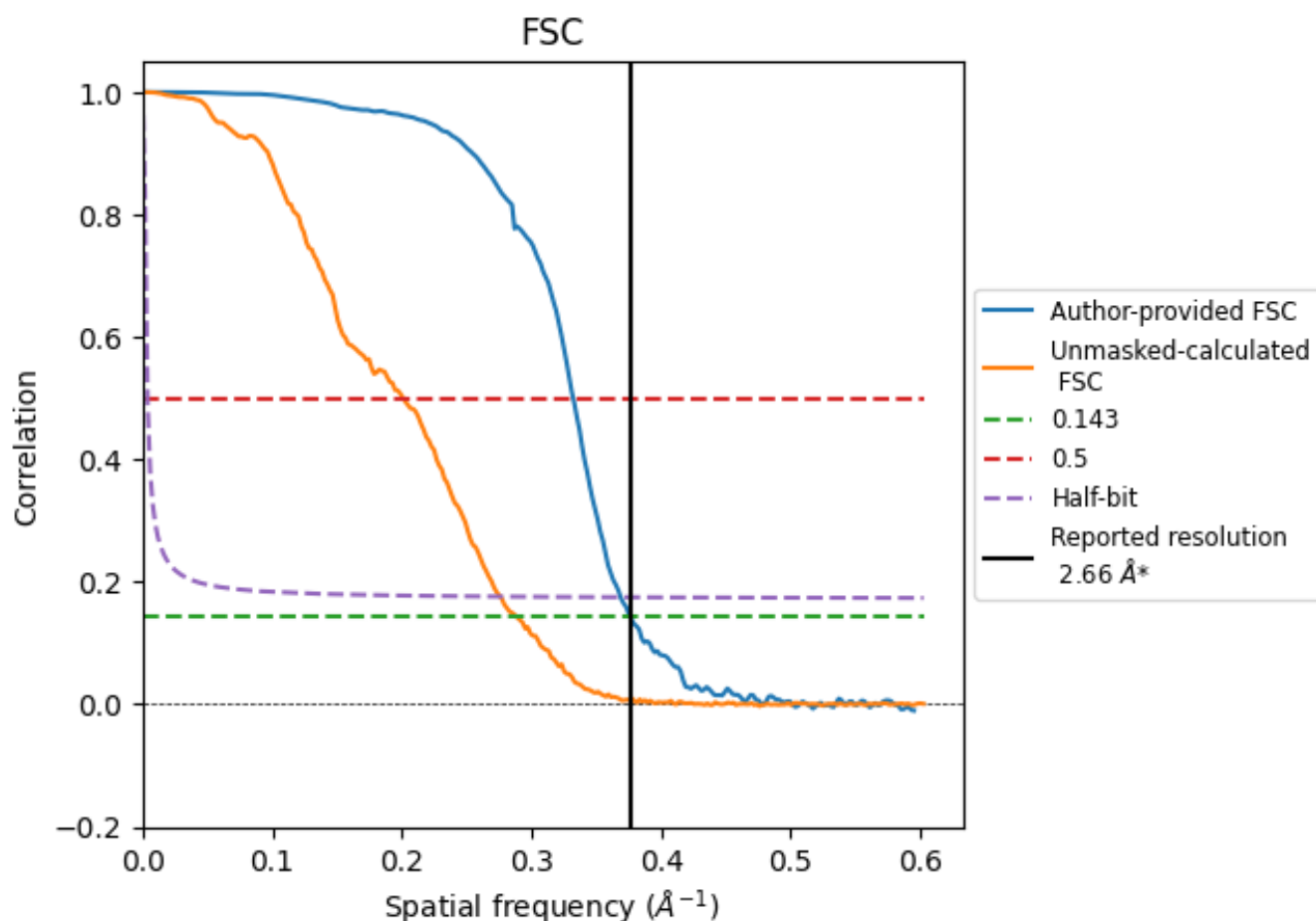


*Reported resolution corresponds to spatial frequency of 0.376 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.376 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

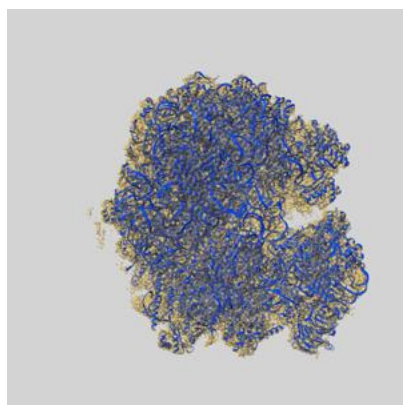
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.66	-	-
Author-provided FSC curve	2.66	3.01	2.71
Unmasked-calculated*	3.47	4.98	3.62

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.47 differs from the reported value 2.66 by more than 10 %

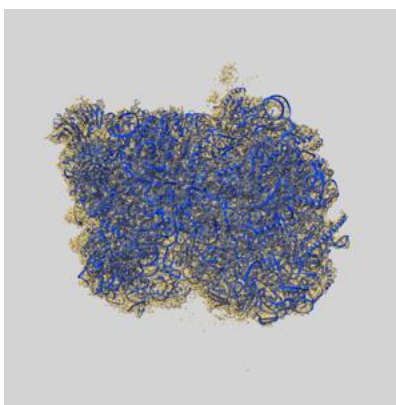
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-72801 and PDB model 9YDD. Per-residue inclusion information can be found in [section 3](#) on page [20](#).

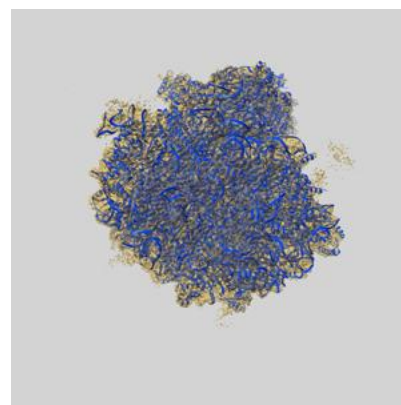
9.1 Map-model overlay [i](#)



X



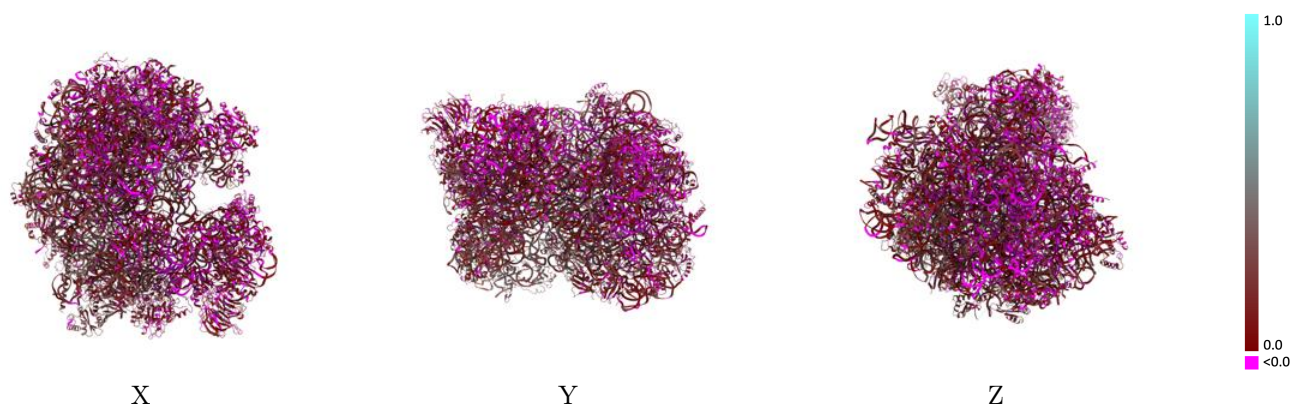
Y



Z

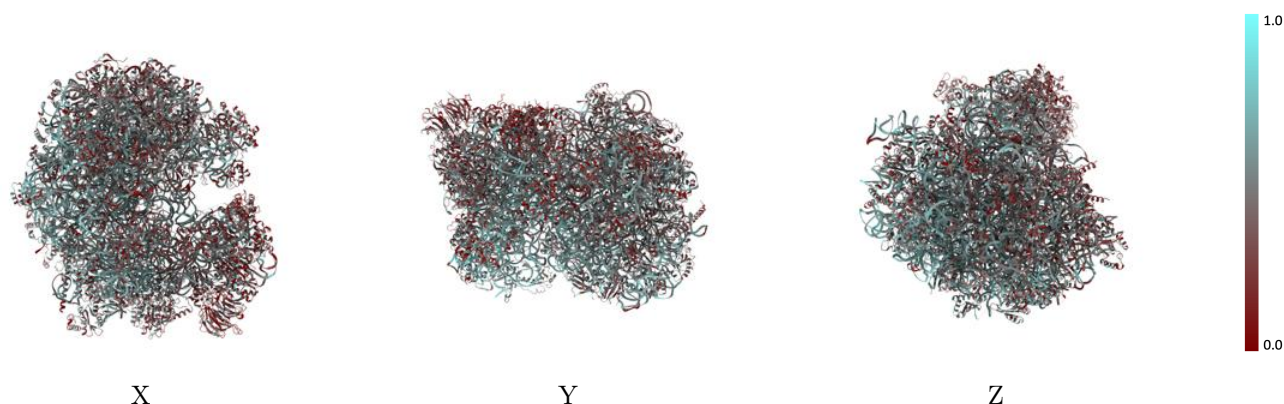
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



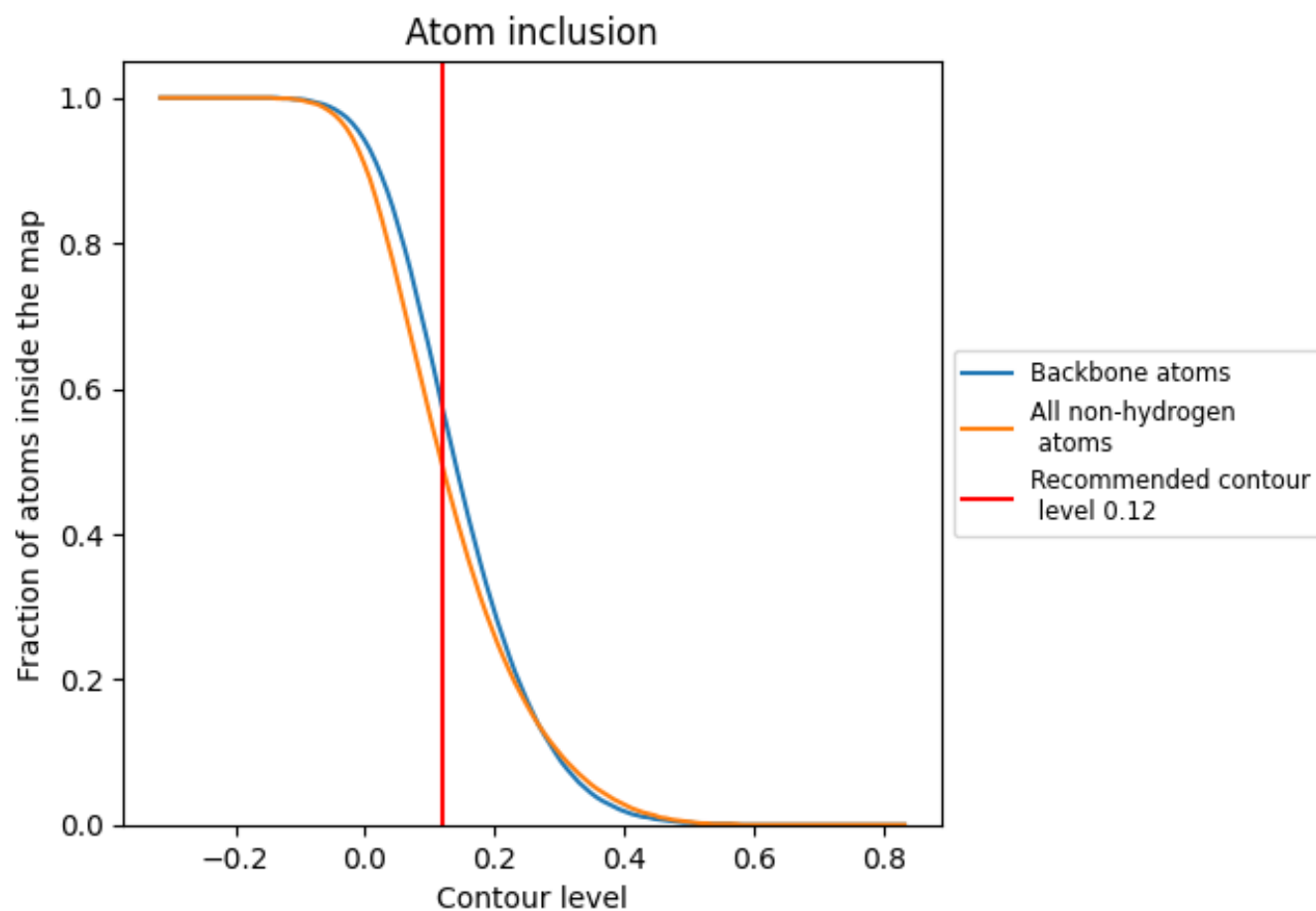
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 49% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4920	 0.1330
A	 0.5450	 0.1300
B	 0.5050	 0.0390
C	 0.5560	 0.1300
D	 0.4720	 0.0770
E	 0.5730	 0.1500
LD	 0.4340	 0.1110
LE	 0.5270	 0.2080
LF	 0.4060	 0.0710
LG	 0.3620	 0.0520
LH	 0.4280	 0.1260
LI	 0.3970	 0.0830
LJ	 0.4100	 0.0950
LK	 0.4440	 0.1500
LL	 0.3810	 0.1080
LM	 0.3480	 0.1270
LN	 0.3750	 0.0370
LO	 0.4340	 0.1180
LP	 0.3810	 0.0450
LQ	 0.4640	 0.1430
LR	 0.4760	 0.1370
LS	 0.3710	 0.0320
LT	 0.5230	 0.2260
LU	 0.4380	 0.1230
LV	 0.3590	 0.0650
LW	 0.4950	 0.2120
LX	 0.4680	 0.1990
LY	 0.5110	 0.2160
LZ	 0.4620	 0.1360
La	 0.4450	 0.0890
Lb	 0.4850	 0.1540
Lc	 0.3760	 0.0490
Ld	 0.3940	 0.0910
Le	 0.4800	 0.1730
Lf	 0.5300	 0.2040



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Chain	Atom inclusion	Q-score
Lg	 0.4020	 0.0820
Lh	 0.4340	 0.1140
Li	 0.4690	 0.1360
Lj	 0.4060	 0.0680
Lk	 0.3500	 0.0630
Ll	 0.4440	 0.0870
Lm	 0.4840	 0.2000
Ln	 0.5080	 0.1700
Lo	 0.4430	 0.1600
Lp	 0.3600	 0.1540
Lq	 0.3700	 0.0660
Lr	 0.4400	 0.1470
SA	 0.3690	 0.1040
SB	 0.3060	 0.0490
SC	 0.4130	 0.1620
SD	 0.2180	 0.1420
SE	 0.3360	 0.1210
SF	 0.3110	 0.0540
SG	 0.3550	 0.1060
SH	 0.2830	 0.0260
SI	 0.2880	 0.0250
SJ	 0.3360	 0.0990
SK	 0.2480	 0.0140
SL	 0.2860	 0.0710
SM	 0.4390	 0.1080
SN	 0.2420	 0.0940
SO	 0.2800	 0.0960
SP	 0.3830	 0.1160
SQ	 0.3240	 0.0860
SR	 0.4850	 0.1880
SS	 0.5410	 0.2630
ST	 0.5230	 0.2680
SU	 0.4580	 0.2410
SV	 0.4870	 0.2220
SW	 0.4980	 0.2100
SX	 0.5170	 0.2390
SY	 0.4510	 0.1940
SZ	 0.3470	 0.0700
Sa	 0.4700	 0.1700
Sb	 0.5010	 0.2080
Sc	 0.4740	 0.2090
Sd	 0.5570	 0.2850

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Chain	Atom inclusion	Q-score
Se	 0.4140	 0.1270
Sf	 0.4030	 0.1580
Sg	 0.4280	 0.1860
m	 0.5140	 0.1960
n	 0.3970	 0.0990