



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 07:33 PM UTC

PDB ID : 6RM3 / pdb_00006rm3
EMDB ID : EMD-4935
Title : Evolutionary compaction and adaptation visualized by the structure of the dormant microsporidian ribosome
Authors : Barandun, J.; Hunziker, M.; Vossbrinck, C.R.; Klinge, S.
Deposited on : 2019-05-05
Resolution : 3.40 Å(reported)
Based on initial model : 4V88

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

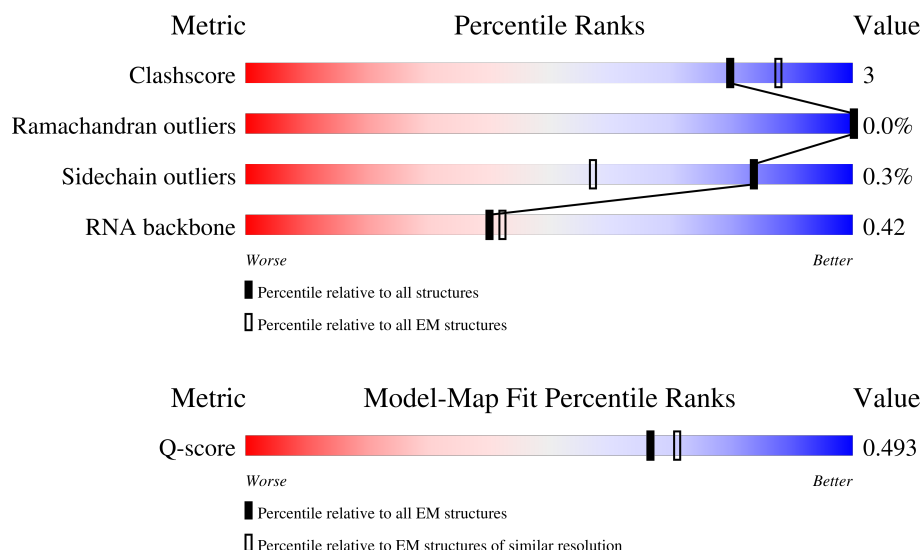
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	S60	1244	9% 66% 30% ••
2	L70	119	75% 22% ••
3	LA0	237	5% 87% 11% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	SA0	264	
5	LAA	148	
6	SAA	104	
7	LB0	384	
8	SB0	237	
9	LBB	55	
10	SBB	94	
11	LC0	334	
12	SC0	237	
13	LCC	108	
14	SCC	67	
15	LD0	295	
16	SD0	215	
17	LDD	111	
18	SDD	68	
19	LE0	172	
20	SE0	262	
21	LEE	139	
22	SEE	60	
23	LF0	239	
24	SF0	189	
25	LFF	98	
26	SFF	151	
27	LG0	200	
28	SG0	217	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	LGG	106	
30	SGG	337	
31	LH0	186	
32	SH0	161	
33	LHH	122	
34	LI0	217	
35	SI0	166	
36	LII	95	
37	LJ0	171	
38	SJ0	189	
39	LJJ	93	
40	LL0	162	
41	SL0	158	
42	LLL	52	
43	LM0	105	
44	LMM	127	
45	SM0	131	
46	LN0	204	
47	SN0	149	
48	LNN	160	
49	SNN	168	
50	LO0	192	
51	SO0	135	
52	LOO	103	
53	LP0	169	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	SP0	143	
55	LPP	89	
56	LQ0	193	
57	SQ0	155	
58	LR0	175	
59	SR0	119	
60	LS0	180	
61	SS0	160	
62	LT0	160	
63	ST0	133	
64	LU0	107	
65	SU0	101	
66	LV0	146	
67	SV0	67	
68	LW0	91	
69	SW0	127	
70	LX0	102	
71	SX0	140	
72	LXX	73	
73	LY0	139	
74	SY0	133	
75	LZ0	126	
76	SZ0	123	
77	SK0	99	
78	L50	2484	

2 Entry composition

There are 80 unique types of molecules in this entry. The entry contains 164223 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 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S60	1231	Total	C	N	O	P	0	0
			26291	11769	4701	8590	1231		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L70	118	Total	C	N	O	P	0	0
			2523	1128	460	817	118		

- Molecule 3 is a protein called uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	LA0	232	Total	C	N	O	S	0	0
			1789	1124	336	321	8		

- Molecule 4 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SA0	197	Total	C	N	O	S	0	0
			1558	1002	262	285	9		

- Molecule 5 is a protein called uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	LAA	148	Total	C	N	O	S	0	0
			1219	778	240	196	5		

- Molecule 6 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SAA	97	Total	C	N	O	S	0	0
			776	481	157	130	8		

- Molecule 7 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LB0	368	Total	C	N	O	S	0	0
			2912	1851	537	515	9		

- Molecule 8 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SB0	210	Total	C	N	O	S	0	0
			1664	1050	297	306	11		

- Molecule 9 is a protein called eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LBB	51	Total	C	N	O	S	0	0
			416	262	84	68	2		

- Molecule 10 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SBB	82	Total	C	N	O	S	0	0
			637	404	107	118	8		

- Molecule 11 is a protein called uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LC0	329	Total	C	N	O	S	0	0
			2624	1656	482	474	12		

- Molecule 12 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SC0	217	Total	C	N	O	S	0	0
			1642	1042	287	308	5		

- Molecule 13 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LCC	104	Total	C	N	O	S	0	0
			797	510	137	146	4		

- Molecule 14 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	SCC	63	Total	C	N	O	S	0	0
			495	305	97	90	3		

- Molecule 15 is a protein called uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LD0	282	Total	C	N	O	S	0	0
			2320	1466	422	425	7		

- Molecule 16 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SD0	210	Total	C	N	O	S	0	0
			1624	1052	279	286	7		

- Molecule 17 is a protein called eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LDD	102	Total	C	N	O	S	0	0
			821	526	150	140	5		

- Molecule 18 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SDD	67	Total	C	N	O	S	0	0
			541	343	96	97	5		

- Molecule 19 is a protein called eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LE0	172	Total	C	N	O	S	0	0
			1410	899	229	274	8		

- Molecule 20 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	SE0	256	Total	C	N	O	S	0	0
			2056	1320	343	386	7		

- Molecule 21 is a protein called eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LEE	123	Total	C	N	O	S	0	0
			1010	643	200	164	3		

- Molecule 22 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	SEE	56	Total	C	N	O	S	0	0
			454	281	92	77	4		

- Molecule 23 is a protein called uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LF0	230	Total	C	N	O	S	0	0
			1884	1209	327	342	6		

- Molecule 24 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	SF0	188	Total	C	N	O	S	0	0
			1457	897	277	277	6		

- Molecule 25 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LFF	96	Total	C	N	O	S	0	0
			771	486	154	129	2		

- Molecule 26 is a protein called eS31.

Mol	Chain	Residues	Atoms			AltConf	Trace
26	SFF	68	Total	C	N	0	0
			266	198	68		

- Molecule 27 is a protein called eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LG0	195	Total	C	N	O	S	0	0
			1573	1010	272	283	8		

- Molecule 28 is a protein called eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	SG0	201	Total	C	N	O	S	0	0
			1587	990	305	286	6		

- Molecule 29 is a protein called eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LGG	100	Total	C	N	O	S	0	0
			814	506	170	133	5		

- Molecule 30 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	SGG	330	Total	C	N	O	S	0	0
			2499	1575	414	497	13		

- Molecule 31 is a protein called uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LH0	184	Total	C	N	O	S	0	0
			1452	930	253	258	11		

- Molecule 32 is a protein called eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	SH0	155	Total	C	N	O	S	0	0
			1265	812	208	239	6		

- Molecule 33 is a protein called uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LHH	120	Total	C	N	O	S	0	0
			1017	640	194	179	4		

- Molecule 34 is a protein called uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LI0	216	Total	C	N	O	S	0	0
			1743	1102	332	298	11		

- Molecule 35 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	SI0	158	Total	C	N	O	S	0	0
			1259	784	238	234	3		

- Molecule 36 is a protein called eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	LII	93	Total	C	N	O	S	0	0
			765	489	148	126	2		

- Molecule 37 is a protein called uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	LJ0	168	Total	C	N	O	S	0	0
			1348	854	246	241	7		

- Molecule 38 is a protein called uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	SJ0	171	Total	C	N	O	S	0	0
			1382	877	245	258	2		

- Molecule 39 is a protein called eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LJJ	90	Total	C	N	O	S	0	0
			719	450	152	110	7		

- Molecule 40 is a protein called eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LL0	162	Total	C	N	O	S	0	0
			1328	831	265	225	7		

- Molecule 41 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	SL0	157	Total	C	N	O	S	0	0
			1269	805	227	231	6		

- Molecule 42 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LLL	51	Total	C	N	O	S	0	0
			445	283	93	68	1		

- Molecule 43 is a protein called eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	LM0	91	Total	C	N	O	S	0	0
			731	471	122	137	1		

- Molecule 44 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	LMM	50	Total	C	N	O	S	0	0
			402	241	87	70	4		

- Molecule 45 is a protein called eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	SM0	119	Total	C	N	O	S	0	0
			929	582	168	174	5		

- Molecule 46 is a protein called eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	LN0	203	Total	C	N	O	S	0	0
			1677	1046	342	280	9		

- Molecule 47 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SN0	147	Total	C	N	O	S	0	0
			1177	748	212	211	6		

- Molecule 48 is a protein called MDF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	LNN	80	Total	C	N	O		0	0
			577	345	125	107			

- Molecule 49 is a protein called MDF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SNN	167	Total	C	N	O	S	0	0
			1336	844	221	261	10		

- Molecule 50 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	LO0	173	Total	C	N	O	S	0	0
			1371	885	249	226	11		

- Molecule 51 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SO0	131	Total	C	N	O	S	0	0
			977	602	191	177	7		

- Molecule 52 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	LOO	98	Total	C	N	O	S	0	0
			792	497	162	126	7		

- Molecule 53 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	LP0	154	Total	C	N	O	S	0	0
			1235	778	242	210	5		

- Molecule 54 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SP0	118	Total	C	N	O	S	0	0
			942	601	174	160	7		

- Molecule 55 is a protein called eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	LPP	83	Total	C	N	O	S	0	0
			642	403	122	111	6		

- Molecule 56 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	LQ0	184	Total	C	N	O	S	0	0
			1460	920	273	260	7		

- Molecule 57 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SQ0	152	Total	C	N	O	S	0	0
			1205	773	208	215	9		

- Molecule 58 is a protein called eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	LR0	165	Total	C	N	O	S	0	0
			1342	840	263	232	7		

- Molecule 59 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SR0	117	Total	C	N	O	S	0	0
			958	604	173	176	5		

- Molecule 60 is a protein called eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	LS0	179	Total	C	N	O	S	0	0
			1472	952	251	265	4		

- Molecule 61 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SS0	151	Total	C	N	O	S	0	0
			1186	731	237	209	9		

- Molecule 62 is a protein called eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	LT0	159	Total	C	N	O	S	0	0
			1310	844	242	223	1		

- Molecule 63 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	ST0	131	Total	C	N	O	S	0	0
			1048	663	173	204	8		

- Molecule 64 is a protein called eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	LU0	97	Total	C	N	O	S	0	0
			790	502	138	148	2		

- Molecule 65 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SU0	96	Total	C	N	O	S	0	0
			764	495	126	141	2		

- Molecule 66 is a protein called uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	LV0	135	Total	C	N	O	S	0	0
			1040	650	203	180	7		

- Molecule 67 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SV0	63	Total	C	N	O	S	0	0
			491	304	88	97	2		

- Molecule 68 is a protein called eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	LW0	90	Total	C	N	O	S	0	0
			667	415	131	120	1		

- Molecule 69 is a protein called uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SW0	127	Total	C	N	O	S	0	0
			1018	645	188	179	6		

- Molecule 70 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	LX0	93	Total	C	N	O	S	0	0
			734	466	137	127	4		

- Molecule 71 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	SX0	138	Total	C	N	O	S	0	0
			1069	687	193	187	2		

- Molecule 72 is a protein called msL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	LXX	55	Total	C	N	O	S	0	0
			462	297	84	80	1		

- Molecule 73 is a protein called uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	LY0	134	Total	C	N	O	S	0	0
			1088	682	203	198	5		

- Molecule 74 is a protein called eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	SY0	125	Total	C	N	O	S	0	0
			1025	637	198	186	4		

- Molecule 75 is a protein called eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	LZ0	125	Total	C	N	O	S	0	0
			1006	647	178	176	5		

- Molecule 76 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	SZ0	91	Total	C	N	O	S	0	0
			724	462	128	131	3		

- Molecule 77 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	SK0	85	Total	C	N	O	S	0	0
			712	456	118	135	3		

- Molecule 78 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	L50	2313	Total	C	N	O	P	0	0
			49259	22082	8715	16149	2313		

- Molecule 79 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
79	S60	49	Total	Mg	0
			49	49	
79	L70	1	Total	Mg	0
			1	1	
79	LJJ	1	Total	Mg	0
			1	1	
79	LV0	1	Total	Mg	0
			1	1	
79	L50	122	Total	Mg	0
			122	122	

- Molecule 80 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
80	SAA	1	Total	Zn	0
			1	1	
80	SBB	1	Total	Zn	0
			1	1	
80	SDD	1	Total	Zn	0
			1	1	
80	LGG	1	Total	Zn	0
			1	1	
80	LJJ	1	Total	Zn	0
			1	1	
80	LMM	1	Total	Zn	0
			1	1	
80	SNN	1	Total	Zn	0
			1	1	
80	LOO	1	Total	Zn	0
			1	1	

Continued on next page...

Continued from previous page...

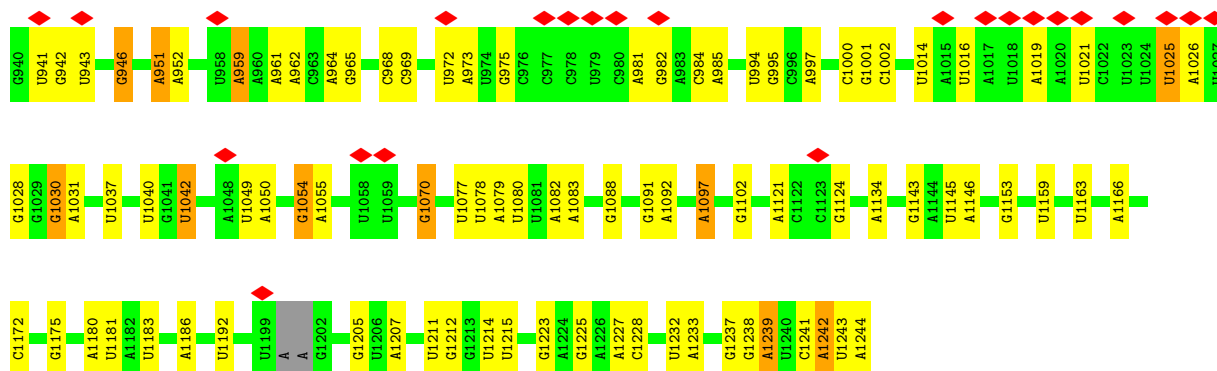
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
80	LPP	1	1	1	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 16S rRNA





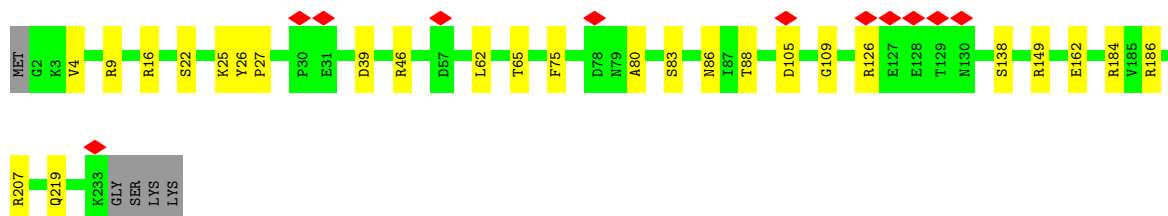
• Molecule 2: 5S rRNA

Chain L70: 75% 22%



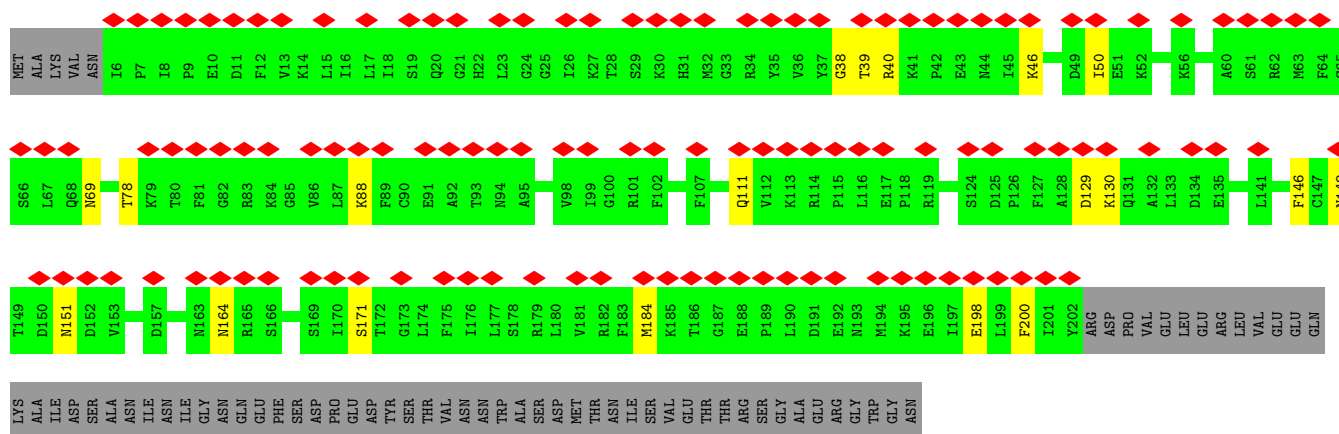
• Molecule 3: uL2

Chain LA0: 5% 87% 11%



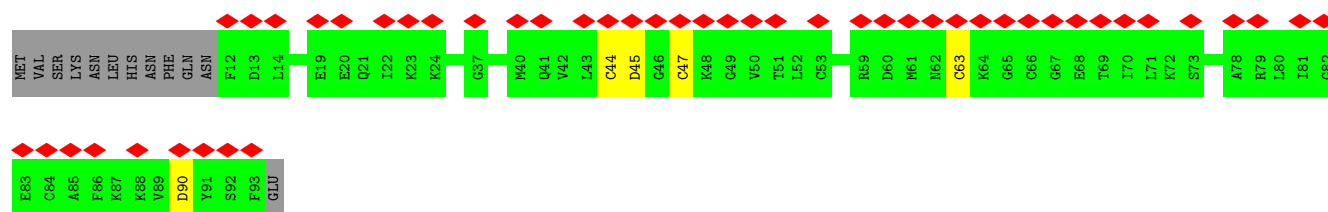
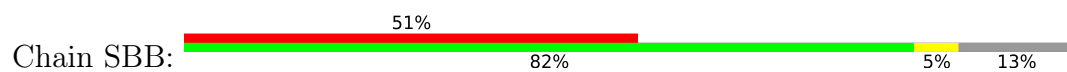
• Molecule 4: uS2

Chain SA0: 46% 67% 7% 25%

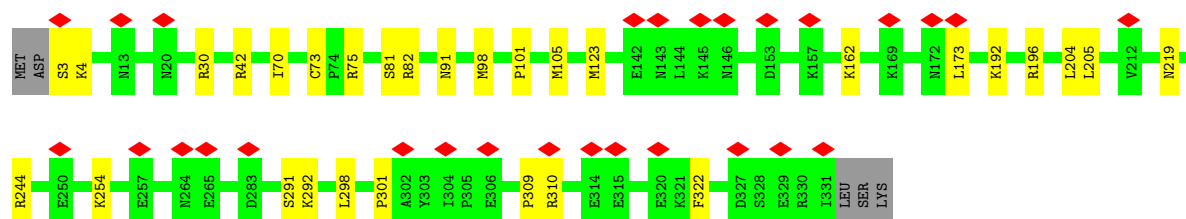
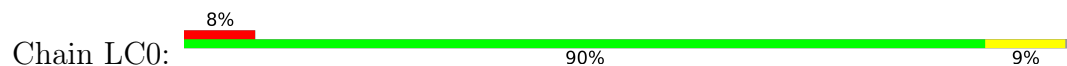


• Molecule 5: uL15

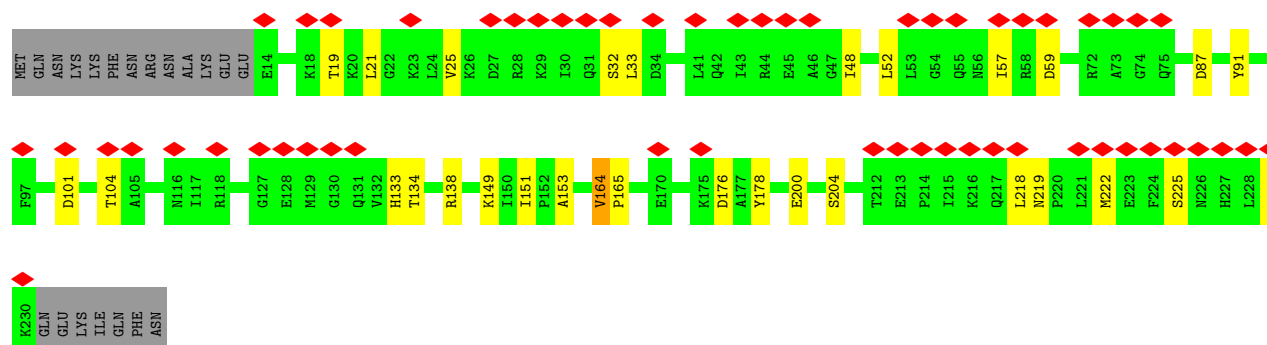
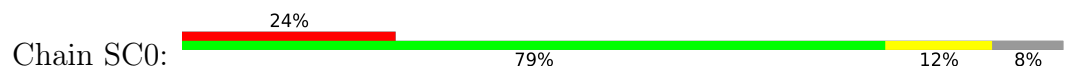
Chain LAA: 95% 5%



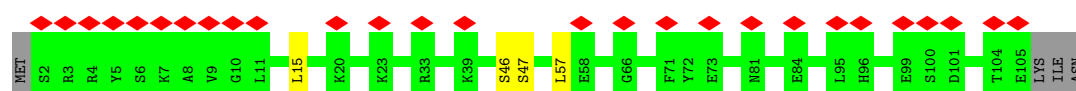
• Molecule 11: uL4



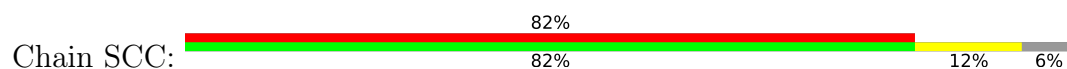
• Molecule 12: uS5



• Molecule 13: eL30

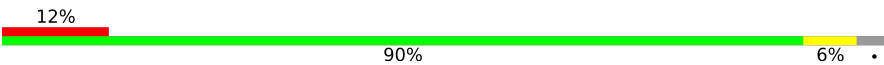


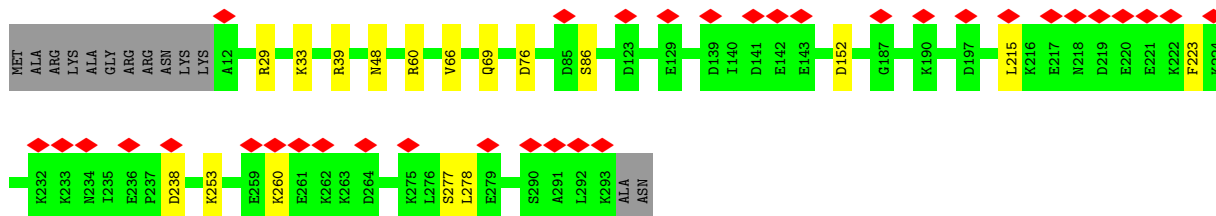
• Molecule 14: eS28



ARG
SER
ARG

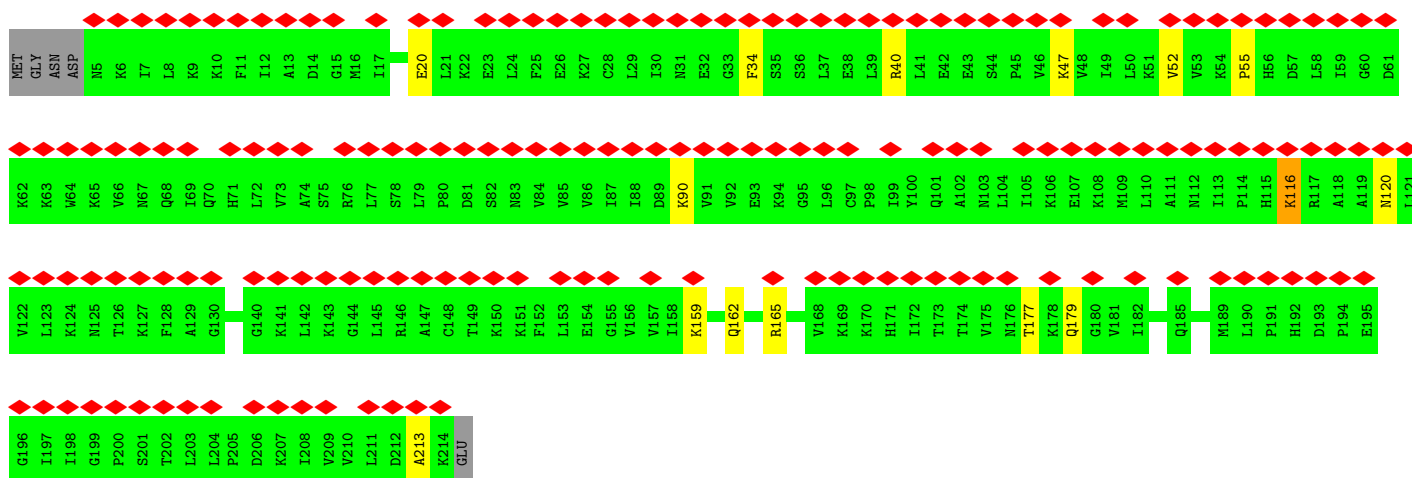
• Molecule 15: uL18

Chain LD0:  12% 90% 6%



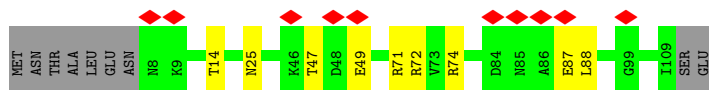
• Molecule 16: uS3

Chain SD0:  79% 91% 7%

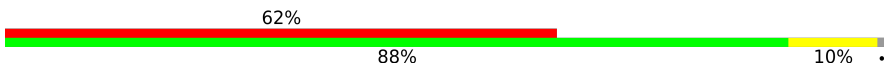


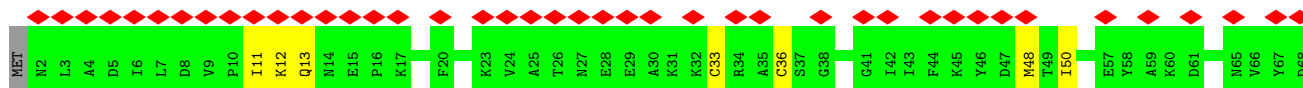
• Molecule 17: eL31

Chain LDD:  9% 84% 8% 8%

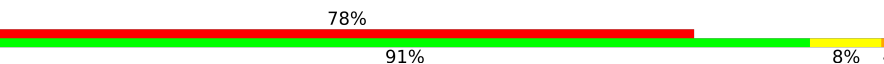


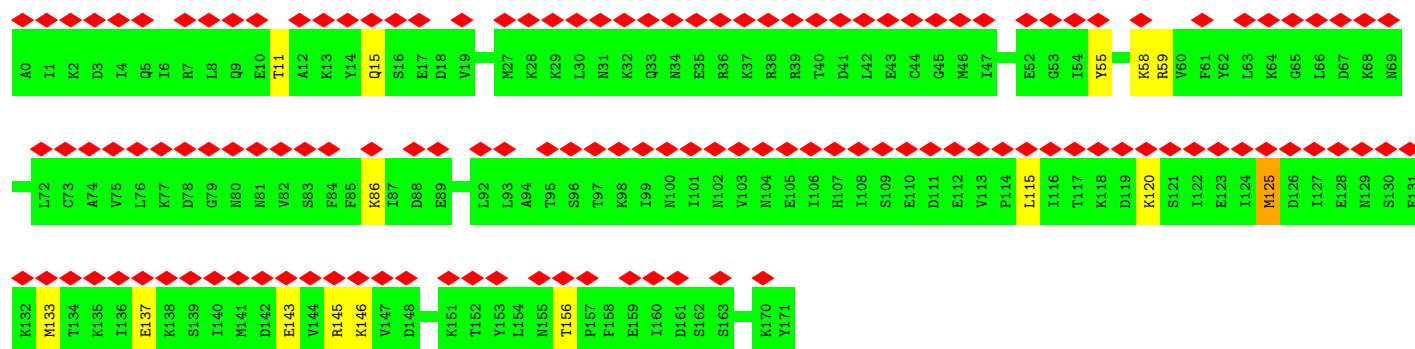
• Molecule 18: uS14

Chain SDD:  62% 88% 10%

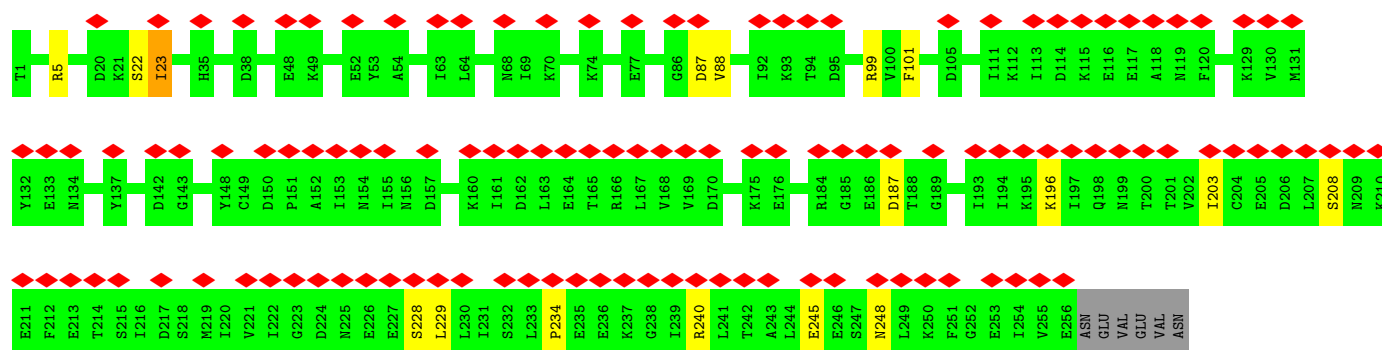


• Molecule 19: eL6

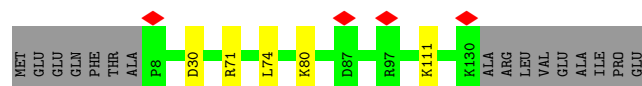
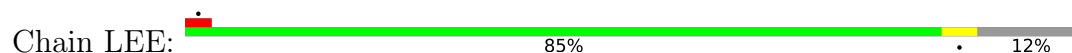
Chain LE0:  78% 91% 8%



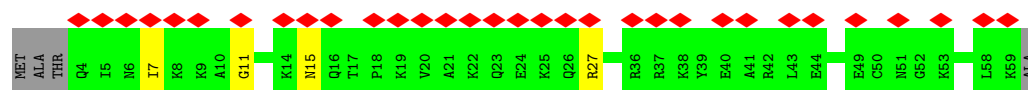
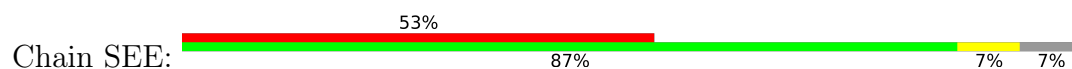
• Molecule 20: eS4



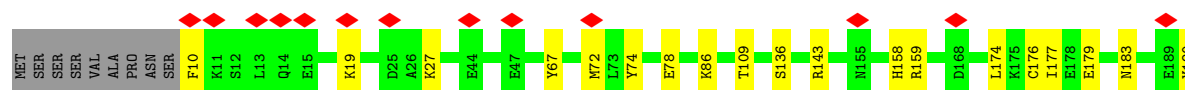
• Molecule 21: eL32



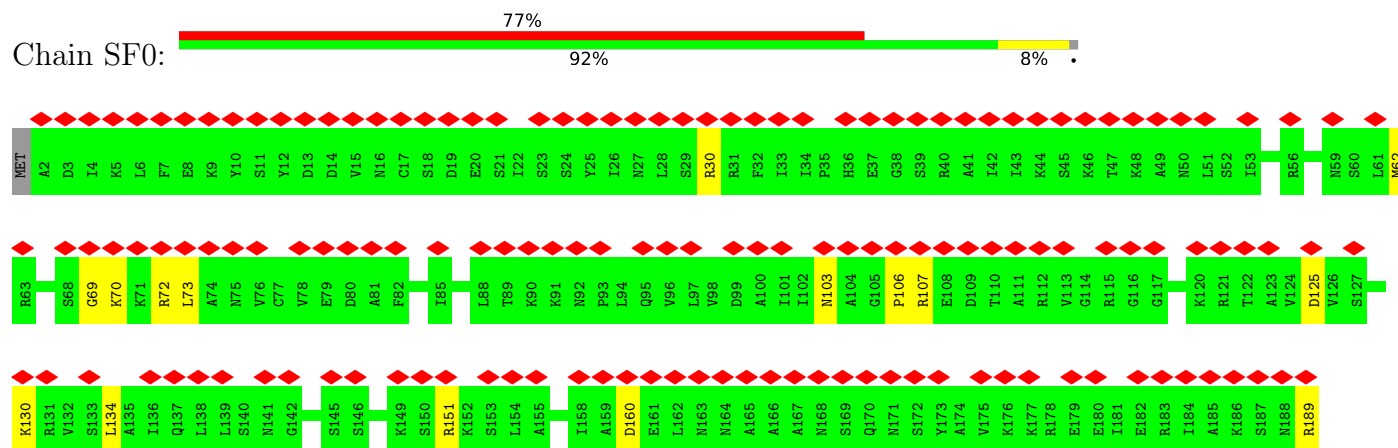
• Molecule 22: eS30



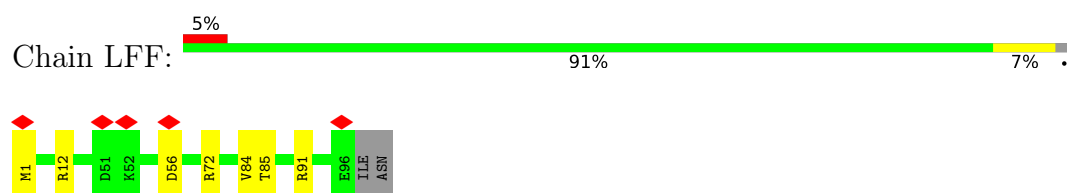
• Molecule 23: uL30



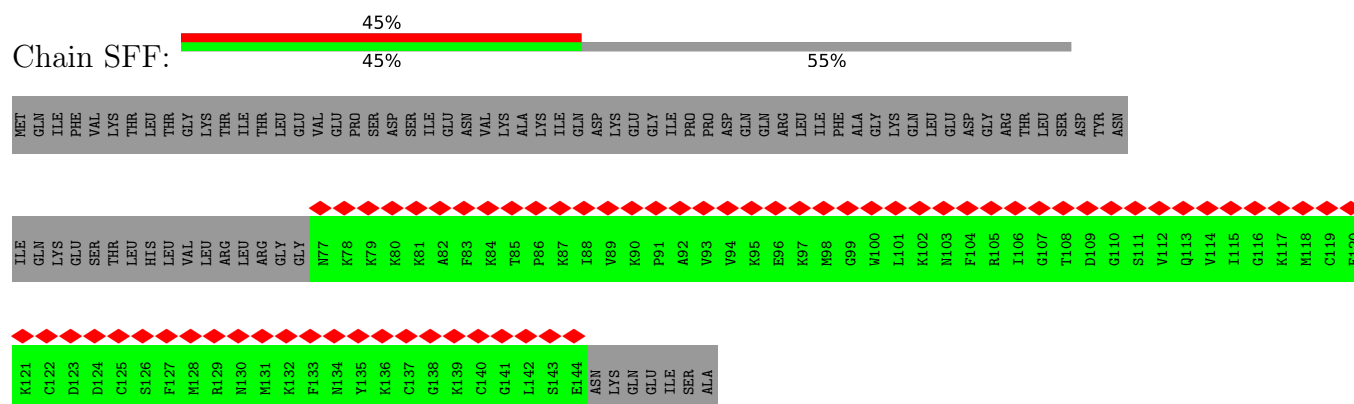
- Molecule 24: uS7



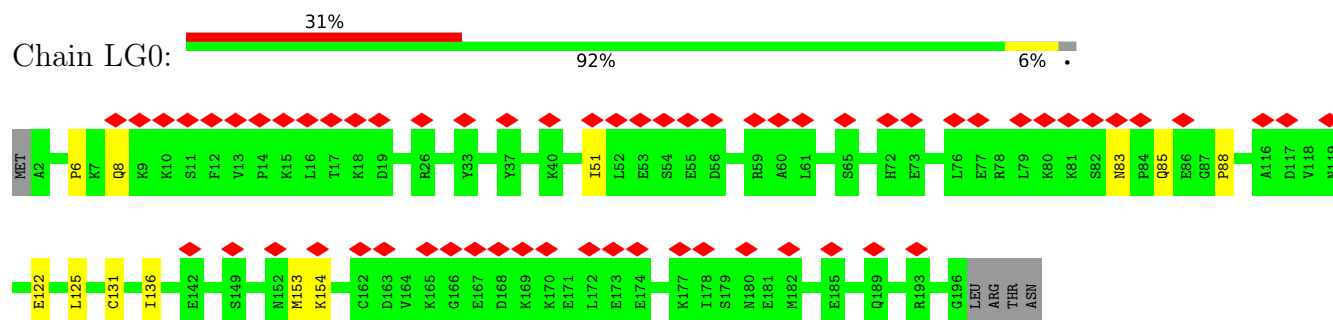
- Molecule 25: eL33



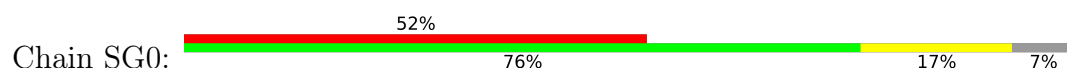
- Molecule 26: eS31

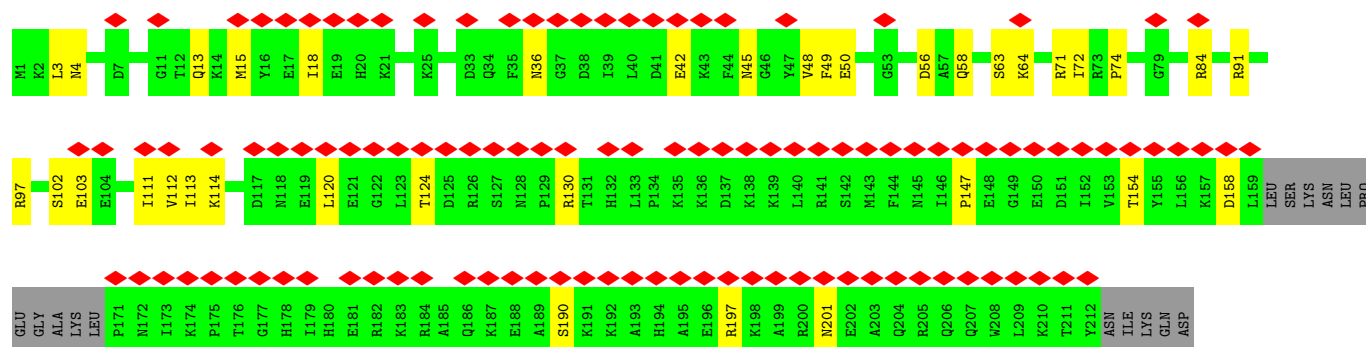


- Molecule 27: eL8

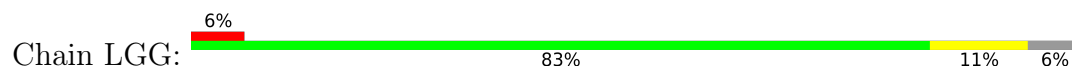


- Molecule 28: eS6

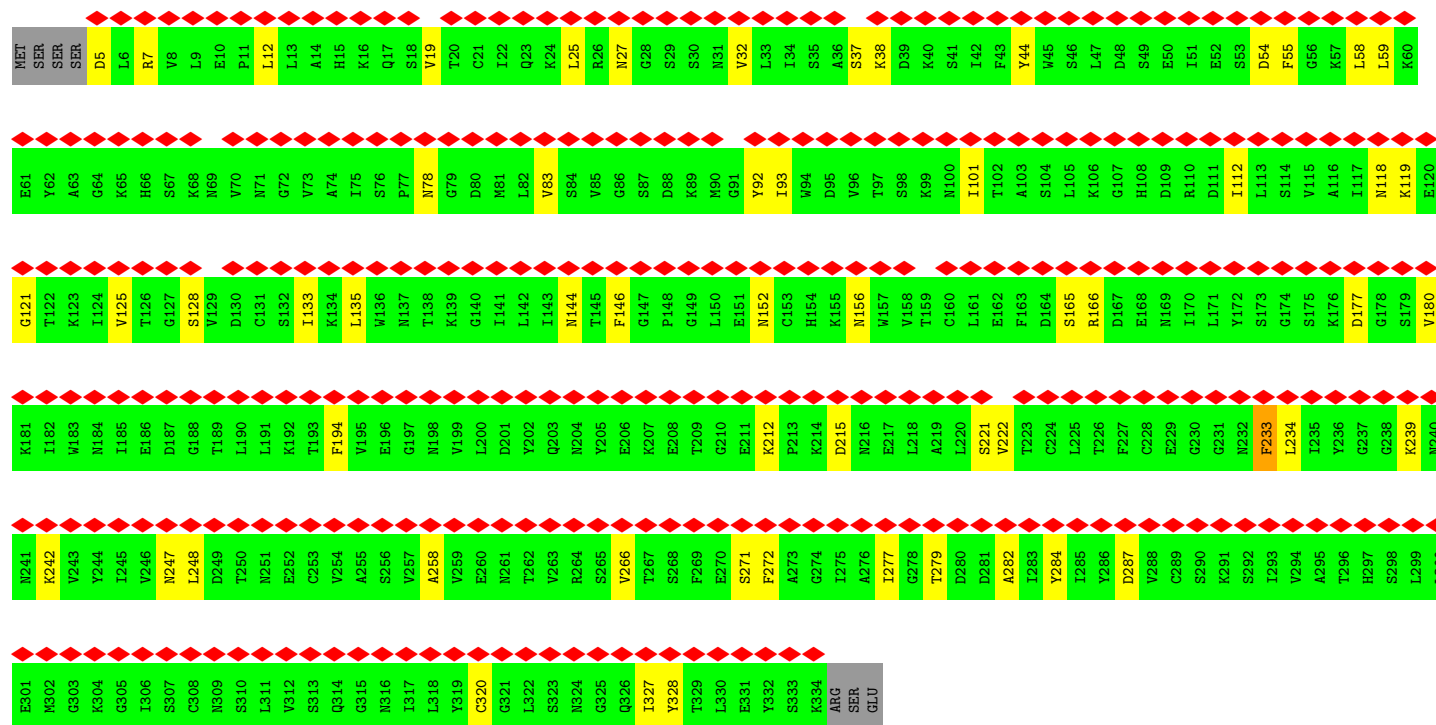
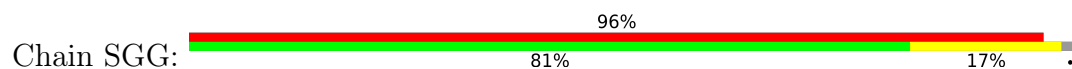




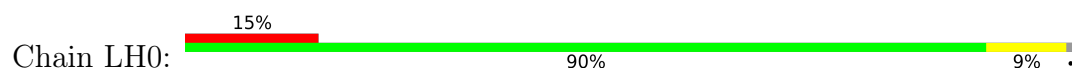
• Molecule 29: eL34



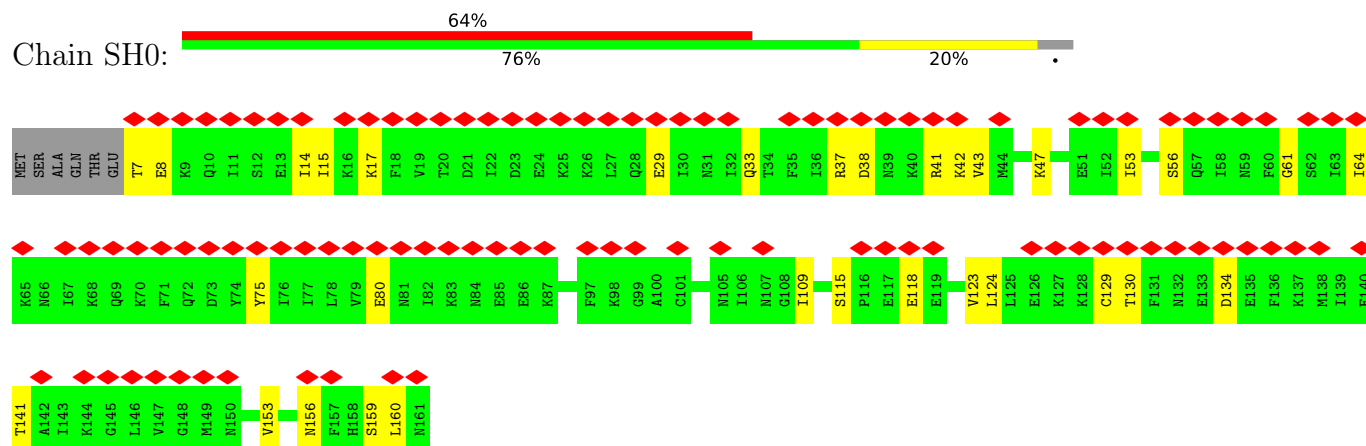
• Molecule 30: RACK1



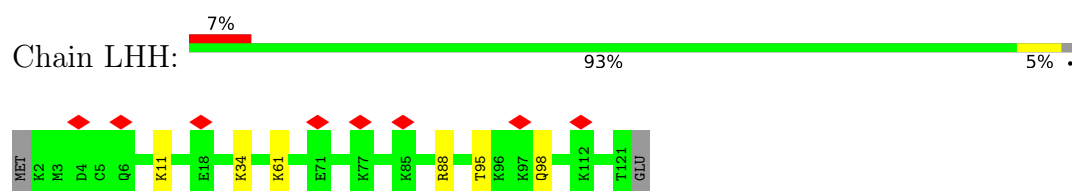
• Molecule 31: uL6



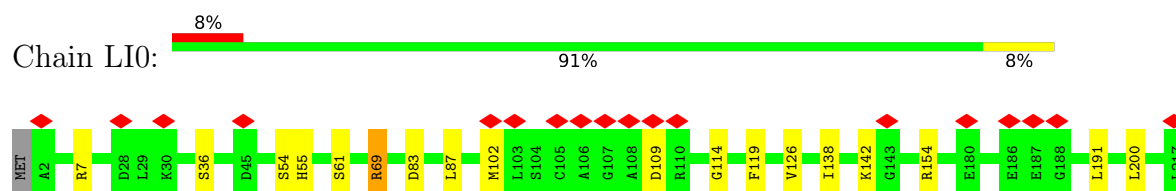
- Molecule 32: eS7



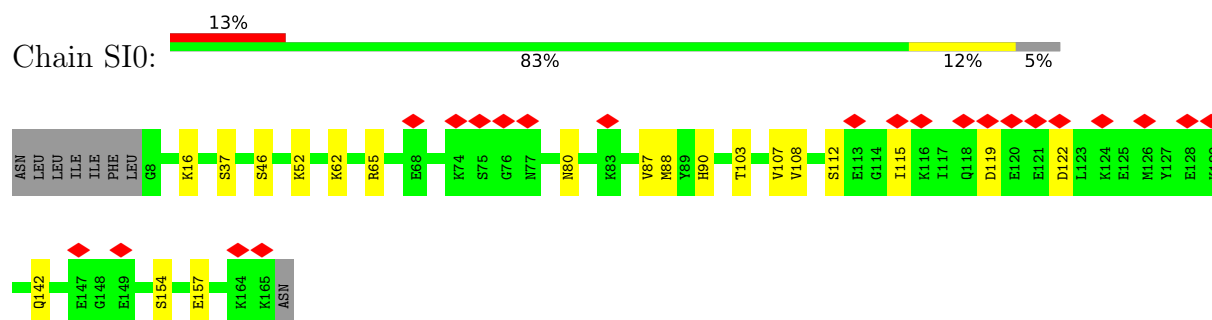
- Molecule 33: uL29



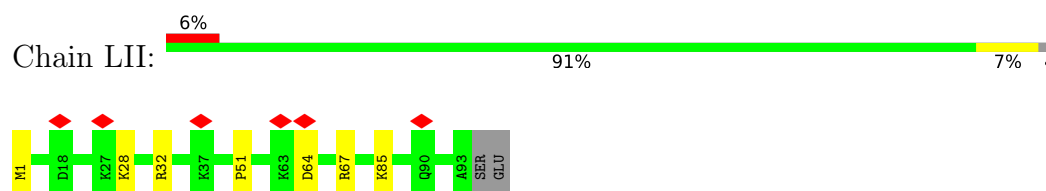
- Molecule 34: uL16



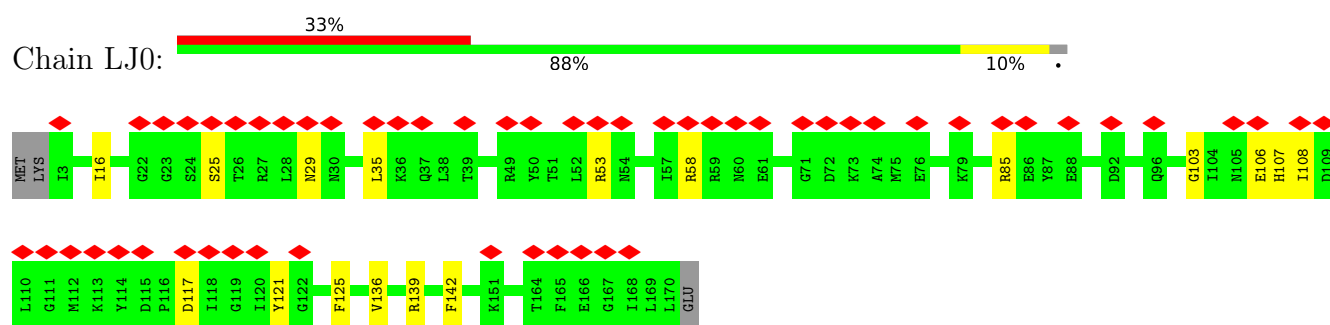
- Molecule 35: eS8



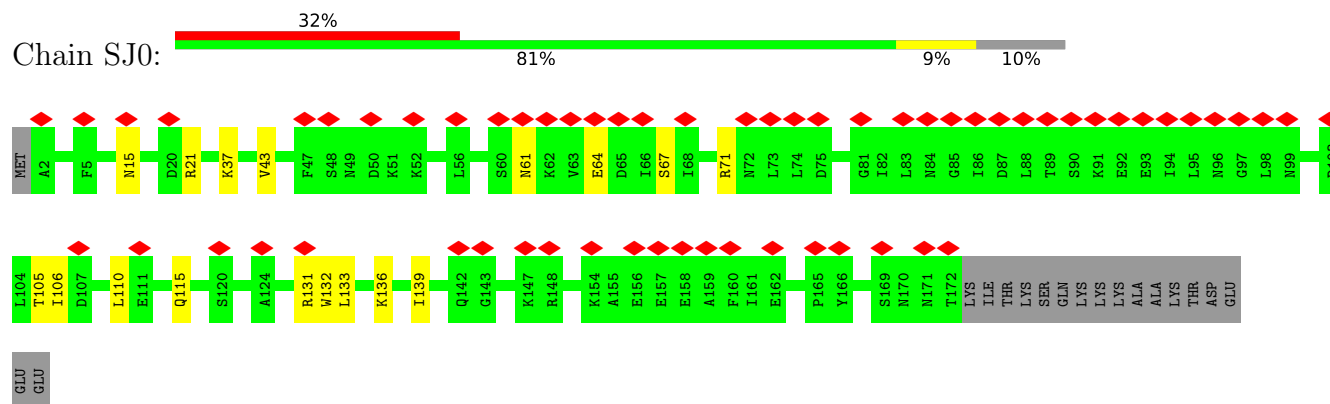
- Molecule 36: eL36



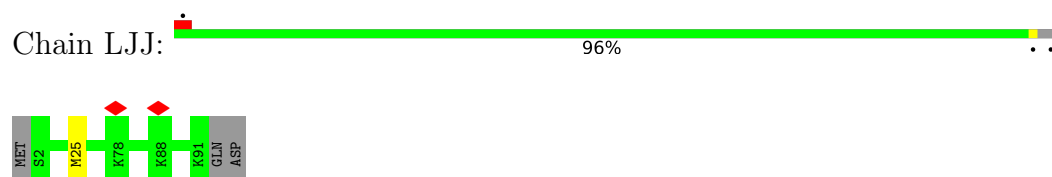
- Molecule 37: uL5



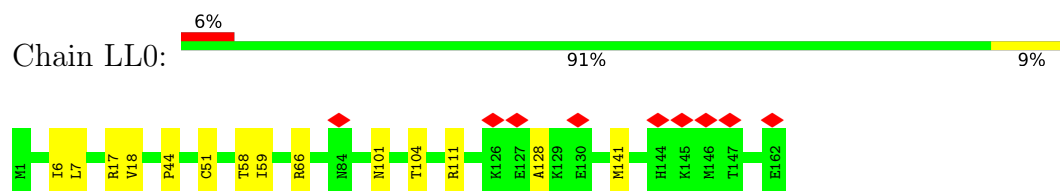
- Molecule 38: uS4



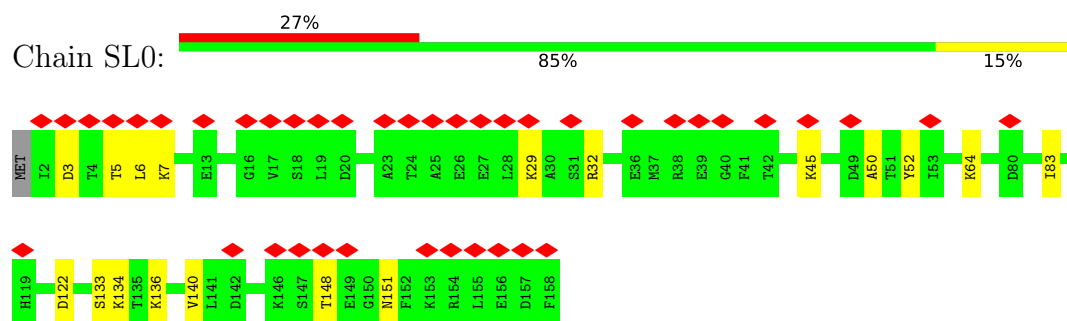
- Molecule 39: eL37



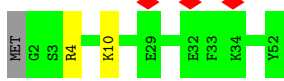
- Molecule 40: eL13



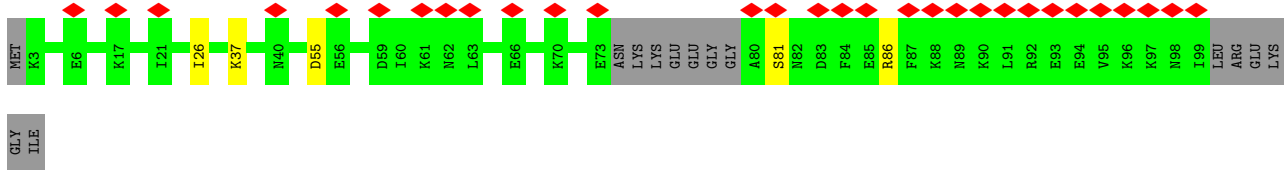
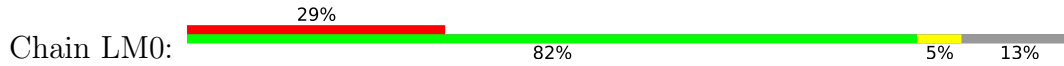
- Molecule 41: uS17



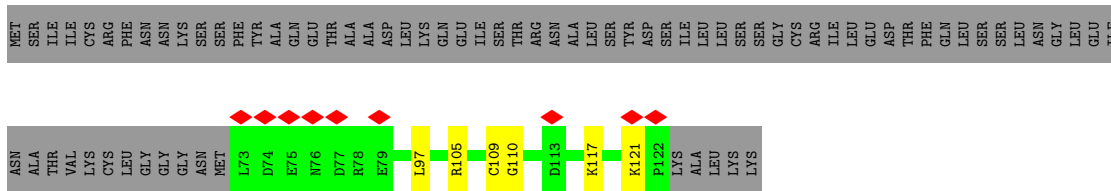
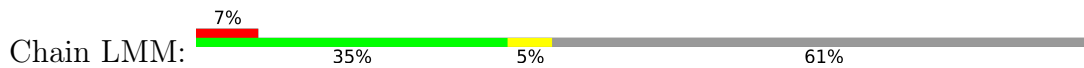
- Molecule 42: eL39



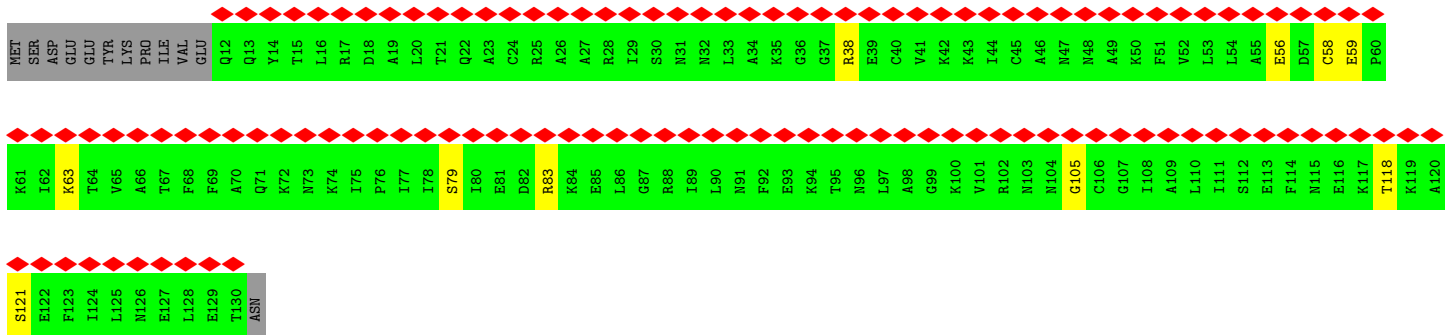
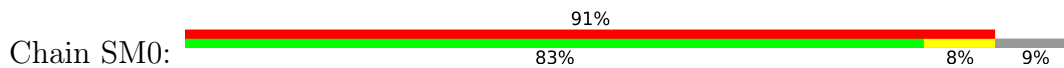
• Molecule 43: eL14



• Molecule 44: eL40



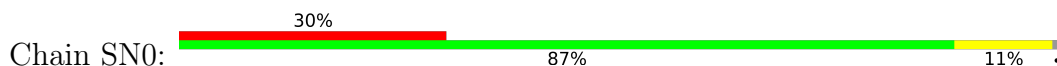
• Molecule 45: eS12

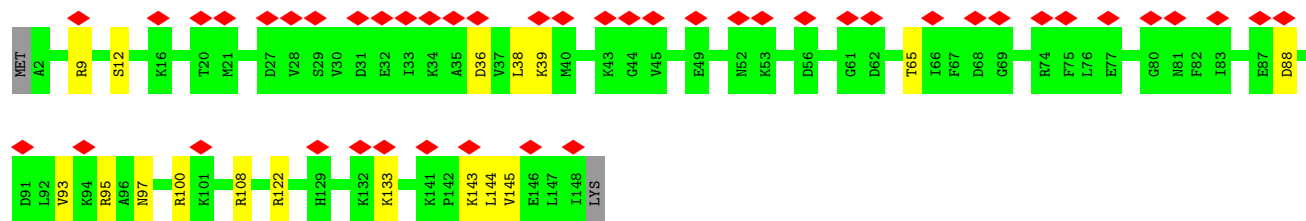


• Molecule 46: eL15

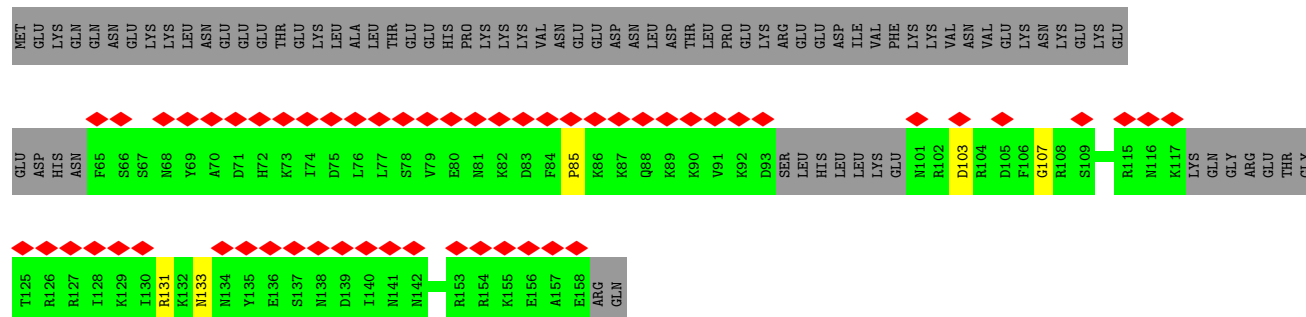


• Molecule 47: uS15

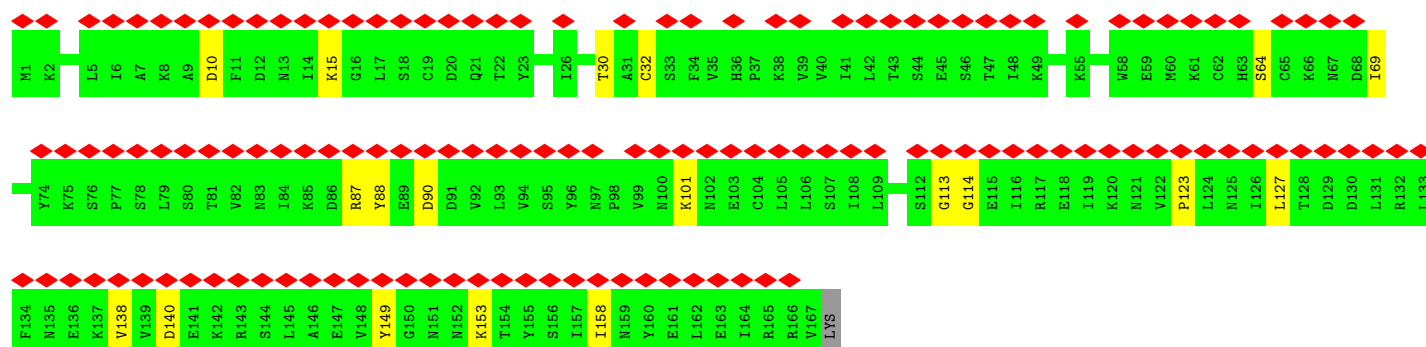
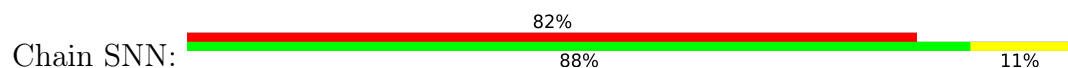




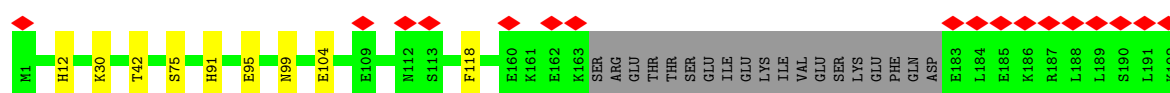
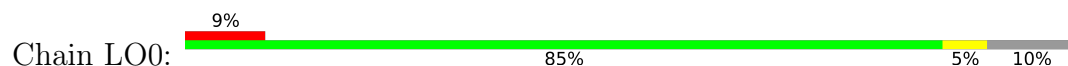
• Molecule 48: MDF2



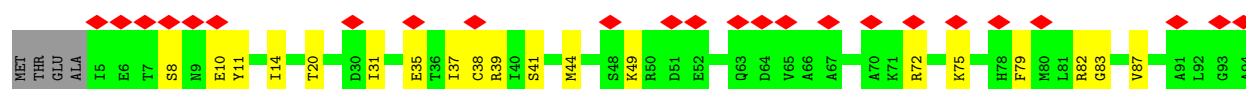
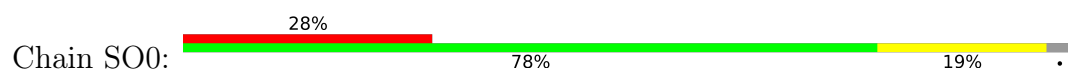
• Molecule 49: MDF1



• Molecule 50: uL13

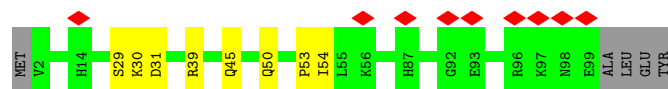


• Molecule 51: uS11





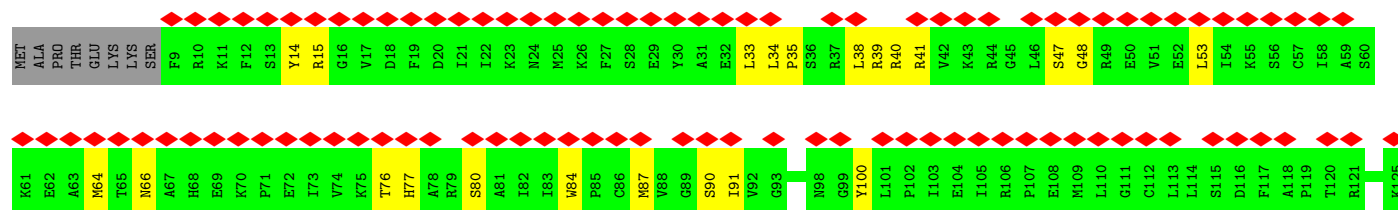
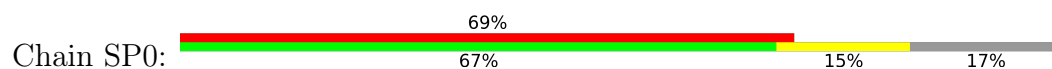
- Molecule 52: eL42



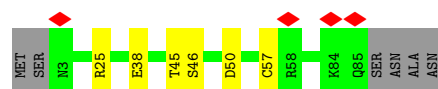
- Molecule 53: uL22



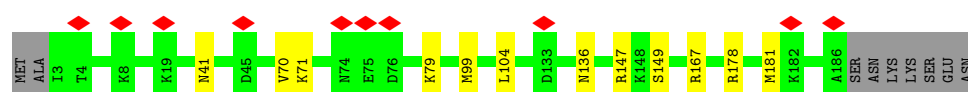
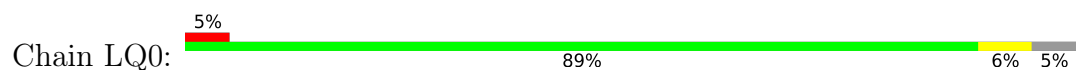
- Molecule 54: uS19



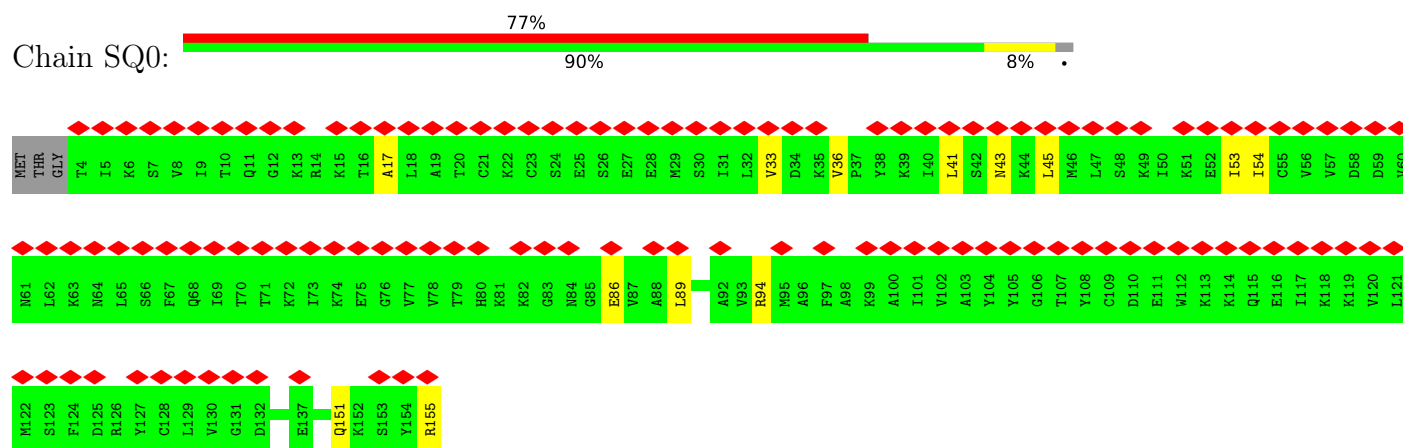
- Molecule 55: eL43



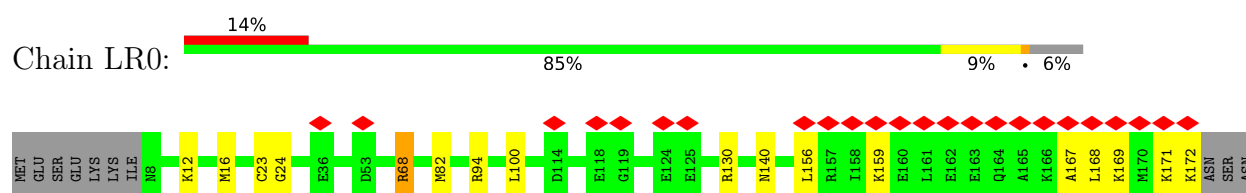
- Molecule 56: eL18



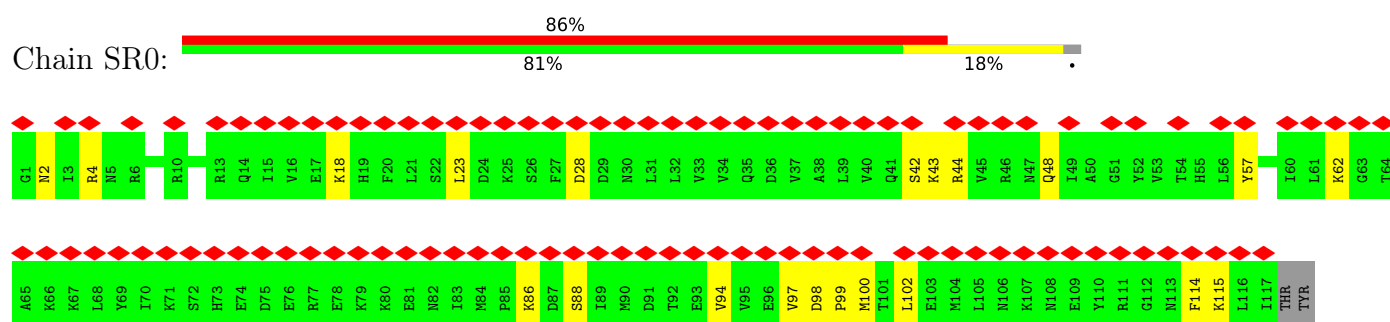
- Molecule 57: uS9



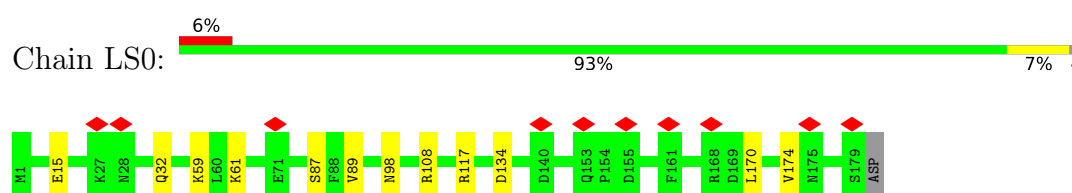
• Molecule 58: eL19



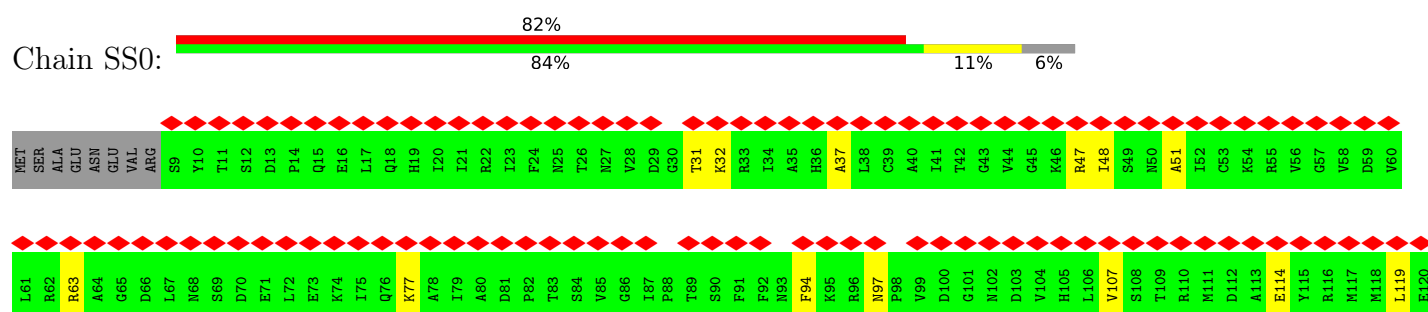
• Molecule 59: eS17

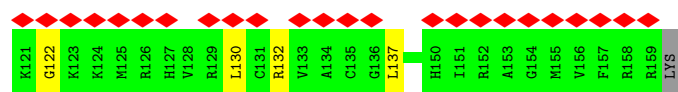


• Molecule 60: eL20

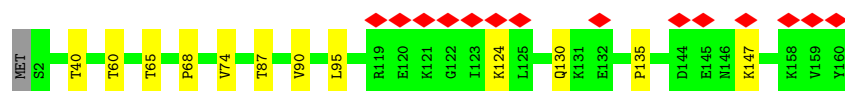


• Molecule 61: uS13

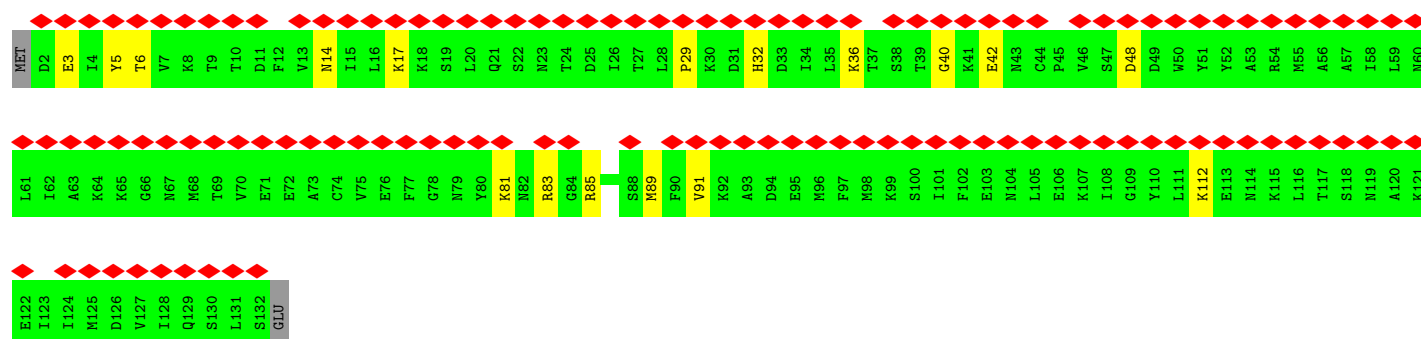




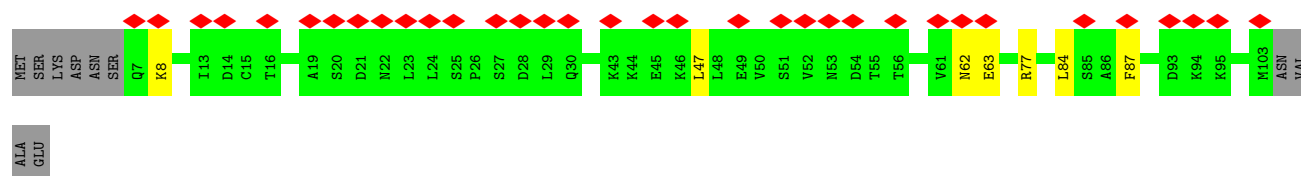
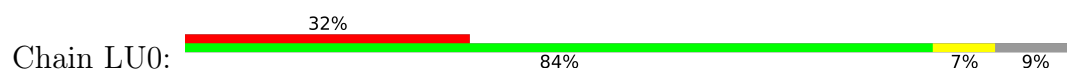
- Molecule 62: eL21



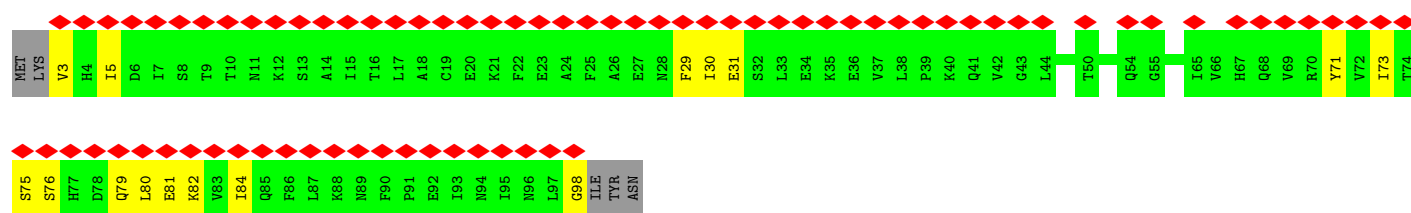
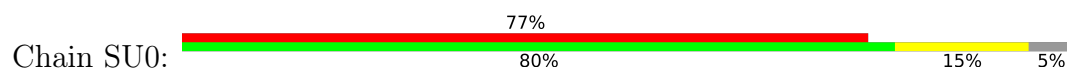
- Molecule 63: eS19



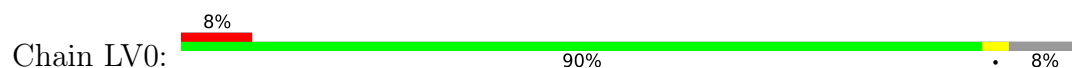
- Molecule 64: eL22

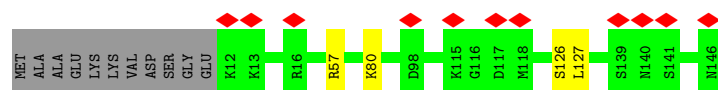


- Molecule 65: uS10

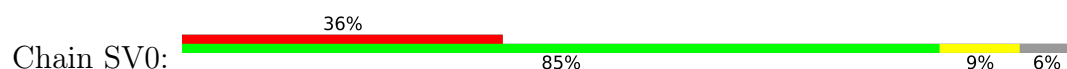


- Molecule 66: uL14

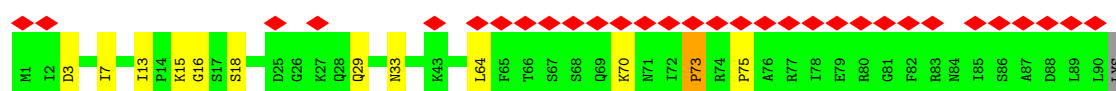
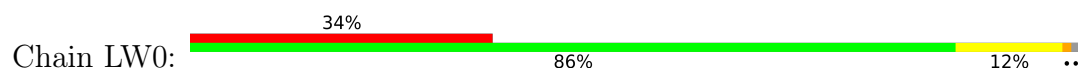




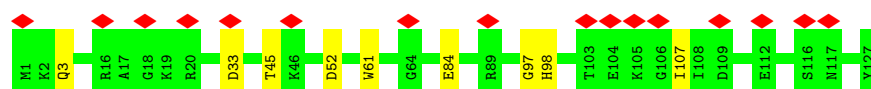
• Molecule 67: eS21



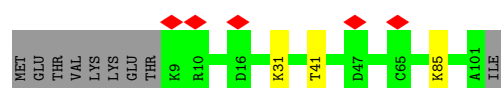
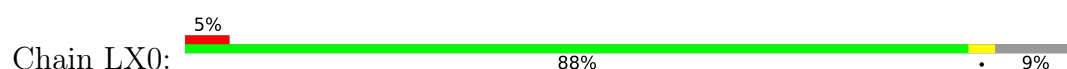
• Molecule 68: eL24



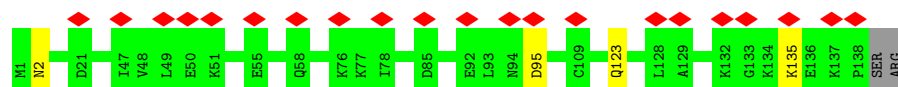
• Molecule 69: uS8



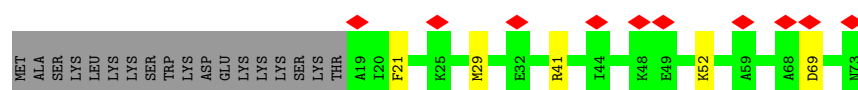
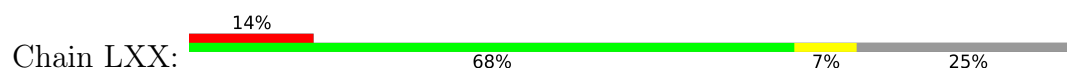
• Molecule 70: uL23



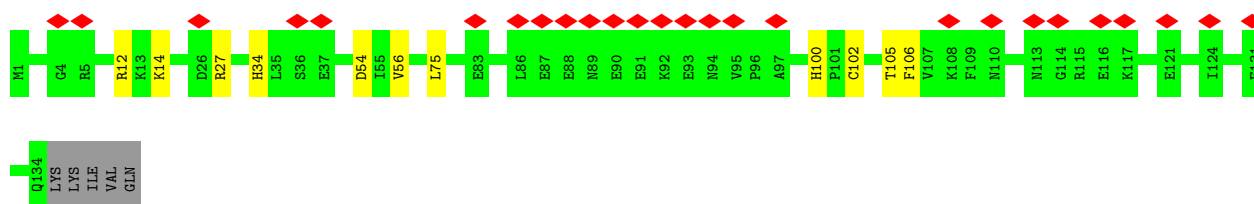
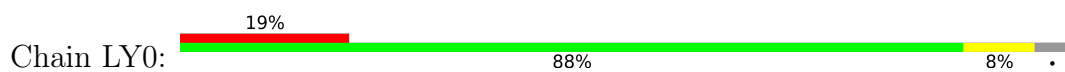
• Molecule 71: uS12



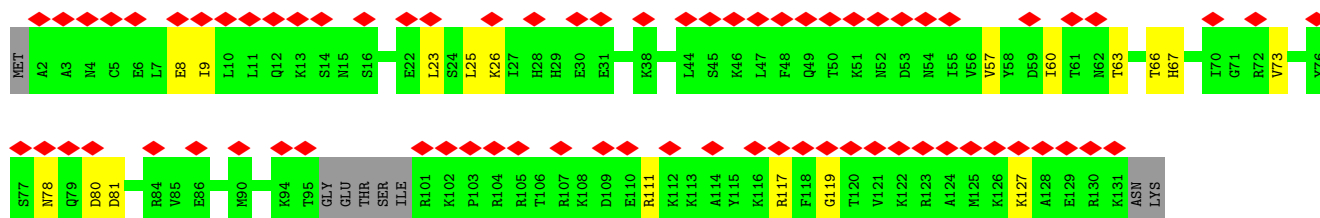
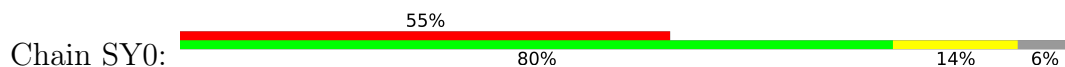
• Molecule 72: msL1



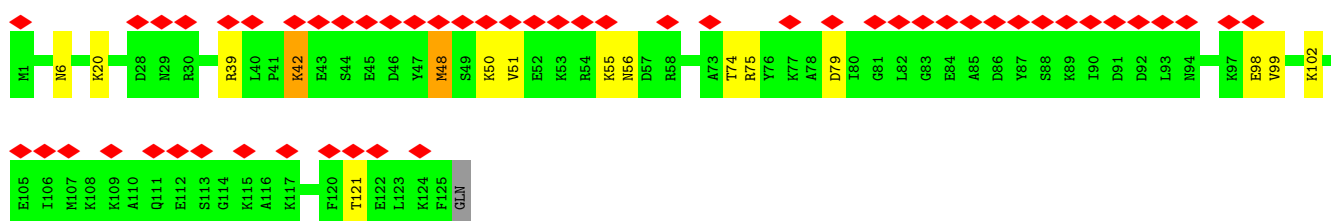
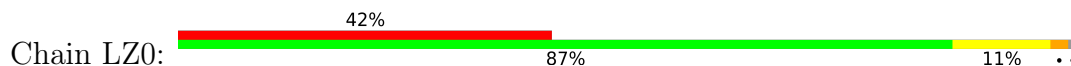
• Molecule 73: uL24



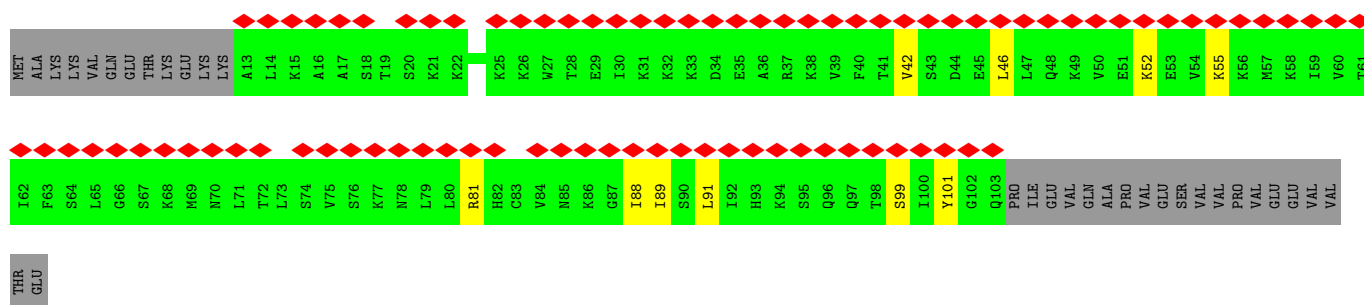
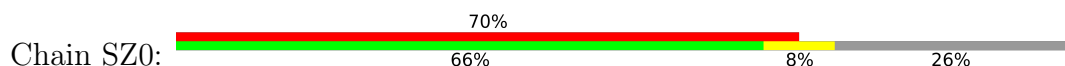
• Molecule 74: eS24



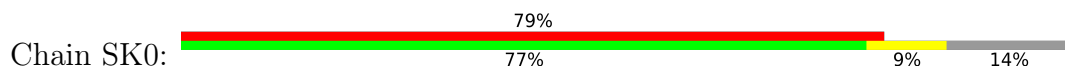
• Molecule 75: eL27



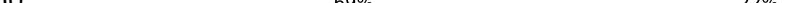
• Molecule 76: eS25

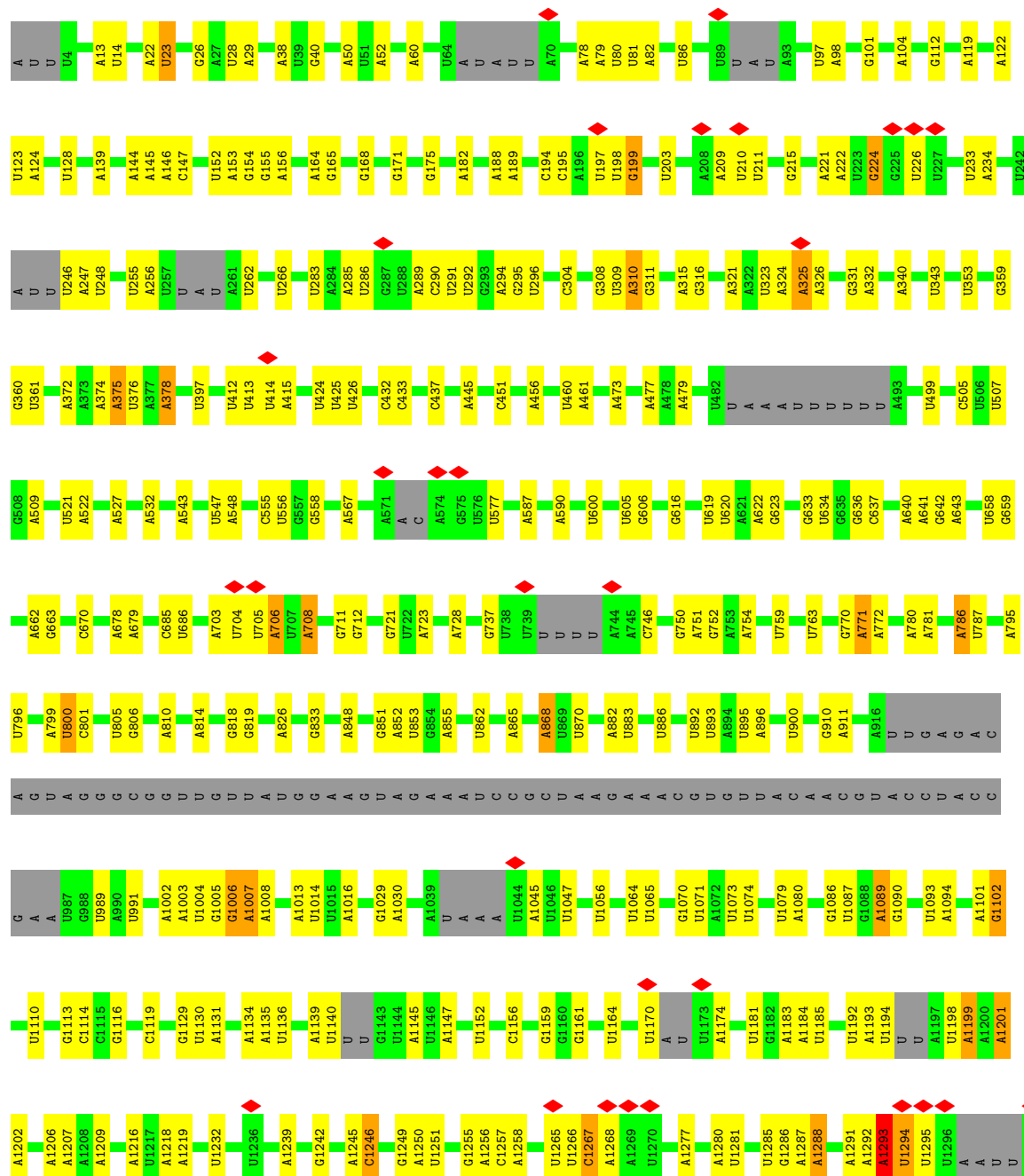


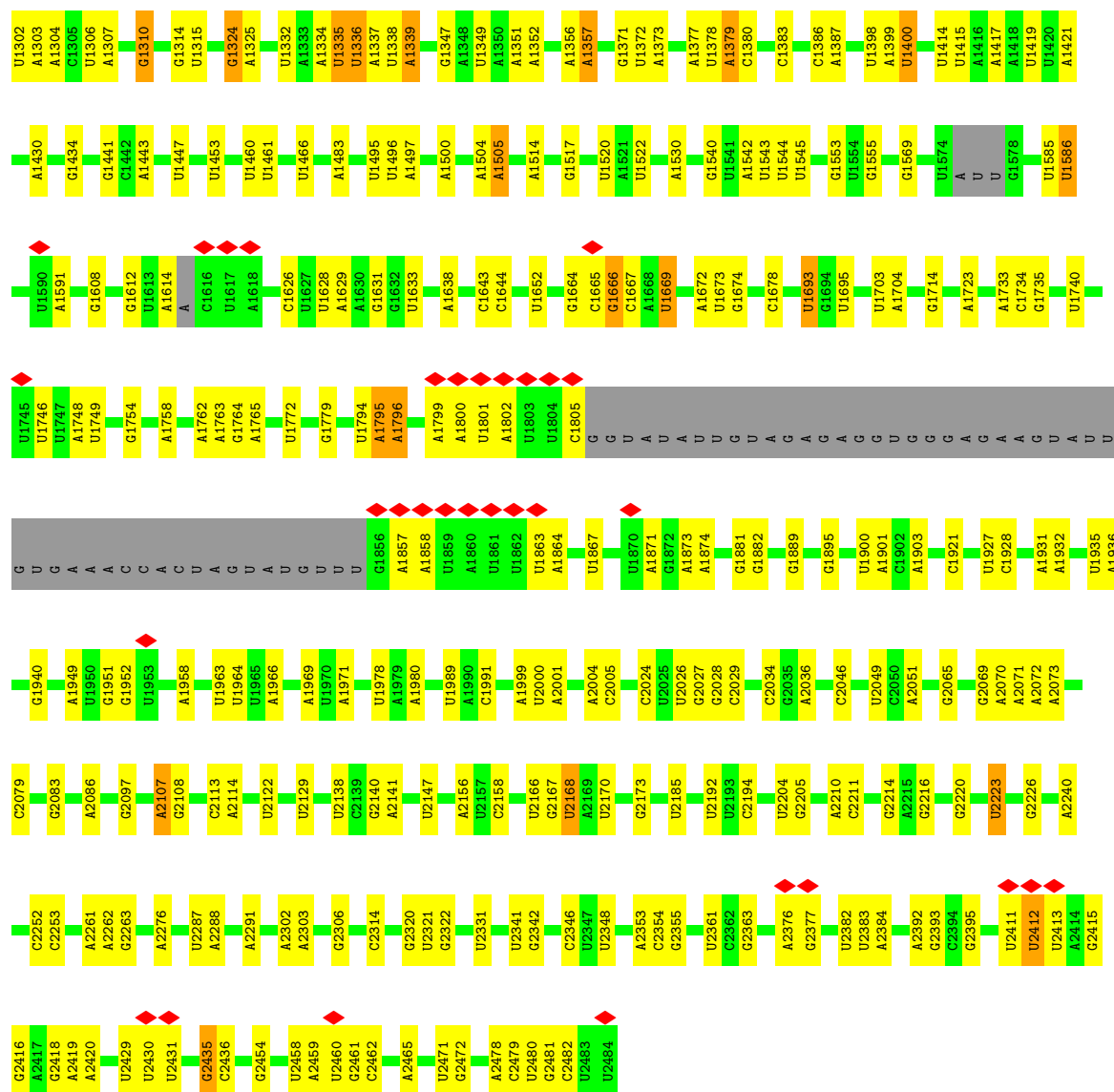
• Molecule 77: eS10



- Molecule 78: 23S rRNA

Chain L50:  69% 22% 7%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	185445	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	5.55	Depositor
Minimum defocus (nm)	4000	Depositor
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.126	Depositor
Minimum map value	-0.072	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0199	Depositor
Map size ($\text{\AA}$)	408.00003, 408.00003, 408.00003	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.2, 1.2, 1.2	Depositor

5 Model quality

5.1 Standard geometry

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

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	S60	0.25	0/29436	0.42	2/45858 (0.0%)
2	L70	0.29	0/2824	0.45	0/4400
3	LA0	0.30	0/1828	0.61	0/2465
4	SA0	0.24	0/1590	0.53	0/2152
5	LAA	0.28	0/1253	0.55	0/1676
6	SAA	0.25	0/788	0.56	0/1049
7	LB0	0.28	0/2966	0.51	0/3977
8	SB0	0.20	0/1687	0.49	0/2259
9	LBB	0.29	0/420	0.59	0/552
10	SBB	0.20	0/649	0.48	0/868
11	LC0	0.27	0/2669	0.53	0/3579
12	SC0	0.22	0/1668	0.54	0/2251
13	LCC	0.22	0/808	0.49	0/1087
14	SCC	0.19	0/497	0.53	0/663
15	LD0	0.24	0/2357	0.50	0/3141
16	SD0	0.20	0/1648	0.55	0/2220
17	LDD	0.27	0/829	0.51	0/1102
18	SDD	0.22	0/552	0.52	0/739
19	LE0	0.21	0/1428	0.59	0/1916
20	SE0	0.22	0/2092	0.58	0/2817
21	LEE	0.29	0/1032	0.58	0/1383
22	SEE	0.19	0/457	0.46	0/600
23	LF0	0.27	0/1914	0.51	0/2557
24	SF0	0.19	0/1470	0.53	0/1971
25	LFF	0.28	0/781	0.59	0/1048
26	SFF	0.23	0/265	0.61	0/326
27	LG0	0.21	0/1599	0.58	2/2142 (0.1%)
28	SG0	0.21	0/1611	0.51	1/2152 (0.0%)
29	LGG	0.25	0/825	0.53	0/1096
30	SGG	0.22	0/2538	0.56	0/3434
31	LH0	0.24	0/1476	0.58	0/1982
32	SH0	0.22	0/1282	0.54	0/1721

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	LHH	0.24	0/1030	0.56	0/1371
34	LI0	0.28	0/1777	0.54	0/2376
35	SI0	0.24	0/1275	0.53	0/1695
36	LII	0.21	0/774	0.50	0/1025
37	LJ0	0.23	0/1367	0.54	0/1823
38	SJ0	0.22	0/1403	0.53	0/1888
39	LJJ	0.31	0/734	0.62	0/973
40	LL0	0.26	0/1350	0.56	0/1803
41	SL0	0.23	0/1291	0.50	0/1731
42	LLL	0.28	0/454	0.53	0/602
43	LM0	0.24	0/736	0.51	0/984
44	LMM	0.23	0/403	0.54	0/532
45	SM0	0.18	0/937	0.55	0/1255
46	LN0	0.29	0/1708	0.55	0/2289
47	SN0	0.22	0/1197	0.50	0/1603
48	LNN	0.21	0/578	0.57	1/770 (0.1%)
49	SNN	0.22	0/1357	0.50	0/1835
50	LO0	0.27	0/1400	0.49	0/1871
51	SO0	0.22	0/987	0.54	0/1322
52	LOO	0.24	0/801	0.52	0/1058
53	LP0	0.29	0/1255	0.55	0/1686
54	SP0	0.20	0/963	0.49	0/1294
55	LPP	0.26	0/651	0.55	0/866
56	LQ0	0.29	0/1478	0.57	0/1975
57	SQ0	0.19	0/1222	0.54	0/1633
58	LR0	0.25	0/1353	0.49	0/1787
59	SR0	0.18	0/969	0.48	0/1297
60	LS0	0.27	0/1504	0.54	2/2024 (0.1%)
61	SS0	0.21	0/1202	0.59	2/1609 (0.1%)
62	LT0	0.29	0/1339	0.56	0/1795
63	ST0	0.20	0/1063	0.57	2/1428 (0.1%)
64	LU0	0.24	0/802	0.57	0/1074
65	SU0	0.21	0/779	0.57	2/1055 (0.2%)
66	LV0	0.28	0/1056	0.56	0/1412
67	SV0	0.23	0/496	0.56	0/667
68	LW0	0.28	0/674	0.67	2/905 (0.2%)
69	SW0	0.23	0/1037	0.49	0/1389
70	LX0	0.25	0/743	0.46	0/994
71	SX0	0.24	0/1086	0.50	0/1450
72	LXX	0.20	0/464	0.48	0/609
73	LY0	0.24	0/1104	0.52	0/1470
74	SY0	0.21	0/1036	0.50	0/1379
75	LZ0	0.23	0/1019	0.60	0/1358

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
76	SZ0	0.18	0/730	0.54	0/969
77	SK0	0.20	0/725	0.52	0/973
78	L50	0.30	0/55133	0.44	2/85837 (0.0%)
All	All	0.26	0/174681	0.48	18/252924 (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
25	LFF	0	1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	LW0	75	PRO	N-CA-CB	7.84	110.62	103.33
68	LW0	73	PRO	N-CA-CB	7.14	110.75	103.25
48	LNN	85	PRO	N-CA-CB	6.61	110.19	103.25
28	SG0	147	PRO	N-CA-CB	6.53	110.11	103.25
61	SS0	107	VAL	CA-C-N	6.43	130.47	120.82
61	SS0	107	VAL	C-N-CA	6.43	130.47	120.82
63	ST0	112	LYS	CA-C-N	6.14	130.03	120.82
63	ST0	112	LYS	C-N-CA	6.14	130.03	120.82
60	LS0	174	VAL	CA-C-N	5.68	134.93	124.82
60	LS0	174	VAL	C-N-CA	5.68	134.93	124.82
27	LG0	51	ILE	CA-C-N	5.59	132.22	121.54
27	LG0	51	ILE	C-N-CA	5.59	132.22	121.54
1	S60	923	A	P-O3'-C3'	5.49	128.44	120.20
78	L50	786	A	P-O3'-C3'	5.39	128.29	120.20
1	S60	309	A	P-O3'-C3'	5.27	128.10	120.20
65	SU0	29	PHE	CA-C-N	-5.13	117.94	122.97
65	SU0	29	PHE	C-N-CA	-5.13	117.94	122.97
78	L50	1293	A	C2'-C3'-O3'	5.10	117.15	109.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	LFF	12	ARG	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S60	26291	0	13176	104	0
2	L70	2523	0	1273	7	0
3	LA0	1789	0	1824	16	0
4	SA0	1558	0	1596	14	0
5	LAA	1219	0	1247	4	0
6	SAA	776	0	814	6	0
7	LB0	2912	0	3040	16	0
8	SB0	1664	0	1734	21	0
9	LBB	416	0	458	2	0
10	SBB	637	0	632	3	0
11	LC0	2624	0	2709	21	0
12	SC0	1642	0	1717	20	0
13	LCC	797	0	844	3	0
14	SCC	495	0	517	9	0
15	LD0	2320	0	2370	14	0
16	SD0	1624	0	1769	10	0
17	LDD	821	0	911	6	0
18	SDD	541	0	532	5	0
19	LE0	1410	0	1449	8	0
20	SE0	2056	0	2113	9	0
21	LEE	1010	0	1072	4	0
22	SEE	454	0	492	2	0
23	LF0	1884	0	1972	12	0
24	SF0	1457	0	1510	14	0
25	LFF	771	0	830	5	0
26	SFF	266	0	145	0	0
27	LG0	1573	0	1679	8	0
28	SG0	1587	0	1605	23	0
29	LGG	814	0	878	8	0
30	SGG	2499	0	2465	33	0
31	LH0	1452	0	1531	9	0
32	SH0	1265	0	1313	18	0
33	LHH	1017	0	1096	5	0
34	LI0	1743	0	1792	12	0
35	SI0	1259	0	1305	13	0
36	LII	765	0	860	7	0
37	LJ0	1348	0	1406	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	SJ0	1382	0	1431	10	0
39	LJJ	719	0	771	1	0
40	LL0	1328	0	1417	10	0
41	SL0	1269	0	1311	18	0
42	LLL	445	0	482	2	0
43	LM0	731	0	785	3	0
44	LMM	402	0	433	5	0
45	SM0	929	0	967	6	0
46	LN0	1677	0	1726	13	0
47	SN0	1177	0	1237	16	0
48	LNN	577	0	496	4	0
49	SNN	1336	0	1349	12	0
50	LO0	1371	0	1424	5	0
51	SO0	977	0	1032	17	0
52	LOO	792	0	889	6	0
53	LP0	1235	0	1300	6	0
54	SP0	942	0	975	14	0
55	LPP	642	0	673	4	0
56	LQ0	1460	0	1579	8	0
57	SQ0	1205	0	1285	9	0
58	LR0	1342	0	1462	12	0
59	SR0	958	0	1002	14	0
60	LS0	1472	0	1503	9	0
61	SS0	1186	0	1224	10	0
62	LT0	1310	0	1368	9	0
63	ST0	1048	0	1062	14	0
64	LU0	790	0	814	4	0
65	SU0	764	0	788	8	0
66	LV0	1040	0	1102	3	0
67	SV0	491	0	492	4	0
68	LW0	667	0	676	7	0
69	SW0	1018	0	1041	6	0
70	LX0	734	0	796	2	0
71	SX0	1069	0	1154	3	0
72	LXX	462	0	518	4	0
73	LY0	1088	0	1124	8	0
74	SY0	1025	0	1090	13	0
75	LZ0	1006	0	1080	9	0
76	SZ0	724	0	800	7	0
77	SK0	712	0	709	6	0
78	L50	49259	0	24706	111	0
79	L50	122	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
79	L70	1	0	0	0	0
79	LJJ	1	0	0	0	0
79	LV0	1	0	0	0	0
79	S60	49	0	0	0	0
80	LGG	1	0	0	0	0
80	LJJ	1	0	0	0	0
80	LMM	1	0	0	0	0
80	LOO	1	0	0	0	0
80	LPP	1	0	0	0	0
80	SAA	1	0	0	0	0
80	SBB	1	0	0	0	0
80	SDD	1	0	0	0	0
80	SNN	1	0	0	0	0
All	All	164223	0	128749	764	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 3.

All (764) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S60:500:G:H1	1:S60:526:U:H3	1.11	0.98
1:S60:124:G:H22	1:S60:135:U:H3	1.40	0.69
7:LB0:283:HIS:HD2	7:LB0:314:GLU:HG3	1.61	0.65
16:SD0:40:ARG:HB2	16:SD0:47:LYS:HB2	1.78	0.65
1:S60:647:U:H3'	1:S60:648:G:H21	1.62	0.65
31:LH0:43:MET:HE1	31:LH0:70:VAL:HG11	1.80	0.64
14:SCC:10:TYR:HB3	14:SCC:34:LEU:HD12	1.80	0.64
45:SM0:58:CYS:SG	45:SM0:59:GLU:N	2.71	0.63
11:LC0:73:CYS:SG	11:LC0:75:ARG:NH1	2.72	0.63
77:SK0:4:THR:H	77:SK0:7:GLN:HE21	1.46	0.63
30:SGG:277:ILE:HB	30:SGG:284:TYR:HB2	1.81	0.63
58:LR0:169:LYS:HA	58:LR0:172:LYS:HD2	1.79	0.63
12:SC0:225:SER:O	12:SC0:229:ASN:ND2	2.32	0.63
1:S60:331:A:OP2	22:SEE:27:ARG:NH2	2.31	0.62
41:SL0:148:THR:HG23	41:SL0:151:ASN:HD22	1.65	0.61
11:LC0:98:MET:HE3	11:LC0:101:PRO:HA	1.81	0.61
58:LR0:23:CYS:SG	58:LR0:24:GLY:N	2.72	0.61
1:S60:772:G:H21	1:S60:997:A:H62	1.48	0.61
14:SCC:8:GLN:HE21	24:SF0:107:ARG:HH12	1.48	0.61
58:LR0:168:LEU:HG	58:LR0:172:LYS:HE3	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:LY0:34:HIS:HB3	73:LY0:105:THR:HG22	1.82	0.60
1:S60:836:G:O6	45:SM0:38:ARG:NH1	2.34	0.60
63:ST0:29:PRO:HG2	63:ST0:32:HIS:HB3	1.82	0.60
30:SGG:180:VAL:HB	30:SGG:194:PHE:HB2	1.83	0.60
56:LQ0:70:VAL:HG22	56:LQ0:99:MET:HE1	1.84	0.60
78:L50:851:G:H5'	78:L50:852:A:H5''	1.84	0.59
19:LE0:125:MET:SD	19:LE0:125:MET:N	2.74	0.59
30:SGG:233:PHE:HB3	30:SGG:247:ASN:HA	1.84	0.59
1:S60:115:A:H2'	1:S60:116:G:H8	1.68	0.59
29:LGG:57:ARG:HD3	29:LGG:58:PRO:HD2	1.83	0.59
45:SM0:118:THR:H	45:SM0:121:SER:HB3	1.68	0.59
61:SS0:122:GLY:HA3	61:SS0:130:LEU:HD22	1.84	0.59
47:SN0:100:ARG:NH1	47:SN0:145:VAL:O	2.36	0.59
67:SV0:45:CYS:SG	67:SV0:46:GLY:N	2.76	0.59
1:S60:1001:G:OP1	57:SQ0:155:ARG:NH1	2.37	0.58
76:SZ0:91:LEU:HD11	76:SZ0:99:SER:HB3	1.85	0.58
64:LU0:77:ARG:NH2	78:L50:1285:U:OP2	2.36	0.58
28:SG0:72:ILE:HG23	28:SG0:74:PRO:HD3	1.86	0.58
40:LL0:111:ARG:NH1	40:LL0:141:MET:O	2.36	0.58
76:SZ0:55:LYS:HD3	76:SZ0:88:ILE:HG23	1.85	0.58
12:SC0:101:ASP:HB2	12:SC0:104:THR:HG22	1.86	0.58
32:SH0:109:ILE:HG12	32:SH0:123:VAL:HG12	1.86	0.58
28:SG0:4:ASN:ND2	28:SG0:15:MET:SD	2.77	0.58
32:SH0:43:VAL:HG12	32:SH0:75:TYR:HB3	1.85	0.58
40:LL0:51:CYS:O	40:LL0:111:ARG:NH2	2.37	0.58
5:LAA:89:GLU:OE2	5:LAA:94:GLN:NE2	2.36	0.57
53:LP0:111:GLU:O	53:LP0:154:ARG:NH2	2.37	0.57
44:LMM:109:CYS:SG	44:LMM:110:GLY:N	2.77	0.57
14:SCC:42:ARG:NH2	14:SCC:61:ARG:O	2.38	0.57
32:SH0:129:CYS:SG	32:SH0:130:THR:N	2.77	0.57
11:LC0:162:LYS:NZ	78:L50:246:U:OP2	2.38	0.57
15:LD0:76:ASP:OD1	15:LD0:76:ASP:N	2.38	0.57
30:SGG:25:LEU:HB2	30:SGG:32:VAL:HG12	1.86	0.57
17:LDD:71:ARG:NH2	78:L50:2322:G:OP1	2.38	0.57
56:LQ0:147:ARG:NH1	56:LQ0:149:SER:OG	2.37	0.57
58:LR0:68:ARG:NH2	78:L50:2331:U:OP2	2.38	0.57
1:S60:15:G:H21	1:S60:731:A:H62	1.51	0.56
1:S60:560:G:OP1	47:SN0:95:ARG:NH2	2.38	0.56
34:LI0:102:MET:HE1	34:LI0:114:GLY:H	1.70	0.56
19:LE0:86:LYS:HE3	19:LE0:115:LEU:HB3	1.86	0.56
25:LFF:72:ARG:NH2	78:L50:868:A:OP1	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:SJ0:67:SER:OG	38:SJ0:71:ARG:NH1	2.38	0.56
52:LOO:50:GLN:HE22	52:LOO:54:ILE:HD11	1.69	0.56
2:L70:74:A:N3	60:LS0:59:LYS:NZ	2.50	0.56
32:SH0:37:ARG:NH2	32:SH0:141:THR:O	2.39	0.56
14:SCC:61:ARG:HG3	24:SF0:189:ARG:HD3	1.88	0.56
30:SGG:221:SER:H	30:SGG:239:LYS:HB2	1.70	0.56
1:S60:911:A:OP1	59:SR0:44:ARG:NH2	2.39	0.56
30:SGG:156:ASN:ND2	30:SGG:177:ASP:OD1	2.38	0.56
71:SX0:95:ASP:OD1	71:SX0:123:GLN:NE2	2.38	0.56
1:S60:1040:U:OP2	54:SP0:40:ARG:NH2	2.39	0.56
11:LC0:42:ARG:NH1	78:L50:1065:U:O2'	2.38	0.56
30:SGG:266:VAL:HG12	30:SGG:277:ILE:HA	1.88	0.56
74:SY0:8:GLU:HB2	74:SY0:26:LYS:HB3	1.88	0.56
12:SC0:133:HIS:ND1	12:SC0:134:THR:OG1	2.35	0.56
1:S60:691:U:OP1	12:SC0:149:LYS:NZ	2.39	0.56
47:SN0:93:VAL:O	47:SN0:97:ASN:ND2	2.39	0.56
58:LR0:94:ARG:HH21	78:L50:1400:U:HO2'	1.54	0.56
14:SCC:4:ASN:HB3	24:SF0:107:ARG:HH21	1.70	0.56
15:LD0:60:ARG:NH2	15:LD0:152:ASP:OD1	2.38	0.56
52:LOO:31:ASP:N	52:LOO:31:ASP:OD1	2.39	0.56
1:S60:55:G:OP1	74:SY0:111:ARG:NH1	2.39	0.55
28:SG0:197:ARG:O	28:SG0:201:ASN:ND2	2.39	0.55
30:SGG:37:SER:OG	30:SGG:38:LYS:N	2.38	0.55
30:SGG:320:CYS:HB3	30:SGG:328:TYR:HB3	1.88	0.55
78:L50:372:A:N6	78:L50:375:A:OP2	2.38	0.55
11:LC0:291:SER:OG	11:LC0:292:LYS:N	2.40	0.55
52:LOO:45:GLN:HE22	52:LOO:50:GLN:HG3	1.71	0.55
53:LP0:46:ILE:O	53:LP0:50:ASN:ND2	2.39	0.55
59:SR0:99:PRO:HA	59:SR0:102:LEU:HD12	1.86	0.55
61:SS0:31:THR:O	61:SS0:63:ARG:NH1	2.39	0.55
65:SU0:3:VAL:HG13	65:SU0:98:GLY:HA2	1.89	0.55
1:S60:75:G:H5'	1:S60:76:A:H5''	1.88	0.55
1:S60:138:C:H5'	1:S60:139:A:H4'	1.89	0.55
75:LZ0:39:ARG:HH12	75:LZ0:55:LYS:HG2	1.71	0.55
36:LII:32:ARG:NH2	46:LN0:5:ASP:OD2	2.39	0.55
9:LBB:35:VAL:HA	62:LT0:65:THR:HG21	1.88	0.55
41:SL0:32:ARG:NH2	41:SL0:52:TYR:O	2.39	0.55
46:LN0:69:GLY:O	46:LN0:71:ARG:NH2	2.39	0.55
65:SU0:79:GLN:HA	65:SU0:82:LYS:HE2	1.88	0.55
73:LY0:56:VAL:HA	73:LY0:106:PHE:HA	1.87	0.55
8:SB0:52:ARG:NH1	8:SB0:57:GLN:O	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:SL0:133:SER:OG	41:SL0:134:LYS:N	2.40	0.55
59:SR0:42:SER:OG	59:SR0:43:LYS:N	2.40	0.55
73:LY0:12:ARG:NH1	78:L50:23:U:OP2	2.39	0.55
76:SZ0:88:ILE:HG22	76:SZ0:89:ILE:HG23	1.88	0.55
1:S60:461:U:OP1	41:SL0:101:ARG:NH1	2.38	0.55
8:SB0:136:ILE:HB	8:SB0:220:VAL:HB	1.88	0.55
22:SEE:11:GLY:O	22:SEE:15:ASN:ND2	2.40	0.55
1:S60:1025:U:OP2	24:SF0:151:ARG:NH2	2.40	0.54
27:LG0:154:LYS:NZ	78:L50:215:G:N7	2.53	0.54
45:SM0:56:GLU:O	45:SM0:63:LYS:NZ	2.40	0.54
73:LY0:56:VAL:HG12	73:LY0:106:PHE:HB3	1.89	0.54
34:LI0:119:PHE:O	48:LNN:133:ASN:ND2	2.39	0.54
54:SP0:34:LEU:O	54:SP0:39:ARG:NH2	2.41	0.54
75:LZ0:6:ASN:ND2	75:LZ0:79:ASP:OD1	2.40	0.54
1:S60:751:C:H42	1:S60:756:A:H61	1.53	0.54
44:LMM:117:LYS:NZ	78:L50:2166:U:OP2	2.40	0.54
37:LJ0:53:ARG:HH21	49:SNN:88:TYR:HB2	1.72	0.54
11:LC0:219:ASN:ND2	78:L50:247:A:N3	2.56	0.54
30:SGG:212:LYS:NZ	30:SGG:215:ASP:OD1	2.41	0.54
38:SJ0:15:ASN:O	38:SJ0:21:ARG:NH2	2.41	0.54
61:SS0:47:ARG:HH21	63:ST0:36:LYS:HG3	1.73	0.54
62:LT0:74:VAL:HG12	62:LT0:87:THR:HG22	1.88	0.54
1:S60:765:U:O2	63:ST0:85:ARG:NH1	2.41	0.54
3:LA0:83:SER:OG	3:LA0:86:ASN:OD1	2.24	0.54
28:SG0:36:ASN:HB2	68:LW0:70:LYS:HE2	1.89	0.54
19:LE0:11:THR:O	19:LE0:15:GLN:NE2	2.40	0.54
49:SNN:69:ILE:HA	49:SNN:113:GLY:HA3	1.88	0.54
1:S60:571:U:OP1	47:SN0:133:LYS:NZ	2.41	0.54
3:LA0:27:PRO:O	3:LA0:149:ARG:NH2	2.41	0.54
13:LCC:46:SER:OG	13:LCC:47:SER:N	2.40	0.54
57:SQ0:43:ASN:HD21	57:SQ0:86:GLU:HB3	1.73	0.54
1:S60:1242:A:H62	6:SAA:84:VAL:HG23	1.72	0.54
41:SL0:122:ASP:OD1	41:SL0:122:ASP:N	2.38	0.54
4:SA0:69:ASN:OD1	12:SC0:229:ASN:ND2	2.41	0.53
18:SDD:48:MET:HB3	18:SDD:50:ILE:HG22	1.88	0.53
19:LE0:59:ARG:NH1	19:LE0:156:THR:O	2.40	0.53
1:S60:111:A:N6	28:SG0:190:SER:OG	2.41	0.53
7:LB0:290:THR:OG1	7:LB0:291:GLU:N	2.42	0.53
10:SBB:44:CYS:SG	10:SBB:45:ASP:N	2.81	0.53
27:LG0:83:ASN:ND2	27:LG0:85:GLN:O	2.42	0.53
64:LU0:8:LYS:HA	64:LU0:62:ASN:HA	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:LA0:105:ASP:OD1	3:LA0:105:ASP:N	2.40	0.53
40:LL0:6:ILE:HG22	56:LQ0:167:ARG:HB3	1.90	0.53
46:LN0:38:ARG:HH22	46:LN0:60:LEU:HB3	1.72	0.53
1:S60:127:U:O4	74:SY0:127:LYS:NZ	2.41	0.53
37:LJ0:85:ARG:HH21	37:LJ0:103:GLY:H	1.56	0.53
41:SL0:29:LYS:NZ	41:SL0:50:ALA:O	2.41	0.53
63:ST0:40:GLY:HA2	63:ST0:81:LYS:HD2	1.91	0.53
68:LW0:13:ILE:HG21	68:LW0:18:SER:HB3	1.89	0.53
30:SGG:54:ASP:OD1	30:SGG:54:ASP:N	2.41	0.53
78:L50:1664:G:OP2	78:L50:1664:G:N2	2.38	0.53
1:S60:500:G:N2	1:S60:526:U:O2	2.35	0.53
21:LEE:111:LYS:NZ	78:L50:1071:U:OP1	2.42	0.53
7:LB0:31:ALA:O	7:LB0:333:ARG:NH1	2.42	0.53
32:SH0:159:SER:OG	32:SH0:160:LEU:N	2.41	0.53
58:LR0:167:ALA:O	58:LR0:171:LYS:NZ	2.39	0.52
73:LY0:14:LYS:NZ	78:L50:361:U:OP2	2.42	0.52
74:SY0:117:ARG:NH1	74:SY0:119:GLY:O	2.42	0.52
1:S60:1031:A:N6	1:S60:1054:G:O2'	2.42	0.52
42:LLL:10:LYS:HD2	78:L50:1371:G:H5''	1.91	0.52
76:SZ0:42:VAL:HG23	76:SZ0:46:LEU:HD22	1.91	0.52
1:S60:352:G:H21	1:S60:357:A:H2	1.58	0.52
28:SG0:42:GLU:O	28:SG0:45:ASN:ND2	2.43	0.52
1:S60:260:U:H2'	1:S60:261:A:H8	1.75	0.52
1:S60:474:A:OP1	47:SN0:122:ARG:NH1	2.43	0.52
12:SC0:176:ASP:N	12:SC0:176:ASP:OD1	2.41	0.52
36:LII:1:MET:N	78:L50:505:C:OP1	2.42	0.52
78:L50:1334:A:H5''	78:L50:1335:U:H5'	1.89	0.52
8:SB0:66:ARG:NH1	51:SO0:35:GLU:OE1	2.43	0.52
19:LE0:55:TYR:HB3	19:LE0:58:LYS:HD2	1.91	0.52
37:LJ0:107:HIS:HD2	37:LJ0:121:TYR:H	1.55	0.52
15:LD0:29:ARG:O	15:LD0:29:ARG:NH1	2.39	0.52
19:LE0:143:GLU:HA	19:LE0:146:LYS:HD2	1.91	0.52
23:LF0:176:CYS:SG	23:LF0:177:ILE:N	2.82	0.52
30:SGG:135:LEU:HD13	30:SGG:144:ASN:HB3	1.90	0.52
32:SH0:61:GLY:HA2	32:SH0:64:ILE:HD12	1.92	0.52
40:LL0:66:ARG:NH2	78:L50:182:A:OP1	2.40	0.52
49:SNN:30:THR:HG23	49:SNN:114:GLY:HA2	1.91	0.52
50:LO0:30:LYS:HG2	50:LO0:99:ASN:HB3	1.91	0.52
55:LPP:38:GLU:HG2	55:LPP:45:THR:HG22	1.92	0.52
65:SU0:75:SER:OG	65:SU0:76:SER:N	2.42	0.52
75:LZ0:50:LYS:HG3	75:LZ0:51:VAL:HG23	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:SB0:173:ILE:HD12	8:SB0:199:ILE:HG13	1.92	0.52
17:LDD:72:ARG:NH1	78:L50:2435:G:OP1	2.43	0.52
54:SP0:35:PRO:HD2	54:SP0:38:LEU:HD12	1.90	0.52
1:S60:951:A:OP2	59:SR0:2:ASN:ND2	2.40	0.52
33:LHH:11:LYS:O	33:LHH:61:LYS:NZ	2.43	0.52
42:LLL:4:ARG:NH1	78:L50:1201:A:O2'	2.43	0.52
46:LN0:155:VAL:O	46:LN0:162:ARG:NH2	2.43	0.52
48:LNN:107:GLY:N	78:L50:2223:U:O2	2.43	0.52
8:SB0:131:THR:OG1	8:SB0:132:LYS:N	2.42	0.52
47:SN0:36:ASP:OD1	47:SN0:36:ASP:N	2.41	0.52
53:LP0:127:PHE:HA	53:LP0:141:ASN:HB3	1.91	0.52
1:S60:464:A:O2'	69:SW0:3:GLN:NE2	2.43	0.52
4:SA0:78:THR:OG1	4:SA0:129:ASP:OD1	2.26	0.51
66:LV0:57:ARG:NH1	78:L50:2306:G:OP1	2.44	0.51
11:LC0:70:ILE:HG12	11:LC0:75:ARG:HH21	1.75	0.51
49:SNN:10:ASP:HB2	49:SNN:158:ILE:HB	1.91	0.51
8:SB0:180:ASP:N	8:SB0:180:ASP:OD1	2.44	0.51
12:SC0:219:ASN:HB3	12:SC0:222:MET:HG2	1.92	0.51
35:SI0:122:ASP:N	35:SI0:122:ASP:OD1	2.44	0.51
56:LQ0:178:ARG:NH2	56:LQ0:181:MET:SD	2.83	0.51
1:S60:124:G:H21	28:SG0:13:GLN:HE22	1.59	0.51
3:LA0:26:TYR:HB3	3:LA0:62:LEU:HD21	1.92	0.51
3:LA0:80:ALA:HB3	3:LA0:88:THR:HG22	1.93	0.51
12:SC0:32:SER:OG	12:SC0:33:LEU:N	2.43	0.51
64:LU0:47:LEU:HD22	64:LU0:63:GLU:HG3	1.92	0.51
1:S60:134:G:OP2	28:SG0:84:ARG:NH1	2.43	0.51
1:S60:351:U:O2'	74:SY0:60:ILE:O	2.27	0.51
37:LJ0:25:SER:OG	37:LJ0:29:ASN:ND2	2.43	0.51
38:SJ0:132:TRP:O	38:SJ0:136:LYS:NZ	2.42	0.51
51:SO0:14:ILE:HD11	51:SO0:31:ILE:HD12	1.92	0.51
2:L70:5:A:O2'	15:LD0:69:GLN:NE2	2.43	0.51
10:SBB:90:ASP:N	10:SBB:90:ASP:OD1	2.42	0.51
16:SD0:20:GLU:OE1	77:SK0:64:TYR:OH	2.27	0.51
36:LII:64:ASP:HB3	36:LII:67:ARG:HB3	1.93	0.51
50:LO0:91:HIS:NE2	50:LO0:95:GLU:OE2	2.43	0.51
73:LY0:27:ARG:NH1	73:LY0:75:LEU:O	2.44	0.51
78:L50:2418:G:O2'	78:L50:2420:A:N7	2.43	0.51
1:S60:600:A:H62	1:S60:618:G:H21	1.58	0.51
20:SE0:245:GLU:HA	20:SE0:248:ASN:HB2	1.91	0.51
1:S60:823:A:N6	1:S60:836:G:O2'	2.44	0.51
20:SE0:196:LYS:HB3	20:SE0:203:ILE:HB	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:SG0:102:SER:OG	28:SG0:103:GLU:N	2.43	0.51
1:S60:814:U:O2	1:S60:842:G:O6	2.29	0.51
8:SB0:2:ALA:N	51:SO0:44:MET:O	2.44	0.51
41:SL0:5:THR:HG23	41:SL0:6:LEU:HG	1.91	0.51
3:LA0:22:SER:OG	3:LA0:46:ARG:NH1	2.43	0.51
30:SGG:233:PHE:HA	30:SGG:248:LEU:HG	1.93	0.51
54:SP0:41:ARG:NH2	54:SP0:80:SER:O	2.44	0.50
78:L50:1267:C:H3'	78:L50:1268:A:H8	1.76	0.50
28:SG0:56:ASP:OD2	28:SG0:97:ARG:NH1	2.45	0.50
29:LGG:69:ARG:HH12	78:L50:1357:A:H8	1.60	0.50
61:SS0:32:LYS:HB2	61:SS0:37:ALA:HB2	1.91	0.50
1:S60:191:G:O2'	35:SI0:16:LYS:NZ	2.44	0.50
35:SI0:46:SER:OG	35:SI0:65:ARG:NH1	2.43	0.50
55:LPP:46:SER:OG	55:LPP:57:CYS:SG	2.70	0.50
41:SL0:52:TYR:OH	41:SL0:113:CYS:SG	2.69	0.50
11:LC0:105:MET:HE1	40:LL0:18:VAL:HG21	1.93	0.50
14:SCC:4:ASN:O	24:SF0:107:ARG:NH2	2.45	0.50
17:LDD:87:GLU:HG2	17:LDD:88:LEU:HD12	1.93	0.50
43:LM0:26:ILE:HD11	43:LM0:37:LYS:HB2	1.94	0.50
6:SAA:44:LEU:HD12	6:SAA:65:PRO:HG2	1.93	0.50
1:S60:1002:C:OP1	57:SQ0:151:GLN:NE2	2.44	0.50
7:LB0:36:ASP:OD2	7:LB0:36:ASP:N	2.45	0.50
11:LC0:81:SER:OG	11:LC0:82:ARG:N	2.45	0.50
11:LC0:91:ASN:OD1	11:LC0:91:ASN:N	2.38	0.50
31:LH0:23:LYS:HE3	31:LH0:39:SER:HA	1.92	0.50
34:LI0:109:ASP:OD1	34:LI0:109:ASP:N	2.43	0.50
54:SP0:47:SER:OG	54:SP0:48:GLY:N	2.45	0.50
3:LA0:25:LYS:HD2	3:LA0:109:GLY:HA3	1.94	0.50
8:SB0:210:GLN:HG3	8:SB0:211:ASN:HB2	1.93	0.50
1:S60:250:G:N2	1:S60:253:A:OP2	2.41	0.49
1:S60:819:A:O2'	1:S60:837:A:N1	2.43	0.49
32:SH0:15:ILE:HG13	32:SH0:29:GLU:HG2	1.93	0.49
51:SO0:41:SER:OG	51:SO0:44:MET:SD	2.69	0.49
52:LOO:39:ARG:NH1	78:L50:310:A:N7	2.60	0.49
65:SU0:30:ILE:HG22	65:SU0:31:GLU:HG2	1.93	0.49
2:L70:6:C:OP1	15:LD0:60:ARG:NH1	2.45	0.49
3:LA0:4:VAL:O	3:LA0:9:ARG:NH2	2.45	0.49
34:LI0:7:ARG:NH2	78:L50:2097:G:OP2	2.44	0.49
43:LM0:81:SER:O	43:LM0:86:ARG:NH1	2.45	0.49
1:S60:509:A:H61	51:SO0:49:LYS:HD3	1.77	0.49
1:S60:927:A:H61	1:S60:946:G:H21	1.60	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:LF0:174:LEU:HD22	23:LF0:179:GLU:HG2	1.95	0.49
38:SJ0:105:THR:OG1	38:SJ0:106:ILE:N	2.43	0.49
4:SA0:198:GLU:OE2	59:SR0:88:SER:OG	2.29	0.49
32:SH0:7:THR:OG1	32:SH0:8:GLU:N	2.43	0.49
51:SO0:37:ILE:HG23	51:SO0:72:ARG:HD2	1.94	0.49
74:SY0:9:ILE:HG23	74:SY0:23:LEU:HD13	1.94	0.49
4:SA0:38:GLY:HA3	59:SR0:100:MET:HE2	1.92	0.49
35:SI0:112:SER:HA	35:SI0:115:ILE:HD12	1.93	0.49
41:SL0:133:SER:HB3	41:SL0:136:LYS:HB2	1.93	0.49
75:LZ0:48:MET:SD	75:LZ0:48:MET:N	2.84	0.49
77:SK0:68:THR:OG1	77:SK0:69:GLU:N	2.45	0.49
12:SC0:151:ILE:HB	12:SC0:178:TYR:HB2	1.94	0.49
25:LFF:1:MET:O	25:LFF:91:ARG:NH1	2.46	0.49
61:SS0:94:PHE:HE2	61:SS0:114:GLU:HG2	1.78	0.49
78:L50:1873:A:H2'	78:L50:1874:A:H8	1.78	0.49
1:S60:870:U:H3	1:S60:906:G:H1	1.61	0.49
30:SGG:112:ILE:HA	30:SGG:128:SER:HA	1.94	0.49
1:S60:138:C:OP1	28:SG0:130:ARG:NH2	2.45	0.49
1:S60:874:U:H1'	4:SA0:111:GLN:HG3	1.95	0.49
8:SB0:47:LYS:NZ	51:SO0:8:SER:OG	2.45	0.49
16:SD0:213:ALA:HB2	59:SR0:18:LYS:HB3	1.95	0.49
23:LF0:183:ASN:HD22	23:LF0:190:TYR:HB2	1.77	0.49
78:L50:1377:A:O2'	78:L50:1379:A:OP2	2.26	0.49
1:S60:961:A:H2'	1:S60:962:A:H8	1.78	0.49
8:SB0:170:MET:HG2	8:SB0:199:ILE:HD11	1.95	0.49
23:LF0:67:TYR:HD2	23:LF0:74:TYR:HB2	1.78	0.49
28:SG0:48:VAL:HG12	28:SG0:113:ILE:HD13	1.95	0.49
78:L50:1005:G:N2	78:L50:1006:G:O6	2.46	0.49
29:LGG:8:LYS:O	29:LGG:19:ARG:NH1	2.46	0.48
12:SC0:164:VAL:HG13	12:SC0:165:PRO:HD3	1.94	0.48
30:SGG:55:PHE:HB2	30:SGG:58:LEU:HD23	1.96	0.48
30:SGG:221:SER:OG	30:SGG:222:VAL:N	2.46	0.48
40:LL0:58:THR:OG1	40:LL0:59:ILE:N	2.46	0.48
2:L70:99:A:N7	60:LS0:61:LYS:NZ	2.54	0.48
68:LW0:7:ILE:HD12	68:LW0:29:GLN:HA	1.93	0.48
78:L50:1857:A:H2'	78:L50:1858:A:H8	1.78	0.48
24:SF0:160:ASP:OD1	24:SF0:160:ASP:N	2.46	0.48
35:SI0:154:SER:HA	35:SI0:157:GLU:HG3	1.96	0.48
37:LJ0:53:ARG:NH2	49:SNN:90:ASP:OD2	2.47	0.48
63:ST0:48:ASP:N	63:ST0:48:ASP:OD1	2.44	0.48
1:S60:811:U:H2'	1:S60:812:A:H8	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:LJ0:117:ASP:OD1	37:LJ0:117:ASP:N	2.46	0.48
51:SO0:83:GLY:H	51:SO0:117:THR:HG22	1.78	0.48
78:L50:1302:U:H2'	78:L50:1303:A:H8	1.79	0.48
1:S60:975:G:O2'	16:SD0:179:GLN:OE1	2.31	0.48
1:S60:1016:U:O4	63:ST0:17:LYS:NZ	2.46	0.48
46:LN0:97:ARG:NH2	78:L50:315:A:OP1	2.45	0.48
47:SN0:143:LYS:NZ	47:SN0:144:LEU:O	2.46	0.48
68:LW0:3:ASP:HB2	68:LW0:15:LYS:HA	1.95	0.48
1:S60:1021:U:H5''	76:SZ0:81:ARG:HH12	1.78	0.48
11:LC0:309:PRO:HG2	11:LC0:310:ARG:HD2	1.95	0.48
30:SGG:25:LEU:HG	30:SGG:27:ASN:HB2	1.95	0.48
30:SGG:118:ASN:HB3	30:SGG:121:GLY:H	1.77	0.48
62:LT0:40:THR:HG22	62:LT0:60:THR:HG22	1.96	0.48
31:LH0:19:ASP:OD1	31:LH0:19:ASP:N	2.47	0.48
34:LI0:83:ASP:OD1	34:LI0:83:ASP:N	2.45	0.48
52:LOO:29:SER:OG	52:LOO:30:LYS:N	2.47	0.48
8:SB0:71:ASN:HD22	51:SO0:112:ARG:HE	1.62	0.48
8:SB0:158:CYS:SG	8:SB0:159:LYS:N	2.87	0.48
25:LFF:56:ASP:OD2	25:LFF:56:ASP:N	2.46	0.48
54:SP0:64:MET:O	54:SP0:66:ASN:ND2	2.47	0.48
54:SP0:77:HIS:HE2	54:SP0:100:TYR:HH	1.59	0.48
60:LS0:32:GLN:NE2	62:LT0:147:LYS:O	2.46	0.47
1:S60:419:C:H2'	1:S60:420:A:H8	1.79	0.47
31:LH0:10:ILE:HD11	31:LH0:71:THR:HG23	1.95	0.47
32:SH0:41:ARG:HH12	32:SH0:134:ASP:HB2	1.79	0.47
46:LN0:23:LEU:HD22	46:LN0:122:ASN:HB3	1.95	0.47
58:LR0:82:MET:SD	58:LR0:94:ARG:NH2	2.87	0.47
7:LB0:159:SER:OG	7:LB0:160:GLN:N	2.45	0.47
8:SB0:84:ARG:NH2	8:SB0:193:GLU:OE1	2.47	0.47
24:SF0:70:LYS:HD3	24:SF0:73:LEU:HD12	1.97	0.47
30:SGG:12:LEU:HB3	30:SGG:327:ILE:HG23	1.96	0.47
32:SH0:53:ILE:HG21	32:SH0:80:GLU:HG2	1.96	0.47
32:SH0:124:LEU:HB3	32:SH0:156:ASN:HB2	1.96	0.47
33:LHH:95:THR:OG1	33:LHH:98:GLN:NE2	2.47	0.47
51:SO0:82:ARG:HB3	51:SO0:116:VAL:HG23	1.95	0.47
52:LOO:53:PRO:HB3	78:L50:2071:A:C8	2.50	0.47
65:SU0:73:ILE:HG21	65:SU0:80:LEU:HD21	1.96	0.47
40:LL0:101:ASN:HB2	40:LL0:104:THR:HG22	1.96	0.47
67:SV0:47:VAL:O	67:SV0:51:ASN:ND2	2.47	0.47
4:SA0:171:SER:HB2	4:SA0:200:PHE:HB3	1.95	0.47
11:LC0:205:LEU:HB2	11:LC0:244:ARG:HD3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:LF0:67:TYR:HB3	23:LF0:72:MET:HB2	1.95	0.47
24:SF0:106:PRO:HG3	24:SF0:134:LEU:HD22	1.96	0.47
31:LH0:133:MET:HA	31:LH0:141:ILE:HG22	1.95	0.47
21:LEE:30:ASP:OD1	21:LEE:30:ASP:N	2.42	0.47
30:SGG:92:TYR:HB3	30:SGG:101:ILE:HD13	1.97	0.47
32:SH0:38:ASP:OD1	32:SH0:38:ASP:N	2.47	0.47
37:LJ0:106:GLU:HG2	37:LJ0:108:ILE:H	1.80	0.47
41:SL0:98:ARG:NH2	71:SX0:2:ASN:OD1	2.48	0.47
69:SW0:97:GLY:O	69:SW0:98:HIS:ND1	2.48	0.47
1:S60:975:G:H1'	16:SD0:179:GLN:HE22	1.80	0.47
12:SC0:138:ARG:HH11	12:SC0:149:LYS:HZ1	1.63	0.47
28:SG0:120:LEU:HB2	28:SG0:124:THR:HG23	1.96	0.47
53:LP0:31:ARG:HH11	53:LP0:63:ARG:HH21	1.62	0.47
59:SR0:94:VAL:HG13	59:SR0:115:LYS:HE2	1.96	0.47
78:L50:1093:U:H2'	78:L50:1094:A:H8	1.80	0.47
1:S60:959:A:H4'	16:SD0:159:LYS:HE3	1.96	0.47
35:SI0:88:MET:HB2	35:SI0:107:VAL:HG23	1.96	0.47
49:SNN:15:LYS:HB3	49:SNN:127:LEU:HD23	1.97	0.47
60:LS0:15:GLU:OE2	60:LS0:108:ARG:NH1	2.47	0.47
7:LB0:91:THR:HG22	7:LB0:105:THR:HG23	1.96	0.47
30:SGG:234:LEU:HG	30:SGG:248:LEU:HD21	1.97	0.47
58:LR0:12:LYS:HG2	58:LR0:16:MET:HE2	1.97	0.47
78:L50:1795:A:H2'	78:L50:1796:A:C8	2.50	0.47
12:SC0:200:GLU:OE1	12:SC0:204:SER:OG	2.33	0.47
66:LV0:80:LYS:NZ	78:L50:1652:U:OP1	2.48	0.47
74:SY0:81:ASP:OD1	74:SY0:81:ASP:N	2.47	0.47
3:LA0:16:ARG:HG2	27:LG0:6:PRO:HG3	1.97	0.46
4:SA0:184:MET:HE1	67:SV0:29:ILE:HG13	1.98	0.46
11:LC0:3:SER:OG	11:LC0:4:LYS:N	2.46	0.46
16:SD0:34:PHE:HA	16:SD0:52:VAL:HA	1.97	0.46
20:SE0:228:SER:OG	20:SE0:229:LEU:N	2.48	0.46
32:SH0:14:ILE:HA	32:SH0:17:LYS:HE2	1.97	0.46
57:SQ0:33:VAL:HG21	57:SQ0:41:LEU:HD11	1.96	0.46
18:SDD:33:CYS:HB3	18:SDD:36:CYS:SG	2.55	0.46
23:LF0:10:PHE:HZ	23:LF0:19:LYS:HD3	1.79	0.46
60:LS0:89:VAL:HG22	60:LS0:98:ASN:HB3	1.96	0.46
68:LW0:33:ASN:OD1	68:LW0:33:ASN:N	2.46	0.46
78:L50:2415:G:H2'	78:L50:2416:G:H8	1.81	0.46
1:S60:553:U:H2'	1:S60:554:A:H8	1.80	0.46
8:SB0:89:ARG:HH12	8:SB0:222:LYS:HG2	1.80	0.46
47:SN0:143:LYS:HD2	47:SN0:143:LYS:HA	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S60:186:U:OP2	35:SI0:142:GLN:NE2	2.43	0.46
1:S60:1030:G:H21	1:S60:1055:A:H2	1.64	0.46
15:LD0:238:ASP:OD2	15:LD0:238:ASP:N	2.45	0.46
63:ST0:29:PRO:O	63:ST0:32:HIS:ND1	2.40	0.46
1:S60:651:A:H4'	8:SB0:155:ARG:HH21	1.81	0.46
1:S60:1239:A:OP2	6:SAA:4:LYS:NZ	2.43	0.46
24:SF0:62:MET:HE3	24:SF0:69:GLY:H	1.80	0.46
45:SM0:83:ARG:NH1	45:SM0:105:GLY:O	2.49	0.46
49:SNN:123:PRO:HB3	49:SNN:138:VAL:HG22	1.98	0.46
76:SZ0:89:ILE:HD12	76:SZ0:101:TYR:HB3	1.97	0.46
1:S60:123:U:H3	1:S60:136:A:H61	1.63	0.46
30:SGG:271:SER:OG	30:SGG:272:PHE:N	2.49	0.46
55:LPP:50:ASP:N	55:LPP:50:ASP:OD1	2.48	0.46
78:L50:1006:G:O2'	78:L50:1007:A:O4'	2.33	0.46
1:S60:1145:U:H2'	1:S60:1146:A:H8	1.79	0.46
3:LA0:162:GLU:O	55:LPP:25:ARG:NH2	2.49	0.46
35:SI0:52:LYS:HE3	35:SI0:62:LYS:HD3	1.97	0.46
35:SI0:87:VAL:HG12	35:SI0:108:VAL:HG12	1.97	0.46
63:ST0:83:ARG:HD2	63:ST0:89:MET:HB2	1.97	0.46
78:L50:771:A:H2'	78:L50:772:A:C8	2.51	0.46
78:L50:1553:G:O2'	78:L50:1673:U:OP2	2.34	0.46
1:S60:625:C:O3'	47:SN0:108:ARG:NH1	2.49	0.46
54:SP0:15:ARG:NE	54:SP0:33:LEU:O	2.42	0.46
59:SR0:28:ASP:N	59:SR0:28:ASP:OD1	2.47	0.46
75:LZ0:20:LYS:NZ	75:LZ0:121:THR:OG1	2.40	0.46
5:LAA:34:ILE:HD13	40:LL0:7:LEU:HD22	1.98	0.46
7:LB0:54:THR:HG22	7:LB0:356:LYS:HE3	1.97	0.46
62:LT0:124:LYS:HA	62:LT0:124:LYS:HD3	1.79	0.46
78:L50:1666:G:O2'	78:L50:1669:U:OP2	2.33	0.46
12:SC0:87:ASP:HB2	12:SC0:91:TYR:HB2	1.98	0.45
15:LD0:260:LYS:HB3	15:LD0:260:LYS:HE2	1.87	0.45
17:LDD:47:THR:HG22	17:LDD:49:GLU:HG3	1.98	0.45
21:LEE:74:LEU:HD11	21:LEE:80:LYS:HB3	1.97	0.45
23:LF0:136:SER:O	23:LF0:136:SER:OG	2.31	0.45
24:SF0:72:ARG:HH21	57:SQ0:45:LEU:HD13	1.81	0.45
30:SGG:44:TYR:HD1	30:SGG:59:LEU:HB2	1.81	0.45
63:ST0:40:GLY:HA3	63:ST0:91:VAL:HG21	1.97	0.45
1:S60:766:U:H2'	1:S60:767:G:H8	1.80	0.45
1:S60:1000:C:H2'	1:S60:1001:G:H8	1.81	0.45
1:S60:1042:U:O3'	18:SDD:12:LYS:NZ	2.50	0.45
1:S60:1070:G:N2	1:S60:1097:A:OP2	2.48	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LB0:154:ARG:HG2	7:LB0:178:GLN:HA	1.99	0.45
78:L50:706:A:H1'	78:L50:708:A:C5	2.51	0.45
8:SB0:183:ILE:HA	8:SB0:186:ILE:HB	1.98	0.45
35:SI0:90:HIS:NE2	35:SI0:103:THR:OG1	2.38	0.45
46:LN0:73:ARG:NH1	78:L50:112:G:OP1	2.48	0.45
78:L50:1161:G:OP2	78:L50:1161:G:N2	2.49	0.45
1:S60:1049:U:H2'	1:S60:1050:A:H8	1.81	0.45
14:SCC:4:ASN:ND2	24:SF0:103:ASN:OD1	2.47	0.45
49:SNN:149:TYR:HB3	49:SNN:153:LYS:HB3	1.97	0.45
78:L50:374:A:N3	78:L50:378:A:O2'	2.48	0.45
1:S60:419:C:H2'	1:S60:420:A:C8	2.52	0.45
1:S60:754:C:H42	1:S60:1102:G:H1	1.63	0.45
21:LEE:71:ARG:NH1	78:L50:1087:U:OP1	2.50	0.45
78:L50:1703:U:H2'	78:L50:1704:A:H8	1.80	0.45
11:LC0:322:PHE:O	23:LF0:143:ARG:NH2	2.39	0.45
23:LF0:158:HIS:O	23:LF0:159:ARG:NH1	2.49	0.45
40:LL0:17:ARG:HB3	46:LN0:197:THR:HG22	1.98	0.45
49:SNN:101:LYS:HB3	49:SNN:101:LYS:HE3	1.79	0.45
50:LO0:42:THR:OG1	78:L50:1014:U:OP2	2.34	0.45
78:L50:28:U:H2'	78:L50:29:A:H8	1.82	0.45
1:S60:897:C:O2'	1:S60:937:U:O2	2.35	0.45
8:SB0:110:ASP:OD1	8:SB0:110:ASP:N	2.39	0.45
23:LF0:86:LYS:HD3	23:LF0:109:THR:HA	1.99	0.45
78:L50:2166:U:H2'	78:L50:2168:U:H5''	1.98	0.45
8:SB0:103:ASP:N	8:SB0:103:ASP:OD1	2.49	0.45
38:SJ0:61:ASN:ND2	69:SW0:84:GLU:OE2	2.50	0.45
58:LR0:130:ARG:NH2	78:L50:1315:U:OP2	2.35	0.45
78:L50:224:G:O2'	78:L50:283:U:O2	2.33	0.45
16:SD0:162:GLN:HA	16:SD0:165:ARG:HD2	1.98	0.45
57:SQ0:36:VAL:HG22	63:ST0:5:TYR:HB3	1.99	0.45
58:LR0:156:LEU:HD23	58:LR0:159:LYS:HD2	1.98	0.45
61:SS0:48:ILE:HD12	61:SS0:51:ALA:HB3	1.99	0.45
78:L50:1310:G:N2	78:L50:1324:G:O2'	2.43	0.45
6:SAA:44:LEU:O	51:SO0:97:GLN:NE2	2.39	0.44
12:SC0:134:THR:HG21	12:SC0:153:ALA:H	1.82	0.44
30:SGG:125:VAL:HG22	30:SGG:135:LEU:HG	1.98	0.44
37:LJ0:58:ARG:HH11	49:SNN:87:ARG:HG3	1.82	0.44
38:SJ0:115:GLN:OE1	38:SJ0:131:ARG:NE	2.43	0.44
62:LT0:130:GLN:HG2	78:L50:800:U:H5'	1.98	0.44
3:LA0:75:PHE:H	3:LA0:86:ASN:ND2	2.16	0.44
12:SC0:25:VAL:HG11	12:SC0:48:ILE:HG23	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:SE0:88:VAL:HG22	20:SE0:99:ARG:HG2	1.99	0.44
28:SG0:50:GLU:HB3	28:SG0:111:ILE:HG22	1.99	0.44
32:SH0:33:GLN:HB2	32:SH0:47:LYS:HD2	2.00	0.44
36:LII:67:ARG:NE	78:L50:1586:U:O2	2.42	0.44
61:SS0:119:LEU:HA	61:SS0:130:LEU:HD21	2.00	0.44
73:LY0:100:HIS:ND1	73:LY0:102:CYS:SG	2.86	0.44
77:SK0:54:ILE:HD11	77:SK0:65:CYS:HB3	1.98	0.44
2:L70:7:G:OP1	15:LD0:39:ARG:NH1	2.50	0.44
27:LG0:153:MET:HE3	27:LG0:153:MET:HB3	1.87	0.44
29:LGG:17:ASN:OD1	29:LGG:19:ARG:NH2	2.50	0.44
66:LV0:126:SER:OG	66:LV0:127:LEU:N	2.49	0.44
78:L50:315:A:H2'	78:L50:316:G:H8	1.81	0.44
78:L50:1857:A:H2'	78:L50:1858:A:C8	2.53	0.44
15:LD0:277:SER:OG	15:LD0:278:LEU:N	2.49	0.44
20:SE0:87:ASP:N	20:SE0:87:ASP:OD1	2.47	0.44
59:SR0:23:LEU:HD23	59:SR0:57:TYR:HB2	2.00	0.44
65:SU0:5:ILE:HG13	65:SU0:71:TYR:HB2	1.99	0.44
1:S60:388:C:H2'	1:S60:389:A:H8	1.82	0.44
1:S60:929:A:OP1	59:SR0:48:GLN:NE2	2.50	0.44
7:LB0:94:GLU:OE1	7:LB0:149:ARG:NH1	2.51	0.44
37:LJ0:16:ILE:HG22	37:LJ0:125:PHE:HD2	1.82	0.44
38:SJ0:64:GLU:H	38:SJ0:64:GLU:HG3	1.66	0.44
41:SL0:3:ASP:OD2	41:SL0:3:ASP:N	2.49	0.44
50:LO0:12:HIS:HE1	50:LO0:118:PHE:HB2	1.83	0.44
53:LP0:31:ARG:HB2	53:LP0:120:ILE:HD11	1.99	0.44
57:SQ0:54:ILE:HD12	57:SQ0:54:ILE:HA	1.91	0.44
68:LW0:16:GLY:O	78:L50:2314:C:O2'	2.36	0.44
69:SW0:52:ASP:OD1	69:SW0:52:ASP:N	2.50	0.44
78:L50:1935:U:H2'	78:L50:1936:A:H8	1.82	0.44
4:SA0:40:ARG:NH2	59:SR0:98:ASP:OD2	2.41	0.44
15:LD0:33:LYS:HE2	37:LJ0:142:PHE:HE1	1.82	0.44
15:LD0:215:LEU:HB3	15:LD0:223:PHE:HB2	1.98	0.44
32:SH0:38:ASP:HB3	32:SH0:42:LYS:HD3	1.99	0.44
1:S60:421:A:OP1	38:SJ0:37:LYS:NZ	2.49	0.44
4:SA0:88:LYS:HD3	4:SA0:88:LYS:HA	1.84	0.44
29:LGG:20:LYS:NZ	78:L50:1336:U:O2'	2.49	0.44
34:LI0:154:ARG:NH1	78:L50:2107:A:OP1	2.46	0.44
51:SO0:87:VAL:HG12	51:SO0:123:LYS:HG2	1.99	0.44
78:L50:521:U:H2'	78:L50:522:A:H8	1.83	0.44
1:S60:776:A:N3	1:S60:803:C:O2'	2.45	0.44
17:LDD:25:ASN:OD1	17:LDD:25:ASN:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:LI0:87:LEU:HD13	34:LI0:138:ILE:HG12	2.00	0.44
54:SP0:84:TRP:HB2	54:SP0:87:MET:HE3	1.99	0.44
63:ST0:3:GLU:O	63:ST0:6:THR:OG1	2.32	0.44
78:L50:1086:G:N2	78:L50:1089:A:OP2	2.45	0.44
3:LA0:186:ARG:NH1	78:L50:1530:A:OP2	2.51	0.44
3:LA0:219:GLN:NE2	78:L50:1882:G:OP1	2.43	0.44
7:LB0:281:ILE:HG12	7:LB0:316:ILE:HG13	2.00	0.44
11:LC0:301:PRO:O	23:LF0:27:LYS:NZ	2.42	0.44
30:SGG:242:LYS:HA	30:SGG:258:ALA:HA	2.00	0.44
31:LH0:49:ASP:OD1	31:LH0:49:ASP:N	2.51	0.44
47:SN0:39:LYS:HB2	47:SN0:39:LYS:HE2	1.80	0.44
74:SY0:57:VAL:HG12	74:SY0:73:VAL:HG22	2.00	0.44
1:S60:1232:U:H2'	1:S60:1233:A:H8	1.83	0.43
1:S60:126:G:H4'	28:SG0:15:MET:HE2	1.99	0.43
1:S60:870:U:O2	1:S60:906:G:N2	2.38	0.43
3:LA0:39:ASP:N	3:LA0:39:ASP:OD1	2.49	0.43
30:SGG:287:ASP:OD1	30:SGG:287:ASP:N	2.47	0.43
1:S60:941:U:H2'	1:S60:942:G:H8	1.82	0.43
8:SB0:91:ASN:OD1	8:SB0:91:ASN:N	2.51	0.43
11:LC0:205:LEU:HB2	11:LC0:244:ARG:HH11	1.82	0.43
32:SH0:56:SER:OG	47:SN0:65:THR:O	2.37	0.43
48:LNN:131:ARG:NH2	78:L50:1921:C:OP2	2.41	0.43
50:LO0:75:SER:N	50:LO0:104:GLU:OE2	2.50	0.43
54:SP0:14:TYR:HE2	54:SP0:33:LEU:HB3	1.83	0.43
54:SP0:64:MET:HE3	54:SP0:66:ASN:H	1.84	0.43
72:LXX:69:ASP:OD1	72:LXX:69:ASP:N	2.51	0.43
74:SY0:63:THR:OG1	74:SY0:66:THR:OG1	2.30	0.43
78:L50:1303:A:H2'	78:L50:1304:A:H8	1.84	0.43
78:L50:2461:G:H2'	78:L50:2462:C:H6	1.83	0.43
27:LG0:88:PRO:O	78:L50:199:G:N2	2.52	0.43
61:SS0:132:ARG:HB3	61:SS0:137:LEU:HB2	2.01	0.43
62:LT0:90:VAL:HG21	62:LT0:95:LEU:HD21	2.00	0.43
78:L50:1242:G:N2	78:L50:1245:A:OP2	2.44	0.43
1:S60:229:A:H2'	1:S60:230:A:H8	1.83	0.43
1:S60:362:A:H5'	74:SY0:67:HIS:HE1	1.83	0.43
2:L70:4:U:H2'	2:L70:5:A:H8	1.83	0.43
13:LCC:57:LEU:HD23	13:LCC:57:LEU:HA	1.90	0.43
15:LD0:66:VAL:HB	15:LD0:86:SER:HB2	2.01	0.43
41:SL0:52:TYR:HH	41:SL0:113:CYS:HG	1.64	0.43
47:SN0:88:ASP:OD1	47:SN0:88:ASP:N	2.49	0.43
78:L50:1291:A:H2'	78:L50:1292:A:H8	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S60:823:A:H3'	1:S60:824:A:H8	1.83	0.43
4:SA0:39:THR:HB	4:SA0:46:LYS:HD3	2.01	0.43
28:SG0:3:LEU:HD23	28:SG0:18:ILE:HD11	2.00	0.43
39:LJJ:25:MET:HE3	39:LJJ:25:MET:HB3	1.83	0.43
59:SR0:97:VAL:HG21	59:SR0:114:PHE:HB3	2.00	0.43
74:SY0:25:LEU:HD23	74:SY0:73:VAL:HG23	2.00	0.43
1:S60:185:G:O3'	35:SI0:37:SER:OG	2.35	0.43
6:SAA:26:CYS:SG	6:SAA:27:GLY:N	2.92	0.43
27:LG0:122:GLU:HA	27:LG0:125:LEU:HD12	2.01	0.43
36:LII:85:LYS:HA	36:LII:85:LYS:HD2	1.85	0.43
37:LJ0:107:HIS:CD2	37:LJ0:121:TYR:H	2.35	0.43
47:SN0:38:LEU:HD23	47:SN0:38:LEU:HA	1.90	0.43
61:SS0:94:PHE:HB3	61:SS0:97:ASN:HB3	2.01	0.43
70:LX0:41:THR:HG22	70:LX0:85:LYS:HA	1.99	0.43
78:L50:1863:U:H2'	78:L50:1864:A:H8	1.84	0.43
4:SA0:130:LYS:HE3	4:SA0:130:LYS:HB3	1.90	0.43
29:LGG:64:GLN:O	29:LGG:69:ARG:NH2	2.52	0.43
30:SGG:78:ASN:OD1	30:SGG:78:ASN:N	2.52	0.43
34:LI0:142:LYS:HB3	34:LI0:142:LYS:HE2	1.75	0.43
64:LU0:84:LEU:HA	64:LU0:87:PHE:HD1	1.84	0.43
73:LY0:54:ASP:OD1	73:LY0:54:ASP:N	2.50	0.43
5:LAA:16:SER:OG	5:LAA:17:HIS:N	2.52	0.43
11:LC0:192:LYS:NZ	78:L50:1102:G:OP2	2.41	0.43
12:SC0:218:LEU:HA	67:SV0:23:GLN:HE22	1.82	0.43
13:LCC:15:LEU:HD23	13:LCC:15:LEU:HA	1.92	0.43
19:LE0:120:LYS:HD3	19:LE0:120:LYS:HA	1.83	0.43
69:SW0:45:THR:OG1	69:SW0:61:TRP:O	2.36	0.43
78:L50:1799:A:H2'	78:L50:1800:A:H8	1.84	0.43
1:S60:642:G:OP2	47:SN0:9:ARG:NH1	2.46	0.43
18:SDD:11:ILE:O	18:SDD:13:GLN:NE2	2.51	0.43
30:SGG:5:ASP:OD2	30:SGG:7:ARG:NH2	2.43	0.43
46:LN0:38:ARG:HH12	46:LN0:60:LEU:HD22	1.83	0.43
53:LP0:7:TYR:OH	53:LP0:116:ASP:OD2	2.29	0.43
59:SR0:86:LYS:HA	59:SR0:86:LYS:HD3	1.94	0.43
60:LS0:87:SER:OG	60:LS0:134:ASP:OD1	2.36	0.43
7:LB0:5:LYS:NZ	78:L50:2147:U:OP1	2.40	0.42
12:SC0:33:LEU:HG	12:SC0:52:LEU:HD13	2.01	0.42
30:SGG:19:VAL:HA	30:SGG:37:SER:HA	2.00	0.42
30:SGG:133:ILE:O	30:SGG:146:PHE:N	2.40	0.42
41:SL0:45:LYS:HA	41:SL0:45:LYS:HD2	1.83	0.42
46:LN0:24:ARG:NH2	78:L50:1795:A:O2'	2.46	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:SO0:11:TYR:OH	51:SO0:72:ARG:O	2.30	0.42
51:SO0:38:CYS:SG	51:SO0:39:ARG:N	2.91	0.42
61:SS0:77:LYS:HD2	61:SS0:77:LYS:HA	1.85	0.42
78:L50:2287:U:H2'	78:L50:2288:A:H8	1.84	0.42
1:S60:961:A:H2'	1:S60:962:A:C8	2.54	0.42
27:LG0:8:GLN:H	27:LG0:8:GLN:HG3	1.71	0.42
28:SG0:49:PHE:HE1	28:SG0:112:VAL:HG22	1.84	0.42
56:LQ0:79:LYS:HA	56:LQ0:136:ASN:HB3	2.01	0.42
60:LS0:98:ASN:OD1	60:LS0:98:ASN:N	2.52	0.42
69:SW0:33:ASP:HB3	69:SW0:107:ILE:HD12	2.00	0.42
75:LZ0:99:VAL:HA	75:LZ0:102:LYS:HD2	1.99	0.42
1:S60:1014:U:OP1	63:ST0:42:GLU:N	2.45	0.42
37:LJ0:16:ILE:HD12	37:LJ0:35:LEU:HD22	2.00	0.42
43:LM0:55:ASP:OD1	43:LM0:55:ASP:N	2.39	0.42
75:LZ0:98:GLU:HG3	75:LZ0:102:LYS:HE3	2.01	0.42
78:L50:1002:A:O2'	78:L50:1003:A:O4'	2.32	0.42
78:L50:1935:U:OP1	78:L50:2024:C:O2'	2.37	0.42
1:S60:499:U:H2'	1:S60:500:G:H8	1.85	0.42
7:LB0:210:ASN:HB3	7:LB0:275:ASN:HA	2.01	0.42
8:SB0:111:LYS:HA	8:SB0:111:LYS:HD3	1.82	0.42
11:LC0:173:LEU:HD21	11:LC0:204:LEU:HD13	1.99	0.42
28:SG0:58:GLN:OE1	28:SG0:71:ARG:NH2	2.48	0.42
48:LNN:103:ASP:HB3	78:L50:2141:A:C8	2.54	0.42
1:S60:348:U:H2'	1:S60:349:A:H8	1.84	0.42
3:LA0:138:SER:OG	78:L50:1540:G:N7	2.46	0.42
10:SBB:44:CYS:HB2	10:SBB:63:CYS:SG	2.60	0.42
28:SG0:103:GLU:H	28:SG0:103:GLU:HG3	1.64	0.42
28:SG0:114:LYS:HB2	28:SG0:114:LYS:HE3	1.83	0.42
78:L50:233:U:H2'	78:L50:234:A:H8	1.85	0.42
78:L50:1292:A:H2'	78:L50:1293:A:C8	2.54	0.42
78:L50:2411:U:H4'	78:L50:2412:U:H5''	2.01	0.42
15:LD0:48:ASN:HD21	62:LT0:68:PRO:HG3	1.83	0.42
24:SF0:130:LYS:HA	24:SF0:130:LYS:HD2	1.90	0.42
29:LGG:50:LEU:HD21	29:LGG:80:CYS:HA	2.00	0.42
33:LHH:34:LYS:NZ	78:L50:50:A:O2'	2.52	0.42
40:LL0:44:PRO:HG2	40:LL0:128:ALA:HB1	2.01	0.42
49:SNN:32:CYS:SG	49:SNN:64:SER:OG	2.71	0.42
75:LZ0:74:THR:OG1	75:LZ0:75:ARG:N	2.52	0.42
78:L50:1801:U:H2'	78:L50:1802:A:H8	1.84	0.42
1:S60:110:A:H2'	1:S60:111:A:C8	2.55	0.42
4:SA0:148:ASN:H	4:SA0:151:ASN:HD22	1.67	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LFF:84:VAL:HG12	25:LFF:85:THR:HG23	2.02	0.42
31:LH0:101:GLU:HB3	31:LH0:110:LEU:HB3	2.02	0.42
32:SH0:123:VAL:HG23	32:SH0:153:VAL:HG13	2.01	0.42
1:S60:1050:A:OP1	63:ST0:36:LYS:NZ	2.52	0.42
33:LHH:98:GLN:O	46:LN0:149:ASN:ND2	2.52	0.42
34:LI0:61:SER:HA	34:LI0:126:VAL:HG12	2.00	0.42
45:SM0:56:GLU:OE2	45:SM0:79:SER:OG	2.36	0.42
1:S60:331:A:H2'	1:S60:332:A:H8	1.85	0.42
1:S60:758:G:H2'	1:S60:759:A:C8	2.55	0.42
1:S60:1242:A:C6	6:SAA:87:ARG:HD2	2.55	0.42
31:LH0:2:THR:HG22	31:LH0:60:LYS:HA	2.01	0.42
68:LW0:64:LEU:HD23	68:LW0:64:LEU:HA	1.90	0.42
74:SY0:127:LYS:HA	74:SY0:127:LYS:HD3	1.81	0.42
78:L50:1447:U:N3	78:L50:1505:A:OP2	2.43	0.42
1:S60:218:U:H2'	1:S60:219:A:C8	2.55	0.42
1:S60:260:U:H2'	1:S60:261:A:C8	2.53	0.42
4:SA0:146:PHE:O	4:SA0:164:ASN:ND2	2.52	0.42
8:SB0:201:LYS:HB2	8:SB0:201:LYS:HE3	1.90	0.42
14:SCC:18:ASP:OD1	14:SCC:18:ASP:N	2.52	0.42
20:SE0:101:PHE:HE2	20:SE0:234:PRO:HG3	1.85	0.42
34:LI0:36:SER:HB2	34:LI0:69:ARG:HH21	1.85	0.42
34:LI0:191:LEU:HD11	34:LI0:200:LEU:HD13	2.02	0.42
56:LQ0:71:LYS:HE2	56:LQ0:71:LYS:HB3	1.79	0.42
24:SF0:30:ARG:HA	24:SF0:30:ARG:HD3	1.87	0.41
37:LJ0:136:VAL:HG13	37:LJ0:139:ARG:HH21	1.85	0.41
65:SU0:81:GLU:HA	65:SU0:84:ILE:HD12	2.00	0.41
76:SZ0:52:LYS:H	76:SZ0:52:LYS:HG2	1.74	0.41
1:S60:806:U:H2'	1:S60:807:A:C8	2.55	0.41
56:LQ0:104:LEU:HD12	56:LQ0:104:LEU:HA	1.88	0.41
1:S60:811:U:O2'	77:SK0:50:ASP:OD2	2.38	0.41
5:LAA:99:PRO:HG2	5:LAA:122:VAL:HG12	2.02	0.41
12:SC0:19:THR:HG22	12:SC0:21:LEU:H	1.86	0.41
14:SCC:44:ILE:HG22	24:SF0:125:ASP:HB2	2.02	0.41
36:LII:51:PRO:HD2	46:LN0:15:GLN:HB3	2.02	0.41
38:SJ0:133:LEU:HD23	38:SJ0:139:ILE:HD11	2.02	0.41
41:SL0:64:LYS:HE3	41:SL0:64:LYS:HB2	1.86	0.41
57:SQ0:53:ILE:HD11	57:SQ0:94:ARG:HG2	2.02	0.41
72:LXX:21:PHE:CG	72:LXX:29:MET:HE1	2.54	0.41
78:L50:1306:U:H2'	78:L50:1307:A:H8	1.84	0.41
1:S60:259:C:O2'	28:SG0:91:ARG:O	2.39	0.41
16:SD0:116:LYS:O	16:SD0:120:ASN:ND2	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:LMM:97:LEU:HD21	44:LMM:105:ARG:HB2	2.03	0.41
54:SP0:53:LEU:HD21	54:SP0:76:THR:HB	2.02	0.41
78:L50:460:U:H2'	78:L50:461:A:H8	1.86	0.41
78:L50:1863:U:H2'	78:L50:1864:A:C8	2.56	0.41
78:L50:1873:A:H2'	78:L50:1874:A:C8	2.55	0.41
3:LA0:126:ARG:HA	3:LA0:126:ARG:HD2	1.77	0.41
29:LGG:73:ARG:NH2	78:L50:1246:C:OP2	2.49	0.41
41:SL0:29:LYS:HA	41:SL0:29:LYS:HD2	1.87	0.41
46:LN0:86:ASN:OD1	46:LN0:86:ASN:N	2.52	0.41
47:SN0:12:SER:O	47:SN0:12:SER:OG	2.30	0.41
54:SP0:90:SER:OG	54:SP0:91:ILE:N	2.52	0.41
11:LC0:298:LEU:HD22	56:LQ0:41:ASN:HB2	2.03	0.41
32:SH0:115:SER:HB3	32:SH0:118:GLU:HB2	2.02	0.41
38:SJ0:43:VAL:HG21	38:SJ0:110:LEU:HD21	2.02	0.41
41:SL0:7:LYS:HD2	41:SL0:7:LYS:HA	1.78	0.41
51:SO0:10:GLU:HG2	51:SO0:75:LYS:HB2	2.02	0.41
54:SP0:77:HIS:NE2	54:SP0:100:TYR:OH	2.49	0.41
74:SY0:78:ASN:HD22	74:SY0:80:ASP:H	1.69	0.41
75:LZ0:42:LYS:HE3	75:LZ0:56:ASN:HD21	1.85	0.41
78:L50:1294:U:H2'	78:L50:1295:U:C6	2.56	0.41
78:L50:1434:G:O2'	78:L50:1693:U:O4	2.30	0.41
2:L70:36:C:H2'	2:L70:37:G:C8	2.55	0.41
7:LB0:81:GLU:OE1	7:LB0:313:ASN:ND2	2.51	0.41
20:SE0:208:SER:O	20:SE0:208:SER:OG	2.32	0.41
23:LF0:78:GLU:HB2	62:LT0:135:PRO:HB2	2.03	0.41
30:SGG:279:THR:OG1	30:SGG:282:ALA:O	2.35	0.41
44:LMM:121:LYS:HE3	44:LMM:121:LYS:HB3	1.88	0.41
77:SK0:54:ILE:HA	77:SK0:67:ALA:HA	2.02	0.41
1:S60:491:U:H2'	1:S60:492:G:H8	1.86	0.41
16:SD0:55:PRO:HG3	16:SD0:90:LYS:HG2	2.03	0.41
19:LE0:133:MET:O	19:LE0:137:GLU:N	2.52	0.41
28:SG0:63:SER:OG	28:SG0:64:LYS:N	2.54	0.41
30:SGG:83:VAL:HG23	30:SGG:93:ILE:HG12	2.03	0.41
35:SI0:80:ASN:OD1	35:SI0:80:ASN:N	2.54	0.41
36:LII:28:LYS:NZ	78:L50:325:A:OP2	2.40	0.41
78:L50:255:U:H2'	78:L50:256:A:C8	2.55	0.41
1:S60:29:C:OP1	71:SX0:135:LYS:NZ	2.53	0.41
1:S60:315:G:H3'	1:S60:316:G:H21	1.85	0.41
1:S60:806:U:H2'	1:S60:807:A:H8	1.86	0.41
7:LB0:41:ILE:HG12	7:LB0:181:GLY:HA3	2.02	0.41
18:SDD:33:CYS:CB	18:SDD:36:CYS:SG	3.08	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:SE0:187:ASP:HA	20:SE0:240:ARG:HH22	1.86	0.41
28:SG0:154:THR:O	28:SG0:158:ASP:N	2.54	0.41
31:LH0:74:LEU:HD12	31:LH0:74:LEU:HA	1.91	0.41
51:SO0:126:MET:HE2	51:SO0:126:MET:HB3	1.92	0.41
60:LS0:170:LEU:HD12	60:LS0:170:LEU:HA	1.94	0.41
63:ST0:14:ASN:HA	63:ST0:17:LYS:HE2	2.03	0.41
70:LX0:31:LYS:NZ	78:L50:1181:U:OP1	2.49	0.41
72:LXX:41:ARG:NH2	78:L50:1199:A:OP1	2.49	0.41
1:S60:626:A:OP1	47:SN0:108:ARG:NE	2.53	0.41
30:SGG:119:LYS:NZ	30:SGG:165:SER:O	2.37	0.41
34:LI0:54:SER:OG	34:LI0:55:HIS:N	2.53	0.41
44:LMM:105:ARG:NH1	78:L50:2382:U:OP2	2.49	0.41
78:L50:1079:U:H2'	78:L50:1080:A:H8	1.86	0.41
78:L50:1935:U:H2'	78:L50:1936:A:C8	2.56	0.41
1:S60:388:C:H2'	1:S60:389:A:C8	2.57	0.40
7:LB0:305:PHE:HB2	7:LB0:308:TYR:HB3	2.02	0.40
17:LDD:14:THR:HG22	17:LDD:74:ARG:HD3	2.03	0.40
35:SI0:80:ASN:HD21	35:SI0:115:ILE:HG23	1.85	0.40
57:SQ0:17:ALA:HB1	57:SQ0:89:LEU:HD23	2.03	0.40
72:LXX:52:LYS:HE3	72:LXX:52:LYS:HB3	1.86	0.40
78:L50:1801:U:H2'	78:L50:1802:A:C8	2.56	0.40
7:LB0:322:ILE:HD13	7:LB0:322:ILE:HA	1.90	0.40
9:LBB:30:LEU:HD13	9:LBB:43:MET:HE1	2.03	0.40
12:SC0:59:ASP:OD1	12:SC0:59:ASP:N	2.54	0.40
15:LD0:253:LYS:HD3	15:LD0:253:LYS:HA	1.90	0.40
27:LG0:131:CYS:HB3	27:LG0:136:ILE:HB	2.03	0.40
33:LHH:88:ARG:NH1	78:L50:38:A:OP2	2.54	0.40
41:SL0:83:ILE:HD11	41:SL0:140:VAL:HG21	2.03	0.40
78:L50:1335:U:O2'	78:L50:1339:A:O2'	2.33	0.40
12:SC0:57:ILE:HD13	12:SC0:57:ILE:HA	1.95	0.40
20:SE0:22:SER:OG	20:SE0:23:ILE:N	2.50	0.40
51:SO0:79:PHE:HB2	51:SO0:113:ILE:HG12	2.04	0.40
58:LR0:140:ASN:OD1	58:LR0:140:ASN:N	2.53	0.40
78:L50:28:U:H2'	78:L50:29:A:C8	2.57	0.40
1:S60:1232:U:H2'	1:S60:1233:A:C8	2.57	0.40
4:SA0:50:ILE:H	4:SA0:50:ILE:HG13	1.78	0.40
11:LC0:30:ARG:HG3	11:LC0:123:MET:HE1	2.04	0.40
11:LC0:254:LYS:HD2	11:LC0:254:LYS:HA	1.80	0.40
25:LFF:91:ARG:HD3	25:LFF:91:ARG:HA	1.85	0.40
41:SL0:91:VAL:HG21	41:SL0:102:ARG:HE	1.87	0.40
49:SNN:140:ASP:N	49:SNN:140:ASP:OD1	2.50	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:LR0:100:LEU:HD12	58:LR0:100:LEU:HA	1.89	0.40
65:SU0:76:SER:HB2	65:SU0:79:GLN:HG2	2.03	0.40
60:LS0:134:ASP:OD1	60:LS0:134:ASP:N	2.55	0.40
78:L50:97:U:H2'	78:L50:98:A:H8	1.86	0.40
78:L50:547:U:H2'	78:L50:548:A:H8	1.87	0.40
78:L50:1287:A:H5''	78:L50:1288:A:H5'	2.04	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	
3	LA0	230/237 (97%)	216 (94%)	14 (6%)	0	100	100
4	SA0	195/264 (74%)	189 (97%)	6 (3%)	0	100	100
5	LAA	146/148 (99%)	135 (92%)	11 (8%)	0	100	100
6	SAA	95/104 (91%)	89 (94%)	6 (6%)	0	100	100
7	LB0	364/384 (95%)	353 (97%)	11 (3%)	0	100	100
8	SB0	206/237 (87%)	195 (95%)	11 (5%)	0	100	100
9	LBB	49/55 (89%)	45 (92%)	4 (8%)	0	100	100
10	SBB	80/94 (85%)	76 (95%)	4 (5%)	0	100	100
11	LC0	327/334 (98%)	312 (95%)	15 (5%)	0	100	100
12	SC0	215/237 (91%)	206 (96%)	9 (4%)	0	100	100
13	LCC	102/108 (94%)	101 (99%)	1 (1%)	0	100	100
14	SCC	61/67 (91%)	58 (95%)	3 (5%)	0	100	100
15	LD0	280/295 (95%)	273 (98%)	7 (2%)	0	100	100
16	SD0	208/215 (97%)	203 (98%)	5 (2%)	0	100	100
17	LDD	100/111 (90%)	91 (91%)	9 (9%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	SDD	65/68 (96%)	59 (91%)	6 (9%)	0	100	100
19	LE0	170/172 (99%)	163 (96%)	7 (4%)	0	100	100
20	SE0	254/262 (97%)	242 (95%)	11 (4%)	1 (0%)	30	59
21	LEE	121/139 (87%)	118 (98%)	3 (2%)	0	100	100
22	SEE	54/60 (90%)	52 (96%)	2 (4%)	0	100	100
23	LF0	228/239 (95%)	216 (95%)	12 (5%)	0	100	100
24	SF0	186/189 (98%)	182 (98%)	4 (2%)	0	100	100
25	LFF	94/98 (96%)	90 (96%)	4 (4%)	0	100	100
26	SFF	66/151 (44%)	65 (98%)	1 (2%)	0	100	100
27	LG0	193/200 (96%)	186 (96%)	7 (4%)	0	100	100
28	SG0	197/217 (91%)	188 (95%)	9 (5%)	0	100	100
29	LGG	98/106 (92%)	94 (96%)	4 (4%)	0	100	100
30	SGG	328/337 (97%)	314 (96%)	14 (4%)	0	100	100
31	LH0	182/186 (98%)	172 (94%)	10 (6%)	0	100	100
32	SH0	153/161 (95%)	145 (95%)	8 (5%)	0	100	100
33	LHH	118/122 (97%)	113 (96%)	5 (4%)	0	100	100
34	LI0	214/217 (99%)	199 (93%)	15 (7%)	0	100	100
35	SI0	156/166 (94%)	150 (96%)	6 (4%)	0	100	100
36	LII	91/95 (96%)	88 (97%)	3 (3%)	0	100	100
37	LJ0	166/171 (97%)	159 (96%)	7 (4%)	0	100	100
38	SJ0	169/189 (89%)	162 (96%)	7 (4%)	0	100	100
39	LJJ	88/93 (95%)	84 (96%)	4 (4%)	0	100	100
40	LL0	160/162 (99%)	150 (94%)	10 (6%)	0	100	100
41	SL0	155/158 (98%)	147 (95%)	8 (5%)	0	100	100
42	LLL	49/52 (94%)	46 (94%)	3 (6%)	0	100	100
43	LM0	87/105 (83%)	83 (95%)	4 (5%)	0	100	100
44	LMM	48/127 (38%)	45 (94%)	3 (6%)	0	100	100
45	SM0	117/131 (89%)	113 (97%)	4 (3%)	0	100	100
46	LN0	201/204 (98%)	191 (95%)	10 (5%)	0	100	100
47	SN0	145/149 (97%)	139 (96%)	6 (4%)	0	100	100
48	LNN	74/160 (46%)	67 (90%)	7 (10%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	SNN	165/168 (98%)	152 (92%)	13 (8%)	0	100	100
50	LO0	169/192 (88%)	165 (98%)	4 (2%)	0	100	100
51	SO0	129/135 (96%)	124 (96%)	5 (4%)	0	100	100
52	LOO	96/103 (93%)	94 (98%)	2 (2%)	0	100	100
53	LP0	152/169 (90%)	147 (97%)	5 (3%)	0	100	100
54	SP0	116/143 (81%)	112 (97%)	4 (3%)	0	100	100
55	LPP	81/89 (91%)	76 (94%)	5 (6%)	0	100	100
56	LQ0	182/193 (94%)	169 (93%)	13 (7%)	0	100	100
57	SQ0	150/155 (97%)	143 (95%)	7 (5%)	0	100	100
58	LR0	163/175 (93%)	160 (98%)	3 (2%)	0	100	100
59	SR0	115/119 (97%)	112 (97%)	3 (3%)	0	100	100
60	LS0	177/180 (98%)	167 (94%)	10 (6%)	0	100	100
61	SS0	149/160 (93%)	142 (95%)	7 (5%)	0	100	100
62	LT0	157/160 (98%)	151 (96%)	6 (4%)	0	100	100
63	ST0	129/133 (97%)	124 (96%)	5 (4%)	0	100	100
64	LU0	95/107 (89%)	91 (96%)	4 (4%)	0	100	100
65	SU0	94/101 (93%)	86 (92%)	8 (8%)	0	100	100
66	LV0	133/146 (91%)	126 (95%)	7 (5%)	0	100	100
67	SV0	61/67 (91%)	56 (92%)	5 (8%)	0	100	100
68	LW0	88/91 (97%)	84 (96%)	3 (3%)	1 (1%)	11	38
69	SW0	125/127 (98%)	121 (97%)	4 (3%)	0	100	100
70	LX0	91/102 (89%)	84 (92%)	7 (8%)	0	100	100
71	SX0	136/140 (97%)	134 (98%)	2 (2%)	0	100	100
72	LXX	53/73 (73%)	53 (100%)	0	0	100	100
73	LY0	132/139 (95%)	126 (96%)	6 (4%)	0	100	100
74	SY0	121/133 (91%)	115 (95%)	6 (5%)	0	100	100
75	LZ0	123/126 (98%)	114 (93%)	9 (7%)	0	100	100
76	SZ0	89/123 (72%)	84 (94%)	5 (6%)	0	100	100
77	SK0	83/99 (84%)	82 (99%)	1 (1%)	0	100	100
All	All	10639/11624 (92%)	10158 (96%)	479 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
68	LW0	73	PRO
20	SE0	23	ILE

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	
3	LA0	193/197 (98%)	190 (98%)	3 (2%)	55	68
4	SA0	179/237 (76%)	179 (100%)	0	100	100
5	LAA	126/126 (100%)	125 (99%)	1 (1%)	73	77
6	SAA	86/93 (92%)	84 (98%)	2 (2%)	44	63
7	LB0	318/334 (95%)	317 (100%)	1 (0%)	86	84
8	SB0	186/210 (89%)	186 (100%)	0	100	100
9	LBB	43/47 (92%)	43 (100%)	0	100	100
10	SBB	70/82 (85%)	69 (99%)	1 (1%)	59	70
11	LC0	287/292 (98%)	286 (100%)	1 (0%)	86	84
12	SC0	179/198 (90%)	178 (99%)	1 (1%)	78	80
13	LCC	88/92 (96%)	88 (100%)	0	100	100
14	SCC	52/56 (93%)	52 (100%)	0	100	100
15	LD0	247/256 (96%)	247 (100%)	0	100	100
16	SD0	185/189 (98%)	183 (99%)	2 (1%)	65	74
17	LDD	93/101 (92%)	93 (100%)	0	100	100
18	SDD	58/59 (98%)	58 (100%)	0	100	100
19	LE0	162/163 (99%)	160 (99%)	2 (1%)	63	72
20	SE0	231/237 (98%)	230 (100%)	1 (0%)	84	83
21	LEE	109/122 (89%)	109 (100%)	0	100	100
22	SEE	47/49 (96%)	46 (98%)	1 (2%)	47	64
23	LF0	208/216 (96%)	208 (100%)	0	100	100
24	SF0	162/163 (99%)	162 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	LFF	86/88 (98%)	86 (100%)	0	100	100
27	LG0	175/180 (97%)	175 (100%)	0	100	100
28	SG0	163/189 (86%)	163 (100%)	0	100	100
29	LGG	90/94 (96%)	89 (99%)	1 (1%)	65	74
30	SGG	280/295 (95%)	277 (99%)	3 (1%)	65	74
31	LH0	162/164 (99%)	161 (99%)	1 (1%)	78	80
32	SH0	148/153 (97%)	148 (100%)	0	100	100
33	LHH	114/116 (98%)	114 (100%)	0	100	100
34	LI0	183/184 (100%)	182 (100%)	1 (0%)	81	81
35	SI0	136/144 (94%)	135 (99%)	1 (1%)	76	78
36	LII	83/85 (98%)	83 (100%)	0	100	100
37	LJ0	148/151 (98%)	148 (100%)	0	100	100
38	SJ0	157/173 (91%)	157 (100%)	0	100	100
39	LJJ	76/79 (96%)	76 (100%)	0	100	100
40	LL0	144/144 (100%)	144 (100%)	0	100	100
41	SL0	141/142 (99%)	141 (100%)	0	100	100
42	LLL	46/47 (98%)	46 (100%)	0	100	100
43	LM0	85/96 (88%)	85 (100%)	0	100	100
44	LMM	46/112 (41%)	46 (100%)	0	100	100
45	SM0	100/112 (89%)	100 (100%)	0	100	100
46	LN0	176/177 (99%)	176 (100%)	0	100	100
47	SN0	134/136 (98%)	134 (100%)	0	100	100
48	LNN	46/153 (30%)	46 (100%)	0	100	100
49	SNN	158/159 (99%)	158 (100%)	0	100	100
50	LO0	148/177 (84%)	148 (100%)	0	100	100
51	SO0	102/105 (97%)	101 (99%)	1 (1%)	68	75
52	LOO	89/93 (96%)	89 (100%)	0	100	100
53	LP0	133/148 (90%)	133 (100%)	0	100	100
54	SP0	103/122 (84%)	103 (100%)	0	100	100
55	LPP	67/72 (93%)	67 (100%)	0	100	100
56	LQ0	166/174 (95%)	166 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	SQ0	132/134 (98%)	132 (100%)	0	100	100
58	LR0	141/151 (93%)	140 (99%)	1 (1%)	76	78
59	SR0	108/110 (98%)	106 (98%)	2 (2%)	50	66
60	LS0	162/163 (99%)	161 (99%)	1 (1%)	78	80
61	SS0	129/137 (94%)	129 (100%)	0	100	100
62	LT0	141/142 (99%)	141 (100%)	0	100	100
63	ST0	119/121 (98%)	119 (100%)	0	100	100
64	LU0	90/99 (91%)	90 (100%)	0	100	100
65	SU0	87/92 (95%)	87 (100%)	0	100	100
66	LV0	110/118 (93%)	110 (100%)	0	100	100
67	SV0	56/60 (93%)	56 (100%)	0	100	100
68	LW0	67/82 (82%)	67 (100%)	0	100	100
69	SW0	111/111 (100%)	111 (100%)	0	100	100
70	LX0	81/90 (90%)	81 (100%)	0	100	100
71	SX0	116/119 (98%)	116 (100%)	0	100	100
72	LXX	49/66 (74%)	49 (100%)	0	100	100
73	LY0	119/124 (96%)	119 (100%)	0	100	100
74	SY0	116/123 (94%)	116 (100%)	0	100	100
75	LZ0	110/111 (99%)	108 (98%)	2 (2%)	51	67
76	SZ0	84/114 (74%)	84 (100%)	0	100	100
77	SK0	80/92 (87%)	80 (100%)	0	100	100
All	All	9402/10142 (93%)	9372 (100%)	30 (0%)	84	84

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	LA0	65	THR
3	LA0	184	ARG
3	LA0	207	ARG
5	LAA	92	ASP
6	SAA	66	ARG
6	SAA	75	ILE
7	LB0	255	ARG
10	SBB	47	CYS
11	LC0	196	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	SC0	164	VAL
16	SD0	116	LYS
16	SD0	177	THR
19	LE0	125	MET
19	LE0	145	ARG
20	SE0	5	ARG
22	SEE	7	ILE
29	LGG	55	ARG
30	SGG	152	ASN
30	SGG	166	ARG
30	SGG	233	PHE
31	LH0	138	LYS
34	LI0	69	ARG
35	SI0	119	ASP
51	SO0	20	THR
58	LR0	68	ARG
59	SR0	4	ARG
59	SR0	62	LYS
60	LS0	117	ARG
75	LZ0	42	LYS
75	LZ0	48	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S60	1224/1244 (98%)	311 (25%)	11 (0%)
2	L70	117/119 (98%)	24 (20%)	2 (1%)
78	L50	2296/2484 (92%)	483 (21%)	17 (0%)
All	All	3637/3847 (94%)	818 (22%)	30 (0%)

All (818) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S60	10	A
1	S60	16	C
1	S60	32	U
1	S60	33	U
1	S60	40	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S60	41	A
1	S60	43	U
1	S60	44	A
1	S60	45	A
1	S60	55	G
1	S60	58	U
1	S60	59	U
1	S60	62	A
1	S60	63	U
1	S60	64	A
1	S60	65	U
1	S60	66	G
1	S60	67	G
1	S60	69	A
1	S60	71	A
1	S60	74	G
1	S60	79	G
1	S60	85	U
1	S60	87	A
1	S60	97	U
1	S60	99	U
1	S60	120	A
1	S60	122	C
1	S60	125	C
1	S60	126	G
1	S60	127	U
1	S60	138	C
1	S60	139	A
1	S60	154	U
1	S60	164	A
1	S60	170	C
1	S60	172	G
1	S60	176	G
1	S60	178	U
1	S60	191	G
1	S60	192	C
1	S60	206	G
1	S60	213	A
1	S60	214	A
1	S60	215	C
1	S60	222	A
1	S60	224	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S60	225	U
1	S60	226	U
1	S60	227	G
1	S60	234	U
1	S60	241	A
1	S60	254	G
1	S60	255	A
1	S60	256	C
1	S60	258	G
1	S60	266	G
1	S60	270	A
1	S60	271	A
1	S60	272	G
1	S60	275	U
1	S60	276	U
1	S60	278	C
1	S60	279	A
1	S60	288	G
1	S60	289	A
1	S60	293	U
1	S60	294	U
1	S60	296	A
1	S60	298	C
1	S60	305	U
1	S60	306	U
1	S60	308	U
1	S60	309	A
1	S60	310	U
1	S60	315	G
1	S60	319	G
1	S60	322	A
1	S60	323	U
1	S60	328	A
1	S60	331	A
1	S60	333	U
1	S60	334	A
1	S60	340	U
1	S60	342	G
1	S60	343	U
1	S60	346	C
1	S60	349	A
1	S60	357	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S60	360	A
1	S60	364	G
1	S60	365	A
1	S60	366	G
1	S60	368	U
1	S60	369	G
1	S60	370	A
1	S60	371	U
1	S60	374	A
1	S60	380	G
1	S60	386	A
1	S60	387	U
1	S60	388	C
1	S60	394	C
1	S60	397	G
1	S60	399	A
1	S60	403	G
1	S60	406	G
1	S60	407	U
1	S60	412	C
1	S60	414	U
1	S60	416	U
1	S60	423	A
1	S60	426	G
1	S60	433	A
1	S60	437	U
1	S60	440	A
1	S60	444	A
1	S60	448	A
1	S60	449	A
1	S60	451	A
1	S60	452	A
1	S60	453	G
1	S60	458	U
1	S60	463	U
1	S60	464	A
1	S60	466	A
1	S60	467	U
1	S60	468	U
1	S60	479	U
1	S60	483	A
1	S60	488	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S60	490	C
1	S60	500	G
1	S60	504	G
1	S60	505	A
1	S60	506	G
1	S60	511	G
1	S60	513	A
1	S60	515	U
1	S60	520	C
1	S60	521	G
1	S60	522	A
1	S60	524	C
1	S60	526	U
1	S60	538	C
1	S60	539	A
1	S60	540	G
1	S60	541	A
1	S60	542	A
1	S60	549	G
1	S60	552	G
1	S60	564	G
1	S60	566	A
1	S60	568	U
1	S60	573	G
1	S60	586	A
1	S60	589	U
1	S60	590	G
1	S60	591	G
1	S60	595	A
1	S60	596	G
1	S60	599	A
1	S60	610	A
1	S60	614	C
1	S60	628	C
1	S60	633	A
1	S60	635	C
1	S60	638	U
1	S60	639	G
1	S60	644	C
1	S60	645	G
1	S60	646	A
1	S60	650	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S60	659	U
1	S60	663	U
1	S60	664	U
1	S60	666	U
1	S60	674	G
1	S60	685	G
1	S60	689	U
1	S60	690	U
1	S60	691	U
1	S60	692	U
1	S60	693	U
1	S60	697	U
1	S60	706	A
1	S60	731	A
1	S60	737	U
1	S60	743	G
1	S60	747	A
1	S60	751	C
1	S60	752	C
1	S60	753	A
1	S60	756	A
1	S60	757	G
1	S60	760	G
1	S60	778	U
1	S60	784	U
1	S60	787	A
1	S60	789	G
1	S60	792	A
1	S60	793	G
1	S60	794	G
1	S60	795	U
1	S60	796	A
1	S60	802	C
1	S60	805	A
1	S60	810	U
1	S60	820	G
1	S60	821	A
1	S60	822	G
1	S60	823	A
1	S60	824	A
1	S60	832	A
1	S60	833	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S60	836	G
1	S60	837	A
1	S60	838	G
1	S60	842	G
1	S60	844	U
1	S60	851	G
1	S60	855	C
1	S60	861	C
1	S60	865	U
1	S60	866	U
1	S60	867	C
1	S60	869	A
1	S60	871	G
1	S60	882	A
1	S60	894	U
1	S60	896	U
1	S60	901	A
1	S60	904	A
1	S60	917	U
1	S60	918	U
1	S60	922	A
1	S60	924	U
1	S60	927	A
1	S60	929	A
1	S60	930	G
1	S60	935	A
1	S60	937	U
1	S60	938	C
1	S60	939	A
1	S60	943	U
1	S60	946	G
1	S60	951	A
1	S60	952	A
1	S60	959	A
1	S60	964	A
1	S60	965	G
1	S60	968	C
1	S60	969	C
1	S60	972	U
1	S60	973	A
1	S60	981	A
1	S60	982	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S60	984	C
1	S60	985	A
1	S60	994	U
1	S60	995	G
1	S60	1019	A
1	S60	1025	U
1	S60	1026	A
1	S60	1028	G
1	S60	1030	G
1	S60	1037	U
1	S60	1042	U
1	S60	1054	G
1	S60	1070	G
1	S60	1077	U
1	S60	1078	U
1	S60	1080	U
1	S60	1082	A
1	S60	1083	A
1	S60	1088	G
1	S60	1091	G
1	S60	1092	A
1	S60	1097	A
1	S60	1121	A
1	S60	1124	G
1	S60	1134	A
1	S60	1143	G
1	S60	1153	G
1	S60	1159	U
1	S60	1163	U
1	S60	1166	A
1	S60	1172	C
1	S60	1175	G
1	S60	1180	A
1	S60	1181	U
1	S60	1183	U
1	S60	1186	A
1	S60	1192	U
1	S60	1205	G
1	S60	1207	A
1	S60	1211	U
1	S60	1212	G
1	S60	1214	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S60	1215	U
1	S60	1223	G
1	S60	1225	G
1	S60	1227	A
1	S60	1228	C
1	S60	1237	G
1	S60	1238	G
1	S60	1239	A
1	S60	1241	C
1	S60	1242	A
1	S60	1243	U
1	S60	1244	A
2	L70	5	A
2	L70	7	G
2	L70	11	A
2	L70	13	A
2	L70	14	U
2	L70	22	A
2	L70	27	A
2	L70	28	C
2	L70	38	U
2	L70	41	G
2	L70	50	A
2	L70	53	U
2	L70	63	A
2	L70	64	G
2	L70	67	C
2	L70	74	A
2	L70	88	A
2	L70	89	G
2	L70	91	C
2	L70	100	A
2	L70	103	G
2	L70	104	C
2	L70	110	G
2	L70	117	U
78	L50	13	A
78	L50	14	U
78	L50	22	A
78	L50	23	U
78	L50	26	G
78	L50	40	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
78	L50	52	A
78	L50	60	A
78	L50	78	A
78	L50	79	A
78	L50	80	U
78	L50	81	U
78	L50	82	A
78	L50	86	U
78	L50	101	G
78	L50	104	A
78	L50	119	A
78	L50	122	A
78	L50	123	U
78	L50	124	A
78	L50	128	U
78	L50	139	A
78	L50	144	A
78	L50	145	A
78	L50	146	A
78	L50	147	C
78	L50	152	U
78	L50	153	A
78	L50	154	G
78	L50	155	G
78	L50	156	A
78	L50	164	A
78	L50	165	G
78	L50	168	G
78	L50	171	G
78	L50	175	G
78	L50	188	A
78	L50	189	A
78	L50	194	C
78	L50	195	C
78	L50	197	U
78	L50	198	U
78	L50	199	G
78	L50	203	U
78	L50	209	A
78	L50	210	U
78	L50	211	U
78	L50	221	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
78	L50	222	A
78	L50	224	G
78	L50	226	U
78	L50	248	U
78	L50	262	U
78	L50	266	U
78	L50	285	A
78	L50	286	U
78	L50	289	A
78	L50	290	C
78	L50	291	U
78	L50	292	U
78	L50	294	A
78	L50	295	G
78	L50	296	U
78	L50	304	C
78	L50	309	U
78	L50	310	A
78	L50	311	G
78	L50	321	A
78	L50	323	U
78	L50	324	A
78	L50	325	A
78	L50	326	A
78	L50	331	G
78	L50	332	A
78	L50	340	A
78	L50	343	U
78	L50	353	U
78	L50	359	G
78	L50	360	G
78	L50	375	A
78	L50	376	U
78	L50	378	A
78	L50	397	U
78	L50	412	U
78	L50	413	U
78	L50	414	U
78	L50	415	A
78	L50	424	U
78	L50	425	U
78	L50	426	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
78	L50	432	C
78	L50	433	C
78	L50	437	C
78	L50	445	A
78	L50	451	C
78	L50	456	A
78	L50	473	A
78	L50	477	A
78	L50	479	A
78	L50	499	U
78	L50	507	U
78	L50	509	A
78	L50	527	A
78	L50	532	A
78	L50	543	A
78	L50	555	C
78	L50	556	U
78	L50	558	G
78	L50	567	A
78	L50	577	U
78	L50	587	A
78	L50	590	A
78	L50	600	U
78	L50	605	U
78	L50	606	G
78	L50	616	G
78	L50	619	U
78	L50	620	U
78	L50	622	A
78	L50	623	G
78	L50	633	G
78	L50	634	U
78	L50	637	C
78	L50	640	A
78	L50	641	A
78	L50	642	G
78	L50	643	A
78	L50	658	U
78	L50	659	G
78	L50	662	A
78	L50	663	G
78	L50	670	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
78	L50	678	A
78	L50	679	A
78	L50	685	C
78	L50	686	U
78	L50	703	A
78	L50	704	U
78	L50	705	U
78	L50	706	A
78	L50	708	A
78	L50	711	G
78	L50	712	G
78	L50	721	G
78	L50	723	A
78	L50	728	A
78	L50	737	G
78	L50	746	C
78	L50	750	G
78	L50	751	A
78	L50	752	G
78	L50	754	A
78	L50	759	U
78	L50	763	U
78	L50	770	G
78	L50	771	A
78	L50	780	A
78	L50	781	A
78	L50	786	A
78	L50	787	U
78	L50	796	U
78	L50	799	A
78	L50	800	U
78	L50	801	C
78	L50	805	U
78	L50	806	G
78	L50	810	A
78	L50	814	A
78	L50	818	G
78	L50	819	G
78	L50	826	A
78	L50	833	G
78	L50	848	A
78	L50	853	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
78	L50	855	A
78	L50	862	U
78	L50	865	A
78	L50	868	A
78	L50	870	U
78	L50	882	A
78	L50	883	U
78	L50	886	U
78	L50	892	U
78	L50	893	U
78	L50	895	U
78	L50	896	A
78	L50	900	U
78	L50	910	G
78	L50	911	A
78	L50	989	U
78	L50	991	U
78	L50	1004	U
78	L50	1006	G
78	L50	1007	A
78	L50	1008	A
78	L50	1013	A
78	L50	1016	A
78	L50	1029	G
78	L50	1030	A
78	L50	1045	A
78	L50	1047	U
78	L50	1056	U
78	L50	1064	U
78	L50	1070	G
78	L50	1073	U
78	L50	1074	U
78	L50	1089	A
78	L50	1090	G
78	L50	1101	A
78	L50	1102	G
78	L50	1110	U
78	L50	1113	G
78	L50	1114	C
78	L50	1116	G
78	L50	1119	C
78	L50	1129	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
78	L50	1130	U
78	L50	1131	A
78	L50	1134	A
78	L50	1135	A
78	L50	1136	U
78	L50	1140	U
78	L50	1145	A
78	L50	1147	A
78	L50	1152	U
78	L50	1156	C
78	L50	1159	G
78	L50	1164	U
78	L50	1170	U
78	L50	1174	A
78	L50	1183	A
78	L50	1184	A
78	L50	1185	U
78	L50	1192	U
78	L50	1193	A
78	L50	1194	U
78	L50	1198	U
78	L50	1199	A
78	L50	1201	A
78	L50	1202	A
78	L50	1206	A
78	L50	1207	A
78	L50	1209	A
78	L50	1216	A
78	L50	1218	A
78	L50	1219	A
78	L50	1232	U
78	L50	1239	A
78	L50	1246	C
78	L50	1249	G
78	L50	1250	A
78	L50	1251	U
78	L50	1255	G
78	L50	1256	A
78	L50	1257	C
78	L50	1258	A
78	L50	1265	U
78	L50	1266	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
78	L50	1267	C
78	L50	1277	A
78	L50	1280	A
78	L50	1281	U
78	L50	1286	G
78	L50	1288	A
78	L50	1293	A
78	L50	1294	U
78	L50	1310	G
78	L50	1314	G
78	L50	1324	G
78	L50	1325	A
78	L50	1332	U
78	L50	1335	U
78	L50	1336	U
78	L50	1337	A
78	L50	1338	U
78	L50	1339	A
78	L50	1347	G
78	L50	1349	U
78	L50	1351	A
78	L50	1352	A
78	L50	1356	A
78	L50	1357	A
78	L50	1372	U
78	L50	1373	A
78	L50	1378	U
78	L50	1379	A
78	L50	1380	C
78	L50	1383	C
78	L50	1386	C
78	L50	1387	A
78	L50	1398	U
78	L50	1399	A
78	L50	1400	U
78	L50	1414	U
78	L50	1415	U
78	L50	1417	A
78	L50	1419	U
78	L50	1421	A
78	L50	1430	A
78	L50	1441	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
78	L50	1443	A
78	L50	1453	U
78	L50	1460	U
78	L50	1461	U
78	L50	1466	U
78	L50	1483	A
78	L50	1495	U
78	L50	1496	U
78	L50	1497	A
78	L50	1500	A
78	L50	1504	A
78	L50	1505	A
78	L50	1514	A
78	L50	1517	G
78	L50	1520	U
78	L50	1522	U
78	L50	1542	A
78	L50	1543	U
78	L50	1544	U
78	L50	1545	U
78	L50	1555	G
78	L50	1569	G
78	L50	1585	U
78	L50	1586	U
78	L50	1591	A
78	L50	1608	G
78	L50	1612	G
78	L50	1614	A
78	L50	1626	C
78	L50	1628	U
78	L50	1629	A
78	L50	1631	G
78	L50	1633	U
78	L50	1638	A
78	L50	1644	C
78	L50	1665	C
78	L50	1666	G
78	L50	1667	C
78	L50	1669	U
78	L50	1672	A
78	L50	1674	G
78	L50	1678	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
78	L50	1693	U
78	L50	1695	U
78	L50	1714	G
78	L50	1723	A
78	L50	1733	A
78	L50	1734	C
78	L50	1735	G
78	L50	1740	U
78	L50	1746	U
78	L50	1748	A
78	L50	1749	U
78	L50	1754	G
78	L50	1758	A
78	L50	1762	A
78	L50	1763	A
78	L50	1764	G
78	L50	1765	A
78	L50	1772	U
78	L50	1779	G
78	L50	1794	U
78	L50	1795	A
78	L50	1796	A
78	L50	1805	C
78	L50	1867	U
78	L50	1871	A
78	L50	1881	G
78	L50	1889	G
78	L50	1895	G
78	L50	1900	U
78	L50	1901	A
78	L50	1903	A
78	L50	1927	U
78	L50	1928	C
78	L50	1931	A
78	L50	1932	A
78	L50	1940	G
78	L50	1949	A
78	L50	1951	G
78	L50	1952	G
78	L50	1958	A
78	L50	1963	U
78	L50	1964	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
78	L50	1966	A
78	L50	1969	A
78	L50	1971	A
78	L50	1978	U
78	L50	1980	A
78	L50	1989	U
78	L50	1991	C
78	L50	1999	A
78	L50	2000	U
78	L50	2001	A
78	L50	2004	A
78	L50	2005	C
78	L50	2026	U
78	L50	2027	G
78	L50	2028	G
78	L50	2029	C
78	L50	2034	C
78	L50	2036	A
78	L50	2046	C
78	L50	2049	U
78	L50	2051	A
78	L50	2065	G
78	L50	2069	G
78	L50	2070	A
78	L50	2072	A
78	L50	2073	A
78	L50	2079	C
78	L50	2083	G
78	L50	2086	A
78	L50	2107	A
78	L50	2108	G
78	L50	2113	C
78	L50	2114	A
78	L50	2122	U
78	L50	2129	U
78	L50	2138	U
78	L50	2140	G
78	L50	2156	A
78	L50	2158	C
78	L50	2167	G
78	L50	2168	U
78	L50	2170	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
78	L50	2173	G
78	L50	2185	U
78	L50	2192	U
78	L50	2194	C
78	L50	2204	U
78	L50	2205	G
78	L50	2210	A
78	L50	2211	C
78	L50	2214	G
78	L50	2216	G
78	L50	2220	G
78	L50	2223	U
78	L50	2226	G
78	L50	2240	A
78	L50	2252	C
78	L50	2253	C
78	L50	2261	A
78	L50	2262	A
78	L50	2263	G
78	L50	2276	A
78	L50	2291	A
78	L50	2302	A
78	L50	2303	A
78	L50	2320	G
78	L50	2321	U
78	L50	2342	G
78	L50	2346	C
78	L50	2348	U
78	L50	2354	C
78	L50	2355	G
78	L50	2361	U
78	L50	2363	G
78	L50	2376	A
78	L50	2377	G
78	L50	2383	U
78	L50	2384	A
78	L50	2392	A
78	L50	2393	G
78	L50	2395	G
78	L50	2412	U
78	L50	2413	U
78	L50	2419	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
78	L50	2429	U
78	L50	2430	U
78	L50	2431	U
78	L50	2436	C
78	L50	2454	G
78	L50	2458	U
78	L50	2459	A
78	L50	2460	U
78	L50	2465	A
78	L50	2471	U
78	L50	2472	G
78	L50	2478	A
78	L50	2479	C
78	L50	2480	U
78	L50	2482	C

All (30) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	S60	307	U
1	S60	309	A
1	S60	339	A
1	S60	342	G
1	S60	499	U
1	S60	503	A
1	S60	690	U
1	S60	832	A
1	S60	836	G
1	S60	923	A
1	S60	1079	A
2	L70	13	A
2	L70	27	A
78	L50	22	A
78	L50	308	G
78	L50	412	U
78	L50	414	U
78	L50	636	G
78	L50	642	G
78	L50	786	A
78	L50	795	A
78	L50	1139	A
78	L50	1265	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
78	L50	1293	A
78	L50	1337	A
78	L50	1643	C
78	L50	2341	U
78	L50	2353	A
78	L50	2435	G
78	L50	2481	G

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](#)

Of 183 ligands modelled in this entry, 183 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

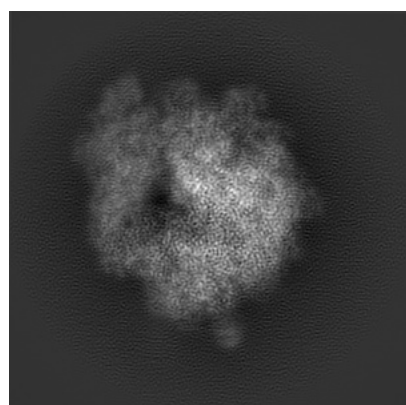
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4935. These allow visual inspection of the internal detail of the map and identification of artifacts.

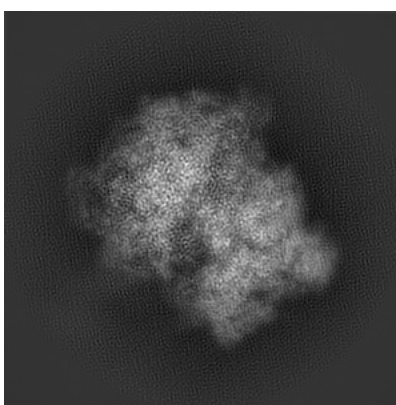
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

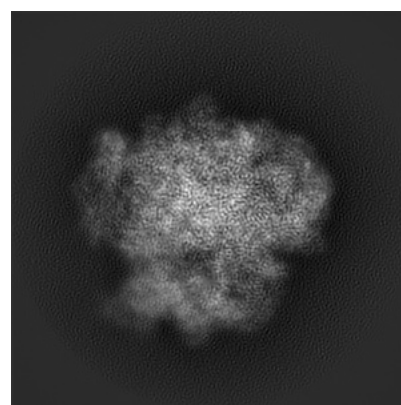
6.1.1 Primary map



X



Y

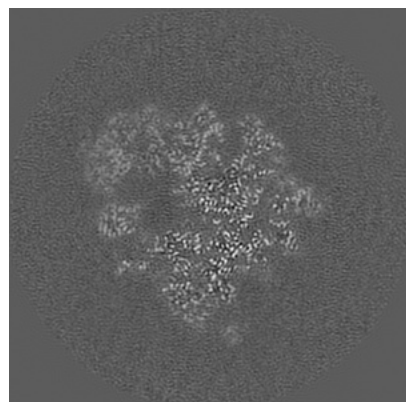


Z

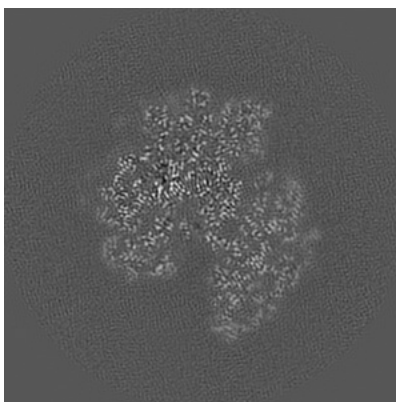
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

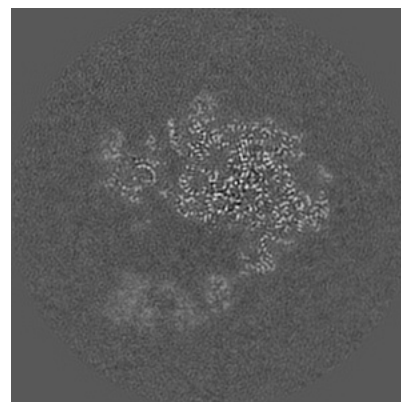
6.2.1 Primary map



X Index: 170



Y Index: 170

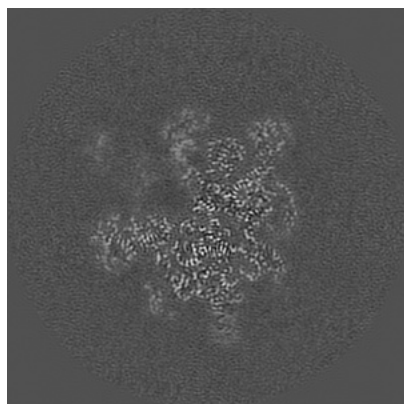


Z Index: 170

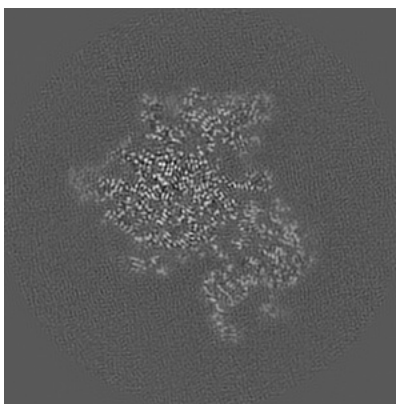
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

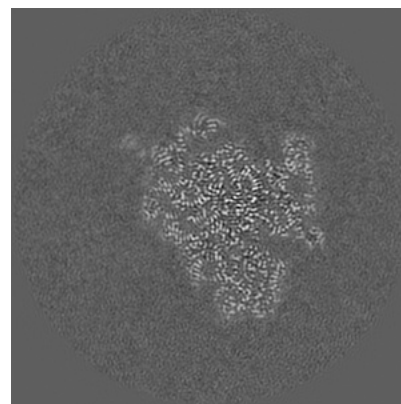
6.3.1 Primary map



X Index: 192



Y Index: 178

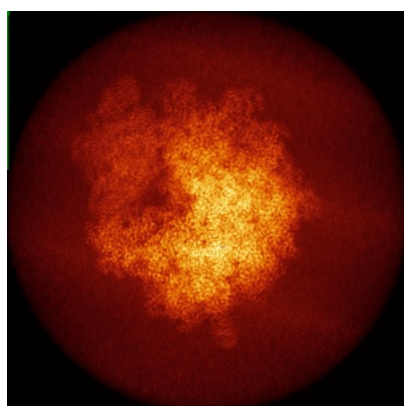


Z Index: 136

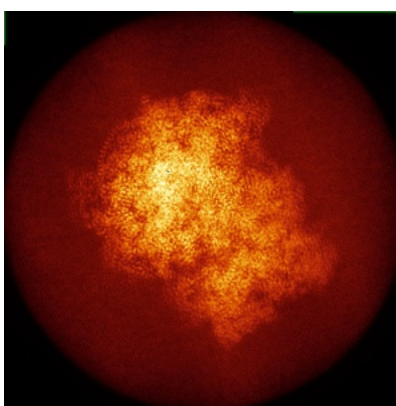
The images above show the largest variance slices of the map in three orthogonal directions.

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

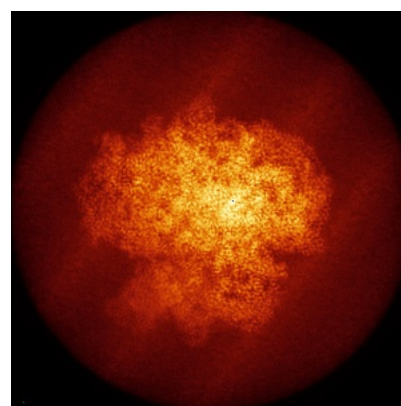
6.4.1 Primary map



X



Y



Z

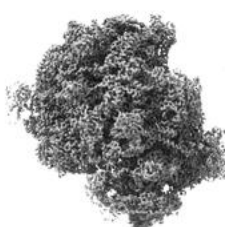
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0199. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

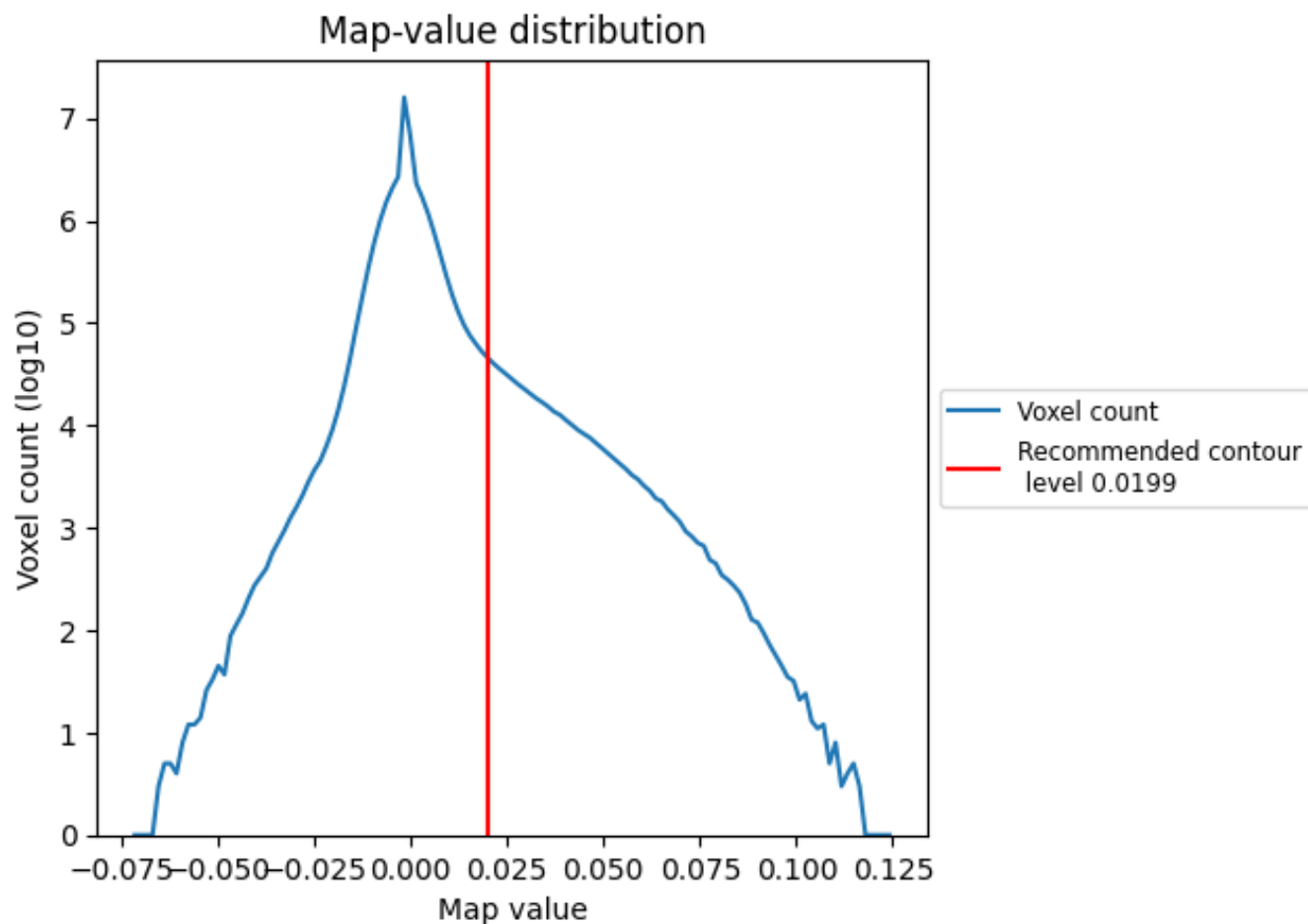
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

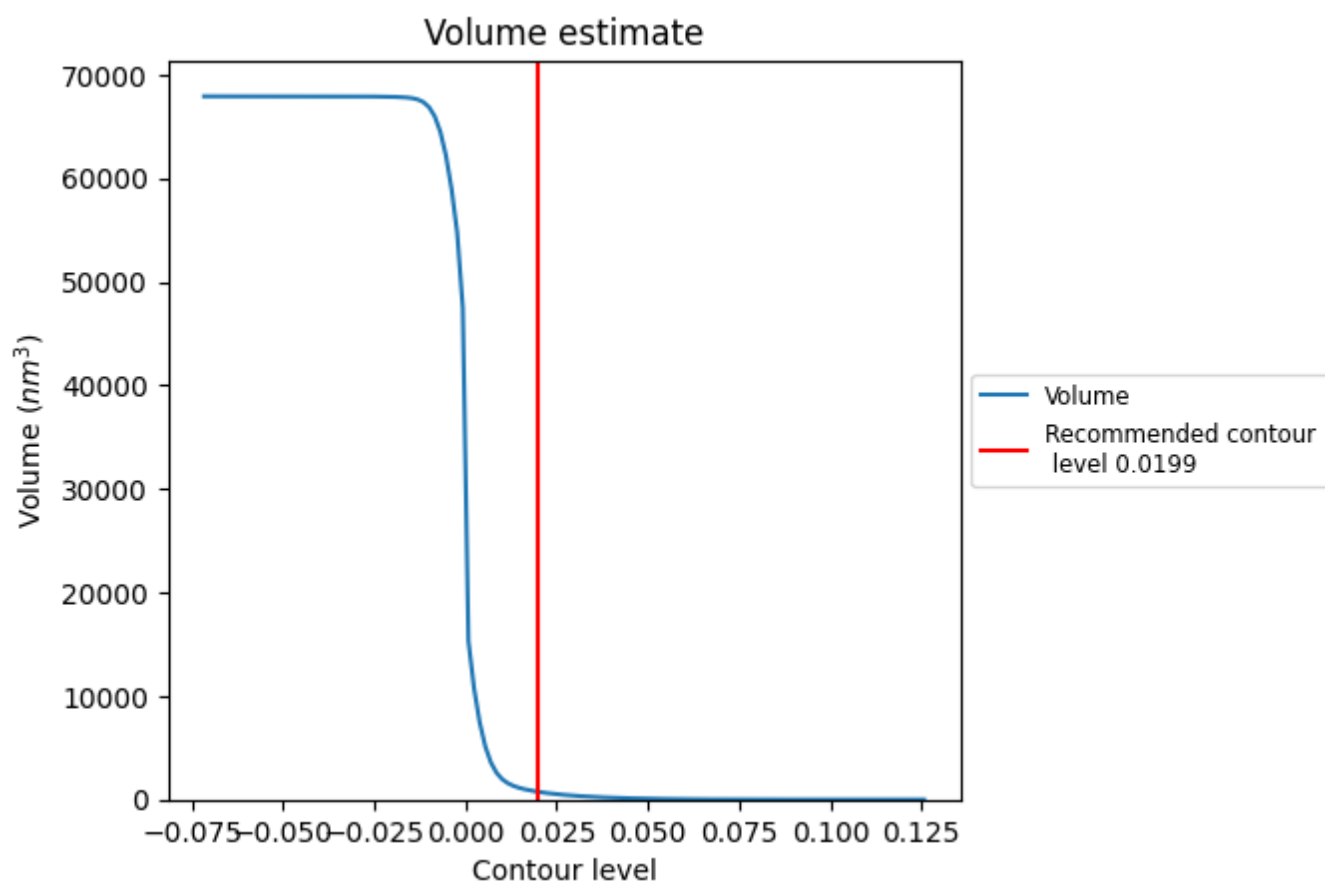
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

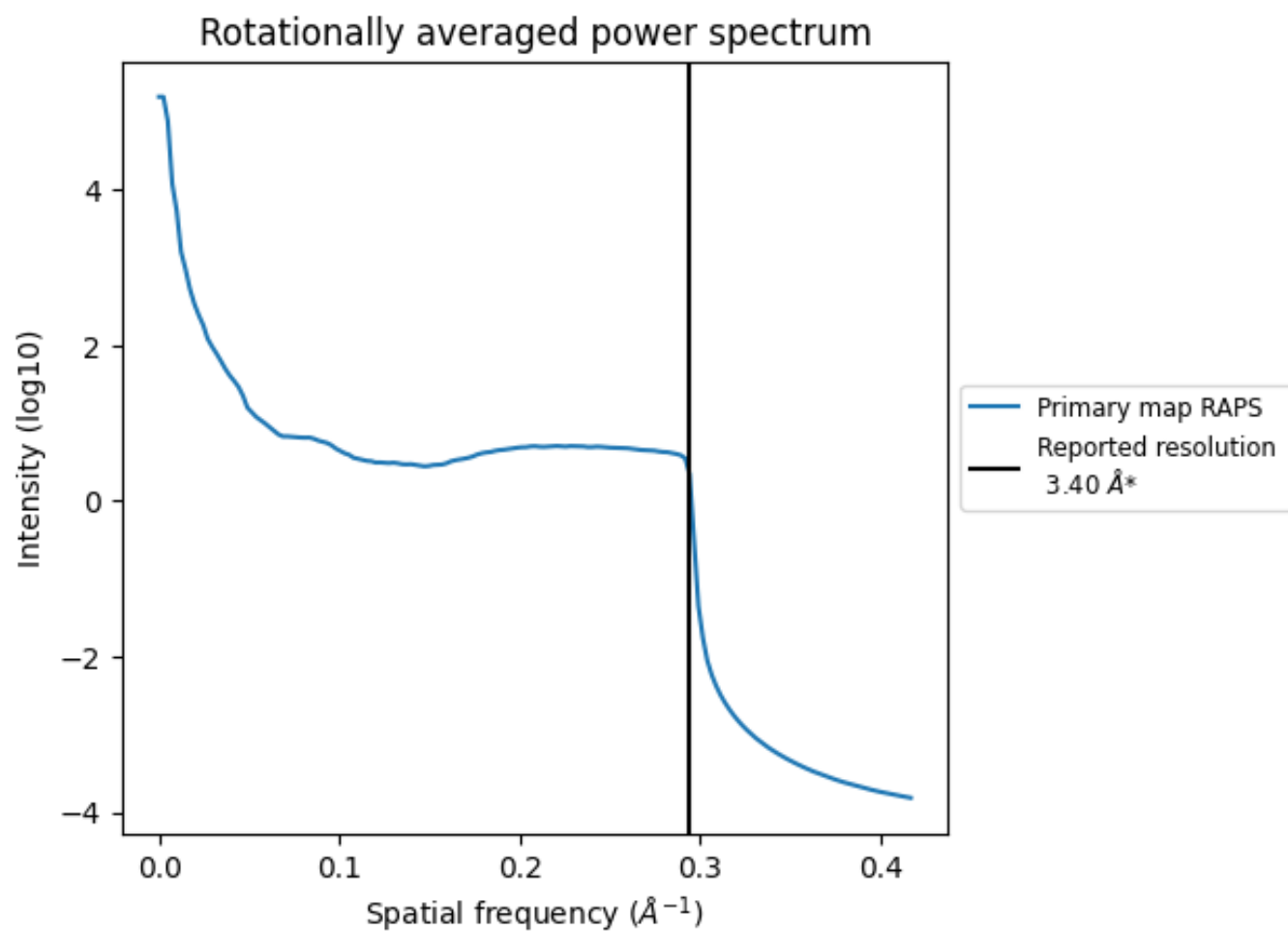
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 750 nm³; this corresponds to an approximate mass of 678 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 ⓘ

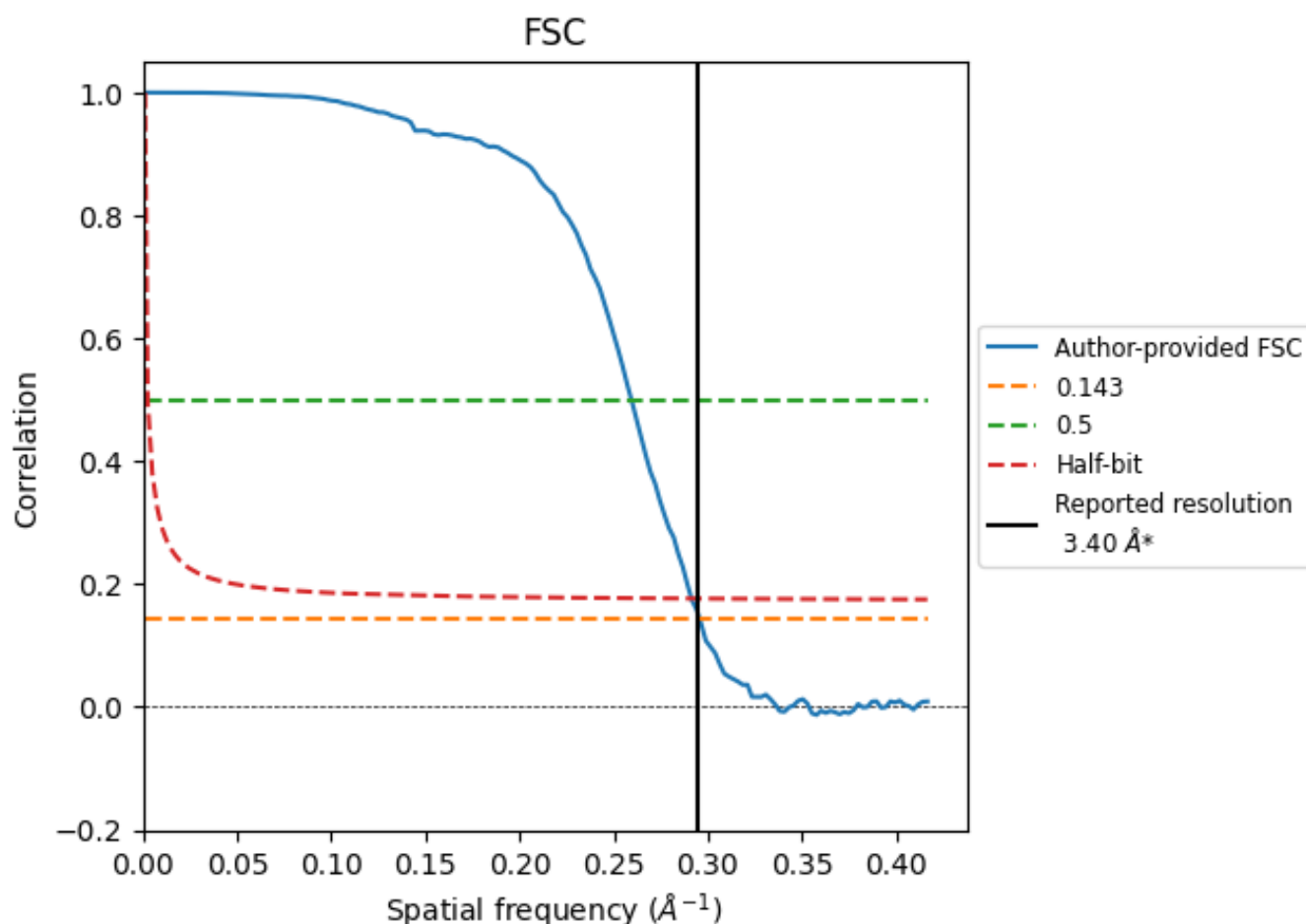


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

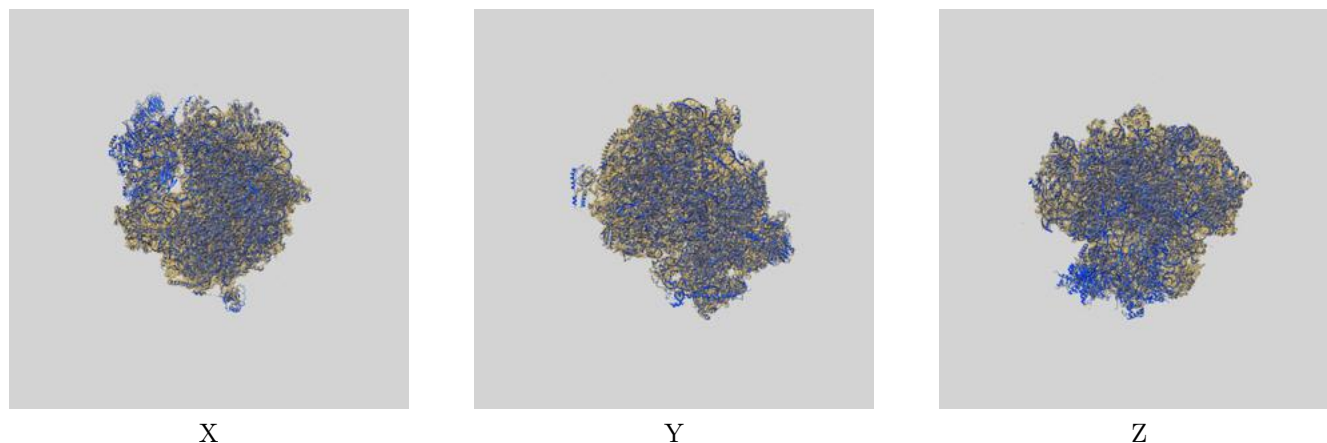
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.38	3.86	3.43
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

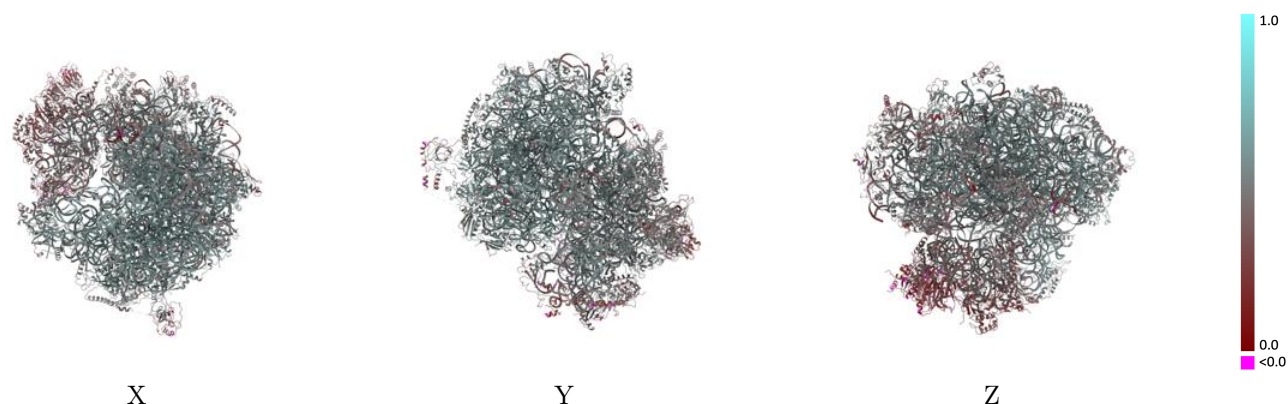
This section contains information regarding the fit between EMDB map EMD-4935 and PDB model 6RM3. Per-residue inclusion information can be found in section 3 on page 19.

9.1 Map-model overlay [i](#)



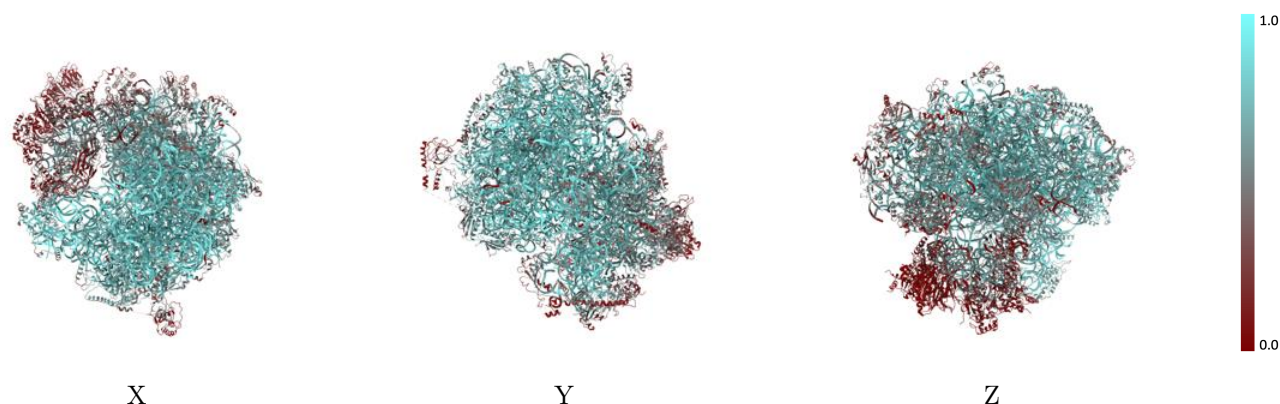
The images above show the 3D surface view of the map at the recommended contour level 0.0199 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



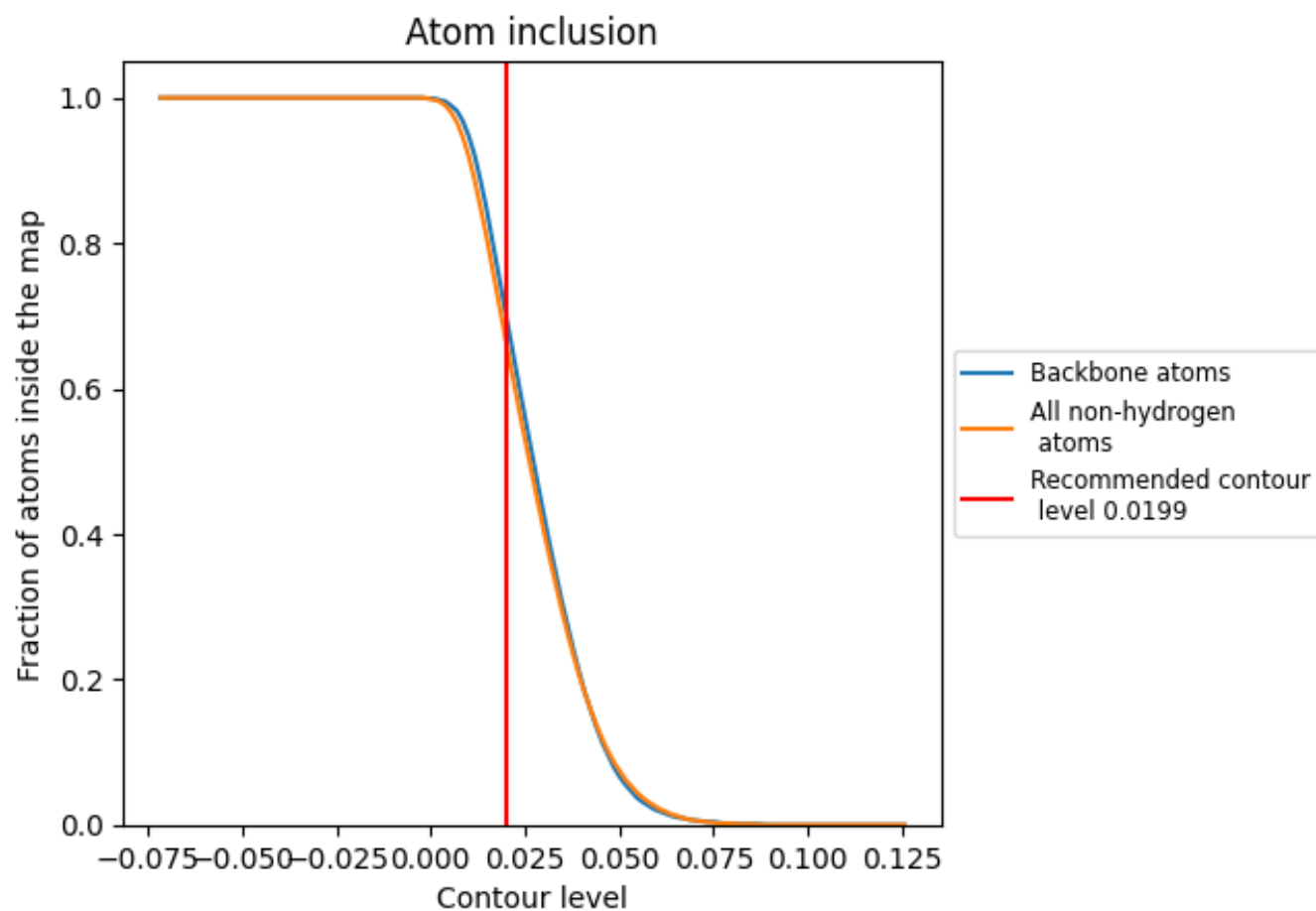
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0199).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 67% 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 (0.0199) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6670	 0.4930
L50	 0.8710	 0.5410
L70	 0.8930	 0.5290
LA0	 0.7610	 0.5440
LAA	 0.7980	 0.5560
LB0	 0.7240	 0.5410
LBB	 0.7190	 0.5300
LC0	 0.7000	 0.5260
LCC	 0.5560	 0.5070
LD0	 0.6750	 0.5050
LDD	 0.6980	 0.5330
LE0	 0.2290	 0.3880
LEE	 0.7640	 0.5400
LF0	 0.7150	 0.5270
LFF	 0.7430	 0.5390
LG0	 0.4980	 0.4720
LGG	 0.7080	 0.5330
LH0	 0.6050	 0.4990
LHH	 0.6750	 0.5190
LI0	 0.7180	 0.5340
LII	 0.6220	 0.5210
LJ0	 0.5170	 0.4740
LJJ	 0.8110	 0.5590
LL0	 0.7100	 0.5370
LLL	 0.7850	 0.5470
LM0	 0.4960	 0.4610
LMM	 0.6450	 0.5130
LN0	 0.8100	 0.5620
LNN	 0.3120	 0.4670
LO0	 0.7140	 0.5400
LOO	 0.6320	 0.5320
LP0	 0.7680	 0.5570
LPP	 0.7210	 0.5460
LQ0	 0.7310	 0.5420
LR0	 0.6390	 0.5080



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
LS0	 0.7180	 0.5300
LT0	 0.7190	 0.5320
LU0	 0.4970	 0.4350
LV0	 0.7070	 0.5410
LW0	 0.5640	 0.4960
LX0	 0.7120	 0.5350
LXX	 0.5510	 0.5010
LY0	 0.5960	 0.4940
LZ0	 0.4350	 0.4490
S60	 0.7430	 0.4810
SA0	 0.3490	 0.4270
SAA	 0.6040	 0.4950
SB0	 0.3890	 0.4220
SBB	 0.3750	 0.4460
SC0	 0.5300	 0.4890
SCC	 0.2060	 0.3790
SD0	 0.2330	 0.3800
SDD	 0.3330	 0.4170
SE0	 0.4290	 0.4410
SEE	 0.3480	 0.4500
SF0	 0.2460	 0.3870
SFF	 0.0040	 0.0910
SG0	 0.3750	 0.4010
SGG	 0.0780	 0.2750
SH0	 0.2880	 0.3830
SI0	 0.6460	 0.5110
SJ0	 0.4880	 0.4450
SK0	 0.1580	 0.3120
SL0	 0.5630	 0.4950
SM0	 0.0190	 0.1750
SN0	 0.5160	 0.4810
SNN	 0.1940	 0.4290
SO0	 0.5120	 0.4770
SP0	 0.2130	 0.3760
SQ0	 0.2450	 0.3710
SR0	 0.1810	 0.3510
SS0	 0.1700	 0.3700
ST0	 0.1520	 0.3520
SU0	 0.1750	 0.2840
SV0	 0.4260	 0.4610
SW0	 0.6140	 0.5060
SX0	 0.6080	 0.5150

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
SY0	 0.3510	 0.3950
SZ0	 0.1030	 0.3420