Full wwPDB EM Validation Report

Feb 12, 2024 – 04:47 pm GMT

PDB ID	:	8BN3
EMDB ID	:	EMD-16127
Title	:	Yeast 80S, ES7s delta, eIF5A, Stm1 containing
Authors	:	Dimitrova-Paternoga, L.; Paternoga, H.; Wilson, D.N.
Deposited on	:	2022-11-12
Resolution	:	2.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

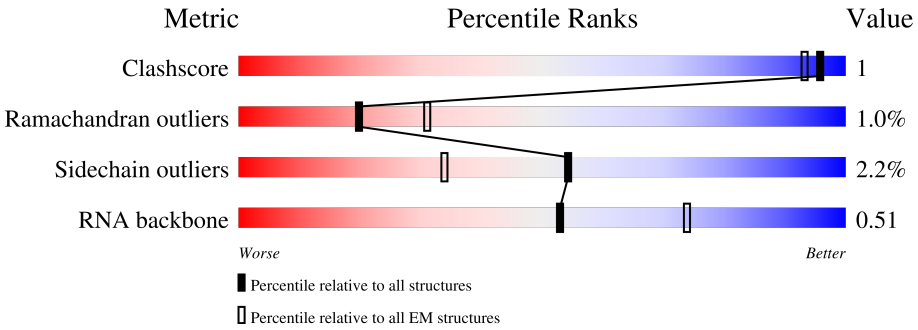
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.40 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	B	217	58% 82% 14% ·
2	S5	206	86% 97% ·
3	C0	96	91% 84% 14% ·
4	C4	127	41% 87% 10% · ·
5	C5	124	64% 85% 7% 7%
6	C8	145	69% 92% 7% ·
7	D0	107	79% 95% 5%

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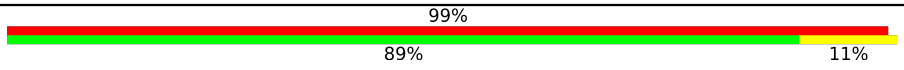
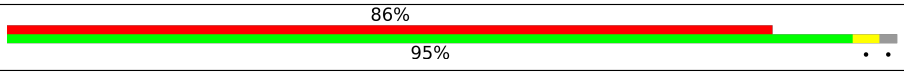
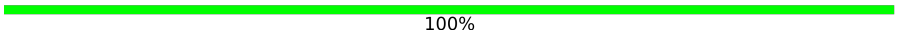
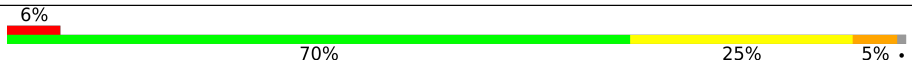
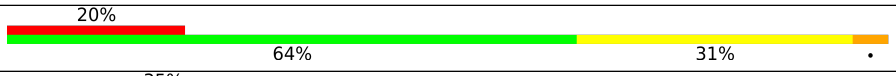
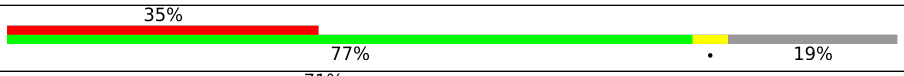
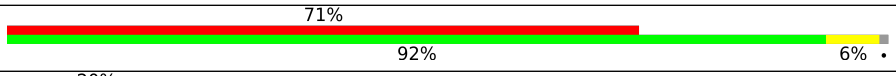
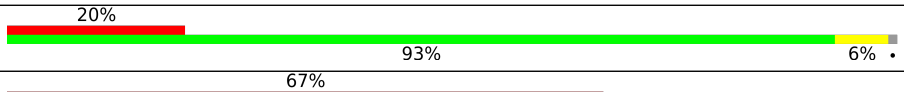
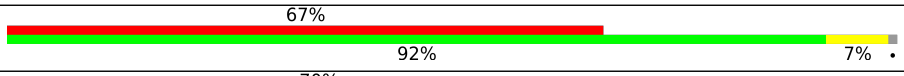
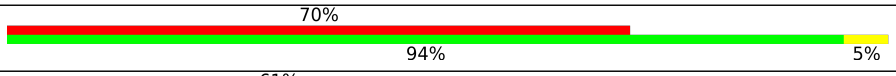
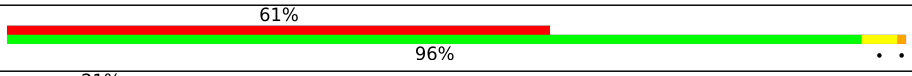
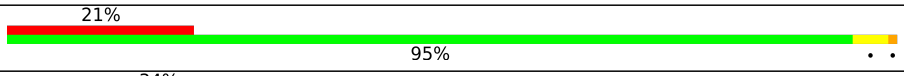
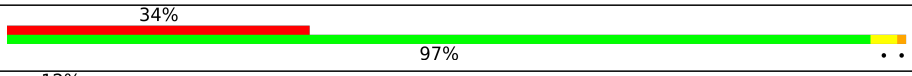
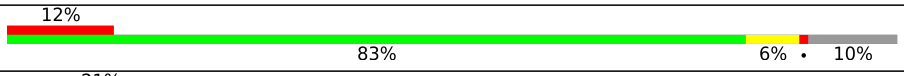
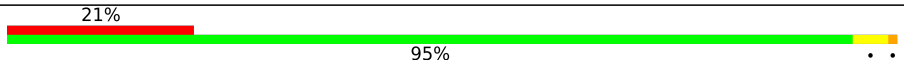
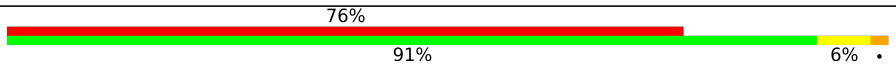
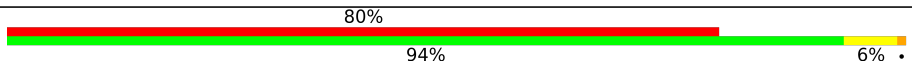
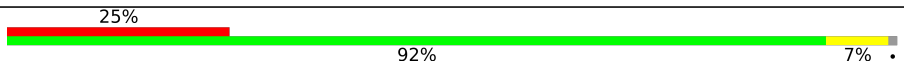
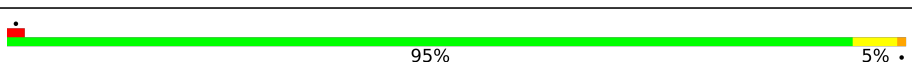
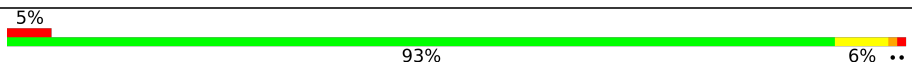
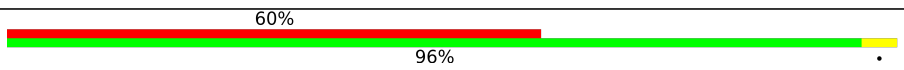
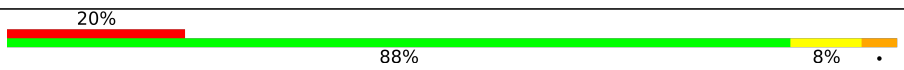
Mol	Chain	Length	Quality of chain
8	D5	70	
9	D8	63	
10	P	15	
11	3	121	
12	4	158	
13	1	3162	
14	2	1737	
15	S0	251	
16	S1	214	
17	S2	217	
18	S3	223	
19	S6	226	
20	S7	184	
21	S8	188	
22	S9	185	
23	C1	155	
24	C3	150	
25	C6	141	
26	C7	120	
27	C9	143	
28	D1	87	
29	D2	129	
30	D3	144	
31	D4	134	
32	D6	97	

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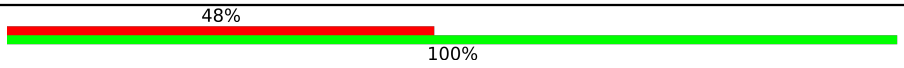
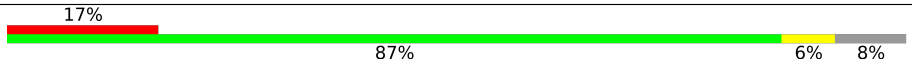
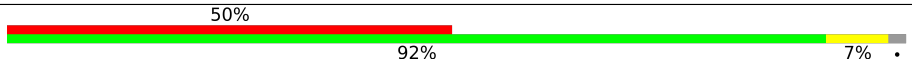
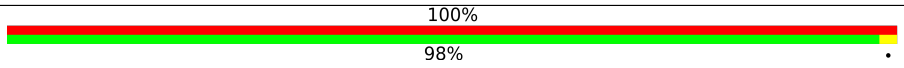
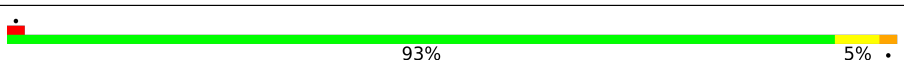
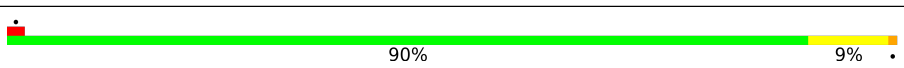
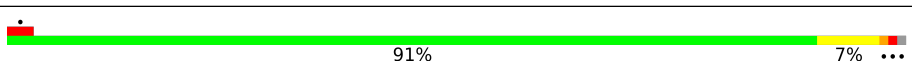
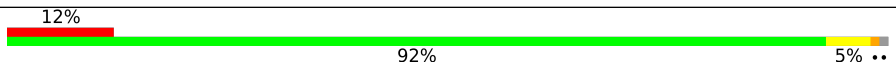
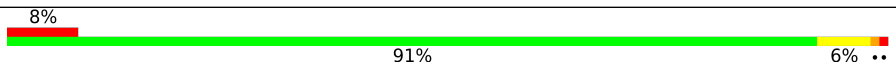
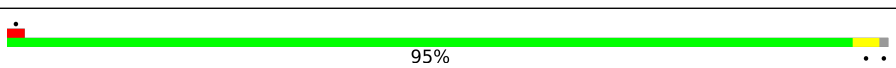
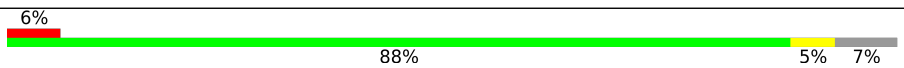
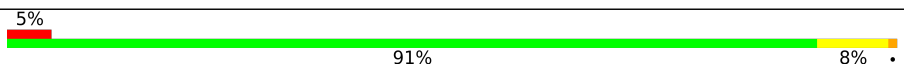
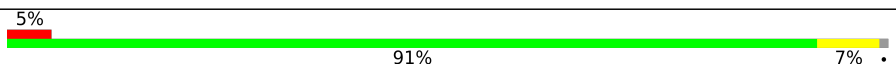
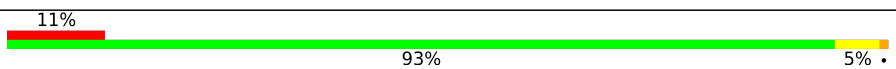
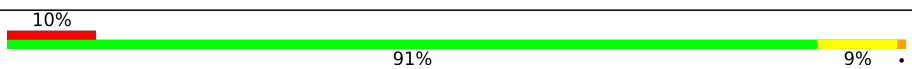
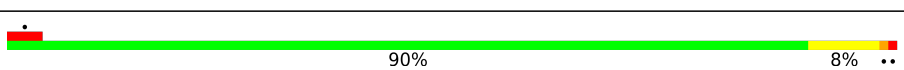
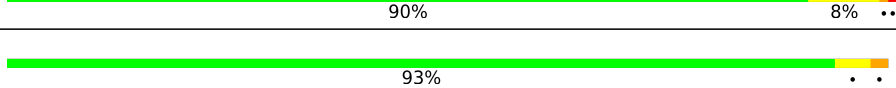
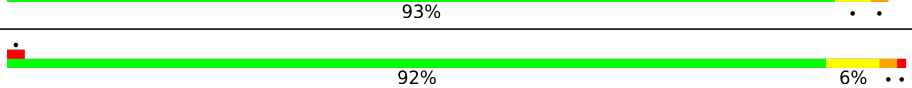
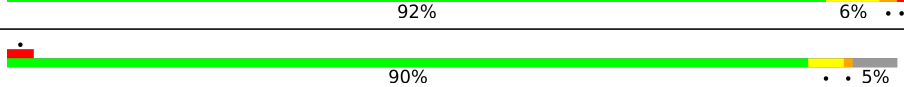
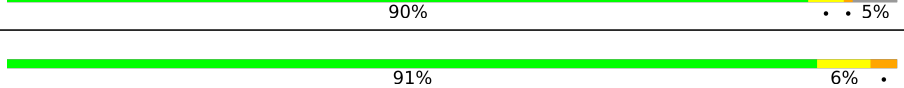
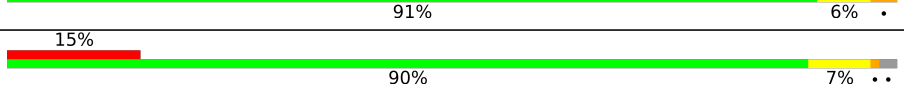
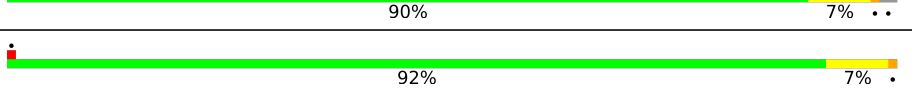
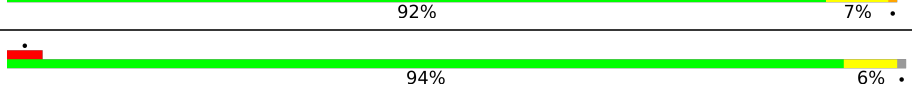
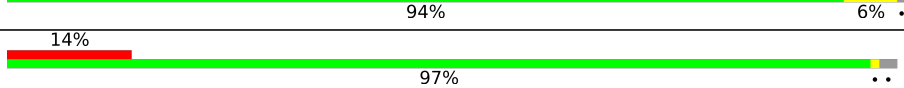
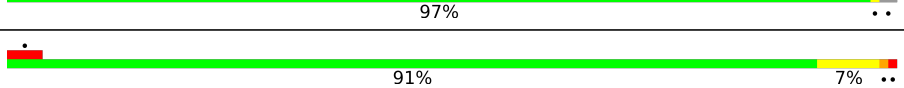
Mol	Chain	Length	Quality of chain
33	D7	81	
34	D9	53	
35	E0	60	
36	SR	318	
37	L2	252	
38	L3	386	
39	L4	361	
40	L5	295	
41	L6	156	
42	L7	222	
43	L8	233	
44	L9	189	
45	M0	209	
46	M1	168	
47	M3	193	
48	M4	136	
49	M5	202	
50	M6	197	
51	M7	183	
52	M8	185	
53	M9	188	
54	N0	172	
55	N1	159	
56	N2	100	
57	N3	136	

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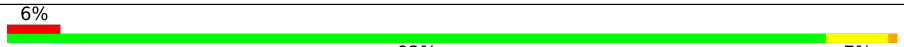
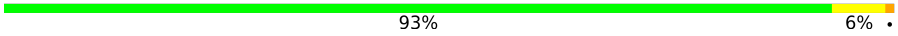
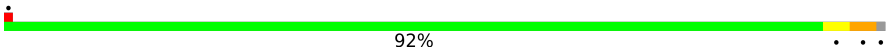
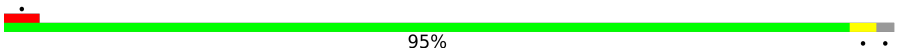
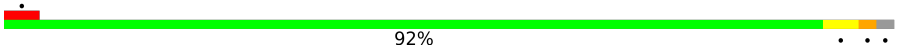
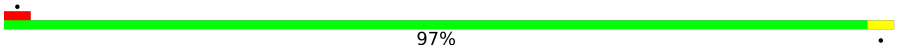
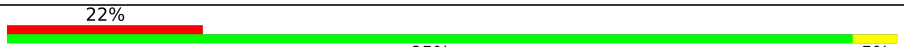
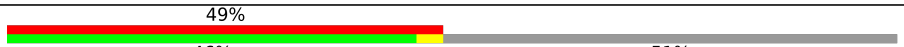
Mol	Chain	Length	Quality of chain
58	N4	98	
59	N5	121	
60	N6	126	
61	N7	135	
62	N8	148	
63	N9	56	
64	O0	97	
65	O1	109	
66	O2	127	
67	O3	106	
68	O4	111	
69	O5	119	
70	O6	99	
71	O7	86	
72	O8	77	
73	O9	50	
74	Q0	52	
75	Q1	25	
76	Q2	105	
77	Q3	91	
78	SM	118	
79	eI	145	
80	S4	260	
81	E1	71	

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 201671 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 protein called 60S ribosomal protein L1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	216	1710	1092	298	311	9	0	0

- Molecule 2 is a protein called Rps5p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	S5	206	1609	1007	300	299	3	0	0

- Molecule 3 is a protein called Small ribosomal subunit protein eS10A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C0	96	818	530	133	153	2	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C0	89	ALA	GLY	conflict	UNP Q08745

- Molecule 4 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C4	126	933	572	185	173	3	0	0

- Molecule 5 is a protein called RPS15 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	C5	115	912	580	170	155	7	0	0

- Molecule 6 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C8	145	Total	C	N	O	S	0	0
			1192	743	237	210	2		

- Molecule 7 is a protein called RPS20 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D0	107	Total	C	N	O	S	0	0
			855	539	156	159	1		

- Molecule 8 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	D5	70	Total	C	N	O	0	0
			563	360	104	99		

- Molecule 9 is a protein called RPS28A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D8	62	Total	C	N	O	S	0	0
			490	302	98	89	1		

- Molecule 10 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	15	Total	C	N	O	S	0	0
			146	89	40	16	1		

- Molecule 11 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	3	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 12 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	4	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 13 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1	3143	Total	C	N	O	P	0	0
			67219	30026	12110	21940	3143		

- Molecule 14 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	2	1737	Total	C	N	O	P	0	0
			37011	16546	6549	12179	1737		

- Molecule 15 is a protein called Small ribosomal subunit protein uS2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S0	204	Total	C	N	O	S	0	0
			1598	1025	283	288	2		

- Molecule 16 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S1	211	Total	C	N	O	S	0	0
			1687	1070	305	308	4		

- Molecule 17 is a protein called RPS2 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S2	214	Total	C	N	O	S	0	0
			1615	1036	285	292	2		

- Molecule 18 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S3	220	Total	C	N	O	S	0	0
			1709	1083	310	310	6		

- Molecule 19 is a protein called Small ribosomal subunit protein eS6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S6	226	Total	C	N	O	S	0	0
			1820	1142	350	325	3		

- Molecule 20 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	S7	184	Total 1481	C 951	N 265	O 265	0	0

- Molecule 21 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S8	188	Total 1489	C 925	N 298	O 264	S 2	0	0

- Molecule 22 is a protein called Small ribosomal subunit protein uS4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S9	185	Total 1494	C 943	N 289	O 261	S 1	0	0

- Molecule 23 is a protein called Small ribosomal subunit protein uS17A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	C1	139	Total 1121	C 721	N 211	O 186	S 3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C1	147	ALA	GLY	conflict	UNP P0CX47

- Molecule 24 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	C3	150	Total 1192	C 759	N 224	O 207	S 2	0	0

- Molecule 25 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	C6	141	Total 1105	C 708	N 203	O 194	0	0

- Molecule 26 is a protein called ES17.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	C7	92	Total	C	N	O	S	0	0
			737	466	140	129	2		

- Molecule 27 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	C9	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 28 is a protein called Small ribosomal subunit protein eS21A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	D1	86	Total	C	N	O	S	0	0
			673	414	121	136	2		

- Molecule 29 is a protein called RPS22A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	D2	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 30 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	D3	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 31 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	D4	134	Total	C	N	O	0	0
			1073	676	208	189		

- Molecule 32 is a protein called RPS26B isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	D6	97	Total	C	N	O	S	0	0
			769	475	160	129	5		

- Molecule 33 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	D7	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 34 is a protein called RPS29A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	D9	49	Total	C	N	O	S	0	0
			404	249	86	65	4		

- Molecule 35 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	E0	59	Total	C	N	O	S	0	0
			469	296	97	75	1		

- Molecule 36 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	SR	318	Total	C	N	O	S	0	0
			2445	1546	419	472	8		

- Molecule 37 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	L2	251	Total	C	N	O	S	0	0
			1909	1188	387	333	1		

- Molecule 38 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	L3	386	Total	C	N	O	S	0	0
			3079	1954	584	533	8		

- Molecule 39 is a protein called RPL4A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	L4	359	Total	C	N	O	S	0	0
			2731	1720	517	491	3		

- Molecule 40 is a protein called RPL5 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	L5	291	Total	C	N	O	S	0	0
			2329	1472	406	449	2		

- Molecule 41 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	L6	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 42 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	L7	219	Total	C	N	O	S	0	0
			1761	1138	320	302	1		

- Molecule 43 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	L8	216	Total	C	N	O	S	0	0
			1706	1095	306	302	3		

- Molecule 44 is a protein called RPL9A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	L9	189	Total	C	N	O	S	0	0
			1502	953	272	273	4		

- Molecule 45 is a protein called RPL10 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	M0	206	Total	C	N	O	S	0	0
			1677	1066	317	289	5		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M0	?	-	LEU	deletion	UNP A0A6A5PUZ5
M0	?	-	SER	deletion	UNP A0A6A5PUZ5
M0	?	-	CYS	deletion	UNP A0A6A5PUZ5
M0	?	-	ALA	deletion	UNP A0A6A5PUZ5
M0	?	-	GLY	deletion	UNP A0A6A5PUZ5
M0	?	-	ALA	deletion	UNP A0A6A5PUZ5

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Chain	Residue	Modelled	Actual	Comment	Reference
M0	?	-	ASP	deletion	UNP A0A6A5PUZ5
M0	?	-	ARG	deletion	UNP A0A6A5PUZ5
M0	?	-	LEU	deletion	UNP A0A6A5PUZ5

- Molecule 46 is a protein called RPL11B isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	M1	168	Total	C	N	O	S	0	0
			1344	841	251	248	4		

- Molecule 47 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	M3	193	Total	C	N	O	0	0
			1543	962	315	266		

- Molecule 48 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	M4	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 49 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	M5	202	Total	C	N	O	S	0	0
			1711	1071	359	280	1		

- Molecule 50 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	M6	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 51 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	M7	174	Total	C	N	O	0	0
			1379	856	275	248		

- Molecule 52 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	M8	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 53 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	M9	184	Total	C	N	O	0	0
			1490	917	321	252		

- Molecule 54 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	N0	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 55 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	N1	158	Total	C	N	O	S	0	0
			1268	799	245	220	4		

- Molecule 56 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	N2	98	Total	C	N	O	0	0
			778	505	127	146		

- Molecule 57 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	N3	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 58 is a protein called RPL24A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	N4	62	Total	C	N	O	S	0	0
			513	330	101	81	1		

- Molecule 59 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	N5	119	Total 954	C 614	N 167	O 171	S 2	0	0

- Molecule 60 is a protein called Large ribosomal subunit protein uL24A.

Mol	Chain	Residues	Atoms				AltConf	Trace
60	N6	126	Total 993	C 625	N 192	O 176	0	0

- Molecule 61 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
61	N7	135	Total 1092	C 710	N 202	O 180	0	0

- Molecule 62 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	N8	148	Total 1173	C 749	N 231	O 190	S 3	0	0

- Molecule 63 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
63	N9	54	Total 434	C 271	N 94	O 69	0	0

- Molecule 64 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	O0	97	Total 743	C 479	N 124	O 139	S 1	0	0

- Molecule 65 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	O1	106	Total 865	C 550	N 165	O 149	S 1	0	0

- Molecule 66 is a protein called RPL32 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	O2	125	Total	C	N	O	S	0	0
			1007	638	203	165	1		

- Molecule 67 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	O3	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 68 is a protein called Large ribosomal subunit protein eL34A.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	O4	109	Total	C	N	O	S	0	0
			861	533	175	149	4		

- Molecule 69 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	O5	118	Total	C	N	O	S	0	0
			964	612	185	166	1		

- Molecule 70 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	O6	97	Total	C	N	O	S	0	0
			750	469	149	130	2		

- Molecule 71 is a protein called Large ribosomal subunit protein eL37A.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	O7	84	Total	C	N	O	S	1	0
			676	411	149	111	5		

- Molecule 72 is a protein called RPL38 isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
72	O8	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 73 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	O9	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 74 is a protein called 60S ribosomal protein L40-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Q0	51	Total	C	N	O	S	0	0
			409	253	85	66	5		

- Molecule 75 is a protein called Large ribosomal subunit protein eL41B.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Q1	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 76 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Q2	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 77 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Q3	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 78 is a protein called STM1 isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
78	SM	118	Total	C	N	O	0	0
			893	527	180	186		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
79	eI	145	Total	C	N	O	S	0	0
			1096	682	183	222	9		

- Molecule 80 is a protein called Small ribosomal subunit protein eS4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	S4	260	Total	C	N	O	S	0	0
			2068	1316	389	360	3		

- Molecule 81 is a protein called RPS31 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	E1	35	Total	C	N	O	S	0	0
			271	165	54	48	4		

- Molecule 82 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
82	3	3	Total	Mg	0
			3	3	
82	4	2	Total	Mg	0
			2	2	
82	1	191	Total	Mg	0
			191	191	
82	2	19	Total	Mg	0
			19	19	
82	L3	1	Total	Mg	0
			1	1	
82	M7	1	Total	Mg	0
			1	1	
82	N3	1	Total	Mg	0
			1	1	
82	O2	1	Total	Mg	0
			1	1	
82	O7	1	Total	Mg	0
			1	1	

- Molecule 83 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
83	1	63	Total	K	0
			63	63	
83	2	1	Total	K	0
			1	1	
83	L2	2	Total	K	0
			2	2	
83	L4	1	Total	K	0
			1	1	

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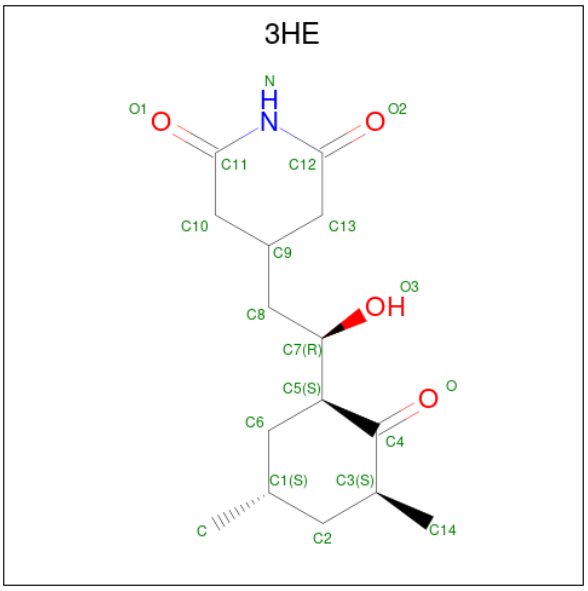
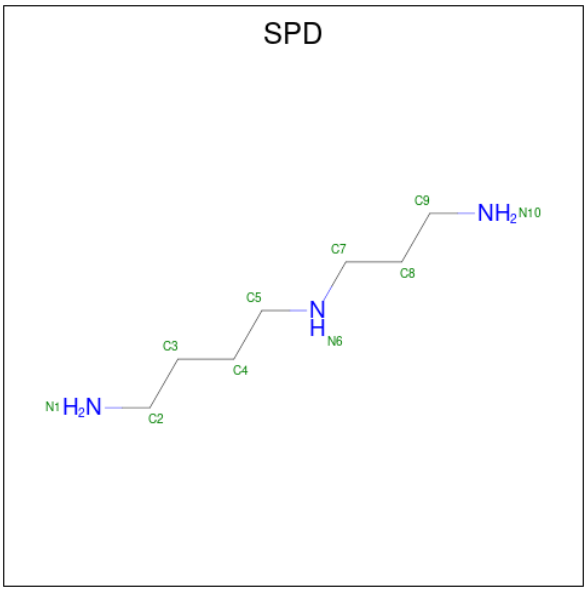
Mol	Chain	Residues	Atoms	AltConf
83	M0	1	Total K 1 1	0
83	M5	1	Total K 1 1	0
83	N9	1	Total K 1 1	0
83	O4	1	Total K 1 1	0
83	O7	1	Total K 1 1	0

- Molecule 84 is 4-{(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl}piperidine-2,6-dione (three-letter code: 3HE) (formula: $C_{15}H_{23}NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
84	1	1	Total C N O 20 15 1 4	0

- Molecule 85 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms	AltConf
85	1	1	Total C N 10 7 3	0
85	1	1	Total C N 10 7 3	0
85	1	1	Total C N 10 7 3	0

- Molecule 86 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
86	D6	1	Total Zn 1 1	0
86	D9	1	Total Zn 1 1	0
86	O4	1	Total Zn 1 1	0
86	O7	1	Total Zn 1 1	0
86	Q0	1	Total Zn 1 1	0
86	Q2	1	Total Zn 1 1	0
86	Q3	1	Total Zn 1 1	0

- Molecule 87 is water.

Mol	Chain	Residues	Atoms	AltConf
87	3	12	Total O 12 12	0
87	4	40	Total O 40 40	0
87	1	1466	Total O 1466 1466	0
87	2	45	Total O 45 45	0
87	C3	2	Total O 2 2	0
87	L2	30	Total O 30 30	0
87	L3	21	Total O 21 21	0
87	L4	16	Total O 16 16	0
87	L5	3	Total O 3 3	0
87	L6	1	Total O 1 1	0
87	L7	10	Total O 10 10	0
87	M0	3	Total O 3 3	0
87	M3	3	Total O 3 3	0
87	M5	19	Total O 19 19	0
87	M6	9	Total O 9 9	0
87	M7	13	Total O 13 13	0
87	M8	10	Total O 10 10	0
87	M9	5	Total O 5 5	0
87	N0	3	Total O 3 3	0
87	N1	6	Total O 6 6	0
87	N3	4	Total O 4 4	0
87	N4	1	Total O 1 1	0

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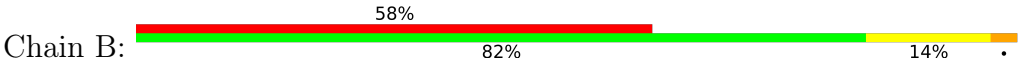
Mol	Chain	Residues	Atoms	AltConf
87	N5	4	Total O 4 4	0
87	N8	15	Total O 15 15	0
87	N9	5	Total O 5 5	0
87	O1	4	Total O 4 4	0
87	O2	20	Total O 20 20	0
87	O3	5	Total O 5 5	0
87	O4	6	Total O 6 6	0
87	O6	1	Total O 1 1	0
87	O7	11	Total O 11 11	0
87	O8	1	Total O 1 1	0
87	O9	1	Total O 1 1	0
87	Q0	1	Total O 1 1	0
87	Q2	9	Total O 9 9	0
87	Q3	4	Total O 4 4	0
87	eI	1	Total O 1 1	0

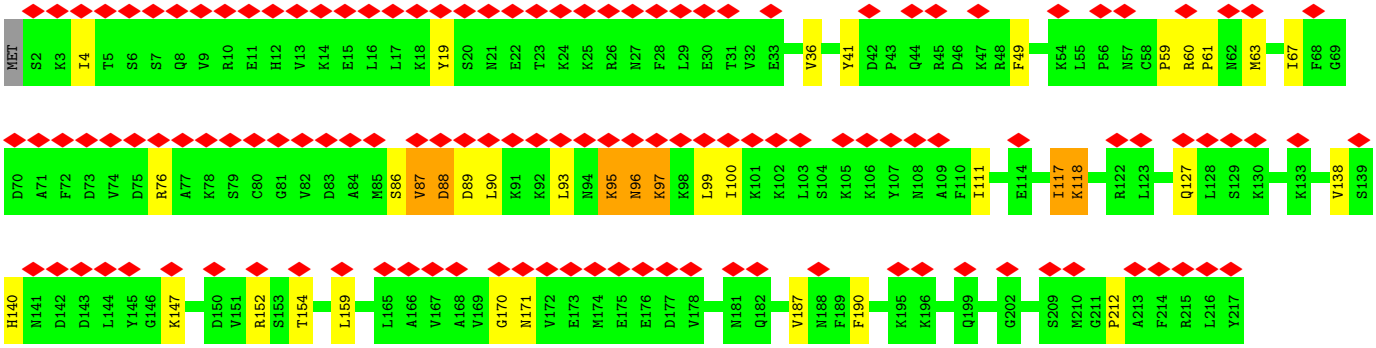
3 Residue-property plots (i)

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

- Molecule 1: 60S ribosomal protein L1-A

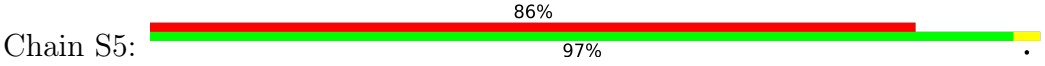
Chain B:

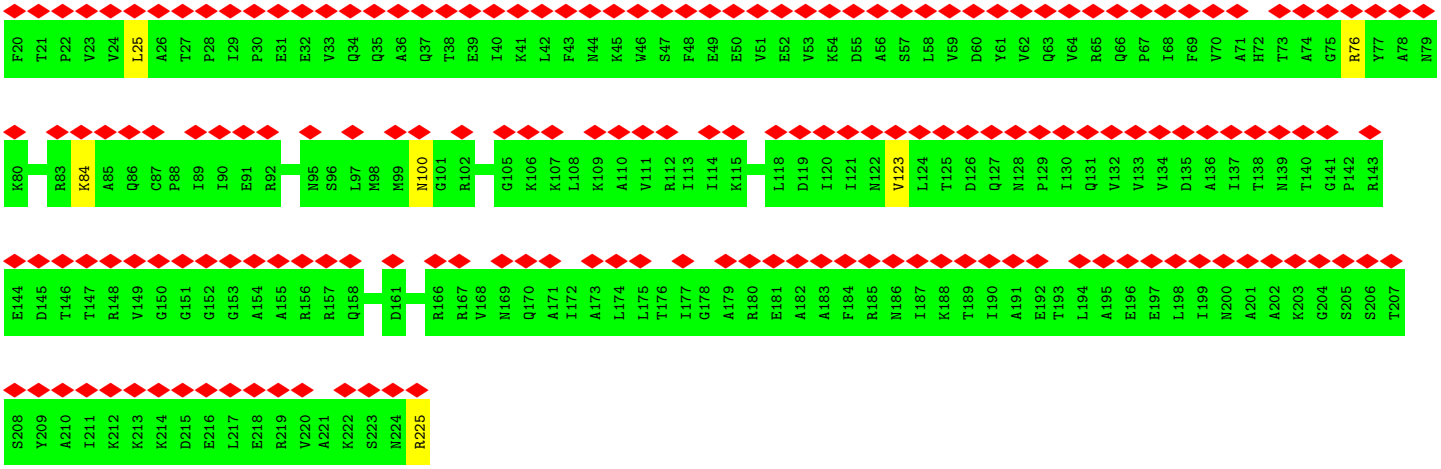




- Molecule 2: Rps5p

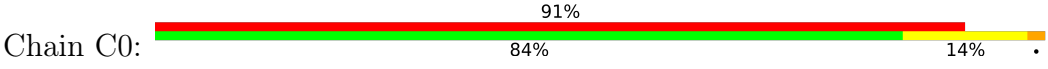
Chain S5:

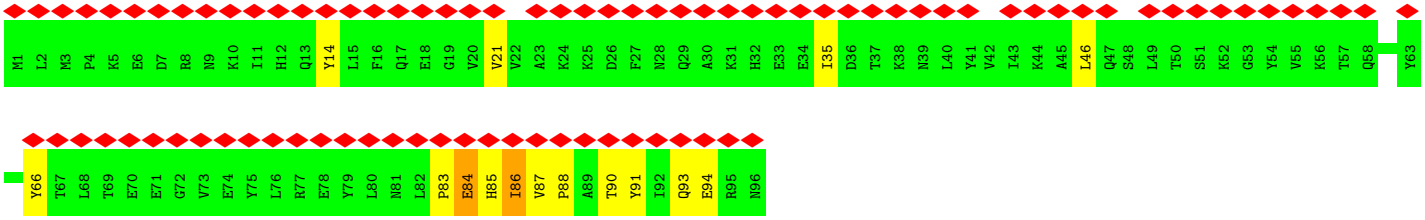




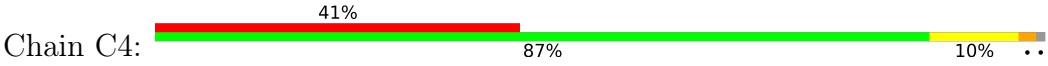
- Molecule 3: Small ribosomal subunit protein eS10A

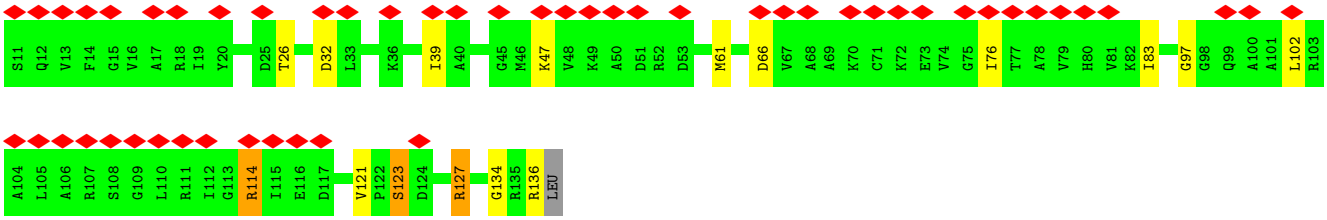
Chain C0:



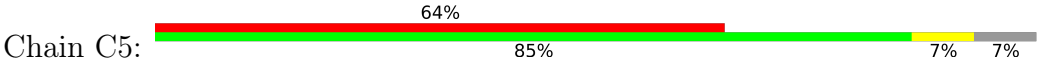


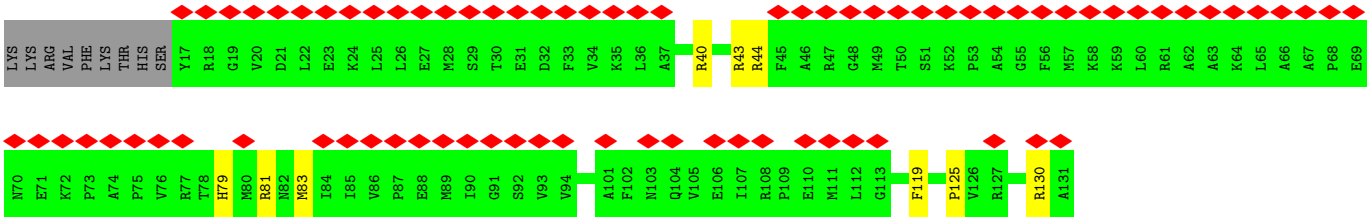
• Molecule 4: 40S ribosomal protein S14-B



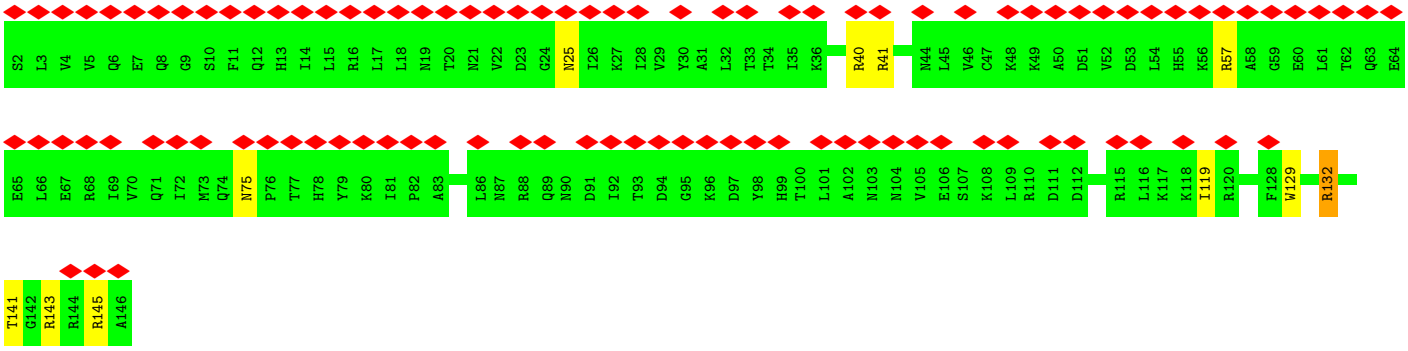


• Molecule 5: RPS15 isoform 1

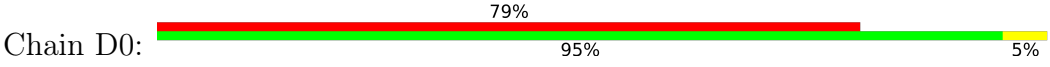


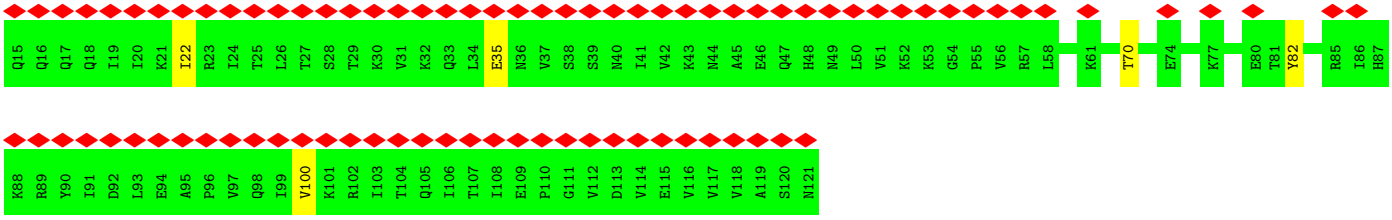


• Molecule 6: 40S ribosomal protein S18-A

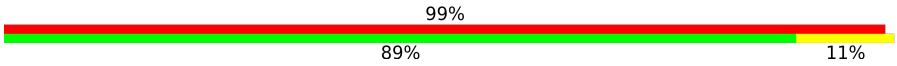


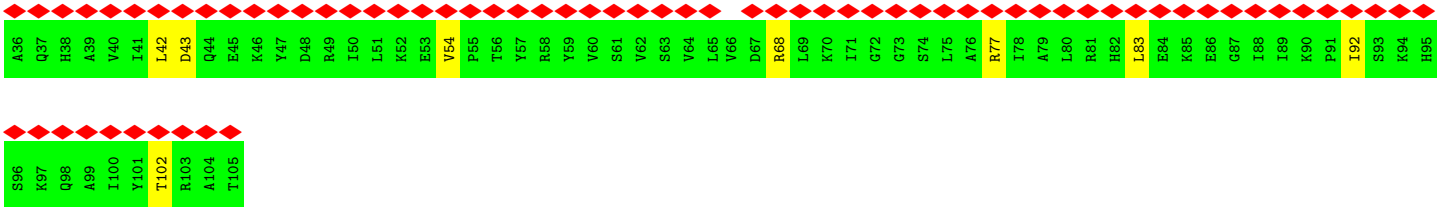
• Molecule 7: RPS20 isoform 1



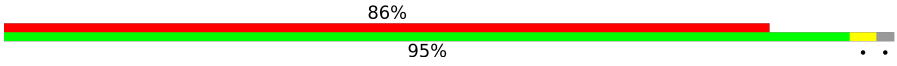


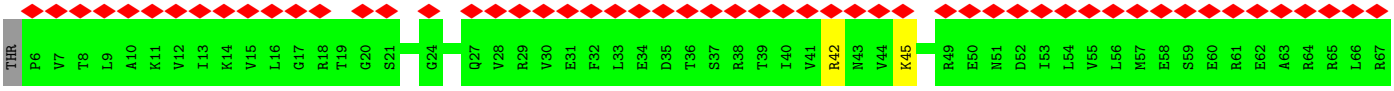
• Molecule 8: 40S ribosomal protein S25



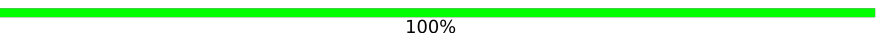


• Molecule 9: RPS28A isoform 1



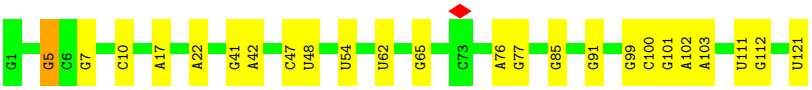


• Molecule 10: 60S ribosomal protein L41-A

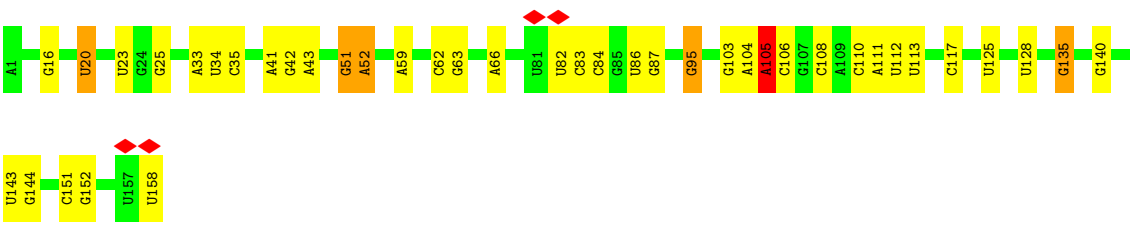


There are no outlier residues recorded for this chain.

• Molecule 11: 5S ribosomal RNA

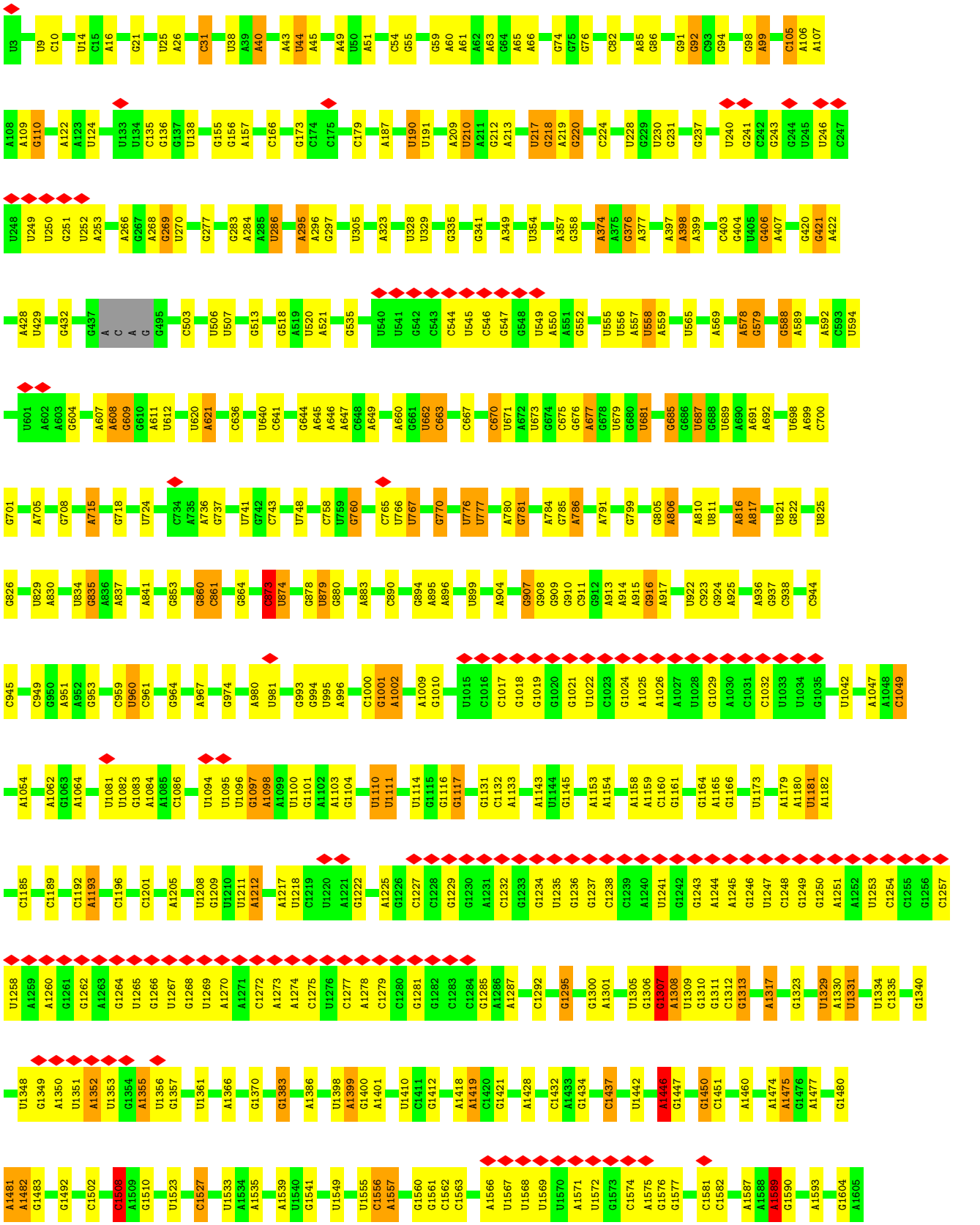


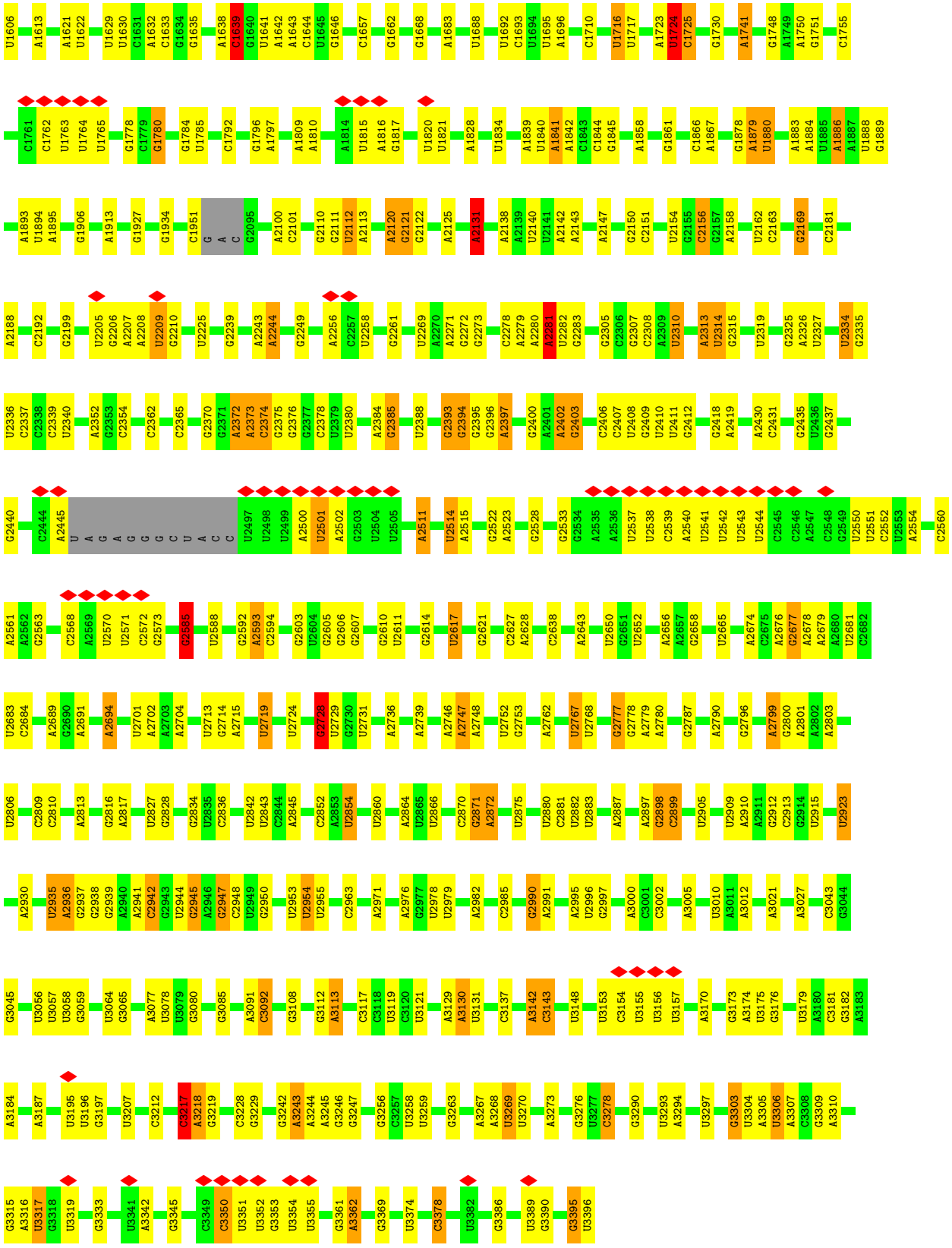
• Molecule 12: 5.8S ribosomal RNA



• Molecule 13: 25S ribosomal RNA

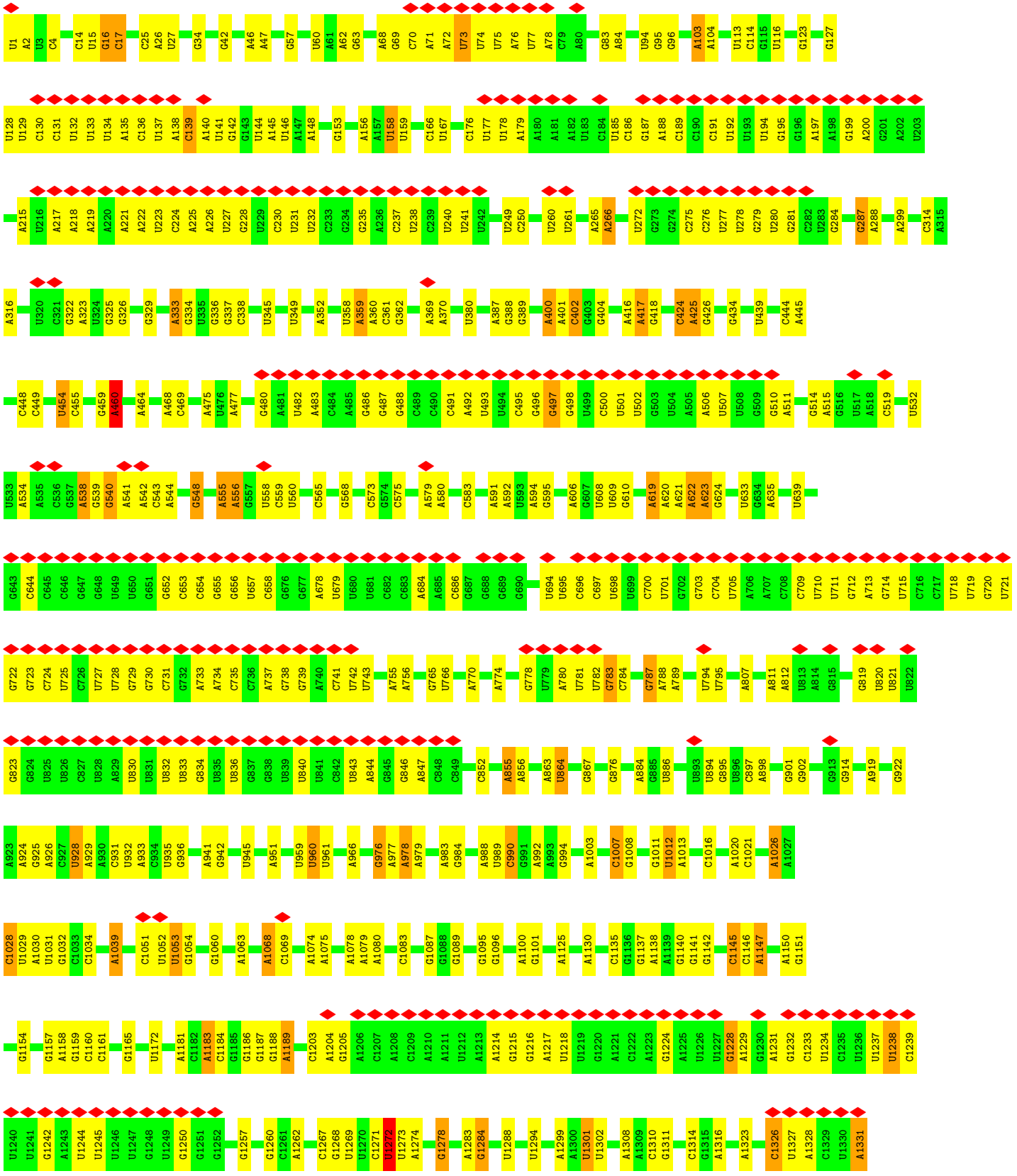
Chain 1:

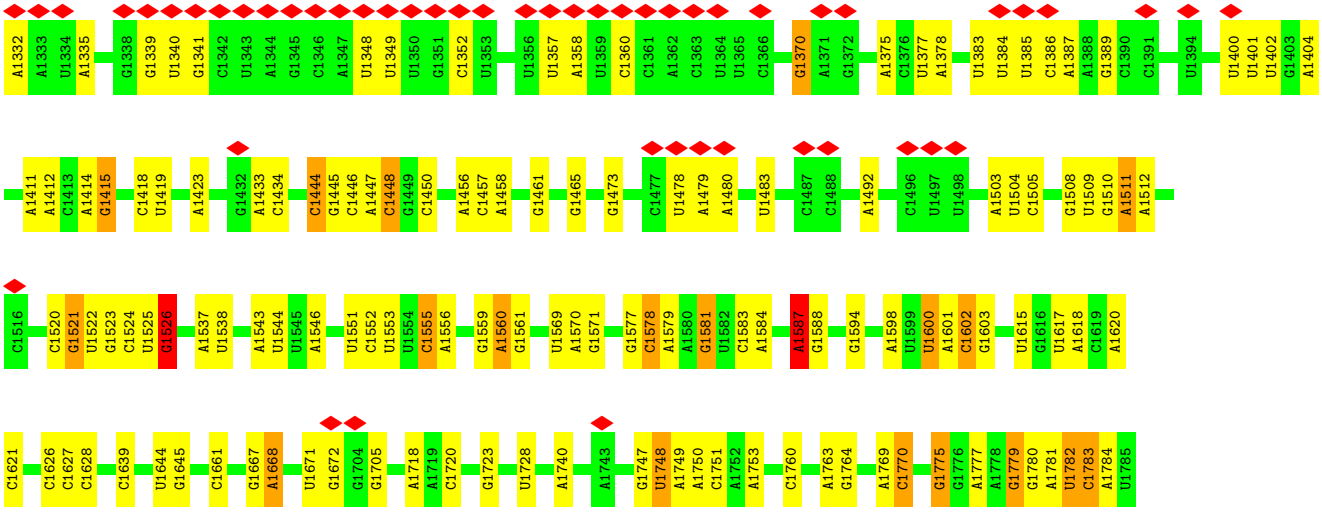




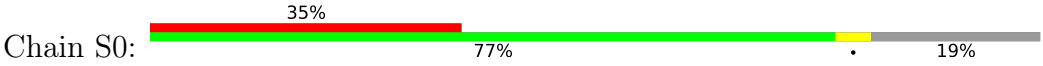
• Molecule 14: 18S ribosomal RNA

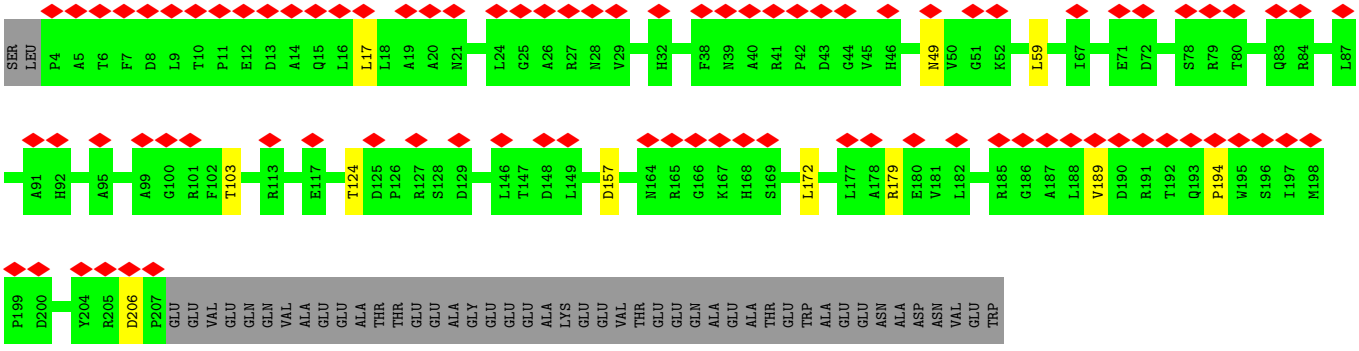
Chain 2:


U1 A2 U3 C4 C14 U15 G16 C17 C25 A26 U27 G34 G42 A46 A47 G57 U60 A61 A62 G63 A68 G69 C70 A71 A72 U73 U74 U75 A76 U77 A78 C79 A80 G83 A84 U94 G95 G96 A103 A104 U113 C114 G115 U116 G123 G127
U128 U129 C130 C131 U132 U133 U134 A135 C136 U137 A138 C139 A140 U141 G142 G143 U144 A145 U146 A147 A148 G153 A156 A157 U158 U159 C166 U167 C176 U177 U178 A179 A180 A181 A182 U183 C184 U185 C186 G187 A188 C189 C190 C191 U192 U193 U194 G195 G196 A197 A198 G199 A200 G201 A202 U203
A215 U216 A217 A218 A219 A220 A221 A222 U223 C224 A225 A226 U227 G228 U229 C230 U231 U232 C233 G234 G235 A236 C237 U238 C239 U240 U241 U242 U249 C250 U260 U261 A265 A266 U272 G273 G274 C275 C276 U277 U278 G279 U280 G281 C282 U283 G284 G287 A288 A299 C314 A315
A316 U320 C321 G322 A323 U324 G325 G326 G329 A333 G334 U335 G336 G337 C338 U345 U349 A352 U358 A359 A360 C361 G362 A369 A370 U380 A387 G388 G389 A400 A401 C402 G403 G404 A416 A417 G418 C424 A425 G426 G434 U439 C444 A445
C448 C449 U454 C455 G459 A460 A464 A468 C469 A475 U476 A477 G480 A481 U482 A483 C484 A485 G486 G487 G488 C489 C490 C491 A492 U493 U494 C495 G496 G497 G498 U499 C500 U501 U502 G503 U504 A505 A506 U507 U508 G509 G510 A511 G514 A515 G516 U517 A518 C519 U532
U533 A534 A535 C536 G537 A538 G539 G540 A541 A542 C543 A544 G548 A555 A556 G557 U558 C559 U560 C565 G568 C573 G574 C575 A579 A580 C583 A591 A592 U593 A594 G595 A606 G607 U608 U609 G610 A619 A620 A621 A622 A623 G624 U633 G634 A635 U639
G643 C644 C645 C646 G647 G648 U649 U650 G651 G652 C653 C654 G655 C656 U657 C658 G676 G677 A678 U679 U680 U681 C682 C683 A684 A685 C686 G687 G688 G689 G690 U694 U695 C696 C697 U698 U699 C700 U701 G702 G703 C704 U705 A706 A707 C708 C709 U710 U711 G712 A713 G714 U715 C716 C717 U718 U719 G720 U721
G722 G723 C724 U725 C726 U727 U728 G729 G730 C731 G732 A733 A734 C735 C736 A737 G738 G739 A740 C741 U742 U743 A755 A756 G765 U766 A770 A774 G778 U779 A780 U781 U782 G783 C784 G787 A788 A789 U794 U795 A807 A811 A812 U813 A814 G815 G819 U820 U821 U822
G823 G824 U825 U826 C827 U828 A829 U830 U831 U832 U833 G834 U835 U836 G837 G838 U839 U840 U841 C842 U843 A844 G845 G846 A847 C848 C849 C852 A855 A856 A863 U864 G867 G876 A884 G885 U886 U893 U894 G895 U896 C897 A898 G901 G902 G913 G914 A919 G922
A923 A924 G925 A926 C927 U928 A929 A930 C931 U932 A933 C934 U935 G936 A941 G942 U945 A951 U959 U960 U961 A966 G976 A977 A978 A979 A983 G984 A988 U989 C990 G991 A992 A993 G994 A1003 C1007 G1008 G1011 U1012 A1013 C1016 A1020 C1021 A1026 A1027
C1028 U1029 A1030 U1031 G1032 C1033 C1034 A1039 C1051 U1052 U1053 G1054 G1060 A1063 A1068 C1069 A1074 A1075 A1078 A1079 A1080 C1083 G1087 G1088 G1089 G1095 G1096 A1100 G1101 A1125 A1130 C1135 G1136 G1137 A1138 A1139 G1140 G1141 G1142 C1145 C1146 A1147 A1150 G1151
G1154 G1157 A1158 G1159 C1160 C1161 G1165 U1172 A1181 C1182 A1183 C1184 G1185 G1186 G1187 G1188 A1189 C1203 A1204 G1205 A1206 C1207 A1208 C1209 A1210 A1211 U1212 A1213 A1214 G1215 G1216 A1217 U1218 U1219 G1220 A1221 C1222 A1223 G1224 A1225 U1226 U1227 G1228 A1229 G1230 A1231 G1232 C1233 U1234 C1235 U1236 U1237 U1238 C1239
U1240 U1241 G1242 A1243 U1244 U1245 U1246 U1247 G1248 U1249 G1250 G1251 G1252 G1257 G1260 C1261 A1262 C1267 G1268 U1269 U1270 C1271 U1272 U1273 A1274 G1278 A1283 G1284 U1288 U1294 A1299 A1300 U1301 U1302 A1308 A1309 C1310 G1311 C1314 G1315 A1316 A1323 C1326 U1327 A1328 C1329 U1330 A1331

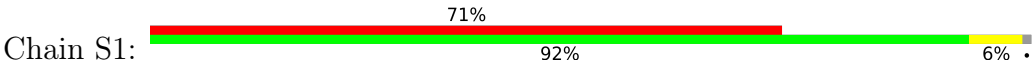


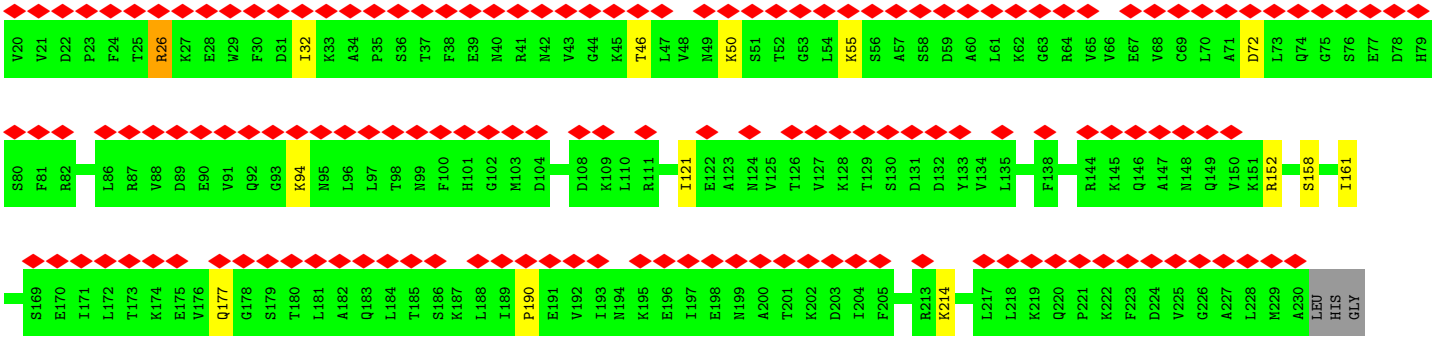
• Molecule 15: Small ribosomal subunit protein uS2A



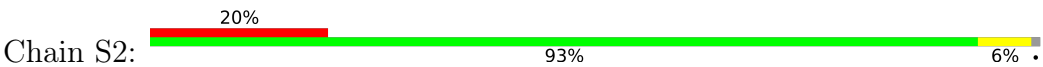


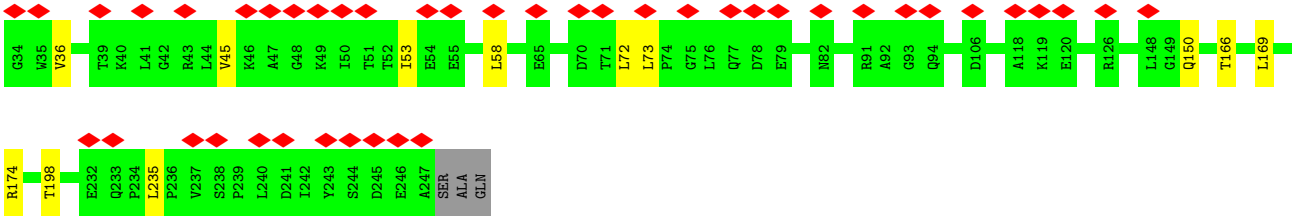
• Molecule 16: Small ribosomal subunit protein eS1





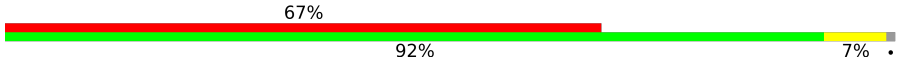
• Molecule 17: RPS2 isoform 1

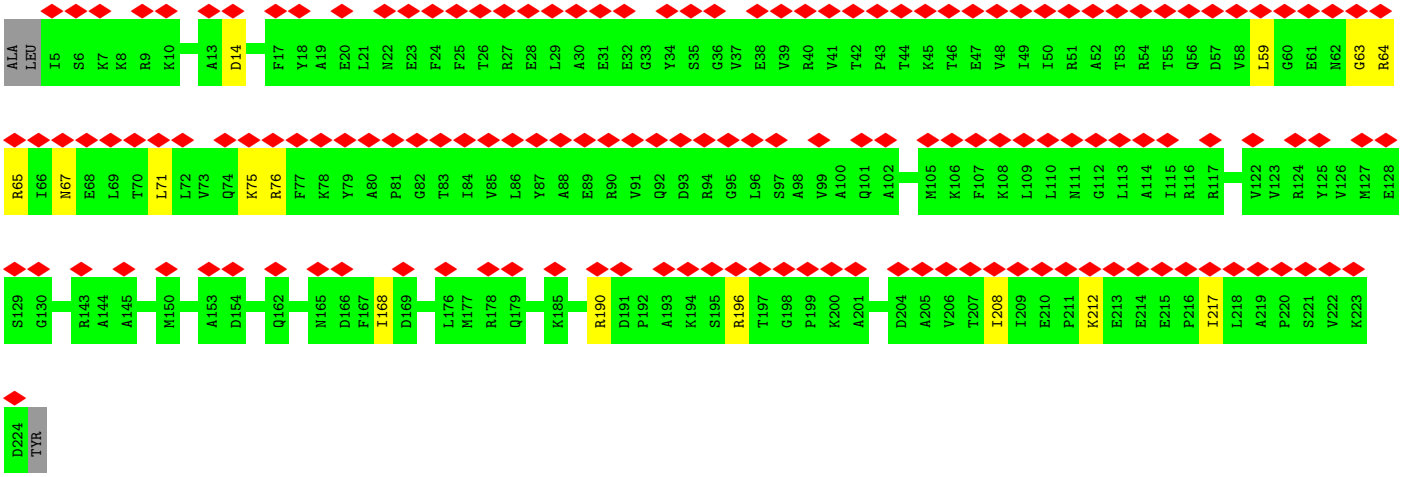




• Molecule 18: 40S ribosomal protein S3

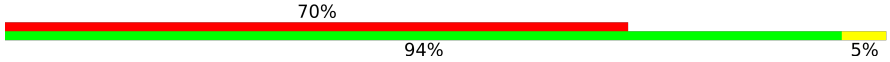
Chain S3:

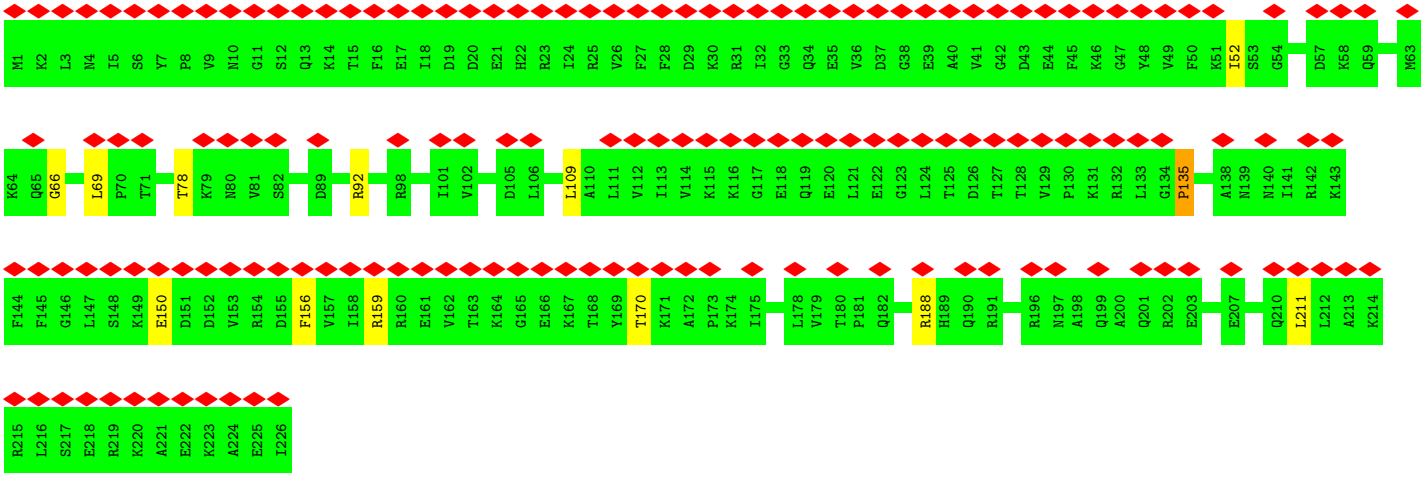




• Molecule 19: Small ribosomal subunit protein eS6A

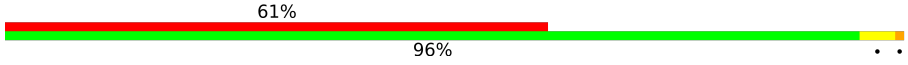
Chain S6:

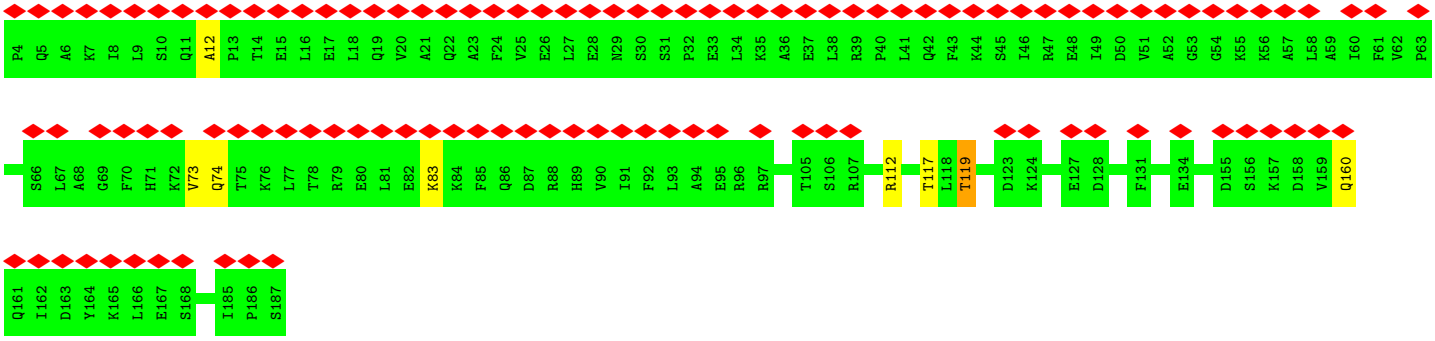




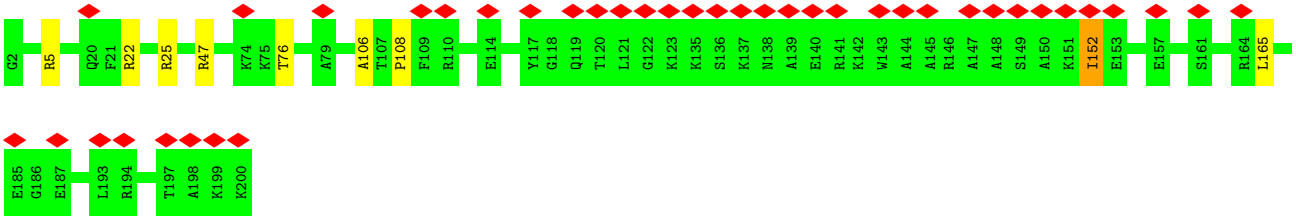
• Molecule 20: 40S ribosomal protein S7-A

Chain S7:

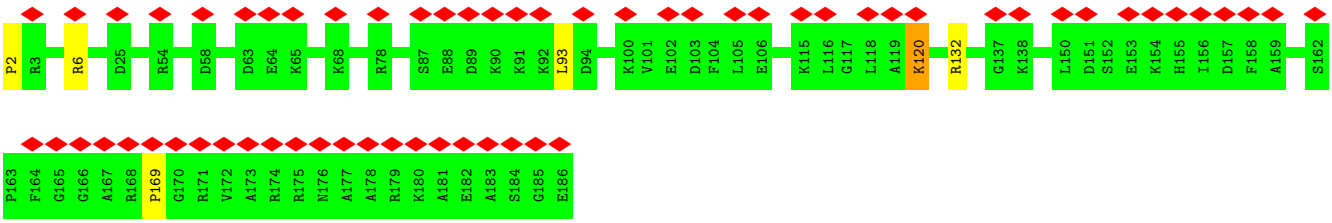




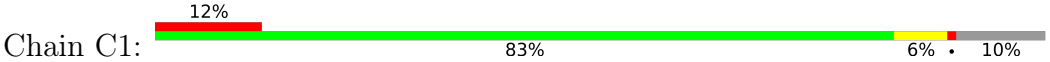
• Molecule 21: 40S ribosomal protein S8

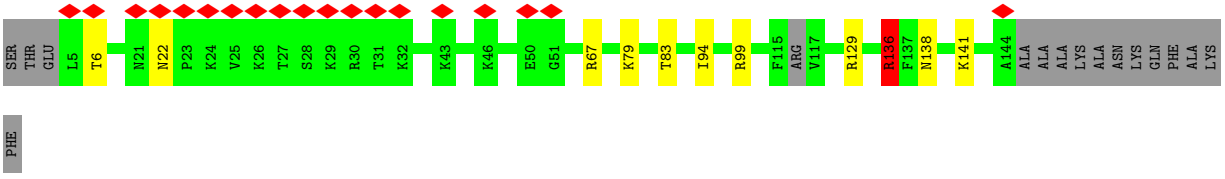


• Molecule 22: Small ribosomal subunit protein uS4A

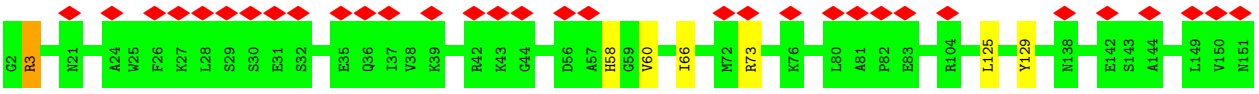


• Molecule 23: Small ribosomal subunit protein uS17A



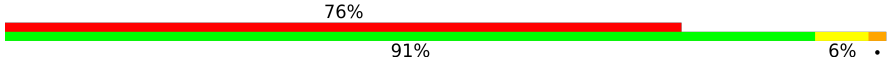


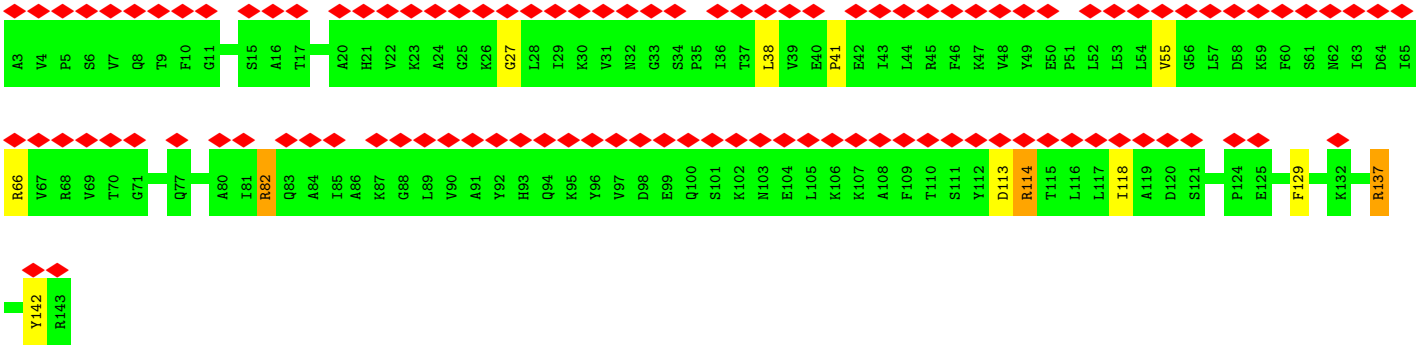
• Molecule 24: 40S ribosomal protein S13



• Molecule 25: 40S ribosomal protein S16-A

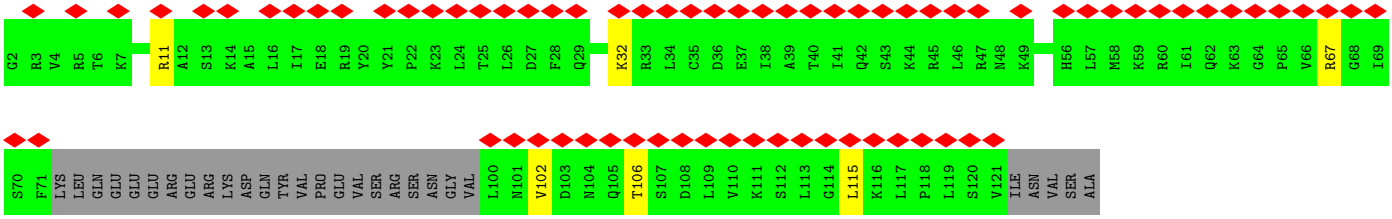
Chain C6:





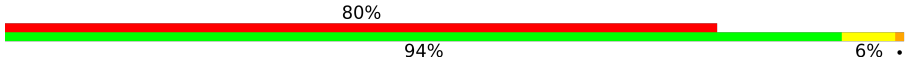
• Molecule 26: ES17

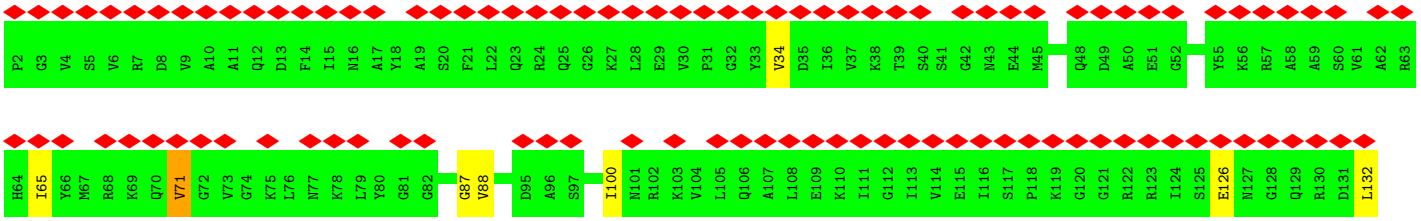
Chain C7:

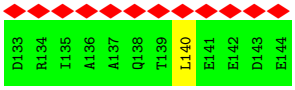


• Molecule 27: 40S ribosomal protein S19-A

Chain C9:

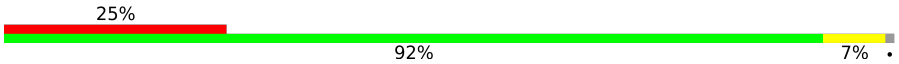


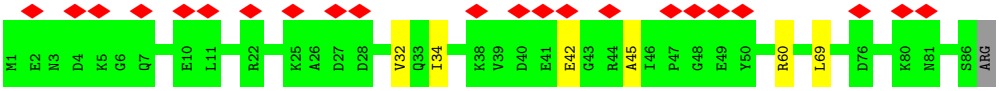




• Molecule 28: Small ribosomal subunit protein eS21A

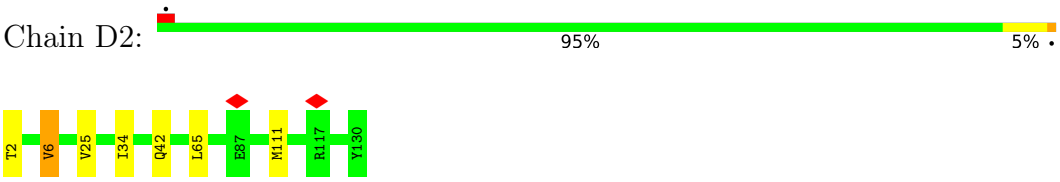
Chain D1:





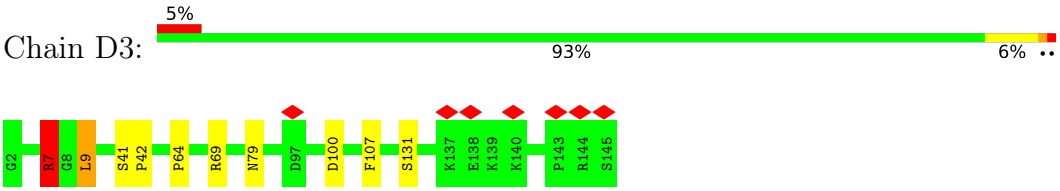
• Molecule 29: RPS22A isoform 1

Chain D2:



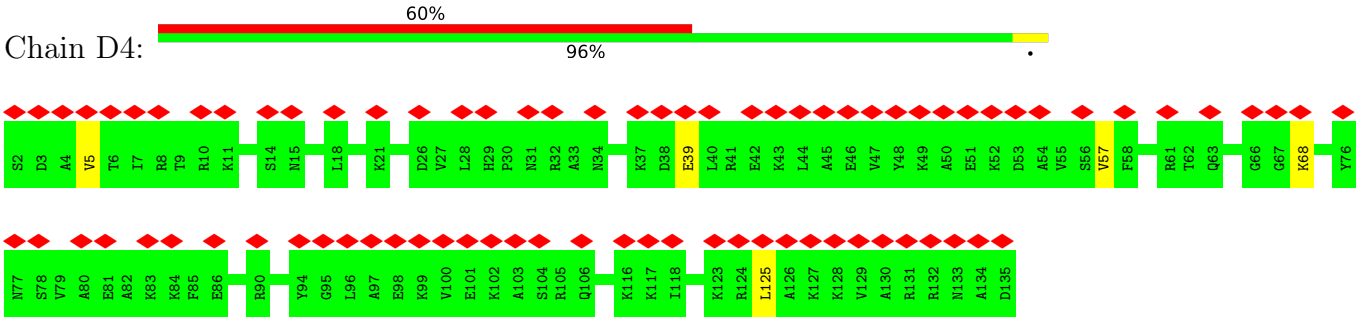
• Molecule 30: 40S ribosomal protein S23-A

Chain D3:



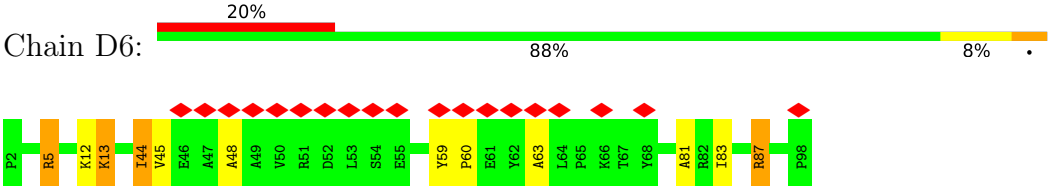
• Molecule 31: 40S ribosomal protein S24-A

Chain D4:



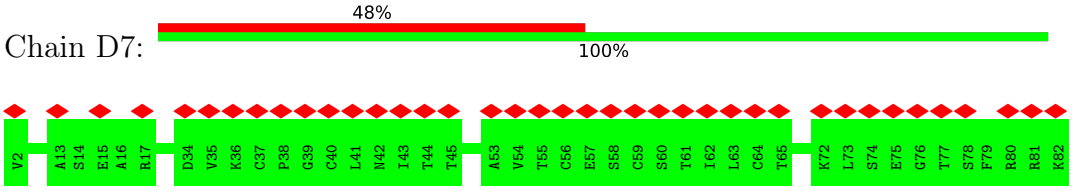
• Molecule 32: RPS26B isoform 1

Chain D6:



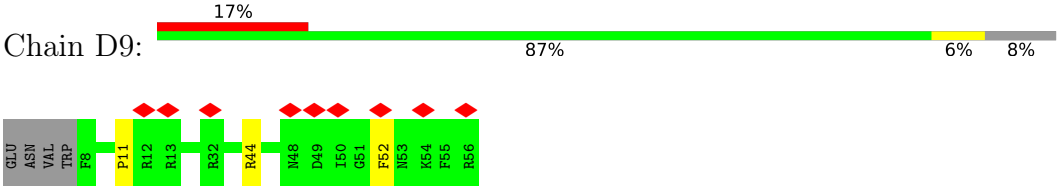
• Molecule 33: 40S ribosomal protein S27-A

Chain D7:



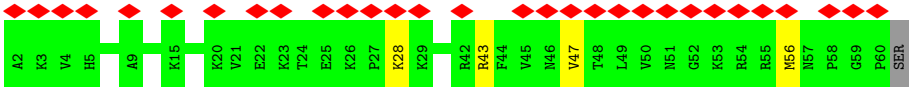
• Molecule 34: RPS29A isoform 1

Chain D9:



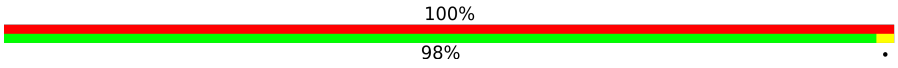
• Molecule 35: 40S ribosomal protein S30-A

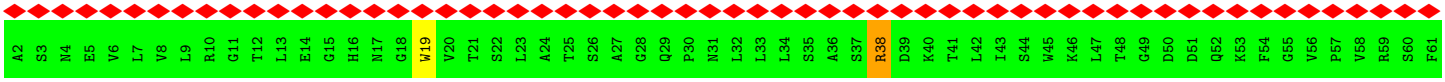
Chain E0:

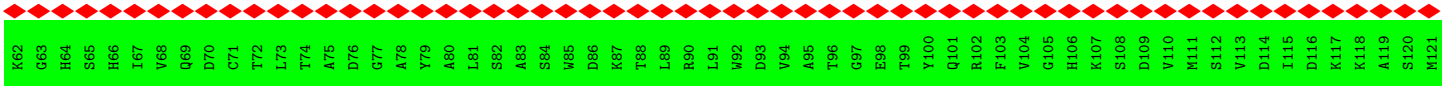


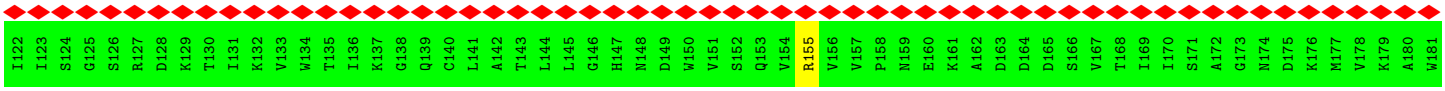
• Molecule 36: Small ribosomal subunit protein RACK1

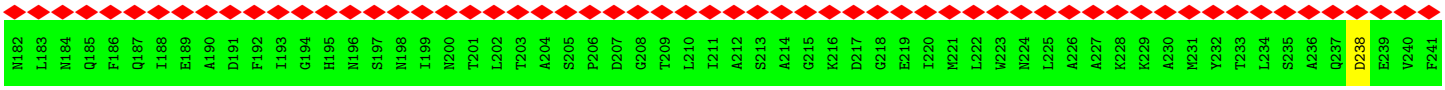
Chain SR:

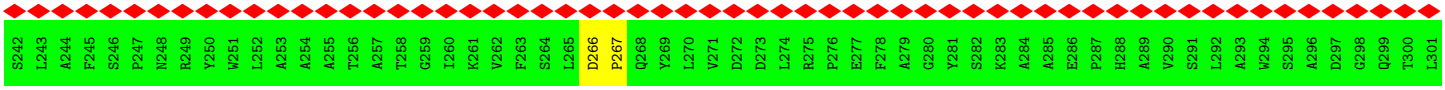


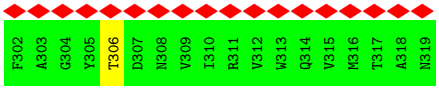






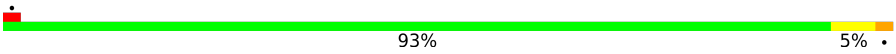






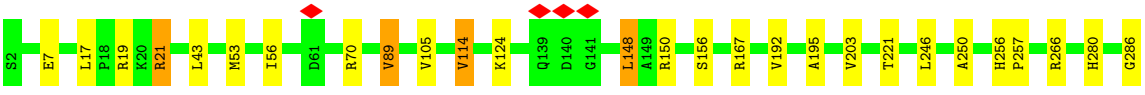
• Molecule 37: 60S ribosomal protein L2-A

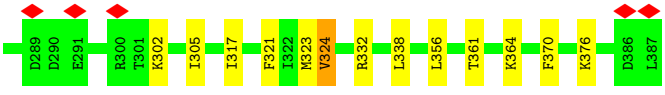
Chain L2:



• Molecule 38: 60S ribosomal protein L3

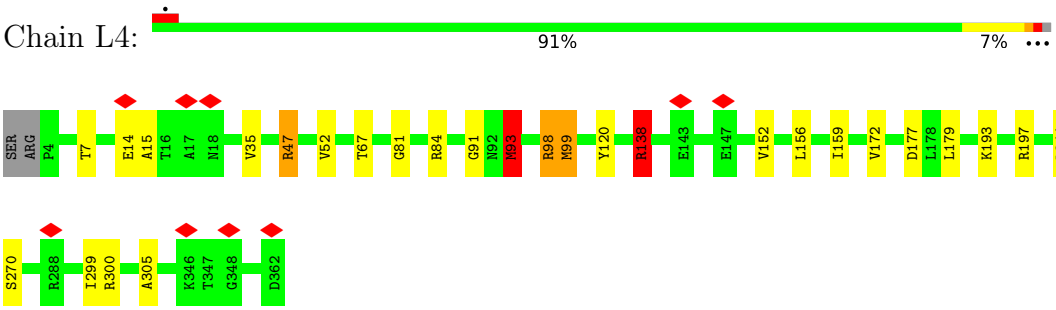
Chain L3:





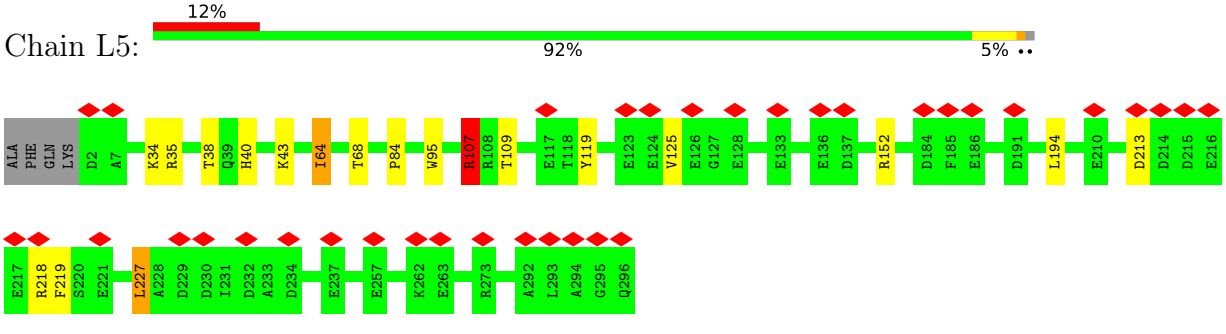
• Molecule 39: RPL4A isoform 1

Chain L4:



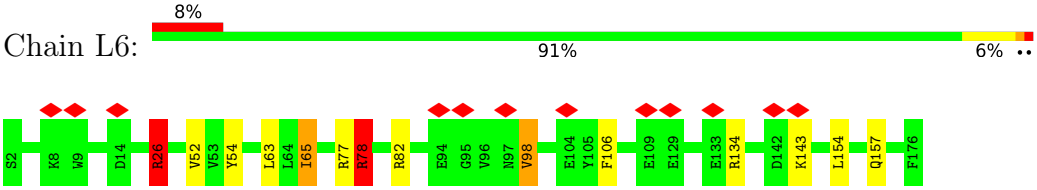
• Molecule 40: RPL5 isoform 1

Chain L5:



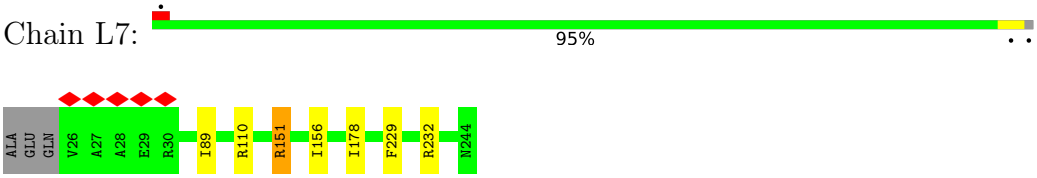
• Molecule 41: 60S ribosomal protein L6-A

Chain L6:



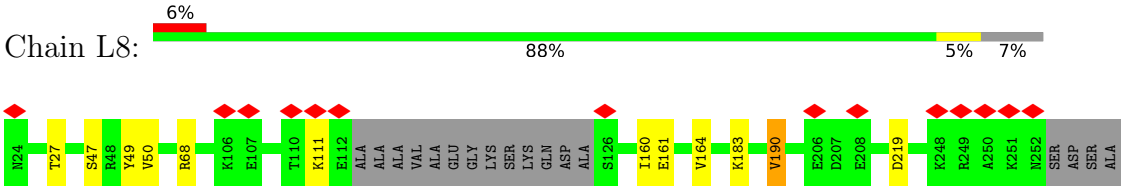
• Molecule 42: 60S ribosomal protein L7-A

Chain L7:



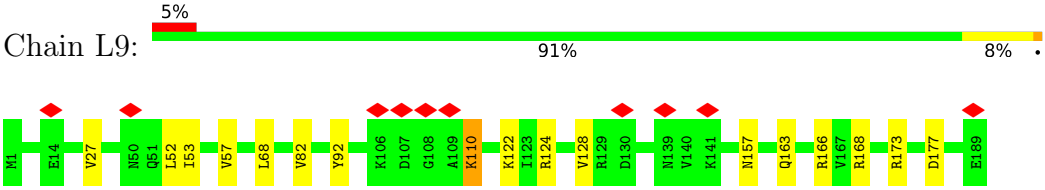
• Molecule 43: 60S ribosomal protein L8-A

Chain L8:



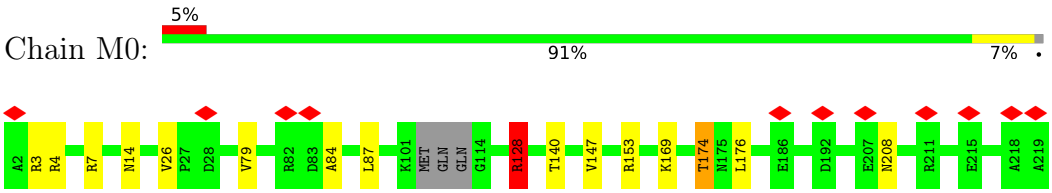
• Molecule 44: RPL9A isoform 1

Chain L9:



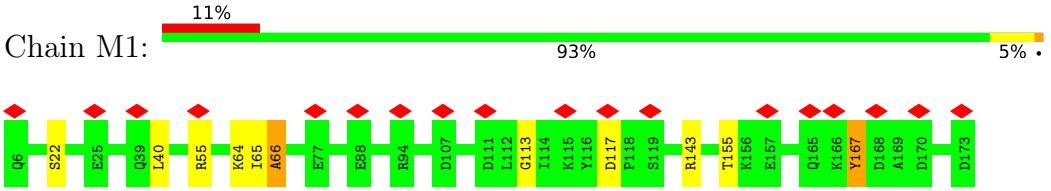
• Molecule 45: RPL10 isoform 1

Chain M0:



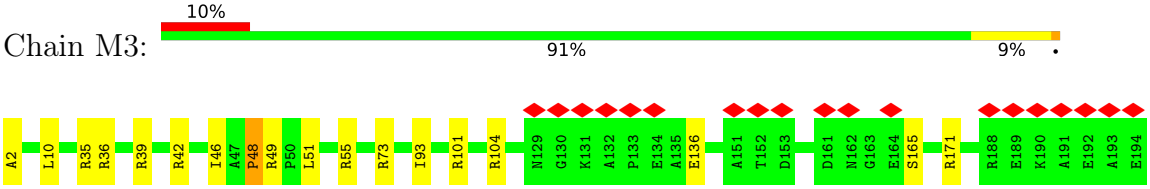
• Molecule 46: RPL11B isoform 1

Chain M1:



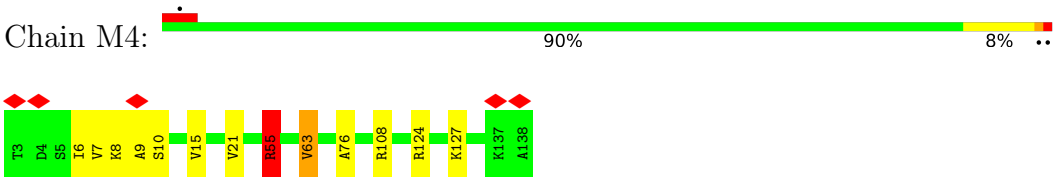
• Molecule 47: 60S ribosomal protein L13-A

Chain M3:



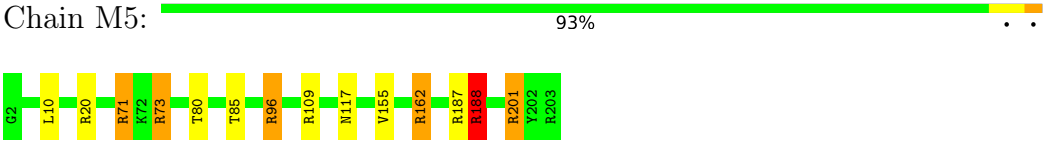
• Molecule 48: 60S ribosomal protein L14-A

Chain M4:



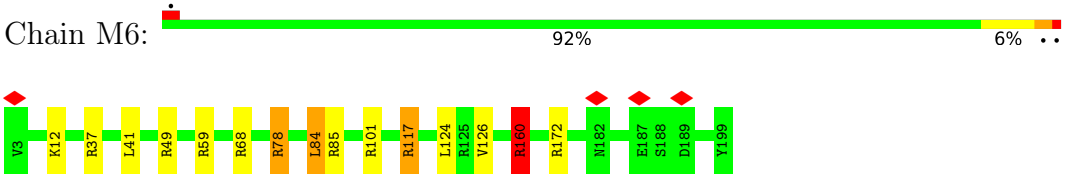
• Molecule 49: Ribosomal protein L15

Chain M5:



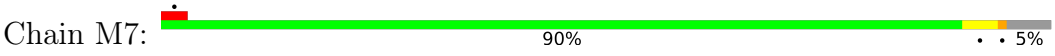
• Molecule 50: 60S ribosomal protein L16-A

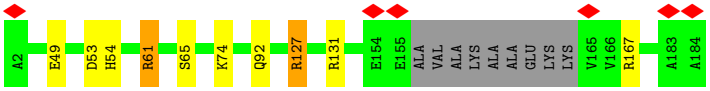
Chain M6:



• Molecule 51: 60S ribosomal protein L17-A

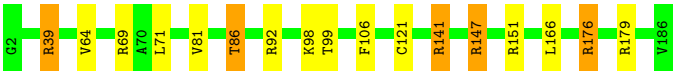
Chain M7:





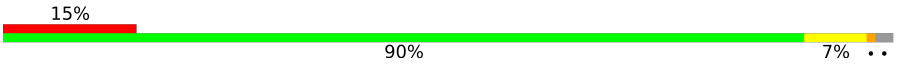
• Molecule 52: 60S ribosomal protein L18-A

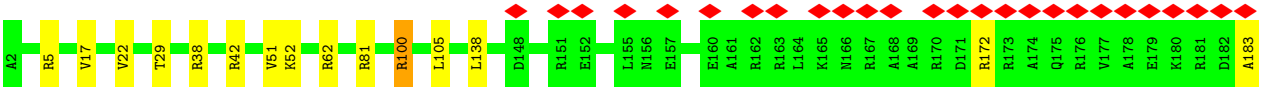
Chain M8:

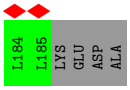


• Molecule 53: 60S ribosomal protein L19-A

Chain M9:





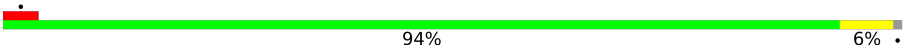


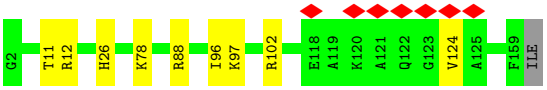
• Molecule 54: 60S ribosomal protein L20-A

Chain N0:

• Molecule 55: 60S ribosomal protein L21-A

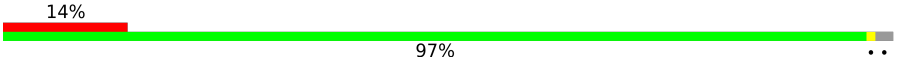
Chain N1:

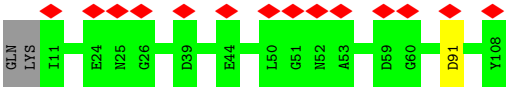




• Molecule 56: 60S ribosomal protein L22-A

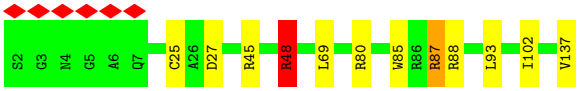
Chain N2:





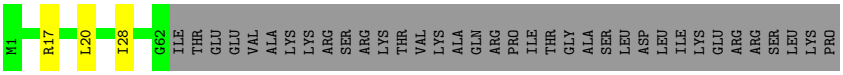
• Molecule 57: 60S ribosomal protein L23-A

Chain N3:



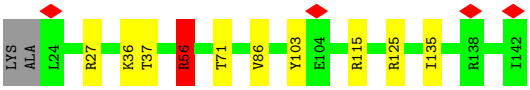
• Molecule 58: RPL24A isoform 1

Chain N4:



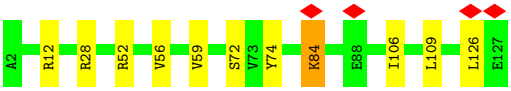
• Molecule 59: 60S ribosomal protein L25

Chain N5:



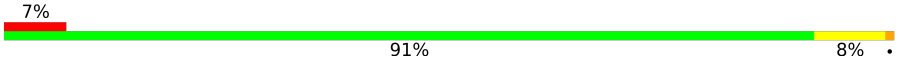
• Molecule 60: Large ribosomal subunit protein uL24A

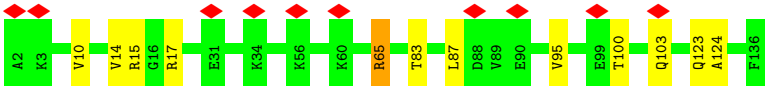
Chain N6:



• Molecule 61: 60S ribosomal protein L27-A

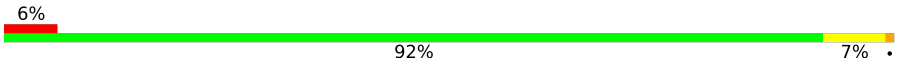
Chain N7:

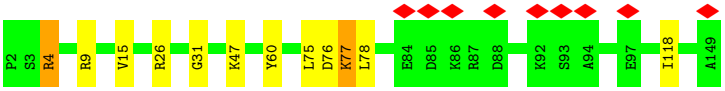




• Molecule 62: 60S ribosomal protein L28

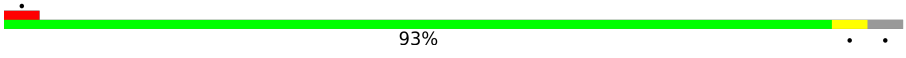
Chain N8:

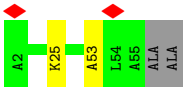




• Molecule 63: 60S ribosomal protein L29

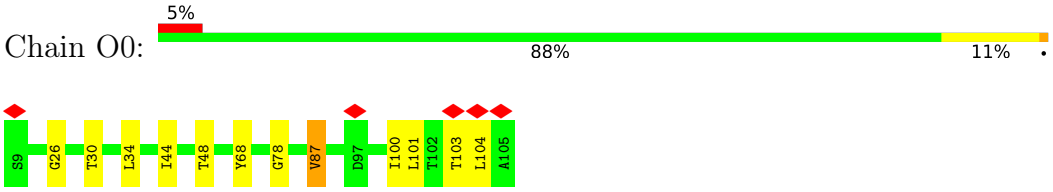
Chain N9:





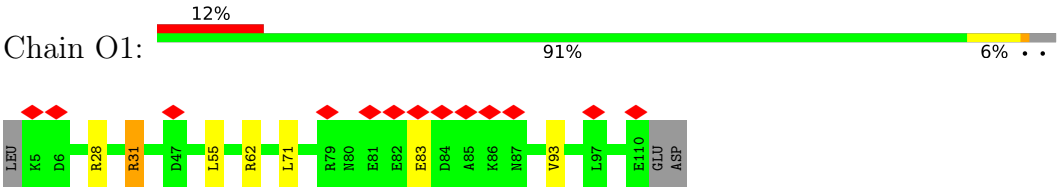
• Molecule 64: 60S ribosomal protein L30

Chain O0:



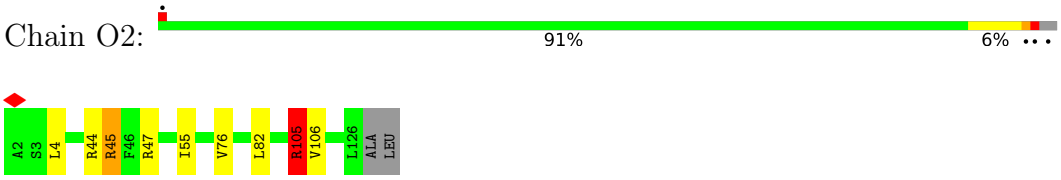
• Molecule 65: 60S ribosomal protein L31-A

Chain O1:



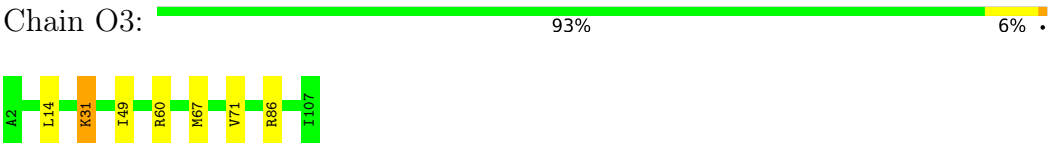
• Molecule 66: RPL32 isoform 1

Chain O2:



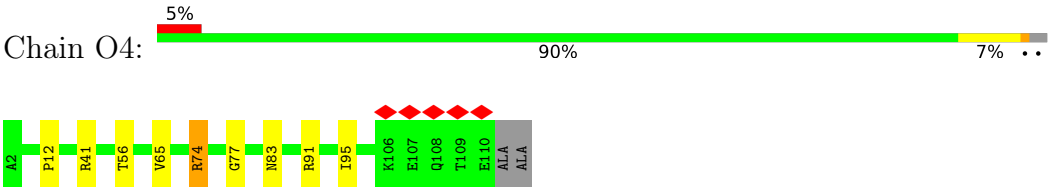
• Molecule 67: 60S ribosomal protein L33-A

Chain O3:



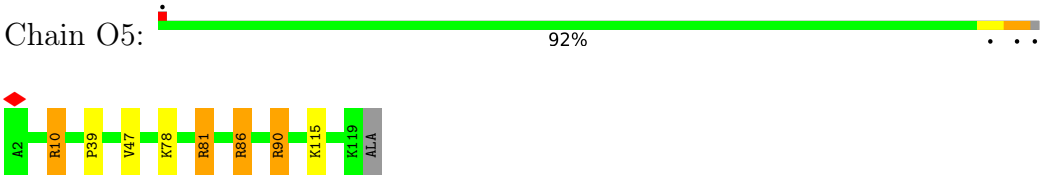
• Molecule 68: Large ribosomal subunit protein eL34A

Chain O4:



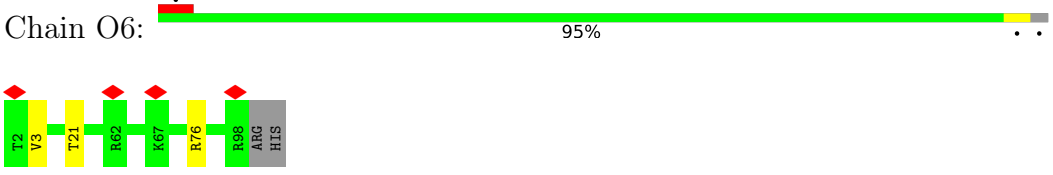
• Molecule 69: 60S ribosomal protein L35-A

Chain O5:



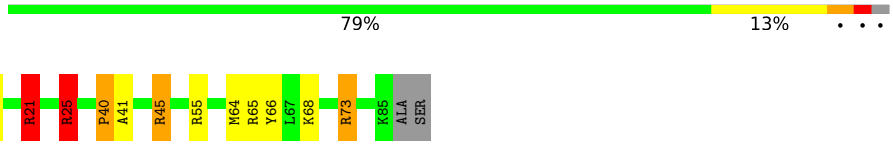
• Molecule 70: 60S ribosomal protein L36-A

Chain O6:



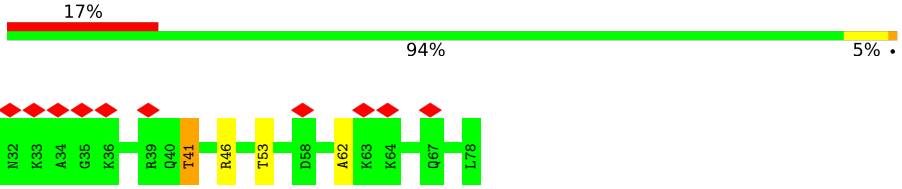
• Molecule 71: Large ribosomal subunit protein eL37A

Chain O7:



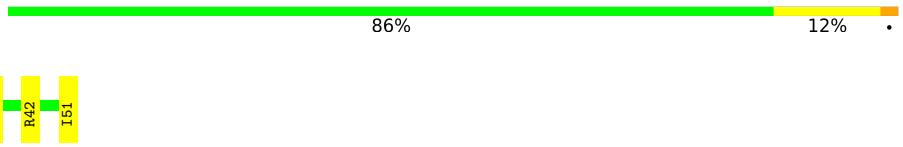
• Molecule 72: RPL38 isoform 1

Chain O8:



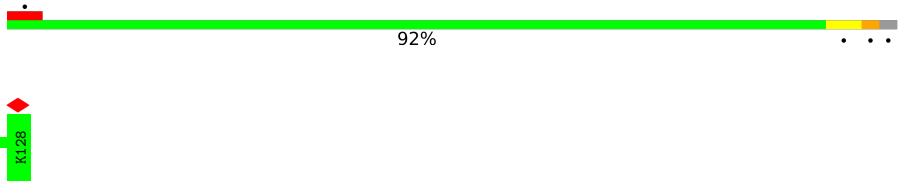
• Molecule 73: 60S ribosomal protein L39

Chain O9:



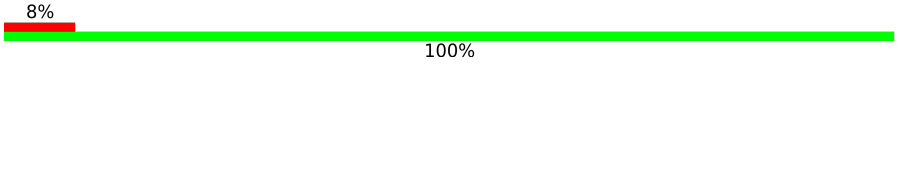
• Molecule 74: 60S ribosomal protein L40-A

Chain Q0:



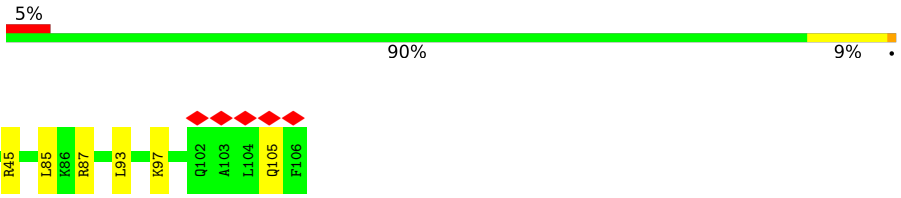
• Molecule 75: Large ribosomal subunit protein eL41B

Chain Q1:



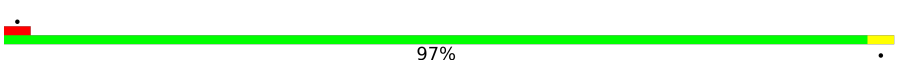
• Molecule 76: 60S ribosomal protein L42-A

Chain Q2:



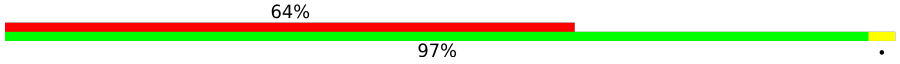
• Molecule 77: 60S ribosomal protein L43-A

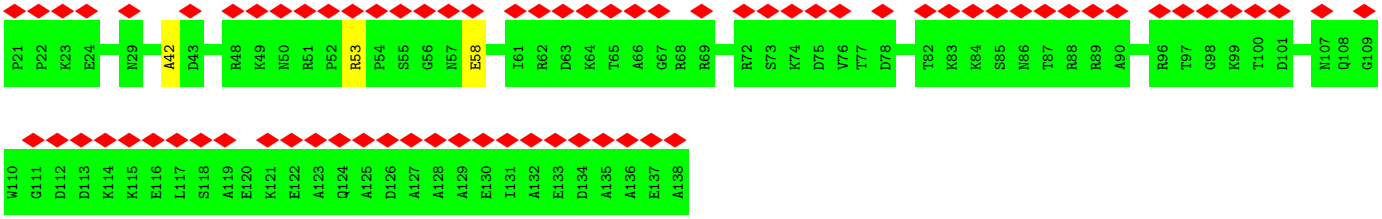
Chain Q3:



• Molecule 78: STM1 isoform 1

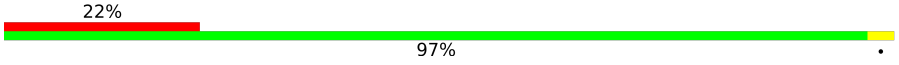
Chain SM:





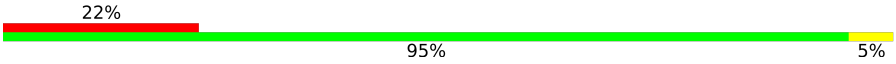
• Molecule 79: Eukaryotic translation initiation factor 5A

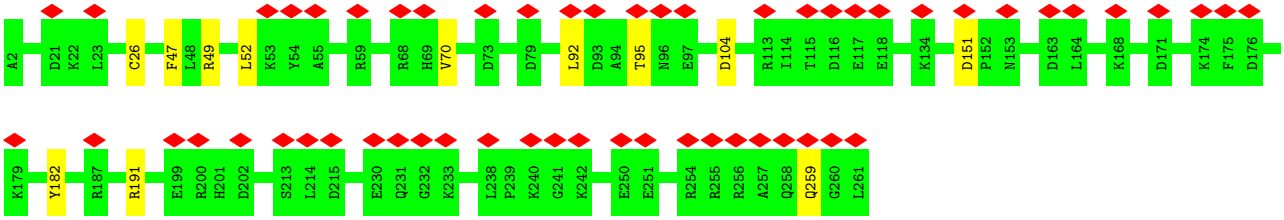
Chain eI:



• Molecule 80: Small ribosomal subunit protein eS4A

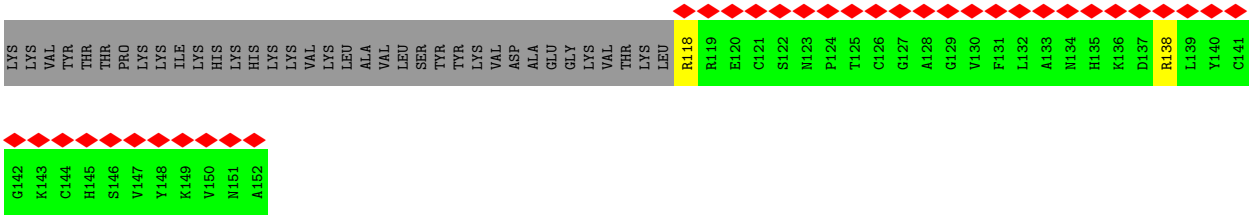
Chain S4:





• Molecule 81: RPS31 isoform 1

Chain E1:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	127945	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	32	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.083	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0143	Depositor
Map size (Å)	375.84, 375.84, 375.84	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.783, 0.783, 0.783	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, SPD, 5CT, 3HE, 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	B	0.35	0/1737	0.74	0/2332
2	S5	0.33	0/1629	0.68	0/2202
3	C0	0.35	0/838	0.74	0/1133
4	C4	0.38	0/944	0.77	1/1268 (0.1%)
5	C5	0.37	0/931	0.77	2/1250 (0.2%)
6	C8	0.33	0/1211	0.74	1/1628 (0.1%)
7	D0	0.31	0/865	0.69	0/1169
8	D5	0.35	0/571	0.75	0/768
9	D8	0.34	0/492	0.80	0/659
10	P	0.35	0/147	1.04	0/189
11	3	0.60	0/2883	1.28	15/4491 (0.3%)
12	4	0.64	0/3746	1.33	20/5832 (0.3%)
13	1	0.69	0/75240	1.39	602/117303 (0.5%)
14	2	0.59	0/41395	1.24	175/64501 (0.3%)
15	S0	0.35	0/1639	0.80	0/2241
16	S1	0.35	0/1712	0.83	1/2304 (0.0%)
17	S2	0.35	0/1645	0.77	0/2236
18	S3	0.35	0/1733	0.82	1/2332 (0.0%)
19	S6	0.35	0/1844	0.80	0/2464
20	S7	0.33	0/1506	0.76	1/2028 (0.0%)
21	S8	0.36	0/1514	0.84	0/2021
22	S9	0.34	0/1519	0.81	1/2035 (0.0%)
23	C1	0.37	0/1146	0.79	0/1544
24	C3	0.34	0/1215	0.75	0/1638
25	C6	0.36	0/1125	0.81	0/1510
26	C7	0.36	0/744	0.76	0/995
27	C9	0.36	0/1130	0.74	0/1517
28	D1	0.35	0/682	0.80	0/921
29	D2	0.34	0/1038	0.78	2/1395 (0.1%)
30	D3	0.37	0/1139	0.92	4/1518 (0.3%)
31	D4	0.34	0/1087	0.80	0/1449
32	D6	0.37	0/782	0.91	1/1047 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	D7	0.34	0/620	0.73	0/838
34	D9	0.38	0/412	0.86	0/544
35	E0	0.35	0/477	0.86	2/635 (0.3%)
36	SR	0.34	0/2498	0.65	0/3398
37	L2	0.49	0/1943	1.02	8/2610 (0.3%)
38	L3	0.48	0/3150	0.97	4/4235 (0.1%)
39	L4	0.45	0/2783	0.91	8/3767 (0.2%)
40	L5	0.36	0/2377	0.79	1/3206 (0.0%)
41	L6	0.37	0/1260	0.81	2/1694 (0.1%)
42	L7	0.44	0/1798	0.85	2/2420 (0.1%)
43	L8	0.36	0/1737	0.80	2/2343 (0.1%)
44	L9	0.36	0/1523	0.84	1/2051 (0.0%)
45	M0	0.41	0/1713	0.91	2/2297 (0.1%)
46	M1	0.36	0/1365	0.85	1/1831 (0.1%)
47	M3	0.44	0/1568	0.94	3/2106 (0.1%)
48	M4	0.36	0/1068	0.84	1/1438 (0.1%)
49	M5	0.52	0/1748	1.08	8/2343 (0.3%)
50	M6	0.49	0/1585	1.05	9/2128 (0.4%)
51	M7	0.51	0/1401	1.01	4/1882 (0.2%)
52	M8	0.44	0/1465	1.03	5/1965 (0.3%)
53	M9	0.45	0/1507	0.90	5/2009 (0.2%)
54	N0	0.43	0/1481	0.91	3/1990 (0.2%)
55	N1	0.47	0/1292	0.88	0/1732
56	N2	0.35	0/794	0.79	0/1076
57	N3	0.47	0/1018	0.98	4/1369 (0.3%)
58	N4	0.44	0/525	0.80	0/696
59	N5	0.40	0/969	0.89	2/1307 (0.2%)
60	N6	0.43	0/1004	0.89	2/1341 (0.1%)
61	N7	0.36	0/1118	0.85	2/1497 (0.1%)
62	N8	0.51	0/1204	0.94	4/1612 (0.2%)
63	N9	0.43	0/445	0.98	0/593
64	O0	0.37	0/751	0.77	0/1008
65	O1	0.45	0/879	0.95	2/1179 (0.2%)
66	O2	0.49	0/1028	1.02	4/1376 (0.3%)
67	O3	0.47	0/868	0.85	1/1168 (0.1%)
68	O4	0.47	0/871	0.96	3/1164 (0.3%)
69	O5	0.38	0/973	0.95	4/1294 (0.3%)
70	O6	0.38	0/756	0.91	0/1005
71	O7	0.57	0/691	1.28	8/915 (0.9%)
72	O8	0.37	0/618	0.78	0/826
73	O9	0.49	0/443	1.07	2/588 (0.3%)
74	Q0	0.39	0/415	0.90	2/551 (0.4%)
75	Q1	0.39	0/234	1.04	0/300

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	Q2	0.41	0/860	0.99	2/1136 (0.2%)
77	Q3	0.45	0/701	0.88	0/934
78	SM	0.35	0/903	0.75	0/1210
79	eI	0.36	0/1095	0.79	0/1473
80	S4	0.34	0/2109	0.79	0/2839
81	E1	0.39	0/276	0.74	1/368 (0.3%)
All	All	0.56	0/214148	1.18	941/314207 (0.3%)

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
1	B	0	2
2	S5	0	2
4	C4	0	3
6	C8	0	2
8	D5	0	1
9	D8	0	1
13	1	0	9
15	S0	0	1
16	S1	0	1
17	S2	0	1
20	S7	0	1
21	S8	0	2
22	S9	0	1
23	C1	0	3
24	C3	0	1
25	C6	0	2
30	D3	0	2
32	D6	0	2
34	D9	0	1
36	SR	0	3
37	L2	0	5
38	L3	0	3
39	L4	0	5
40	L5	0	3
41	L6	0	5
42	L7	0	3
43	L8	0	1
44	L9	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
45	M0	0	2
47	M3	0	6
48	M4	0	1
49	M5	0	7
50	M6	0	6
51	M7	0	3
52	M8	0	4
53	M9	0	3
54	N0	0	5
55	N1	0	2
57	N3	0	3
58	N4	0	1
59	N5	0	2
60	N6	0	2
61	N7	0	2
62	N8	0	3
65	O1	0	2
66	O2	0	4
67	O3	0	2
69	O5	0	3
71	O7	0	4
73	O9	0	1
76	Q2	0	1
80	S4	0	2
All	All	0	141

There are no bond length outliers.

All (941) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	1	2403	G	O5'-P-OP2	-23.53	82.47	110.70
13	1	806	A	O5'-P-OP1	-19.93	86.78	110.70
13	1	1639	C	O5'-P-OP2	-19.57	87.22	110.70
13	1	2373	A	O5'-P-OP1	-17.61	89.57	110.70
13	1	1117	G	O5'-P-OP1	-17.14	90.13	110.70
13	1	861	C	O5'-P-OP2	-16.72	90.64	110.70
14	2	1760	C	O5'-P-OP2	-15.74	91.53	105.70
13	1	2923	U	O5'-P-OP1	-15.39	91.85	105.70
13	1	2945	G	O5'-P-OP2	15.27	129.02	110.70
13	1	295	A	O5'-P-OP1	-15.25	91.98	105.70
13	1	99	A	O5'-P-OP2	-15.04	92.16	105.70
13	1	2393	G	O5'-P-OP2	-14.98	92.22	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	1	2244	A	O5'-P-OP1	14.58	128.19	110.70
13	1	92	G	O5'-P-OP1	-14.46	92.69	105.70
12	4	112	U	O3'-P-O5'	-14.36	76.72	104.00
13	1	1313	G	O5'-P-OP2	-14.20	92.92	105.70
13	1	609	G	O5'-P-OP2	-13.95	93.15	105.70
13	1	817	A	O5'-P-OP1	-13.40	93.64	105.70
13	1	2314	U	O5'-P-OP2	-13.26	93.77	105.70
13	1	1447	G	O5'-P-OP2	-13.18	93.84	105.70
13	1	1792	C	O5'-P-OP2	-13.05	93.96	105.70
13	1	2945	G	O5'-P-OP1	-12.99	94.01	105.70
13	1	890	C	O5'-P-OP2	-12.68	94.29	105.70
13	1	2334	U	O5'-P-OP2	-12.42	94.52	105.70
71	O7	45	ARG	NE-CZ-NH2	-11.82	114.39	120.30
13	1	671	U	O5'-P-OP2	-11.72	95.15	105.70
13	1	110	G	O5'-P-OP2	-11.68	95.19	105.70
13	1	406	G	O4'-C1'-N9	11.62	117.50	108.20
13	1	2728	G	O5'-P-OP2	-11.25	95.57	105.70
13	1	92	G	O5'-P-OP2	11.22	124.17	110.70
13	1	2243	A	O3'-P-O5'	-11.16	82.79	104.00
13	1	3361	G	O3'-P-O5'	-11.13	82.85	104.00
14	2	287	G	O4'-C1'-N9	10.95	116.96	108.20
76	Q2	41	ARG	NE-CZ-NH2	-10.94	114.83	120.30
13	1	429	U	O5'-P-OP2	-10.80	95.98	105.70
13	1	816	A	O3'-P-O5'	10.78	124.49	104.00
13	1	1508	C	O5'-P-OP1	-10.75	96.02	105.70
38	L3	266	ARG	NE-CZ-NH2	-10.71	114.94	120.30
14	2	1415	G	O5'-P-OP1	-10.59	96.17	105.70
14	2	623	A	O5'-P-OP1	10.53	123.33	110.70
13	1	3143	C	O5'-P-OP2	-10.52	96.23	105.70
13	1	2314	U	O5'-P-OP1	10.31	123.07	110.70
13	1	2995	A	O5'-P-OP2	-10.26	96.46	105.70
13	1	1724	U	O3'-P-O5'	-10.19	84.65	104.00
38	L3	53	MET	CG-SD-CE	-10.09	84.05	100.20
68	O4	74	ARG	NE-CZ-NH1	10.07	125.33	120.30
14	2	402	C	O5'-P-OP1	-10.05	96.65	105.70
13	1	98	G	OP2-P-O3'	10.04	127.29	105.20
13	1	1632	A	O3'-P-O5'	-9.94	85.12	104.00
51	M7	127	ARG	NE-CZ-NH2	-9.88	115.36	120.30
13	1	98	G	O3'-P-O5'	-9.80	85.37	104.00
69	O5	86	ARG	NE-CZ-NH2	-9.79	115.40	120.30
13	1	1398	U	O3'-P-O5'	-9.74	85.50	104.00
13	1	2935	U	O3'-P-O5'	-9.71	85.55	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
71	O7	55	ARG	NE-CZ-NH1	9.66	125.13	120.30
13	1	770	G	O4'-C1'-N9	9.62	115.89	108.20
13	1	2621	G	O5'-P-OP2	-9.60	97.06	105.70
13	1	2142	A	C6-N1-C2	-9.56	112.86	118.60
13	1	835	G	O4'-C1'-N9	9.55	115.84	108.20
13	1	2409	G	O5'-P-OP2	-9.55	97.10	105.70
13	1	1212	A	O5'-P-OP2	-9.51	97.14	105.70
13	1	2610	G	O5'-P-OP2	-9.46	97.19	105.70
13	1	2860	U	O5'-P-OP2	-9.34	97.30	105.70
13	1	1841	A	O5'-P-OP2	-9.33	97.30	105.70
14	2	16	G	O5'-P-OP2	-9.28	97.34	105.70
13	1	1662	G	O5'-P-OP2	-9.24	97.38	105.70
13	1	209	A	O3'-P-O5'	-9.23	86.45	104.00
13	1	936	A	O3'-P-O5'	-9.23	86.46	104.00
13	1	1419	A	O5'-P-OP2	-9.11	97.50	105.70
48	M4	55	ARG	NE-CZ-NH2	-9.11	115.75	120.30
51	M7	127	ARG	NE-CZ-NH1	9.10	124.85	120.30
13	1	31	C	O5'-P-OP2	-9.08	97.53	105.70
14	2	1274	A	O3'-P-O5'	-9.06	86.78	104.00
57	N3	48	ARG	NE-CZ-NH2	-9.06	115.77	120.30
13	1	1450	G	O5'-P-OP2	-9.06	97.54	105.70
13	1	2713	U	O3'-P-O5'	-9.04	86.83	104.00
14	2	425	A	O5'-P-OP1	8.96	121.46	110.70
14	2	359	A	O3'-P-O5'	-8.95	87.00	104.00
13	1	2327	U	O5'-P-OP2	-8.95	97.65	105.70
11	3	48	U	O5'-P-OP2	-8.85	97.73	105.70
13	1	1049	C	O5'-P-OP2	-8.81	97.77	105.70
13	1	681	U	O5'-P-OP1	8.77	121.23	110.70
14	2	424	C	O3'-P-O5'	-8.76	87.35	104.00
13	1	645	A	C6-N1-C2	-8.65	113.41	118.60
52	M8	147	ARG	NE-CZ-NH2	-8.65	115.98	120.30
13	1	2121	G	O5'-P-OP2	-8.63	97.93	105.70
13	1	1724	U	O5'-P-OP2	-8.61	97.95	105.70
13	1	909	G	O5'-P-OP1	-8.60	97.96	105.70
13	1	2736	A	O5'-P-OP2	-8.60	97.96	105.70
52	M8	176	ARG	NE-CZ-NH1	-8.60	116.00	120.30
13	1	2790	A	O5'-P-OP2	-8.60	97.96	105.70
13	1	109	A	O5'-P-OP2	-8.59	97.97	105.70
71	O7	55	ARG	NE-CZ-NH2	-8.56	116.02	120.30
13	1	328	U	O5'-P-OP2	-8.55	98.00	105.70
13	1	2393	G	O5'-P-OP1	8.55	120.96	110.70
68	O4	74	ARG	NE-CZ-NH2	-8.54	116.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	2	17	C	O5'-P-OP2	-8.51	98.04	105.70
50	M6	84	LEU	CB-CG-CD2	-8.50	96.56	111.00
14	2	460	A	O5'-P-OP1	-8.44	98.11	105.70
37	L2	30	ARG	NE-CZ-NH2	-8.44	116.08	120.30
13	1	2514	U	O5'-P-OP2	-8.43	98.11	105.70
39	L4	93	MET	CG-SD-CE	-8.36	86.82	100.20
13	1	2372	A	O3'-P-O5'	8.30	119.77	104.00
14	2	113	U	O3'-P-O5'	-8.30	88.23	104.00
13	1	91	G	O3'-P-O5'	-8.28	88.26	104.00
13	1	2748	A	O3'-P-O5'	-8.24	88.34	104.00
37	L2	9	ARG	NE-CZ-NH1	-8.24	116.18	120.30
13	1	2431	C	O5'-P-OP2	-8.24	98.28	105.70
14	2	1748	U	C2'-C3'-O3'	8.24	127.63	109.50
14	2	1617	U	O5'-P-OP2	-8.23	98.29	105.70
13	1	1097	G	C2'-C3'-O3'	8.23	127.61	109.50
14	2	1039	A	O4'-C1'-N9	8.22	114.78	108.20
12	4	108	C	O5'-P-OP2	-8.20	98.32	105.70
13	1	2402	A	O3'-P-O5'	8.17	119.53	104.00
39	L4	99	MET	CG-SD-CE	-8.16	87.14	100.20
13	1	1638	A	O3'-P-O5'	8.11	119.41	104.00
73	O9	13	MET	CG-SD-CE	-8.04	87.34	100.20
13	1	1527	C	O3'-P-O5'	-8.03	88.75	104.00
12	4	33	A	O3'-P-O5'	-8.00	88.81	104.00
13	1	2143	A	O5'-P-OP1	-7.99	98.51	105.70
14	2	1760	C	N3-C4-C5	-7.99	118.71	121.90
50	M6	160	ARG	NE-CZ-NH2	-7.96	116.32	120.30
13	1	1437	C	O5'-P-OP1	-7.96	98.54	105.70
13	1	2982	A	O3'-P-O5'	-7.93	88.93	104.00
13	1	3315	G	O3'-P-O5'	-7.93	88.94	104.00
13	1	2704	A	O5'-P-OP1	-7.92	98.57	105.70
14	2	1028	C	O5'-P-OP1	-7.92	98.57	105.70
13	1	3362	A	O5'-P-OP2	7.90	120.18	110.70
13	1	2402	A	OP1-P-O3'	7.89	122.55	105.20
49	M5	71	ARG	NE-CZ-NH2	-7.86	116.37	120.30
13	1	2872	A	O5'-P-OP2	-7.86	98.63	105.70
14	2	1748	U	P-O3'-C3'	7.84	129.11	119.70
13	1	2271	A	O3'-P-O5'	-7.82	89.14	104.00
13	1	105	C	O5'-P-OP2	-7.81	98.67	105.70
13	1	961	C	O5'-P-OP2	-7.81	98.67	105.70
13	1	2944	U	O3'-P-O5'	-7.81	89.16	104.00
13	1	2806	U	O5'-P-OP2	-7.79	98.69	105.70
13	1	692	A	O5'-P-OP1	-7.78	98.70	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	1	2156	C	O5'-P-OP2	-7.78	98.70	105.70
14	2	389	G	O5'-P-OP2	-7.76	98.71	105.70
13	1	810	A	O5'-P-OP2	-7.76	98.72	105.70
13	1	428	A	O5'-P-OP2	-7.75	98.73	105.70
62	N8	4	ARG	NE-CZ-NH2	-7.75	116.43	120.30
13	1	1084	A	O3'-P-O5'	-7.74	89.30	104.00
12	4	135	G	O5'-P-OP2	-7.72	98.75	105.70
14	2	1272	U	P-O3'-C3'	7.71	128.95	119.70
13	1	1312	C	O3'-P-O5'	7.70	118.63	104.00
13	1	2665	U	O3'-P-O5'	-7.69	89.38	104.00
50	M6	68	ARG	NE-CZ-NH1	7.65	124.12	120.30
12	4	110	C	O3'-P-O5'	-7.63	89.50	104.00
71	O7	45	ARG	NE-CZ-NH1	7.59	124.09	120.30
49	M5	201	ARG	NE-CZ-NH1	7.58	124.09	120.30
66	O2	105	ARG	NE-CZ-NH2	-7.57	116.51	120.30
13	1	2313	A	O3'-P-O5'	-7.56	89.63	104.00
13	1	407	A	O3'-P-O5'	-7.56	89.63	104.00
13	1	1158	A	O5'-P-OP2	-7.56	98.89	105.70
13	1	1399	A	O5'-P-OP1	7.55	119.76	110.70
13	1	1307	G	O3'-P-O5'	-7.54	89.67	104.00
14	2	932	U	O5'-P-OP1	7.54	119.75	110.70
13	1	86	G	O5'-P-OP1	7.51	119.72	110.70
14	2	1748	U	O3'-P-O5'	7.49	118.23	104.00
13	1	1101	G	O5'-P-OP2	-7.48	98.96	105.70
71	O7	73	ARG	NE-CZ-NH1	7.48	124.04	120.30
13	1	1934	G	O3'-P-O5'	-7.47	89.81	104.00
11	3	103	A	O5'-P-OP2	-7.44	99.00	105.70
13	1	1132	C	O5'-P-OP2	-7.44	99.01	105.70
13	1	2728	G	C1'-O4'-C4'	-7.43	103.95	109.90
13	1	21	G	O4'-C1'-N9	7.43	114.15	108.20
76	Q2	41	ARG	NE-CZ-NH1	7.41	124.00	120.30
71	O7	21	ARG	NE-CZ-NH2	-7.40	116.60	120.30
42	L7	151	ARG	NE-CZ-NH2	-7.39	116.61	120.30
49	M5	71	ARG	NE-CZ-NH1	7.39	123.99	120.30
14	2	635	A	O5'-P-OP2	-7.38	99.06	105.70
13	1	3045	G	O3'-P-O5'	-7.37	89.99	104.00
13	1	3043	C	O5'-P-OP2	-7.37	99.07	105.70
13	1	2100	A	O3'-P-O5'	-7.34	90.05	104.00
13	1	1179	A	O5'-P-OP1	-7.34	99.09	105.70
13	1	1419	A	O5'-P-OP1	7.34	119.51	110.70
13	1	85	A	O3'-P-O5'	-7.33	90.06	104.00
13	1	1049	C	O5'-P-OP1	7.33	119.50	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	4	43	A	O5'-P-OP2	-7.33	99.11	105.70
13	1	1165	A	O5'-P-OP2	-7.32	99.11	105.70
14	2	988	A	OP1-P-O3'	7.30	121.26	105.20
14	2	925	G	O3'-P-O5'	-7.29	90.14	104.00
13	1	829	U	O5'-P-OP2	-7.28	99.14	105.70
13	1	2852	C	O3'-P-O5'	-7.28	90.18	104.00
14	2	1060	G	O3'-P-O5'	-7.27	90.18	104.00
12	4	25	G	O5'-P-OP2	-7.25	99.17	105.70
13	1	708	G	O5'-P-OP2	-7.24	99.18	105.70
13	1	354	U	O5'-P-OP2	-7.23	99.19	105.70
13	1	1317	A	O3'-P-O5'	-7.21	90.29	104.00
13	1	1097	G	O3'-P-O5'	-7.20	90.32	104.00
14	2	46	A	O3'-P-O5'	-7.20	90.32	104.00
13	1	2746	A	O3'-P-O5'	-7.20	90.33	104.00
13	1	3307	A	OP1-P-O3'	7.17	120.98	105.20
13	1	913	A	O3'-P-O5'	-7.17	90.38	104.00
13	1	2768	U	O5'-P-OP2	-7.15	99.27	105.70
13	1	578	A	O3'-P-O5'	-7.14	90.44	104.00
13	1	1477	A	O5'-P-OP1	-7.13	99.28	105.70
13	1	2694	A	O3'-P-O5'	-7.12	90.46	104.00
13	1	86	G	O5'-P-OP2	-7.12	99.30	105.70
13	1	2430	A	OP2-P-O3'	7.12	120.85	105.20
30	D3	7	ARG	CB-CA-C	7.09	124.59	110.40
13	1	879	U	O5'-P-OP1	-7.09	99.32	105.70
13	1	822	G	O5'-P-OP2	-7.08	99.33	105.70
54	N0	155	ARG	NE-CZ-NH1	-7.07	116.77	120.30
66	O2	45	ARG	NE-CZ-NH2	-7.06	116.77	120.30
53	M9	100	ARG	NE-CZ-NH1	7.05	123.83	120.30
13	1	1561	G	O4'-C1'-N9	7.04	113.83	108.20
13	1	2779	A	O5'-P-OP2	-7.03	99.37	105.70
13	1	284	A	OP1-P-O3'	7.03	120.66	105.20
13	1	210	U	O5'-P-OP1	7.02	119.13	110.70
12	4	52	A	O3'-P-O5'	-7.01	90.67	104.00
14	2	619	A	O3'-P-O5'	-7.01	90.67	104.00
13	1	220	G	O5'-P-OP2	-6.98	99.42	105.70
14	2	1278	G	N3-C4-N9	-6.97	121.81	126.00
13	1	2319	U	O5'-P-OP2	-6.96	99.43	105.70
13	1	2280	A	O4'-C1'-N9	-6.95	102.64	108.20
13	1	3218	A	P-O3'-C3'	6.95	128.04	119.70
13	1	107	A	O5'-P-OP2	-6.93	99.46	105.70
42	L7	151	ARG	NE-CZ-NH1	6.93	123.76	120.30
13	1	1009	A	O3'-P-O5'	-6.91	90.87	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	1	2402	A	OP2-P-O3'	-6.89	90.03	105.20
49	M5	201	ARG	NE-CZ-NH2	-6.89	116.85	120.30
13	1	1311	G	O5'-P-OP2	-6.89	99.50	105.70
13	1	2936	A	O5'-P-OP2	6.89	118.97	110.70
13	1	2326	A	OP2-P-O3'	6.88	120.34	105.20
13	1	518	G	O4'-C1'-N9	6.87	113.69	108.20
14	2	1183	A	P-O3'-C3'	6.87	127.94	119.70
13	1	92	G	O4'-C1'-N9	6.86	113.69	108.20
14	2	1720	C	O3'-P-O5'	-6.86	90.96	104.00
13	1	1541	G	O3'-P-O5'	-6.86	90.96	104.00
13	1	3244	A	O3'-P-O5'	-6.86	90.97	104.00
13	1	2827	U	O4'-C1'-N1	6.85	113.68	108.20
13	1	1693	C	O3'-P-O5'	-6.84	91.00	104.00
13	1	3148	U	O5'-P-OP2	-6.84	99.54	105.70
12	4	16	G	O4'-C1'-N9	6.83	113.67	108.20
14	2	1100	A	O3'-P-O5'	-6.83	91.03	104.00
13	1	2985	C	O5'-P-OP2	-6.83	99.56	105.70
13	1	860	G	O5'-P-OP2	-6.82	99.56	105.70
13	1	873	C	P-O3'-C3'	6.82	127.89	119.70
13	1	1641	U	O4'-C1'-N1	6.82	113.65	108.20
13	1	2278	C	O5'-P-OP2	-6.82	99.57	105.70
14	2	329	G	OP1-P-O3'	6.80	120.16	105.20
13	1	2945	G	C5'-C4'-O4'	-6.80	100.94	109.10
13	1	861	C	O5'-P-OP1	6.80	118.86	110.70
13	1	2384	A	O3'-P-O5'	-6.80	91.09	104.00
13	1	1428	A	O5'-P-OP2	-6.78	99.60	105.70
13	1	1646	G	O4'-C1'-N9	6.77	113.62	108.20
13	1	1589	A	O4'-C1'-N9	-6.77	102.78	108.20
14	2	103	A	P-O3'-C3'	6.77	127.82	119.70
13	1	55	G	O5'-P-OP2	-6.75	99.63	105.70
13	1	212	G	OP1-P-O3'	6.74	120.03	105.20
11	3	100	C	O5'-P-OP2	-6.74	99.64	105.70
65	O1	28	ARG	NE-CZ-NH1	6.73	123.67	120.30
14	2	621	A	O3'-P-O5'	-6.73	91.22	104.00
14	2	1283	A	O3'-P-O5'	-6.72	91.24	104.00
53	M9	100	ARG	NE-CZ-NH2	-6.69	116.95	120.30
13	1	110	G	O5'-P-OP1	6.68	118.72	110.70
39	L4	47	ARG	NE-CZ-NH2	-6.68	116.96	120.30
53	M9	5	ARG	NE-CZ-NH1	6.67	123.64	120.30
13	1	3130	A	O5'-P-OP1	-6.66	99.71	105.70
14	2	349	U	O5'-P-OP2	-6.66	99.71	105.70
14	2	619	A	OP2-P-O3'	6.65	119.84	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	2	548	G	O3'-P-O5'	-6.64	91.38	104.00
37	L2	242	ARG	NE-CZ-NH2	-6.64	116.98	120.30
13	1	1100	U	OP2-P-O3'	6.64	119.80	105.20
65	O1	28	ARG	NE-CZ-NH2	-6.64	116.98	120.30
13	1	1300	G	OP1-P-O3'	6.63	119.79	105.20
14	2	323	A	O3'-P-O5'	-6.63	91.40	104.00
69	O5	86	ARG	NE-CZ-NH1	6.62	123.61	120.30
13	1	1116	G	O5'-P-OP1	-6.61	99.75	105.70
32	D6	5	ARG	NE-CZ-NH1	6.61	123.61	120.30
13	1	1295	G	O5'-P-OP1	-6.61	99.75	105.70
13	1	1110	U	OP2-P-O3'	6.60	119.72	105.20
66	O2	105	ARG	NE-CZ-NH1	6.60	123.60	120.30
13	1	2939	G	O5'-P-OP2	-6.60	99.76	105.70
12	4	108	C	O3'-P-O5'	-6.59	91.47	104.00
14	2	989	U	O3'-P-O5'	-6.59	91.47	104.00
13	1	2112	U	P-O3'-C3'	6.59	127.61	119.70
13	1	1193	A	O5'-P-OP2	-6.58	99.78	105.70
13	1	2272	G	O4'-C1'-N9	6.57	113.46	108.20
13	1	2395	G	O5'-P-OP2	-6.57	99.78	105.70
13	1	2813	A	O3'-P-O5'	-6.57	91.52	104.00
13	1	860	G	OP1-P-O3'	6.57	119.64	105.20
13	1	266	A	O3'-P-O5'	-6.56	91.53	104.00
14	2	1783	C	O5'-P-OP2	6.56	118.57	110.70
73	O9	42	ARG	NE-CZ-NH2	-6.55	117.02	120.30
13	1	673	U	O5'-P-OP2	-6.55	99.81	105.70
14	2	1404	A	O3'-P-O5'	-6.55	91.56	104.00
13	1	2963	C	O5'-P-OP2	-6.54	99.81	105.70
13	1	960	U	C1'-O4'-C4'	-6.54	104.67	109.90
13	1	2913	C	O3'-P-O5'	-6.54	91.58	104.00
13	1	404	G	O5'-P-OP2	-6.54	99.82	105.70
13	1	817	A	C3'-C2'-C1'	-6.53	96.28	101.50
13	1	1693	C	O5'-P-OP2	-6.53	99.83	105.70
13	1	3395	G	O3'-P-O5'	-6.53	91.60	104.00
13	1	2511	A	O3'-P-O5'	-6.51	91.62	104.00
46	M1	167	TYR	N-CA-CB	6.50	122.31	110.60
13	1	335	G	O3'-P-O5'	-6.50	91.65	104.00
14	2	1101	G	O3'-P-O5'	-6.49	91.66	104.00
13	1	2354	C	O5'-P-OP2	-6.49	99.86	105.70
14	2	1278	G	C8-N9-C1'	6.49	135.43	127.00
71	O7	40	PRO	N-CA-CB	-6.48	95.47	102.60
13	1	2385	G	O5'-P-OP1	-6.48	99.87	105.70
13	1	701	G	OP2-P-O3'	6.48	119.45	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	1	1002	A	O5'-P-OP1	6.47	118.47	110.70
13	1	2188	A	O5'-P-OP1	-6.47	99.88	105.70
13	1	155	G	O3'-P-O5'	-6.46	91.72	104.00
50	M6	78	ARG	CG-CD-NE	6.46	125.36	111.80
69	O5	10	ARG	NE-CZ-NH2	-6.46	117.07	120.30
14	2	1012	U	O3'-P-O5'	-6.45	91.74	104.00
50	M6	68	ARG	NE-CZ-NH2	-6.45	117.08	120.30
13	1	786	A	O5'-P-OP1	6.45	118.44	110.70
13	1	3170	A	O4'-C1'-N9	6.45	113.36	108.20
67	O3	67	MET	CG-SD-CE	-6.45	89.89	100.20
45	M0	128	ARG	NE-CZ-NH2	-6.44	117.08	120.30
13	1	3092	C	C1'-O4'-C4'	-6.43	104.75	109.90
14	2	960	U	O3'-P-O5'	-6.43	91.77	104.00
11	3	17	A	O3'-P-O5'	-6.43	91.79	104.00
13	1	916	G	P-O3'-C3'	6.42	127.41	119.70
13	1	825	U	O5'-P-OP2	-6.42	99.92	105.70
14	2	770	A	O3'-P-O5'	-6.39	91.85	104.00
13	1	1828	A	OP2-P-O3'	6.38	119.23	105.20
13	1	2181	C	O5'-P-OP2	-6.38	99.96	105.70
49	M5	162	ARG	NE-CZ-NH2	-6.36	117.12	120.30
13	1	2131	A	O5'-P-OP2	-6.36	99.98	105.70
14	2	984	G	O3'-P-O5'	-6.35	91.94	104.00
14	2	983	A	O3'-P-O5'	-6.34	91.95	104.00
13	1	2731	U	O3'-P-O5'	-6.34	91.96	104.00
13	1	2813	A	O5'-P-OP2	-6.33	100.00	105.70
13	1	2281	A	O5'-P-OP2	-6.33	100.00	105.70
37	L2	30	ARG	NE-CZ-NH1	6.33	123.46	120.30
13	1	1716	U	C2'-C3'-O3'	6.32	123.82	113.70
14	2	1147	A	O5'-P-OP2	-6.32	100.01	105.70
14	2	1274	A	OP1-P-O3'	6.31	119.08	105.20
12	4	51	G	O3'-P-O5'	-6.30	92.03	104.00
13	1	1688	U	OP2-P-O3'	6.30	119.05	105.20
13	1	907	G	O4'-C1'-N9	6.29	113.23	108.20
13	1	2370	G	O5'-P-OP2	-6.29	100.04	105.70
14	2	1598	A	O4'-C1'-N9	6.28	113.22	108.20
13	1	3184	A	O5'-P-OP2	-6.28	100.05	105.70
13	1	1117	G	O5'-P-OP2	6.27	118.23	110.70
13	1	3143	C	O5'-P-OP1	6.27	118.22	110.70
13	1	2352	A	O5'-P-OP2	-6.27	100.06	105.70
13	1	2305	G	O4'-C1'-N9	6.26	113.21	108.20
14	2	976	G	O3'-P-O5'	-6.26	92.10	104.00
13	1	2163	C	O5'-P-OP2	-6.26	100.07	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	1	1098	A	O5'-P-OP1	6.25	118.20	110.70
13	1	2325	G	O3'-P-O5'	-6.25	92.13	104.00
14	2	1026	A	OP2-P-O3'	6.24	118.93	105.20
11	3	77	G	O5'-P-OP1	6.23	118.18	110.70
13	1	1383	G	O5'-P-OP2	-6.22	100.10	105.70
13	1	2799	A	O3'-P-O5'	-6.22	92.19	104.00
14	2	1639	C	OP1-P-O3'	6.20	118.83	105.20
13	1	1002	A	O5'-P-OP2	-6.19	100.13	105.70
37	L2	128	ARG	NE-CZ-NH2	-6.19	117.20	120.30
13	1	558	U	P-O3'-C3'	6.19	127.12	119.70
13	1	3021	A	O3'-P-O5'	-6.18	92.25	104.00
13	1	1523	U	C3'-C2'-C1'	-6.18	96.56	101.50
13	1	2162	U	OP2-P-O3'	6.18	118.79	105.20
13	1	687	U	O5'-P-OP2	6.18	118.11	110.70
14	2	1555	C	P-O3'-C3'	6.17	127.10	119.70
13	1	2909	U	O3'-P-O5'	-6.17	92.29	104.00
13	1	54	C	OP2-P-O3'	6.15	118.73	105.20
14	2	73	U	P-O3'-C3'	6.15	127.08	119.70
13	1	349	A	O4'-C1'-N9	-6.15	103.28	108.20
13	1	2400	G	OP2-P-O3'	6.15	118.72	105.20
13	1	218	G	O3'-P-O5'	-6.15	92.32	104.00
37	L2	37	ARG	NE-CZ-NH2	6.14	123.37	120.30
13	1	715	A	O5'-P-OP2	-6.14	100.17	105.70
59	N5	56	ARG	NE-CZ-NH2	-6.14	117.23	120.30
13	1	1724	U	O4'-C1'-N1	6.13	113.11	108.20
13	1	2676	A	O3'-P-O5'	-6.12	92.36	104.00
39	L4	138	ARG	NE-CZ-NH2	-6.12	117.24	120.30
13	1	2374	C	OP2-P-O3'	6.12	118.66	105.20
13	1	2976	A	O3'-P-O5'	-6.11	92.38	104.00
14	2	573	C	O3'-P-O5'	-6.11	92.39	104.00
13	1	2728	G	O4'-C1'-N9	6.11	113.09	108.20
13	1	269	G	O5'-P-OP1	-6.10	100.21	105.70
13	1	3170	A	O3'-P-O5'	-6.10	92.40	104.00
13	1	1741	A	O4'-C1'-N9	6.09	113.08	108.20
13	1	1845	G	OP1-P-O3'	6.09	118.59	105.20
13	1	10	C	O5'-P-OP2	-6.08	100.22	105.70
13	1	1086	C	O3'-P-O5'	-6.08	92.44	104.00
13	1	2314	U	O3'-P-O5'	-6.08	92.44	104.00
14	2	1011	G	O3'-P-O5'	-6.08	92.45	104.00
13	1	3085	G	O3'-P-O5'	-6.07	92.48	104.00
13	1	1111	U	O5'-P-OP2	-6.06	100.24	105.70
13	1	1306	G	O5'-P-OP2	-6.05	100.25	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	2	1007	C	OP1-P-O3'	6.05	118.52	105.20
13	1	1329	U	P-O3'-C3'	6.05	126.96	119.70
14	2	1760	C	C6-N1-C2	-6.05	117.88	120.30
13	1	1888	U	O3'-P-O5'	-6.03	92.54	104.00
13	1	1730	G	O3'-P-O5'	-6.03	92.55	104.00
13	1	2747	A	O3'-P-O5'	-6.03	92.55	104.00
30	D3	7	ARG	N-CA-CB	-6.03	99.75	110.60
13	1	432	G	OP2-P-O3'	6.02	118.45	105.20
44	L9	110	LYS	N-CA-CB	6.01	121.42	110.60
13	1	3258	U	O3'-P-O5'	-6.00	92.59	104.00
13	1	2739	A	O3'-P-O5'	-6.00	92.60	104.00
13	1	760	G	O4'-C1'-N9	5.99	112.99	108.20
4	C4	61	MET	CG-SD-CE	5.98	109.78	100.20
13	1	428	A	OP2-P-O3'	5.98	118.36	105.20
14	2	622	A	O3'-P-O5'	-5.98	92.63	104.00
13	1	2143	A	O5'-P-OP2	-5.98	100.32	105.70
13	1	2396	G	O5'-P-OP2	-5.98	100.32	105.70
13	1	2281	A	O4'-C1'-N9	5.97	112.98	108.20
13	1	1305	U	OP2-P-O3'	5.97	118.34	105.20
13	1	2955	U	OP1-P-O3'	5.97	118.34	105.20
13	1	2937	G	O3'-P-O5'	-5.97	92.66	104.00
13	1	2941	A	O4'-C1'-N9	-5.96	103.43	108.20
13	1	61	A	OP1-P-O3'	5.96	118.31	105.20
13	1	1840	U	OP1-P-O3'	5.95	118.29	105.20
49	M5	73	ARG	NE-CZ-NH2	-5.95	117.33	120.30
13	1	1451	C	OP1-P-O3'	5.95	118.29	105.20
14	2	1007	C	O3'-P-O5'	-5.95	92.70	104.00
13	1	1181	U	C1'-O4'-C4'	-5.94	105.15	109.90
13	1	2913	C	OP2-P-O3'	5.94	118.26	105.20
13	1	1858	A	O4'-C1'-N9	5.93	112.95	108.20
14	2	454	U	P-O3'-C3'	5.93	126.82	119.70
13	1	1111	U	OP2-P-O3'	5.93	118.25	105.20
13	1	2131	A	N9-C1'-C2'	-5.93	105.48	112.00
13	1	841	A	O5'-P-OP2	-5.93	100.36	105.70
13	1	1668	G	OP2-P-O3'	5.92	118.23	105.20
14	2	123	G	O3'-P-O5'	-5.92	92.75	104.00
52	M8	147	ARG	NE-CZ-NH1	5.92	123.26	120.30
13	1	3142	A	OP1-P-O3'	5.92	118.22	105.20
14	2	1030	A	O5'-P-OP2	-5.92	100.38	105.70
13	1	503	C	O3'-P-O5'	-5.91	92.77	104.00
13	1	1164	G	OP2-P-O3'	5.91	118.19	105.20
13	1	2337	C	C3'-C2'-C1'	-5.91	96.78	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	1	3268	A	O3'-P-O5'	-5.91	92.78	104.00
13	1	3374	U	O3'-P-O5'	-5.91	92.78	104.00
14	2	1602	C	P-O3'-C3'	5.90	126.78	119.70
14	2	1775	G	O5'-P-OP2	-5.90	100.39	105.70
13	1	1886	A	O5'-P-OP2	-5.90	100.39	105.70
13	1	1432	C	O5'-P-OP2	-5.89	100.40	105.70
13	1	895	A	O3'-P-O5'	-5.88	92.82	104.00
13	1	899	U	O5'-P-OP2	-5.88	100.41	105.70
13	1	1696	A	O5'-P-OP2	-5.87	100.42	105.70
11	3	5	G	O5'-P-OP1	5.87	117.74	110.70
13	1	911	C	O5'-P-OP2	-5.87	100.42	105.70
13	1	269	G	O3'-P-O5'	-5.85	92.89	104.00
13	1	588	G	O5'-P-OP2	-5.85	100.44	105.70
13	1	2724	U	OP1-P-O3'	5.85	118.06	105.20
14	2	990	C	OP1-P-O3'	5.85	118.06	105.20
13	1	873	C	C4'-C3'-O3'	5.84	124.68	113.00
13	1	1366	A	OP1-P-O3'	5.84	118.05	105.20
13	1	2408	U	OP2-P-O3'	5.84	118.05	105.20
13	1	821	U	OP2-P-O3'	5.84	118.04	105.20
14	2	1299	A	O3'-P-O5'	-5.84	92.91	104.00
12	4	105	A	OP1-P-O3'	5.83	118.03	105.20
35	E0	43	ARG	CG-CD-NE	5.83	124.05	111.80
13	1	2412	G	N3-C4-C5	-5.83	125.69	128.60
14	2	1260	G	P-O3'-C3'	5.83	126.70	119.70
13	1	40	A	O5'-P-OP2	-5.83	100.46	105.70
13	1	138	U	O3'-P-O5'	-5.82	92.94	104.00
13	1	217	U	OP1-P-O3'	5.82	118.00	105.20
13	1	1480	G	O4'-C1'-N9	5.82	112.86	108.20
13	1	3315	G	OP2-P-O3'	5.82	118.00	105.20
53	M9	38	ARG	NE-CZ-NH1	5.81	123.21	120.30
13	1	2593	A	O3'-P-O5'	-5.81	92.97	104.00
13	1	1097	G	P-O3'-C3'	5.81	126.67	119.70
69	O5	10	ARG	NE-CZ-NH1	5.80	123.20	120.30
14	2	1301	U	O3'-P-O5'	-5.80	92.98	104.00
13	1	268	A	O3'-P-O5'	-5.79	92.99	104.00
13	1	911	C	N3-C4-C5	-5.79	119.58	121.90
13	1	663	C	C3'-C2'-C1'	-5.79	96.87	101.50
14	2	1553	U	O3'-P-O5'	-5.79	93.01	104.00
57	N3	48	ARG	CD-NE-CZ	5.78	131.69	123.60
14	2	1671	U	O4'-C1'-N1	5.78	112.82	108.20
14	2	1587	A	OP1-P-O3'	5.78	117.90	105.20
13	1	269	G	O5'-P-OP2	5.77	117.62	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	1	864	G	OP2-P-O3'	5.77	117.89	105.20
14	2	609	U	O5'-P-OP2	-5.76	100.51	105.70
14	2	1026	A	O4'-C1'-N9	-5.76	103.59	108.20
12	4	20	U	O4'-C1'-N1	5.76	112.81	108.20
13	1	155	G	OP1-P-O3'	5.76	117.88	105.20
13	1	2385	G	OP1-P-O3'	5.76	117.88	105.20
14	2	388	G	O5'-P-OP1	-5.75	100.52	105.70
49	M5	162	ARG	NE-CZ-NH1	5.75	123.18	120.30
14	2	608	U	O3'-P-O5'	-5.75	93.08	104.00
13	1	2704	A	O4'-C1'-N9	5.74	112.79	108.20
13	1	2787	G	O3'-P-O5'	-5.74	93.09	104.00
13	1	1502	C	O3'-P-O5'	-5.74	93.10	104.00
13	1	3378	C	O5'-P-OP1	-5.74	100.54	105.70
47	M3	101	ARG	NE-CZ-NH1	5.74	123.17	120.30
13	1	1934	G	OP2-P-O3'	5.73	117.81	105.20
13	1	3000	A	OP2-P-O3'	5.73	117.81	105.20
13	1	2978	U	P-O3'-C3'	5.73	126.58	119.70
13	1	2397	A	OP1-P-O3'	5.72	117.79	105.20
13	1	2528	G	O3'-P-O5'	-5.72	93.13	104.00
13	1	1549	U	O5'-P-OP2	5.72	117.56	110.70
13	1	724	U	O3'-P-O5'	-5.71	93.15	104.00
14	2	1526	G	O3'-P-O5'	-5.71	93.16	104.00
35	E0	43	ARG	CD-NE-CZ	5.71	131.59	123.60
13	1	266	A	O5'-P-OP2	-5.70	100.57	105.70
14	2	619	A	O5'-P-OP1	-5.70	100.57	105.70
13	1	1861	G	O5'-P-OP2	-5.69	100.58	105.70
13	1	2131	A	O5'-P-OP1	5.69	117.53	110.70
14	2	1617	U	OP2-P-O3'	5.69	117.71	105.20
13	1	2327	U	C4'-C3'-C2'	-5.68	96.92	102.60
14	2	1779	G	O4'-C1'-N9	5.68	112.75	108.20
13	1	2142	A	N3-C4-C5	-5.68	122.82	126.80
13	1	398	A	C1'-O4'-C4'	-5.68	105.36	109.90
13	1	2617	U	C5-C6-N1	-5.68	119.86	122.70
14	2	1238	U	O3'-P-O5'	-5.67	93.23	104.00
14	2	1770	C	OP2-P-O3'	5.67	117.67	105.20
11	3	62	U	O3'-P-O5'	-5.66	93.24	104.00
14	2	686	C	O3'-P-O5'	-5.66	93.24	104.00
12	4	151	C	O3'-P-O5'	-5.66	93.24	104.00
13	1	2407	C	O5'-P-OP2	-5.66	100.61	105.70
14	2	978	A	OP2-P-O3'	5.66	117.64	105.20
13	1	2650	U	O3'-P-O5'	-5.65	93.26	104.00
14	2	1618	A	O3'-P-O5'	-5.65	93.27	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	1	953	G	OP1-P-O3'	5.64	117.62	105.20
13	1	2715	A	O5'-P-OP1	-5.64	100.62	105.70
43	L8	183	LYS	CB-CA-C	5.64	121.69	110.40
13	1	1475	A	OP2-P-O3'	5.64	117.61	105.20
14	2	608	U	OP2-P-O3'	5.64	117.61	105.20
13	1	507	U	O5'-P-OP2	-5.64	100.62	105.70
37	L2	9	ARG	NE-CZ-NH2	5.64	123.12	120.30
13	1	9	U	OP2-P-O3'	5.64	117.60	105.20
13	1	883	A	O5'-P-OP2	5.64	117.46	110.70
13	1	1884	A	O5'-P-OP1	5.64	117.47	110.70
14	2	941	A	O5'-P-OP1	5.64	117.46	110.70
14	2	1763	A	OP2-P-O3'	5.64	117.60	105.20
52	M8	179	ARG	NE-CZ-NH2	-5.63	117.48	120.30
13	1	296	A	O5'-P-OP2	-5.63	100.63	105.70
50	M6	68	ARG	CD-NE-CZ	5.63	131.48	123.60
14	2	1581	G	O3'-P-O5'	-5.63	93.31	104.00
54	N0	155	ARG	NE-CZ-NH2	5.63	123.11	120.30
13	1	2142	A	OP1-P-O3'	5.63	117.58	105.20
14	2	787	G	O3'-P-O5'	-5.63	93.31	104.00
13	1	3217	C	C2-N1-C1'	5.62	124.99	118.80
14	2	417	A	P-O3'-C3'	5.62	126.45	119.70
13	1	2728	G	C5-C6-O6	-5.62	125.23	128.60
61	N7	65	ARG	NE-CZ-NH2	-5.62	117.49	120.30
13	1	938	C	OP2-P-O3'	5.62	117.55	105.20
13	1	1143	A	O3'-P-O5'	-5.62	93.33	104.00
47	M3	101	ARG	NE-CZ-NH2	-5.61	117.49	120.30
13	1	25	U	O3'-P-O5'	-5.61	93.34	104.00
13	1	964	G	OP2-P-O3'	5.61	117.54	105.20
14	2	610	G	O3'-P-O5'	-5.61	93.35	104.00
13	1	822	G	C4'-C3'-C2'	-5.60	97.00	102.60
13	1	1723	A	OP1-P-O3'	5.60	117.52	105.20
13	1	1446	A	OP1-P-O3'	5.60	117.52	105.20
74	Q0	122	ARG	NE-CZ-NH1	5.59	123.10	120.30
14	2	1269	U	O3'-P-O5'	-5.59	93.37	104.00
13	1	805	G	OP2-P-O3'	5.59	117.50	105.20
13	1	1205	A	O3'-P-O5'	-5.59	93.38	104.00
13	1	644	G	OP2-P-O3'	5.59	117.49	105.20
13	1	1879	A	O3'-P-O5'	-5.59	93.39	104.00
13	1	3077	A	OP1-P-O3'	5.58	117.48	105.20
13	1	741	U	O3'-P-O5'	-5.58	93.40	104.00
13	1	1796	G	OP1-P-O3'	5.58	117.47	105.20
14	2	158	U	P-O3'-C3'	5.58	126.39	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	2	1189	A	OP2-P-O3'	5.58	117.47	105.20
14	2	358	U	O3'-P-O5'	-5.57	93.41	104.00
13	1	1185	C	O3'-P-O5'	-5.57	93.41	104.00
13	1	3005	A	O3'-P-O5'	-5.57	93.42	104.00
13	1	3350	C	P-O3'-C3'	5.57	126.38	119.70
14	2	287	G	C1'-O4'-C4'	-5.57	105.45	109.90
50	M6	49	ARG	CB-CA-C	-5.57	99.27	110.40
54	N0	113	ARG	NE-CZ-NH2	-5.57	117.52	120.30
62	N8	4	ARG	CG-CD-NE	-5.56	100.11	111.80
14	2	960	U	OP1-P-O3'	5.56	117.44	105.20
13	1	662	U	OP2-P-O3'	5.56	117.43	105.20
13	1	811	U	O5'-P-OP1	-5.56	100.70	105.70
13	1	2870	C	C3'-C2'-C1'	5.56	105.94	101.50
13	1	59	G	P-O3'-C3'	5.55	126.36	119.70
45	M0	4	ARG	CB-CA-C	-5.55	99.30	110.40
22	S9	120	LYS	N-CA-CB	5.55	120.58	110.60
13	1	894	G	OP1-P-O3'	5.54	117.39	105.20
13	1	2406	C	OP2-P-O3'	5.54	117.39	105.20
43	L8	190	VAL	N-CA-CB	-5.54	99.31	111.50
13	1	2588	U	O3'-P-O5'	-5.54	93.48	104.00
13	1	1355	A	P-O3'-C3'	5.54	126.34	119.70
13	1	1370	G	C4'-C3'-C2'	-5.54	97.06	102.60
13	1	3305	A	OP2-P-O3'	5.53	117.38	105.20
13	1	945	C	O5'-P-OP2	-5.53	100.73	105.70
13	1	1189	C	OP1-P-O3'	5.52	117.35	105.20
13	1	2864	A	OP2-P-O3'	5.52	117.35	105.20
13	1	2898	G	O4'-C1'-N9	-5.52	103.78	108.20
13	1	377	A	O3'-P-O5'	-5.52	93.52	104.00
13	1	2283	G	C5-C6-O6	-5.52	125.29	128.60
71	O7	25	ARG	NE-CZ-NH2	-5.52	117.54	120.30
13	1	670	C	OP2-P-O3'	5.51	117.33	105.20
14	2	1404	A	C2'-C3'-O3'	5.51	122.51	113.70
13	1	3119	U	OP2-P-O3'	5.50	117.31	105.20
41	L6	78	ARG	NE-CZ-NH2	-5.50	117.55	120.30
13	1	270	U	P-O5'-C5'	-5.50	112.10	120.90
13	1	1211	U	O5'-P-OP2	-5.50	100.75	105.70
14	2	936	G	O3'-P-O5'	-5.50	93.55	104.00
13	1	2866	U	O3'-P-O5'	-5.50	93.55	104.00
13	1	1884	A	O5'-P-OP2	-5.50	100.75	105.70
13	1	2150	G	O4'-C1'-N9	5.50	112.60	108.20
13	1	1334	U	O5'-P-OP2	-5.49	100.76	105.70
13	1	1133	A	C3'-C2'-C1'	-5.48	97.11	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	N3	48	ARG	NE-CZ-NH1	5.48	123.04	120.30
13	1	1158	A	O5'-P-OP1	-5.47	100.77	105.70
14	2	345	U	O3'-P-O5'	-5.47	93.60	104.00
13	1	916	G	OP1-P-O3'	5.47	117.24	105.20
14	2	977	A	O3'-P-O5'	-5.47	93.60	104.00
13	1	1301	A	O4'-C1'-N9	-5.47	103.83	108.20
13	1	2313	A	O5'-P-OP1	-5.47	100.78	105.70
14	2	1278	G	C4-N9-C1'	-5.47	119.39	126.50
59	N5	56	ARG	NE-CZ-NH1	5.47	123.03	120.30
14	2	459	G	O3'-P-O5'	5.46	114.38	104.00
13	1	86	G	C3'-C2'-C1'	-5.46	97.13	101.50
39	L4	138	ARG	NE-CZ-NH1	5.46	123.03	120.30
13	1	1880	U	OP2-P-O3'	5.46	117.21	105.20
13	1	2611	U	O5'-P-OP2	-5.46	100.79	105.70
13	1	2950	G	O4'-C1'-N9	5.46	112.56	108.20
13	1	2605	G	O3'-P-O5'	-5.45	93.64	104.00
14	2	942	G	O5'-P-OP1	5.45	117.24	110.70
13	1	1111	U	C4'-C3'-C2'	-5.45	97.15	102.60
13	1	1165	A	C4'-C3'-C2'	-5.45	97.15	102.60
13	1	681	U	O3'-P-O5'	-5.44	93.66	104.00
50	M6	117	ARG	NE-CZ-NH2	-5.44	117.58	120.30
13	1	2380	U	O3'-P-O5'	-5.44	93.67	104.00
13	1	2617	U	N1-C2-N3	5.44	118.16	114.90
14	2	623	A	O3'-P-O5'	-5.44	93.67	104.00
13	1	700	C	O5'-P-OP1	-5.44	100.81	105.70
13	1	1340	G	O5'-P-OP2	-5.44	100.81	105.70
13	1	565	U	O3'-P-O5'	-5.44	93.67	104.00
13	1	2767	U	OP2-P-O3'	5.44	117.16	105.20
14	2	1760	C	N3-C4-N4	5.44	121.81	118.00
13	1	786	A	O5'-P-OP2	-5.43	100.81	105.70
13	1	1173	U	OP2-P-O3'	5.43	117.15	105.20
13	1	1861	G	OP2-P-O3'	5.43	117.15	105.20
14	2	855	A	O4'-C1'-N9	5.43	112.55	108.20
11	3	47	C	O5'-P-OP2	-5.42	100.82	105.70
13	1	224	C	OP1-P-O3'	5.42	117.12	105.20
13	1	646	A	O5'-P-OP1	-5.41	100.83	105.70
13	1	1695	U	OP2-P-O3'	5.41	117.11	105.20
51	M7	92	GLN	N-CA-CB	5.41	120.34	110.60
13	1	374	A	C3'-C2'-C1'	-5.41	97.17	101.50
13	1	791	A	OP2-P-O3'	5.41	117.10	105.20
13	1	74	G	O3'-P-O5'	-5.41	93.73	104.00
13	1	1879	A	C1'-O4'-C4'	-5.40	105.58	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	1	2643	A	O3'-P-O5'	-5.40	93.73	104.00
13	1	2963	C	OP2-P-O3'	5.40	117.08	105.20
5	C5	40	ARG	NE-CZ-NH2	-5.40	117.60	120.30
13	1	1508	C	O4'-C1'-N1	5.40	112.52	108.20
13	1	2713	U	OP1-P-O3'	5.40	117.08	105.20
13	1	2942	C	OP1-P-O3'	5.40	117.08	105.20
13	1	799	G	O5'-P-OP1	-5.40	100.84	105.70
13	1	1927	G	O5'-P-OP1	-5.39	100.84	105.70
14	2	158	U	C2'-C3'-O3'	5.39	122.33	113.70
14	2	1560	A	P-O3'-C3'	5.39	126.17	119.70
13	1	2990	G	OP1-P-O3'	5.39	117.06	105.20
14	2	400	A	OP1-P-O3'	5.39	117.05	105.20
13	1	3333	G	O4'-C1'-N9	5.38	112.51	108.20
13	1	3269	U	P-O3'-C3'	5.38	126.16	119.70
11	3	85	G	O3'-P-O5'	-5.38	93.78	104.00
14	2	1294	U	O4'-C1'-N1	5.38	112.50	108.20
13	1	1482	A	P-O3'-C3'	5.38	126.16	119.70
13	1	3278	C	C2-N1-C1'	5.38	124.72	118.80
11	3	99	G	OP2-P-O3'	5.38	117.03	105.20
13	1	1557	A	O3'-P-O5'	-5.38	93.79	104.00
13	1	2701	U	O5'-P-OP2	-5.38	100.86	105.70
13	1	1143	A	OP2-P-O3'	5.38	117.03	105.20
11	3	7	G	O5'-P-OP1	5.37	117.14	110.70
14	2	555	A	C2'-C3'-O3'	5.37	122.29	113.70
13	1	1606	U	C1'-O4'-C4'	-5.36	105.61	109.90
14	2	1053	U	P-O3'-C3'	5.36	126.14	119.70
14	2	1068	A	P-O3'-C3'	5.36	126.14	119.70
14	2	1628	C	OP2-P-O3'	5.36	117.00	105.20
13	1	38	U	O3'-P-O5'	-5.36	93.81	104.00
13	1	2142	A	C5-C6-N1	5.36	120.38	117.70
13	1	2979	U	O3'-P-O5'	-5.36	93.82	104.00
13	1	228	U	O3'-P-O5'	-5.36	93.82	104.00
11	3	101	G	OP2-P-O3'	5.36	116.98	105.20
13	1	915	A	O5'-P-OP1	-5.36	100.88	105.70
14	2	1274	A	P-O3'-C3'	5.36	126.13	119.70
13	1	341	G	O5'-P-OP2	-5.35	100.88	105.70
13	1	1510	G	OP2-P-O3'	5.35	116.98	105.20
14	2	1783	C	OP1-P-O3'	5.35	116.97	105.20
14	2	387	A	O5'-P-OP2	-5.35	100.89	105.70
14	2	556	A	O3'-P-O5'	-5.35	93.84	104.00
13	1	821	U	O5'-P-OP2	-5.34	100.89	105.70
6	C8	132	ARG	NE-CZ-NH2	-5.34	117.63	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	1	2154	U	O3'-P-O5'	-5.34	93.85	104.00
13	1	780	A	OP1-P-O3'	5.34	116.95	105.20
14	2	1008	G	OP1-P-O3'	5.34	116.94	105.20
13	1	3218	A	OP2-P-O3'	5.34	116.94	105.20
14	2	1779	G	O3'-P-O5'	-5.33	93.86	104.00
50	M6	41	LEU	N-CA-CB	-5.33	99.73	110.40
11	3	48	U	O3'-P-O5'	-5.33	93.87	104.00
13	1	3064	U	OP2-P-O3'	5.33	116.93	105.20
14	2	1415	G	O5'-P-OP2	5.33	117.10	110.70
20	S7	119	THR	N-CA-CB	5.33	120.43	110.30
13	1	99	A	C5'-C4'-O4'	5.33	115.49	109.10
13	1	421	G	O3'-P-O5'	-5.33	93.88	104.00
13	1	608	A	O3'-P-O5'	5.33	114.12	104.00
81	E1	138	ARG	NE-CZ-NH1	5.32	122.96	120.30
14	2	1314	C	OP2-P-O3'	5.32	116.91	105.20
13	1	681	U	O5'-P-OP2	-5.32	100.91	105.70
13	1	2112	U	O5'-P-OP2	-5.32	100.92	105.70
13	1	2120	A	O3'-P-O5'	5.32	114.10	104.00
13	1	2406	C	N3-C4-C5	-5.32	119.77	121.90
66	O2	82	LEU	CB-CG-CD2	5.32	120.03	111.00
13	1	63	A	OP2-P-O3'	5.31	116.89	105.20
13	1	579	G	O3'-P-O5'	-5.31	93.90	104.00
29	D2	111	MET	CG-SD-CE	-5.31	91.70	100.20
14	2	1011	G	OP1-P-O3'	5.31	116.89	105.20
13	1	641	C	N1-C1'-C2'	-5.31	106.16	112.00
13	1	82	C	O3'-P-O5'	-5.31	93.91	104.00
13	1	1556	C	P-O3'-C3'	5.31	126.07	119.70
13	1	1755	C	O3'-P-O5'	-5.30	93.93	104.00
14	2	1751	C	OP2-P-O3'	5.30	116.86	105.20
13	1	2777	G	O3'-P-O5'	-5.30	93.93	104.00
13	1	270	U	C5'-C4'-C3'	-5.30	107.53	116.00
13	1	1310	G	OP2-P-O3'	5.30	116.85	105.20
13	1	1688	U	O3'-P-O5'	-5.30	93.94	104.00
13	1	1695	U	O4'-C1'-N1	5.30	112.44	108.20
13	1	2412	G	N9-C4-C5	5.29	107.52	105.40
57	N3	87	ARG	NE-CZ-NH2	-5.29	117.65	120.30
13	1	2930	A	C4'-C3'-C2'	-5.29	97.31	102.60
13	1	1604	G	O3'-P-O5'	-5.29	93.95	104.00
13	1	1844	C	O5'-P-OP2	-5.29	100.94	105.70
14	2	497	G	P-O3'-C3'	5.28	126.04	119.70
74	Q0	79	GLU	N-CA-CB	5.28	120.11	110.60
13	1	878	G	OP1-P-O3'	5.28	116.81	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	1	1730	G	O5'-P-OP2	-5.28	100.95	105.70
13	1	2991	A	OP2-P-O3'	5.28	116.81	105.20
14	2	1775	G	O3'-P-O5'	-5.28	93.97	104.00
51	M7	61	ARG	NE-CZ-NH2	-5.28	117.66	120.30
13	1	2400	G	O3'-P-O5'	-5.27	93.98	104.00
12	4	117	C	OP2-P-O3'	5.27	116.80	105.20
13	1	810	A	OP1-P-O3'	5.27	116.80	105.20
13	1	1145	G	C5-C6-O6	-5.27	125.44	128.60
13	1	1361	U	OP2-P-O3'	5.27	116.79	105.20
14	2	73	U	OP1-P-O3'	5.26	116.78	105.20
12	4	42	G	OP2-P-O3'	5.26	116.77	105.20
13	1	1401	A	O5'-P-OP1	-5.26	100.97	105.70
13	1	2912	G	P-O3'-C3'	5.26	126.01	119.70
13	1	2991	A	O3'-P-O5'	-5.26	94.01	104.00
13	1	1894	U	O5'-P-OP2	-5.25	100.97	105.70
14	2	633	U	O5'-P-OP2	-5.25	100.97	105.70
13	1	904	A	OP2-P-O3'	5.25	116.75	105.20
13	1	3175	U	O5'-P-OP2	-5.25	100.97	105.70
13	1	2125	A	OP2-P-O3'	5.25	116.75	105.20
13	1	2585	G	C1'-O4'-C4'	-5.25	105.70	109.90
13	1	1334	U	OP1-P-O3'	5.25	116.75	105.20
13	1	1895	A	OP1-P-O3'	5.25	116.75	105.20
13	1	922	U	OP2-P-O3'	5.25	116.74	105.20
38	L3	192	VAL	N-CA-CB	5.25	123.04	111.50
14	2	1029	U	OP1-P-O3'	5.24	116.73	105.20
14	2	1615	U	OP2-P-O3'	5.24	116.73	105.20
14	2	994	G	C4'-C3'-C2'	-5.24	97.36	102.60
13	1	286	U	OP1-P-O3'	5.24	116.73	105.20
13	1	1692	U	OP2-P-O3'	5.24	116.72	105.20
53	M9	81	ARG	NE-CZ-NH1	5.24	122.92	120.30
14	2	329	G	O3'-P-O5'	-5.23	94.06	104.00
13	1	2394	G	OP2-P-O3'	5.23	116.71	105.20
14	2	1331	A	P-O3'-C3'	5.23	125.98	119.70
14	2	1284	G	C5'-C4'-O4'	5.23	115.38	109.10
13	1	297	G	O4'-C1'-N9	5.23	112.38	108.20
49	M5	188	ARG	NE-CZ-NH2	-5.23	117.69	120.30
13	1	880	G	C1'-O4'-C4'	-5.22	105.73	109.90
13	1	3317	U	O4'-C1'-N1	5.22	112.37	108.20
14	2	14	C	C6-N1-C2	-5.22	118.21	120.30
13	1	1535	A	O3'-P-O5'	-5.21	94.09	104.00
13	1	2665	U	OP1-P-O3'	5.21	116.66	105.20
13	1	2169	G	OP2-P-O3'	5.21	116.65	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	1	2373	A	C5'-C4'-O4'	-5.20	102.86	109.10
14	2	1728	U	O3'-P-O5'	-5.20	94.12	104.00
13	1	2780	A	O3'-P-O5'	-5.20	94.12	104.00
13	1	2938	G	OP2-P-O3'	5.20	116.63	105.20
13	1	784	A	OP2-P-O3'	5.20	116.63	105.20
13	1	3091	A	OP2-P-O3'	5.20	116.63	105.20
13	1	777	U	O5'-P-OP2	-5.19	101.03	105.70
13	1	59	G	O3'-P-O5'	-5.19	94.14	104.00
13	1	949	C	O5'-P-OP2	-5.19	101.03	105.70
13	1	2151	C	OP2-P-O3'	5.19	116.62	105.20
13	1	1834	U	O4'-C1'-N1	5.19	112.35	108.20
13	1	190	U	C1'-O4'-C4'	-5.18	105.75	109.90
13	1	2384	A	OP2-P-O3'	5.18	116.61	105.20
61	N7	65	ARG	CG-CD-NE	-5.18	100.92	111.80
13	1	667	C	O4'-C1'-N1	5.18	112.34	108.20
13	1	3143	C	OP1-P-O3'	5.18	116.60	105.20
13	1	685	G	OP2-P-O3'	5.18	116.59	105.20
13	1	1639	C	O5'-P-OP1	5.18	116.92	110.70
14	2	1012	U	OP1-P-O3'	5.18	116.59	105.20
13	1	951	A	OP1-P-O3'	5.18	116.59	105.20
13	1	1166	G	O5'-P-OP2	-5.18	101.04	105.70
13	1	506	U	OP2-P-O3'	5.17	116.59	105.20
13	1	708	G	C4'-C3'-C2'	-5.17	97.43	102.60
13	1	3121	U	P-O3'-C3'	5.17	125.91	119.70
12	4	42	G	O4'-C1'-N9	5.17	112.34	108.20
13	1	1335	C	C6-N1-C2	-5.17	118.23	120.30
13	1	3092	C	O5'-P-OP2	-5.17	101.05	105.70
13	1	277	G	C4'-C3'-C2'	-5.17	97.43	102.60
13	1	1635	G	O5'-P-OP2	-5.17	101.05	105.70
14	2	924	A	O3'-P-O5'	-5.17	94.18	104.00
13	1	1062	A	OP1-P-O3'	5.17	116.57	105.20
13	1	3065	G	O5'-P-OP2	-5.17	101.05	105.70
38	L3	114	VAL	N-CA-CB	5.17	122.86	111.50
13	1	1447	G	OP2-P-O3'	5.17	116.56	105.20
14	2	424	C	OP2-P-O3'	5.16	116.56	105.20
18	S3	76	ARG	NE-CZ-NH1	5.16	122.88	120.30
13	1	2910	A	C5'-C4'-C3'	-5.16	107.74	116.00
13	1	1331	U	OP2-P-O3'	5.16	116.55	105.20
14	2	961	U	OP1-P-O3'	5.16	116.55	105.20
13	1	834	U	O5'-P-OP2	-5.16	101.06	105.70
13	1	1211	U	OP2-P-O3'	5.16	116.55	105.20
13	1	609	G	O5'-P-OP1	5.16	116.89	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	L4	98	ARG	NE-CZ-NH2	-5.16	117.72	120.30
13	1	406	G	C1'-O4'-C4'	-5.16	105.78	109.90
14	2	867	G	O3'-P-O5'	-5.16	94.20	104.00
14	2	1444	C	C1'-O4'-C4'	-5.16	105.78	109.90
13	1	503	C	OP1-P-O3'	5.15	116.54	105.20
13	1	2816	G	O4'-C1'-C2'	-5.15	100.65	105.80
13	1	2870	C	C6-N1-C1'	5.15	126.98	120.80
13	1	3113	A	OP2-P-O3'	5.15	116.53	105.20
60	N6	12	ARG	NE-CZ-NH2	-5.15	117.72	120.30
13	1	1710	C	OP2-P-O3'	5.15	116.53	105.20
13	1	2199	G	O3'-P-O5'	-5.15	94.22	104.00
13	1	2269	U	O4'-C1'-N1	5.15	112.32	108.20
13	1	2393	G	O3'-P-O5'	-5.15	94.22	104.00
13	1	99	A	O5'-P-OP1	5.14	116.87	110.70
13	1	2881	C	O4'-C1'-N1	5.14	112.31	108.20
13	1	677	A	P-O3'-C3'	5.14	125.87	119.70
13	1	1481	A	O3'-P-O5'	5.14	113.77	104.00
13	1	3002	C	O3'-P-O5'	-5.14	94.23	104.00
14	2	555	A	P-O3'-C3'	5.14	125.87	119.70
30	D3	9	LEU	CB-CG-CD2	5.14	119.74	111.00
68	O4	12	PRO	N-CA-CB	-5.14	96.95	102.60
13	1	2702	A	OP1-P-O3'	5.14	116.50	105.20
13	1	1839	A	O4'-C1'-N9	-5.14	104.09	108.20
13	1	3112	G	O3'-P-O5'	-5.14	94.24	104.00
13	1	2209	U	P-O3'-C3'	5.13	125.86	119.70
52	M8	147	ARG	CB-CA-C	-5.13	100.13	110.40
13	1	2378	C	O3'-P-O5'	-5.13	94.25	104.00
14	2	1316	A	OP2-P-O3'	5.13	116.49	105.20
41	L6	26	ARG	NE-CZ-NH2	-5.13	117.73	120.30
13	1	645	A	OP2-P-O3'	5.13	116.49	105.20
13	1	974	G	O3'-P-O5'	-5.13	94.25	104.00
13	1	1042	U	O3'-P-O5'	-5.13	94.25	104.00
12	4	140	G	OP2-P-O3'	5.13	116.48	105.20
13	1	1442	U	O5'-P-OP2	-5.13	101.08	105.70
13	1	2410	U	OP1-P-O3'	5.13	116.48	105.20
30	D3	7	ARG	CG-CD-NE	5.13	122.57	111.80
40	L5	107	ARG	NE-CZ-NH1	5.13	122.86	120.30
13	1	2638	C	OP1-P-O3'	5.13	116.48	105.20
12	4	95	G	O3'-P-O5'	-5.12	94.27	104.00
13	1	1001	G	O3'-P-O5'	-5.12	94.27	104.00
13	1	1889	G	OP2-P-O3'	5.12	116.47	105.20
13	1	2948	C	N3-C4-C5	-5.12	119.85	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	2	449	C	O3'-P-O5'	-5.12	94.27	104.00
13	1	748	U	O5'-P-OP2	-5.12	101.09	105.70
13	1	767	U	O3'-P-O5'	-5.12	94.28	104.00
14	2	864	U	O4'-C1'-N1	5.11	112.29	108.20
13	1	3129	A	OP2-P-O3'	5.11	116.45	105.20
14	2	619	A	O4'-C1'-N9	-5.11	104.11	108.20
14	2	1764	G	O5'-P-OP2	-5.11	101.10	105.70
13	1	3217	C	C1'-O4'-C4'	-5.11	105.81	109.90
14	2	555	A	C4'-C3'-C2'	-5.11	97.49	102.60
13	1	3293	U	OP1-P-O3'	5.11	116.43	105.20
14	2	326	G	OP2-P-O3'	5.11	116.43	105.20
13	1	1895	A	OP2-P-O3'	5.10	116.43	105.20
13	1	640	U	O5'-P-OP2	-5.10	101.11	105.70
11	3	10	C	O5'-P-OP2	-5.10	101.11	105.70
12	4	25	G	OP1-P-O3'	5.10	116.42	105.20
13	1	1189	C	O5'-P-OP2	-5.10	101.11	105.70
13	1	3306	U	N3-C2-O2	-5.10	118.63	122.20
37	L2	242	ARG	NE-CZ-NH1	5.10	122.85	120.30
39	L4	193	LYS	CB-CA-C	-5.10	100.21	110.40
13	1	645	A	C5-C6-N1	5.09	120.25	117.70
13	1	1114	U	O3'-P-O5'	-5.09	94.32	104.00
14	2	783	G	O4'-C1'-N9	5.09	112.28	108.20
13	1	2340	U	O5'-P-OP2	5.09	116.81	110.70
13	1	2365	C	O3'-P-O5'	-5.09	94.33	104.00
13	1	2854	U	O5'-P-OP2	-5.09	101.12	105.70
13	1	2870	C	C6-N1-C2	-5.09	118.27	120.30
14	2	1553	U	OP1-P-O3'	5.09	116.39	105.20
14	2	1777	A	O5'-P-OP1	5.09	116.81	110.70
13	1	2110	G	OP2-P-O3'	5.09	116.39	105.20
13	1	2702	A	O5'-P-OP2	-5.08	101.13	105.70
13	1	718	G	C5-N7-C8	-5.08	101.76	104.30
13	1	3243	A	O3'-P-O5'	-5.08	94.35	104.00
47	M3	48	PRO	N-CA-CB	-5.08	97.01	102.60
13	1	2125	A	O3'-P-O5'	-5.08	94.35	104.00
14	2	400	A	O3'-P-O5'	-5.08	94.35	104.00
16	S1	26	ARG	N-CA-CB	5.08	119.74	110.60
13	1	910	G	OP2-P-O3'	5.08	116.37	105.20
13	1	2866	U	OP1-P-O3'	5.07	116.36	105.20
13	1	283	G	O4'-C1'-N9	-5.07	104.14	108.20
14	2	568	G	O5'-P-OP2	5.07	116.78	110.70
13	1	2809	C	O4'-C1'-N1	5.07	112.25	108.20
39	L4	138	ARG	CG-CD-NE	-5.07	101.16	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	1	2362	C	O5'-P-OP2	-5.07	101.14	105.70
13	1	2550	U	O4'-C1'-N1	5.07	112.25	108.20
14	2	1587	A	P-O3'-C3'	5.07	125.78	119.70
13	1	1329	U	O4'-C1'-N1	5.06	112.25	108.20
13	1	1410	U	OP2-P-O3'	5.06	116.33	105.20
13	1	295	A	OP2-P-O3'	5.06	116.33	105.20
14	2	1617	U	O5'-P-OP1	5.06	116.77	110.70
13	1	641	C	O5'-P-OP2	-5.06	101.15	105.70
14	2	1278	G	N3-C4-C5	5.06	131.13	128.60
62	N8	4	ARG	NE-CZ-NH1	5.05	122.83	120.30
13	1	513	G	OP2-P-O3'	5.05	116.32	105.20
13	1	3137	C	OP2-P-O3'	5.05	116.31	105.20
13	1	2501	U	P-O3'-C3'	5.05	125.76	119.70
14	2	103	A	OP2-P-O3'	5.05	116.31	105.20
13	1	1460	A	O5'-P-OP2	-5.05	101.16	105.70
13	1	853	G	O3'-P-O5'	-5.04	94.42	104.00
13	1	1883	A	OP2-P-O3'	5.04	116.30	105.20
14	2	1775	G	OP2-P-O3'	5.04	116.30	105.20
5	C5	81	ARG	NE-CZ-NH1	5.04	122.82	120.30
29	D2	42	GLN	CB-CA-C	-5.04	100.31	110.40
13	1	1165	A	OP2-P-O3'	5.04	116.29	105.20
11	3	85	G	OP2-P-O3'	5.04	116.28	105.20
14	2	1782	U	O5'-P-OP1	5.04	116.75	110.70
13	1	76	G	OP1-P-O3'	5.03	116.28	105.20
13	1	2816	G	C3'-C2'-C1'	-5.03	97.47	101.50
14	2	1323	A	O3'-P-O5'	-5.03	94.44	104.00
14	2	928	U	C3'-C2'-C1'	-5.03	97.47	101.50
13	1	51	A	O5'-P-OP2	-5.03	101.17	105.70
13	1	2592	G	O5'-P-OP2	-5.03	101.17	105.70
13	1	621	A	O3'-P-O5'	-5.03	94.45	104.00
14	2	1003	A	O4'-C1'-N9	5.03	112.22	108.20
14	2	1740	A	O3'-P-O5'	-5.03	94.45	104.00
13	1	106	A	OP2-P-O3'	5.03	116.26	105.20
13	1	3010	U	OP2-P-O3'	5.03	116.26	105.20
13	1	1323	G	OP1-P-O3'	5.02	116.24	105.20
13	1	1352	A	P-O3'-C3'	5.02	125.72	119.70
13	1	2147	A	OP2-P-O3'	5.02	116.24	105.20
13	1	2871	G	OP1-P-O3'	5.02	116.23	105.20
13	1	3303	G	OP1-P-O3'	5.01	116.22	105.20
13	1	1474	A	OP2-P-O3'	5.01	116.22	105.20
62	N8	77	LYS	CB-CA-C	5.01	120.42	110.40
13	1	2905	U	OP2-P-O3'	5.01	116.22	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	2	1101	G	C3'-C2'-C1'	-5.01	97.49	101.50
14	2	1145	C	OP2-P-O3'	5.01	116.21	105.20
60	N6	84	LYS	N-CA-CB	5.01	119.61	110.60
13	1	1895	A	P-O3'-C3'	5.00	125.70	119.70
14	2	1326	C	P-O3'-C3'	5.00	125.70	119.70

There are no chirality outliers.

All (141) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	1	1589	A	Sidechain
13	1	2131	A	Sidechain
13	1	2281	A	Sidechain
13	1	2376	G	Sidechain
13	1	358	G	Sidechain
13	1	406	G	Sidechain
13	1	770	G	Sidechain
13	1	835	G	Sidechain
13	1	94	G	Sidechain
1	B	117	ILE	Peptide
1	B	60	ARG	Sidechain
23	C1	129	ARG	Sidechain
23	C1	136	ARG	Sidechain
23	C1	99	ARG	Sidechain
24	C3	3	ARG	Sidechain
4	C4	114	ARG	Sidechain
4	C4	123	SER	Peptide
4	C4	127	ARG	Sidechain
25	C6	137	ARG	Sidechain
25	C6	82	ARG	Sidechain
6	C8	40	ARG	Sidechain
6	C8	41	ARG	Sidechain
30	D3	69	ARG	Sidechain
30	D3	7	ARG	Sidechain
8	D5	68	ARG	Sidechain
32	D6	5	ARG	Sidechain
32	D6	87	ARG	Sidechain
9	D8	42	ARG	Sidechain
34	D9	44	ARG	Sidechain
37	L2	21	ARG	Sidechain
37	L2	227	ARG	Sidechain
37	L2	3	ARG	Sidechain

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Mol	Chain	Res	Type	Group
37	L2	30	ARG	Sidechain
37	L2	9	ARG	Sidechain
38	L3	19	ARG	Sidechain
38	L3	21	ARG	Sidechain
38	L3	70	ARG	Sidechain
39	L4	138	ARG	Sidechain
39	L4	197	ARG	Sidechain
39	L4	47	ARG	Sidechain
39	L4	84	ARG	Sidechain
39	L4	98	ARG	Sidechain
40	L5	107	ARG	Sidechain
40	L5	218	ARG	Sidechain
40	L5	35	ARG	Sidechain
41	L6	134	ARG	Sidechain
41	L6	26	ARG	Sidechain
41	L6	77	ARG	Sidechain
41	L6	78	ARG	Sidechain
41	L6	82	ARG	Sidechain
42	L7	110	ARG	Sidechain
42	L7	151	ARG	Sidechain
42	L7	232	ARG	Sidechain
43	L8	68	ARG	Sidechain
44	L9	124	ARG	Sidechain
44	L9	166	ARG	Sidechain
44	L9	168	ARG	Sidechain
44	L9	173	ARG	Sidechain
45	M0	128	ARG	Sidechain
45	M0	153	ARG	Sidechain
47	M3	104	ARG	Sidechain
47	M3	171	ARG	Sidechain
47	M3	39	ARG	Sidechain
47	M3	49	ARG	Sidechain
47	M3	55	ARG	Sidechain
47	M3	73	ARG	Sidechain
48	M4	55	ARG	Sidechain
49	M5	187	ARG	Sidechain
49	M5	188	ARG	Sidechain
49	M5	20	ARG	Sidechain
49	M5	201	ARG	Sidechain
49	M5	71	ARG	Sidechain
49	M5	73	ARG	Sidechain
49	M5	96	ARG	Sidechain

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Mol	Chain	Res	Type	Group
50	M6	101	ARG	Sidechain
50	M6	117	ARG	Sidechain
50	M6	160	ARG	Sidechain
50	M6	37	ARG	Sidechain
50	M6	59	ARG	Sidechain
50	M6	78	ARG	Sidechain
51	M7	131	ARG	Sidechain
51	M7	167	ARG	Sidechain
51	M7	61	ARG	Sidechain
52	M8	141	ARG	Sidechain
52	M8	176	ARG	Sidechain
52	M8	39	ARG	Sidechain
52	M8	92	ARG	Sidechain
53	M9	100	ARG	Sidechain
53	M9	42	ARG	Sidechain
53	M9	62	ARG	Sidechain
54	N0	113	ARG	Sidechain
54	N0	117	ARG	Sidechain
54	N0	137	ARG	Sidechain
54	N0	155	ARG	Sidechain
54	N0	95	ARG	Sidechain
55	N1	102	ARG	Sidechain
55	N1	88	ARG	Sidechain
57	N3	45	ARG	Sidechain
57	N3	48	ARG	Sidechain
57	N3	80	ARG	Sidechain
58	N4	17	ARG	Sidechain
59	N5	115	ARG	Sidechain
59	N5	56	ARG	Sidechain
60	N6	28	ARG	Sidechain
60	N6	52	ARG	Sidechain
61	N7	17	ARG	Sidechain
61	N7	65	ARG	Sidechain
62	N8	26	ARG	Sidechain
62	N8	4	ARG	Sidechain
62	N8	9	ARG	Sidechain
65	O1	31	ARG	Sidechain
65	O1	62	ARG	Sidechain
66	O2	105	ARG	Sidechain
66	O2	44	ARG	Sidechain
66	O2	45	ARG	Sidechain
66	O2	47	ARG	Sidechain

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Mol	Chain	Res	Type	Group
67	O3	60	ARG	Sidechain
67	O3	86	ARG	Sidechain
69	O5	81	ARG	Sidechain
69	O5	86	ARG	Sidechain
69	O5	90	ARG	Sidechain
71	O7	21	ARG	Sidechain
71	O7	25	ARG	Sidechain
71	O7	45	ARG	Sidechain
71	O7	65	ARG	Sidechain
73	O9	30	ARG	Sidechain
76	Q2	87	ARG	Sidechain
15	S0	179	ARG	Sidechain
16	S1	152	ARG	Sidechain
17	S2	174	ARG	Sidechain
80	S4	191	ARG	Sidechain
80	S4	49	ARG	Sidechain
2	S5	225	ARG	Sidechain
2	S5	76	ARG	Sidechain
20	S7	112	ARG	Sidechain
21	S8	47	ARG	Sidechain
21	S8	5	ARG	Sidechain
22	S9	6	ARG	Sidechain
36	SR	155	ARG	Sidechain
36	SR	266	ASP	Peptide
36	SR	38	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1710	0	1799	22	0
2	S5	1609	0	1675	2	0
3	C0	818	0	806	10	0
4	C4	933	0	968	12	0
5	C5	912	0	946	6	0
6	C8	1192	0	1222	7	0
7	D0	855	0	917	6	0
8	D5	563	0	603	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	D8	490	0	529	0	0
10	P	146	0	174	0	0
11	3	2579	0	1303	1	0
12	4	3353	0	1695	7	0
13	1	67219	0	33762	72	0
14	2	37011	0	18622	55	0
15	S0	1598	0	1608	2	0
16	S1	1687	0	1763	4	0
17	S2	1615	0	1705	3	0
18	S3	1709	0	1792	2	0
19	S6	1820	0	1918	5	0
20	S7	1481	0	1572	0	0
21	S8	1489	0	1525	3	0
22	S9	1494	0	1573	1	0
23	C1	1121	0	1188	2	0
24	C3	1192	0	1255	2	0
25	C6	1105	0	1166	2	0
26	C7	737	0	802	1	0
27	C9	1112	0	1124	1	0
28	D1	673	0	659	2	0
29	D2	1021	0	1060	3	0
30	D3	1121	0	1196	3	0
31	D4	1073	0	1132	0	0
32	D6	769	0	814	6	0
33	D7	610	0	633	0	0
34	D9	404	0	397	1	0
35	E0	469	0	520	0	0
36	SR	2445	0	2401	2	0
37	L2	1909	0	1979	8	0
38	L3	3079	0	3157	15	0
39	L4	2731	0	2842	13	0
40	L5	2329	0	2279	6	0
41	L6	1239	0	1326	5	0
42	L7	1761	0	1843	1	0
43	L8	1706	0	1802	5	0
44	L9	1502	0	1572	5	0
45	M0	1677	0	1715	7	0
46	M1	1344	0	1370	2	0
47	M3	1543	0	1608	5	0
48	M4	1053	0	1149	4	0
49	M5	1711	0	1765	6	0
50	M6	1555	0	1659	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	M7	1379	0	1410	3	0
52	M8	1441	0	1543	11	0
53	M9	1490	0	1589	1	0
54	N0	1445	0	1487	3	0
55	N1	1268	0	1312	3	0
56	N2	778	0	791	0	0
57	N3	1003	0	1048	4	0
58	N4	513	0	540	1	0
59	N5	954	0	1018	3	0
60	N6	993	0	1081	1	0
61	N7	1092	0	1155	3	0
62	N8	1173	0	1215	3	0
63	N9	434	0	454	0	0
64	O0	743	0	797	4	0
65	O1	865	0	917	2	0
66	O2	1007	0	1074	2	0
67	O3	850	0	880	2	0
68	O4	861	0	918	4	0
69	O5	964	0	1073	3	0
70	O6	750	0	829	0	0
71	O7	676	0	678	8	0
72	O8	612	0	682	6	0
73	O9	436	0	475	4	0
74	Q0	409	0	444	0	0
75	Q1	233	0	284	0	0
76	Q2	847	0	914	3	0
77	Q3	694	0	734	2	0
78	SM	893	0	895	0	0
79	eI	1096	0	1094	0	0
80	S4	2068	0	2154	2	0
81	E1	271	0	263	2	0
82	1	191	0	0	0	0
82	2	19	0	0	0	0
82	3	3	0	0	0	0
82	4	2	0	0	0	0
82	L3	1	0	0	0	0
82	M7	1	0	0	0	0
82	N3	1	0	0	0	0
82	O2	1	0	0	0	0
82	O7	1	0	0	0	0
83	1	63	0	0	0	0
83	2	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
83	L2	2	0	0	0	0
83	L4	1	0	0	0	0
83	M0	1	0	0	0	0
83	M5	1	0	0	0	0
83	N9	1	0	0	0	0
83	O4	1	0	0	0	0
83	O7	1	0	0	0	0
84	1	20	0	23	0	0
85	1	30	0	57	0	0
86	D6	1	0	0	0	0
86	D9	1	0	0	0	0
86	O4	1	0	0	0	0
86	O7	1	0	0	0	0
86	Q0	1	0	0	0	0
86	Q2	1	0	0	0	0
86	Q3	1	0	0	0	0
87	1	1466	0	0	0	0
87	2	45	0	0	0	0
87	3	12	0	0	0	0
87	4	40	0	0	1	0
87	C3	2	0	0	0	0
87	L2	30	0	0	0	0
87	L3	21	0	0	0	0
87	L4	16	0	0	0	0
87	L5	3	0	0	0	0
87	L6	1	0	0	0	0
87	L7	10	0	0	0	0
87	M0	3	0	0	0	0
87	M3	3	0	0	0	0
87	M5	19	0	0	0	0
87	M6	9	0	0	0	0
87	M7	13	0	0	0	0
87	M8	10	0	0	0	0
87	M9	5	0	0	0	0
87	N0	3	0	0	0	0
87	N1	6	0	0	0	0
87	N3	4	0	0	0	0
87	N4	1	0	0	0	0
87	N5	4	0	0	0	0
87	N8	15	0	0	0	0
87	N9	5	0	0	0	0
87	O1	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	O2	20	0	0	0	0
87	O3	5	0	0	0	0
87	O4	6	0	0	0	0
87	O6	1	0	0	0	0
87	O7	11	0	0	0	0
87	O8	1	0	0	0	0
87	O9	1	0	0	0	0
87	Q0	1	0	0	0	0
87	Q2	9	0	0	1	0
87	Q3	4	0	0	0	0
87	eI	1	0	0	0	0
All	All	201671	0	148718	320	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 1.

All (320) 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:B:87:VAL:O	1:B:89:ASP:N	1.88	1.06
13:1:1639:C:OP2	68:O4:74:ARG:NH2	1.99	0.94
52:M8:71:LEU:HD13	52:M8:99:THR:HG21	1.48	0.93
4:C4:39:ILE:HD13	4:C4:76:ILE:HD11	1.60	0.83
1:B:76:ARG:HH22	1:B:140:HIS:HA	1.49	0.78
1:B:87:VAL:O	1:B:88:ASP:C	2.23	0.75
8:D5:92:ILE:HD11	8:D5:102:THR:HG23	1.70	0.72
12:4:41:A:OP1	71:O7:64:MET:O	2.07	0.71
5:C5:79:HIS:HD1	14:2:1228:G:C1'	2.04	0.71
6:C8:132:ARG:NH2	14:2:1160:C:OP1	2.24	0.70
4:C4:47:LYS:NZ	4:C4:66:ASP:OD2	2.24	0.70
50:M6:12:LYS:O	54:N0:167:ARG:NH2	2.26	0.69
1:B:36:VAL:HG11	1:B:190:PHE:CE1	2.29	0.67
1:B:95:LYS:O	1:B:96:ASN:O	2.13	0.67
3:C0:88:PRO:HD2	3:C0:91:TYR:CD2	2.31	0.66
13:1:776:U:H5	13:1:2719:U:O2	1.77	0.66
39:L4:52:VAL:HG11	39:L4:99:MET:CE	2.26	0.65
14:2:1034:C:HO2'	29:D2:2:THR:N	1.95	0.65
52:M8:71:LEU:CD1	52:M8:99:THR:HG21	2.26	0.64
14:2:1239:C:P	81:E1:118:ARG:HH12	2.20	0.64
54:N0:1:MET:HE1	54:N0:36:ILE:HG21	1.81	0.63
13:1:860:G:OP1	77:Q3:17:ARG:NH1	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:676:G:O6	52:M8:86:THR:HG21	1.99	0.61
19:S6:52:ILE:HG23	19:S6:109:LEU:HD21	1.82	0.61
13:1:2767:U:O2'	76:Q2:30:ALA:O	2.16	0.60
13:1:3306:U:O2	13:1:3306:U:O5'	2.19	0.60
5:C5:79:HIS:ND1	14:2:1228:G:O4'	2.33	0.59
6:C8:141:THR:HG21	14:2:1161:C:OP2	2.03	0.59
45:M0:14:ASN:O	45:M0:128:ARG:NH2	2.36	0.58
7:D0:22:ILE:HD12	7:D0:100:VAL:HG21	1.86	0.58
73:O9:9:ILE:HG22	73:O9:13:MET:HE3	1.85	0.58
25:C6:129:PHE:O	25:C6:137:ARG:NH2	2.35	0.57
1:B:61:PRO:HD2	1:B:171:ASN:HD21	1.67	0.57
13:1:1778:G:O2'	13:1:1780:G:OP2	2.20	0.57
14:2:284:G:N7	19:S6:188:ARG:NH1	2.51	0.57
73:O9:9:ILE:HG22	73:O9:13:MET:CE	2.33	0.57
49:M5:155:VAL:O	49:M5:162:ARG:NH2	2.37	0.57
54:N0:1:MET:HG3	54:N0:118:PHE:CE1	2.39	0.57
40:L5:107:ARG:NH2	40:L5:119:TYR:O	2.37	0.57
13:1:1724:U:H1'	13:1:1725:C:C6	2.40	0.57
21:S8:106:ALA:HB2	21:S8:165:LEU:HD23	1.86	0.56
14:2:1239:C:O5'	81:E1:118:ARG:NH1	2.39	0.56
13:1:44:U:H5"	49:M5:85:THR:HG23	1.88	0.55
14:2:325:G:H4'	23:C1:83:THR:HG21	1.87	0.55
14:2:1278:G:H22	14:2:1311:G:H22	1.53	0.55
3:C0:87:VAL:HB	3:C0:88:PRO:CD	2.37	0.55
13:1:2828:G:OP1	45:M0:7:ARG:NH1	2.39	0.55
57:N3:87:ARG:HH22	57:N3:137:VAL:HG21	1.73	0.54
7:D0:70:THR:HG22	14:2:1267:C:O2'	2.07	0.54
2:S5:84:LYS:NZ	14:2:1600:U:OP2	2.40	0.54
13:1:687:U:OP2	47:M3:36:ARG:NH2	2.40	0.53
4:C4:83:ILE:HD12	32:D6:44:ILE:HG22	1.90	0.53
14:2:1278:G:H2'	14:2:1278:G:N3	2.23	0.53
44:L9:57:VAL:HG23	44:L9:68:LEU:HD13	1.90	0.53
72:O8:46:ARG:O	72:O8:46:ARG:NE	2.41	0.53
13:1:873:C:H3'	13:1:874:U:H4'	1.90	0.53
13:1:1383:G:O3'	39:L4:138:ARG:NH2	2.41	0.53
14:2:1146:C:N4	14:2:1272:U:OP1	2.41	0.53
18:S3:67:ASN:HD22	18:S3:71:LEU:HG	1.73	0.53
13:1:2156:C:P	37:L2:241:ARG:HH22	2.32	0.53
1:B:95:LYS:O	1:B:96:ASN:C	2.45	0.53
29:D2:6:VAL:HG13	29:D2:34:ILE:HD11	1.91	0.53
47:M3:10:LEU:HD23	52:M8:166:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:45:A:P	49:M5:85:THR:HG21	2.48	0.53
71:O7:21:ARG:NH2	71:O7:41:ALA:O	2.41	0.53
13:1:607:A:OP1	41:L6:26:ARG:NH2	2.41	0.52
29:D2:25:VAL:CG2	29:D2:65:LEU:HD11	2.40	0.52
64:O0:68:TYR:CE1	64:O0:104:LEU:HD12	2.44	0.52
14:2:1551:U:H2'	14:2:1552:C:C6	2.44	0.52
14:2:142:G:C8	14:2:266:A:C2	2.97	0.52
41:L6:52:VAL:HG21	41:L6:65:ILE:HG13	1.92	0.52
53:M9:105:LEU:HD23	53:M9:138:LEU:HD23	1.90	0.52
39:L4:35:VAL:HG21	39:L4:244:LEU:HD21	1.91	0.52
71:O7:17:THR:HG22	71:O7:18:LEU:H	1.73	0.52
14:2:538:A:N3	14:2:540:G:N1	2.58	0.52
13:1:743:C:O2	52:M8:141:ARG:HD3	2.10	0.51
14:2:1158:A:H2'	14:2:1159:G:C8	2.45	0.51
6:C8:132:ARG:HH12	14:2:1160:C:H5"	1.74	0.51
12:4:66:A:OP1	69:O5:10:ARG:NH2	2.43	0.51
39:L4:52:VAL:HG11	39:L4:99:MET:HE3	1.92	0.51
4:C4:134:GLY:O	4:C4:136:ARG:HG3	2.10	0.51
43:L8:161:GLU:HA	43:L8:164:VAL:HG22	1.93	0.51
37:L2:104:LEU:CD2	37:L2:158:ILE:HD11	2.41	0.51
1:B:63:MET:HB3	1:B:152:ARG:HG2	1.92	0.51
38:L3:286:GLY:HA3	38:L3:321:PHE:CE2	2.46	0.51
13:1:1446:A:H5"	51:M7:65:SER:OG	2.11	0.50
13:1:2953:U:H2'	13:1:2954:U:H2'	1.91	0.50
3:C0:90:THR:O	3:C0:94:GLU:HG3	2.11	0.50
36:SR:19:TRP:CE3	36:SR:306:THR:HG22	2.45	0.50
80:S4:70:VAL:HG12	80:S4:92:LEU:HD22	1.91	0.50
8:D5:77:ARG:NH2	14:2:1521:G:N7	2.60	0.50
41:L6:78:ARG:HD2	41:L6:106:PHE:CD2	2.47	0.50
69:O5:78:LYS:HA	69:O5:81:ARG:HD3	1.93	0.50
1:B:61:PRO:HD2	1:B:171:ASN:ND2	2.27	0.50
13:1:670:C:P	52:M8:147:ARG:HH22	2.35	0.50
40:L5:34:LYS:O	40:L5:38:THR:HG23	2.11	0.50
7:D0:35:GLU:OE1	14:2:1370:G:H4'	2.11	0.50
68:O4:41:ARG:HG2	68:O4:56:THR:HG21	1.93	0.49
13:1:31:C:OP2	49:M5:188:ARG:NH2	2.32	0.49
13:1:2854:U:OP2	45:M0:3:ARG:NH2	2.45	0.49
23:C1:136:ARG:HG2	23:C1:136:ARG:HH11	1.77	0.49
13:1:2138:A:HO2'	71:O7:2:GLY:N	2.10	0.49
71:O7:14:LYS:HD2	73:O9:51:ILE:HD11	1.94	0.49
1:B:95:LYS:O	1:B:100:ILE:HG13	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C4:123:SER:O	14:2:929:A:C8	2.66	0.49
13:1:45:A:OP2	49:M5:85:THR:HG21	2.13	0.48
14:2:1074:A:H2'	14:2:1075:A:C8	2.48	0.48
64:O0:78:GLY:HA2	64:O0:87:VAL:HG13	1.96	0.48
3:C0:46:LEU:HD13	3:C0:66:TYR:CD2	2.48	0.48
3:C0:84:GLU:O	3:C0:86:ILE:N	2.47	0.48
44:L9:53:ILE:HD12	48:M4:7:VAL:HG21	1.95	0.48
13:1:996:A:C2	13:1:1054:A:C4	3.02	0.48
24:C3:125:LEU:HD22	24:C3:129:TYR:CE2	2.48	0.48
4:C4:121:VAL:O	14:2:886:U:O2'	2.31	0.48
61:N7:15:ARG:NH2	68:O4:83:ASN:OD1	2.47	0.48
13:1:2828:G:P	45:M0:7:ARG:HH12	2.37	0.48
14:2:1267:C:H2'	14:2:1268:G:H8	1.77	0.48
1:B:67:ILE:HA	1:B:111:ILE:O	2.13	0.48
13:1:1809:A:H2'	13:1:1810:A:O4'	2.14	0.48
13:1:2282:U:O2	13:1:2310:U:H4'	2.13	0.48
30:D3:7:ARG:HH11	30:D3:7:ARG:HG2	1.79	0.48
13:1:1613:A:OP1	72:O8:2:ALA:HB2	2.14	0.47
7:D0:70:THR:CG2	14:2:1267:C:O2'	2.62	0.47
16:S1:32:ILE:HD11	16:S1:46:THR:HG23	1.94	0.47
36:SR:19:TRP:CE3	36:SR:38:ARG:NH1	2.83	0.47
59:N5:103:TYR:HB3	59:N5:135:ILE:HD11	1.96	0.47
3:C0:94:GLU:HB3	18:S3:67:ASN:H	1.79	0.47
6:C8:25:ASN:O	6:C8:57:ARG:NH1	2.48	0.47
64:O0:44:ILE:CG2	64:O0:48:THR:HG21	2.44	0.47
13:1:967:A:OP1	62:N8:47:LYS:NZ	2.47	0.47
48:M4:55:ARG:NH2	48:M4:76:ALA:O	2.37	0.47
52:M8:69:ARG:HG3	52:M8:69:ARG:HH11	1.79	0.47
64:O0:26:GLY:O	64:O0:30:THR:HG23	2.14	0.47
38:L3:370:PHE:CD2	38:L3:376:LYS:HG3	2.49	0.47
46:M1:65:ILE:O	46:M1:66:ALA:O	2.33	0.47
14:2:1520:C:H4'	14:2:1526:G:N1	2.30	0.47
6:C8:143:ARG:O	14:2:1448:C:OP1	2.32	0.47
17:S2:169:LEU:HD23	17:S2:198:THR:HG22	1.96	0.47
13:1:698:U:H2'	13:1:699:A:O4'	2.15	0.47
38:L3:246:LEU:HD12	38:L3:246:LEU:C	2.35	0.46
39:L4:91:GLY:HA3	39:L4:93:MET:CE	2.46	0.46
14:2:1188:G:C2	14:2:1587:A:C2	3.03	0.46
37:L2:27:ALA:O	37:L2:128:ARG:NH2	2.43	0.46
1:B:138:VAL:HG23	1:B:147:LYS:HG3	1.97	0.46
13:1:2585:G:N7	43:L8:47:SER:HB3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:374:A:HO2'	13:1:376:G:H8	1.63	0.46
67:O3:14:LEU:HD11	67:O3:31:LYS:HB2	1.96	0.46
4:C4:83:ILE:HD12	32:D6:44:ILE:CG2	2.45	0.46
28:D1:34:ILE:HD13	28:D1:69:LEU:HD11	1.98	0.46
13:1:3278:C:H2'	13:1:3278:C:O2	2.16	0.46
3:C0:14:TYR:CD2	3:C0:35:ILE:HD11	2.50	0.46
13:1:2947:G:N3	38:L3:250:ALA:HB1	2.31	0.46
15:S0:157:ASP:OD1	28:D1:60:ARG:NH2	2.46	0.46
38:L3:323:MET:CE	38:L3:356:LEU:HD11	2.47	0.46
1:B:59:PRO:HA	1:B:170:GLY:HA2	1.98	0.45
4:C4:114:ARG:HH12	16:S1:72:ASP:CG	2.20	0.45
38:L3:280:HIS:HB3	38:L3:324:VAL:HG13	1.98	0.45
13:1:685:G:P	47:M3:35:ARG:HH11	2.40	0.45
14:2:1310:C:H2'	14:2:1311:G:O4'	2.17	0.45
3:C0:87:VAL:HB	3:C0:88:PRO:HD3	1.99	0.45
4:C4:39:ILE:CD1	4:C4:76:ILE:HD11	2.41	0.45
13:1:2339:C:OP2	57:N3:48:ARG:HG3	2.17	0.45
30:D3:42:PRO:O	30:D3:79:ASN:ND2	2.50	0.45
45:M0:79:VAL:CG2	45:M0:147:VAL:HG13	2.46	0.45
48:M4:21:VAL:HB	48:M4:63:VAL:HG13	1.98	0.45
4:C4:26:THR:HG21	4:C4:97:GLY:HA3	1.98	0.45
13:1:2677:G:H2'	13:1:2679:A:C2	2.52	0.45
14:2:1278:G:H22	14:2:1311:G:N2	2.15	0.45
32:D6:12:LYS:O	32:D6:13:LYS:C	2.55	0.45
38:L3:256:HIS:HA	38:L3:257:PRO:C	2.36	0.45
13:1:2523:A:H2'	43:L8:49:TYR:O	2.17	0.45
13:1:2563:G:H5"	43:L8:27:THR:CG2	2.46	0.45
14:2:1626:C:O2	14:2:1750:A:N1	2.50	0.45
13:1:230:U:H2'	13:1:231:G:O4'	2.16	0.45
13:1:675:C:O2'	13:1:679:U:OP1	2.34	0.45
14:2:978:A:H2'	14:2:979:A:O4'	2.16	0.45
39:L4:300:ARG:O	52:M8:39:ARG:NH1	2.48	0.45
13:1:2728:G:O6	55:N1:78:LYS:HE3	2.17	0.45
11:3:5:G:OP1	46:M1:143:ARG:NH2	2.50	0.44
14:2:1661:C:OP1	19:S6:92:ARG:NH2	2.46	0.44
25:C6:82:ARG:HH12	25:C6:114:ARG:CZ	2.30	0.44
41:L6:154:LEU:HA	41:L6:157:GLN:HE21	1.81	0.44
1:B:49:PHE:CE1	1:B:159:LEU:HB2	2.52	0.44
5:C5:43:ARG:HH12	14:2:1538:U:H3'	1.81	0.44
38:L3:150:ARG:HG2	38:L3:150:ARG:HH11	1.81	0.44
42:L7:156:ILE:HD12	42:L7:156:ILE:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:N7:123:GLN:O	61:N7:124:ALA:HB3	2.16	0.44
4:C4:32:ASP:OD1	4:C4:39:ILE:HD11	2.18	0.44
12:4:135:G:OP2	59:N5:56:ARG:NH2	2.48	0.44
13:1:2617:U:O2	13:1:2617:U:O5'	2.36	0.44
13:1:2880:U:H1'	38:L3:250:ALA:HB3	1.99	0.44
13:1:3212:C:OP2	48:M4:124:ARG:NH2	2.50	0.44
12:4:103:G:H4'	71:O7:21:ARG:HG3	2.00	0.44
38:L3:105:VAL:HG21	38:L3:148:LEU:HD13	1.99	0.44
58:N4:20:LEU:HD21	58:N4:28:ILE:HG23	1.99	0.44
1:B:117:ILE:O	1:B:118:LYS:C	2.56	0.44
13:1:2836:C:O2	13:1:2836:C:O5'	2.35	0.44
15:S0:17:LEU:HD23	15:S0:172:LEU:HD11	2.00	0.44
1:B:4:ILE:HD12	1:B:187:VAL:HG11	1.99	0.44
1:B:19:TYR:CD1	1:B:212:PRO:HD3	2.53	0.44
37:L2:7:ASN:C	37:L2:7:ASN:HD22	2.21	0.44
39:L4:156:LEU:HD12	39:L4:159:ILE:HD12	2.00	0.44
40:L5:34:LYS:HE2	40:L5:38:THR:HG21	2.00	0.44
7:D0:22:ILE:CD1	7:D0:100:VAL:HG21	2.47	0.44
13:1:1412:G:OP1	66:O2:105:ARG:NH2	2.51	0.44
69:O5:90:ARG:HG3	69:O5:90:ARG:HH11	1.83	0.44
14:2:95:G:O2'	14:2:460:A:O2'	2.30	0.43
14:2:1587:A:H2'	14:2:1587:A:N3	2.33	0.43
27:C9:65:ILE:HG12	27:C9:71:VAL:HG22	2.00	0.43
39:L4:52:VAL:HG11	39:L4:99:MET:HE1	2.00	0.43
1:B:96:ASN:O	1:B:97:LYS:C	2.56	0.43
2:S5:123:VAL:HG21	8:D5:92:ILE:CD1	2.48	0.43
37:L2:30:ARG:NH2	37:L2:33:ASP:OD1	2.52	0.43
49:M5:96:ARG:HG2	49:M5:96:ARG:HH11	1.83	0.43
38:L3:43:LEU:HD22	38:L3:203:VAL:HG11	1.99	0.43
55:N1:11:THR:O	55:N1:12:ARG:C	2.56	0.43
14:2:1089:G:OP2	30:D3:7:ARG:NH1	2.52	0.43
13:1:1784:G:H2'	13:1:1785:U:O4'	2.18	0.43
39:L4:7:THR:HG21	39:L4:15:ALA:HB1	1.99	0.43
37:L2:30:ARG:HG2	37:L2:74:GLU:HG2	2.01	0.43
40:L5:40:HIS:HB3	40:L5:43:LYS:HD3	2.00	0.43
13:1:2897:A:H2'	13:1:2899:C:H5"	2.01	0.43
21:S8:76:THR:HG22	21:S8:108:PRO:HG2	2.01	0.43
67:O3:49:ILE:HD11	67:O3:71:VAL:HG22	2.01	0.43
8:D5:54:VAL:HG11	8:D5:83:LEU:HD13	2.01	0.43
13:1:2728:G:O6	55:N1:78:LYS:CE	2.67	0.43
14:2:591:A:H2'	14:2:592:A:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S2:45:VAL:HG13	17:S2:72:LEU:CD1	2.49	0.43
5:C5:44:ARG:HH12	5:C5:83:MET:HA	1.83	0.43
12:4:104:A:C8	12:4:105:A:C8	3.07	0.42
13:1:3182:G:OP1	50:M6:160:ARG:NH2	2.51	0.42
47:M3:2:ALA:HB2	62:N8:31:GLY:O	2.19	0.42
13:1:1508:C:P	51:M7:127:ARG:HH22	2.41	0.42
14:2:139:C:C4	14:2:266:A:C2	3.06	0.42
14:2:333:A:C6	14:2:334:G:C6	3.07	0.42
21:S8:106:ALA:CB	21:S8:165:LEU:HD23	2.49	0.42
13:1:662:U:H2'	13:1:663:C:C6	2.54	0.42
3:C0:14:TYR:CD2	3:C0:21:VAL:HG22	2.54	0.42
14:2:15:U:H2'	14:2:16:G:O4'	2.20	0.42
38:L3:89:VAL:HG13	38:L3:195:ALA:HB1	2.02	0.42
39:L4:52:VAL:HG21	39:L4:99:MET:HE3	2.00	0.42
65:O1:55:LEU:HD22	65:O1:93:VAL:HG12	2.01	0.42
12:4:20:U:OP1	87:4:301:HOH:O	2.22	0.42
13:1:3217:C:O2	13:1:3217:C:H2'	2.18	0.42
14:2:1456:A:H2'	14:2:1457:C:C6	2.55	0.42
44:L9:27:VAL:HG12	44:L9:82:VAL:HG11	2.00	0.42
5:C5:119:PHE:HE1	6:C8:119:ILE:CG2	2.33	0.42
13:1:2207:A:H2'	13:1:2208:A:O4'	2.19	0.42
13:1:2915:U:C5	38:L3:7:GLU:HG2	2.55	0.42
13:1:2683:U:H2'	13:1:2684:C:C6	2.55	0.42
13:1:3297:U:O4	38:L3:124:LYS:NZ	2.52	0.42
14:2:532:U:OP1	22:S9:132:ARG:NH2	2.52	0.42
14:2:1511:A:H2'	14:2:1512:A:C8	2.54	0.42
72:O8:41:THR:HG21	72:O8:62:ALA:CB	2.49	0.42
16:S1:158:SER:HA	16:S1:161:ILE:HG12	2.01	0.42
32:D6:81:ALA:HB3	32:D6:83:ILE:HG12	2.01	0.42
62:N8:75:LEU:HB3	62:N8:118:ILE:HG23	2.01	0.42
71:O7:17:THR:HG22	71:O7:18:LEU:N	2.35	0.42
1:B:86:SER:N	1:B:89:ASP:OD2	2.52	0.42
13:1:1110:U:H2'	13:1:1111:U:C6	2.54	0.42
13:1:1492:G:N7	73:O9:2:ALA:CB	2.83	0.42
60:N6:106:ILE:HG21	60:N6:109:LEU:HD23	2.01	0.42
13:1:826:G:OP1	13:1:1590:G:O2'	2.32	0.41
13:1:1613:A:OP1	72:O8:2:ALA:CB	2.68	0.41
1:B:96:ASN:CB	1:B:99:LEU:HD23	2.50	0.41
40:L5:64:ILE:HD12	40:L5:109:THR:HG21	2.02	0.41
68:O4:91:ARG:HG2	68:O4:95:ILE:HD12	2.02	0.41
72:O8:41:THR:HG21	72:O8:62:ALA:HB1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:1784:A:C6	32:D6:87:ARG:HD2	2.56	0.41
24:C3:60:VAL:HG13	24:C3:66:ILE:CD1	2.50	0.41
39:L4:152:VAL:HG12	39:L4:172:VAL:HG21	2.02	0.41
43:L8:50:VAL:HG21	59:N5:27:ARG:HD3	2.03	0.41
44:L9:128:VAL:HA	44:L9:157:ASN:HD21	1.85	0.41
52:M8:106:PHE:CE1	52:M8:121:CYS:HB3	2.55	0.41
13:1:781:G:OP1	52:M8:151:ARG:HD2	2.20	0.41
13:1:1913:A:N3	13:1:2120:A:H2'	2.36	0.41
13:1:3309:G:O6	38:L3:21:ARG:NH2	2.48	0.41
17:S2:53:ILE:HD11	17:S2:73:LEU:HD13	2.03	0.41
19:S6:159:ARG:HH21	19:S6:170:THR:HG23	1.86	0.41
61:N7:10:VAL:O	61:N7:83:THR:HG22	2.20	0.41
13:1:2882:U:H2'	13:1:2883:U:O4'	2.21	0.41
37:L2:168:VAL:HG13	77:Q3:79:VAL:HG21	2.03	0.41
47:M3:42:ARG:NH1	47:M3:51:LEU:O	2.54	0.41
14:2:148:A:N6	14:2:167:U:O2	2.53	0.41
1:B:93:LEU:C	1:B:95:LYS:H	2.24	0.41
13:1:1748:G:OP1	72:O8:53:THR:HG21	2.21	0.41
14:2:901:G:N1	14:2:902:G:C6	2.89	0.41
14:2:1668:A:H1'	19:S6:66:GLY:HA2	2.03	0.41
26:C7:102:VAL:HG13	26:C7:106:THR:HB	2.03	0.41
65:O1:31:ARG:HH21	65:O1:31:ARG:HG2	1.85	0.41
76:Q2:45:ARG:NH2	87:Q2:302:HOH:O	2.53	0.41
3:C0:88:PRO:HG2	3:C0:91:TYR:CE2	2.56	0.41
5:C5:125:PRO:HG3	6:C8:129:TRP:CH2	2.55	0.41
7:D0:82:TYR:HB3	34:D9:52:PHE:HB3	2.03	0.41
66:O2:55:ILE:HD12	66:O2:55:ILE:HA	1.90	0.41
71:O7:66:TYR:OH	71:O7:73:ARG:NH2	2.54	0.41
76:Q2:4:VAL:HG22	76:Q2:93:LEU:HD12	2.03	0.41
1:B:87:VAL:O	1:B:90:LEU:N	2.54	0.40
57:N3:85:TRP:CE2	57:N3:93:LEU:HD21	2.56	0.40
13:1:357:A:O4'	39:L4:81:GLY:HA3	2.21	0.40
13:1:1307:G:C2	13:1:1308:A:C2	3.09	0.40
13:1:3310:A:OP1	51:M7:74:LYS:NZ	2.48	0.40
14:2:1278:G:N3	14:2:1278:G:C2'	2.82	0.40
14:2:1626:C:H2'	14:2:1627:C:O4'	2.21	0.40
14:2:1267:C:H2'	14:2:1268:G:C8	2.55	0.40
16:S1:121:ILE:HD11	16:S1:161:ILE:HG22	2.04	0.40
39:L4:299:ILE:HG23	52:M8:39:ARG:HB3	2.02	0.40
40:L5:219:PHE:CE2	40:L5:227:LEU:HD21	2.57	0.40
41:L6:54:TYR:CE1	41:L6:63:LEU:HD22	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:1581:G:OP2	14:2:1583:C:N4	2.54	0.40
45:M0:84:ALA:O	45:M0:140:THR:HG22	2.21	0.40
80:S4:47:PHE:CE2	80:S4:52:LEU:HD11	2.57	0.40
4:C4:102:LEU:HD21	32:D6:45:VAL:HG12	2.03	0.40
12:4:143:U:H2'	12:4:144:G:O4'	2.22	0.40
13:1:3108:G:H21	44:L9:163:GLN:HE22	1.68	0.40
14:2:1150:A:H2'	14:2:1151:G:O4'	2.21	0.40
14:2:1578:C:H2'	14:2:1579:A:C8	2.57	0.40
37:L2:158:ILE:HD13	37:L2:158:ILE:HG21	1.85	0.40
45:M0:174:THR:HG23	45:M0:176:LEU:H	1.86	0.40
57:N3:25:CYS:SG	57:N3:27:ASP:OD1	2.79	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
1	B	214/217 (99%)	195 (91%)	14 (6%)	5 (2%)	6 7
2	S5	204/206 (99%)	193 (95%)	10 (5%)	1 (0%)	29 41
3	C0	94/96 (98%)	85 (90%)	5 (5%)	4 (4%)	2 2
4	C4	124/127 (98%)	123 (99%)	1 (1%)	0	100 100
5	C5	113/124 (91%)	110 (97%)	2 (2%)	1 (1%)	17 25
6	C8	143/145 (99%)	138 (96%)	4 (3%)	1 (1%)	22 32
7	D0	105/107 (98%)	104 (99%)	1 (1%)	0	100 100
8	D5	68/70 (97%)	65 (96%)	1 (2%)	2 (3%)	4 4
9	D8	60/63 (95%)	57 (95%)	2 (3%)	1 (2%)	9 11
10	P	13/15 (87%)	13 (100%)	0	0	100 100
15	S0	202/251 (80%)	179 (89%)	19 (9%)	4 (2%)	7 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
16	S1	209/214 (98%)	185 (88%)	20 (10%)	4 (2%)	8 10
17	S2	212/217 (98%)	196 (92%)	13 (6%)	3 (1%)	11 15
18	S3	218/223 (98%)	195 (89%)	19 (9%)	4 (2%)	8 10
19	S6	224/226 (99%)	198 (88%)	24 (11%)	2 (1%)	17 25
20	S7	182/184 (99%)	155 (85%)	23 (13%)	4 (2%)	6 7
21	S8	184/188 (98%)	168 (91%)	14 (8%)	2 (1%)	14 20
22	S9	183/185 (99%)	164 (90%)	17 (9%)	2 (1%)	14 20
23	C1	135/155 (87%)	122 (90%)	10 (7%)	3 (2%)	6 7
24	C3	148/150 (99%)	136 (92%)	12 (8%)	0	100 100
25	C6	139/141 (99%)	115 (83%)	19 (14%)	5 (4%)	3 3
26	C7	88/120 (73%)	79 (90%)	8 (9%)	1 (1%)	14 20
27	C9	141/143 (99%)	131 (93%)	8 (6%)	2 (1%)	11 15
28	D1	84/87 (97%)	72 (86%)	10 (12%)	2 (2%)	6 6
29	D2	127/129 (98%)	123 (97%)	4 (3%)	0	100 100
30	D3	142/144 (99%)	132 (93%)	9 (6%)	1 (1%)	22 32
31	D4	132/134 (98%)	121 (92%)	9 (7%)	2 (2%)	10 14
32	D6	95/97 (98%)	81 (85%)	9 (10%)	5 (5%)	2 1
33	D7	79/81 (98%)	74 (94%)	5 (6%)	0	100 100
34	D9	47/53 (89%)	41 (87%)	5 (11%)	1 (2%)	7 8
35	E0	57/60 (95%)	50 (88%)	5 (9%)	2 (4%)	3 3
36	SR	316/318 (99%)	304 (96%)	11 (4%)	1 (0%)	41 55
37	L2	249/252 (99%)	238 (96%)	11 (4%)	0	100 100
38	L3	384/386 (100%)	368 (96%)	15 (4%)	1 (0%)	41 55
39	L4	357/361 (99%)	335 (94%)	18 (5%)	4 (1%)	14 20
40	L5	288/295 (98%)	275 (96%)	11 (4%)	2 (1%)	22 32
41	L6	152/156 (97%)	144 (95%)	7 (5%)	1 (1%)	22 32
42	L7	217/222 (98%)	214 (99%)	2 (1%)	1 (0%)	29 41
43	L8	212/233 (91%)	203 (96%)	9 (4%)	0	100 100
44	L9	187/189 (99%)	180 (96%)	6 (3%)	1 (0%)	29 41
45	M0	202/209 (97%)	193 (96%)	9 (4%)	0	100 100
46	M1	166/168 (99%)	152 (92%)	8 (5%)	6 (4%)	3 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
47	M3	191/193 (99%)	180 (94%)	9 (5%)	2 (1%)	15 23
48	M4	134/136 (98%)	127 (95%)	3 (2%)	4 (3%)	4 3
49	M5	200/202 (99%)	195 (98%)	5 (2%)	0	100 100
50	M6	195/197 (99%)	193 (99%)	2 (1%)	0	100 100
51	M7	170/183 (93%)	163 (96%)	7 (4%)	0	100 100
52	M8	183/185 (99%)	175 (96%)	7 (4%)	1 (0%)	29 41
53	M9	182/188 (97%)	180 (99%)	1 (0%)	1 (0%)	29 41
54	N0	170/172 (99%)	165 (97%)	4 (2%)	1 (1%)	25 36
55	N1	156/159 (98%)	149 (96%)	6 (4%)	1 (1%)	25 36
56	N2	96/100 (96%)	86 (90%)	9 (9%)	1 (1%)	15 23
57	N3	134/136 (98%)	129 (96%)	5 (4%)	0	100 100
58	N4	60/98 (61%)	59 (98%)	1 (2%)	0	100 100
59	N5	117/121 (97%)	113 (97%)	4 (3%)	0	100 100
60	N6	124/126 (98%)	117 (94%)	5 (4%)	2 (2%)	9 13
61	N7	133/135 (98%)	129 (97%)	3 (2%)	1 (1%)	19 29
62	N8	146/148 (99%)	134 (92%)	9 (6%)	3 (2%)	7 8
63	N9	52/56 (93%)	48 (92%)	2 (4%)	2 (4%)	3 2
64	O0	95/97 (98%)	92 (97%)	2 (2%)	1 (1%)	14 20
65	O1	104/109 (95%)	99 (95%)	4 (4%)	1 (1%)	15 23
66	O2	123/127 (97%)	117 (95%)	6 (5%)	0	100 100
67	O3	104/106 (98%)	103 (99%)	1 (1%)	0	100 100
68	O4	107/111 (96%)	104 (97%)	2 (2%)	1 (1%)	17 25
69	O5	116/119 (98%)	114 (98%)	1 (1%)	1 (1%)	17 25
70	O6	95/99 (96%)	89 (94%)	4 (4%)	2 (2%)	7 8
71	O7	83/86 (96%)	77 (93%)	6 (7%)	0	100 100
72	O8	75/77 (97%)	73 (97%)	2 (3%)	0	100 100
73	O9	48/50 (96%)	48 (100%)	0	0	100 100
74	Q0	49/52 (94%)	47 (96%)	0	2 (4%)	3 2
75	Q1	23/25 (92%)	23 (100%)	0	0	100 100
76	Q2	103/105 (98%)	97 (94%)	6 (6%)	0	100 100
77	Q3	89/91 (98%)	83 (93%)	5 (6%)	1 (1%)	14 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
78	SM	116/118 (98%)	102 (88%)	12 (10%)	2 (2%)	9 11
79	eI	142/145 (98%)	127 (89%)	13 (9%)	2 (1%)	11 15
80	S4	258/260 (99%)	240 (93%)	16 (6%)	2 (1%)	19 29
81	E1	33/71 (46%)	33 (100%)	0	0	100 100
All	All	11102/11524 (96%)	10416 (94%)	571 (5%)	115 (1%)	20 23

All (115) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	88	ASP
1	B	118	LYS
3	C0	85	HIS
16	S1	26	ARG
16	S1	50	LYS
16	S1	177	GLN
20	S7	12	ALA
20	S7	119	THR
21	S8	152	ILE
22	S9	93	LEU
25	C6	55	VAL
39	L4	269	SER
46	M1	55	ARG
46	M1	64	LYS
46	M1	66	ALA
74	Q0	81	SER
80	S4	26	CYS
1	B	97	LYS
3	C0	93	GLN
5	C5	130	ARG
18	S3	59	LEU
18	S3	217	ILE
20	S7	73	VAL
20	S7	74	GLN
22	S9	120	LYS
25	C6	27	GLY
27	C9	34	VAL
28	D1	42	GLU
31	D4	39	GLU
32	D6	13	LYS
32	D6	48	ALA
36	SR	267	PRO

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Mol	Chain	Res	Type
39	L4	305	ALA
40	L5	213	ASP
46	M1	167	TYR
48	M4	8	LYS
48	M4	9	ALA
52	M8	98	LYS
55	N1	124	VAL
56	N2	91	ASP
62	N8	76	ASP
62	N8	77	LYS
63	N9	53	ALA
68	O4	77	GLY
79	eI	114	LYS
1	B	95	LYS
6	C8	145	ARG
9	D8	45	LYS
25	C6	118	ILE
25	C6	142	TYR
32	D6	63	ALA
39	L4	270	SER
41	L6	98	VAL
44	L9	110	LYS
47	M3	136	GLU
48	M4	10	SER
53	M9	183	ALA
3	C0	84	GLU
8	D5	43	ASP
16	S1	94	LYS
17	S2	150	GLN
18	S3	63	GLY
19	S6	69	LEU
23	C1	141	LYS
25	C6	41	PRO
27	C9	87	GLY
30	D3	41	SER
35	E0	56	MET
46	M1	117	ASP
47	M3	165	SER
60	N6	126	LEU
61	N7	103	GLN
74	Q0	79	GLU
2	S5	100	ASN

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Mol	Chain	Res	Type
3	C0	83	PRO
8	D5	42	LEU
15	S0	103	THR
17	S2	235	LEU
18	S3	196	ARG
19	S6	135	PRO
21	S8	22	ARG
23	C1	6	THR
23	C1	22	ASN
26	C7	115	LEU
28	D1	45	ALA
35	E0	47	VAL
38	L3	317	ILE
40	L5	125	VAL
48	M4	6	ILE
54	N0	2	ALA
60	N6	84	LYS
63	N9	25	LYS
65	O1	83	GLU
69	O5	39	PRO
70	O6	3	VAL
77	Q3	51	ALA
78	SM	42	ALA
78	SM	53	ARG
1	B	87	VAL
17	S2	36	VAL
31	D4	5	VAL
39	L4	14	GLU
42	L7	178	ILE
46	M1	113	GLY
64	O0	103	THR
70	O6	21	THR
80	S4	95	THR
15	S0	194	PRO
32	D6	59	TYR
32	D6	60	PRO
34	D9	11	PRO
62	N8	15	VAL
15	S0	189	VAL
15	S0	206	ASP
79	eI	115	ALA

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	197/198 (100%)	193 (98%)	4 (2%)	55	74
2	S5	173/173 (100%)	172 (99%)	1 (1%)	86	94
3	C0	89/89 (100%)	88 (99%)	1 (1%)	73	87
4	C4	95/96 (99%)	94 (99%)	1 (1%)	73	87
5	C5	95/104 (91%)	95 (100%)	0	100	100
6	C8	128/128 (100%)	127 (99%)	1 (1%)	81	91
7	D0	100/100 (100%)	100 (100%)	0	100	100
8	D5	61/61 (100%)	61 (100%)	0	100	100
9	D8	55/56 (98%)	55 (100%)	0	100	100
10	P	14/14 (100%)	14 (100%)	0	100	100
15	S0	171/209 (82%)	168 (98%)	3 (2%)	59	76
16	S1	189/191 (99%)	186 (98%)	3 (2%)	62	79
17	S2	174/176 (99%)	172 (99%)	2 (1%)	73	87
18	S3	180/182 (99%)	172 (96%)	8 (4%)	28	45
19	S6	193/193 (100%)	188 (97%)	5 (3%)	46	66
20	S7	165/165 (100%)	162 (98%)	3 (2%)	59	76
21	S8	150/150 (100%)	148 (99%)	2 (1%)	69	84
22	S9	158/158 (100%)	156 (99%)	2 (1%)	69	84
23	C1	125/136 (92%)	120 (96%)	5 (4%)	31	49
24	C3	127/127 (100%)	124 (98%)	3 (2%)	49	68
25	C6	117/117 (100%)	113 (97%)	4 (3%)	37	56
26	C7	83/109 (76%)	80 (96%)	3 (4%)	35	54
27	C9	115/115 (100%)	109 (95%)	6 (5%)	23	38
28	D1	73/74 (99%)	72 (99%)	1 (1%)	67	82
29	D2	110/110 (100%)	109 (99%)	1 (1%)	78	90
30	D3	119/119 (100%)	114 (96%)	5 (4%)	30	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	D4	112/112 (100%)	109 (97%)	3 (3%)	44	65
32	D6	83/83 (100%)	82 (99%)	1 (1%)	71	85
33	D7	70/70 (100%)	70 (100%)	0	100	100
34	D9	43/47 (92%)	43 (100%)	0	100	100
35	E0	50/51 (98%)	49 (98%)	1 (2%)	55	74
36	SR	261/261 (100%)	260 (100%)	1 (0%)	91	96
37	L2	193/194 (100%)	190 (98%)	3 (2%)	62	79
38	L3	322/322 (100%)	307 (95%)	15 (5%)	26	42
39	L4	286/288 (99%)	280 (98%)	6 (2%)	53	72
40	L5	239/243 (98%)	232 (97%)	7 (3%)	42	62
41	L6	134/134 (100%)	131 (98%)	3 (2%)	52	71
42	L7	184/186 (99%)	182 (99%)	2 (1%)	73	87
43	L8	181/191 (95%)	177 (98%)	4 (2%)	52	71
44	L9	169/169 (100%)	165 (98%)	4 (2%)	49	68
45	M0	176/179 (98%)	171 (97%)	5 (3%)	43	63
46	M1	146/146 (100%)	143 (98%)	3 (2%)	53	72
47	M3	154/154 (100%)	151 (98%)	3 (2%)	57	75
48	M4	107/107 (100%)	103 (96%)	4 (4%)	34	53
49	M5	174/174 (100%)	170 (98%)	4 (2%)	50	70
50	M6	160/160 (100%)	155 (97%)	5 (3%)	40	60
51	M7	140/145 (97%)	137 (98%)	3 (2%)	53	72
52	M8	150/150 (100%)	147 (98%)	3 (2%)	55	74
53	M9	150/153 (98%)	144 (96%)	6 (4%)	31	49
54	N0	156/156 (100%)	152 (97%)	4 (3%)	46	66
55	N1	135/136 (99%)	132 (98%)	3 (2%)	52	71
56	N2	85/87 (98%)	85 (100%)	0	100	100
57	N3	104/104 (100%)	101 (97%)	3 (3%)	42	62
58	N4	54/86 (63%)	54 (100%)	0	100	100
59	N5	104/105 (99%)	99 (95%)	5 (5%)	25	41
60	N6	109/109 (100%)	105 (96%)	4 (4%)	34	53
61	N7	115/115 (100%)	111 (96%)	4 (4%)	36	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
62	N8	118/118 (100%)	116 (98%)	2 (2%)	60 78
63	N9	44/44 (100%)	44 (100%)	0	100 100
64	O0	81/81 (100%)	77 (95%)	4 (5%)	25 40
65	O1	93/96 (97%)	92 (99%)	1 (1%)	73 87
66	O2	108/109 (99%)	105 (97%)	3 (3%)	43 63
67	O3	90/90 (100%)	89 (99%)	1 (1%)	73 87
68	O4	94/94 (100%)	93 (99%)	1 (1%)	73 87
69	O5	104/104 (100%)	102 (98%)	2 (2%)	57 75
70	O6	79/81 (98%)	78 (99%)	1 (1%)	69 84
71	O7	70/70 (100%)	66 (94%)	4 (6%)	20 33
72	O8	68/68 (100%)	67 (98%)	1 (2%)	65 80
73	O9	45/45 (100%)	44 (98%)	1 (2%)	52 71
74	Q0	46/47 (98%)	46 (100%)	0	100 100
75	Q1	23/23 (100%)	23 (100%)	0	100 100
76	Q2	90/90 (100%)	85 (94%)	5 (6%)	21 34
77	Q3	71/71 (100%)	71 (100%)	0	100 100
78	SM	95/95 (100%)	94 (99%)	1 (1%)	73 87
79	eI	120/120 (100%)	118 (98%)	2 (2%)	60 78
80	S4	221/221 (100%)	217 (98%)	4 (2%)	59 76
81	E1	29/62 (47%)	29 (100%)	0	100 100
All	All	9491/9696 (98%)	9285 (98%)	206 (2%)	54 71

All (206) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	41	TYR
1	B	96	ASN
1	B	127	GLN
1	B	154	THR
2	S5	25	LEU
3	C0	86	ILE
4	C4	127	ARG
6	C8	75	ASN
15	S0	49	ASN
15	S0	59	LEU

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Mol	Chain	Res	Type
15	S0	124	THR
16	S1	55	LYS
16	S1	190	PRO
16	S1	214	LYS
17	S2	58	LEU
17	S2	166	THR
18	S3	14	ASP
18	S3	64	ARG
18	S3	65	ARG
18	S3	75	LYS
18	S3	168	ILE
18	S3	190	ARG
18	S3	208	ILE
18	S3	212	LYS
19	S6	78	THR
19	S6	135	PRO
19	S6	150	GLU
19	S6	156	PHE
19	S6	211	LEU
20	S7	83	LYS
20	S7	117	THR
20	S7	160	GLN
21	S8	25	ARG
21	S8	152	ILE
22	S9	2	PRO
22	S9	169	PRO
23	C1	67	ARG
23	C1	79	LYS
23	C1	94	ILE
23	C1	136	ARG
23	C1	138	ASN
24	C3	3	ARG
24	C3	58	HIS
24	C3	73	ARG
25	C6	38	LEU
25	C6	66	ARG
25	C6	113	ASP
25	C6	114	ARG
26	C7	11	ARG
26	C7	32	LYS
26	C7	67	ARG
27	C9	71	VAL

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Mol	Chain	Res	Type
27	C9	88	VAL
27	C9	100	ILE
27	C9	126	GLU
27	C9	132	LEU
27	C9	140	LEU
28	D1	32	VAL
29	D2	6	VAL
30	D3	9	LEU
30	D3	64	PRO
30	D3	100	ASP
30	D3	107	PHE
30	D3	131	SER
31	D4	57	VAL
31	D4	68	LYS
31	D4	125	LEU
32	D6	44	ILE
35	E0	28	LYS
36	SR	238	ASP
37	L2	7	ASN
37	L2	74	GLU
37	L2	122	ASP
38	L3	17	LEU
38	L3	56	ILE
38	L3	89	VAL
38	L3	114	VAL
38	L3	148	LEU
38	L3	156	SER
38	L3	167	ARG
38	L3	221	THR
38	L3	302	LYS
38	L3	305	ILE
38	L3	324	VAL
38	L3	332	ARG
38	L3	338	LEU
38	L3	361	THR
38	L3	364	LYS
39	L4	67	THR
39	L4	93	MET
39	L4	120	TYR
39	L4	138	ARG
39	L4	177	ASP
39	L4	179	LEU

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Mol	Chain	Res	Type
40	L5	64	ILE
40	L5	68	THR
40	L5	84	PRO
40	L5	95	TRP
40	L5	152	ARG
40	L5	194	LEU
40	L5	227	LEU
41	L6	65	ILE
41	L6	98	VAL
41	L6	143	LYS
42	L7	89	ILE
42	L7	229	PHE
43	L8	111	LYS
43	L8	160	ILE
43	L8	190	VAL
43	L8	219	ASP
44	L9	52	LEU
44	L9	92	TYR
44	L9	122	LYS
44	L9	177	ASP
45	M0	26	VAL
45	M0	87	LEU
45	M0	169	LYS
45	M0	174	THR
45	M0	208	ASN
46	M1	22	SER
46	M1	40	LEU
46	M1	155	THR
47	M3	46	ILE
47	M3	48	PRO
47	M3	93	ILE
48	M4	15	VAL
48	M4	63	VAL
48	M4	108	ARG
48	M4	127	LYS
49	M5	10	LEU
49	M5	80	THR
49	M5	109	ARG
49	M5	117	ASN
50	M6	84	LEU
50	M6	85	ARG
50	M6	124	LEU

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Mol	Chain	Res	Type
50	M6	126	VAL
50	M6	172	ARG
51	M7	49	GLU
51	M7	53	ASP
51	M7	54	HIS
52	M8	64	VAL
52	M8	81	VAL
52	M8	86	THR
53	M9	17	VAL
53	M9	22	VAL
53	M9	29	THR
53	M9	51	VAL
53	M9	52	LYS
53	M9	172	ARG
54	N0	96	ASP
54	N0	162	THR
54	N0	169	SER
54	N0	172	TYR
55	N1	26	HIS
55	N1	96	ILE
55	N1	97	LYS
57	N3	69	LEU
57	N3	88	ARG
57	N3	102	ILE
59	N5	36	LYS
59	N5	37	THR
59	N5	71	THR
59	N5	86	VAL
59	N5	125	ARG
60	N6	56	VAL
60	N6	59	VAL
60	N6	72	SER
60	N6	74	TYR
61	N7	14	VAL
61	N7	87	LEU
61	N7	95	VAL
61	N7	100	THR
62	N8	60	TYR
62	N8	78	LEU
64	O0	34	LEU
64	O0	87	VAL
64	O0	100	ILE

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Mol	Chain	Res	Type
64	O0	101	LEU
65	O1	71	LEU
66	O2	4	LEU
66	O2	76	VAL
66	O2	106	VAL
67	O3	31	LYS
68	O4	65	VAL
69	O5	47	VAL
69	O5	115	LYS
70	O6	76	ARG
71	O7	7	SER
71	O7	25	ARG
71	O7	40	PRO
71	O7	68	LYS
72	O8	41	THR
73	O9	29	LEU
76	Q2	2	VAL
76	Q2	4	VAL
76	Q2	85	LEU
76	Q2	97	LYS
76	Q2	105	GLN
78	SM	58	GLU
79	eI	138	ILE
79	eI	142	MET
80	S4	104	ASP
80	S4	151	ASP
80	S4	182	TYR
80	S4	259	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	12	HIS
1	B	140	HIS
1	B	200	ASN
2	S5	35	GLN
2	S5	104	ASN
3	C0	96	ASN
15	S0	92	HIS
16	S1	92	GLN
19	S6	201	GLN
20	S7	74	GLN

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Mol	Chain	Res	Type
22	S9	38	ASN
26	C7	48	ASN
26	C7	101	ASN
27	C9	64	HIS
27	C9	129	GLN
28	D1	75	ASN
30	D3	79	ASN
32	D6	8	ASN
36	SR	187	GLN
37	L2	7	ASN
37	L2	205	ASN
38	L3	371	GLN
39	L4	5	GLN
39	L4	87	GLN
39	L4	307	GLN
40	L5	32	GLN
40	L5	40	HIS
40	L5	206	GLN
41	L6	157	GLN
41	L6	167	ASN
44	L9	157	ASN
44	L9	163	GLN
46	M1	6	GLN
46	M1	39	GLN
46	M1	95	ASN
47	M3	19	GLN
47	M3	120	GLN
49	M5	15	GLN
49	M5	87	GLN
49	M5	95	GLN
49	M5	194	GLN
49	M5	195	ASN
50	M6	31	GLN
50	M6	90	HIS
53	M9	130	ASN
54	N0	138	GLN
57	N3	98	ASN
60	N6	42	GLN
60	N6	100	HIS
61	N7	57	HIS
62	N8	39	HIS
63	N9	19	ASN

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Mol	Chain	Res	Type
71	O7	79	GLN
77	Q3	34	HIS
78	SM	86	ASN
80	S4	130	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	3	120/121 (99%)	10 (8%)	2 (1%)
12	4	157/158 (99%)	21 (13%)	2 (1%)
13	1	3139/3162 (99%)	495 (15%)	93 (2%)
14	2	1735/1737 (99%)	467 (26%)	90 (5%)
All	All	5151/5178 (99%)	993 (19%)	187 (3%)

All (993) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	3	22	A
11	3	41	G
11	3	42	A
11	3	54	U
11	3	65	G
11	3	76	A
11	3	91	G
11	3	102	A
11	3	112	G
11	3	121	U
12	4	23	U
12	4	34	U
12	4	35	C
12	4	51	G
12	4	52	A
12	4	59	A
12	4	62	C
12	4	63	G
12	4	82	U
12	4	83	C
12	4	84	C
12	4	86	U
12	4	87	G
12	4	95	G

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Mol	Chain	Res	Type
12	4	105	A
12	4	106	C
12	4	111	A
12	4	113	U
12	4	125	U
12	4	152	G
12	4	158	U
13	1	14	U
13	1	16	A
13	1	26	A
13	1	40	A
13	1	43	A
13	1	44	U
13	1	49	A
13	1	60	A
13	1	65	A
13	1	66	A
13	1	92	G
13	1	99	A
13	1	105	C
13	1	110	G
13	1	122	A
13	1	124	U
13	1	135	C
13	1	136	G
13	1	156	G
13	1	157	A
13	1	166	C
13	1	173	G
13	1	179	C
13	1	187	A
13	1	190	U
13	1	191	U
13	1	210	U
13	1	213	A
13	1	218	G
13	1	219	A
13	1	220	G
13	1	237	G
13	1	240	U
13	1	241	G
13	1	243	G

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Mol	Chain	Res	Type
13	1	246	U
13	1	249	U
13	1	250	U
13	1	251	G
13	1	252	U
13	1	253	A
13	1	269	G
13	1	286	U
13	1	295	A
13	1	305	U
13	1	323	A
13	1	329	U
13	1	376	G
13	1	397	A
13	1	398	A
13	1	399	A
13	1	403	C
13	1	421	G
13	1	422	A
13	1	520	U
13	1	521	A
13	1	544	C
13	1	545	U
13	1	546	C
13	1	547	G
13	1	549	U
13	1	550	A
13	1	552	G
13	1	555	U
13	1	556	U
13	1	557	A
13	1	558	U
13	1	559	A
13	1	569	A
13	1	578	A
13	1	579	G
13	1	588	G
13	1	589	A
13	1	592	A
13	1	604	G
13	1	608	A
13	1	609	G

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Mol	Chain	Res	Type
13	1	611	A
13	1	612	U
13	1	620	U
13	1	621	A
13	1	636	C
13	1	649	A
13	1	660	A
13	1	677	A
13	1	681	U
13	1	689	U
13	1	691	A
13	1	705	A
13	1	715	A
13	1	736	A
13	1	737	G
13	1	758	C
13	1	760	G
13	1	765	C
13	1	766	U
13	1	767	U
13	1	776	U
13	1	777	U
13	1	781	G
13	1	785	G
13	1	786	A
13	1	806	A
13	1	816	A
13	1	817	A
13	1	830	A
13	1	837	A
13	1	861	C
13	1	874	U
13	1	879	U
13	1	907	G
13	1	908	G
13	1	914	A
13	1	916	G
13	1	917	A
13	1	923	C
13	1	924	G
13	1	925	A
13	1	937	G

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Mol	Chain	Res	Type
13	1	944	C
13	1	959	C
13	1	960	U
13	1	980	A
13	1	981	U
13	1	993	G
13	1	994	G
13	1	995	U
13	1	1000	C
13	1	1001	G
13	1	1002	A
13	1	1010	G
13	1	1017	C
13	1	1018	G
13	1	1019	G
13	1	1021	G
13	1	1022	U
13	1	1024	G
13	1	1025	A
13	1	1026	A
13	1	1029	G
13	1	1032	C
13	1	1047	A
13	1	1049	C
13	1	1064	A
13	1	1081	U
13	1	1082	U
13	1	1083	G
13	1	1094	U
13	1	1095	U
13	1	1096	U
13	1	1097	G
13	1	1098	A
13	1	1103	A
13	1	1104	G
13	1	1117	G
13	1	1131	G
13	1	1153	A
13	1	1159	A
13	1	1160	C
13	1	1161	G
13	1	1180	A

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Mol	Chain	Res	Type
13	1	1181	U
13	1	1182	A
13	1	1192	C
13	1	1193	A
13	1	1201	C
13	1	1208	U
13	1	1209	G
13	1	1212	A
13	1	1217	A
13	1	1218	U
13	1	1222	G
13	1	1225	A
13	1	1227	C
13	1	1229	G
13	1	1232	C
13	1	1234	G
13	1	1235	U
13	1	1236	G
13	1	1237	G
13	1	1238	C
13	1	1241	U
13	1	1243	G
13	1	1245	A
13	1	1246	G
13	1	1247	U
13	1	1248	C
13	1	1249	G
13	1	1250	G
13	1	1251	A
13	1	1253	U
13	1	1254	C
13	1	1257	C
13	1	1258	U
13	1	1260	A
13	1	1262	G
13	1	1264	G
13	1	1265	U
13	1	1266	G
13	1	1267	U
13	1	1268	G
13	1	1269	U
13	1	1270	A

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Mol	Chain	Res	Type
13	1	1272	C
13	1	1273	A
13	1	1274	A
13	1	1275	C
13	1	1277	C
13	1	1278	A
13	1	1279	C
13	1	1281	G
13	1	1285	G
13	1	1287	A
13	1	1292	C
13	1	1295	G
13	1	1307	G
13	1	1308	A
13	1	1309	U
13	1	1313	G
13	1	1329	U
13	1	1330	A
13	1	1348	U
13	1	1349	G
13	1	1350	A
13	1	1351	U
13	1	1352	A
13	1	1353	U
13	1	1355	A
13	1	1356	U
13	1	1357	G
13	1	1386	A
13	1	1399	A
13	1	1400	G
13	1	1418	A
13	1	1419	A
13	1	1421	G
13	1	1434	G
13	1	1437	C
13	1	1446	A
13	1	1450	G
13	1	1481	A
13	1	1482	A
13	1	1483	G
13	1	1508	C
13	1	1527	C

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Mol	Chain	Res	Type
13	1	1533	U
13	1	1539	A
13	1	1555	U
13	1	1557	A
13	1	1560	G
13	1	1562	C
13	1	1563	C
13	1	1566	A
13	1	1567	U
13	1	1568	U
13	1	1569	U
13	1	1571	A
13	1	1572	U
13	1	1574	C
13	1	1575	A
13	1	1576	G
13	1	1577	G
13	1	1581	C
13	1	1582	C
13	1	1587	A
13	1	1589	A
13	1	1593	A
13	1	1621	A
13	1	1622	U
13	1	1629	U
13	1	1633	C
13	1	1639	C
13	1	1642	A
13	1	1643	A
13	1	1644	C
13	1	1657	C
13	1	1683	A
13	1	1716	U
13	1	1717	U
13	1	1724	U
13	1	1725	C
13	1	1750	A
13	1	1751	G
13	1	1762	C
13	1	1763	U
13	1	1764	U
13	1	1765	U

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Mol	Chain	Res	Type
13	1	1780	G
13	1	1797	A
13	1	1815	U
13	1	1816	A
13	1	1817	G
13	1	1821	U
13	1	1841	A
13	1	1842	A
13	1	1866	C
13	1	1867	A
13	1	1879	A
13	1	1880	U
13	1	1886	A
13	1	1893	A
13	1	1906	G
13	1	1951	C
13	1	2101	C
13	1	2111	G
13	1	2112	U
13	1	2113	A
13	1	2121	G
13	1	2122	G
13	1	2131	A
13	1	2140	U
13	1	2158	A
13	1	2169	G
13	1	2192	C
13	1	2205	U
13	1	2206	G
13	1	2209	U
13	1	2210	G
13	1	2225	U
13	1	2239	G
13	1	2244	A
13	1	2249	G
13	1	2256	A
13	1	2258	U
13	1	2273	G
13	1	2279	A
13	1	2281	A
13	1	2307	G
13	1	2308	C

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Mol	Chain	Res	Type
13	1	2310	U
13	1	2313	A
13	1	2314	U
13	1	2315	G
13	1	2334	U
13	1	2335	G
13	1	2336	U
13	1	2374	C
13	1	2375	G
13	1	2385	G
13	1	2388	U
13	1	2393	G
13	1	2394	G
13	1	2397	A
13	1	2402	A
13	1	2403	G
13	1	2411	U
13	1	2418	G
13	1	2419	A
13	1	2435	G
13	1	2437	G
13	1	2440	G
13	1	2445	A
13	1	2500	A
13	1	2501	U
13	1	2502	A
13	1	2511	A
13	1	2514	U
13	1	2515	A
13	1	2533	G
13	1	2537	U
13	1	2538	U
13	1	2539	C
13	1	2540	A
13	1	2541	U
13	1	2542	U
13	1	2543	U
13	1	2544	U
13	1	2551	U
13	1	2552	C
13	1	2554	A
13	1	2560	C

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Mol	Chain	Res	Type
13	1	2561	A
13	1	2568	C
13	1	2570	U
13	1	2571	U
13	1	2572	C
13	1	2573	G
13	1	2585	G
13	1	2593	A
13	1	2594	C
13	1	2603	G
13	1	2606	G
13	1	2607	G
13	1	2614	G
13	1	2628	A
13	1	2652	U
13	1	2656	A
13	1	2658	G
13	1	2674	A
13	1	2677	G
13	1	2678	A
13	1	2681	U
13	1	2689	A
13	1	2691	A
13	1	2694	A
13	1	2714	G
13	1	2719	U
13	1	2728	G
13	1	2729	U
13	1	2747	A
13	1	2752	U
13	1	2753	G
13	1	2762	A
13	1	2777	G
13	1	2778	G
13	1	2796	G
13	1	2799	A
13	1	2800	G
13	1	2801	A
13	1	2803	A
13	1	2810	C
13	1	2817	A
13	1	2834	G

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Mol	Chain	Res	Type
13	1	2842	U
13	1	2843	U
13	1	2845	A
13	1	2871	G
13	1	2872	A
13	1	2875	U
13	1	2887	A
13	1	2899	C
13	1	2923	U
13	1	2935	U
13	1	2936	A
13	1	2942	C
13	1	2945	G
13	1	2947	G
13	1	2954	U
13	1	2971	A
13	1	2990	G
13	1	2996	U
13	1	2997	G
13	1	3012	A
13	1	3027	A
13	1	3057	U
13	1	3058	U
13	1	3059	G
13	1	3078	U
13	1	3080	G
13	1	3092	C
13	1	3113	A
13	1	3117	C
13	1	3130	A
13	1	3131	U
13	1	3142	A
13	1	3143	C
13	1	3153	U
13	1	3154	C
13	1	3155	U
13	1	3156	U
13	1	3157	U
13	1	3173	G
13	1	3174	A
13	1	3176	G
13	1	3179	U

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Mol	Chain	Res	Type
13	1	3181	C
13	1	3187	A
13	1	3195	U
13	1	3196	U
13	1	3197	G
13	1	3207	U
13	1	3217	C
13	1	3218	A
13	1	3219	G
13	1	3228	C
13	1	3229	G
13	1	3243	A
13	1	3245	A
13	1	3246	G
13	1	3247	G
13	1	3256	G
13	1	3259	U
13	1	3263	G
13	1	3269	U
13	1	3270	U
13	1	3273	A
13	1	3276	G
13	1	3290	G
13	1	3294	A
13	1	3304	U
13	1	3316	A
13	1	3317	U
13	1	3319	U
13	1	3342	A
13	1	3345	G
13	1	3351	U
13	1	3352	U
13	1	3354	U
13	1	3355	U
13	1	3362	A
13	1	3369	G
13	1	3378	C
13	1	3386	G
13	1	3390	G
13	1	3396	U
14	2	2	A
14	2	4	C

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Mol	Chain	Res	Type
14	2	17	C
14	2	25	C
14	2	26	A
14	2	27	U
14	2	34	G
14	2	42	G
14	2	47	A
14	2	57	G
14	2	60	U
14	2	62	A
14	2	63	G
14	2	68	A
14	2	69	G
14	2	70	C
14	2	71	A
14	2	72	A
14	2	73	U
14	2	74	U
14	2	75	U
14	2	76	A
14	2	77	U
14	2	78	A
14	2	83	G
14	2	84	A
14	2	94	U
14	2	96	G
14	2	104	A
14	2	114	C
14	2	116	U
14	2	127	G
14	2	129	U
14	2	130	C
14	2	131	C
14	2	132	U
14	2	133	U
14	2	134	U
14	2	135	A
14	2	136	C
14	2	137	U
14	2	138	A
14	2	140	A
14	2	141	U

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Mol	Chain	Res	Type
14	2	144	U
14	2	145	A
14	2	146	U
14	2	153	G
14	2	156	A
14	2	158	U
14	2	159	U
14	2	166	C
14	2	176	C
14	2	177	U
14	2	178	U
14	2	179	A
14	2	185	U
14	2	186	C
14	2	187	G
14	2	188	A
14	2	189	C
14	2	191	C
14	2	192	U
14	2	194	U
14	2	195	G
14	2	197	A
14	2	199	G
14	2	200	A
14	2	215	A
14	2	217	A
14	2	218	A
14	2	219	A
14	2	221	A
14	2	222	A
14	2	223	U
14	2	224	C
14	2	225	A
14	2	226	A
14	2	227	U
14	2	228	G
14	2	230	C
14	2	231	U
14	2	232	U
14	2	235	G
14	2	237	C
14	2	238	U

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Mol	Chain	Res	Type
14	2	240	U
14	2	241	U
14	2	250	C
14	2	260	U
14	2	261	U
14	2	265	A
14	2	266	A
14	2	272	U
14	2	275	C
14	2	277	U
14	2	278	U
14	2	279	G
14	2	280	U
14	2	281	G
14	2	288	A
14	2	299	A
14	2	314	C
14	2	316	A
14	2	322	G
14	2	333	A
14	2	336	G
14	2	337	G
14	2	338	C
14	2	352	A
14	2	359	A
14	2	360	A
14	2	361	C
14	2	362	G
14	2	369	A
14	2	370	A
14	2	400	A
14	2	401	A
14	2	402	C
14	2	404	G
14	2	416	A
14	2	417	A
14	2	418	G
14	2	424	C
14	2	425	A
14	2	426	G
14	2	434	G
14	2	439	U

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Mol	Chain	Res	Type
14	2	444	C
14	2	445	A
14	2	448	C
14	2	455	C
14	2	460	A
14	2	464	A
14	2	468	A
14	2	469	C
14	2	475	A
14	2	477	A
14	2	480	G
14	2	482	U
14	2	483	A
14	2	486	G
14	2	487	G
14	2	488	G
14	2	491	C
14	2	492	A
14	2	493	U
14	2	495	C
14	2	496	G
14	2	498	G
14	2	500	C
14	2	501	U
14	2	502	U
14	2	506	A
14	2	507	U
14	2	510	G
14	2	511	A
14	2	514	G
14	2	515	A
14	2	519	C
14	2	534	A
14	2	538	A
14	2	539	G
14	2	541	A
14	2	542	A
14	2	543	C
14	2	544	A
14	2	548	G
14	2	555	A
14	2	556	A

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Mol	Chain	Res	Type
14	2	558	U
14	2	559	C
14	2	560	U
14	2	565	C
14	2	575	C
14	2	579	A
14	2	580	A
14	2	583	C
14	2	594	A
14	2	595	G
14	2	606	A
14	2	619	A
14	2	620	A
14	2	622	A
14	2	623	A
14	2	624	G
14	2	639	U
14	2	644	C
14	2	652	G
14	2	653	C
14	2	654	C
14	2	655	G
14	2	656	G
14	2	657	U
14	2	658	C
14	2	678	A
14	2	679	U
14	2	684	A
14	2	694	U
14	2	695	U
14	2	696	C
14	2	697	C
14	2	698	U
14	2	700	C
14	2	701	U
14	2	703	G
14	2	704	C
14	2	705	U
14	2	709	C
14	2	710	U
14	2	711	U
14	2	712	G

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Mol	Chain	Res	Type
14	2	713	A
14	2	714	G
14	2	715	U
14	2	718	U
14	2	719	U
14	2	720	G
14	2	721	U
14	2	722	G
14	2	723	G
14	2	724	C
14	2	725	U
14	2	727	U
14	2	728	U
14	2	729	G
14	2	730	G
14	2	731	C
14	2	733	A
14	2	734	A
14	2	735	C
14	2	737	A
14	2	738	G
14	2	739	G
14	2	741	C
14	2	742	U
14	2	743	U
14	2	755	A
14	2	756	A
14	2	765	G
14	2	766	U
14	2	774	A
14	2	778	G
14	2	780	A
14	2	781	U
14	2	782	U
14	2	783	G
14	2	784	C
14	2	787	G
14	2	788	A
14	2	789	A
14	2	794	U
14	2	795	U
14	2	807	A

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Mol	Chain	Res	Type
14	2	811	A
14	2	812	A
14	2	819	G
14	2	820	U
14	2	821	U
14	2	823	G
14	2	830	U
14	2	832	U
14	2	833	U
14	2	834	G
14	2	836	U
14	2	840	U
14	2	843	U
14	2	844	A
14	2	846	G
14	2	847	A
14	2	852	C
14	2	856	A
14	2	863	A
14	2	864	U
14	2	876	G
14	2	884	A
14	2	894	U
14	2	895	G
14	2	897	C
14	2	898	A
14	2	914	G
14	2	919	A
14	2	922	G
14	2	926	A
14	2	928	U
14	2	931	C
14	2	933	A
14	2	935	U
14	2	945	U
14	2	951	A
14	2	960	U
14	2	966	A
14	2	976	G
14	2	990	C
14	2	992	A
14	2	1007	C

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Mol	Chain	Res	Type
14	2	1012	U
14	2	1013	A
14	2	1016	C
14	2	1020	A
14	2	1021	C
14	2	1026	A
14	2	1028	C
14	2	1031	U
14	2	1032	G
14	2	1039	A
14	2	1051	C
14	2	1052	U
14	2	1054	G
14	2	1063	A
14	2	1069	C
14	2	1078	A
14	2	1079	A
14	2	1080	A
14	2	1083	C
14	2	1096	G
14	2	1125	A
14	2	1130	A
14	2	1135	C
14	2	1137	G
14	2	1138	A
14	2	1140	G
14	2	1141	G
14	2	1142	G
14	2	1145	C
14	2	1147	A
14	2	1154	G
14	2	1157	G
14	2	1165	G
14	2	1172	U
14	2	1181	A
14	2	1183	A
14	2	1184	C
14	2	1186	G
14	2	1187	G
14	2	1189	A
14	2	1203	C
14	2	1204	A

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Mol	Chain	Res	Type
14	2	1205	G
14	2	1214	A
14	2	1215	G
14	2	1216	G
14	2	1217	A
14	2	1218	U
14	2	1224	G
14	2	1228	G
14	2	1229	A
14	2	1231	A
14	2	1232	G
14	2	1233	C
14	2	1234	U
14	2	1238	U
14	2	1242	G
14	2	1244	U
14	2	1245	U
14	2	1250	G
14	2	1257	G
14	2	1262	A
14	2	1273	U
14	2	1284	G
14	2	1288	U
14	2	1301	U
14	2	1302	U
14	2	1308	A
14	2	1327	U
14	2	1328	A
14	2	1331	A
14	2	1332	A
14	2	1335	A
14	2	1339	G
14	2	1340	U
14	2	1341	G
14	2	1348	U
14	2	1349	U
14	2	1352	C
14	2	1357	U
14	2	1358	A
14	2	1360	C
14	2	1370	G
14	2	1375	A

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Mol	Chain	Res	Type
14	2	1377	U
14	2	1378	A
14	2	1383	U
14	2	1384	U
14	2	1385	U
14	2	1386	C
14	2	1387	A
14	2	1389	G
14	2	1400	U
14	2	1401	U
14	2	1402	U
14	2	1411	A
14	2	1412	A
14	2	1414	A
14	2	1415	G
14	2	1418	C
14	2	1419	U
14	2	1423	A
14	2	1433	A
14	2	1434	C
14	2	1444	C
14	2	1445	G
14	2	1446	C
14	2	1447	A
14	2	1448	C
14	2	1450	C
14	2	1458	A
14	2	1461	G
14	2	1465	G
14	2	1473	G
14	2	1478	U
14	2	1479	A
14	2	1480	A
14	2	1483	U
14	2	1492	A
14	2	1503	A
14	2	1504	U
14	2	1505	C
14	2	1508	G
14	2	1509	U
14	2	1510	G
14	2	1511	A

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Mol	Chain	Res	Type
14	2	1522	U
14	2	1523	G
14	2	1524	C
14	2	1525	U
14	2	1526	G
14	2	1537	A
14	2	1543	A
14	2	1544	U
14	2	1546	A
14	2	1555	C
14	2	1556	A
14	2	1560	A
14	2	1561	G
14	2	1569	U
14	2	1570	A
14	2	1571	G
14	2	1577	G
14	2	1578	C
14	2	1584	A
14	2	1588	G
14	2	1594	G
14	2	1600	U
14	2	1601	A
14	2	1602	C
14	2	1603	G
14	2	1620	A
14	2	1621	C
14	2	1644	U
14	2	1645	G
14	2	1667	G
14	2	1668	A
14	2	1672	G
14	2	1705	G
14	2	1718	A
14	2	1723	G
14	2	1747	G
14	2	1749	A
14	2	1753	A
14	2	1769	A
14	2	1770	C
14	2	1779	G
14	2	1780	G

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Mol	Chain	Res	Type
14	2	1781	A
14	2	1782	U
14	2	1783	C

All (187) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	3	41	G
11	3	111	U
12	4	111	A
12	4	128	U
13	1	43	A
13	1	210	U
13	1	217	U
13	1	397	A
13	1	398	A
13	1	420	G
13	1	535	G
13	1	544	C
13	1	549	U
13	1	555	U
13	1	557	A
13	1	558	U
13	1	588	G
13	1	594	U
13	1	647	A
13	1	806	A
13	1	816	A
13	1	873	C
13	1	896	A
13	1	908	G
13	1	916	G
13	1	993	G
13	1	1000	C
13	1	1097	G
13	1	1154	A
13	1	1160	C
13	1	1181	U
13	1	1196	C
13	1	1208	U
13	1	1234	G
13	1	1244	A

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Mol	Chain	Res	Type
13	1	1274	A
13	1	1285	G
13	1	1317	A
13	1	1329	U
13	1	1331	U
13	1	1348	U
13	1	1352	A
13	1	1355	A
13	1	1475	A
13	1	1482	A
13	1	1556	C
13	1	1568	U
13	1	1630	U
13	1	1643	A
13	1	1716	U
13	1	1741	A
13	1	1763	U
13	1	1815	U
13	1	1820	U
13	1	1841	A
13	1	1842	A
13	1	1878	G
13	1	1879	A
13	1	2112	U
13	1	2209	U
13	1	2261	G
13	1	2281	A
13	1	2372	A
13	1	2373	A
13	1	2374	C
13	1	2418	G
13	1	2501	U
13	1	2522	G
13	1	2538	U
13	1	2542	U
13	1	2585	G
13	1	2593	A
13	1	2627	C
13	1	2656	A
13	1	2677	G
13	1	2689	A
13	1	2728	G

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Mol	Chain	Res	Type
13	1	2801	A
13	1	2817	A
13	1	2898	G
13	1	3056	U
13	1	3057	U
13	1	3196	U
13	1	3217	C
13	1	3218	A
13	1	3228	C
13	1	3242	G
13	1	3246	G
13	1	3259	U
13	1	3267	A
13	1	3269	U
13	1	3303	G
13	1	3350	C
13	1	3351	U
13	1	3353	G
13	1	3389	U
13	1	3395	G
14	2	1	U
14	2	68	A
14	2	72	A
14	2	73	U
14	2	74	U
14	2	103	A
14	2	114	C
14	2	128	U
14	2	131	C
14	2	139	C
14	2	158	U
14	2	159	U
14	2	177	U
14	2	192	U
14	2	218	A
14	2	226	A
14	2	227	U
14	2	249	U
14	2	260	U
14	2	265	A
14	2	276	C
14	2	277	U

Continued on next page...

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Mol	Chain	Res	Type
14	2	280	U
14	2	287	G
14	2	322	G
14	2	359	A
14	2	380	U
14	2	400	A
14	2	417	A
14	2	454	U
14	2	468	A
14	2	492	A
14	2	497	G
14	2	501	U
14	2	538	A
14	2	540	G
14	2	543	C
14	2	555	A
14	2	652	G
14	2	656	G
14	2	700	C
14	2	710	U
14	2	721	U
14	2	727	U
14	2	742	U
14	2	765	G
14	2	794	U
14	2	811	A
14	2	812	A
14	2	819	G
14	2	832	U
14	2	855	A
14	2	933	A
14	2	959	U
14	2	1031	U
14	2	1053	U
14	2	1068	A
14	2	1087	G
14	2	1095	G
14	2	1137	G
14	2	1183	A
14	2	1203	C
14	2	1205	G
14	2	1232	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	2	1237	U
14	2	1271	C
14	2	1272	U
14	2	1284	G
14	2	1326	C
14	2	1331	A
14	2	1357	U
14	2	1401	U
14	2	1414	A
14	2	1418	C
14	2	1444	C
14	2	1504	U
14	2	1521	G
14	2	1523	G
14	2	1524	C
14	2	1543	A
14	2	1555	C
14	2	1559	G
14	2	1560	A
14	2	1569	U
14	2	1587	A
14	2	1602	C
14	2	1644	U
14	2	1667	G
14	2	1748	U
14	2	1775	G

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
79	5CT	eI	51	79	13,14,15	0.45	0	9,15,17	1.09	1 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
79	5CT	eI	51	79	-	6/13/14/16	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
79	eI	51	5CT	C4-C3-C2	2.76	119.29	113.47

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
79	eI	51	5CT	C1-C2-C3-C4
79	eI	51	5CT	O1-C2-C3-C4
79	eI	51	5CT	C2-C1-NZ-CE
79	eI	51	5CT	C2-C3-C4-N1
79	eI	51	5CT	NZ-C1-C2-O1
79	eI	51	5CT	CE-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 303 ligands modelled in this entry, 299 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
85	SPD	1	3467	-	9,9,9	0.24	0	8,8,8	0.32	0
85	SPD	1	3466	-	9,9,9	0.48	0	8,8,8	0.88	0
85	SPD	1	3465	-	9,9,9	0.26	0	8,8,8	0.34	0
84	3HE	1	3464	-	21,21,21	0.72	0	19,30,30	0.82	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	SPD	1	3467	-	-	1/7/7/7	-
85	SPD	1	3466	-	-	3/7/7/7	-
85	SPD	1	3465	-	-	0/7/7/7	-
84	3HE	1	3464	-	-	0/8/36/36	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
85	1	3466	SPD	N6-C7-C8-C9
85	1	3466	SPD	C3-C4-C5-N6
85	1	3466	SPD	C8-C7-N6-C5
85	1	3467	SPD	C7-C8-C9-N10

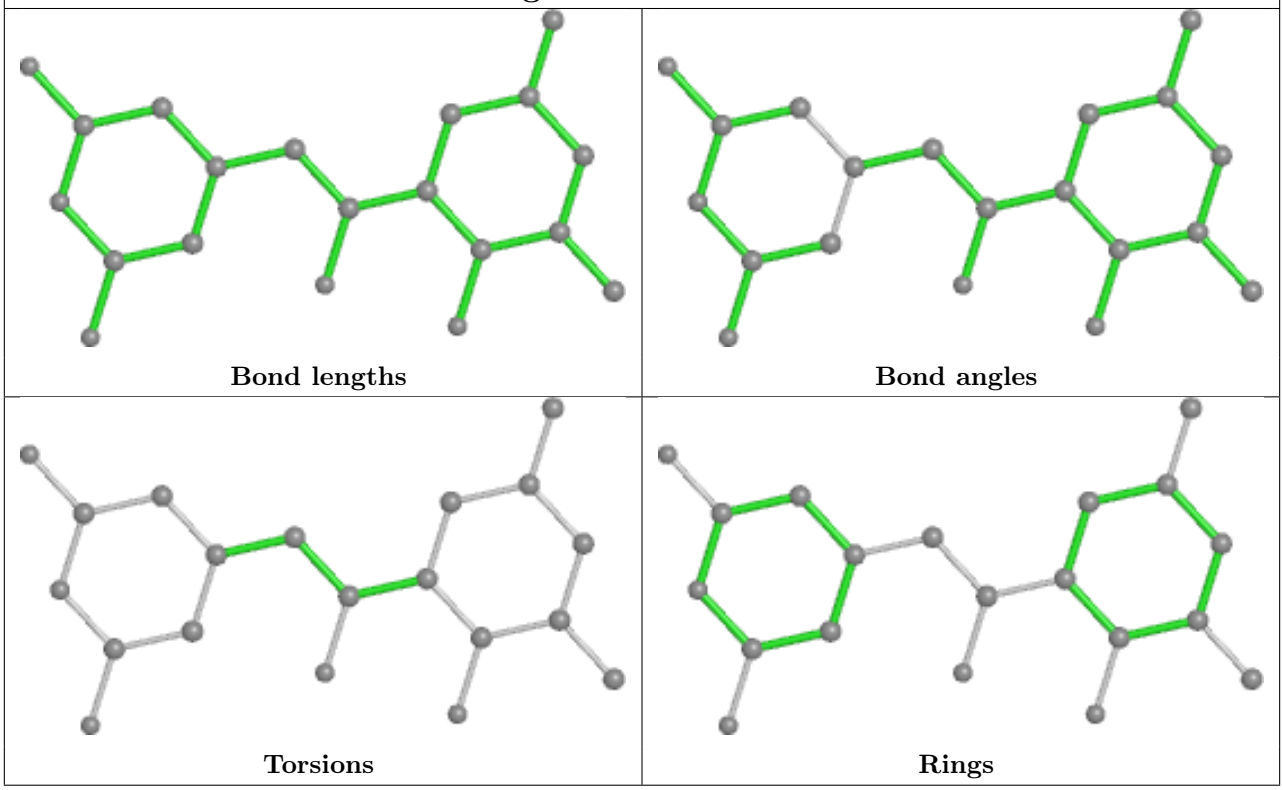
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 3HE 1 3464



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
14	2	2
21	S8	1
41	L6	1
40	L5	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S8	123:LYS	C	135:LYS	N	22.02
1	L6	109:GLU	C	129:GLU	N	15.02
1	L5	2:ASP	C	7:ALA	N	7.28
1	2	658:C	O3'	676:G	P	4.28
1	2	1672:G	O3'	1704:G	P	3.36

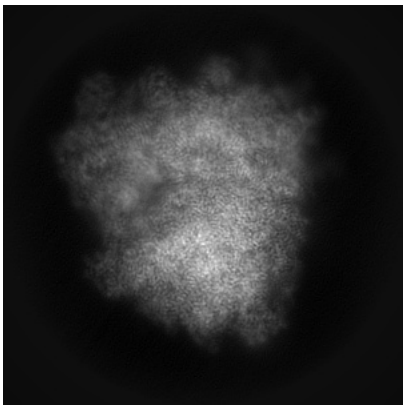
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16127. These allow visual inspection of the internal detail of the map and identification of artifacts.

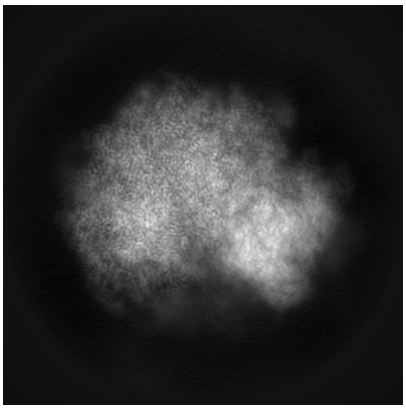
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

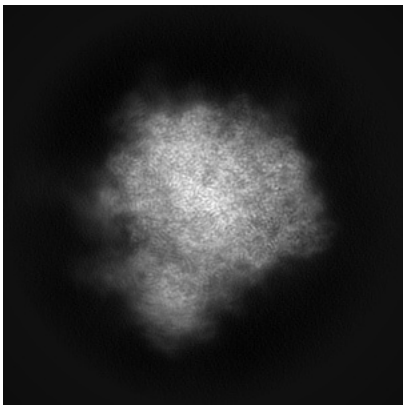
6.1.1 Primary map



X

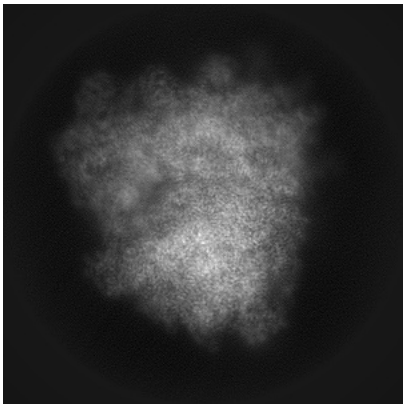


Y

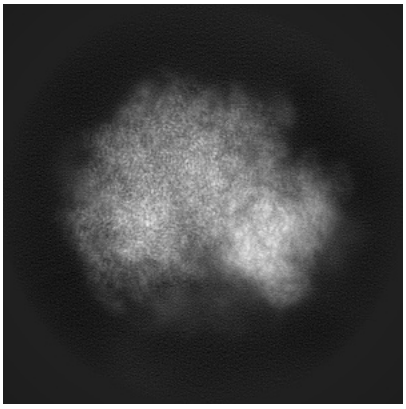


Z

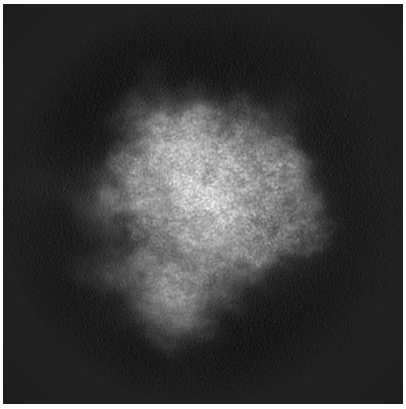
6.1.2 Raw map



X



Y

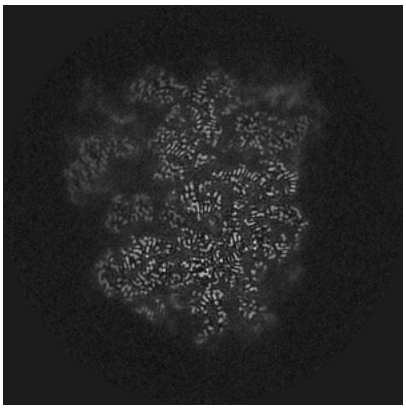


Z

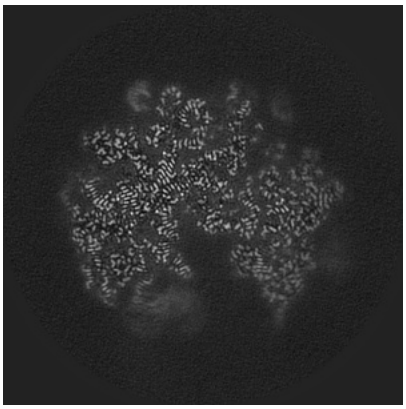
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

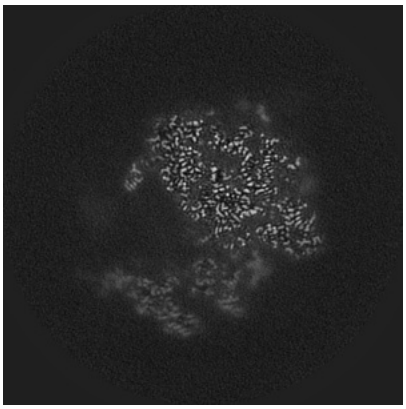
6.2.1 Primary map



X Index: 240

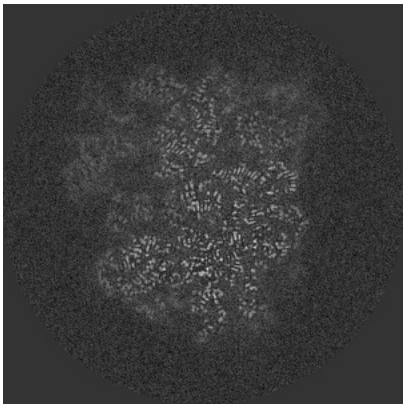


Y Index: 240

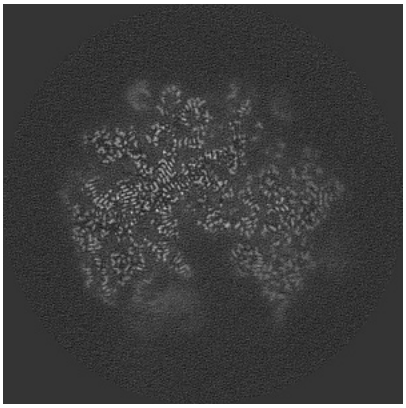


Z Index: 240

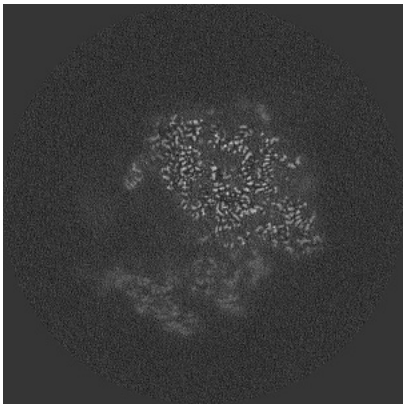
6.2.2 Raw map



X Index: 240



Y Index: 240

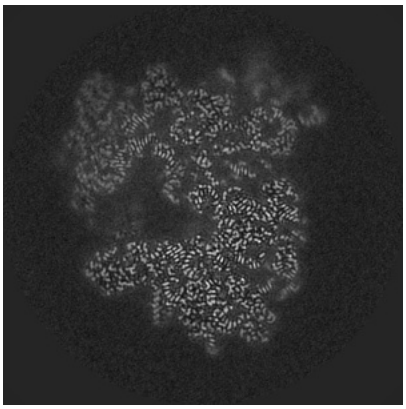


Z Index: 240

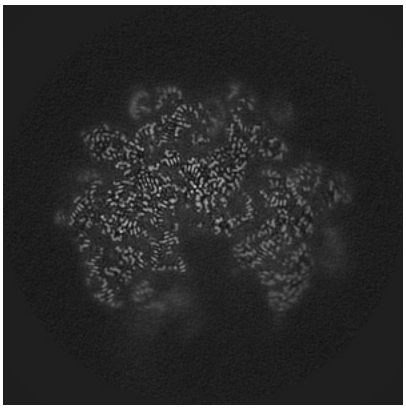
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

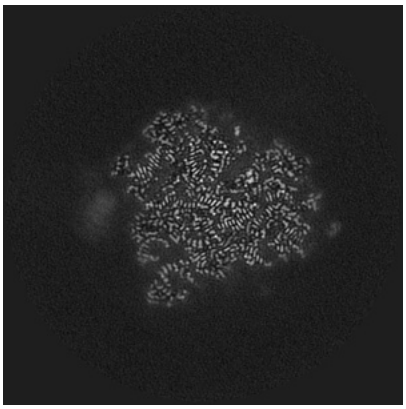
6.3.1 Primary map



X Index: 222

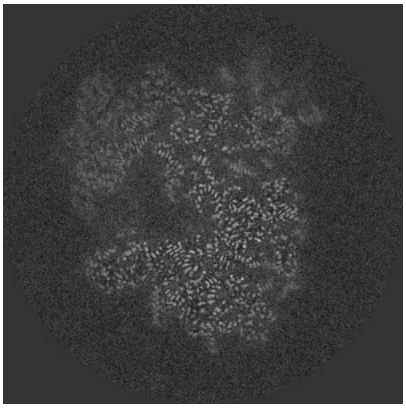


Y Index: 247

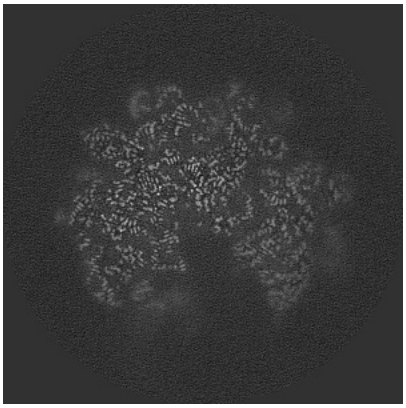


Z Index: 193

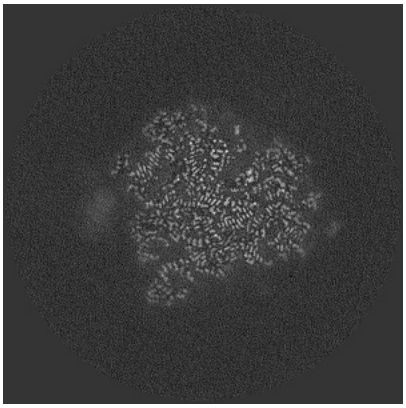
6.3.2 Raw map



X Index: 221



Y Index: 247

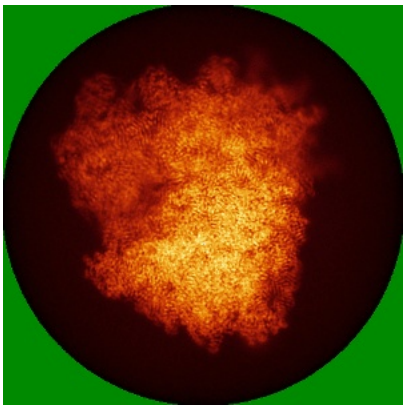


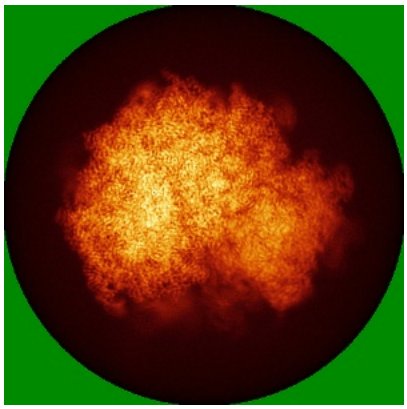
Z Index: 193

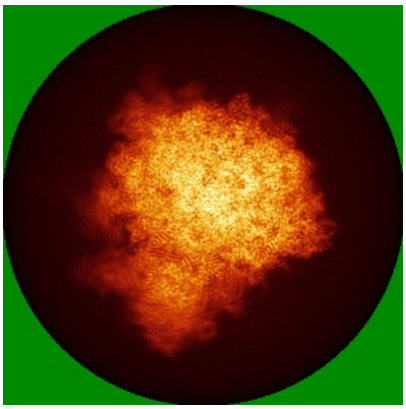
The images above show the largest variance slices of the map in three orthogonal directions.

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

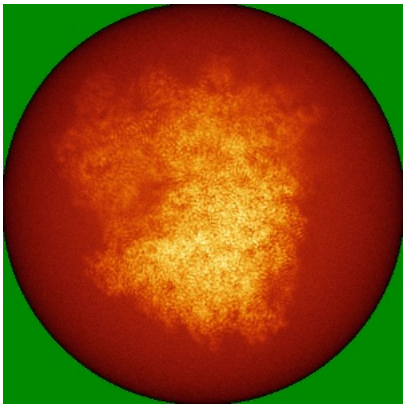
6.4.1 Primary map

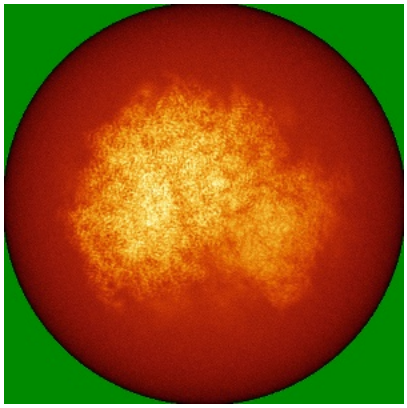

X

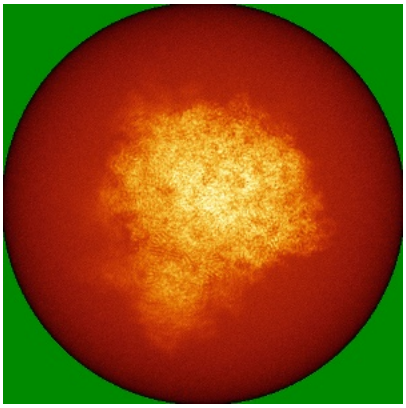

Y


Z

6.4.2 Raw map


X

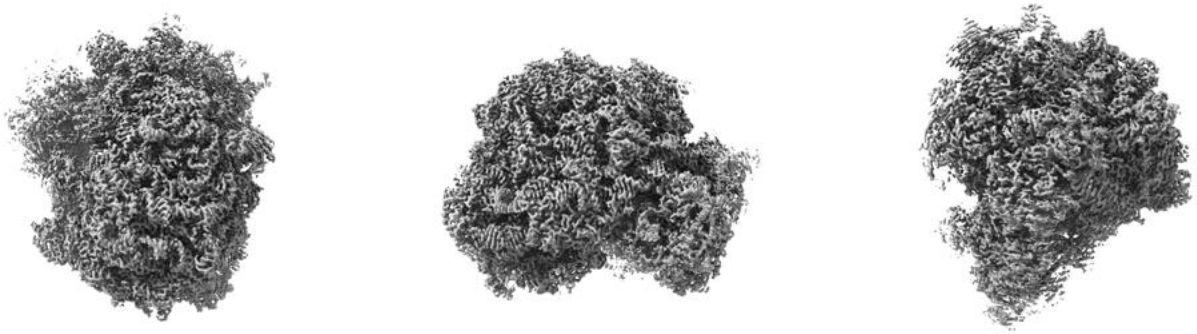

Y


Z

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

6.5 Orthogonal surface views (i)

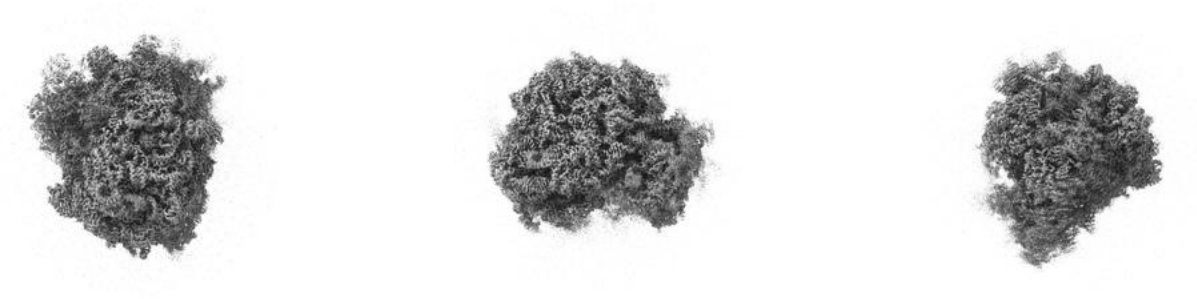
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0143. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

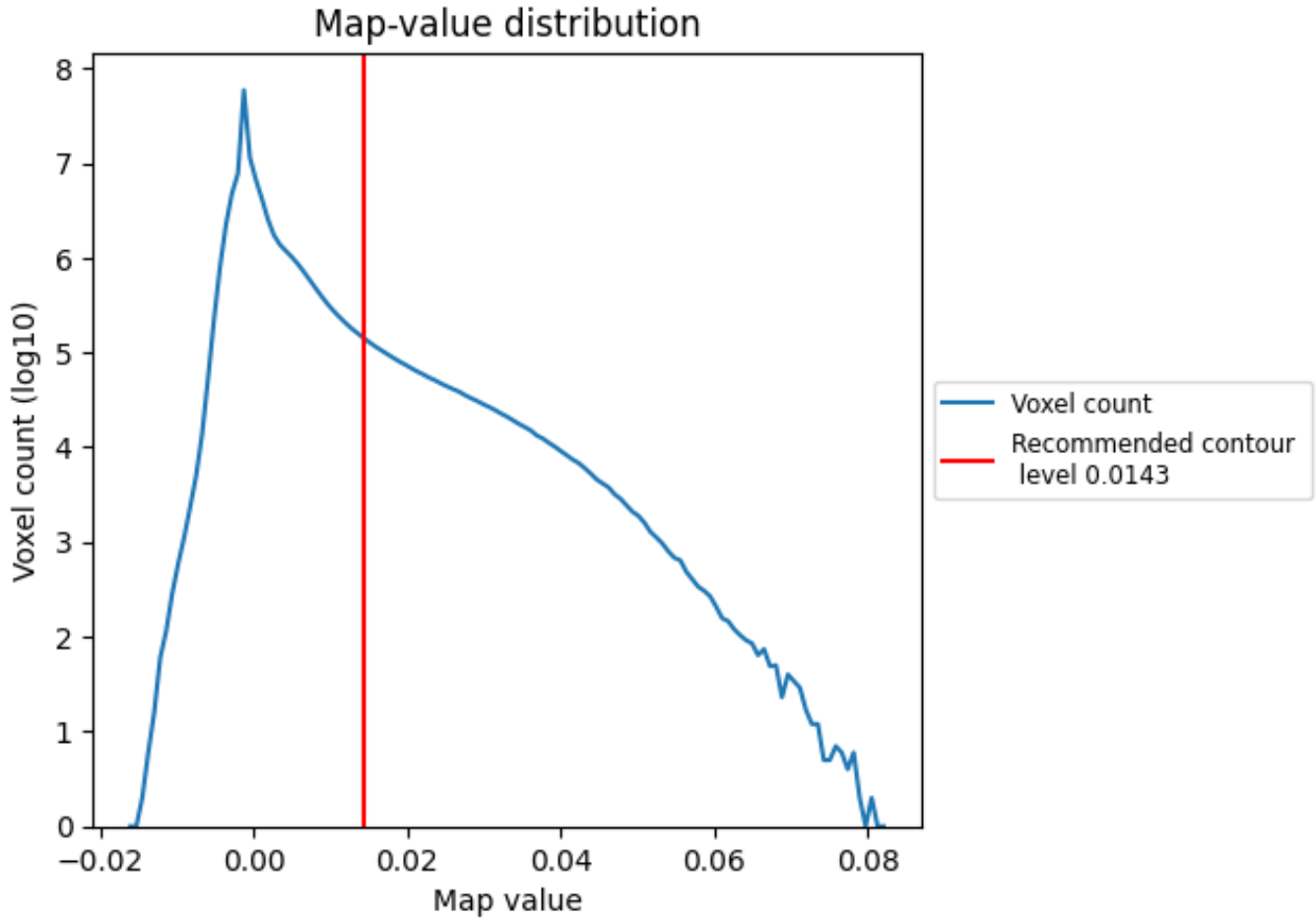
6.6 Mask visualisation (i)

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

7 Map analysis

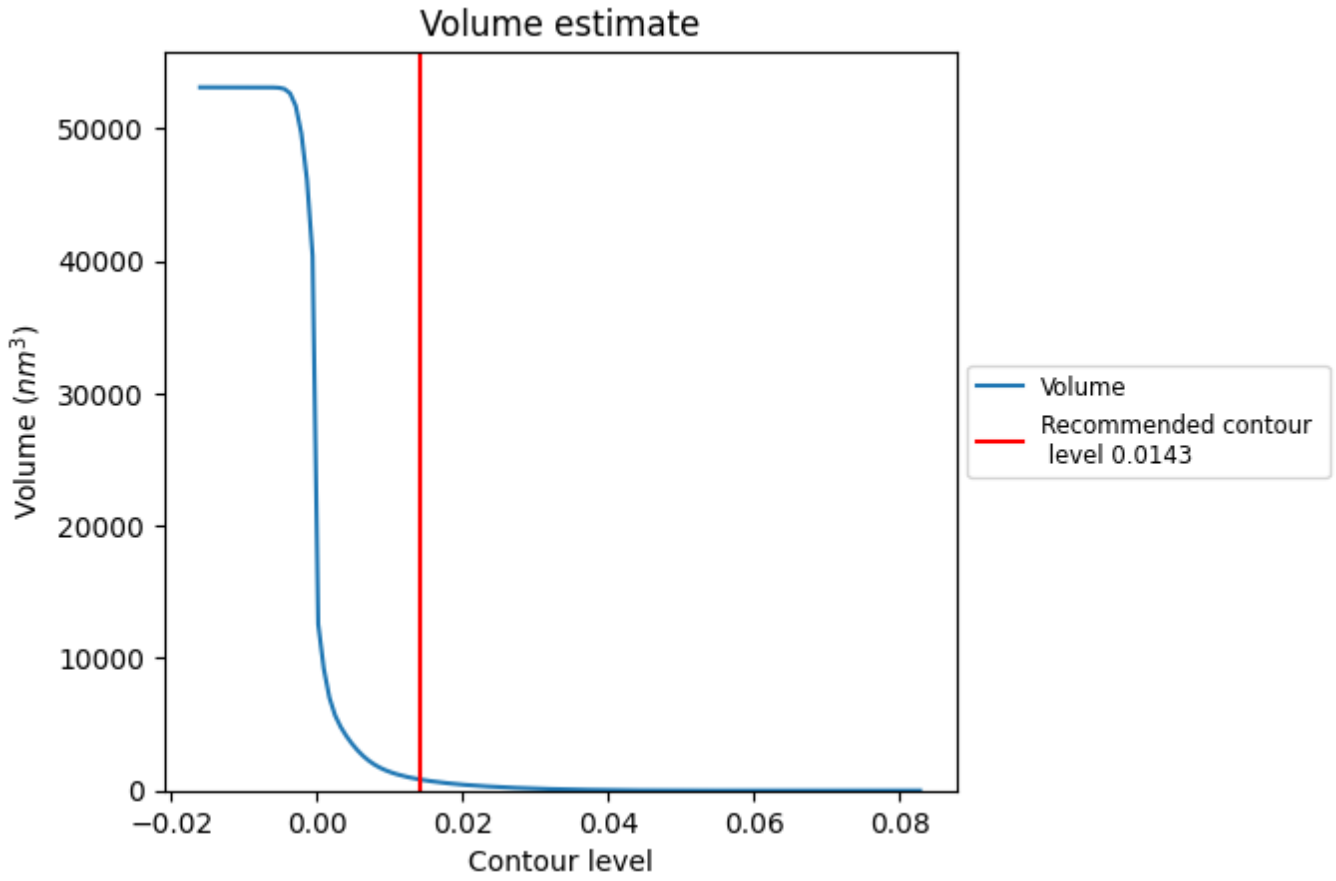
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

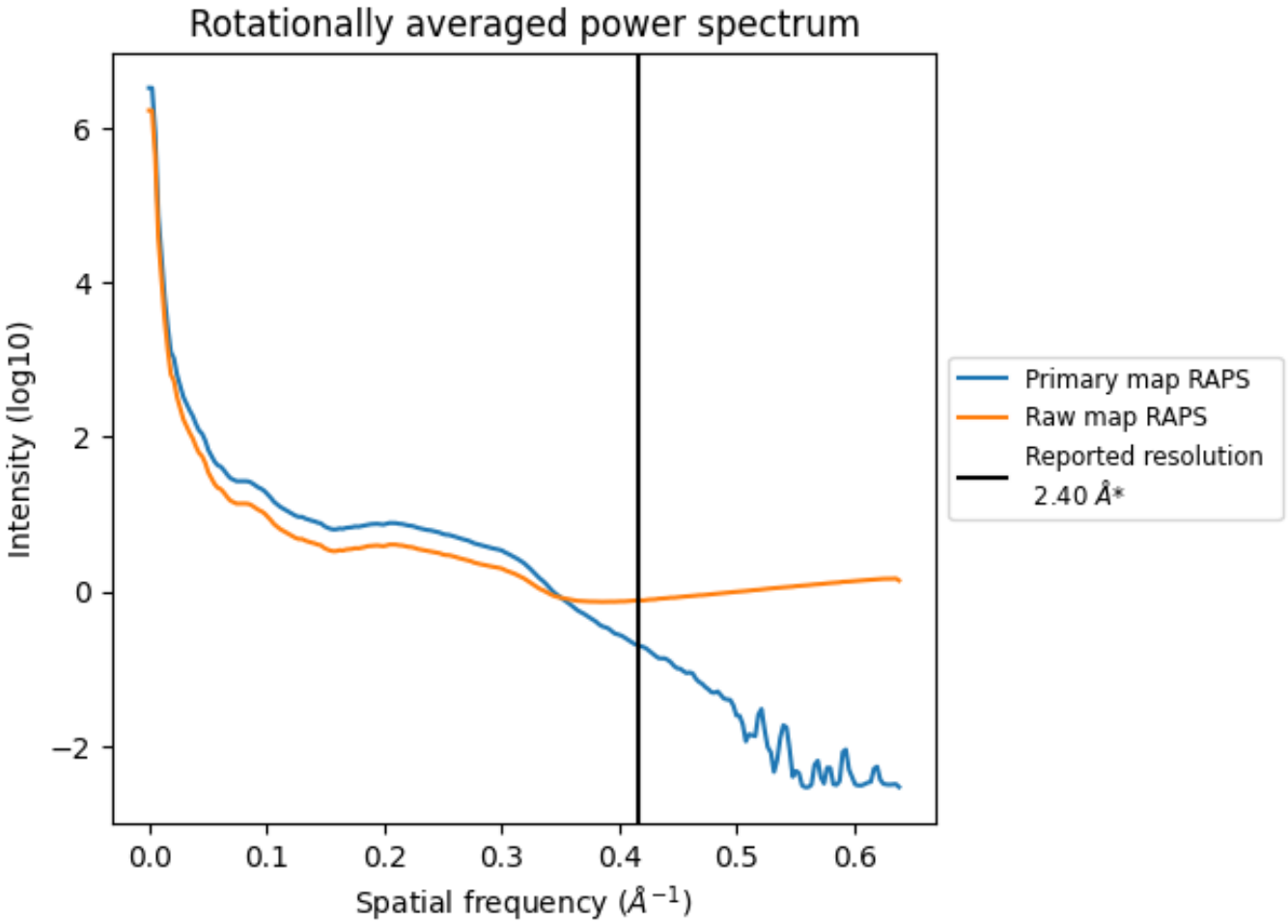
7.2 Volume estimate



The volume at the recommended contour level is 825 nm^3; this corresponds to an approximate mass of 745 kDa.

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

7.3 Rotationally averaged power spectrum (i)

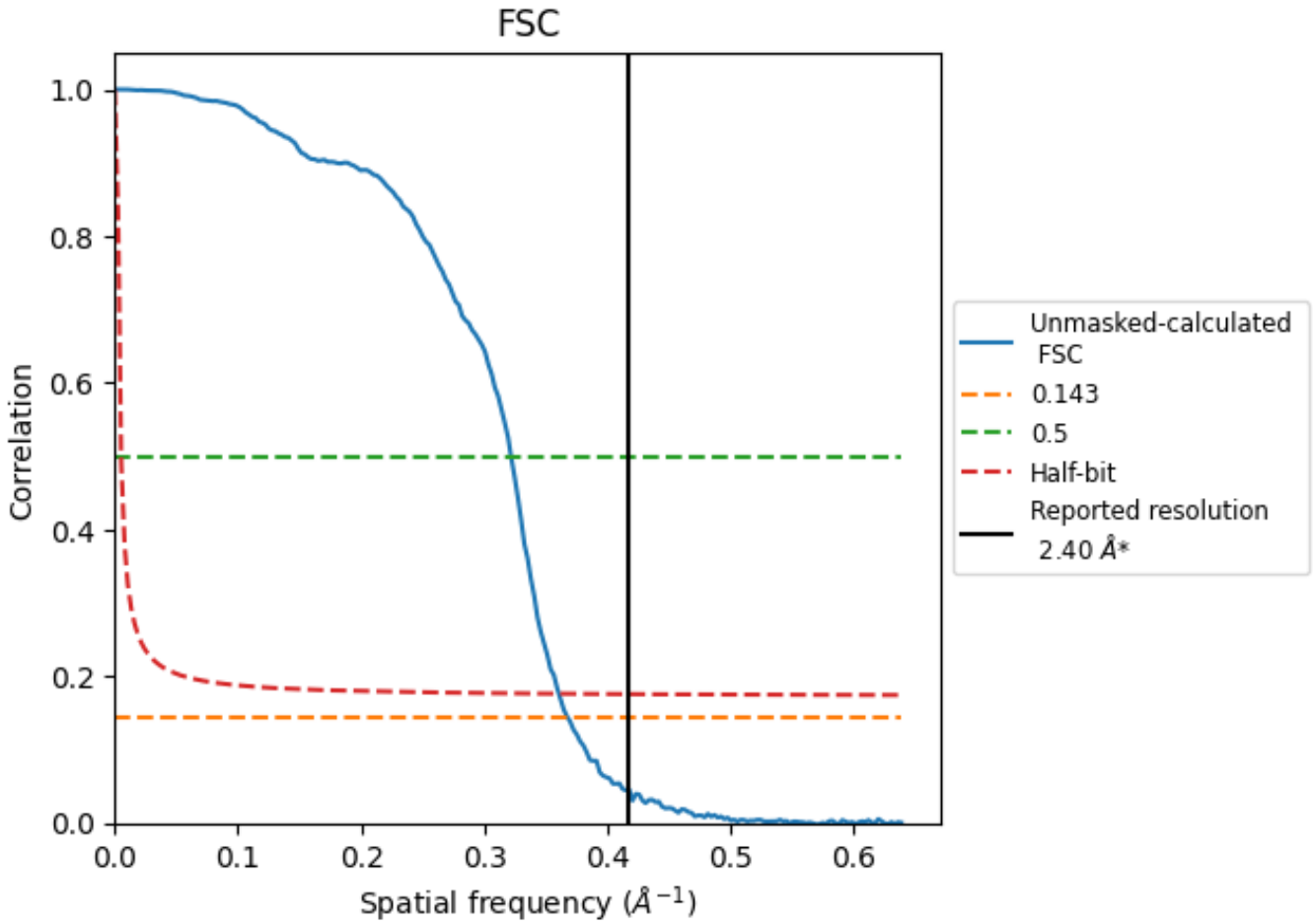


*Reported resolution corresponds to spatial frequency of 0.417 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.417 Å^{-1}

8.2 Resolution estimates (i)

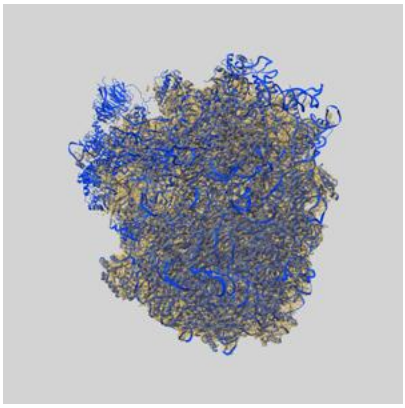
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.72	3.11	2.77

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.72 differs from the reported value 2.4 by more than 10 %

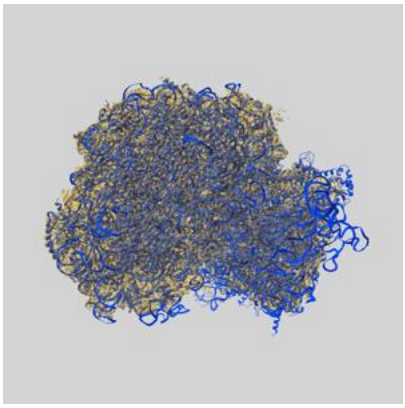
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16127 and PDB model 8BN3. Per-residue inclusion information can be found in section 3 on page 23.

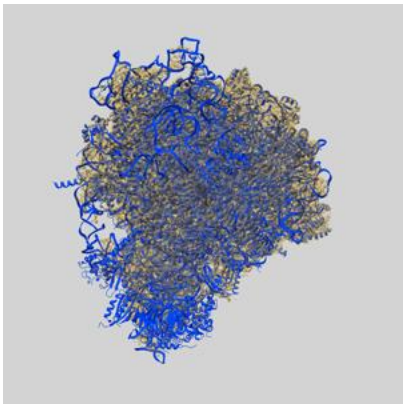
9.1 Map-model overlay



X



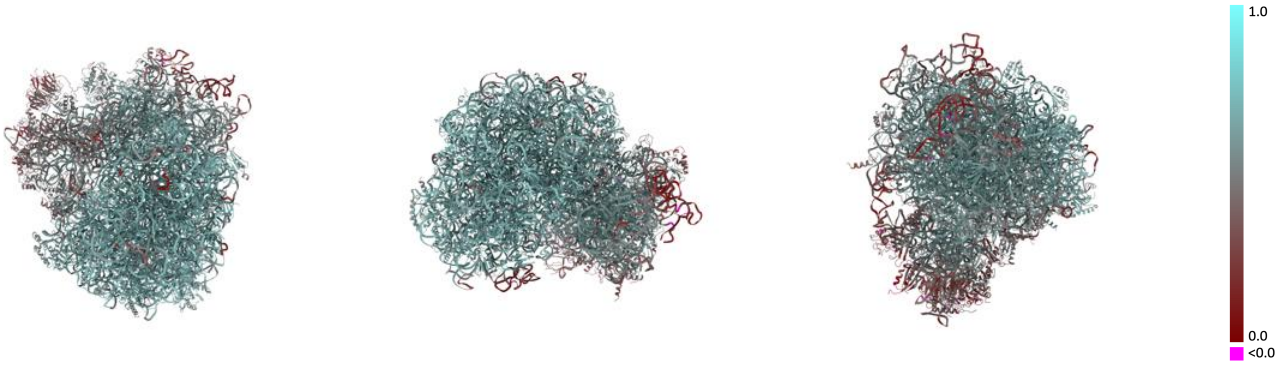
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0143 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

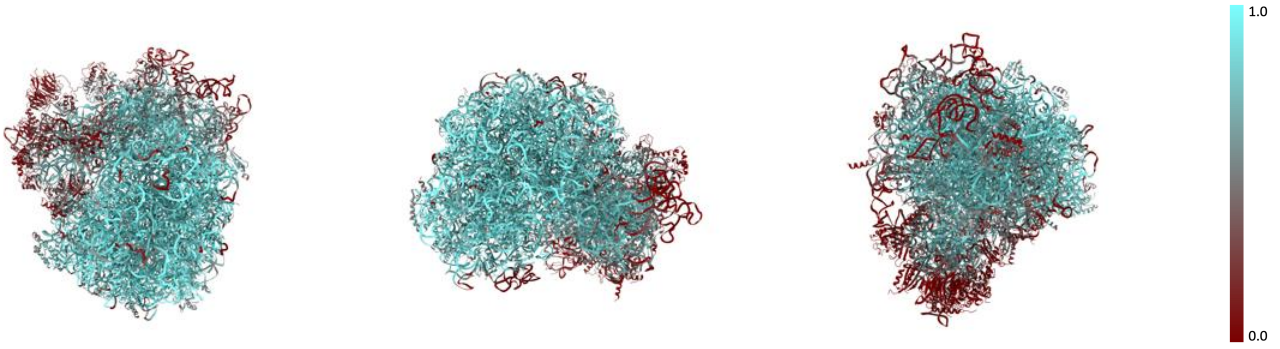
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

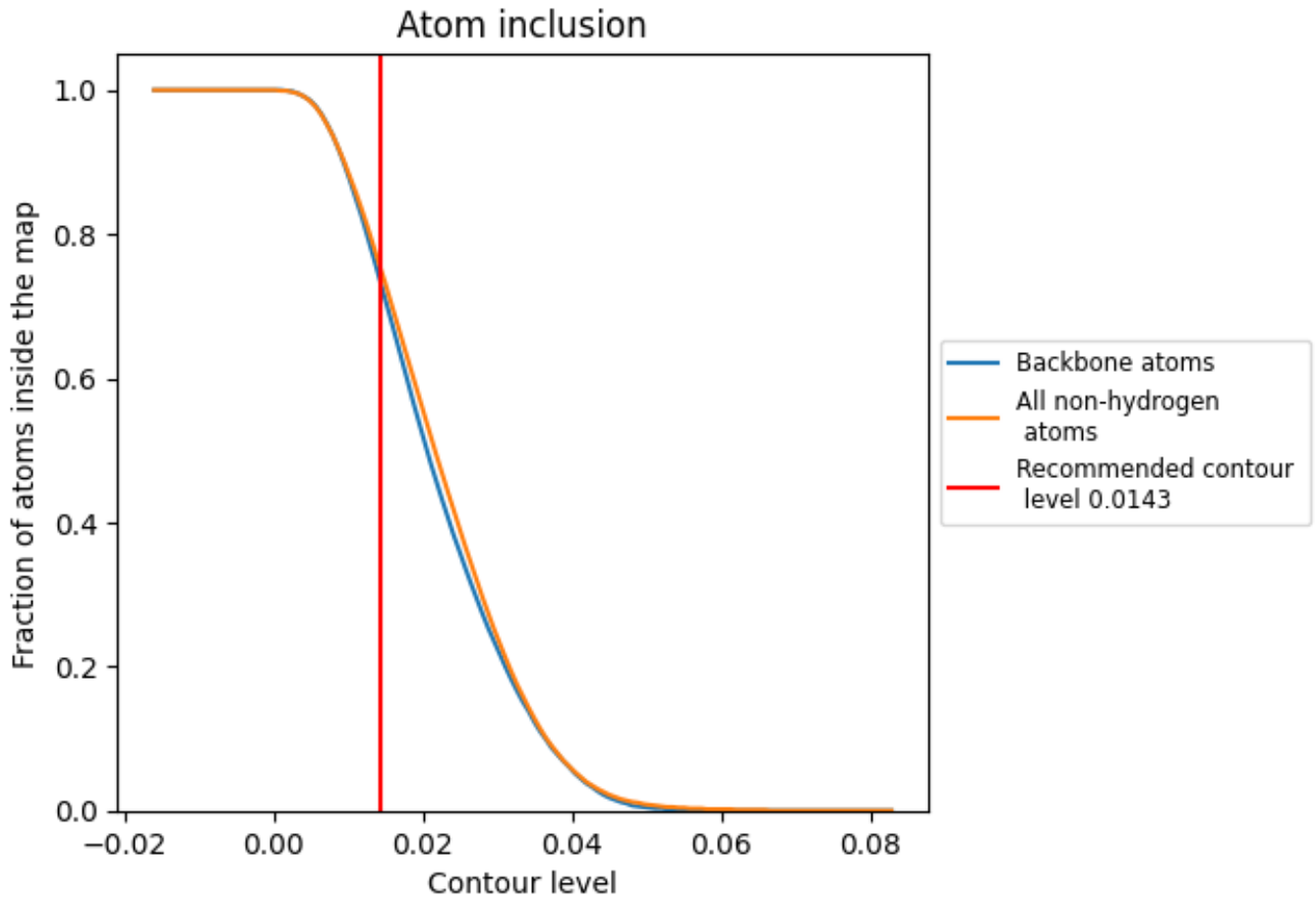
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0143).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 75% 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 (0.0143) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7530	0.5970
1	0.9120	0.6480
2	0.7180	0.5400
3	0.9590	0.6580
4	0.9540	0.6630
B	0.3520	0.5050
C0	0.1250	0.3300
C1	0.7230	0.6110
C3	0.6180	0.5680
C4	0.4530	0.4760
C5	0.3120	0.4430
C6	0.2180	0.4240
C7	0.2290	0.4630
C8	0.3150	0.4440
C9	0.2290	0.4460
D0	0.1860	0.3210
D1	0.5430	0.5690
D2	0.7950	0.6270
D3	0.7600	0.6160
D4	0.3480	0.4840
D5	0.0440	0.3270
D6	0.6580	0.5600
D7	0.4230	0.5350
D8	0.1340	0.3520
D9	0.6100	0.5490
E0	0.3860	0.4790
E1	0.0000	0.1990
L2	0.9260	0.6860
L3	0.8880	0.6770
L4	0.8610	0.6660
L5	0.7360	0.6130
L6	0.7470	0.6230
L7	0.9010	0.6750
L8	0.7650	0.6300
L9	0.7840	0.6440

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Chain	Atom inclusion	Q-score
M0	0.8280	0.6490
M1	0.6910	0.6020
M3	0.8140	0.6470
M4	0.8210	0.6470
M5	0.9700	0.6950
M6	0.9070	0.6780
M7	0.8960	0.6770
M8	0.9060	0.6740
M9	0.7880	0.6200
N0	0.8860	0.6690
N1	0.8640	0.6620
N2	0.6530	0.5870
N3	0.8630	0.6600
N4	0.8890	0.6600
N5	0.8460	0.6510
N6	0.8050	0.6480
N7	0.7580	0.6310
N8	0.8890	0.6790
N9	0.8570	0.6520
O0	0.7820	0.6240
O1	0.8160	0.6530
O2	0.9000	0.6790
O3	0.9390	0.6920
O4	0.8790	0.6700
O5	0.8110	0.6440
O6	0.7950	0.6350
O7	0.9640	0.6970
O8	0.6230	0.5970
O9	0.9420	0.6740
P	0.7790	0.6370
Q0	0.8540	0.6560
Q1	0.7030	0.6310
Q2	0.8470	0.6630
Q3	0.8810	0.6720
S0	0.4310	0.5260
S1	0.2870	0.4610
S2	0.6110	0.5750
S3	0.2640	0.4220
S4	0.5900	0.5700
S5	0.1720	0.3780
S6	0.2900	0.4500
S7	0.3050	0.4690

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Chain	Atom inclusion	Q-score
S8	0.6280	0.5720
S9	0.5100	0.5230
SM	0.3070	0.4810
SR	0.0130	0.3020
eI	0.6020	0.5930