Full wwPDB EM Validation Report ⓘ

Apr 30, 2024 – 05:33 pm BST

PDB ID	:	6ZQA
EMDB ID	:	EMD-11357
Title	:	Cryo-EM structure of the 90S pre-ribosome from Saccharomyces cerevisiae, state A (Poly-Ala)
Authors	:	Cheng, J.; Lau, B.; Venuta, G.L.; Berninghausen, O.; Hurt, E.; Beckmann, R.
Deposited on	:	2020-07-09
Resolution	:	4.40 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:

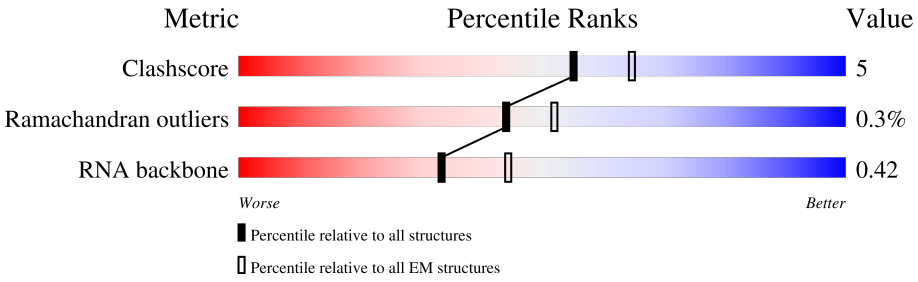
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.40 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
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	UA	923	88% · 10%
2	UB	810	9% 61% · 38%
3	UC	610	· 21% 79%
4	UD	776	· 84% · 13%
5	UE	643	73% · 26%
6	UF	440	· 66% · 33%
7	UG	554	6% 95% · ·
8	UH	713	11% 52% 8% · 38%

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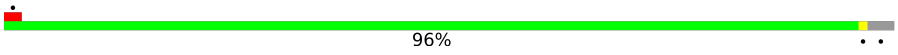
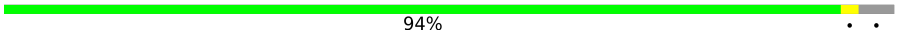
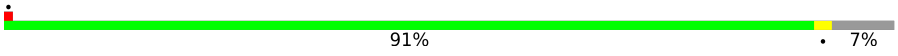
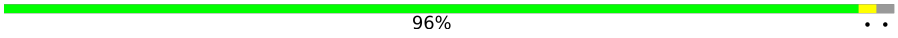
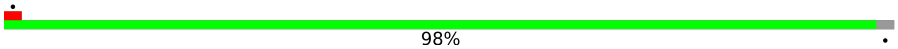
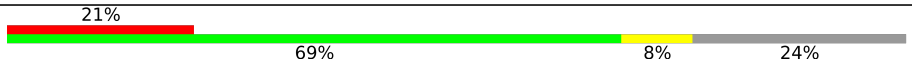
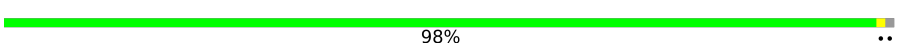
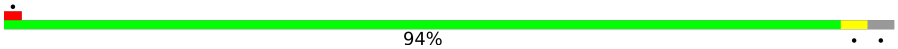
Mol	Chain	Length	Quality of chain
9	UI	575	
10	UJ	1769	
11	UK	250	
12	UL	943	
13	UM	817	
14	UN	899	
15	UO	513	
16	UP	214	
17	UQ	896	
18	UR	594	
19	US	552	
20	UU	939	
21	UV	1237	
22	UX	189	
23	UZ	274	
24	CA	327	
24	CB	327	
25	CD	504	
26	CE	511	
27	CF	126	
27	CG	126	
28	CH	573	
29	CI	183	
30	CJ	290	
31	CK	593	

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Mol	Chain	Length	Quality of chain
32	CL	1183	64% 34%
33	CM	367	95%
34	CN	297	72% 76% 22%
35	JF	252	83% 14%
35	JG	252	87% 9%
36	JH	483	42% 53% 46%
37	JJ	274	66% 34%
38	JM	217	62% 38%
39	JN	346	51% 46%
40	JO	316	59% 41%
41	JP	489	91% 6%
42	JQ	206	20% 31% 69%
43	DA	255	21% 89% 5% 6%
44	DF	225	94% 5%
45	DH	190	45% 94%
46	DJ	197	8% 93% 6%
47	DN	151	37% 98%
48	DO	137	85% 12%
49	DQ	143	87% 13%
50	DS	146	45% 70% 28%
51	DW	130	97%
52	DX	145	66% 5% 29%
53	Db	82	88% 99%
54	Dc	67	94% 6%
55	D2	700	24% 40% 10% 25%

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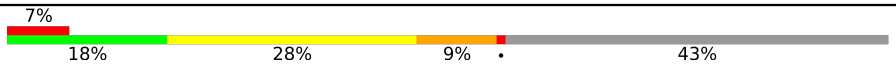
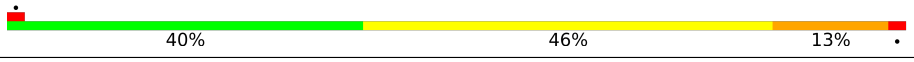
Mol	Chain	Length	Quality of chain
56	D3	1379	
57	D4	175	

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 125991 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 Periodic tryptophan protein 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	UA	834	Total 4121	C 2453	N 834	O 834	0	0

- Molecule 2 is a protein called Nucleolar complex protein 14.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	UB	504	Total 2512	C 1504	N 504	O 504	0	0

- Molecule 3 is a protein called Something about silencing protein 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	UC	128	Total 628	C 372	N 128	O 128	0	0

- Molecule 4 is a protein called U3 small nucleolar RNA-associated protein 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	UD	675	Total 3339	C 1989	N 675	O 675	0	0

- Molecule 5 is a protein called U3 small nucleolar RNA-associated protein 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	UE	475	Total 2353	C 1403	N 475	O 475	0	0

- Molecule 6 is a protein called U3 small nucleolar RNA-associated protein 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	UF	293	Total 1456	C 870	N 293	O 293	0	0

- Molecule 7 is a protein called U3 small nucleolar RNA-associated protein 7.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	UG	533	Total	C	N	O	0	0
			2629	1563	533	533		

- Molecule 8 is a protein called U3 small nucleolar RNA-associated protein 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	UH	442	Total	C	N	O	0	0
			2190	1306	442	442		

- Molecule 9 is a protein called U3 small nucleolar RNA-associated protein 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	UI	104	Total	C	N	O	0	0
			517	309	104	104		

- Molecule 10 is a protein called U3 small nucleolar RNA-associated protein 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	UJ	726	Total	C	N	O	0	0
			3621	2169	726	726		

- Molecule 11 is a protein called U3 small nucleolar RNA-associated protein 11.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	UK	242	Total	C	N	O	0	0
			1203	719	242	242		

- Molecule 12 is a protein called U3 small nucleolar RNA-associated protein 12.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	UL	842	Total	C	N	O	0	0
			4163	2479	842	842		

- Molecule 13 is a protein called U3 small nucleolar RNA-associated protein 13.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	UM	762	Total	C	N	O	0	0
			3763	2239	762	762		

- Molecule 14 is a protein called U3 small nucleolar RNA-associated protein 14.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	UN	147	Total 733	C 439	N 147	O 147	0	0

- Molecule 15 is a protein called U3 small nucleolar RNA-associated protein 15.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	UO	493	Total 2441	C 1455	N 493	O 493	0	0

- Molecule 16 is a protein called Bud site selection protein 21.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	UP	60	Total 298	C 178	N 60	O 60	0	0

- Molecule 17 is a protein called NET1-associated nuclear protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	UQ	832	Total 4122	C 2458	N 832	O 832	0	0

- Molecule 18 is a protein called U3 small nucleolar RNA-associated protein 18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	UR	482	Total 2377	C 1413	N 482	O 482	0	0

- Molecule 19 is a protein called Nucleolar complex protein 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	US	473	Total 2357	C 1411	N 473	O 473	0	0

- Molecule 20 is a protein called U3 small nucleolar RNA-associated protein 21.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	UU	848	Total 4181	C 2485	N 848	O 848	0	0

- Molecule 21 is a protein called U3 small nucleolar RNA-associated protein 22.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	UV	1098	Total 5442	C 3246	N 1098	O 1098	0	0

- Molecule 22 is a protein called rRNA-processing protein FCF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	UX	174	Total 862	C 514	N 174	O 174	0	0

- Molecule 23 is a protein called Ribosome biogenesis protein UTP30.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	UZ	247	Total 1224	C 730	N 247	O 247	0	0

- Molecule 24 is a protein called rRNA 2'-O-methyltransferase fibrillarin.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	CA	242	Total 1190	C 706	N 242	O 242	0	0
24	CB	228	Total 1122	C 666	N 228	O 228	0	0

- Molecule 25 is a protein called Nucleolar protein 56.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	CD	380	Total 1880	C 1120	N 380	O 380	0	0

- Molecule 26 is a protein called Nucleolar protein 58.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	CE	435	Total 2155	C 1285	N 435	O 435	0	0

- Molecule 27 is a protein called 13 kDa ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	CF	123	Total 611	C 365	N 123	O 123	0	0
27	CG	123	Total 611	C 365	N 123	O 123	0	0

- Molecule 28 is a protein called Ribosomal RNA-processing protein 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	CH	438	Total 2158	C 1282	N 438	O 438	0	0

- Molecule 29 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	CI	182	Total 905	C 541	N 182	O 182	0	0

- Molecule 30 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	CJ	282	Total 1397	C 833	N 282	O 282	0	0

- Molecule 31 is a protein called U3 small nucleolar RNA-associated protein MPP10.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	CK	207	Total 1031	C 617	N 207	O 207	0	0

- Molecule 32 is a protein called Ribosome biogenesis protein BMS1.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	CL	781	Total 3859	C 2298	N 781	O 780	0	0

- Molecule 33 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	CM	360	Total 1767	C 1047	N 360	O 360	0	0

- Molecule 34 is a protein called Ribosomal RNA-processing protein 7.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	CN	232	Total 1154	C 690	N 232	O 232	0	0

- Molecule 35 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	JF	216	Total 1071	C 639	N 216	O 216	0	0
35	JG	230	Total 1141	C 681	N 230	O 230	0	0

- Molecule 36 is a protein called Essential nuclear protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	JH	261	Total 1295	C 773	N 261	O 261	0	0

- Molecule 37 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	JJ	182	Total 898	C 534	N 182	O 182	0	0

- Molecule 38 is a protein called rRNA-processing protein FCF2.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	JM	135	Total 671	C 401	N 135	O 135	0	0

- Molecule 39 is a protein called Protein FAF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	JN	186	Total 918	C 546	N 186	O 186	0	0

- Molecule 40 is a protein called KRR1 small subunit processome component.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	JO	188	Total 933	C 557	N 188	O 188	0	0

- Molecule 41 is a protein called Protein SOF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	JP	461	Total 2283	C 1361	N 461	O 461	0	0

- Molecule 42 is a protein called Regulator of rDNA transcription protein 14.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	JQ	63	Total 312	C 186	N 63	O 63	0	0

- Molecule 43 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	DA	240	Total 1187	C 707	N 240	O 240	0	0

- Molecule 44 is a protein called Rps5p.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	DF	213	Total 1055	C 629	N 213	O 213	0	0

- Molecule 45 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	DH	184	Total 913	C 545	N 184	O 184	0	0

- Molecule 46 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	DJ	185	Total 915	C 545	N 185	O 185	0	0

- Molecule 47 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	DN	150	Total 742	C 442	N 150	O 150	0	0

- Molecule 48 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	DO	120	Total 587	C 347	N 120	O 120	0	0

- Molecule 49 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	DQ	125	Total 616	C 366	N 125	O 125	0	0

- Molecule 50 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	DS	105	Total 521	C 311	N 105	O 105	0	0

- Molecule 51 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	DW	129	Total 634	C 376	N 129	O 129	0	0

- Molecule 52 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	DX	103	Total 503	C 297	N 103	O 103	0	0

- Molecule 53 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	Db	81	Total 400	C 238	N 81	O 81	0	0

- Molecule 54 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	Dc	63	Total 310	C 184	N 63	O 63	0	0

- Molecule 55 is a RNA chain called 5ETS RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	D2	523	Total 11160	C 4987	N 1981	O 3669	P 523	0	0

- Molecule 56 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	D3	787	Total	C	N	O	P	0	0
			16806	7509	3018	5492	787		

- Molecule 57 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	D4	175	Total	C	N	O	P	0	0
			3712	1661	648	1228	175		

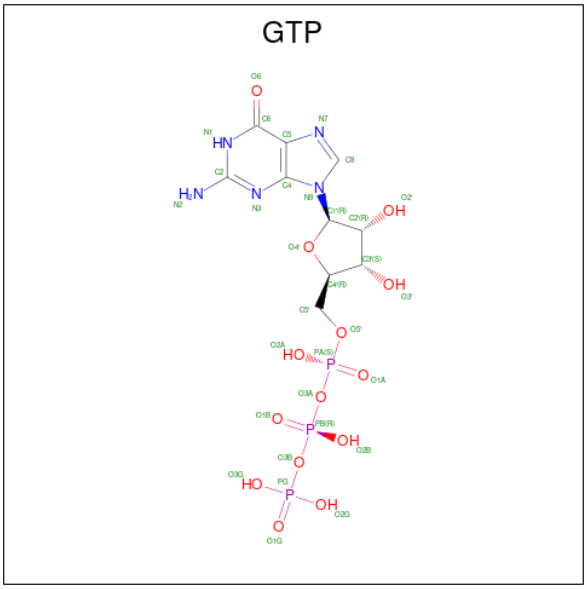
- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
58	UX	1	Total	Zn	0
			1	1	
58	Db	1	Total	Zn	0
			1	1	

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
59	UX	1	Total	Mg	0
			1	1	
59	CL	1	Total	Mg	0
			1	1	

- Molecule 60 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



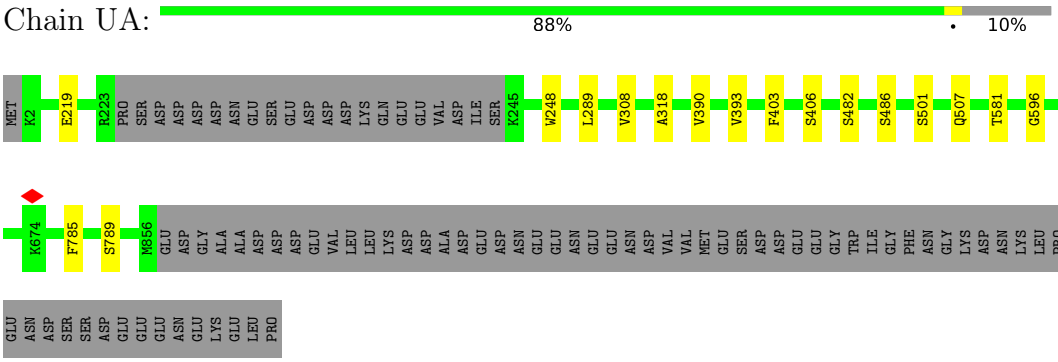
Mol	Chain	Residues	Atoms					AltConf
60	CL	1	Total	C	N	O	P	0
			32	10	5	14	3	

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.

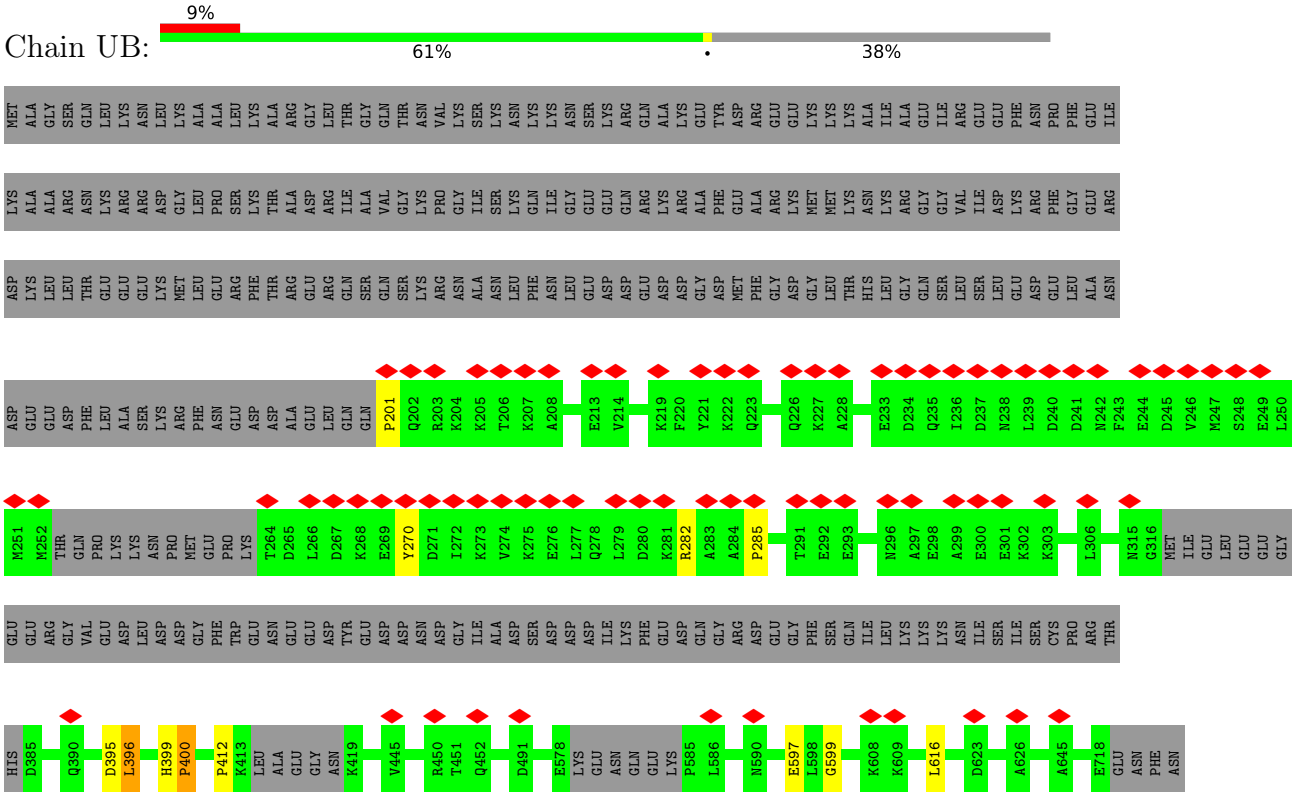
• Molecule 1: Periodic tryptophan protein 2

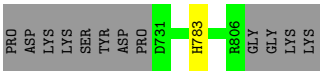
Chain UA:



• Molecule 2: Nucleolar complex protein 14

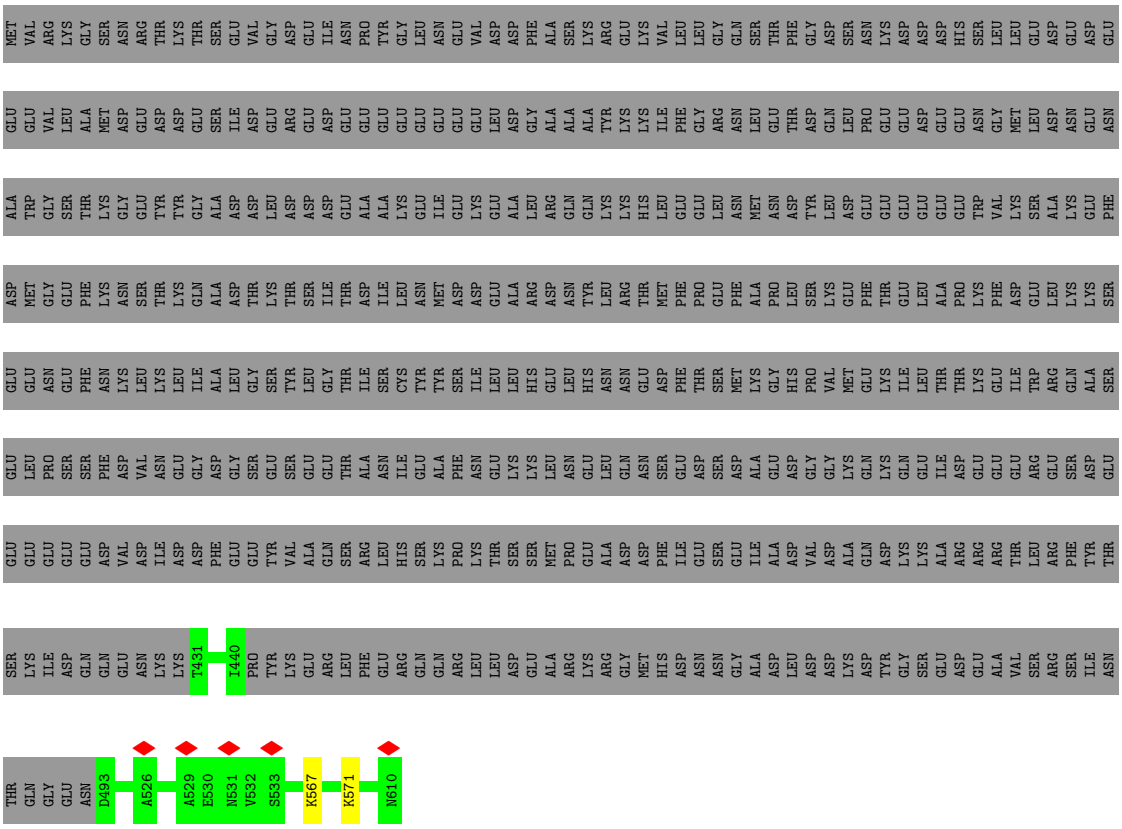
Chain UB:





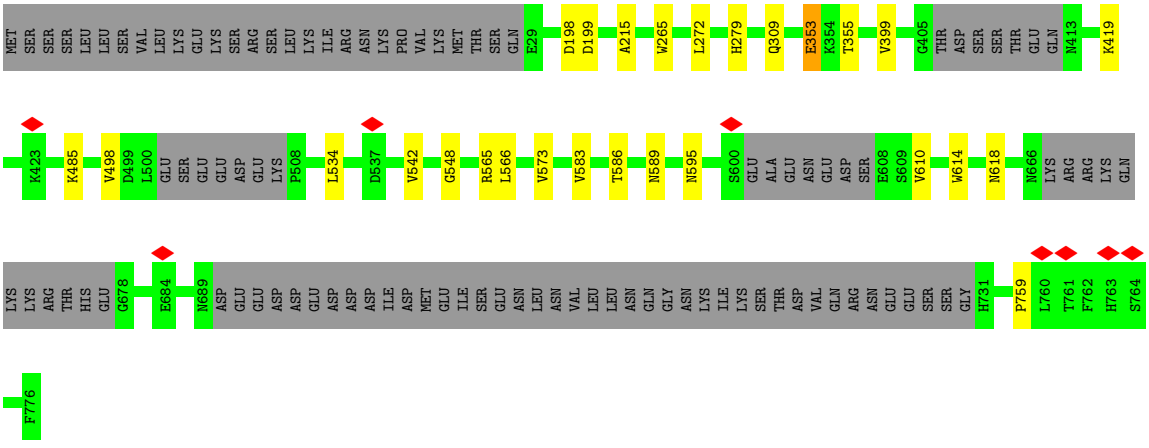
• Molecule 3: Something about silencing protein 10

Chain UC:



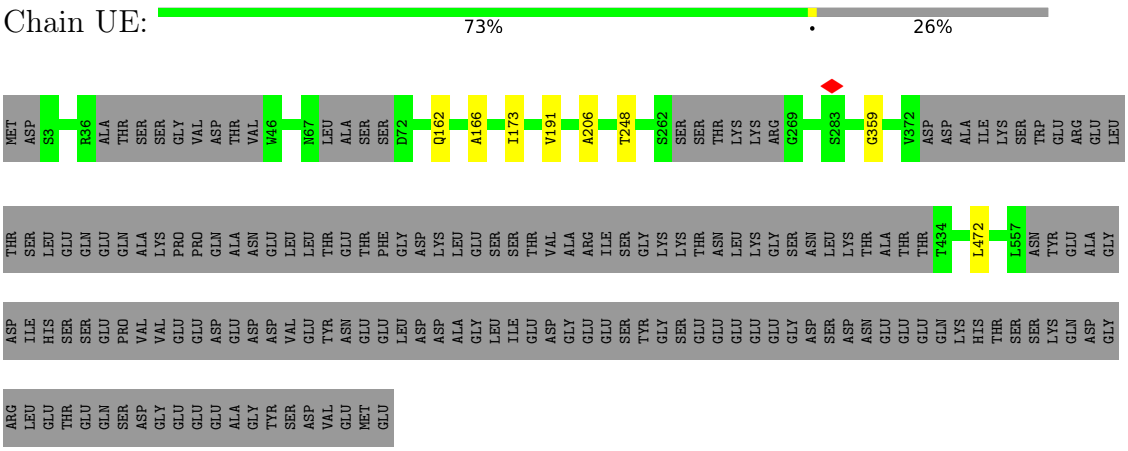
• Molecule 4: U3 small nucleolar RNA-associated protein 4

Chain UD:



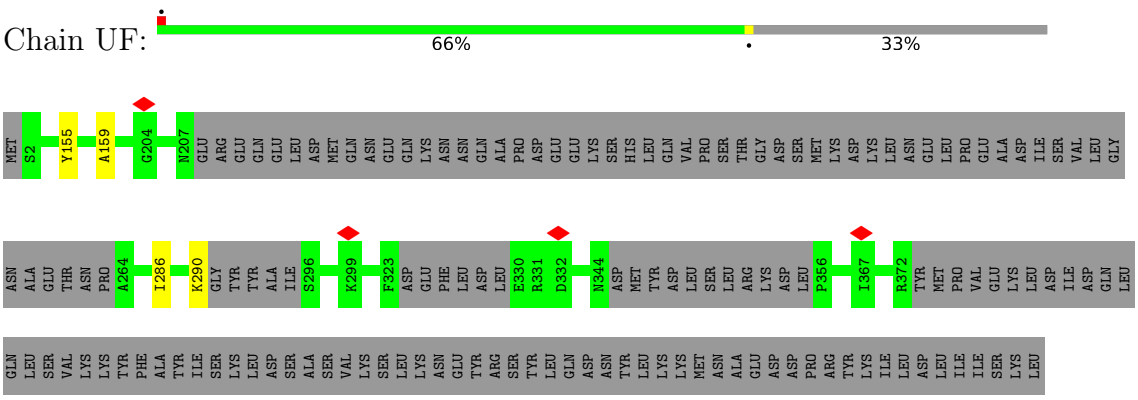
• Molecule 5: U3 small nucleolar RNA-associated protein 5

Chain UE:



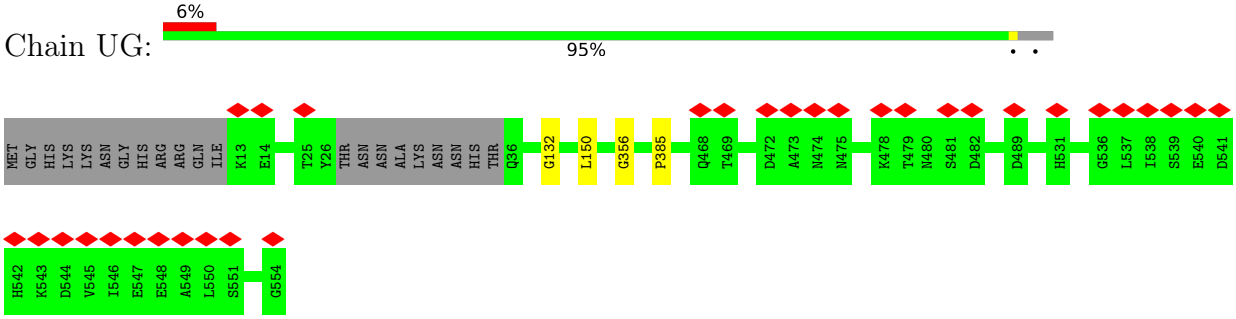
• Molecule 6: U3 small nucleolar RNA-associated protein 6

Chain UF:



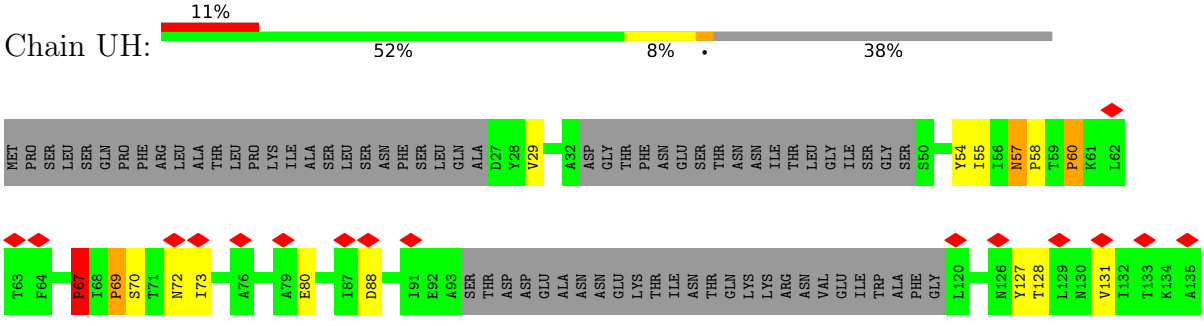
• Molecule 7: U3 small nucleolar RNA-associated protein 7

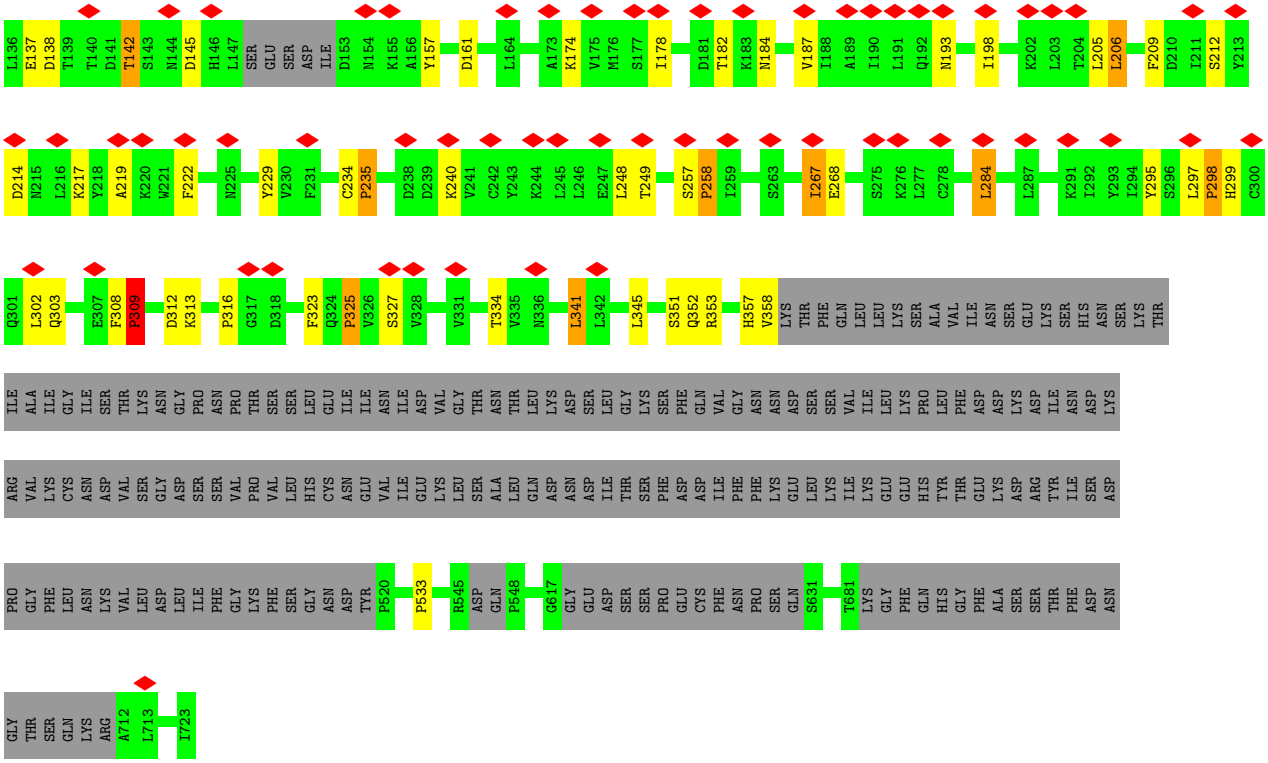
Chain UG:



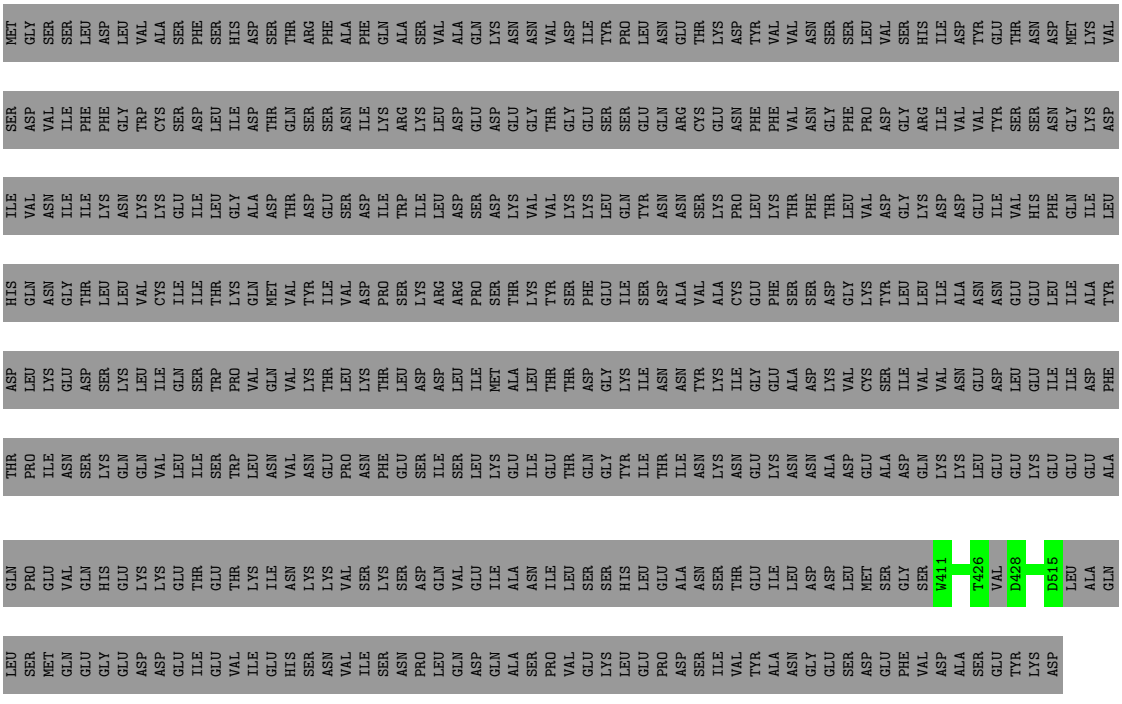
• Molecule 8: U3 small nucleolar RNA-associated protein 8

Chain UH:

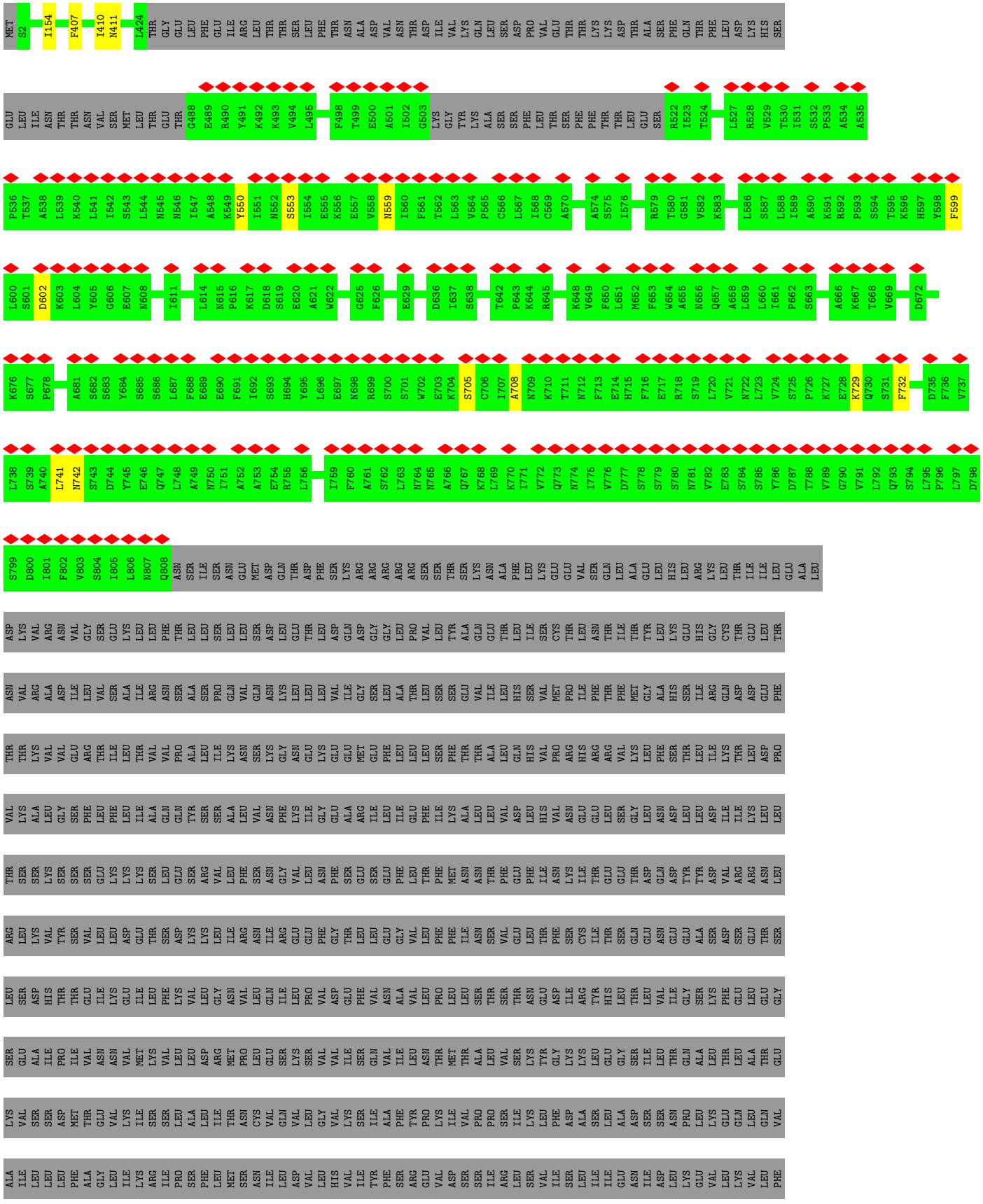




• Molecule 9: U3 small nucleolar RNA-associated protein 9



• Molecule 10: U3 small nucleolar RNA-associated protein 10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GLU LEU ILE ASN THR THR ASN VAL SER MET LEU THR GLU THR G488 E489 R490 Y491 K492 K493 V494 L495 F498 T499 E500 A501 I502 G503 LYS GLY TYR LYS ALA SER SER PHE LEU THR SER PHE PHE THR THR LEU GLU SER R522 I523 T524 L527 R528 V529 T530 I531 S532 P533 A534 A535
P536 T537 A538 L539 K540 L541 I542 S543 L544 N545 N546 I547 A548 K549 Y550 I551 N552 S553 I554 E555 K556 E557 V558 N559 I560 F561 T562 L563 V564 P565 C566 L567 I568 C569 A570 A574 S575 I576 R579 T580 G581 V582 K583 L586 S587 L588 I589 A590 K591 R592 P593 S594 T595 K596 H597 Y598 F599
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K676 S677 P678 A681 S682 S683 Y684 S685 S686 L687 F688 E689 E690 F691 I692 S693 H694 Y695 L696 E697 N698 R699 S700 S701 W702 E703 K704 S705 C706 I707 A708 N709 K710 T711 N712 F713 E714 H715 F716 E717 R718 S719 L720 V721 N722 L723 V724 S725 P726 K727 E728 K729 Q730 S731 F732 D735 F736 V737
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S799 D800 I801 F802 V803 S804 I805 L806 N807 Q808 ASN SER ILE SER ASN GLU MET ASP GLN THR ASP PHE SER LYS ARG ARG ARG ARG ARG SER SER THR SER LYS ASN ALA PHE LEU LYS GLU GLU VAL SER GLN LEU ALA GLU LEU HIS LEU ARG LYS LEU THR ILE ILE LEU GLU ALA LEU
ASP LYS VAL ARG ASN VAL GLY SER GLU LYS LEU LEU PHE THR LEU LEU LEU SER LEU LEU SER ASP GLU LEU SER ASP GLN ASP GLY GLY LEU PRO VAL LEU TYR ALA GLN GLU THR LEU ILE SER CYS THR LEU ASN THR ILE THR TYR LEU LYS GLU HIS GLY CYS THR LEU GLU LEU THR
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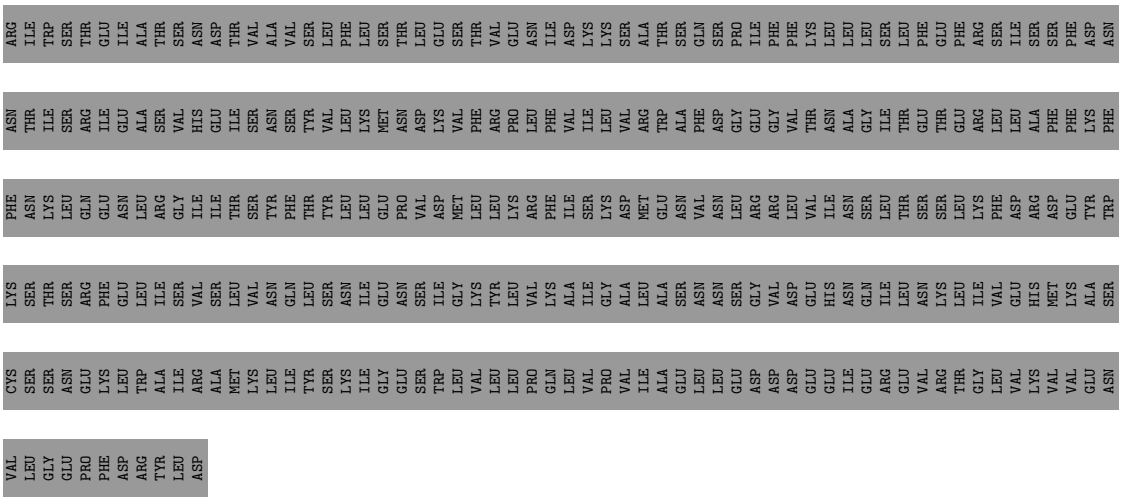
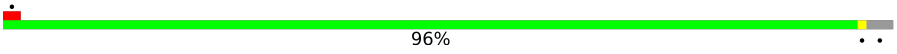
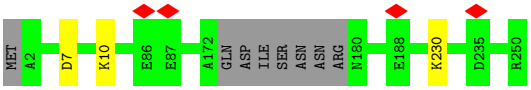


• Molecule 11: U3 small nucleolar RNA-associated protein 11

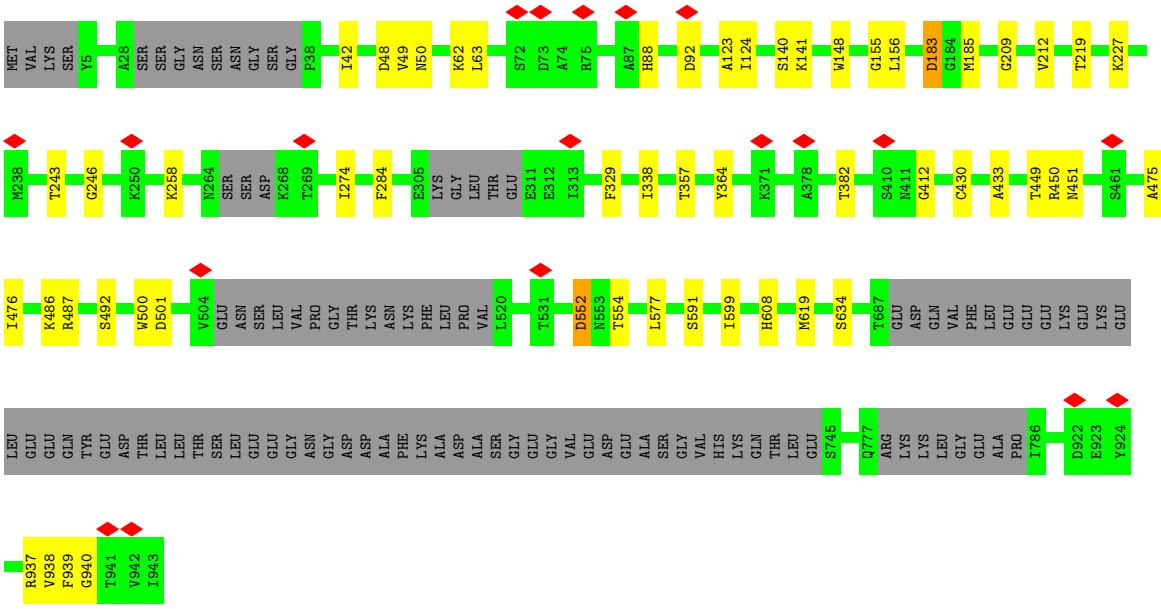
Chain UK:





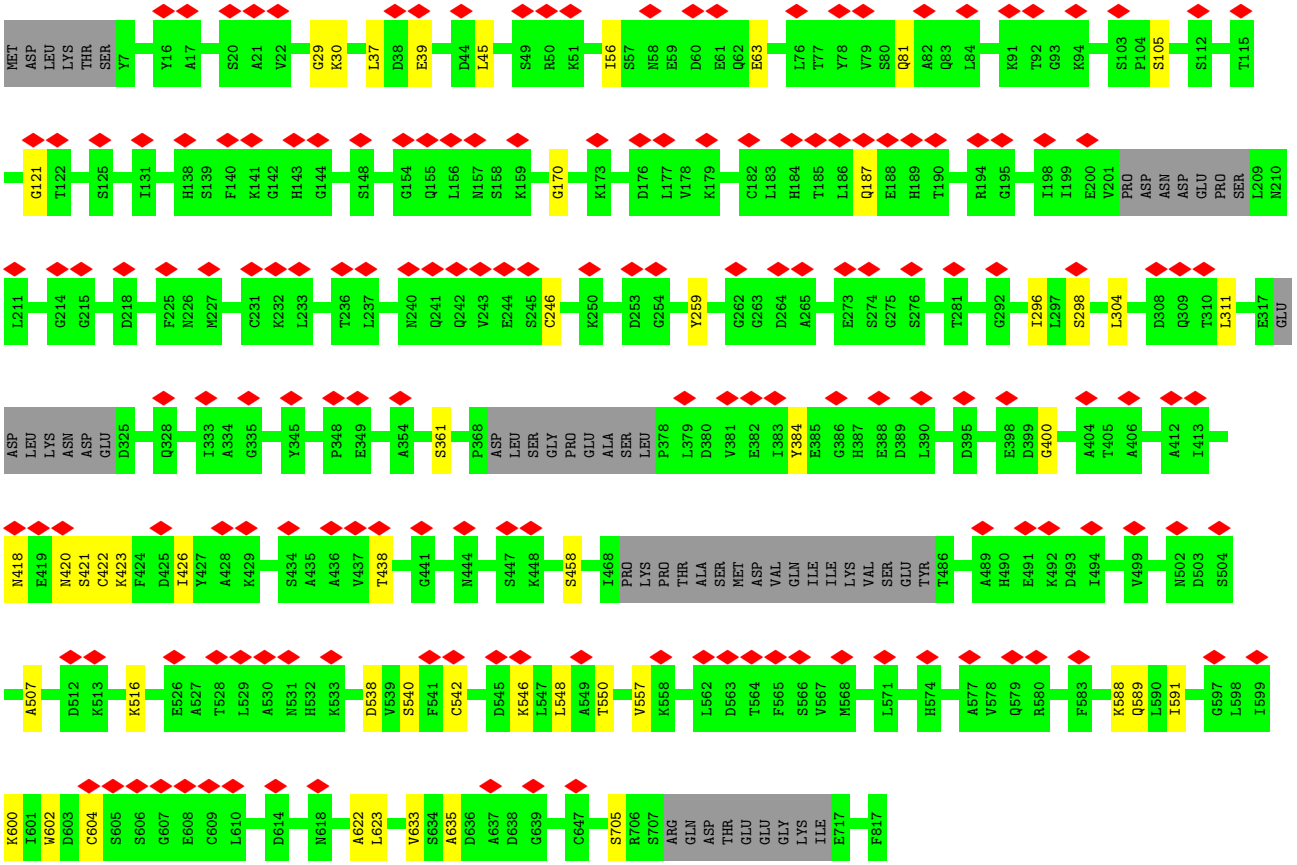
• Molecule 12: U3 small nucleolar RNA-associated protein 12

Chain UL:



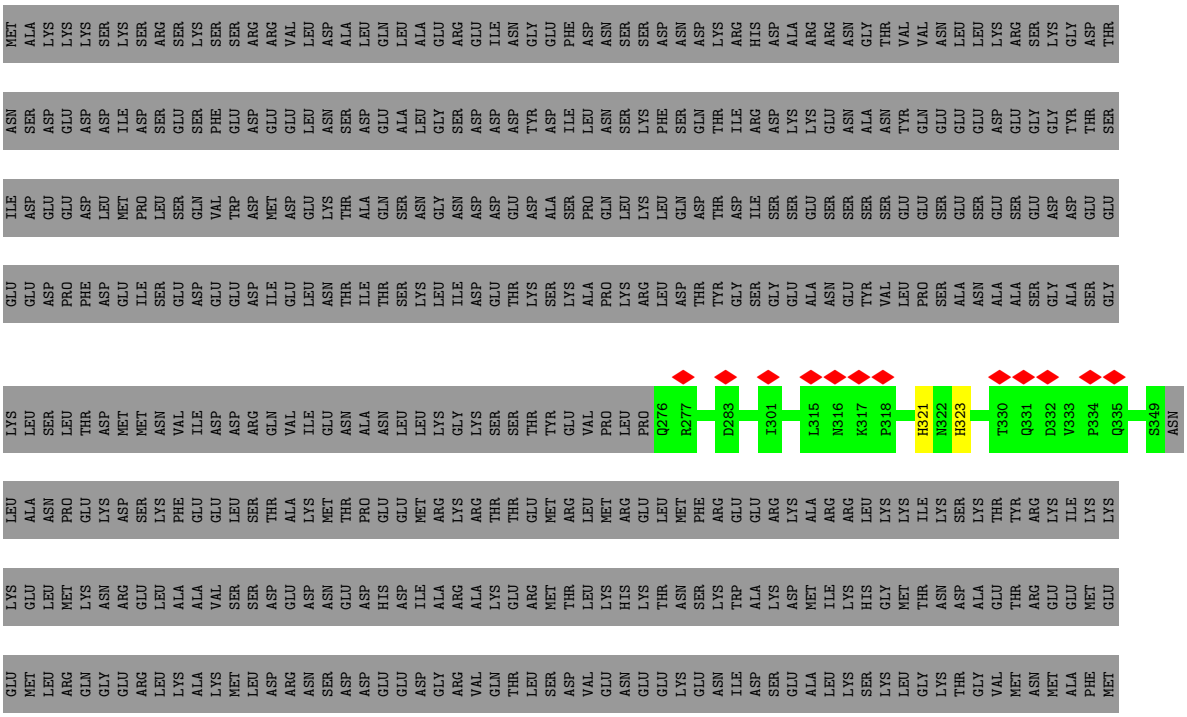
• Molecule 13: U3 small nucleolar RNA-associated protein 13

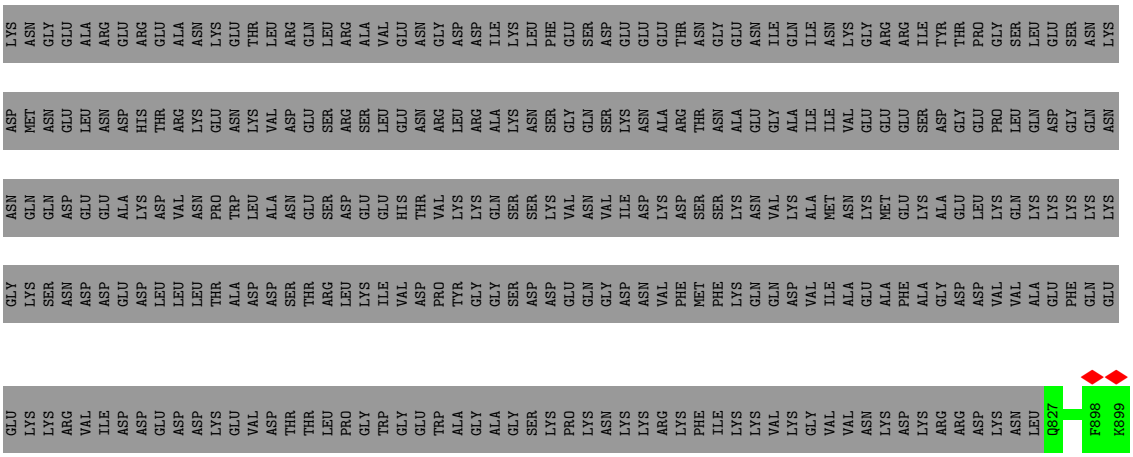
Chain UM:



• Molecule 14: U3 small nucleolar RNA-associated protein 14

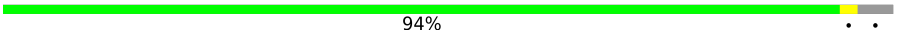
Chain UN:

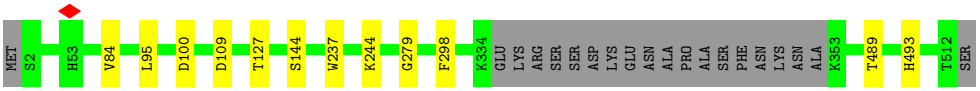




• Molecule 15: U3 small nucleolar RNA-associated protein 15

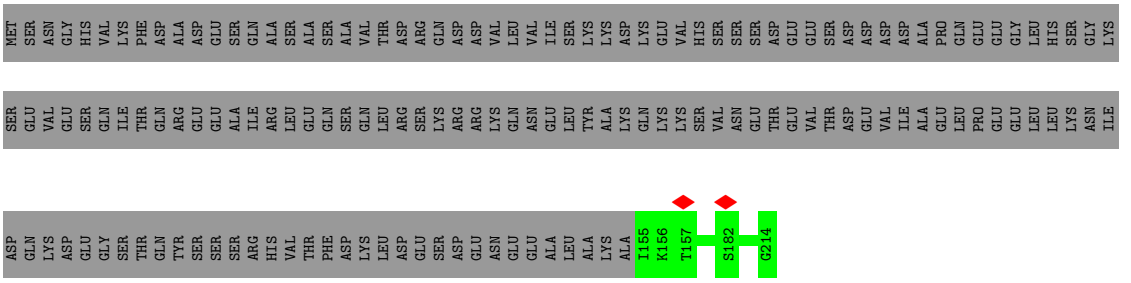
Chain UO:





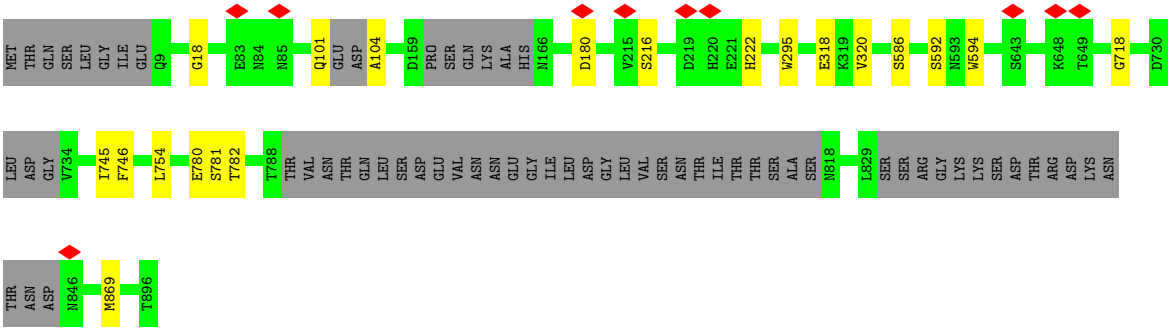
• Molecule 16: Bud site selection protein 21

Chain UP:



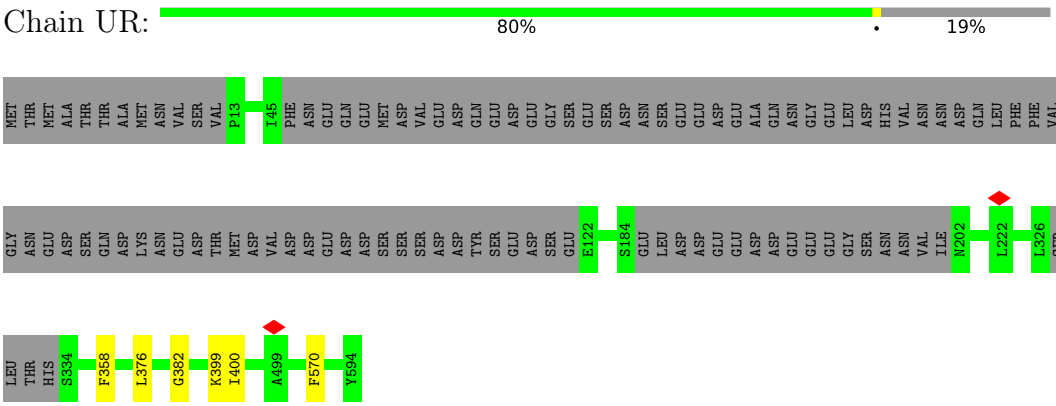
• Molecule 17: NET1-associated nuclear protein 1

Chain UQ:



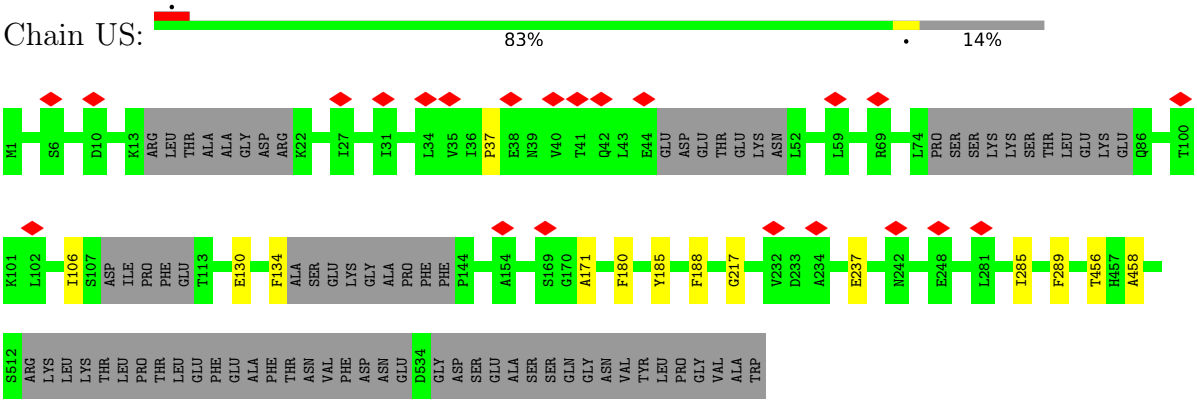
• Molecule 18: U3 small nucleolar RNA-associated protein 18

Chain UR:



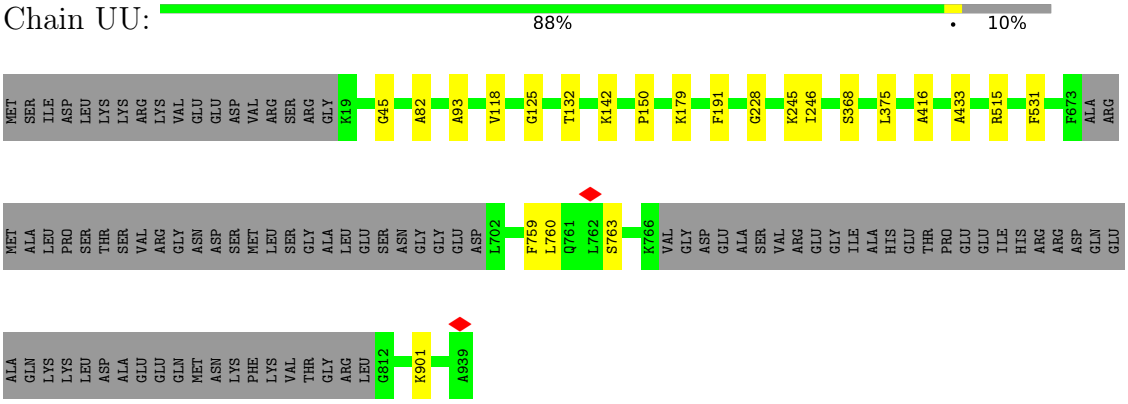
• Molecule 19: Nucleolar complex protein 4

Chain US:



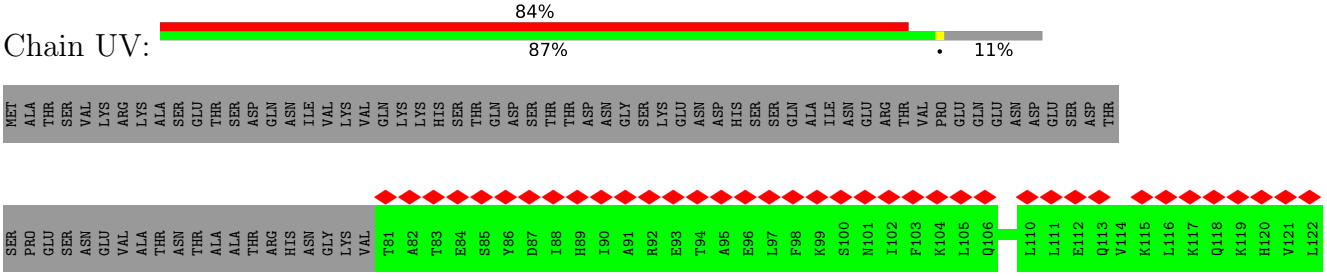
• Molecule 20: U3 small nucleolar RNA-associated protein 21

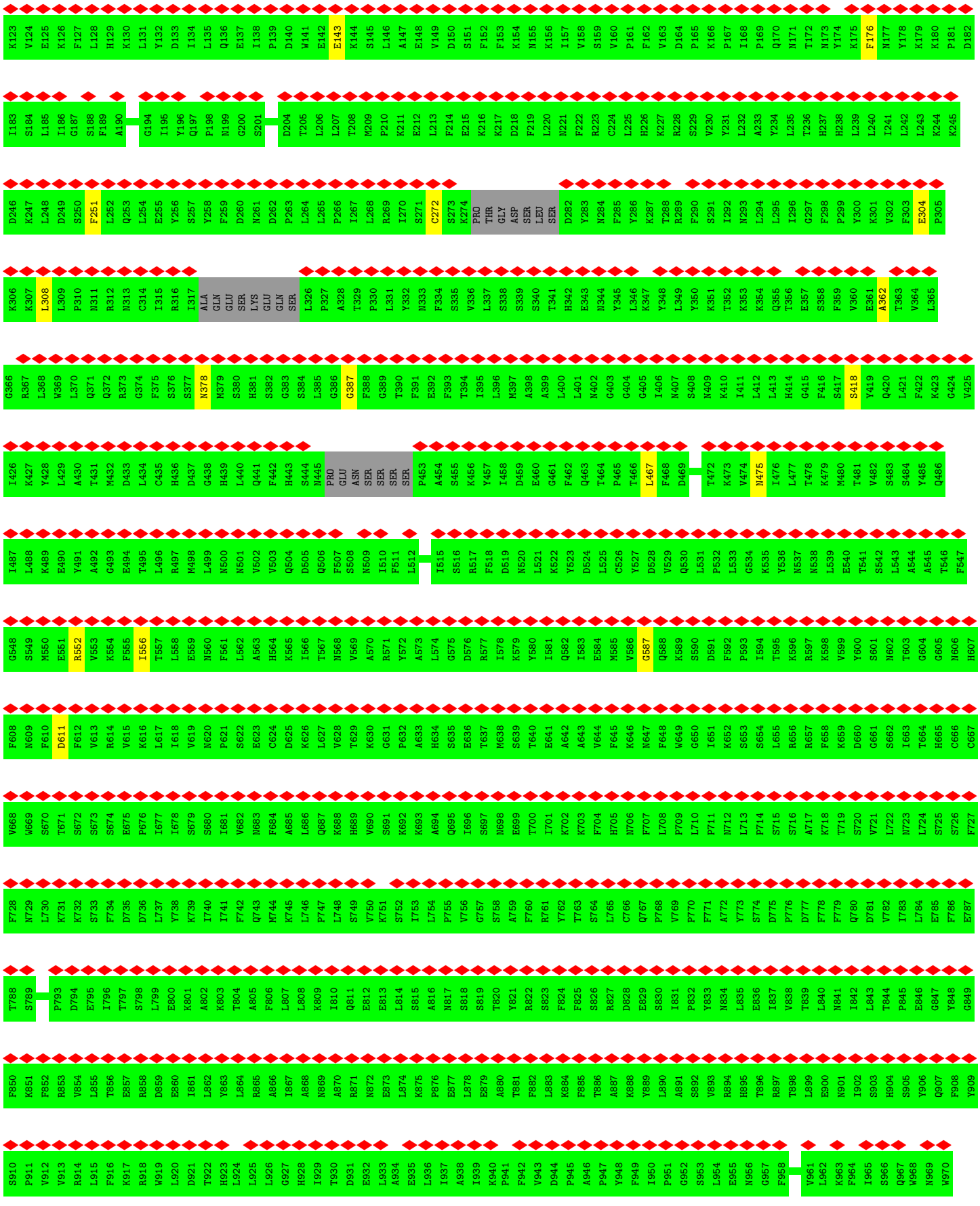
Chain UU:



• Molecule 21: U3 small nucleolar RNA-associated protein 22

Chain UV:

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I183 S184 L185 I186 G187 S188 F189 A190 G194 I195 Y196 Q197 P198 N199 C200 S201 D204 T205 L206 L207 T208 M209 P210 K211 E212 L213 F214 E215 K216 K217 D218 F219 L220 N221 F222 R223 C224 L225 H226 K227 R228 S229 V230 Y231 L232 A233 Y234 L235 T236 H237 H238 L239 L240 I241 L242 L243 K244 K245
D246 K247 L248 D249 S250 F251 L252 Q253 L254 E255 Y256 S257 Y258 F259 D260 N261 D262 P263 L264 L265 P266 I267 L268 R269 I270 S271 C272 S273 K274 PRO THR GLY ASP SER LEU SER D282 Y283 N284 F285 Y286 K287 T288 R289 F290 S291 I292 N293 L294 L295 I296 G297 F298 P299 Y300 K301 V302 F303 E304 P305
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T788 S789 P793 D794 E795 I796 T797 S798 L799 E800 K801 A802 K803 T804 A805 F806 L807 L808 K809 I810 Q811 E812 E813 L814 S815 A816 N817 S818 S819 T820 Y821 R822 S823 F824 F825 S826 R827 D828 E829 S830 I831 P832 Y833 N834 L835 E836 I837 V838 T839 L840 N841 I842 L843 T844 P845 E846 G847 Y848 G849
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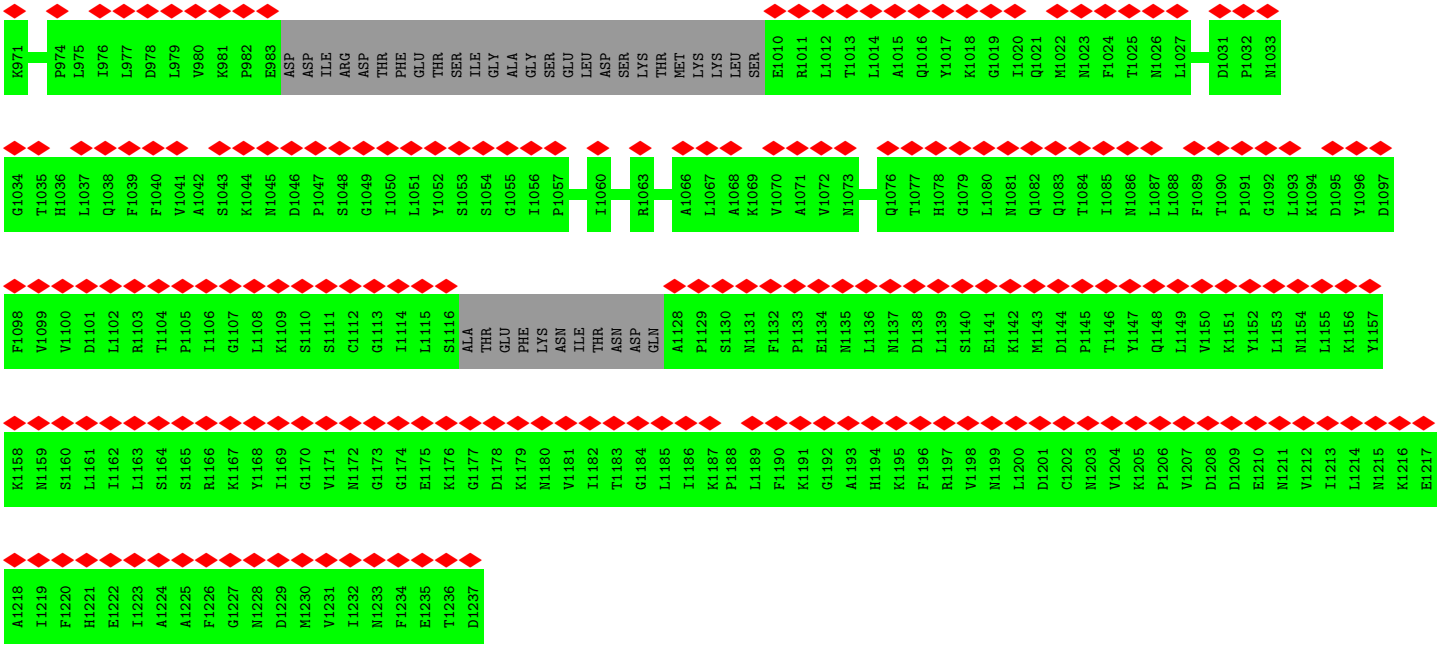
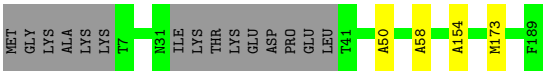


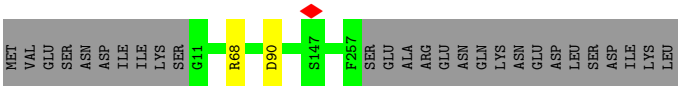
• Molecule 22: rRNA-processing protein FCF1

Chain UX:



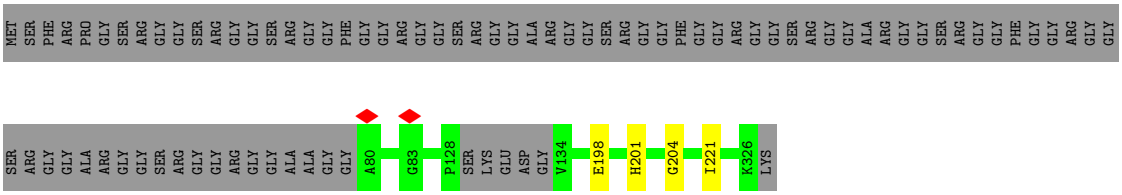
• Molecule 23: Ribosome biogenesis protein UTP30

Chain UZ:



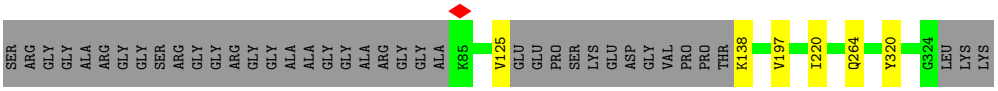
• Molecule 24: rRNA 2'-O-methyltransferase fibrillarin

Chain CA:



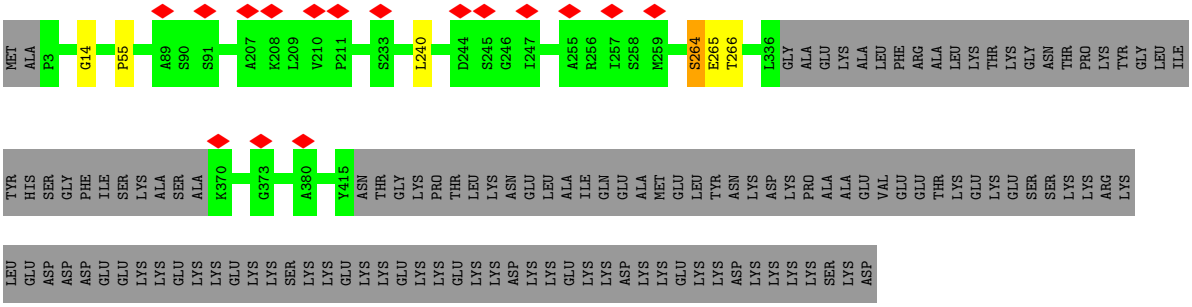
• Molecule 24: rRNA 2'-O-methyltransferase fibrillarin

Chain CB:



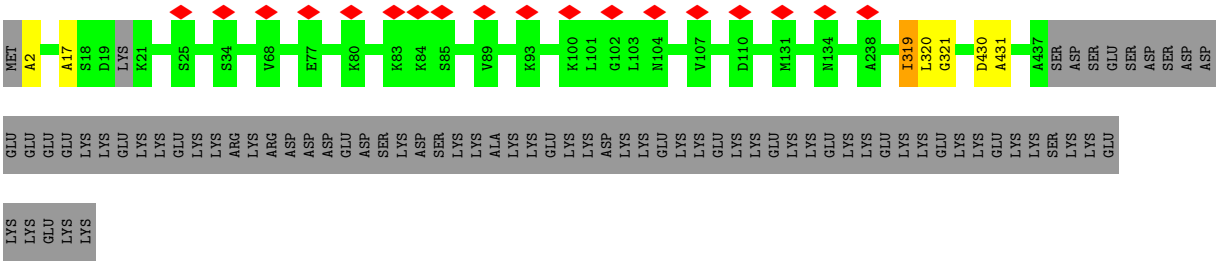
• Molecule 25: Nucleolar protein 56

Chain CD:



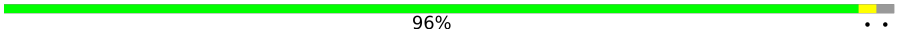
• Molecule 26: Nucleolar protein 58

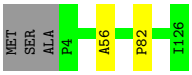
Chain CE:



• Molecule 27: 13 kDa ribonucleoprotein-associated protein

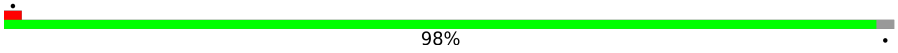
Chain CF:

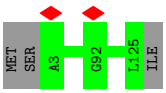




• Molecule 27: 13 kDa ribonucleoprotein-associated protein

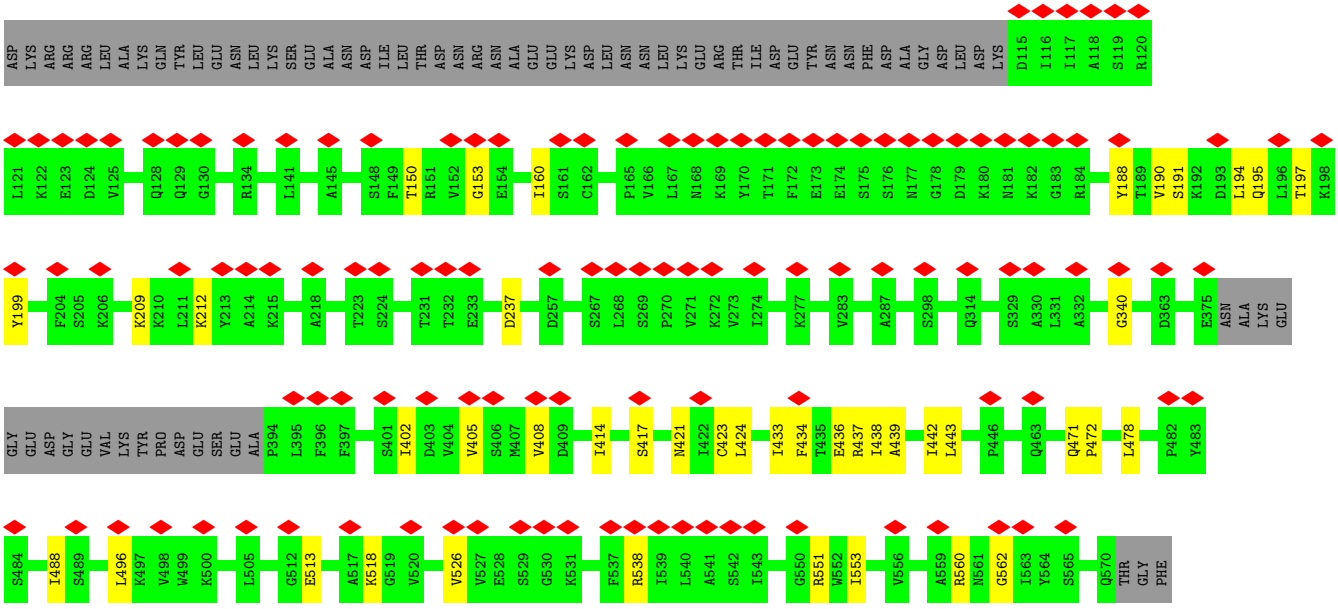
Chain CG:





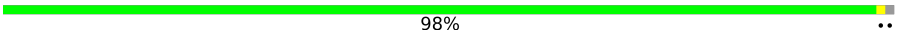
• Molecule 28: Ribosomal RNA-processing protein 9

Chain CH:



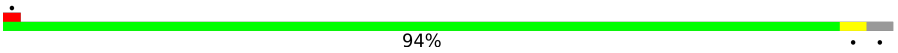
• Molecule 29: U3 small nucleolar ribonucleoprotein protein IMP3

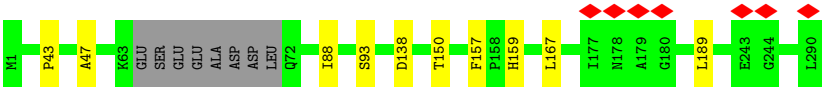
Chain CI:



• Molecule 30: U3 small nucleolar ribonucleoprotein protein IMP4

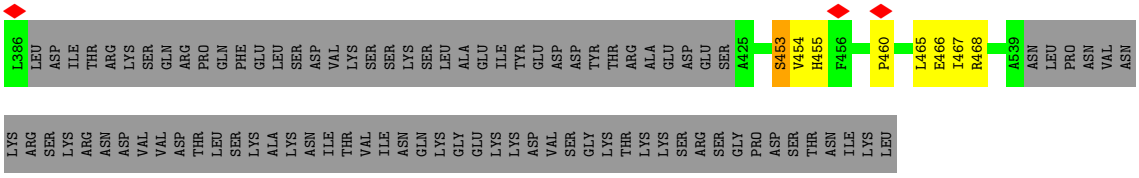
Chain CJ:





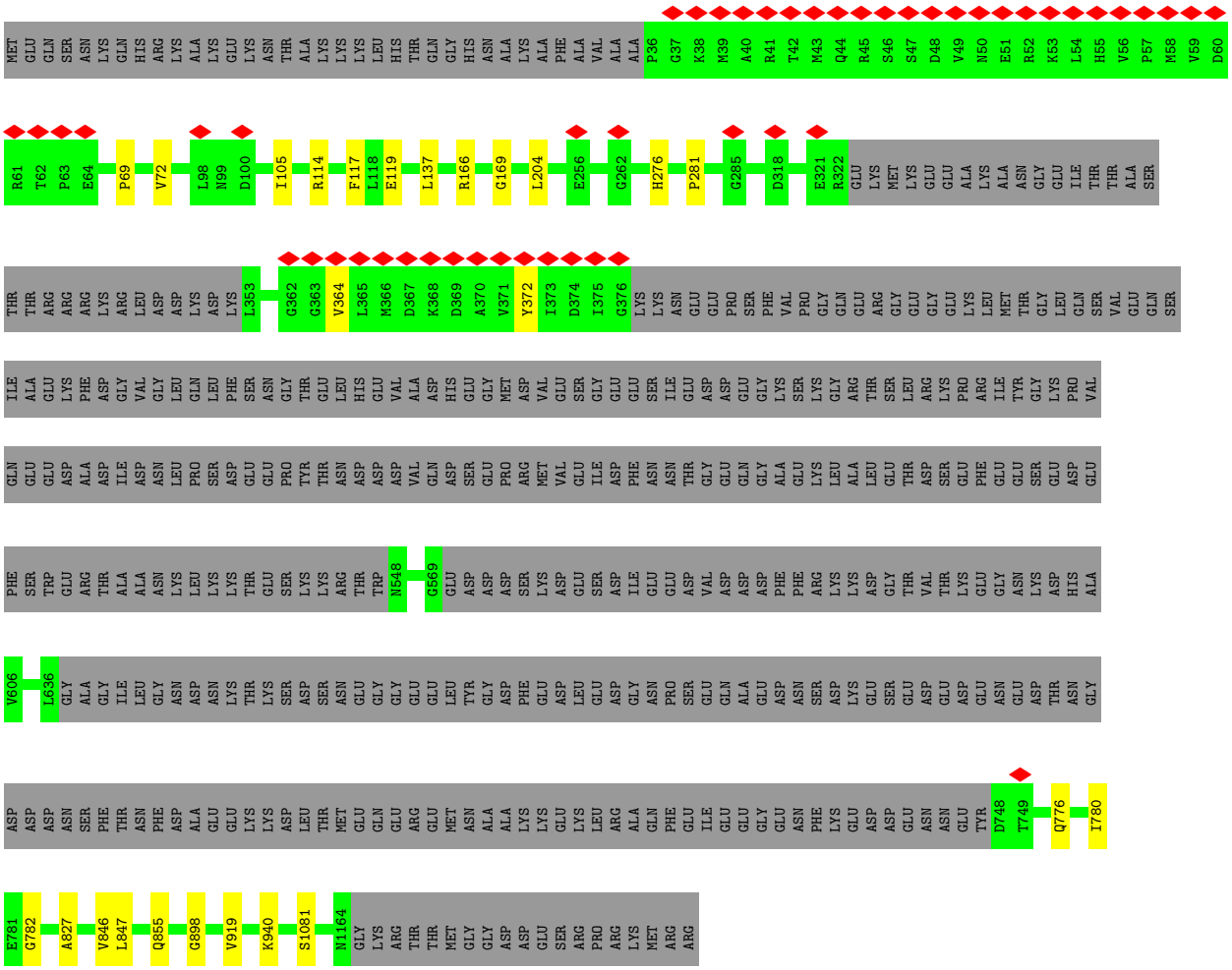
• Molecule 31: U3 small nucleolar RNA-associated protein MPP10

Chain CK:



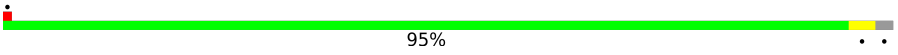
• Molecule 32: Ribosome biogenesis protein BMS1

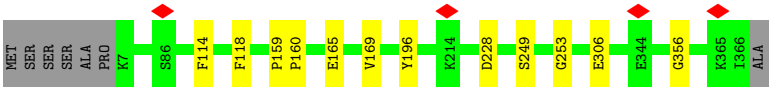
Chain CL:



• Molecule 33: RNA 3'-terminal phosphate cyclase-like protein

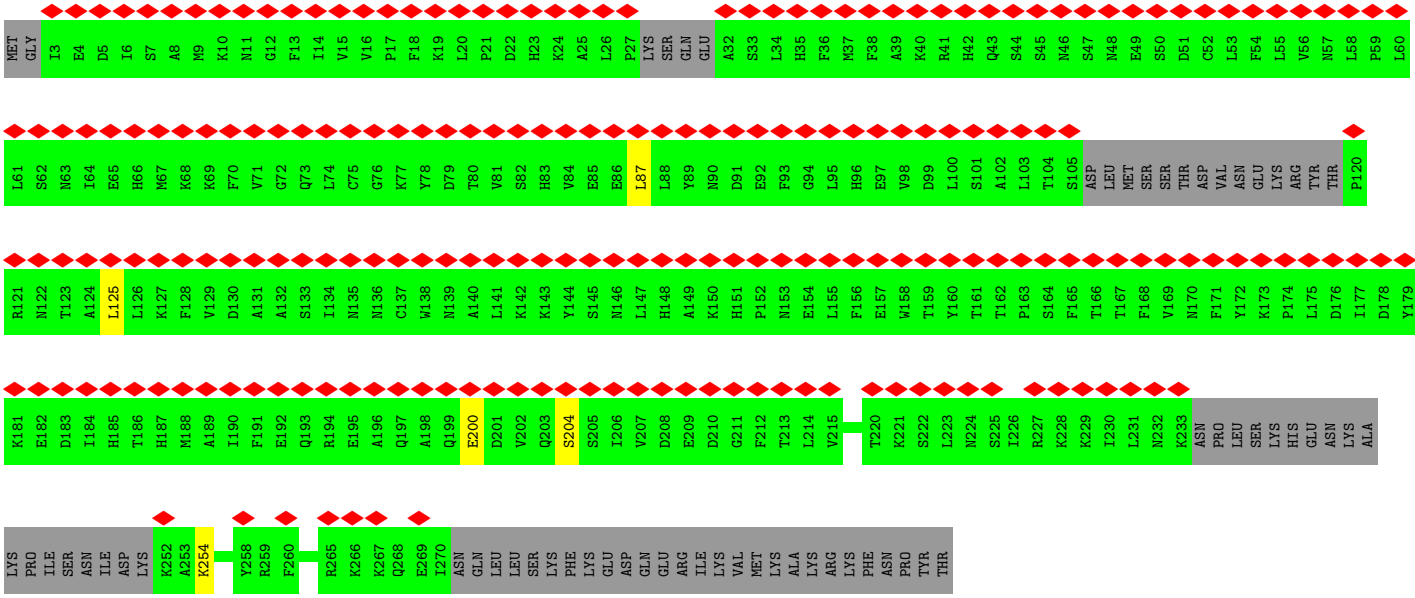
Chain CM:





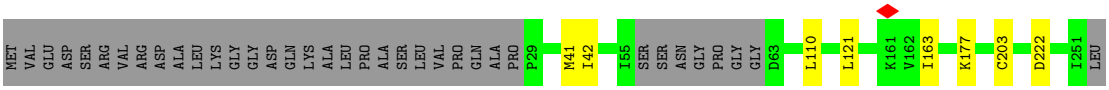
• Molecule 34: Ribosomal RNA-processing protein 7

Chain CN:



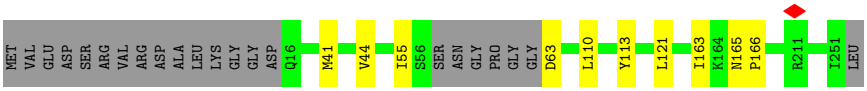
• Molecule 35: Ribosomal RNA small subunit methyltransferase NEP1

Chain JF:



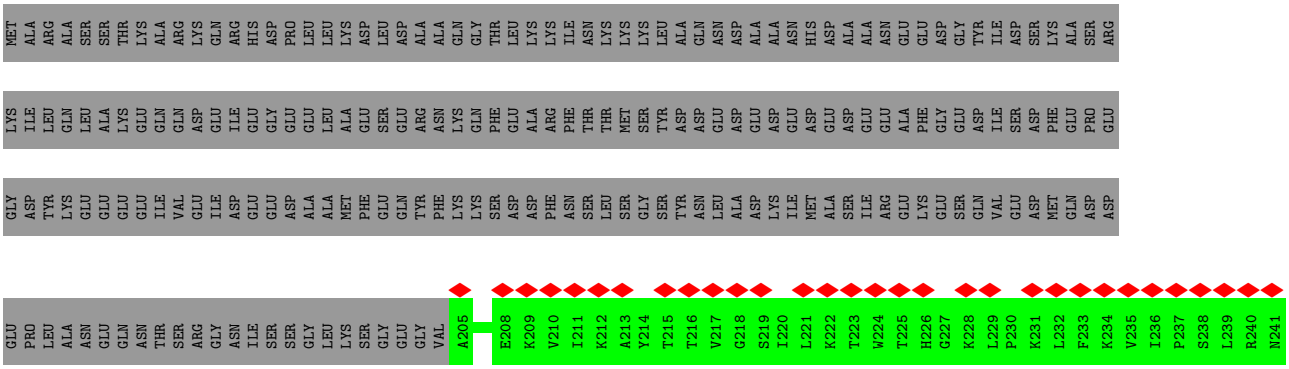
• Molecule 35: Ribosomal RNA small subunit methyltransferase NEP1

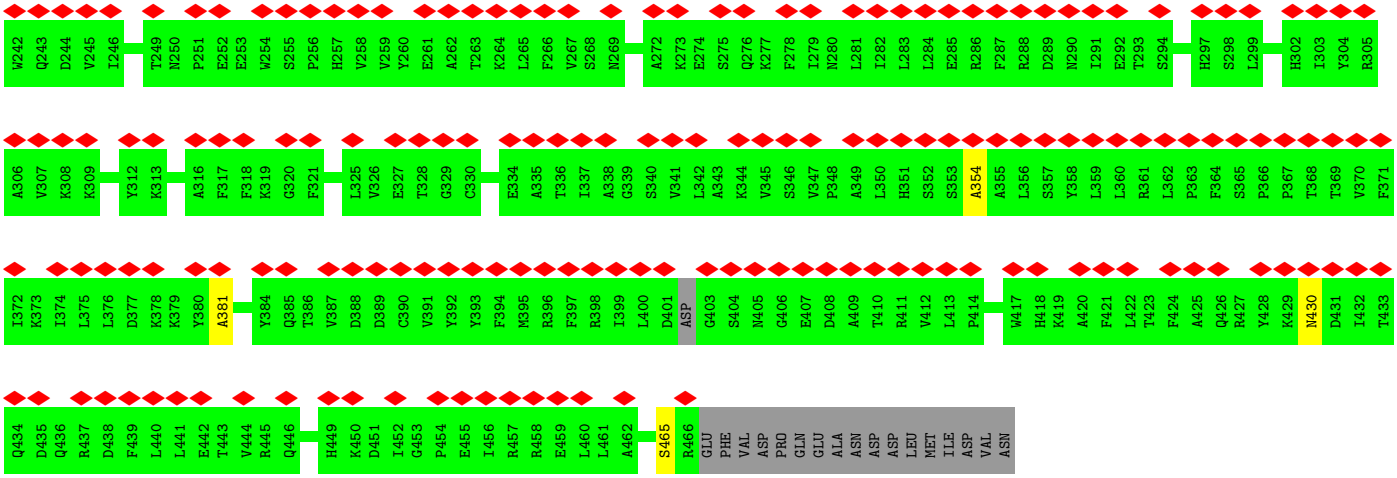
Chain JG:



• Molecule 36: Essential nuclear protein 1

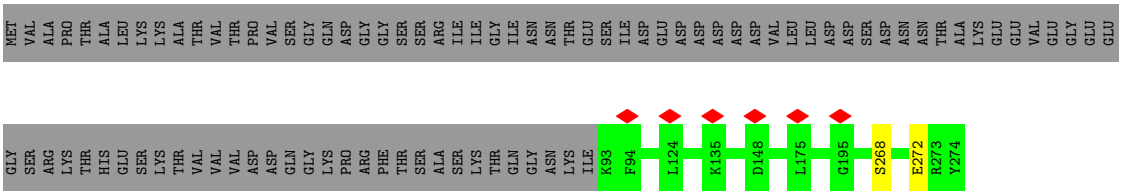
Chain JH:





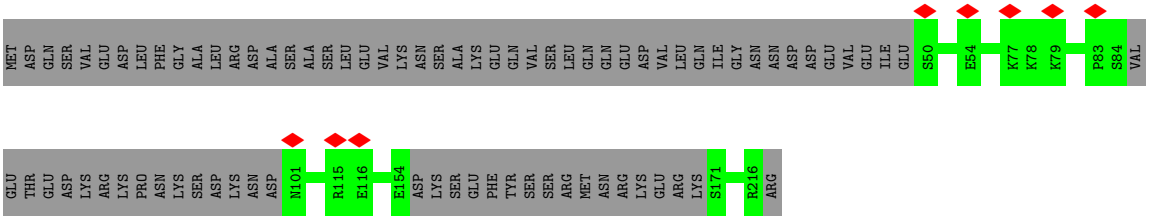
• Molecule 37: Pre-rRNA-processing protein PNO1

Chain JJ:



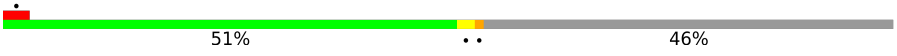
• Molecule 38: rRNA-processing protein FCF2

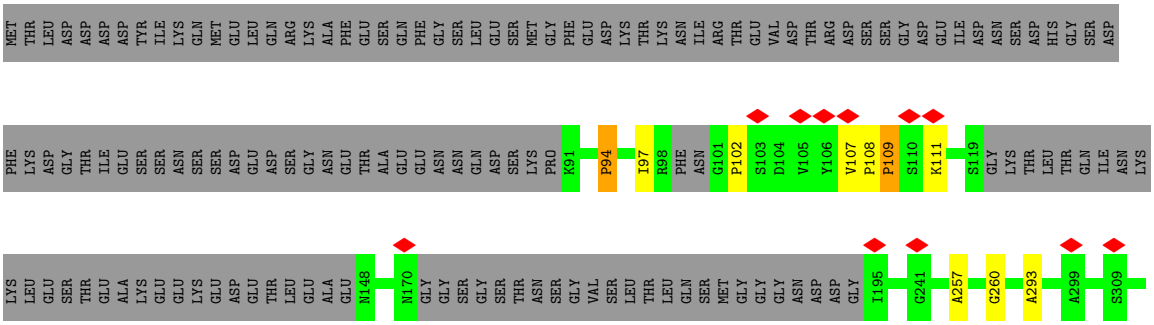
Chain JM:

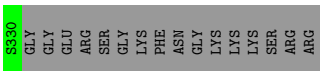


• Molecule 39: Protein FAF1

Chain JN:

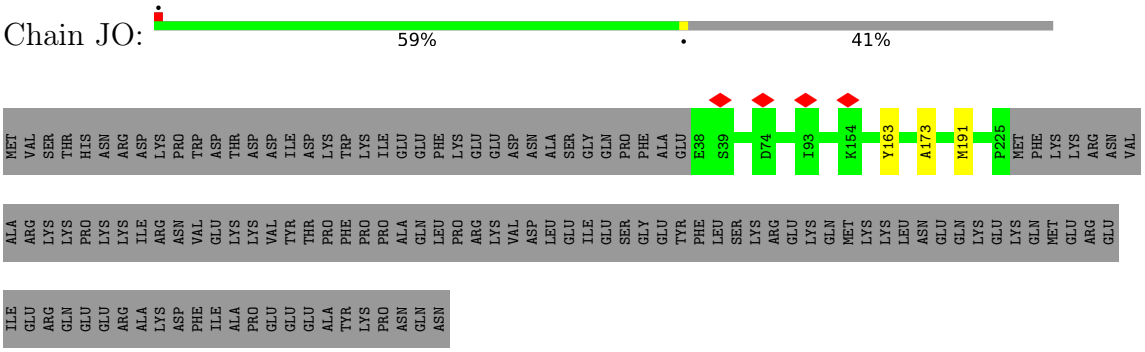






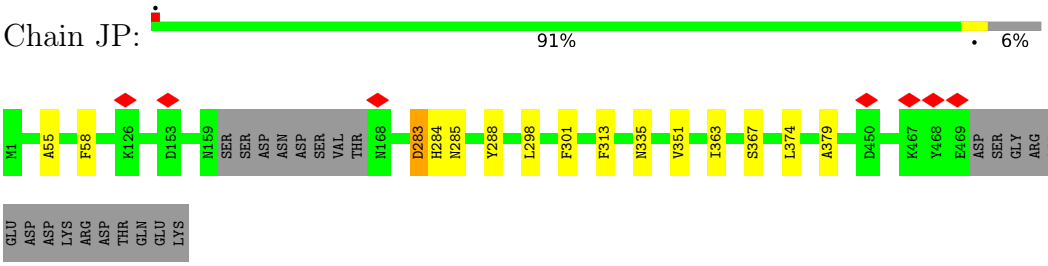
• Molecule 40: KRR1 small subunit processome component

Chain JO:



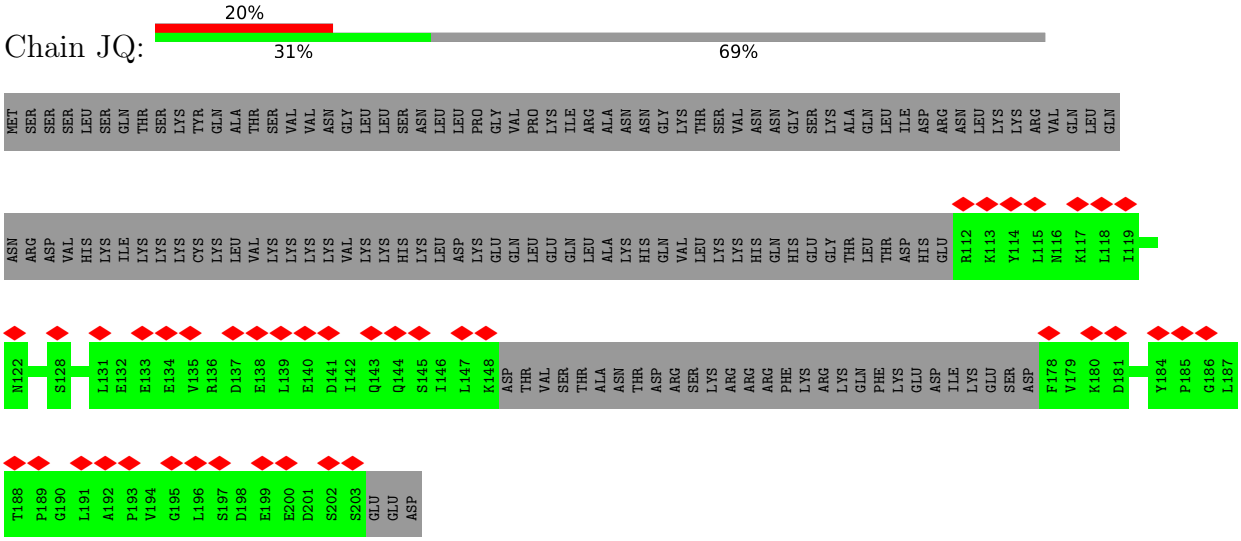
• Molecule 41: Protein SOF1

Chain JP:



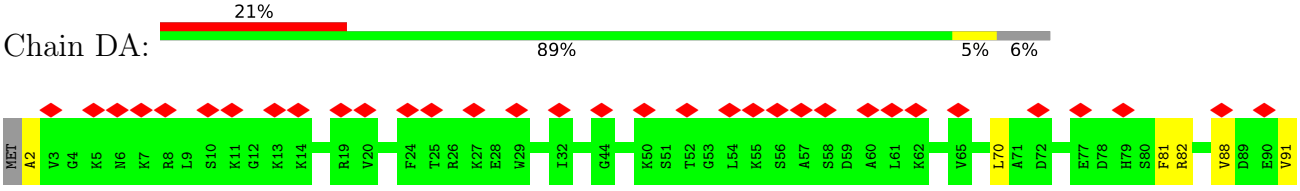
• Molecule 42: Regulator of rDNA transcription protein 14

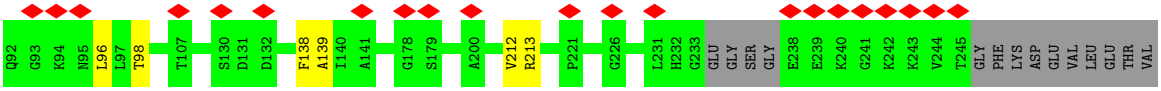
Chain JQ:



• Molecule 43: 40S ribosomal protein S1-A

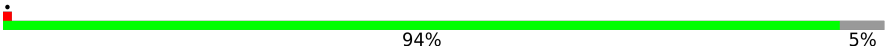
Chain DA:

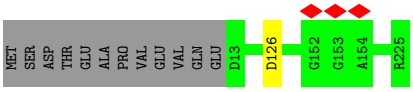




• Molecule 44: Rps5p

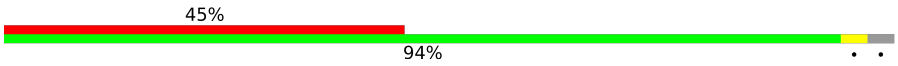
Chain DF:

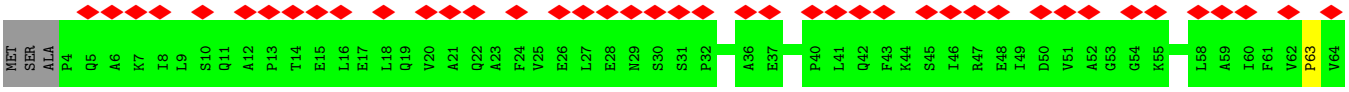


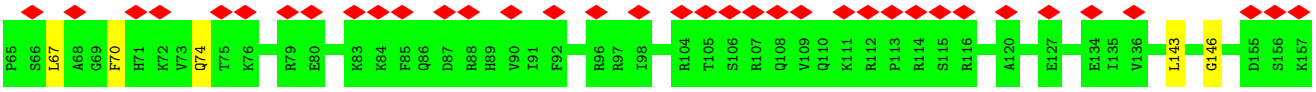


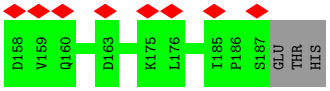
• Molecule 45: 40S ribosomal protein S7-A

Chain DH:



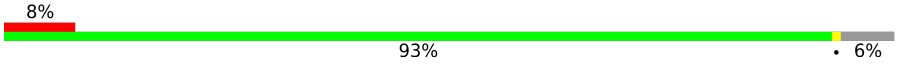


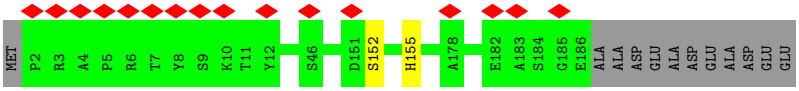




• Molecule 46: 40S ribosomal protein S9-A

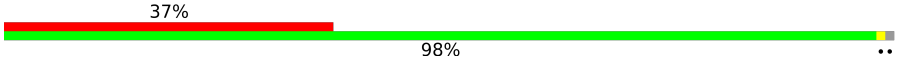
Chain DJ:

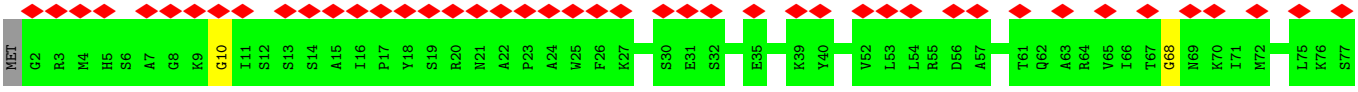


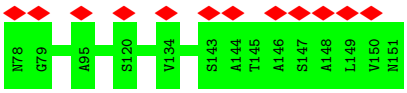


• Molecule 47: 40S ribosomal protein S13

Chain DN:

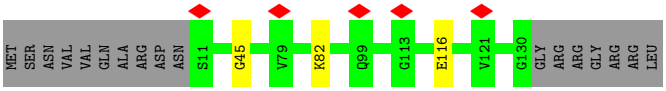






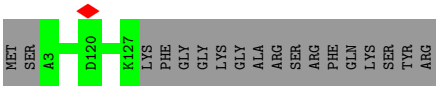
• Molecule 48: 40S ribosomal protein S14-A

Chain DO:



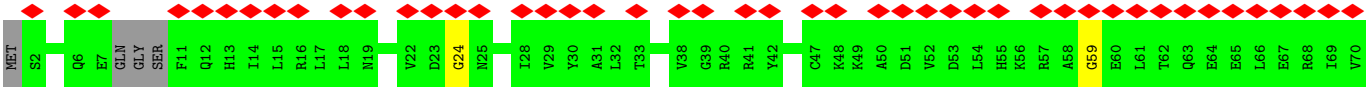
• Molecule 49: 40S ribosomal protein S16-A

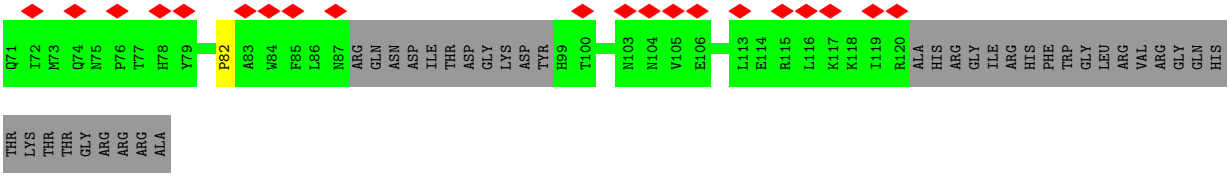
Chain DQ:



• Molecule 50: 40S ribosomal protein S18-A

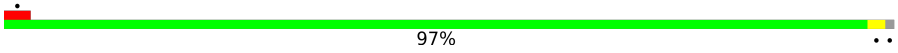
Chain DS:

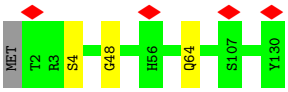




• Molecule 51: 40S ribosomal protein S22-A

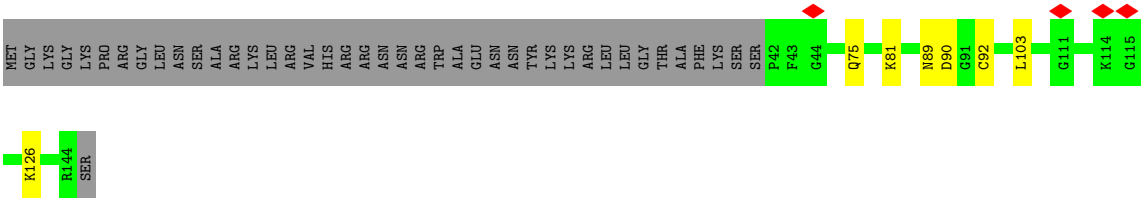
Chain DW:





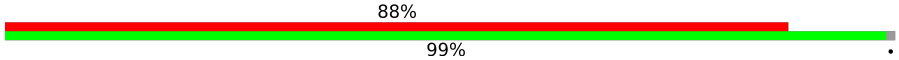
• Molecule 52: 40S ribosomal protein S23-A

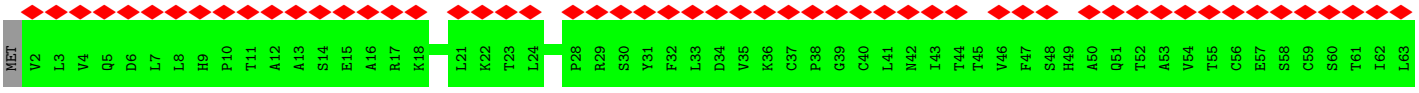
Chain DX:

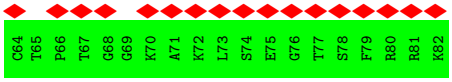


• Molecule 53: 40S ribosomal protein S27-A

Chain Db:

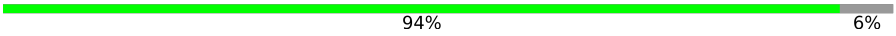


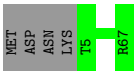




• Molecule 54: 40S ribosomal protein S28-A

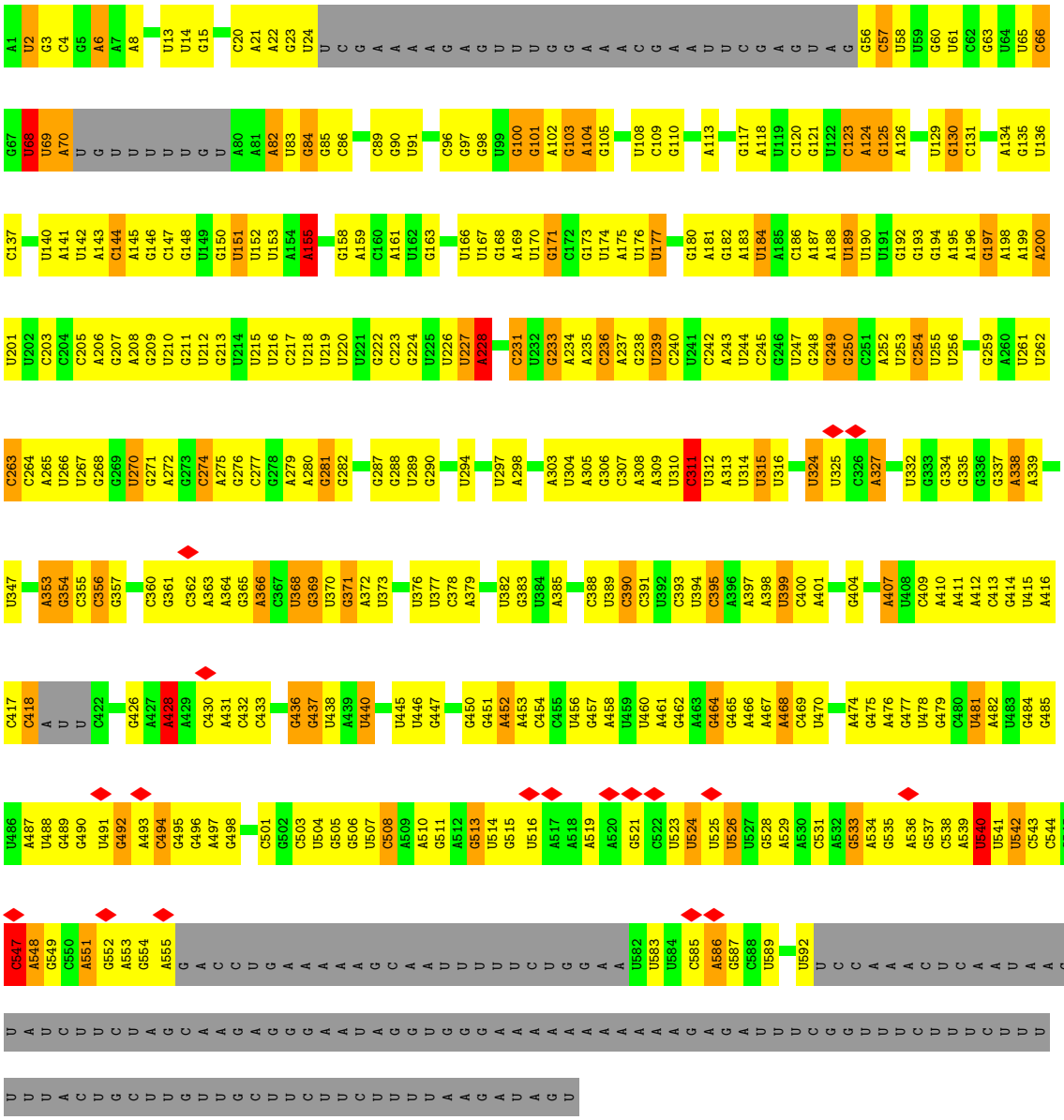
Chain Dc:





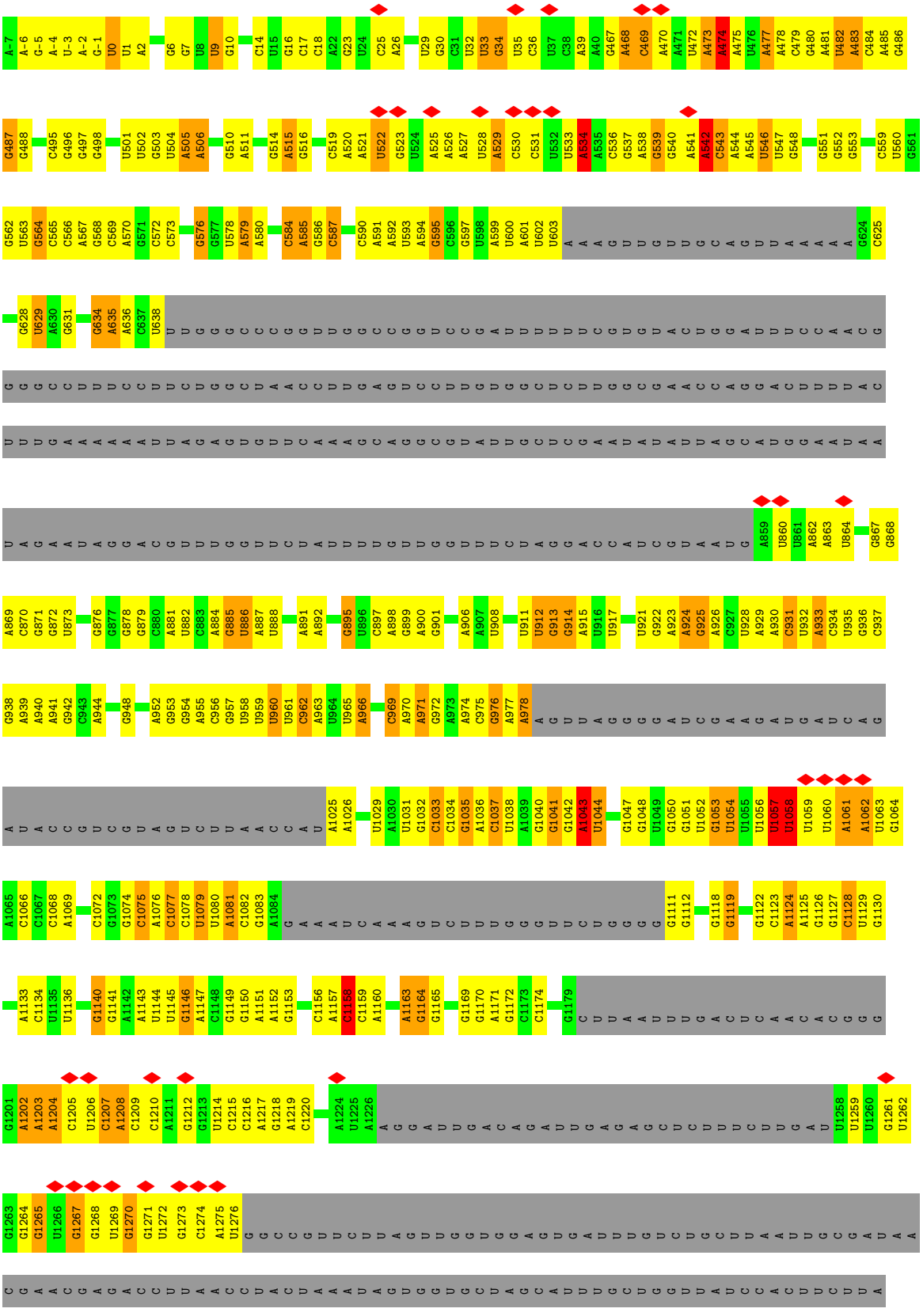
• Molecule 55: 5ETS RNA

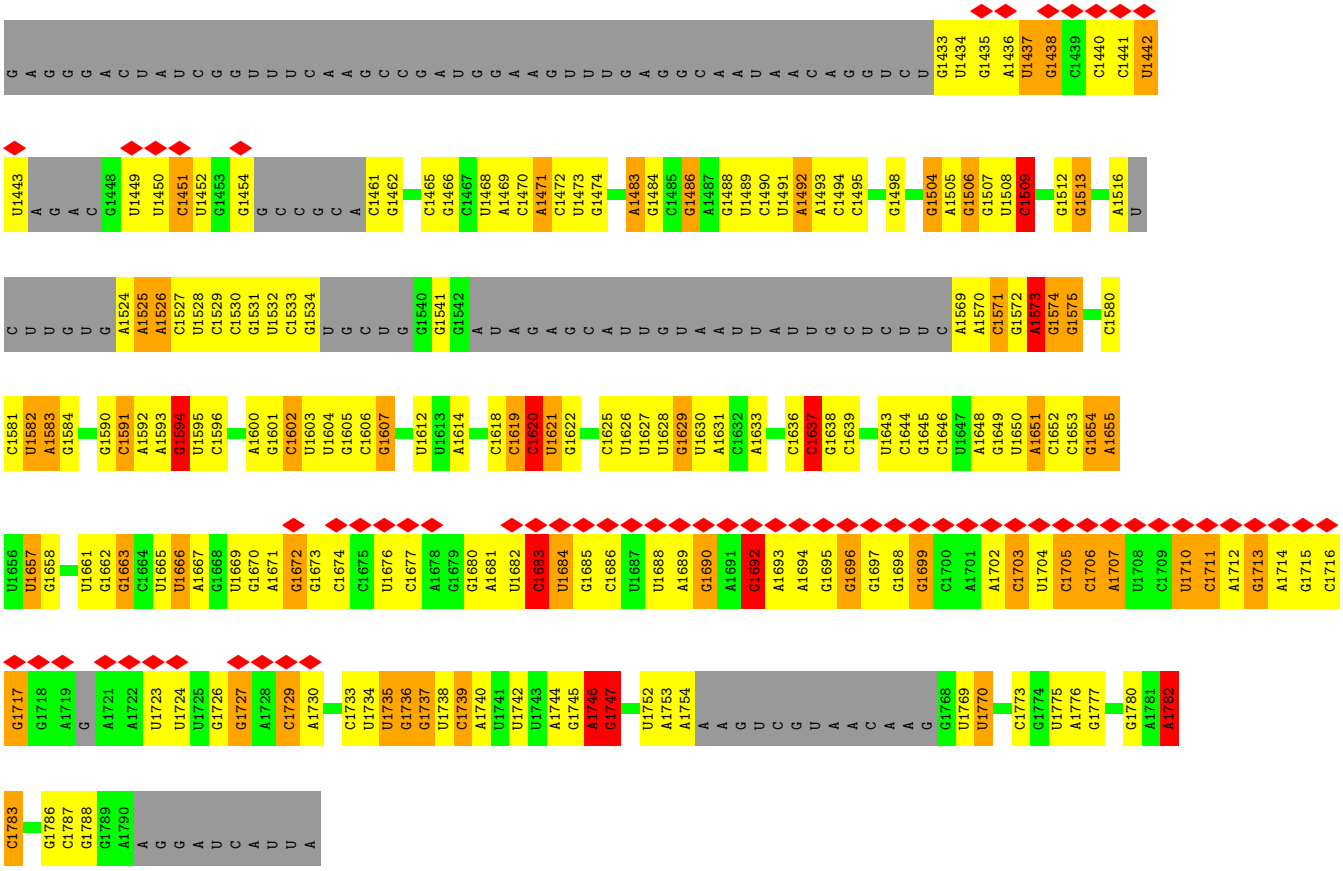
Chain D2:



• Molecule 56: 18S rRNA

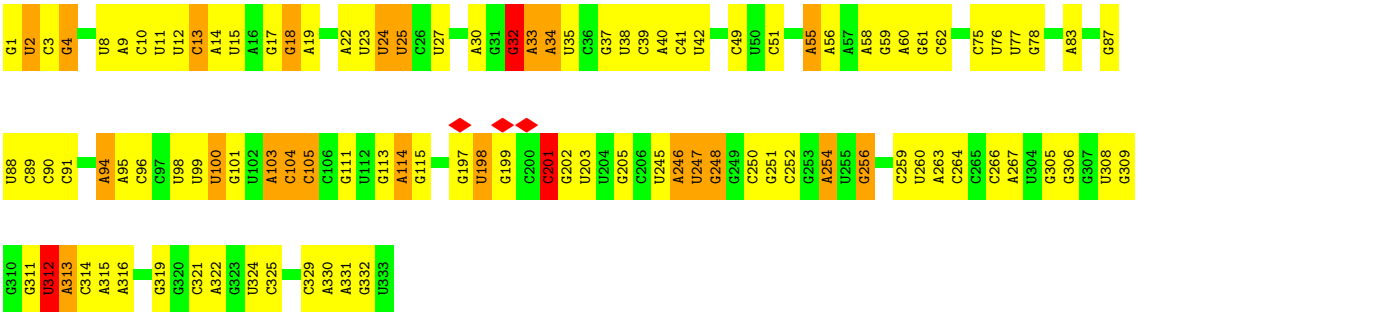
Chain D3:





• Molecule 57: U3 snoRNA

Chain D4:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11194	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	44, 44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k), GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.062	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	508.32, 508.32, 508.32	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, 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	UA	0.42	0/4119	0.64	0/5734
2	UB	0.33	0/2506	0.57	4/3494 (0.1%)
3	UC	0.35	0/626	0.56	0/866
4	UD	0.39	0/3333	0.64	0/4635
5	UE	0.40	0/2348	0.64	1/3266 (0.0%)
6	UF	0.36	0/1451	0.50	0/2018
7	UG	0.44	0/2627	0.61	0/3653
8	UH	0.32	0/2182	0.67	10/3030 (0.3%)
9	UI	0.32	0/515	0.50	0/716
10	UJ	0.34	0/3618	0.53	0/5055
11	UK	0.37	0/1201	0.52	0/1674
12	UL	0.34	0/4156	0.61	0/5779
13	UM	0.32	0/3757	0.61	0/5222
14	UN	0.34	0/731	0.57	0/1019
15	UO	0.39	0/2439	0.59	0/3397
16	UP	0.33	0/297	0.53	0/413
17	UQ	0.37	0/4116	0.61	1/5730 (0.0%)
18	UR	0.45	1/2373 (0.0%)	0.61	0/3296
19	US	0.34	0/2350	0.55	1/3274 (0.0%)
20	UU	0.41	0/4178	0.61	0/5809
21	UV	0.25	0/5436	0.51	0/7572
22	UX	0.38	0/860	0.56	0/1196
23	UZ	0.34	0/1223	0.56	0/1704
24	CA	0.42	0/1188	0.59	0/1648
24	CB	0.37	0/1120	0.64	0/1554
25	CD	0.34	0/1878	0.54	0/2614
26	CE	0.34	0/2153	0.55	0/2999
27	CF	0.39	0/610	0.58	0/850
27	CG	0.37	0/610	0.58	0/850
28	CH	0.30	0/2156	0.66	0/2996
29	CI	0.42	0/904	0.60	0/1261
30	CJ	0.40	0/1395	0.61	0/1942

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	CK	0.36	0/1029	0.58	0/1435
32	CL	0.37	1/3854 (0.0%)	0.56	1/5361 (0.0%)
33	CM	0.33	0/1766	0.58	0/2451
34	CN	0.25	0/1150	0.50	0/1600
35	JF	0.33	0/1069	0.55	0/1488
35	JG	0.36	0/1139	0.59	0/1586
36	JH	0.29	0/1293	0.54	0/1801
37	JJ	0.31	0/897	0.54	0/1247
38	JM	0.36	0/668	0.54	0/928
39	JN	0.32	0/914	0.65	4/1266 (0.3%)
40	JO	0.32	0/932	0.56	0/1299
41	JP	0.42	1/2281 (0.0%)	0.63	0/3177
42	JQ	0.33	0/310	0.52	0/429
43	DA	0.29	0/1185	0.57	0/1648
44	DF	0.38	0/1054	0.54	0/1468
45	DH	0.29	0/912	0.56	0/1271
46	DJ	0.34	0/914	0.55	0/1272
47	DN	0.28	0/741	0.55	0/1031
48	DO	0.34	0/586	0.57	0/811
49	DQ	0.37	0/615	0.60	0/854
50	DS	0.28	0/518	0.52	0/718
51	DW	0.32	0/633	0.58	0/878
52	DX	0.34	0/502	0.56	0/694
53	Db	0.26	0/399	0.54	0/554
54	Dc	0.40	0/309	0.56	0/428
55	D2	0.89	2/12482 (0.0%)	1.28	112/19446 (0.6%)
56	D3	0.76	3/18789 (0.0%)	1.36	243/29248 (0.8%)
57	D4	0.91	1/4142 (0.0%)	1.28	27/6435 (0.4%)
All	All	0.53	9/129539 (0.0%)	0.87	404/186090 (0.2%)

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	UA	0	1
2	UB	0	1
4	UD	0	3
5	UE	0	2
10	UJ	0	2
12	UL	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	UM	0	4
14	UN	0	1
17	UQ	0	2
20	UU	0	1
23	UZ	0	1
25	CD	0	1
26	CE	0	1
28	CH	0	3
31	CK	0	1
32	CL	0	1
34	CN	0	1
40	JO	0	1
41	JP	0	3
44	DF	0	1
All	All	0	36

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	D3	1158	C	N3-C4	-8.09	1.28	1.33
56	D3	1164	G	C6-O6	-7.08	1.17	1.24
41	JP	313	PHE	C-N	-5.88	1.20	1.34
57	D4	83	A	N9-C4	-5.55	1.34	1.37
55	D2	388	C	C2-O2	-5.50	1.19	1.24
56	D3	553	G	C2-N3	-5.49	1.28	1.32
32	CL	1081	SER	CA-CB	-5.47	1.44	1.52
55	D2	298	A	N9-C4	-5.12	1.34	1.37
18	UR	570	PHE	C-N	-5.12	1.22	1.34

All (404) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	D3	1164	G	N1-C6-O6	-29.76	102.04	119.90
56	D3	1158	C	N3-C4-N4	-24.46	100.88	118.00
56	D3	1158	C	C5-C4-N4	19.67	133.97	120.20
56	D3	1164	G	C5-C6-O6	17.37	139.02	128.60
56	D3	1705	C	N3-C2-O2	-12.32	113.28	121.90
55	D2	394	U	C2-N1-C1'	11.55	131.56	117.70
56	D3	1164	G	C5-C6-N1	11.40	117.20	111.50
57	D4	13	C	N1-C2-O2	11.34	125.70	118.90
5	UE	472	LEU	C-N-CA	11.18	149.66	121.70
57	D4	13	C	N3-C2-O2	-10.96	114.23	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	D2	356	C	N3-C2-O2	-10.36	114.65	121.90
56	D3	474	A	N1-C6-N6	-10.35	112.39	118.60
56	D3	553	G	N3-C4-N9	-10.28	119.83	126.00
56	D3	1705	C	N1-C2-O2	10.02	124.91	118.90
55	D2	394	U	N1-C2-O2	9.65	129.55	122.80
55	D2	524	U	OP1-P-O3'	-9.61	84.05	105.20
55	D2	151	U	C2-N1-C1'	9.59	129.21	117.70
56	D3	1703	C	N3-C2-O2	-9.49	115.25	121.90
55	D2	524	U	OP2-P-O3'	-9.31	84.72	105.20
55	D2	418	C	N3-C2-O2	-9.29	115.39	121.90
56	D3	1739	C	C6-N1-C2	-9.24	116.60	120.30
56	D3	563	U	N1-C2-O2	9.21	129.24	122.80
55	D2	394	U	N3-C2-O2	-9.13	115.81	122.20
56	D3	553	G	N9-C4-C5	9.12	109.05	105.40
56	D3	1066	C	N3-C2-O2	-8.95	115.64	121.90
56	D3	563	U	C2-N1-C1'	8.93	128.42	117.70
56	D3	1077	C	N3-C2-O2	-8.91	115.67	121.90
56	D3	553	G	C8-N9-C1'	8.86	138.52	127.00
55	D2	356	C	C6-N1-C2	-8.85	116.76	120.30
55	D2	151	U	N1-C2-O2	8.78	128.95	122.80
56	D3	551	G	N3-C4-N9	8.78	131.27	126.00
55	D2	144	C	N1-C2-O2	8.73	124.14	118.90
55	D2	108	U	N1-C2-O2	8.53	128.77	122.80
56	D3	976	G	C4-N9-C1'	8.45	137.49	126.50
55	D2	481	U	N1-C2-O2	8.42	128.70	122.80
56	D3	1128	C	N3-C2-O2	-8.38	116.03	121.90
56	D3	1729	C	N3-C2-O2	-8.36	116.05	121.90
55	D2	263	C	N3-C2-O2	-8.26	116.12	121.90
55	D2	108	U	C2-N1-C1'	8.19	127.53	117.70
56	D3	1653	C	N3-C2-O2	-8.16	116.19	121.90
56	D3	563	U	N3-C2-O2	-8.14	116.50	122.20
56	D3	553	G	C6-C5-N7	8.13	135.28	130.40
56	D3	1066	C	N1-C2-O2	8.10	123.76	118.90
2	UB	400	PRO	N-CA-CB	8.09	113.01	103.30
56	D3	1075	C	C6-N1-C2	-7.96	117.12	120.30
55	D2	123	C	C2-N1-C1'	7.94	127.53	118.80
56	D3	1158	C	N3-C4-C5	7.93	125.07	121.90
55	D2	151	U	N3-C2-O2	-7.92	116.66	122.20
55	D2	355	C	N1-C2-O2	7.92	123.65	118.90
56	D3	1746	A	N1-C6-N6	-7.82	113.91	118.60
56	D3	1495	C	N3-C2-O2	-7.80	116.44	121.90
56	D3	553	G	N3-C2-N2	-7.77	114.46	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	D2	394	U	C6-N1-C1'	-7.76	110.33	121.20
55	D2	123	C	N1-C2-O2	7.74	123.54	118.90
55	D2	356	C	N1-C2-O2	7.70	123.52	118.90
56	D3	1163	A	C6-N1-C2	-7.70	113.98	118.60
57	D4	55	A	O4'-C1'-N9	7.67	114.33	108.20
56	D3	1123	C	N1-C2-O2	7.64	123.49	118.90
55	D2	68	U	N3-C2-O2	-7.58	116.89	122.20
56	D3	553	G	C4-N9-C1'	-7.55	116.68	126.50
55	D2	123	C	C6-N1-C2	-7.54	117.28	120.30
56	D3	1449	U	N1-C2-O2	7.50	128.05	122.80
55	D2	481	U	N3-C2-O2	-7.50	116.95	122.20
57	D4	100	U	N3-C2-O2	-7.49	116.96	122.20
55	D2	231	C	C2-N1-C1'	7.48	127.02	118.80
56	D3	976	G	C8-N9-C1'	-7.47	117.29	127.00
56	D3	1727	G	N3-C4-N9	7.47	130.48	126.00
56	D3	1692	G	C2-N3-C4	7.42	115.61	111.90
55	D2	355	C	C2-N1-C1'	7.42	126.96	118.80
56	D3	1210	C	C5-C6-N1	7.42	124.71	121.00
56	D3	551	G	C6-C5-N7	-7.42	125.95	130.40
56	D3	536	C	C2-N1-C1'	7.41	126.95	118.80
56	D3	551	G	C8-N9-C1'	-7.31	117.50	127.00
56	D3	551	G	C4-N9-C1'	7.28	135.97	126.50
56	D3	587	C	N3-C2-O2	-7.28	116.81	121.90
56	D3	1220	C	C5-C6-N1	7.27	124.64	121.00
56	D3	1440	C	C5-C6-N1	7.27	124.64	121.00
56	D3	1705	C	C6-N1-C2	-7.25	117.40	120.30
56	D3	885	G	C4-N9-C1'	7.21	135.87	126.50
56	D3	553	G	N1-C6-O6	-7.20	115.58	119.90
57	D4	100	U	N1-C2-O2	7.17	127.82	122.80
56	D3	1739	C	N3-C2-O2	-7.11	116.92	121.90
57	D4	312	U	C5-C6-N1	7.07	126.23	122.70
56	D3	1747	G	N3-C4-N9	7.02	130.21	126.00
56	D3	1654	G	N9-C4-C5	-7.02	102.59	105.40
56	D3	542	A	N7-C8-N9	7.01	117.30	113.80
56	D3	486	G	O4'-C1'-N9	6.98	113.78	108.20
56	D3	1637	C	N3-C2-O2	-6.98	117.01	121.90
56	D3	14	C	N3-C2-O2	-6.97	117.02	121.90
56	D3	551	G	C4-C5-N7	6.96	113.59	110.80
55	D2	66	C	C5-C6-N1	6.95	124.47	121.00
55	D2	525	U	OP1-P-OP2	6.95	130.02	119.60
55	D2	274	C	N3-C2-O2	-6.94	117.04	121.90
56	D3	551	G	N9-C4-C5	-6.94	102.62	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	D2	144	C	C2-N1-C1'	6.92	126.41	118.80
57	D4	312	U	C6-N1-C2	-6.91	116.86	121.00
55	D2	108	U	C6-N1-C1'	-6.88	111.56	121.20
55	D2	231	C	C6-N1-C2	-6.86	117.56	120.30
56	D3	1449	U	N3-C2-O2	-6.85	117.41	122.20
55	D2	481	U	C2-N1-C1'	6.83	125.90	117.70
55	D2	369	G	N3-C4-N9	6.78	130.07	126.00
56	D3	1433	G	C4-N9-C1'	6.78	135.31	126.50
56	D3	1747	G	C6-C5-N7	-6.78	126.33	130.40
55	D2	391	C	C2-N1-C1'	6.77	126.24	118.80
39	JN	108	PRO	N-CA-CB	6.76	111.42	103.30
56	D3	579	A	P-O3'-C3'	6.76	127.81	119.70
55	D2	250	G	C2-N3-C4	-6.74	108.53	111.90
56	D3	1033	C	N1-C2-O2	6.74	122.94	118.90
55	D2	390	C	N3-C2-O2	-6.70	117.21	121.90
56	D3	885	G	C8-N9-C1'	-6.70	118.29	127.00
56	D3	14	C	C6-N1-C2	-6.68	117.63	120.30
56	D3	1056	U	C5-C6-N1	6.68	126.04	122.70
55	D2	123	C	C5-C6-N1	6.66	124.33	121.00
8	UH	235	PRO	N-CA-CB	6.64	111.27	103.30
56	D3	1696	G	C5-C6-O6	6.61	132.57	128.60
55	D2	68	U	N1-C2-O2	6.60	127.42	122.80
56	D3	564	G	C4-C5-N7	6.58	113.43	110.80
56	D3	1164	G	C6-N1-C2	-6.57	121.16	125.10
57	D4	314	C	N3-C2-O2	-6.54	117.32	121.90
56	D3	1527	C	C2-N1-C1'	6.53	125.98	118.80
56	D3	1440	C	C6-N1-C2	-6.50	117.70	120.30
56	D3	1215	C	C6-N1-C2	-6.49	117.70	120.30
55	D2	151	U	C5-C6-N1	6.49	125.95	122.70
56	D3	1033	C	N3-C2-O2	-6.49	117.36	121.90
55	D2	356	C	C2-N1-C1'	6.45	125.90	118.80
57	D4	13	C	C2-N1-C1'	6.45	125.89	118.80
8	UH	325	PRO	N-CA-CB	6.44	111.03	103.30
57	D4	89	C	C6-N1-C2	-6.43	117.73	120.30
39	JN	109	PRO	N-CA-CB	6.42	111.01	103.30
55	D2	508	C	C5-C6-N1	6.41	124.20	121.00
55	D2	144	C	N3-C2-O2	-6.40	117.42	121.90
56	D3	1673	G	C8-N9-C4	-6.40	103.84	106.40
56	D3	563	U	C6-N1-C1'	-6.38	112.26	121.20
56	D3	1674	C	N1-C2-O2	6.38	122.73	118.90
19	US	37	PRO	N-CA-CB	6.37	110.94	103.30
56	D3	912	U	P-O3'-C3'	6.36	127.33	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	D3	1128	C	C6-N1-C2	-6.35	117.76	120.30
56	D3	908	U	C5-C6-N1	6.34	125.87	122.70
56	D3	913	G	N3-C4-N9	6.34	129.80	126.00
55	D2	123	C	N3-C2-O2	-6.33	117.47	121.90
56	D3	1077	C	N1-C2-O2	6.33	122.70	118.90
56	D3	1220	C	C2-N1-C1'	6.33	125.76	118.80
56	D3	1746	A	O4'-C1'-N9	6.32	113.26	108.20
56	D3	975	C	C6-N1-C2	-6.31	117.78	120.30
55	D2	547	C	N1-C2-O2	6.31	122.69	118.90
55	D2	216	U	C5-C6-N1	6.30	125.85	122.70
56	D3	1692	G	N3-C4-C5	-6.27	125.47	128.60
56	D3	1729	C	N1-C2-O2	6.26	122.66	118.90
8	UH	67	PRO	N-CA-CB	6.25	110.80	103.30
56	D3	482	U	C2-N1-C1'	6.24	125.19	117.70
56	D3	1079	U	N3-C2-O2	-6.23	117.84	122.20
55	D2	311	C	P-O3'-C3'	6.21	127.15	119.70
55	D2	418	C	C6-N1-C2	-6.21	117.81	120.30
8	UH	309	PRO	N-CA-CB	6.19	110.72	103.30
39	JN	102	PRO	N-CA-CB	6.18	110.72	103.30
56	D3	587	C	N1-C2-O2	6.18	122.61	118.90
56	D3	976	G	N3-C4-N9	6.18	129.71	126.00
55	D2	501	C	C2-N1-C1'	6.17	125.59	118.80
55	D2	393	C	C6-N1-C1'	6.17	128.21	120.80
2	UB	412	PRO	N-CA-CB	6.17	110.70	103.30
56	D3	553	G	C5-C6-O6	6.16	132.29	128.60
56	D3	1060	U	C2-N1-C1'	6.13	125.06	117.70
56	D3	553	G	N1-C2-N2	6.12	121.71	116.20
55	D2	388	C	N3-C2-O2	-6.11	117.62	121.90
56	D3	1433	G	N3-C4-N9	6.10	129.66	126.00
56	D3	1747	G	N7-C8-N9	6.10	116.15	113.10
56	D3	1674	C	C2-N1-C1'	6.08	125.48	118.80
56	D3	1729	C	C6-N1-C2	-6.06	117.87	120.30
39	JN	94	PRO	N-CA-CB	6.06	110.57	103.30
56	D3	1591	C	N1-C2-O2	6.05	122.53	118.90
56	D3	1683	C	C5-C6-N1	6.04	124.02	121.00
56	D3	1653	C	C6-N1-C2	-6.03	117.89	120.30
55	D2	151	U	C6-N1-C1'	-6.03	112.76	121.20
56	D3	1057	U	P-O3'-C3'	6.03	126.93	119.70
57	D4	266	C	N3-C2-O2	-6.02	117.68	121.90
55	D2	369	G	C6-C5-N7	-6.02	126.79	130.40
2	UB	201	PRO	N-CA-CB	6.00	110.50	103.30
56	D3	1692	G	C8-N9-C4	-5.99	104.00	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	D3	1037	C	C6-N1-C2	5.98	122.69	120.30
55	D2	394	U	C5-C6-N1	5.96	125.68	122.70
8	UH	258	PRO	N-CA-CB	5.96	110.45	103.30
55	D2	89	C	N1-C2-O2	5.94	122.46	118.90
8	UH	298	PRO	N-CA-CB	5.93	110.42	103.30
56	D3	14	C	N1-C2-N3	5.93	123.36	119.20
56	D3	1513	G	C5-C6-O6	5.93	132.16	128.60
56	D3	469	C	N1-C2-O2	5.93	122.46	118.90
56	D3	1686	C	C2-N1-C1'	5.93	125.33	118.80
55	D2	347	U	N3-C2-O2	-5.93	118.05	122.20
56	D3	1607	G	O5'-P-OP2	-5.93	100.36	105.70
56	D3	1654	G	N3-C2-N2	5.92	124.05	119.90
56	D3	1163	A	N1-C2-N3	5.91	132.26	129.30
55	D2	68	U	C2-N1-C1'	5.91	124.79	117.70
56	D3	1059	U	C2-N1-C1'	5.91	124.79	117.70
56	D3	1056	U	C2-N1-C1'	5.91	124.79	117.70
56	D3	1043	A	N1-C6-N6	-5.90	115.06	118.60
55	D2	91	U	C5-C6-N1	5.89	125.65	122.70
56	D3	1220	C	N1-C2-O2	5.89	122.43	118.90
56	D3	1513	G	C2-N3-C4	-5.88	108.96	111.90
56	D3	1582	U	N3-C2-O2	5.87	126.31	122.20
56	D3	1620	C	N1-C2-O2	5.86	122.42	118.90
56	D3	1207	C	N1-C2-O2	5.85	122.41	118.90
56	D3	1495	C	C6-N1-C2	-5.85	117.96	120.30
56	D3	542	A	C5-N7-C8	-5.84	100.98	103.90
57	D4	89	C	C2-N1-C1'	5.84	125.22	118.80
55	D2	540	U	C2-N1-C1'	5.84	124.70	117.70
56	D3	1696	G	N1-C6-O6	-5.82	116.41	119.90
55	D2	270	U	N3-C2-O2	-5.81	118.13	122.20
56	D3	1727	G	C6-C5-N7	-5.81	126.91	130.40
2	UB	285	PRO	N-CA-CB	5.80	110.26	103.30
55	D2	437	G	C2-N3-C4	-5.80	109.00	111.90
56	D3	1433	G	N3-C4-C5	-5.79	125.70	128.60
56	D3	1747	G	C4-N9-C1'	5.79	134.03	126.50
56	D3	1056	U	N1-C2-O2	5.79	126.85	122.80
56	D3	536	C	N1-C2-O2	5.78	122.37	118.90
56	D3	1449	U	C2-N1-C1'	5.78	124.64	117.70
56	D3	895	G	C5-C6-O6	5.78	132.07	128.60
56	D3	536	C	C6-N1-C1'	-5.76	113.89	120.80
56	D3	1747	G	C4-C5-N7	5.76	113.10	110.80
55	D2	108	U	N3-C2-O2	-5.76	118.17	122.20
56	D3	1620	C	N3-C2-O2	-5.75	117.88	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	D3	962	C	N1-C2-O2	5.74	122.34	118.90
55	D2	395	C	N1-C2-O2	5.73	122.34	118.90
56	D3	1451	C	N3-C2-O2	-5.72	117.90	121.90
56	D3	1672	G	N3-C4-N9	5.71	129.43	126.00
56	D3	1433	G	C8-N9-C1'	-5.70	119.58	127.00
8	UH	69	PRO	N-CA-CB	5.70	110.13	103.30
55	D2	355	C	C6-N1-C1'	-5.70	113.97	120.80
56	D3	1746	A	C5-C6-N6	5.69	128.25	123.70
55	D2	436	G	N3-C4-N9	5.68	129.41	126.00
55	D2	66	C	C2-N1-C1'	5.68	125.05	118.80
55	D2	417	C	N1-C2-O2	5.68	122.31	118.90
56	D3	584	C	C6-N1-C1'	5.67	127.61	120.80
57	D4	89	C	N1-C2-O2	5.67	122.30	118.90
55	D2	391	C	N1-C2-O2	5.67	122.30	118.90
56	D3	948	G	C4-N9-C1'	5.66	133.86	126.50
56	D3	933	A	C2-N3-C4	5.66	113.43	110.60
56	D3	960	U	C2-N1-C1'	5.65	124.48	117.70
56	D3	1210	C	C6-N1-C2	-5.65	118.04	120.30
56	D3	1674	C	C5-C6-N1	5.64	123.82	121.00
32	CL	119	GLU	C-N-CA	-5.64	107.60	121.70
57	D4	306	G	C5-C6-O6	5.64	131.98	128.60
56	D3	1746	A	N9-C4-C5	5.63	108.05	105.80
55	D2	184	U	C2-N1-C1'	5.62	124.45	117.70
55	D2	184	U	N1-C2-O2	5.62	126.73	122.80
8	UH	58	PRO	N-CA-CB	5.61	110.03	103.30
55	D2	250	G	C5-C6-O6	5.60	131.96	128.60
55	D2	501	C	N1-C2-O2	5.60	122.26	118.90
56	D3	1209	C	C6-N1-C2	-5.59	118.06	120.30
56	D3	948	G	C8-N9-C1'	-5.59	119.73	127.00
55	D2	390	C	C6-N1-C2	-5.58	118.07	120.30
56	D3	1747	G	N3-C4-C5	-5.58	125.81	128.60
56	D3	1059	U	O4'-C1'-N1	5.58	112.66	108.20
56	D3	1637	C	C6-N1-C2	-5.58	118.07	120.30
56	D3	584	C	C2-N1-C1'	-5.57	112.67	118.80
57	D4	89	C	C5-C6-N1	5.56	123.78	121.00
56	D3	1216	C	N3-C2-O2	-5.56	118.01	121.90
55	D2	250	G	N1-C2-N3	5.56	127.23	123.90
56	D3	1123	C	N3-C2-O2	-5.56	118.01	121.90
56	D3	1673	G	C5-C6-O6	5.55	131.93	128.60
56	D3	553	G	O4'-C1'-N9	5.55	112.64	108.20
56	D3	1075	C	N3-C2-O2	-5.53	118.03	121.90
55	D2	89	C	C2-N1-C1'	5.52	124.88	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	D2	338	A	N1-C2-N3	5.52	132.06	129.30
56	D3	1081	A	N7-C8-N9	5.52	116.56	113.80
56	D3	1207	C	N3-C2-O2	-5.52	118.04	121.90
56	D3	534	A	C2-N3-C4	5.52	113.36	110.60
56	D3	1451	C	C6-N1-C2	-5.51	118.09	120.30
56	D3	1637	C	N1-C2-O2	5.50	122.20	118.90
56	D3	1056	U	N3-C2-O2	-5.49	118.36	122.20
55	D2	233	G	C6-C5-N7	-5.48	127.11	130.40
55	D2	492	G	P-O3'-C3'	5.48	126.28	119.70
56	D3	1081	A	C8-N9-C4	-5.48	103.61	105.80
56	D3	1452	U	C2-N1-C1'	5.47	124.27	117.70
57	D4	32	G	C4-N9-C1'	5.46	133.60	126.50
55	D2	369	G	C4-C5-N7	5.46	112.98	110.80
56	D3	542	A	C6-C5-N7	-5.45	128.48	132.30
56	D3	1265	G	N3-C4-N9	5.45	129.27	126.00
56	D3	1209	C	C5-C6-N1	5.44	123.72	121.00
55	D2	57	C	C5-C6-N1	5.43	123.71	121.00
56	D3	1654	G	N3-C4-N9	5.42	129.25	126.00
8	UH	60	PRO	N-CA-CB	5.42	109.80	103.30
55	D2	355	C	N3-C2-O2	-5.41	118.11	121.90
56	D3	976	G	N7-C8-N9	5.41	115.80	113.10
56	D3	1657	U	P-O3'-C3'	5.41	126.19	119.70
57	D4	13	C	C6-N1-C2	-5.40	118.14	120.30
55	D2	508	C	C6-N1-C2	-5.40	118.14	120.30
56	D3	1452	U	C5-C6-N1	5.40	125.40	122.70
56	D3	1654	G	N1-C2-N2	-5.39	111.35	116.20
57	D4	2	U	N3-C2-O2	-5.39	118.43	122.20
56	D3	1591	C	C5-C6-N1	5.38	123.69	121.00
56	D3	1737	G	C6-C5-N7	-5.38	127.17	130.40
56	D3	474	A	C5-C6-N6	5.38	128.00	123.70
56	D3	1571	C	N3-C2-O2	-5.37	118.14	121.90
56	D3	1594	G	P-O3'-C3'	5.37	126.14	119.70
56	D3	1629	G	C5-C6-O6	5.37	131.82	128.60
56	D3	1056	U	C6-N1-C2	-5.37	117.78	121.00
56	D3	1654	G	C4-C5-N7	5.37	112.95	110.80
56	D3	1782	A	N1-C6-N6	-5.37	115.38	118.60
56	D3	1054	U	C2-N1-C1'	5.36	124.13	117.70
55	D2	338	A	C2-N3-C4	-5.36	107.92	110.60
56	D3	962	C	N3-C2-O2	-5.36	118.15	121.90
55	D2	189	U	N1-C2-O2	5.35	126.55	122.80
57	D4	264	C	C6-N1-C2	-5.34	118.16	120.30
56	D3	1620	C	P-O3'-C3'	5.34	126.11	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	D3	1452	U	N1-C2-O2	5.34	126.54	122.80
56	D3	1770	U	N3-C2-O2	-5.33	118.47	122.20
55	D2	418	C	N1-C2-O2	5.33	122.10	118.90
55	D2	65	U	N1-C2-O2	5.33	126.53	122.80
56	D3	1058	U	N3-C2-O2	-5.33	118.47	122.20
56	D3	483	A	C6-N1-C2	-5.32	115.41	118.60
56	D3	1727	G	N9-C4-C5	-5.32	103.27	105.40
55	D2	393	C	C2-N1-C1'	-5.32	112.95	118.80
56	D3	564	G	C6-C5-N7	-5.32	127.21	130.40
56	D3	1686	C	C6-N1-C2	-5.31	118.17	120.30
57	D4	18	G	N3-C4-N9	-5.31	122.81	126.00
56	D3	1696	G	N1-C2-N2	-5.31	111.42	116.20
56	D3	960	U	N3-C2-O2	-5.30	118.49	122.20
56	D3	895	G	N1-C6-O6	-5.30	116.72	119.90
56	D3	530	C	C6-N1-C2	-5.30	118.18	120.30
57	D4	27	U	N1-C2-O2	5.29	126.50	122.80
56	D3	1128	C	N1-C2-O2	5.29	122.07	118.90
56	D3	1621	U	N3-C2-O2	-5.28	118.50	122.20
57	D4	105	C	C6-N1-C2	-5.28	118.19	120.30
55	D2	66	C	C6-N1-C2	-5.27	118.19	120.30
55	D2	356	C	C5-C6-N1	5.27	123.64	121.00
56	D3	573	C	N1-C2-O2	5.26	122.06	118.90
56	D3	1652	C	N1-C2-O2	5.24	122.04	118.90
56	D3	962	C	C2-N1-C1'	5.23	124.56	118.80
56	D3	1673	G	N1-C6-O6	-5.23	116.76	119.90
56	D3	1509	C	C6-N1-C2	-5.22	118.21	120.30
56	D3	1654	G	C6-C5-N7	-5.22	127.27	130.40
56	D3	1727	G	C4-N9-C1'	5.22	133.28	126.50
56	D3	1058	U	C2-N1-C1'	5.21	123.95	117.70
55	D2	120	C	C2-N1-C1'	5.21	124.53	118.80
57	D4	306	G	C8-N9-C4	-5.21	104.32	106.40
56	D3	913	G	N3-C4-C5	-5.20	126.00	128.60
56	D3	1058	U	N1-C2-O2	5.19	126.43	122.80
56	D3	885	G	C6-C5-N7	-5.19	127.29	130.40
55	D2	428	A	C8-N9-C4	-5.18	103.73	105.80
55	D2	464	G	C5-C6-O6	5.18	131.71	128.60
55	D2	501	C	C6-N1-C2	-5.18	118.23	120.30
55	D2	144	C	C6-N1-C1'	-5.18	114.58	120.80
56	D3	564	G	C5-N7-C8	-5.17	101.72	104.30
56	D3	1206	U	N3-C2-O2	-5.17	118.58	122.20
8	UH	316	PRO	N-CA-CB	5.17	109.50	103.30
56	D3	469	C	C2-N1-C1'	5.17	124.48	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	D3	495	C	C6-N1-C2	-5.17	118.23	120.30
56	D3	1265	G	N3-C4-C5	-5.15	126.02	128.60
55	D2	347	U	N1-C2-O2	5.15	126.41	122.80
55	D2	388	C	C6-N1-C2	-5.15	118.24	120.30
55	D2	249	G	C5-C6-N1	5.14	114.07	111.50
55	D2	86	C	N1-C2-O2	-5.13	115.82	118.90
56	D3	1210	C	C2-N3-C4	5.13	122.47	119.90
57	D4	201	C	C6-N1-C2	-5.13	118.25	120.30
56	D3	1494	C	N3-C2-O2	-5.13	118.31	121.90
55	D2	228	A	N7-C8-N9	5.13	116.36	113.80
56	D3	1209	C	C2-N1-C1'	5.12	124.44	118.80
56	D3	1034	C	C6-N1-C2	-5.12	118.25	120.30
56	D3	573	C	N3-C2-O2	-5.12	118.32	121.90
56	D3	551	G	N3-C2-N2	5.11	123.48	119.90
56	D3	1582	U	C5-C4-O4	-5.11	122.83	125.90
56	D3	1703	C	N1-C2-O2	5.11	121.97	118.90
56	D3	1057	U	OP1-P-O3'	5.10	116.43	105.20
56	D3	542	A	C4-C5-N7	5.10	113.25	110.70
56	D3	1673	G	N9-C4-C5	5.10	107.44	105.40
56	D3	552	G	C2-N3-C4	-5.10	109.35	111.90
55	D2	155	A	C8-N9-C4	-5.10	103.76	105.80
55	D2	355	C	C5-C4-N4	-5.09	116.64	120.20
56	D3	1513	G	N1-C2-N3	5.09	126.96	123.90
56	D3	1140	G	N1-C6-O6	-5.09	116.85	119.90
57	D4	201	C	C2-N1-C1'	5.08	124.39	118.80
56	D3	976	G	C6-C5-N7	-5.08	127.35	130.40
56	D3	1054	U	N1-C2-O2	5.08	126.35	122.80
17	UQ	869	MET	CA-C-N	5.08	128.37	117.20
55	D2	501	C	C5-C6-N1	5.07	123.53	121.00
56	D3	542	A	C4-N9-C1'	5.07	135.42	126.30
56	D3	924	A	C6-C5-N7	-5.07	128.75	132.30
55	D2	369	G	C4-N9-C1'	5.06	133.08	126.50
56	D3	1174	C	N1-C2-O2	5.06	121.94	118.90
56	D3	1534	G	C8-N9-C4	-5.06	104.38	106.40
56	D3	1727	G	C8-N9-C1'	-5.06	120.42	127.00
56	D3	886	U	N3-C2-O2	-5.05	118.66	122.20
55	D2	233	G	C8-N9-C1'	-5.05	120.44	127.00
56	D3	573	C	C6-N1-C2	-5.05	118.28	120.30
56	D3	1573	A	P-O3'-C3'	5.05	125.76	119.70
57	D4	314	C	N1-C2-O2	5.04	121.93	118.90
57	D4	308	U	N3-C2-O2	-5.04	118.67	122.20
56	D3	1262	U	N3-C2-O2	-5.04	118.67	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	D3	1174	C	N3-C2-O2	-5.03	118.38	121.90
56	D3	1703	C	C6-N1-C2	-5.03	118.29	120.30
55	D2	231	C	N3-C2-O2	-5.03	118.38	121.90
55	D2	189	U	N3-C2-O2	-5.02	118.68	122.20
56	D3	913	G	C4-N9-C1'	5.02	133.02	126.50
56	D3	0	U	P-O3'-C3'	5.01	125.72	119.70
56	D3	553	G	N3-C4-C5	5.01	131.11	128.60
55	D2	66	C	N1-C2-O2	5.01	121.91	118.90
56	D3	551	G	N3-C4-C5	-5.01	126.09	128.60
56	D3	908	U	N1-C2-O2	5.01	126.31	122.80
55	D2	388	C	N1-C2-N3	5.01	122.71	119.20
56	D3	1696	G	N3-C4-N9	-5.01	123.00	126.00
55	D2	369	G	N9-C4-C5	-5.01	103.40	105.40
55	D2	369	G	C8-N9-C1'	-5.00	120.50	127.00
55	D2	82	A	P-O3'-C3'	5.00	125.70	119.70
55	D2	391	C	C6-N1-C1'	-5.00	114.80	120.80

There are no chirality outliers.

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	CD	264	SER	Peptide
26	CE	319	ILE	Peptide
28	CH	237	ASP	Peptide
28	CH	340	GLY	Peptide
28	CH	408	VAL	Peptide
31	CK	453	SER	Peptide
32	CL	276	HIS	Peptide
34	CN	254	LYS	Peptide
44	DF	126	ASP	Peptide
40	JO	191	MET	Peptide
41	JP	283	ASP	Peptide
41	JP	301	PHE	Peptide
41	JP	335	ASN	Peptide
1	UA	289	LEU	Peptide
2	UB	616	LEU	Peptide
4	UD	279	HIS	Peptide
4	UD	309	GLN	Peptide
4	UD	353	GLU	Peptide
5	UE	166	ALA	Peptide
5	UE	248	THR	Peptide
10	UJ	154	ILE	Peptide

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Mol	Chain	Res	Type	Group
10	UJ	602	ASP	Peptide
12	UL	183	ASP	Peptide
12	UL	212	VAL	Peptide
12	UL	243	THR	Peptide
12	UL	451	ASN	Peptide
12	UL	552	ASP	Peptide
13	UM	400	GLY	Peptide
13	UM	421	SER	Peptide
13	UM	426	ILE	Peptide
13	UM	705	SER	Peptide
14	UN	321	HIS	Peptide
17	UQ	180	ASP	Peptide
17	UQ	592	SER	Peptide
20	UU	901	LYS	Peptide
23	UZ	90	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	UA	4121	0	1858	11	0
2	UB	2512	0	1079	5	0
3	UC	628	0	292	1	0
4	UD	3339	0	1434	15	0
5	UE	2353	0	1028	3	0
6	UF	1456	0	606	2	0
7	UG	2629	0	1182	4	0
8	UH	2190	0	916	23	0
9	UI	517	0	211	0	0
10	UJ	3621	0	1585	8	0
11	UK	1203	0	513	2	0
12	UL	4163	0	1851	31	0
13	UM	3763	0	1688	29	0
14	UN	733	0	308	1	0
15	UO	2441	0	1083	8	0
16	UP	298	0	122	0	0
17	UQ	4122	0	1749	9	0
18	UR	2377	0	1045	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	US	2357	0	1007	6	0
20	UU	4181	0	1864	14	0
21	UV	5442	0	2336	8	0
22	UX	862	0	375	2	0
23	UZ	1224	0	510	1	0
24	CA	1190	0	547	2	0
24	CB	1122	0	514	4	0
25	CD	1880	0	871	2	0
26	CE	2155	0	1051	5	0
27	CF	611	0	293	1	0
27	CG	611	0	295	0	0
28	CH	2158	0	965	19	0
29	CI	905	0	380	1	0
30	CJ	1397	0	620	6	0
31	CK	1031	0	456	7	0
32	CL	3859	0	1693	12	0
33	CM	1767	0	795	8	0
34	CN	1154	0	501	3	0
35	JF	1071	0	467	4	0
35	JG	1141	0	500	5	0
36	JH	1295	0	570	3	0
37	JJ	898	0	399	1	0
38	JM	671	0	286	0	0
39	JN	918	0	396	2	0
40	JO	933	0	406	1	0
41	JP	2283	0	999	6	0
42	JQ	312	0	127	0	0
43	DA	1187	0	531	6	0
44	DF	1055	0	496	0	0
45	DH	913	0	400	3	0
46	DJ	915	0	422	1	0
47	DN	742	0	345	1	0
48	DO	587	0	295	2	0
49	DQ	616	0	285	0	0
50	DS	521	0	224	2	0
51	DW	634	0	289	2	0
52	DX	503	0	231	3	0
53	Db	400	0	180	0	0
54	Dc	310	0	134	0	0
55	D2	11160	0	5609	239	0
56	D3	16806	0	8479	350	0
57	D4	3712	0	1882	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	Db	1	0	0	0	0
58	UX	1	0	0	0	0
59	CL	1	0	0	0	0
59	UX	1	0	0	0	0
60	CL	32	0	12	0	0
All	All	125991	0	57587	924	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (924) 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)
56:D3:1541:G:N2	56:D3:1569:A:C6	1.99	1.31
34:CN:87:LEU:HA	34:CN:125:LEU:O	1.23	1.30
20:UU:228:GLY:HA3	20:UU:246:ILE:O	1.28	1.28
13:UM:30:LYS:HA	13:UM:45:LEU:O	1.22	1.28
7:UG:132:GLY:HA3	7:UG:150:LEU:O	1.26	1.26
18:UR:382:GLY:HA3	18:UR:400:ILE:O	1.35	1.21
56:D3:1541:G:C2	56:D3:1570:A:N6	2.10	1.19
8:UH:341:LEU:HA	8:UH:358:VAL:O	1.02	1.17
8:UH:341:LEU:CA	8:UH:358:VAL:O	1.93	1.17
4:UD:548:GLY:O	4:UD:565:ARG:HA	1.43	1.16
56:D3:1541:G:N2	56:D3:1570:A:C6	2.15	1.14
7:UG:132:GLY:CA	7:UG:150:LEU:O	1.98	1.12
55:D2:101:G:C8	55:D2:103:G:N2	2.17	1.10
56:D3:1677:C:N4	56:D3:1724:U:H3	1.53	1.07
56:D3:1699:G:H21	56:D3:1702:A:N6	1.53	1.06
56:D3:1043:A:H61	56:D3:1075:C:N4	1.53	1.05
56:D3:625:C:H42	56:D3:974:A:N6	1.54	1.05
56:D3:1541:G:C2	56:D3:1569:A:N6	2.26	1.03
56:D3:1654:G:H21	56:D3:1746:A:N6	1.56	1.02
56:D3:1267:G:C6	56:D3:1442:U:N3	2.28	1.01
56:D3:1699:G:N2	56:D3:1702:A:H62	1.58	1.01
56:D3:625:C:N4	56:D3:974:A:H61	1.58	1.01
56:D3:1267:G:O6	56:D3:1442:U:C4	2.14	1.01
56:D3:1158:C:H42	56:D3:1163:A:H61	1.03	1.01
56:D3:1646:C:N4	56:D3:1754:A:H61	1.58	0.99
56:D3:628:G:N2	56:D3:971:A:H62	1.60	0.98
56:D3:1654:G:N2	56:D3:1746:A:N6	2.13	0.96
55:D2:174:U:H3	55:D2:222:G:H1	0.96	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:D3:1043:A:N6	56:D3:1075:C:H42	1.61	0.96
56:D3:1646:C:H42	56:D3:1754:A:N6	1.61	0.96
56:D3:628:G:H21	56:D3:971:A:N6	1.65	0.95
57:D4:95:A:H61	57:D4:321:C:H42	0.97	0.95
56:D3:625:C:H42	56:D3:974:A:H61	0.96	0.94
57:D4:205:G:N1	57:D4:245:U:C2	2.36	0.94
56:D3:1044:U:H3	56:D3:1074:G:H1	1.04	0.94
56:D3:1654:G:N2	56:D3:1746:A:H62	1.64	0.94
55:D2:254:C:N4	55:D2:440:U:H3	1.65	0.93
56:D3:477:A:N6	56:D3:539:G:H21	1.65	0.93
55:D2:182:G:H1	55:D2:215:U:H3	1.12	0.93
56:D3:1655:A:N6	56:D3:1745:G:H1	1.68	0.92
56:D3:1775:U:H3	56:D3:1786:G:H1	1.13	0.92
56:D3:477:A:H61	56:D3:539:G:H21	1.13	0.91
56:D3:477:A:H61	56:D3:539:G:N2	1.67	0.91
56:D3:867:G:H1	56:D3:961:U:H3	1.14	0.91
56:D3:1655:A:H61	56:D3:1745:G:N2	1.68	0.91
56:D3:895:G:H1	56:D3:917:U:H3	1.16	0.90
15:UO:279:GLY:CA	15:UO:298:PHE:O	2.20	0.90
55:D2:360:C:N4	55:D2:366:A:H61	1.70	0.89
55:D2:254:C:H42	55:D2:440:U:H3	0.91	0.89
56:D3:1267:G:C6	56:D3:1442:U:C4	2.61	0.89
15:UO:279:GLY:HA3	15:UO:298:PHE:O	1.72	0.88
56:D3:976:G:N2	56:D3:978:A:N6	2.21	0.87
33:CM:306:GLU:HA	33:CM:356:GLY:O	1.74	0.87
56:D3:1541:G:N2	56:D3:1570:A:N6	2.18	0.86
56:D3:1689:A:N6	56:D3:1713:G:N2	2.23	0.86
55:D2:546:G:C6	55:D2:592:U:O2	2.28	0.86
56:D3:1541:G:C2	56:D3:1570:A:C6	2.60	0.85
55:D2:467:A:H61	57:D4:49:C:N4	1.73	0.85
56:D3:1541:G:C2	56:D3:1569:A:C6	2.64	0.85
21:UV:143:GLU:HA	21:UV:176:PHE:O	1.76	0.85
55:D2:184:U:H3	55:D2:213:G:H1	1.20	0.85
56:D3:1158:C:N4	56:D3:1163:A:H61	1.74	0.85
56:D3:1582:U:C2	56:D3:1614:A:N7	2.45	0.84
56:D3:1655:A:N6	56:D3:1745:G:H22	1.74	0.84
28:CH:190:VAL:HA	28:CH:195:GLN:O	1.77	0.84
8:UH:57:ASN:O	8:UH:70:SER:HA	1.78	0.83
55:D2:101:G:C5	55:D2:103:G:C2	2.65	0.83
13:UM:542:CYS:O	13:UM:546:LYS:HA	1.77	0.83
56:D3:628:G:H21	56:D3:971:A:H62	0.86	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:UM:589:GLN:HA	13:UM:602:TRP:O	1.81	0.81
55:D2:498:G:O6	55:D2:540:U:C4	2.34	0.81
18:UR:382:GLY:O	18:UR:399:LYS:HA	1.81	0.81
56:D3:1541:G:N2	56:D3:1569:A:C5	2.49	0.81
55:D2:121:G:H21	55:D2:124:A:H62	1.28	0.80
56:D3:1646:C:H42	56:D3:1754:A:H61	0.82	0.80
4:UD:548:GLY:O	4:UD:565:ARG:CA	2.26	0.80
56:D3:1677:C:H42	56:D3:1724:U:H3	0.82	0.80
56:D3:1699:G:H21	56:D3:1702:A:H62	0.81	0.79
55:D2:516:U:O2	55:D2:519:A:N7	2.17	0.78
56:D3:1043:A:H61	56:D3:1075:C:H42	0.81	0.78
30:CJ:150:THR:HA	30:CJ:167:LEU:O	1.83	0.77
56:D3:1158:C:H42	56:D3:1163:A:N6	1.81	0.77
55:D2:101:G:H3'	55:D2:103:G:H21	1.49	0.77
13:UM:30:LYS:CA	13:UM:45:LEU:O	2.19	0.76
1:UA:390:VAL:HA	1:UA:406:SER:HA	1.68	0.76
57:D4:95:A:N6	57:D4:321:C:H42	1.81	0.75
26:CE:2:ALA:HB3	26:CE:17:ALA:O	1.87	0.75
55:D2:24:U:H3	55:D2:56:G:H1	1.31	0.75
56:D3:1267:G:N1	56:D3:1442:U:C2	2.55	0.75
55:D2:506:G:N2	55:D2:531:C:O2	2.21	0.74
55:D2:360:C:N4	55:D2:366:A:N6	2.35	0.74
57:D4:114:A:C6	57:D4:254:A:C2	2.76	0.73
4:UD:199:ASP:HA	4:UD:215:ALA:O	1.88	0.73
28:CH:421:ASN:HA	28:CH:436:GLU:O	1.88	0.73
56:D3:1655:A:N6	56:D3:1745:G:N2	2.35	0.73
56:D3:1270:G:N2	56:D3:1441:C:O2	2.22	0.73
55:D2:101:G:N7	55:D2:103:G:N2	2.36	0.73
12:UL:412:GLY:HA3	12:UL:430:CYS:H	1.54	0.72
34:CN:87:LEU:CA	34:CN:125:LEU:O	2.19	0.72
56:D3:1734:U:H2'	56:D3:1735:U:C5'	2.20	0.72
20:UU:125:GLY:HA2	26:CE:430:ASP:HA	1.72	0.72
15:UO:279:GLY:HA2	15:UO:298:PHE:O	1.89	0.71
56:D3:872:G:N2	56:D3:956:C:O2	2.22	0.71
12:UL:364:TYR:O	12:UL:382:THR:O	2.09	0.71
55:D2:238:G:O6	55:D2:275:A:C6	2.43	0.71
56:D3:1663:G:H1	56:D3:1738:U:H3	1.37	0.71
55:D2:121:G:N2	55:D2:124:A:H62	1.88	0.71
56:D3:867:G:N2	56:D3:961:U:O2	2.23	0.71
20:UU:416:ALA:HB3	20:UU:433:ALA:HB3	1.73	0.71
55:D2:121:G:H21	55:D2:124:A:N6	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:JG:41:MET:O	35:JG:110:LEU:HA	1.91	0.70
56:D3:23:G:C2	56:D3:603:U:O2	2.44	0.70
56:D3:34:G:O6	56:D3:474:A:C5	2.45	0.70
57:D4:114:A:C5	57:D4:254:A:C6	2.79	0.70
56:D3:868:G:H1	56:D3:960:U:H3	1.39	0.69
57:D4:263:A:C6	57:D4:309:G:C2	2.80	0.69
56:D3:473:A:C6	56:D3:474:A:N6	2.60	0.69
56:D3:1689:A:N6	56:D3:1713:G:C2	2.60	0.69
55:D2:554:G:N2	55:D2:583:U:O2	2.25	0.69
56:D3:1164:G:H2'	56:D3:1165:G:H8	1.57	0.69
56:D3:1530:C:H2'	56:D3:1531:G:H8	1.58	0.69
56:D3:1582:U:O2	56:D3:1614:A:C5	2.46	0.69
56:D3:1273:G:O6	56:D3:1437:U:O2	2.11	0.68
19:US:180:PHE:O	19:US:185:TYR:N	2.27	0.68
56:D3:1273:G:O6	56:D3:1437:U:C2	2.47	0.68
12:UL:209:GLY:O	12:UL:219:THR:HA	1.94	0.68
56:D3:625:C:N3	56:D3:974:A:N1	2.42	0.68
24:CB:264:GLN:HA	24:CB:320:TYR:O	1.94	0.68
13:UM:540:SER:O	13:UM:548:LEU:HA	1.93	0.68
55:D2:514:U:H3	55:D2:521:G:H1	1.41	0.68
56:D3:868:G:N2	56:D3:960:U:O2	2.25	0.68
56:D3:1734:U:H2'	56:D3:1735:U:H5'	1.76	0.68
55:D2:101:G:N7	55:D2:103:G:C2	2.62	0.67
55:D2:168:G:H22	55:D2:227:U:H3	1.42	0.67
55:D2:360:C:H42	55:D2:366:A:N6	1.91	0.67
56:D3:1541:G:N2	56:D3:1569:A:N1	2.41	0.67
56:D3:519:C:N4	56:D3:534:A:C8	2.63	0.67
55:D2:554:G:N1	55:D2:583:U:N3	2.43	0.67
56:D3:33:U:O2	56:D3:468:A:C5	2.49	0.66
56:D3:1698:G:C6	56:D3:1704:U:N3	2.64	0.66
55:D2:161:A:N6	55:D2:233:G:C5	2.64	0.66
55:D2:6:A:N6	55:D2:8:A:N3	2.43	0.66
55:D2:103:G:O2'	55:D2:104:A:N7	2.26	0.66
10:UJ:407:PHE:O	10:UJ:410:ILE:O	2.14	0.65
57:D4:312:U:H2'	57:D4:313:A:C8	2.32	0.65
55:D2:467:A:N6	57:D4:49:C:N4	2.44	0.65
56:D3:479:C:O2	56:D3:510:G:N2	2.30	0.65
56:D3:1541:G:N1	56:D3:1569:A:N6	2.44	0.65
41:JP:351:VAL:HA	41:JP:367:SER:HA	1.78	0.65
55:D2:361:G:N2	55:D2:364:A:OP2	2.29	0.65
55:D2:498:G:O6	55:D2:540:U:O4	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:D3:477:A:N6	56:D3:539:G:N2	2.35	0.64
56:D3:1782:A:OP2	56:D3:1783:C:N4	2.30	0.64
57:D4:113:G:O2'	57:D4:256:G:N2	2.29	0.64
56:D3:23:G:N1	56:D3:603:U:C2	2.65	0.64
10:UJ:550:TYR:O	10:UJ:553:SER:C	2.36	0.64
55:D2:254:C:N3	55:D2:440:U:O4	2.30	0.64
52:DX:89:ASN:O	52:DX:92:CYS:N	2.28	0.64
56:D3:1267:G:C6	56:D3:1442:U:C2	2.85	0.64
35:JG:44:VAL:HA	35:JG:113:TYR:O	1.98	0.64
56:D3:1068:C:H2'	56:D3:1069:A:H8	1.62	0.63
55:D2:125:G:H2'	55:D2:126:A:H8	1.62	0.63
13:UM:304:LEU:O	13:UM:311:LEU:HA	1.97	0.63
55:D2:489:G:N2	55:D2:495:G:O3'	2.31	0.63
56:D3:1663:G:O6	56:D3:1738:U:O4	2.16	0.63
20:UU:118:VAL:HA	20:UU:132:THR:HA	1.81	0.63
57:D4:205:G:N1	57:D4:245:U:N3	2.47	0.63
56:D3:897:C:O2'	56:D3:914:G:N2	2.31	0.63
56:D3:1468:U:H2'	56:D3:1469:A:H8	1.64	0.63
8:UH:312:ASP:HA	8:UH:323:PHE:O	1.98	0.63
20:UU:179:LYS:HA	20:UU:191:PHE:O	1.98	0.63
56:D3:1690:G:N2	56:D3:1711:C:C2	2.65	0.63
41:JP:363:ILE:O	41:JP:374:LEU:HA	1.98	0.63
56:D3:1471:A:OP2	56:D3:1573:A:N6	2.32	0.62
56:D3:1663:G:N1	56:D3:1738:U:N3	2.43	0.62
55:D2:197:G:N2	55:D2:200:A:OP2	2.31	0.62
56:D3:634:G:C2	56:D3:966:A:N6	2.68	0.62
56:D3:1272:U:O2	56:D3:1438:G:O6	2.18	0.62
56:D3:1541:G:N1	56:D3:1570:A:N6	2.47	0.62
12:UL:364:TYR:O	12:UL:382:THR:C	2.37	0.62
12:UL:476:ILE:HA	12:UL:492:SER:HA	1.81	0.62
55:D2:171:G:O6	55:D2:226:U:C4	2.53	0.62
56:D3:1665:U:C2	56:D3:1737:G:N1	2.68	0.62
13:UM:418:ASN:O	13:UM:422:CYS:C	2.38	0.61
33:CM:249:SER:O	33:CM:253:GLY:CA	2.48	0.61
55:D2:353:A:H4'	55:D2:354:G:H5'	1.81	0.61
56:D3:1270:G:C2	56:D3:1441:C:O2	2.52	0.61
21:UV:251:PHE:O	21:UV:272:CYS:HA	2.00	0.61
32:CL:776:GLN:O	32:CL:780:ILE:N	2.30	0.61
5:UE:191:VAL:HA	5:UE:206:ALA:HA	1.81	0.61
56:D3:1164:G:H2'	56:D3:1165:G:C8	2.35	0.61
56:D3:1707:A:H8	56:D3:1707:A:P	2.22	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:UM:418:ASN:O	13:UM:422:CYS:HA	2.01	0.61
33:CM:249:SER:O	33:CM:253:GLY:N	2.33	0.61
56:D3:936:G:OP1	56:D3:1074:G:N2	2.30	0.61
55:D2:20:C:H2'	55:D2:21:A:H8	1.65	0.61
55:D2:123:C:OP2	55:D2:124:A:N6	2.33	0.61
57:D4:8:U:H2'	57:D4:9:A:H8	1.65	0.61
8:UH:212:SER:HA	8:UH:219:ALA:HA	1.83	0.60
55:D2:242:C:H2'	55:D2:243:A:H8	1.65	0.60
56:D3:634:G:N2	56:D3:965:U:OP2	2.34	0.60
1:UA:482:SER:O	1:UA:486:SER:N	2.35	0.60
31:CK:453:SER:O	31:CK:455:HIS:N	2.35	0.60
43:DA:91:VAL:HA	43:DA:96:LEU:HA	1.83	0.60
56:D3:480:G:H2'	56:D3:481:A:H8	1.66	0.60
57:D4:205:G:N2	57:D4:245:U:O2	2.34	0.60
55:D2:436:G:H2'	55:D2:437:G:C8	2.37	0.60
56:D3:32:U:O2	56:D3:595:G:C2	2.55	0.60
57:D4:8:U:H2'	57:D4:9:A:C8	2.37	0.60
57:D4:111:G:O6	57:D4:260:U:O4	2.20	0.60
8:UH:67:PRO:HA	8:UH:80:GLU:O	2.01	0.60
17:UQ:745:ILE:O	17:UQ:754:LEU:N	2.35	0.59
55:D2:184:U:O2	55:D2:213:G:N2	2.32	0.59
8:UH:341:LEU:O	8:UH:357:HIS:HA	2.02	0.59
56:D3:1775:U:H2'	56:D3:1776:A:H8	1.67	0.59
28:CH:518:LYS:O	28:CH:560:ARG:N	2.34	0.59
57:D4:250:C:H2'	57:D4:251:G:C8	2.38	0.59
12:UL:227:LYS:HA	12:UL:246:GLY:O	2.03	0.59
57:D4:3:C:H2'	57:D4:4:G:H8	1.68	0.59
1:UA:581:THR:H	1:UA:596:GLY:HA2	1.68	0.59
56:D3:1715:G:H5'	56:D3:1716:C:OP2	2.03	0.59
13:UM:622:ALA:HB3	13:UM:635:ALA:HB3	1.85	0.59
17:UQ:101:GLN:O	17:UQ:104:ALA:N	2.36	0.59
41:JP:288:TYR:O	41:JP:298:LEU:N	2.36	0.59
55:D2:238:G:H4'	55:D2:239:U:H5'	1.82	0.59
4:UD:595:ASN:N	4:UD:610:VAL:O	2.36	0.59
28:CH:402:ILE:HA	28:CH:417:SER:HA	1.85	0.59
12:UL:940:GLY:HA2	31:CK:465:LEU:HA	1.85	0.59
35:JF:41:MET:O	35:JF:110:LEU:HA	2.02	0.59
56:D3:1707:A:H8	56:D3:1707:A:O5'	1.84	0.59
57:D4:114:A:N6	57:D4:254:A:C2	2.71	0.59
12:UL:88:HIS:O	12:UL:92:ASP:N	2.36	0.58
56:D3:566:C:H2'	56:D3:567:A:H8	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:UD:534:LEU:HA	4:UD:542:VAL:O	2.02	0.58
56:D3:1202:A:H3'	56:D3:1203:A:H8	1.67	0.58
43:DA:2:ALA:N	48:DO:45:GLY:O	2.36	0.58
13:UM:29:GLY:O	13:UM:45:LEU:O	2.22	0.58
56:D3:629:U:OP2	56:D3:969:C:N4	2.36	0.58
56:D3:1082:C:H2'	56:D3:1083:G:H8	1.68	0.58
1:UA:482:SER:O	1:UA:486:SER:HA	2.04	0.58
56:D3:519:C:N4	56:D3:534:A:N7	2.52	0.58
55:D2:158:G:H2'	55:D2:159:A:H8	1.68	0.58
55:D2:174:U:O4	55:D2:222:G:O6	2.22	0.58
56:D3:1041:G:H2'	56:D3:1042:G:C8	2.38	0.58
57:D4:197:G:N1	57:D4:246:A:OP2	2.37	0.58
28:CH:526:VAL:HA	28:CH:538:ARG:O	2.03	0.58
56:D3:519:C:C4	56:D3:534:A:C5	2.92	0.58
12:UL:48:ASP:HA	12:UL:63:LEU:O	2.02	0.58
13:UM:588:LYS:O	13:UM:604:CYS:N	2.35	0.58
56:D3:1692:G:C6	56:D3:1710:U:C4	2.91	0.58
15:UO:95:LEU:HA	15:UO:109:ASP:HA	1.85	0.57
55:D2:490:G:H1'	55:D2:495:G:H5'	1.86	0.57
55:D2:117:G:H2'	55:D2:118:A:C8	2.39	0.57
57:D4:114:A:C8	57:D4:254:A:N6	2.73	0.57
13:UM:105:SER:HA	13:UM:121:GLY:HA2	1.86	0.57
12:UL:599:ILE:O	12:UL:608:HIS:N	2.38	0.57
28:CH:191:SER:O	28:CH:194:LEU:N	2.37	0.57
30:CJ:43:PRO:O	30:CJ:47:ALA:HB2	2.05	0.57
56:D3:1461:C:H2'	56:D3:1462:G:H8	1.70	0.57
13:UM:550:THR:O	13:UM:557:VAL:HA	2.04	0.57
57:D4:114:A:C6	57:D4:254:A:N1	2.71	0.57
55:D2:210:U:H2'	55:D2:211:G:H8	1.70	0.56
55:D2:490:G:N3	55:D2:494:C:O2'	2.36	0.56
56:D3:1688:U:H2'	56:D3:1689:A:H8	1.68	0.56
13:UM:542:CYS:O	13:UM:546:LYS:CA	2.52	0.56
55:D2:24:U:O4	55:D2:56:G:O6	2.23	0.56
55:D2:334:G:H2'	55:D2:335:G:H8	1.70	0.56
56:D3:467:G:O2'	56:D3:469:C:OP2	2.20	0.56
56:D3:1692:G:O6	56:D3:1710:U:O4	2.23	0.56
56:D3:1716:C:H6	56:D3:1716:C:O5'	1.88	0.56
57:D4:18:G:H2'	57:D4:19:A:H8	1.70	0.56
25:CD:264:SER:O	25:CD:266:THR:N	2.33	0.56
56:D3:1082:C:H2'	56:D3:1083:G:C8	2.39	0.56
56:D3:1204:A:O2'	56:D3:1208:A:N3	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:CL:72:VAL:HA	32:CL:137:LEU:O	2.05	0.56
41:JP:283:ASP:O	41:JP:285:ASN:N	2.37	0.56
56:D3:937:C:H2'	56:D3:938:G:C8	2.41	0.56
11:UK:230:LYS:O	55:D2:236:C:N4	2.27	0.56
55:D2:456:U:H2'	55:D2:457:G:C8	2.41	0.56
56:D3:871:G:H2'	56:D3:872:G:C8	2.41	0.56
57:D4:114:A:N7	57:D4:254:A:C6	2.74	0.56
56:D3:868:G:H2'	56:D3:869:A:H8	1.71	0.56
56:D3:1688:U:H2'	56:D3:1689:A:C8	2.41	0.56
20:UU:228:GLY:CA	20:UU:246:ILE:O	2.24	0.56
26:CE:431:ALA:HB3	55:D2:309:A:H61	1.71	0.56
55:D2:2:U:H2'	55:D2:3:G:H8	1.71	0.56
55:D2:193:G:H2'	55:D2:194:G:H8	1.71	0.56
55:D2:189:U:C2	55:D2:209:G:N1	2.74	0.56
55:D2:540:U:O2'	55:D2:542:U:OP2	2.23	0.56
56:D3:478:A:N1	56:D3:510:G:O6	2.39	0.56
56:D3:1655:A:N6	56:D3:1745:G:N1	2.32	0.56
4:UD:198:ASP:O	4:UD:215:ALA:O	2.24	0.56
28:CH:160:ILE:HA	28:CH:188:TYR:O	2.05	0.56
56:D3:23:G:C6	56:D3:603:U:N3	2.74	0.56
56:D3:1506:G:H2'	56:D3:1507:G:H8	1.71	0.56
13:UM:30:LYS:C	13:UM:45:LEU:H	2.09	0.56
55:D2:177:U:H3	55:D2:220:U:H3	1.53	0.55
56:D3:34:G:O6	56:D3:474:A:N7	2.39	0.55
12:UL:258:LYS:O	12:UL:274:ILE:HA	2.05	0.55
31:CK:328:GLY:N	56:D3:576:G:OP1	2.37	0.55
55:D2:117:G:H2'	55:D2:118:A:H8	1.71	0.55
55:D2:515:G:N2	55:D2:521:G:N7	2.54	0.55
28:CH:150:THR:O	28:CH:562:GLY:HA3	2.05	0.55
55:D2:467:A:N6	57:D4:49:C:H42	2.04	0.55
55:D2:554:G:N1	55:D2:583:U:C2	2.74	0.55
4:UD:265:TRP:HA	4:UD:272:LEU:HA	1.88	0.55
28:CH:424:LEU:O	28:CH:433:ILE:N	2.38	0.55
55:D2:2:U:H2'	55:D2:3:G:C8	2.42	0.55
28:CH:405:VAL:HA	28:CH:414:ILE:O	2.07	0.55
56:D3:976:G:N2	56:D3:978:A:H61	2.01	0.55
7:UG:132:GLY:HA2	7:UG:150:LEU:O	2.01	0.55
55:D2:24:U:N3	55:D2:56:G:N1	2.43	0.55
1:UA:482:SER:O	1:UA:486:SER:CA	2.55	0.55
56:D3:1270:G:H2'	56:D3:1271:G:H8	1.71	0.55
8:UH:209:PHE:CB	8:UH:222:PHE:O	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:CM:249:SER:O	33:CM:253:GLY:HA2	2.07	0.55
34:CN:200:GLU:O	34:CN:204:SER:CB	2.55	0.55
55:D2:238:G:C6	55:D2:275:A:C6	2.95	0.55
56:D3:1736:G:H2'	56:D3:1737:G:C8	2.42	0.55
4:UD:614:TRP:O	4:UD:618:ASN:CB	2.55	0.55
24:CA:201:HIS:O	24:CA:204:GLY:N	2.40	0.55
28:CH:442:ILE:HA	28:CH:472:PRO:HA	1.89	0.55
55:D2:22:A:H2'	55:D2:23:G:C8	2.41	0.55
56:D3:33:U:C2	56:D3:468:A:N7	2.75	0.55
43:DA:139:ALA:HA	43:DA:212:VAL:HA	1.89	0.54
55:D2:171:G:C6	55:D2:226:U:N3	2.75	0.54
55:D2:223:C:H2'	55:D2:224:G:C8	2.42	0.54
55:D2:271:G:H2'	55:D2:272:A:H8	1.71	0.54
55:D2:389:U:H2'	55:D2:390:C:C6	2.42	0.54
56:D3:884:A:H2'	56:D3:885:G:H8	1.72	0.54
56:D3:897:C:N4	56:D3:914:G:O2'	2.40	0.54
56:D3:1111:G:H2'	56:D3:1112:G:C8	2.43	0.54
56:D3:1274:C:C4	56:D3:1275:A:N6	2.75	0.54
56:D3:1582:U:C2	56:D3:1614:A:C8	2.94	0.54
56:D3:923:A:H2'	56:D3:924:A:C8	2.42	0.54
56:D3:938:G:N2	56:D3:941:A:OP2	2.35	0.54
19:US:171:ALA:HB1	19:US:217:GLY:HA2	1.90	0.54
4:UD:485:LYS:HA	4:UD:498:VAL:O	2.08	0.54
30:CJ:43:PRO:O	30:CJ:47:ALA:CB	2.56	0.54
30:CJ:189:LEU:O	31:CK:379:ASP:N	2.41	0.54
55:D2:210:U:H2'	55:D2:211:G:C8	2.43	0.54
56:D3:1512:G:H2'	56:D3:1513:G:C8	2.42	0.54
55:D2:503:C:H2'	55:D2:504:U:H6	1.72	0.54
56:D3:537:G:O2'	56:D3:543:C:N4	2.41	0.54
57:D4:114:A:C5	57:D4:254:A:N1	2.75	0.54
32:CL:281:PRO:HA	32:CL:782:GLY:HA3	1.89	0.54
41:JP:58:PHE:O	57:D4:32:G:N1	2.35	0.54
56:D3:1528:U:H2'	56:D3:1529:C:C6	2.43	0.54
55:D2:101:G:C8	55:D2:103:G:C2	2.94	0.54
56:D3:1044:U:O4	56:D3:1074:G:O6	2.25	0.54
56:D3:1057:U:O2'	56:D3:1058:U:O4'	2.26	0.54
56:D3:1202:A:H3'	56:D3:1203:A:C8	2.43	0.54
18:UR:358:PHE:HA	18:UR:376:LEU:O	2.08	0.54
56:D3:1267:G:H22	56:D3:1442:U:H2'	1.73	0.54
12:UL:284:PHE:HA	12:UL:329:PHE:H	1.72	0.53
55:D2:445:U:H2'	55:D2:446:U:C6	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:D4:77:U:H2'	57:D4:78:G:H8	1.72	0.53
1:UA:785:PHE:O	1:UA:789:SER:CB	2.57	0.53
10:UJ:407:PHE:O	10:UJ:410:ILE:C	2.47	0.53
55:D2:334:G:H2'	55:D2:335:G:C8	2.44	0.53
55:D2:467:A:H61	57:D4:49:C:H42	1.55	0.53
56:D3:1080:U:H2'	56:D3:1081:A:H8	1.74	0.53
55:D2:404:G:N2	55:D2:452:A:OP2	2.41	0.53
56:D3:477:A:C6	56:D3:539:G:N2	2.76	0.53
56:D3:1129:U:O4	56:D3:1140:G:O6	2.27	0.53
56:D3:1698:G:N1	56:D3:1704:U:N3	2.56	0.53
13:UM:438:THR:H	13:UM:458:SER:HA	1.73	0.53
28:CH:478:LEU:HA	28:CH:488:ILE:O	2.08	0.53
55:D2:411:A:H2'	55:D2:412:A:C8	2.44	0.53
55:D2:413:C:H2'	55:D2:414:G:H8	1.73	0.53
56:D3:32:U:C2	56:D3:595:G:N1	2.77	0.53
55:D2:249:G:H2'	55:D2:250:G:C8	2.44	0.53
21:UV:362:ALA:HB2	21:UV:418:SER:HA	1.90	0.53
37:JJ:268:SER:O	37:JJ:272:GLU:CB	2.57	0.53
55:D2:192:G:H2'	55:D2:193:G:H8	1.74	0.53
55:D2:546:G:O6	55:D2:592:U:C2	2.62	0.53
56:D3:931:C:H5"	56:D3:932:U:H2'	1.91	0.53
56:D3:1665:U:O2	56:D3:1737:G:C2	2.61	0.53
21:UV:467:LEU:O	21:UV:475:ASN:HA	2.09	0.53
56:D3:505:A:O2'	56:D3:585:A:N6	2.35	0.53
12:UL:938:VAL:HA	31:CK:467:ILE:HA	1.90	0.52
55:D2:101:G:C5	55:D2:103:G:N1	2.77	0.52
55:D2:136:U:H2'	55:D2:137:C:H6	1.74	0.52
55:D2:446:U:H2'	55:D2:447:G:H8	1.74	0.52
56:D3:862:A:O2'	56:D3:963:A:N1	2.34	0.52
25:CD:14:GLY:HA3	25:CD:55:PRO:HA	1.91	0.52
28:CH:423:CYS:HA	28:CH:434:PHE:O	2.10	0.52
56:D3:1450:U:H2'	56:D3:1451:C:C6	2.45	0.52
13:UM:30:LYS:HA	13:UM:45:LEU:C	2.18	0.52
55:D2:446:U:H2'	55:D2:447:G:C8	2.43	0.52
55:D2:524:U:O2'	55:D2:526:U:OP1	2.18	0.52
56:D3:1061:A:H2'	56:D3:1062:A:H4'	1.90	0.52
56:D3:1068:C:H2'	56:D3:1069:A:C8	2.43	0.52
8:UH:334:THR:HA	8:UH:345:LEU:HA	1.91	0.52
39:JN:293:ALA:N	56:D3:9:U:OP2	2.41	0.52
55:D2:494:C:H2'	55:D2:495:G:H8	1.74	0.52
56:D3:32:U:N3	56:D3:595:G:N1	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:D3:522:U:H2'	56:D3:523:G:C8	2.44	0.52
56:D3:1606:C:H2'	56:D3:1607:G:C8	2.45	0.52
5:UE:162:GLN:HA	5:UE:173:ILE:O	2.08	0.52
55:D2:182:G:H2'	55:D2:183:A:H8	1.74	0.52
56:D3:1151:A:H2'	56:D3:1152:A:H8	1.74	0.52
55:D2:182:G:H2'	55:D2:183:A:C8	2.44	0.52
56:D3:1270:G:N2	56:D3:1441:C:C2	2.78	0.52
56:D3:1582:U:O2	56:D3:1614:A:N7	2.43	0.52
57:D4:33:A:O2'	57:D4:34:A:O4'	2.24	0.52
2:UB:282:ARG:H	36:JH:381:ALA:HB1	1.74	0.52
55:D2:411:A:H2'	55:D2:412:A:H8	1.73	0.52
56:D3:1171:A:H2'	56:D3:1172:G:H8	1.75	0.52
4:UD:586:THR:O	4:UD:589:ASN:N	2.42	0.52
56:D3:1275:A:N1	56:D3:1435:G:C2	2.78	0.52
17:UQ:18:GLY:HA3	17:UQ:781:SER:O	2.10	0.52
19:US:285:ILE:O	19:US:289:PHE:N	2.43	0.52
35:JG:55:ILE:O	35:JG:63:ASP:N	2.43	0.52
56:D3:1080:U:H2'	56:D3:1081:A:C8	2.45	0.52
56:D3:1734:U:C2'	56:D3:1735:U:C5'	2.86	0.52
55:D2:217:C:H2'	55:D2:218:U:H6	1.73	0.51
55:D2:289:U:H2'	55:D2:290:G:H8	1.75	0.51
56:D3:540:G:O2'	56:D3:542:A:OP2	2.28	0.51
56:D3:483:A:H2'	56:D3:484:C:C6	2.45	0.51
56:D3:1746:A:O2'	56:D3:1747:G:O4'	2.29	0.51
20:UU:45:GLY:O	55:D2:308:A:O2'	2.28	0.51
55:D2:238:G:N1	55:D2:275:A:C5	2.78	0.51
55:D2:400:C:H2'	55:D2:401:A:H8	1.75	0.51
56:D3:1716:C:H2'	56:D3:1717:G:H5"	1.91	0.51
1:UA:308:VAL:HA	1:UA:318:ALA:O	2.10	0.51
2:UB:270:TYR:HA	36:JH:354:ALA:HB1	1.92	0.51
55:D2:184:U:O4	55:D2:213:G:O6	2.29	0.51
56:D3:1739:C:H2'	56:D3:1740:A:H8	1.75	0.51
56:D3:1775:U:H2'	56:D3:1776:A:C8	2.44	0.51
1:UA:501:SER:O	1:UA:507:GLN:HA	2.11	0.51
20:UU:142:LYS:HA	20:UU:150:PRO:HA	1.91	0.51
32:CL:846:VAL:HA	32:CL:855:GLN:HA	1.92	0.51
55:D2:378:C:H2'	55:D2:379:A:H8	1.75	0.51
55:D2:495:G:H2'	55:D2:496:G:C8	2.45	0.51
55:D2:513:G:N1	55:D2:523:U:N3	2.58	0.51
56:D3:590:C:H2'	56:D3:591:A:C8	2.46	0.51
57:D4:202:G:O6	57:D4:247:U:O2	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:UL:552:ASP:O	12:UL:554:THR:N	2.43	0.51
56:D3:924:A:H2'	56:D3:925:G:C8	2.45	0.51
56:D3:1144:U:O2'	56:D3:1146:G:OP2	2.21	0.51
8:UH:303:GLN:HA	8:UH:313:LYS:HA	1.93	0.51
56:D3:868:G:H2'	56:D3:869:A:C8	2.45	0.51
22:UX:50:ALA:HB1	22:UX:58:ALA:HB2	1.93	0.51
30:CJ:88:ILE:HA	30:CJ:138:ASP:O	2.10	0.51
55:D2:456:U:H2'	55:D2:457:G:H8	1.76	0.51
57:D4:95:A:H61	57:D4:321:C:N4	1.83	0.51
56:D3:1689:A:N6	56:D3:1690:G:O6	2.44	0.51
56:D3:1787:C:H2'	56:D3:1788:G:H8	1.76	0.51
4:UD:353:GLU:O	4:UD:355:THR:N	2.44	0.51
55:D2:145:A:H2'	55:D2:146:G:H8	1.74	0.51
55:D2:436:G:H2'	55:D2:437:G:H8	1.75	0.51
56:D3:1267:G:C5	56:D3:1442:U:N3	2.75	0.51
56:D3:1650:U:H2'	56:D3:1651:A:C8	2.45	0.51
56:D3:1683:C:O2'	56:D3:1684:U:O5'	2.29	0.51
55:D2:495:G:H2'	55:D2:496:G:H8	1.76	0.50
56:D3:1715:G:C5'	56:D3:1716:C:OP2	2.59	0.50
56:D3:1746:A:HO2'	56:D3:1747:G:H8	1.57	0.50
7:UG:356:GLY:HA3	55:D2:315:U:H5'	1.92	0.50
8:UH:295:TYR:HA	8:UH:302:LEU:HA	1.92	0.50
17:UQ:295:TRP:O	55:D2:84:G:O2'	2.30	0.50
55:D2:262:U:C4	55:D2:263:C:N4	2.79	0.50
12:UL:123:ALA:O	12:UL:141:LYS:N	2.45	0.50
13:UM:361:SER:HA	13:UM:384:TYR:O	2.11	0.50
15:UO:84:VAL:HA	15:UO:100:ASP:HA	1.93	0.50
55:D2:20:C:H2'	55:D2:21:A:C8	2.46	0.50
55:D2:24:U:O2	55:D2:56:G:N2	2.42	0.50
56:D3:1541:G:N2	56:D3:1569:A:N6	2.34	0.50
33:CM:114:PHE:O	33:CM:169:VAL:HA	2.11	0.50
56:D3:1594:G:N1	56:D3:1603:U:N3	2.60	0.50
56:D3:1735:U:C2	56:D3:1736:G:H1'	2.46	0.50
12:UL:49:VAL:O	12:UL:62:LYS:HA	2.11	0.50
17:UQ:318:GLU:O	17:UQ:320:VAL:N	2.43	0.50
21:UV:552:ARG:O	21:UV:556:ILE:HA	2.11	0.50
55:D2:533:G:H2'	55:D2:534:A:C8	2.47	0.50
56:D3:1170:G:O6	56:D3:1469:A:N1	2.45	0.50
56:D3:1692:G:C6	56:D3:1710:U:N3	2.79	0.50
55:D2:180:G:H2'	55:D2:181:A:H8	1.76	0.50
55:D2:205:C:H2'	55:D2:206:A:C8	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:D3:1140:G:H2'	56:D3:1141:G:C8	2.46	0.50
47:DN:10:GLY:HA3	56:D3:955:A:H5"	1.93	0.50
55:D2:22:A:H2'	55:D2:23:G:H8	1.77	0.50
55:D2:101:G:C6	55:D2:103:G:C6	3.00	0.50
55:D2:445:U:H2'	55:D2:446:U:H6	1.76	0.50
56:D3:1052:U:H2'	56:D3:1053:G:C8	2.47	0.50
12:UL:487:ARG:HA	12:UL:500:TRP:O	2.12	0.49
55:D2:145:A:H2'	55:D2:146:G:C8	2.47	0.49
55:D2:100:G:C2	55:D2:101:G:H1'	2.47	0.49
56:D3:1267:G:O6	56:D3:1442:U:C5	2.64	0.49
56:D3:1665:U:C2	56:D3:1737:G:C2	3.00	0.49
8:UH:341:LEU:CB	8:UH:358:VAL:O	2.57	0.49
45:DH:70:PHE:O	45:DH:74:GLN:CB	2.60	0.49
20:UU:760:LEU:O	20:UU:763:SER:N	2.45	0.49
55:D2:255:U:N3	55:D2:262:U:O2'	2.45	0.49
55:D2:398:A:H2'	55:D2:399:U:C6	2.47	0.49
56:D3:480:G:H2'	56:D3:481:A:C8	2.45	0.49
56:D3:566:C:H2'	56:D3:567:A:C8	2.47	0.49
56:D3:1698:G:O6	56:D3:1704:U:C4	2.65	0.49
24:CB:197:VAL:HA	24:CB:220:ILE:O	2.13	0.49
43:DA:138:PHE:O	43:DA:213:ARG:N	2.44	0.49
55:D2:249:G:H2'	55:D2:250:G:H8	1.76	0.49
57:D4:330:A:H2'	57:D4:331:A:H8	1.77	0.49
57:D4:315:A:H2'	57:D4:316:A:C8	2.47	0.49
55:D2:189:U:O2	55:D2:209:G:C2	2.66	0.49
56:D3:1163:A:H2'	56:D3:1164:G:O4'	2.13	0.49
56:D3:1698:G:N1	56:D3:1704:U:C2	2.81	0.49
56:D3:1706:C:H3'	56:D3:1706:C:H6	1.78	0.49
56:D3:1733:C:H2'	56:D3:1734:U:H6	1.78	0.49
56:D3:1744:A:H2'	56:D3:1745:G:C8	2.48	0.49
56:D3:634:G:C2	56:D3:966:A:C6	3.00	0.49
56:D3:1636:C:C4	56:D3:1637:C:N4	2.81	0.49
57:D4:10:C:H2'	57:D4:11:U:C6	2.48	0.49
55:D2:426:G:C2	55:D2:428:A:H5"	2.47	0.49
56:D3:1646:C:N3	56:D3:1754:A:N1	2.60	0.49
56:D3:1707:A:P	56:D3:1707:A:C8	3.05	0.49
55:D2:140:U:H2'	55:D2:143:A:H2	1.76	0.49
55:D2:186:C:H2'	55:D2:187:A:H8	1.78	0.49
17:UQ:586:SER:O	17:UQ:594:TRP:HA	2.13	0.48
55:D2:549:G:N1	55:D2:589:U:N3	2.60	0.48
56:D3:1047:G:H2'	56:D3:1048:G:H8	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:UO:489:THR:O	15:UO:493:HIS:N	2.37	0.48
55:D2:208:A:H2'	55:D2:209:G:H8	1.78	0.48
56:D3:519:C:C4	56:D3:534:A:N7	2.81	0.48
56:D3:547:U:H2'	56:D3:548:G:C8	2.48	0.48
56:D3:600:U:H2'	56:D3:601:A:C8	2.49	0.48
56:D3:1735:U:C5'	56:D3:1735:U:H6	2.26	0.48
6:UF:155:TYR:HA	6:UF:159:ALA:HA	1.94	0.48
12:UL:937:ARG:O	31:CK:468:ARG:N	2.45	0.48
24:CB:264:GLN:CA	24:CB:320:TYR:O	2.61	0.48
28:CH:199:TYR:HA	28:CH:209:LYS:O	2.14	0.48
56:D3:1735:U:H5'	56:D3:1735:U:H6	1.79	0.48
32:CL:940:LYS:HA	56:D3:1492:A:C8	2.49	0.48
55:D2:238:G:C6	55:D2:275:A:C5	3.01	0.48
56:D3:891:A:H2'	56:D3:892:A:C8	2.48	0.48
8:UH:80:GLU:HA	8:UH:88:ASP:HA	1.95	0.48
56:D3:1505:A:C5	56:D3:1506:G:H1'	2.48	0.48
55:D2:21:A:H2'	55:D2:22:A:H8	1.79	0.48
55:D2:96:C:H2'	55:D2:97:G:C8	2.48	0.48
55:D2:186:C:H2'	55:D2:187:A:C8	2.48	0.48
56:D3:1666:U:O2	56:D3:1735:U:O4	2.32	0.48
57:D4:103:A:H2'	57:D4:104:C:C6	2.49	0.48
12:UL:486:LYS:O	12:UL:501:ASP:HA	2.14	0.48
32:CL:827:ALA:HA	32:CL:919:VAL:HA	1.95	0.48
55:D2:551:A:H2'	55:D2:552:G:H8	1.78	0.48
56:D3:35:U:H3	56:D3:474:A:H62	1.60	0.48
20:UU:759:PHE:O	20:UU:763:SER:CB	2.62	0.48
22:UX:154:ALA:HA	22:UX:173:MET:O	2.14	0.48
39:JN:257:ALA:O	39:JN:260:GLY:O	2.32	0.48
55:D2:289:U:H2'	55:D2:290:G:C8	2.49	0.48
6:UF:286:ILE:O	6:UF:290:LYS:HA	2.13	0.48
8:UH:229:TYR:HA	8:UH:240:LYS:O	2.14	0.48
56:D3:1151:A:H2'	56:D3:1152:A:C8	2.49	0.48
56:D3:1698:G:O6	56:D3:1704:U:O4	2.31	0.48
8:UH:182:THR:HA	8:UH:206:LEU:HA	1.95	0.47
55:D2:494:C:H2'	55:D2:495:G:C8	2.49	0.47
56:D3:1654:G:N2	56:D3:1746:A:C6	2.76	0.47
56:D3:1690:G:N1	56:D3:1711:C:C2	2.82	0.47
27:CF:56:ALA:HB3	27:CF:82:PRO:HA	1.95	0.47
56:D3:1704:U:H2'	56:D3:1705:C:C6	2.49	0.47
57:D4:41:C:H2'	57:D4:42:U:C6	2.50	0.47
55:D2:97:G:H1'	55:D2:155:A:N3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:D2:166:U:H2'	55:D2:167:U:H6	1.79	0.47
57:D4:12:U:H2'	57:D4:13:C:C5	2.48	0.47
57:D4:104:C:H2'	57:D4:105:C:C6	2.49	0.47
35:JF:42:ILE:O	35:JF:203:CYS:HA	2.14	0.47
55:D2:101:G:N7	55:D2:103:G:N1	2.62	0.47
56:D3:32:U:C2	56:D3:595:G:C2	3.03	0.47
55:D2:60:G:H2'	55:D2:61:U:C6	2.49	0.47
56:D3:1592:A:H2'	56:D3:1593:A:C8	2.50	0.47
10:UJ:550:TYR:O	10:UJ:553:SER:O	2.32	0.47
12:UL:433:ALA:HA	12:UL:449:THR:HA	1.96	0.47
13:UM:418:ASN:O	13:UM:422:CYS:CA	2.63	0.47
55:D2:158:G:H2'	55:D2:159:A:C8	2.48	0.47
55:D2:180:G:H2'	55:D2:181:A:C8	2.50	0.47
55:D2:212:U:H2'	55:D2:213:G:H8	1.79	0.47
55:D2:237:A:N7	55:D2:274:C:O2'	2.47	0.47
55:D2:407:A:C6	55:D2:450:G:N1	2.82	0.47
56:D3:1158:C:N4	56:D3:1164:G:N1	2.63	0.47
56:D3:1524:A:H2'	56:D3:1525:A:C8	2.49	0.47
56:D3:924:A:H2'	56:D3:925:G:H8	1.80	0.47
30:CJ:157:PHE:O	30:CJ:159:HIS:N	2.47	0.47
52:DX:75:GLN:HA	52:DX:81:LYS:O	2.14	0.47
57:D4:205:G:C6	57:D4:245:U:N3	2.83	0.47
12:UL:412:GLY:HA3	12:UL:430:CYS:N	2.28	0.47
26:CE:319:ILE:O	26:CE:321:GLY:N	2.48	0.47
32:CL:69:PRO:HA	32:CL:114:ARG:O	2.14	0.47
55:D2:101:G:O6	55:D2:103:G:C6	2.69	0.47
55:D2:338:A:O2'	55:D2:339:A:N7	2.44	0.47
10:UJ:729:LYS:O	10:UJ:732:PHE:N	2.46	0.46
55:D2:400:C:H2'	55:D2:401:A:C8	2.50	0.46
56:D3:559:C:H2'	56:D3:560:U:H6	1.81	0.46
56:D3:1582:U:N3	56:D3:1614:A:C8	2.83	0.46
13:UM:39:GLU:HA	13:UM:56:ILE:O	2.15	0.46
55:D2:56:G:H2'	55:D2:57:C:C6	2.50	0.46
56:D3:34:G:C6	56:D3:474:A:N7	2.84	0.46
56:D3:1163:A:N6	56:D3:1164:G:C6	2.84	0.46
15:UO:237:TRP:HA	15:UO:244:LYS:HA	1.96	0.46
28:CH:496:LEU:O	28:CH:513:GLU:HA	2.15	0.46
56:D3:976:G:C2	56:D3:978:A:N6	2.83	0.46
56:D3:1752:U:H2'	56:D3:1753:A:H8	1.81	0.46
13:UM:538:ASP:O	13:UM:550:THR:HA	2.15	0.46
18:UR:382:GLY:CA	18:UR:400:ILE:O	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:D2:546:G:O6	55:D2:592:U:O2	2.31	0.46
56:D3:1043:A:N6	56:D3:1075:C:N4	2.36	0.46
56:D3:1169:G:N1	56:D3:1575:G:OP2	2.49	0.46
56:D3:1699:G:N2	56:D3:1702:A:N6	2.36	0.46
11:UK:7:ASP:O	11:UK:10:LYS:N	2.49	0.46
55:D2:195:A:H2'	55:D2:196:A:C8	2.51	0.46
55:D2:506:G:N2	55:D2:531:C:C2	2.83	0.46
55:D2:549:G:N1	55:D2:589:U:C4	2.84	0.46
56:D3:1663:G:N2	56:D3:1738:U:O2	2.49	0.46
3:UC:567:LYS:O	3:UC:571:LYS:N	2.46	0.46
12:UL:183:ASP:O	12:UL:185:MET:N	2.48	0.46
12:UL:939:PHE:O	31:CK:466:GLU:N	2.38	0.46
56:D3:519:C:N3	56:D3:534:A:C5	2.83	0.46
56:D3:521:A:N1	56:D3:531:C:N4	2.63	0.46
56:D3:1270:G:H2'	56:D3:1271:G:C8	2.49	0.46
55:D2:474:A:H2'	55:D2:475:G:H8	1.79	0.46
56:D3:502:U:H2'	56:D3:503:G:C8	2.50	0.46
56:D3:547:U:H2'	56:D3:548:G:H8	1.80	0.46
56:D3:591:A:H2'	56:D3:592:A:C8	2.50	0.46
2:UB:783:HIS:HA	56:D3:1119:G:H5"	1.98	0.46
45:DH:143:LEU:O	45:DH:146:GLY:N	2.47	0.46
56:D3:485:A:N1	56:D3:503:G:C6	2.84	0.46
56:D3:497:G:H2'	56:D3:498:G:H8	1.81	0.46
56:D3:884:A:H2'	56:D3:885:G:C8	2.51	0.46
56:D3:1736:G:H2'	56:D3:1737:G:H8	1.81	0.46
2:UB:396:LEU:O	2:UB:400:PRO:N	2.49	0.46
12:UL:577:LEU:N	12:UL:591:SER:O	2.39	0.46
55:D2:219:U:H2'	55:D2:220:U:H6	1.81	0.46
55:D2:452:A:H2'	55:D2:453:A:H8	1.80	0.46
56:D3:1124:A:H1'	57:D4:1:G:N1	2.31	0.46
57:D4:75:C:H2'	57:D4:76:U:C6	2.51	0.46
55:D2:217:C:H2'	55:D2:218:U:C6	2.50	0.46
55:D2:409:C:H2'	55:D2:410:A:C8	2.51	0.46
56:D3:592:A:H2'	56:D3:593:U:O4'	2.16	0.46
56:D3:1733:C:H2'	56:D3:1734:U:C6	2.51	0.46
2:UB:597:GLU:O	2:UB:599:GLY:N	2.49	0.45
35:JF:177:LYS:O	35:JF:222:ASP:N	2.49	0.45
56:D3:1530:C:H2'	56:D3:1531:G:C8	2.44	0.45
56:D3:1604:U:H2'	56:D3:1605:G:H8	1.80	0.45
57:D4:3:C:H2'	57:D4:4:G:C8	2.48	0.45
13:UM:507:ALA:HA	13:UM:516:LYS:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:CA:198:GLU:O	24:CA:221:ILE:HA	2.16	0.45
55:D2:212:U:H2'	55:D2:213:G:C8	2.52	0.45
55:D2:507:U:H2'	55:D2:508:C:C6	2.52	0.45
55:D2:514:U:N3	55:D2:521:G:N1	2.56	0.45
56:D3:1606:C:H2'	56:D3:1607:G:H8	1.80	0.45
56:D3:1665:U:N3	56:D3:1737:G:C6	2.84	0.45
57:D4:198:U:H3	57:D4:201:C:H41	1.64	0.45
57:D4:315:A:H2'	57:D4:316:A:H8	1.81	0.45
55:D2:262:U:N3	55:D2:263:C:N4	2.63	0.45
56:D3:23:G:C2	56:D3:603:U:C2	3.03	0.45
56:D3:1594:G:O2'	56:D3:1600:A:N6	2.35	0.45
8:UH:178:ILE:HA	8:UH:187:VAL:O	2.15	0.45
19:US:130:GLU:O	19:US:134:PHE:CB	2.65	0.45
55:D2:516:U:O2'	55:D2:519:A:N6	2.49	0.45
56:D3:1025:A:H2'	56:D3:1026:A:H8	1.80	0.45
56:D3:1437:U:H2'	56:D3:1438:G:C8	2.51	0.45
57:D4:17:G:H2'	57:D4:18:G:C8	2.51	0.45
12:UL:42:ILE:HA	12:UL:50:ASN:O	2.17	0.45
12:UL:148:TRP:HA	12:UL:156:LEU:H	1.81	0.45
20:UU:82:ALA:HB3	20:UU:93:ALA:HB3	1.98	0.45
20:UU:368:SER:O	20:UU:375:LEU:HA	2.15	0.45
32:CL:847:LEU:HA	32:CL:898:GLY:HA2	1.98	0.45
56:D3:953:G:H2'	56:D3:954:G:C8	2.52	0.45
57:D4:205:G:C6	57:D4:245:U:C4	3.05	0.45
19:US:188:PHE:HA	19:US:237:GLU:O	2.17	0.45
56:D3:1602:C:H2'	56:D3:1603:U:C6	2.52	0.45
56:D3:1677:C:N3	56:D3:1724:U:O2	2.50	0.45
57:D4:94:A:H2'	57:D4:95:A:H8	1.80	0.45
56:D3:1569:A:H2'	56:D3:1570:A:C8	2.52	0.45
55:D2:199:A:H2'	55:D2:200:A:C8	2.51	0.45
57:D4:95:A:H2'	57:D4:96:C:H6	1.82	0.45
55:D2:223:C:H2'	55:D2:224:G:H8	1.79	0.45
55:D2:409:C:H2'	55:D2:410:A:H8	1.82	0.45
55:D2:457:G:H2'	55:D2:458:A:C8	2.52	0.45
56:D3:961:U:H2'	56:D3:962:C:C6	2.52	0.45
56:D3:1666:U:C4	56:D3:1736:G:N1	2.85	0.45
56:D3:1272:U:O2	56:D3:1438:G:C6	2.70	0.45
56:D3:1583:A:N6	56:D3:1612:U:OP2	2.50	0.45
56:D3:1692:G:N1	56:D3:1710:U:N3	2.64	0.45
56:D3:1729:C:H2'	56:D3:1730:A:O4'	2.17	0.45
21:UV:587:GLY:HA3	21:UV:611:ASP:H	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:CI:137:ARG:HA	29:CI:142:LEU:HA	1.98	0.44
56:D3:1486:G:H21	56:D3:1592:A:H4'	1.82	0.44
56:D3:1592:A:H2'	56:D3:1593:A:H8	1.82	0.44
56:D3:1665:U:N3	56:D3:1737:G:N1	2.66	0.44
56:D3:1267:G:C2	56:D3:1442:U:C2	3.05	0.44
56:D3:1643:U:H2'	56:D3:1644:C:H6	1.82	0.44
57:D4:58:A:H2'	57:D4:59:G:C8	2.52	0.44
13:UM:170:GLY:O	13:UM:187:GLN:HA	2.17	0.44
32:CL:364:VAL:HA	32:CL:372:TYR:O	2.18	0.44
55:D2:287:G:H2'	55:D2:288:G:H8	1.82	0.44
55:D2:476:A:H2'	55:D2:477:G:H8	1.82	0.44
56:D3:516:G:O6	56:D3:537:G:C2	2.70	0.44
56:D3:1532:U:H2'	56:D3:1533:C:C6	2.52	0.44
56:D3:1699:G:N2	56:D3:1702:A:C5	2.85	0.44
17:UQ:216:SER:N	17:UQ:222:HIS:O	2.50	0.44
40:JO:163:TYR:O	40:JO:173:ALA:HA	2.17	0.44
55:D2:410:A:H2'	55:D2:411:A:C8	2.53	0.44
55:D2:464:G:H2'	55:D2:465:G:H8	1.82	0.44
55:D2:466:A:N6	57:D4:51:C:N4	2.66	0.44
56:D3:1707:A:C8	56:D3:1707:A:OP2	2.70	0.44
55:D2:21:A:H2'	55:D2:22:A:C8	2.53	0.44
55:D2:353:A:C6	55:D2:371:G:C6	3.05	0.44
55:D2:378:C:H2'	55:D2:379:A:C8	2.52	0.44
56:D3:1580:C:H2'	56:D3:1581:C:C6	2.52	0.44
4:UD:399:VAL:O	4:UD:419:LYS:HA	2.17	0.44
8:UH:351:SER:O	8:UH:353:ARG:N	2.51	0.44
55:D2:264:C:H2'	55:D2:265:A:C8	2.53	0.44
56:D3:900:A:H3'	56:D3:901:G:H21	1.82	0.44
56:D3:1625:C:H2'	56:D3:1626:U:C6	2.52	0.44
55:D2:182:G:O6	55:D2:215:U:O4	2.35	0.44
57:D4:202:G:H2'	57:D4:203:U:H6	1.82	0.44
35:JF:121:LEU:CB	35:JF:163:ILE:O	2.65	0.44
55:D2:161:A:N6	55:D2:233:G:C6	2.86	0.44
56:D3:1508:U:H2'	56:D3:1509:C:C6	2.53	0.44
21:UV:378:ASN:O	21:UV:387:GLY:N	2.51	0.44
28:CH:197:THR:HA	28:CH:212:LYS:O	2.18	0.44
32:CL:137:LEU:HA	32:CL:166:ARG:O	2.17	0.44
33:CM:196:TYR:HA	33:CM:228:ASP:O	2.18	0.44
55:D2:357:G:O6	55:D2:368:U:O2	2.36	0.44
56:D3:1050:G:H2'	56:D3:1051:G:C8	2.53	0.44
4:UD:573:VAL:HA	4:UD:583:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:UQ:780:GLU:O	17:UQ:782:THR:N	2.51	0.43
33:CM:118:PHE:O	33:CM:165:GLU:HA	2.18	0.43
55:D2:173:G:H2'	55:D2:174:U:C6	2.53	0.43
55:D2:208:A:H2'	55:D2:209:G:C8	2.52	0.43
55:D2:360:C:N3	55:D2:366:A:N1	2.66	0.43
55:D2:407:A:C6	55:D2:450:G:C2	3.06	0.43
56:D3:546:U:H2'	56:D3:547:U:C6	2.52	0.43
56:D3:568:G:H2'	56:D3:569:C:C6	2.53	0.43
4:UD:199:ASP:CA	4:UD:215:ALA:O	2.62	0.43
36:JH:430:ASN:HA	36:JH:465:SER:HA	1.99	0.43
55:D2:166:U:H2'	55:D2:167:U:C6	2.53	0.43
55:D2:324:U:H2'	55:D2:327:A:C8	2.53	0.43
55:D2:464:G:H2'	55:D2:465:G:C8	2.52	0.43
56:D3:953:G:H2'	56:D3:954:G:H8	1.82	0.43
56:D3:1156:C:H2'	56:D3:1157:A:C8	2.52	0.43
56:D3:881:A:H2'	56:D3:882:U:O4'	2.18	0.43
57:D4:95:A:H2'	57:D4:96:C:C6	2.52	0.43
57:D4:205:G:O6	57:D4:245:U:C4	2.71	0.43
56:D3:1152:A:H2'	56:D3:1153:G:C8	2.54	0.43
56:D3:1484:G:H1	56:D3:1591:C:H1'	1.82	0.43
56:D3:1752:U:H2'	56:D3:1753:A:C8	2.53	0.43
57:D4:98:U:H2'	57:D4:99:U:H6	1.82	0.43
10:UJ:559:ASN:O	10:UJ:599:PHE:N	2.34	0.43
43:DA:88:VAL:HA	43:DA:98:THR:HA	2.00	0.43
46:DJ:152:SER:O	46:DJ:155:HIS:N	2.42	0.43
1:UA:600:SER:HA	1:UA:615:PHE:O	2.19	0.43
13:UM:246:CYS:HA	13:UM:259:TYR:O	2.19	0.43
13:UM:623:LEU:HA	13:UM:633:VAL:O	2.19	0.43
51:DW:4:SER:O	56:D3:634:G:H5'	2.19	0.43
56:D3:1264:G:N2	56:D3:1265:G:N7	2.65	0.43
15:UO:127:THR:HA	15:UO:144:SER:HA	2.01	0.43
55:D2:415:U:H2'	55:D2:416:A:H8	1.84	0.43
55:D2:468:A:N6	57:D4:49:C:N3	2.67	0.43
56:D3:870:C:H2'	56:D3:871:G:C8	2.54	0.43
13:UM:418:ASN:CB	13:UM:423:LYS:O	2.67	0.43
56:D3:1736:G:H2'	56:D3:1736:G:N3	2.34	0.43
10:UJ:741:LEU:HA	10:UJ:742:ASN:HA	1.69	0.43
55:D2:188:A:H2	55:D2:209:G:H22	1.67	0.43
56:D3:939:A:H2'	56:D3:940:A:C8	2.53	0.43
8:UH:131:VAL:H	8:UH:145:ASP:C	2.22	0.43
10:UJ:705:SER:HA	10:UJ:708:ALA:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:D2:134:A:H2'	55:D2:135:G:H8	1.84	0.43
55:D2:476:A:H2'	55:D2:477:G:C8	2.53	0.43
55:D2:586:A:H2'	55:D2:587:G:H8	1.84	0.43
56:D3:891:A:H2'	56:D3:892:A:H8	1.84	0.43
56:D3:957:G:H2'	56:D3:958:U:C6	2.54	0.43
56:D3:1267:G:C2	56:D3:1442:U:O2	2.72	0.43
56:D3:1666:U:C2	56:D3:1735:U:O4	2.72	0.43
56:D3:1726:G:H2'	56:D3:1727:G:H8	1.84	0.43
56:D3:1739:C:H2'	56:D3:1740:A:C8	2.53	0.43
55:D2:478:U:H2'	55:D2:479:G:C8	2.54	0.42
56:D3:523:G:H21	56:D3:529:A:H62	1.66	0.42
56:D3:1111:G:H2'	56:D3:1112:G:H8	1.84	0.42
57:D4:331:A:H2'	57:D4:332:G:H8	1.83	0.42
45:DH:63:PRO:O	45:DH:67:LEU:CB	2.67	0.42
55:D2:554:G:C6	55:D2:583:U:N3	2.86	0.42
56:D3:1619:C:H2'	56:D3:1620:C:H6	1.85	0.42
57:D4:76:U:H2'	57:D4:77:U:C6	2.54	0.42
20:UU:515:ARG:O	20:UU:531:PHE:N	2.52	0.42
51:DW:48:GLY:HA3	51:DW:64:GLN:O	2.18	0.42
55:D2:2:U:O2'	55:D2:69:U:O2'	2.18	0.42
55:D2:247:U:H2'	55:D2:248:G:H8	1.83	0.42
55:D2:276:G:H2'	55:D2:277:C:H6	1.85	0.42
55:D2:362:C:H3'	55:D2:363:A:C8	2.55	0.42
55:D2:504:U:H2'	55:D2:505:G:C8	2.55	0.42
56:D3:887:A:H2'	56:D3:888:U:H6	1.85	0.42
56:D3:1047:G:H2'	56:D3:1048:G:C8	2.54	0.42
56:D3:1077:C:H2'	56:D3:1078:C:H6	1.84	0.42
55:D2:397:A:H2'	55:D2:398:A:C8	2.54	0.42
56:D3:485:A:C2	56:D3:503:G:N1	2.88	0.42
56:D3:601:A:H2'	56:D3:602:U:C6	2.54	0.42
56:D3:1483:A:C6	56:D3:1524:A:C5	3.07	0.42
26:CE:431:ALA:HB3	55:D2:309:A:N6	2.34	0.42
55:D2:227:U:H2'	55:D2:228:A:C8	2.55	0.42
55:D2:398:A:H2'	55:D2:399:U:H6	1.85	0.42
57:D4:263:A:N6	57:D4:309:G:C2	2.87	0.42
12:UL:148:TRP:HA	12:UL:155:GLY:HA2	2.00	0.42
41:JP:55:ALA:HA	41:JP:379:ALA:HB1	2.01	0.42
55:D2:134:A:H2'	55:D2:135:G:C8	2.55	0.42
55:D2:489:G:O2'	55:D2:490:G:H8	2.02	0.42
4:UD:548:GLY:O	4:UD:566:LEU:N	2.53	0.42
12:UL:450:ARG:O	12:UL:475:ALA:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:D2:171:G:C6	55:D2:226:U:C4	3.07	0.42
56:D3:1643:U:H2'	56:D3:1644:C:C6	2.54	0.42
57:D4:104:C:H2'	57:D4:105:C:H6	1.85	0.42
57:D4:311:G:O2'	57:D4:312:U:O4'	2.35	0.42
24:CB:125:VAL:O	24:CB:138:LYS:HA	2.20	0.42
56:D3:1170:G:C6	56:D3:1574:G:N1	2.88	0.42
56:D3:1573:A:H5'	56:D3:1574:G:N3	2.34	0.42
57:D4:202:G:C6	57:D4:248:G:C5	3.07	0.42
12:UL:338:ILE:HA	12:UL:357:THR:HA	2.02	0.42
17:UQ:718:GLY:HA3	17:UQ:746:PHE:O	2.20	0.42
23:UZ:68:ARG:O	50:DS:82:PRO:HA	2.20	0.42
35:JG:121:LEU:CB	35:JG:163:ILE:O	2.67	0.42
55:D2:13:U:H1'	55:D2:70:A:N7	2.35	0.42
55:D2:174:U:H2'	55:D2:175:A:C8	2.55	0.42
55:D2:496:G:H2'	55:D2:497:A:C8	2.55	0.42
56:D3:1506:G:H2'	56:D3:1507:G:C8	2.53	0.42
57:D4:17:G:H2'	57:D4:18:G:H8	1.85	0.42
55:D2:453:A:H2'	55:D2:454:C:C6	2.55	0.42
56:D3:514:G:HO2'	56:D3:515:A:H8	1.68	0.42
56:D3:599:A:H2'	56:D3:600:U:C6	2.55	0.42
56:D3:1648:A:H2'	56:D3:1649:G:H8	1.84	0.42
12:UL:124:ILE:HA	12:UL:140:SER:HA	2.01	0.41
12:UL:619:MET:H	12:UL:634:SER:HA	1.85	0.41
32:CL:105:ILE:O	32:CL:117:PHE:N	2.50	0.41
56:D3:1525:A:H2'	56:D3:1526:A:C8	2.55	0.41
56:D3:1787:C:H2'	56:D3:1788:G:C8	2.55	0.41
50:DS:24:GLY:O	50:DS:59:GLY:N	2.52	0.41
56:D3:487:G:H2'	56:D3:488:G:H8	1.85	0.41
56:D3:1661:U:H2'	56:D3:1662:G:H8	1.85	0.41
56:D3:1692:G:C6	56:D3:1710:U:O4	2.73	0.41
56:D3:1693:A:O2'	56:D3:1694:A:O4'	2.21	0.41
14:UN:323:HIS:N	55:D2:534:A:O2'	2.53	0.41
20:UU:228:GLY:O	20:UU:245:LYS:HA	2.21	0.41
55:D2:147:C:H2'	55:D2:148:G:C8	2.55	0.41
55:D2:281:G:H2'	55:D2:282:G:H8	1.86	0.41
56:D3:1684:U:H2'	56:D3:1685:G:H8	1.85	0.41
57:D4:330:A:H2'	57:D4:331:A:C8	2.55	0.41
52:DX:103:LEU:N	52:DX:126:LYS:O	2.54	0.41
55:D2:547:C:H2'	55:D2:548:A:C8	2.54	0.41
56:D3:961:U:H2'	56:D3:962:C:H6	1.85	0.41
8:UH:309:PRO:O	8:UH:327:SER:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:US:456:THR:O	19:US:458:ALA:N	2.50	0.41
48:DO:82:LYS:HA	48:DO:116:GLU:O	2.21	0.41
55:D2:60:G:H2'	55:D2:61:U:H6	1.85	0.41
55:D2:192:G:H2'	55:D2:193:G:C8	2.53	0.41
56:D3:29:U:H2'	56:D3:30:G:C8	2.55	0.41
56:D3:1693:A:H2'	56:D3:1694:A:C8	2.55	0.41
56:D3:1723:U:H2'	56:D3:1724:U:C6	2.55	0.41
56:D3:1782:A:H3'	56:D3:1783:C:C6	2.55	0.41
43:DA:70:LEU:N	43:DA:82:ARG:O	2.47	0.41
55:D2:3:G:H2'	55:D2:4:C:C6	2.56	0.41
56:D3:504:U:HO2'	56:D3:506:A:H8	1.67	0.41
8:UH:55:ILE:HA	8:UH:72:ASN:HA	2.02	0.41
28:CH:153:GLY:O	57:D4:251:G:N1	2.48	0.41
55:D2:244:U:H2'	55:D2:245:C:C6	2.55	0.41
55:D2:353:A:N1	55:D2:371:G:C6	2.88	0.41
56:D3:33:U:O2	56:D3:468:A:N7	2.53	0.41
56:D3:472:U:H2'	56:D3:473:A:C8	2.55	0.41
56:D3:559:C:H2'	56:D3:560:U:C6	2.55	0.41
56:D3:1124:A:H1'	57:D4:1:G:C2	2.56	0.41
5:UE:359:GLY:HA2	55:D2:147:C:H4'	2.03	0.41
33:CM:159:PRO:HA	33:CM:160:PRO:HA	1.75	0.41
55:D2:376:U:H2'	55:D2:377:U:C6	2.56	0.41
56:D3:1602:C:H2'	56:D3:1603:U:H6	1.86	0.41
8:UH:142:THR:N	8:UH:157:TYR:O	2.35	0.41
13:UM:296:ILE:C	13:UM:298:SER:H	2.24	0.41
28:CH:551:ARG:O	28:CH:553:ILE:N	2.54	0.41
55:D2:262:U:H2'	55:D2:263:C:C6	2.55	0.41
55:D2:497:A:H2'	55:D2:498:G:C8	2.56	0.41
55:D2:528:G:H2'	55:D2:529:A:C8	2.56	0.41
56:D3:1707:A:O5'	56:D3:1707:A:C8	2.70	0.41
57:D4:263:A:N6	57:D4:309:G:N1	2.69	0.41
55:D2:397:A:H2'	55:D2:398:A:H8	1.86	0.41
55:D2:538:C:H2'	55:D2:539:A:C8	2.56	0.41
56:D3:1158:C:N4	56:D3:1164:G:H1	2.19	0.41
57:D4:101:G:C6	57:D4:315:A:C6	3.09	0.41
57:D4:205:G:N1	57:D4:245:U:O2	2.53	0.41
8:UH:54:TYR:O	8:UH:73:ILE:N	2.54	0.40
13:UM:63:GLU:O	13:UM:81:GLN:N	2.54	0.40
21:UV:304:GLU:O	21:UV:308:LEU:CB	2.69	0.40
28:CH:443:LEU:N	28:CH:471:GLN:O	2.41	0.40
55:D2:306:G:H2'	55:D2:307:C:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:D2:307:C:O2'	55:D2:311:C:OP2	2.24	0.40
55:D2:552:G:H2'	55:D2:553:A:H8	1.85	0.40
56:D3:1504:G:H3'	56:D3:1505:A:H8	1.86	0.40
32:CL:169:GLY:O	32:CL:204:LEU:HA	2.21	0.40
35:JG:165:ASN:HA	35:JG:166:PRO:HA	1.80	0.40
55:D2:554:G:C2	55:D2:583:U:O2	2.74	0.40
56:D3:478:A:C6	56:D3:510:G:O6	2.73	0.40
56:D3:590:C:H2'	56:D3:591:A:H8	1.86	0.40
56:D3:1484:G:H22	56:D3:1591:C:H1'	1.86	0.40
56:D3:1723:U:H2'	56:D3:1724:U:H6	1.87	0.40
56:D3:1776:A:H2'	56:D3:1777:G:C8	2.55	0.40
8:UH:267:ILE:O	8:UH:284:LEU:HA	2.21	0.40
55:D2:96:C:H2'	55:D2:97:G:H8	1.85	0.40
55:D2:130:G:H2'	55:D2:131:C:C6	2.56	0.40
55:D2:147:C:H2'	55:D2:148:G:H8	1.85	0.40
55:D2:437:G:H2'	55:D2:438:U:C6	2.57	0.40
55:D2:543:C:H2'	55:D2:544:C:C6	2.56	0.40
56:D3:635:A:H2'	56:D3:636:A:H8	1.86	0.40
56:D3:1050:G:H2'	56:D3:1051:G:H8	1.87	0.40
56:D3:1684:U:H3	56:D3:1717:G:H1	1.69	0.40
57:D4:24:U:HO2'	57:D4:25:U:P	2.45	0.40
13:UM:591:ILE:HA	13:UM:600:LYS:O	2.21	0.40
55:D2:506:G:C2	55:D2:531:C:O2	2.75	0.40
55:D2:510:A:H2'	55:D2:511:G:H8	1.87	0.40
56:D3:34:G:H2'	56:D3:35:U:O4'	2.21	0.40
56:D3:1274:C:N3	56:D3:1275:A:N6	2.70	0.40
1:UA:219:GLU:O	1:UA:248:TRP:HA	2.21	0.40
1:UA:393:VAL:HA	1:UA:403:PHE:O	2.22	0.40
55:D2:68:U:H5	55:D2:70:A:H2'	1.87	0.40
55:D2:123:C:H3'	55:D2:124:A:C8	2.56	0.40
56:D3:878:G:H2'	56:D3:879:G:C8	2.56	0.40
56:D3:1035:G:H3'	56:D3:1037:C:H41	1.87	0.40
56:D3:1541:G:N3	56:D3:1570:A:N1	2.68	0.40
56:D3:1707:A:H8	56:D3:1707:A:OP2	2.03	0.40
57:D4:103:A:N1	57:D4:313:A:N6	2.70	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	UA	830/923 (90%)	750 (90%)	80 (10%)	0	100	100
2	UB	492/810 (61%)	451 (92%)	38 (8%)	3 (1%)	25	65
3	UC	124/610 (20%)	116 (94%)	8 (6%)	0	100	100
4	UD	663/776 (85%)	581 (88%)	81 (12%)	1 (0%)	47	81
5	UE	465/643 (72%)	407 (88%)	58 (12%)	0	100	100
6	UF	283/440 (64%)	277 (98%)	6 (2%)	0	100	100
7	UG	529/554 (96%)	472 (89%)	56 (11%)	1 (0%)	47	81
8	UH	426/713 (60%)	305 (72%)	84 (20%)	37 (9%)	1	13
9	UI	100/575 (17%)	94 (94%)	6 (6%)	0	100	100
10	UJ	720/1769 (41%)	665 (92%)	54 (8%)	1 (0%)	51	85
11	UK	238/250 (95%)	222 (93%)	16 (7%)	0	100	100
12	UL	828/943 (88%)	737 (89%)	91 (11%)	0	100	100
13	UM	750/817 (92%)	661 (88%)	87 (12%)	2 (0%)	41	76
14	UN	143/899 (16%)	130 (91%)	13 (9%)	0	100	100
15	UO	489/513 (95%)	435 (89%)	54 (11%)	0	100	100
16	UP	58/214 (27%)	55 (95%)	3 (5%)	0	100	100
17	UQ	820/896 (92%)	720 (88%)	100 (12%)	0	100	100
18	UR	474/594 (80%)	418 (88%)	56 (12%)	0	100	100
19	US	460/552 (83%)	419 (91%)	40 (9%)	1 (0%)	47	81
20	UU	842/939 (90%)	756 (90%)	86 (10%)	0	100	100
21	UV	1086/1237 (88%)	1037 (96%)	49 (4%)	0	100	100
22	UX	170/189 (90%)	160 (94%)	10 (6%)	0	100	100
23	UZ	245/274 (89%)	223 (91%)	22 (9%)	0	100	100
24	CA	238/327 (73%)	218 (92%)	20 (8%)	0	100	100
24	CB	224/327 (68%)	198 (88%)	26 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
25	CD	376/504 (75%)	343 (91%)	31 (8%)	2 (0%)	29 68
26	CE	431/511 (84%)	392 (91%)	38 (9%)	1 (0%)	47 81
27	CF	121/126 (96%)	110 (91%)	11 (9%)	0	100 100
27	CG	121/126 (96%)	116 (96%)	5 (4%)	0	100 100
28	CH	434/573 (76%)	385 (89%)	46 (11%)	3 (1%)	22 62
29	CI	180/183 (98%)	163 (91%)	17 (9%)	0	100 100
30	CJ	278/290 (96%)	248 (89%)	29 (10%)	1 (0%)	34 72
31	CK	203/593 (34%)	192 (95%)	9 (4%)	2 (1%)	15 54
32	CL	771/1183 (65%)	716 (93%)	55 (7%)	0	100 100
33	CM	358/367 (98%)	328 (92%)	30 (8%)	0	100 100
34	CN	224/297 (75%)	215 (96%)	9 (4%)	0	100 100
35	JF	212/252 (84%)	199 (94%)	13 (6%)	0	100 100
35	JG	226/252 (90%)	209 (92%)	17 (8%)	0	100 100
36	JH	257/483 (53%)	234 (91%)	23 (9%)	0	100 100
37	JJ	180/274 (66%)	169 (94%)	11 (6%)	0	100 100
38	JM	129/217 (59%)	122 (95%)	7 (5%)	0	100 100
39	JN	178/346 (51%)	162 (91%)	11 (6%)	5 (3%)	5 33
40	JO	186/316 (59%)	177 (95%)	9 (5%)	0	100 100
41	JP	457/489 (94%)	412 (90%)	44 (10%)	1 (0%)	47 81
42	JQ	59/206 (29%)	54 (92%)	5 (8%)	0	100 100
43	DA	236/255 (92%)	217 (92%)	18 (8%)	1 (0%)	34 72
44	DF	211/225 (94%)	192 (91%)	19 (9%)	0	100 100
45	DH	182/190 (96%)	163 (90%)	19 (10%)	0	100 100
46	DJ	183/197 (93%)	169 (92%)	14 (8%)	0	100 100
47	DN	148/151 (98%)	132 (89%)	15 (10%)	1 (1%)	22 62
48	DO	118/137 (86%)	108 (92%)	10 (8%)	0	100 100
49	DQ	123/143 (86%)	110 (89%)	13 (11%)	0	100 100
50	DS	99/146 (68%)	88 (89%)	11 (11%)	0	100 100
51	DW	127/130 (98%)	107 (84%)	20 (16%)	0	100 100
52	DX	101/145 (70%)	86 (85%)	14 (14%)	1 (1%)	15 54
53	Db	79/82 (96%)	70 (89%)	9 (11%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
54	Dc	61/67 (91%)	52 (85%)	9 (15%)	0	100 100
All	All	18746/26240 (71%)	16947 (90%)	1735 (9%)	64 (0%)	44 76

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	UB	395	ASP
8	UH	67	PRO
8	UH	184	ASN
8	UH	234	CYS
8	UH	258	PRO
8	UH	267	ILE
8	UH	298	PRO
8	UH	309	PRO
8	UH	325	PRO
25	CD	265	GLU
28	CH	438	ILE
31	CK	454	VAL
39	JN	94	PRO
39	JN	97	ILE
8	UH	29	VAL
8	UH	127	TYR
8	UH	214	ASP
8	UH	235	PRO
8	UH	248	LEU
8	UH	268	GLU
8	UH	352	GLN
39	JN	107	VAL
39	JN	109	PRO
8	UH	128	THR
8	UH	174	LYS
8	UH	198	ILE
8	UH	205	LEU
8	UH	206	LEU
8	UH	217	LYS
8	UH	299	HIS
8	UH	308	PHE
8	UH	533	PRO
13	UM	420	ASN
26	CE	320	LEU
28	CH	437	ARG
28	CH	439	ALA

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Mol	Chain	Res	Type
39	JN	111	LYS
52	DX	90	ASP
8	UH	137	GLU
8	UH	138	ASP
8	UH	142	THR
8	UH	284	LEU
8	UH	341	LEU
30	CJ	93	SER
43	DA	81	PHE
2	UB	396	LEU
4	UD	759	PRO
8	UH	161	ASP
8	UH	249	THR
10	UJ	411	ASN
13	UM	37	LEU
19	US	106	ILE
25	CD	240	LEU
41	JP	284	HIS
2	UB	399	HIS
8	UH	57	ASN
8	UH	69	PRO
8	UH	193	ASN
8	UH	257	SER
8	UH	297	LEU
31	CK	460	PRO
47	DN	68	GLY
7	UG	385	PRO
8	UH	60	PRO

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
55	D2	519/700 (74%)	146 (28%)	6 (1%)
56	D3	770/1379 (55%)	264 (34%)	17 (2%)
57	D4	169/175 (96%)	51 (30%)	0
All	All	1458/2254 (64%)	461 (31%)	23 (1%)

All (461) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
55	D2	2	U
55	D2	6	A
55	D2	14	U
55	D2	15	G
55	D2	58	U
55	D2	63	G
55	D2	66	C
55	D2	68	U
55	D2	69	U
55	D2	70	A
55	D2	82	A
55	D2	83	U
55	D2	84	G
55	D2	85	G
55	D2	90	G
55	D2	98	G
55	D2	100	G
55	D2	101	G
55	D2	102	A
55	D2	103	G
55	D2	104	A
55	D2	105	G
55	D2	109	C
55	D2	110	G
55	D2	113	A
55	D2	124	A
55	D2	125	G
55	D2	129	U
55	D2	130	G
55	D2	141	A
55	D2	142	U
55	D2	144	C
55	D2	150	G
55	D2	151	U
55	D2	152	U
55	D2	153	U
55	D2	155	A
55	D2	163	G
55	D2	169	A
55	D2	170	U
55	D2	171	G
55	D2	176	U

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Mol	Chain	Res	Type
55	D2	177	U
55	D2	190	U
55	D2	197	G
55	D2	198	A
55	D2	200	A
55	D2	201	U
55	D2	203	C
55	D2	207	G
55	D2	227	U
55	D2	228	A
55	D2	231	C
55	D2	234	A
55	D2	235	A
55	D2	236	C
55	D2	239	U
55	D2	240	C
55	D2	252	A
55	D2	253	U
55	D2	254	C
55	D2	256	U
55	D2	259	G
55	D2	261	U
55	D2	266	U
55	D2	267	U
55	D2	268	G
55	D2	270	U
55	D2	279	A
55	D2	280	A
55	D2	281	G
55	D2	294	U
55	D2	297	U
55	D2	303	A
55	D2	304	U
55	D2	305	A
55	D2	310	U
55	D2	311	C
55	D2	312	U
55	D2	313	A
55	D2	314	U
55	D2	315	U
55	D2	316	U
55	D2	324	U

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Mol	Chain	Res	Type
55	D2	325	U
55	D2	327	A
55	D2	332	U
55	D2	337	G
55	D2	353	A
55	D2	354	G
55	D2	356	C
55	D2	365	G
55	D2	366	A
55	D2	368	U
55	D2	369	G
55	D2	370	U
55	D2	371	G
55	D2	372	A
55	D2	373	U
55	D2	382	U
55	D2	383	G
55	D2	385	A
55	D2	395	C
55	D2	399	U
55	D2	407	A
55	D2	418	C
55	D2	428	A
55	D2	430	C
55	D2	431	A
55	D2	432	C
55	D2	433	C
55	D2	440	U
55	D2	451	G
55	D2	452	A
55	D2	460	U
55	D2	461	A
55	D2	462	G
55	D2	468	A
55	D2	469	C
55	D2	470	U
55	D2	481	U
55	D2	482	A
55	D2	484	G
55	D2	485	G
55	D2	487	A
55	D2	488	U

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Mol	Chain	Res	Type
55	D2	491	U
55	D2	492	G
55	D2	493	A
55	D2	494	C
55	D2	513	G
55	D2	526	U
55	D2	533	G
55	D2	535	G
55	D2	536	A
55	D2	537	G
55	D2	540	U
55	D2	541	U
55	D2	542	U
55	D2	546	G
55	D2	547	C
55	D2	548	A
55	D2	551	A
55	D2	555	A
55	D2	585	C
55	D2	586	A
56	D3	-6	A
56	D3	-5	G
56	D3	-4	A
56	D3	-3	U
56	D3	-2	A
56	D3	-1	G
56	D3	1	U
56	D3	2	A
56	D3	6	G
56	D3	7	G
56	D3	9	U
56	D3	10	G
56	D3	16	G
56	D3	17	C
56	D3	18	C
56	D3	25	C
56	D3	26	A
56	D3	33	U
56	D3	34	G
56	D3	36	C
56	D3	39	A
56	D3	468	A

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Mol	Chain	Res	Type
56	D3	470	A
56	D3	473	A
56	D3	474	A
56	D3	475	A
56	D3	477	A
56	D3	482	U
56	D3	487	G
56	D3	496	G
56	D3	501	U
56	D3	505	A
56	D3	506	A
56	D3	511	A
56	D3	515	A
56	D3	520	A
56	D3	522	U
56	D3	525	A
56	D3	526	A
56	D3	527	A
56	D3	528	U
56	D3	529	A
56	D3	533	U
56	D3	534	A
56	D3	538	A
56	D3	539	G
56	D3	541	A
56	D3	542	A
56	D3	543	C
56	D3	544	A
56	D3	545	A
56	D3	546	U
56	D3	562	G
56	D3	564	G
56	D3	565	C
56	D3	570	A
56	D3	572	C
56	D3	576	G
56	D3	578	U
56	D3	579	A
56	D3	580	A
56	D3	584	C
56	D3	585	A
56	D3	586	G

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Mol	Chain	Res	Type
56	D3	587	C
56	D3	594	A
56	D3	595	G
56	D3	597	G
56	D3	629	U
56	D3	631	G
56	D3	634	G
56	D3	635	A
56	D3	638	U
56	D3	860	U
56	D3	863	A
56	D3	864	U
56	D3	873	U
56	D3	876	G
56	D3	886	U
56	D3	898	A
56	D3	899	G
56	D3	906	A
56	D3	911	U
56	D3	912	U
56	D3	913	G
56	D3	914	G
56	D3	915	A
56	D3	921	U
56	D3	922	G
56	D3	926	A
56	D3	928	U
56	D3	929	A
56	D3	930	A
56	D3	931	C
56	D3	933	A
56	D3	934	C
56	D3	935	U
56	D3	942	G
56	D3	944	A
56	D3	952	A
56	D3	959	U
56	D3	966	A
56	D3	969	C
56	D3	970	A
56	D3	971	A
56	D3	972	G

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Mol	Chain	Res	Type
56	D3	977	A
56	D3	978	A
56	D3	1029	U
56	D3	1031	U
56	D3	1032	G
56	D3	1033	C
56	D3	1035	G
56	D3	1036	A
56	D3	1038	U
56	D3	1040	G
56	D3	1041	G
56	D3	1043	A
56	D3	1044	U
56	D3	1053	G
56	D3	1054	U
56	D3	1058	U
56	D3	1061	A
56	D3	1062	A
56	D3	1063	U
56	D3	1064	G
56	D3	1072	C
56	D3	1076	A
56	D3	1079	U
56	D3	1118	G
56	D3	1119	G
56	D3	1122	G
56	D3	1124	A
56	D3	1125	A
56	D3	1126	G
56	D3	1127	G
56	D3	1128	C
56	D3	1130	G
56	D3	1133	A
56	D3	1134	C
56	D3	1136	U
56	D3	1143	A
56	D3	1145	U
56	D3	1146	G
56	D3	1147	A
56	D3	1149	G
56	D3	1150	G
56	D3	1158	C

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Mol	Chain	Res	Type
56	D3	1159	C
56	D3	1160	A
56	D3	1202	A
56	D3	1203	A
56	D3	1204	A
56	D3	1205	C
56	D3	1207	C
56	D3	1208	A
56	D3	1212	G
56	D3	1214	U
56	D3	1217	A
56	D3	1218	G
56	D3	1219	A
56	D3	1259	U
56	D3	1261	G
56	D3	1267	G
56	D3	1268	G
56	D3	1269	U
56	D3	1270	G
56	D3	1276	U
56	D3	1434	U
56	D3	1436	A
56	D3	1437	U
56	D3	1438	G
56	D3	1442	U
56	D3	1443	U
56	D3	1454	G
56	D3	1465	C
56	D3	1466	G
56	D3	1470	C
56	D3	1471	A
56	D3	1472	C
56	D3	1473	U
56	D3	1474	G
56	D3	1483	A
56	D3	1486	G
56	D3	1488	G
56	D3	1489	U
56	D3	1490	C
56	D3	1491	U
56	D3	1492	A
56	D3	1493	A

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Mol	Chain	Res	Type
56	D3	1498	G
56	D3	1504	G
56	D3	1506	G
56	D3	1509	C
56	D3	1516	A
56	D3	1526	A
56	D3	1571	C
56	D3	1572	G
56	D3	1573	A
56	D3	1574	G
56	D3	1575	G
56	D3	1583	A
56	D3	1584	G
56	D3	1590	G
56	D3	1595	U
56	D3	1596	C
56	D3	1601	G
56	D3	1602	C
56	D3	1618	C
56	D3	1619	C
56	D3	1621	U
56	D3	1622	G
56	D3	1627	U
56	D3	1628	U
56	D3	1629	G
56	D3	1630	U
56	D3	1631	A
56	D3	1633	A
56	D3	1637	C
56	D3	1638	G
56	D3	1639	C
56	D3	1645	G
56	D3	1651	A
56	D3	1655	A
56	D3	1657	U
56	D3	1658	G
56	D3	1663	G
56	D3	1666	U
56	D3	1667	A
56	D3	1670	G
56	D3	1671	A
56	D3	1672	G

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Mol	Chain	Res	Type
56	D3	1676	U
56	D3	1680	G
56	D3	1681	A
56	D3	1682	U
56	D3	1683	C
56	D3	1684	U
56	D3	1690	G
56	D3	1692	G
56	D3	1695	G
56	D3	1696	G
56	D3	1697	G
56	D3	1699	G
56	D3	1703	C
56	D3	1706	C
56	D3	1707	A
56	D3	1710	U
56	D3	1711	C
56	D3	1712	A
56	D3	1713	G
56	D3	1714	A
56	D3	1717	G
56	D3	1735	U
56	D3	1736	G
56	D3	1742	U
56	D3	1746	A
56	D3	1747	G
56	D3	1769	U
56	D3	1770	U
56	D3	1773	C
56	D3	1780	G
56	D3	1782	A
56	D3	1783	C
57	D4	2	U
57	D4	4	G
57	D4	14	A
57	D4	15	U
57	D4	22	A
57	D4	23	U
57	D4	24	U
57	D4	25	U
57	D4	30	A
57	D4	32	G

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Mol	Chain	Res	Type
57	D4	33	A
57	D4	34	A
57	D4	35	U
57	D4	37	G
57	D4	38	U
57	D4	39	C
57	D4	40	A
57	D4	55	A
57	D4	56	A
57	D4	60	A
57	D4	61	G
57	D4	62	C
57	D4	87	G
57	D4	88	U
57	D4	90	C
57	D4	91	C
57	D4	94	A
57	D4	100	U
57	D4	103	A
57	D4	104	C
57	D4	114	A
57	D4	115	G
57	D4	198	U
57	D4	199	G
57	D4	201	C
57	D4	246	A
57	D4	247	U
57	D4	248	G
57	D4	252	C
57	D4	254	A
57	D4	256	G
57	D4	259	C
57	D4	267	A
57	D4	305	G
57	D4	312	U
57	D4	313	A
57	D4	319	G
57	D4	322	A
57	D4	324	U
57	D4	325	C
57	D4	329	C

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
55	D2	82	A
55	D2	311	C
55	D2	314	U
55	D2	370	U
55	D2	451	G
55	D2	492	G
56	D3	0	U
56	D3	474	A
56	D3	579	A
56	D3	586	G
56	D3	912	U
56	D3	925	G
56	D3	934	C
56	D3	1057	U
56	D3	1525	A
56	D3	1573	A
56	D3	1594	G
56	D3	1620	C
56	D3	1638	G
56	D3	1657	U
56	D3	1669	U
56	D3	1706	C
56	D3	1746	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
60	GTP	CL	2001	59	26,34,34	0.93	1 (3%)	32,54,54	1.49	5 (15%)

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
60	GTP	CL	2001	59	-	3/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	CL	2001	GTP	C6-N1	-2.43	1.34	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	CL	2001	GTP	PB-O3B-PG	-3.79	119.82	132.83
60	CL	2001	GTP	PA-O3A-PB	-3.57	120.58	132.83
60	CL	2001	GTP	C3'-C2'-C1'	3.18	105.77	100.98
60	CL	2001	GTP	C8-N7-C5	2.42	107.60	102.99
60	CL	2001	GTP	C5-C6-N1	2.31	118.03	113.95

There are no chirality outliers.

All (3) torsion outliers are listed below:

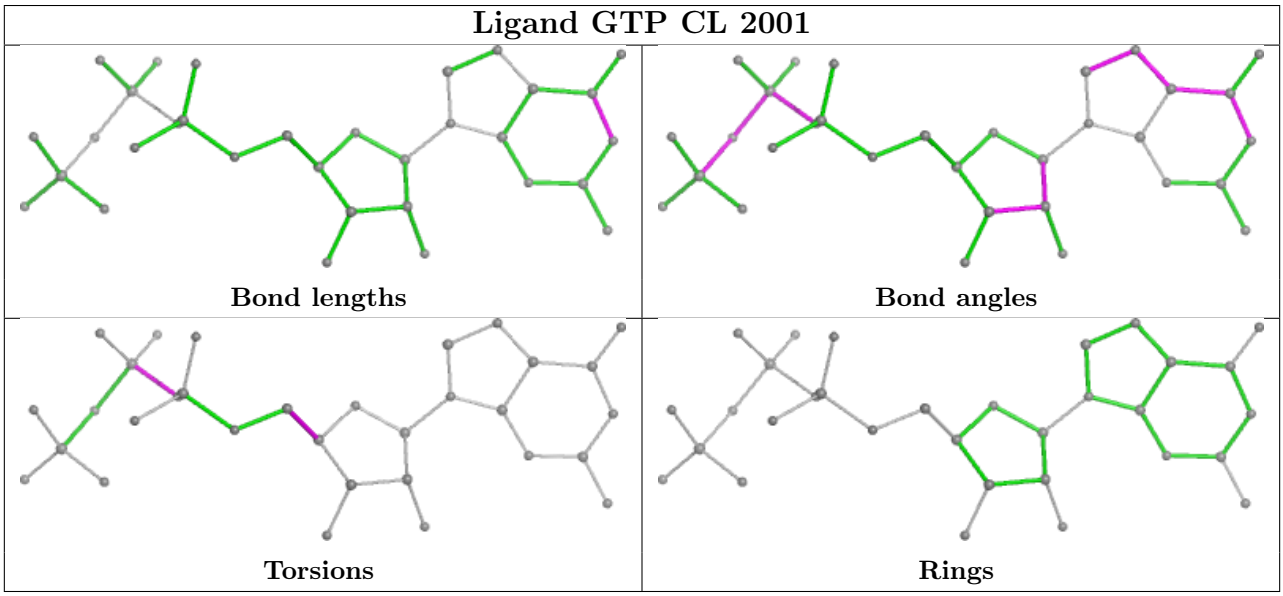
Mol	Chain	Res	Type	Atoms
60	CL	2001	GTP	O4'-C4'-C5'-O5'
60	CL	2001	GTP	C3'-C4'-C5'-O5'
60	CL	2001	GTP	PA-O3A-PB-O2B

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.



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
57	D4	5
56	D3	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D4	118:A	O3'	197:G	P	26.63
1	D4	106:C	O3'	111:G	P	20.40
1	D3	40:A	O3'	467:G	P	18.14

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D4	267:A	O3'	304:U	P	18.02
1	D4	206:C	O3'	245:U	P	17.13
1	D4	260:U	O3'	263:A	P	9.74
1	D3	18:C	O3'	22:A	P	8.80

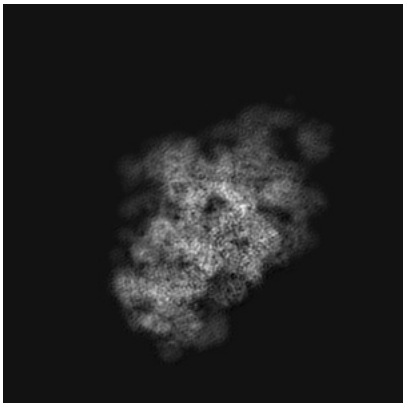
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11357. These allow visual inspection of the internal detail of the map and identification of artifacts.

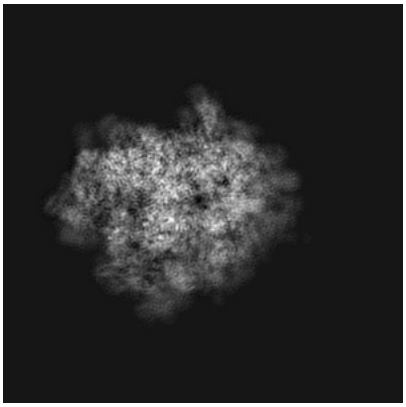
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

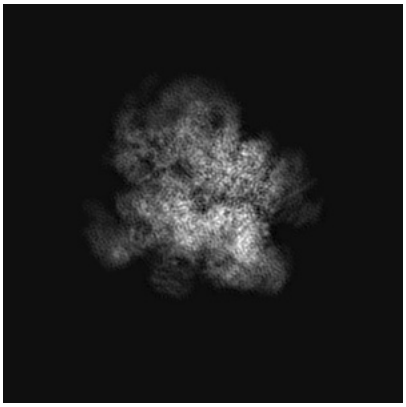
6.1.1 Primary map



X



Y

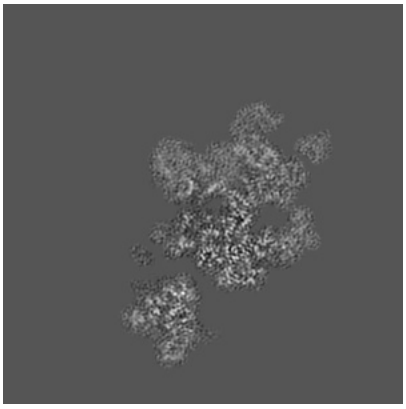


Z

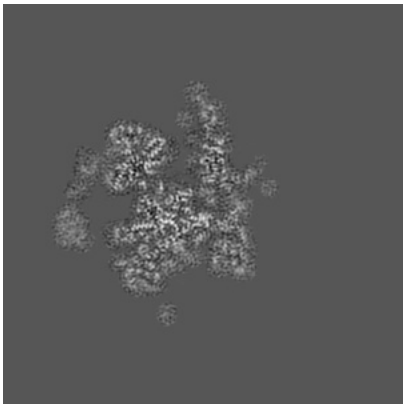
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 240



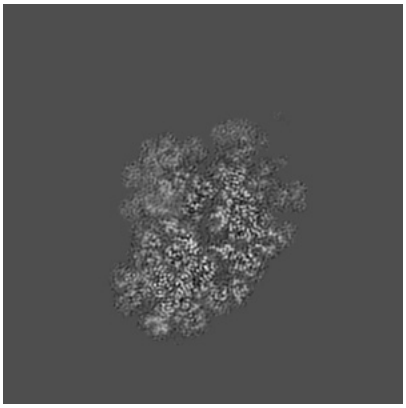
Y Index: 240

Z Index: 240

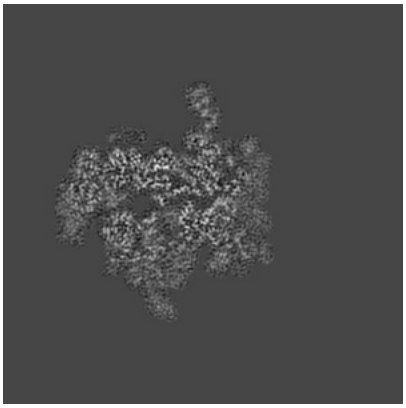
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

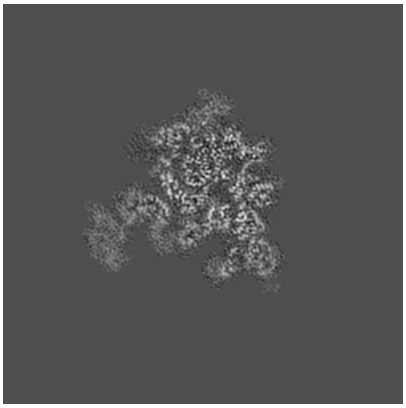
6.3.1 Primary map



X Index: 283



Y Index: 225

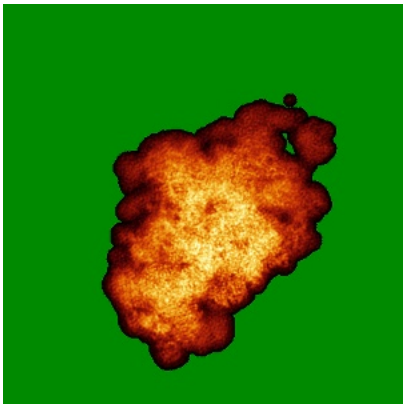


Z Index: 187

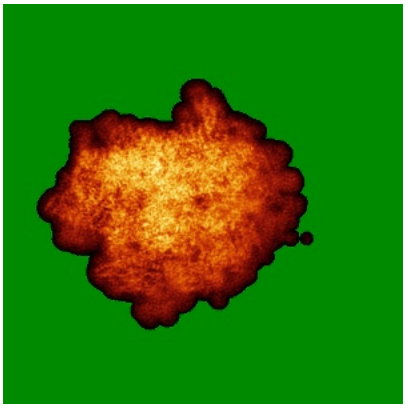
The images above show the largest variance slices of the map in three orthogonal directions.

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

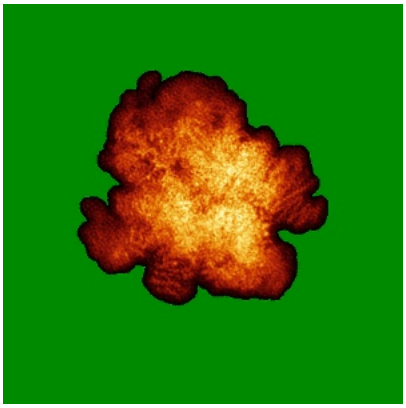
6.4.1 Primary map



X



Y

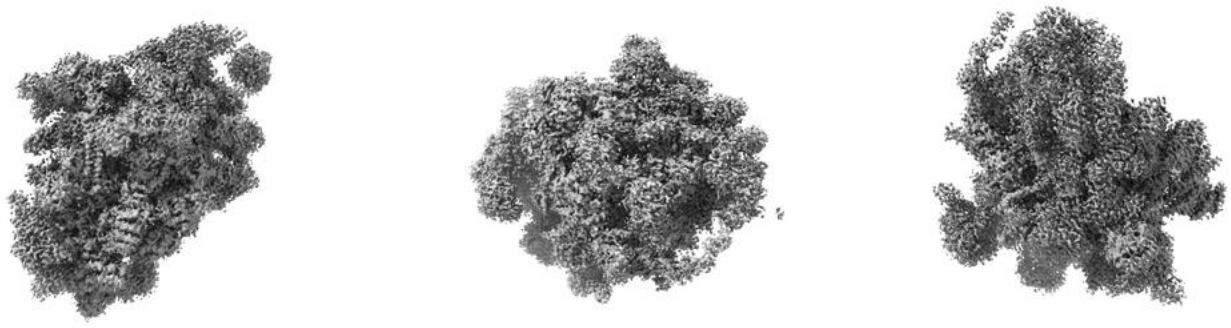


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

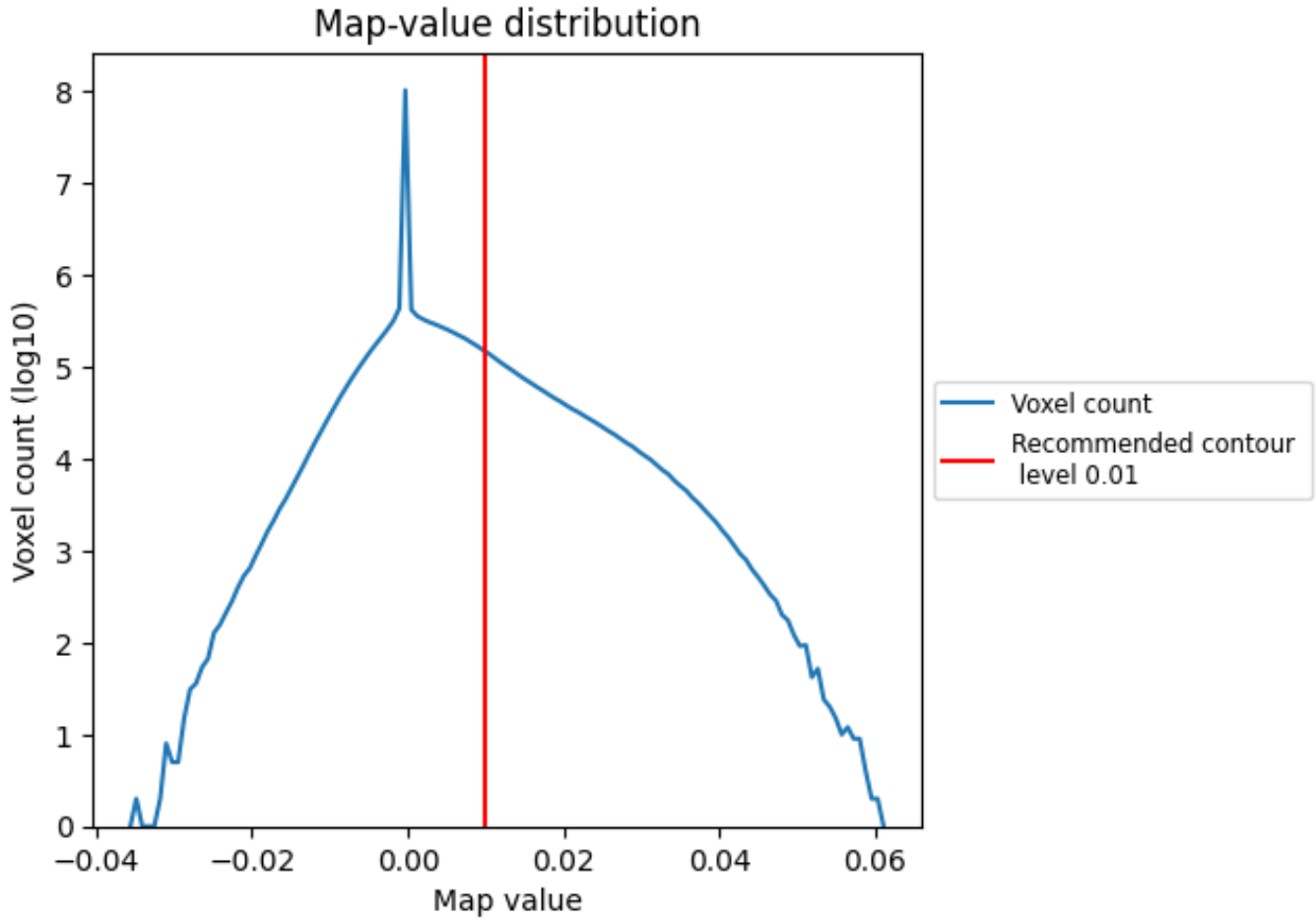
6.6 Mask visualisation (i)

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

7 Map analysis

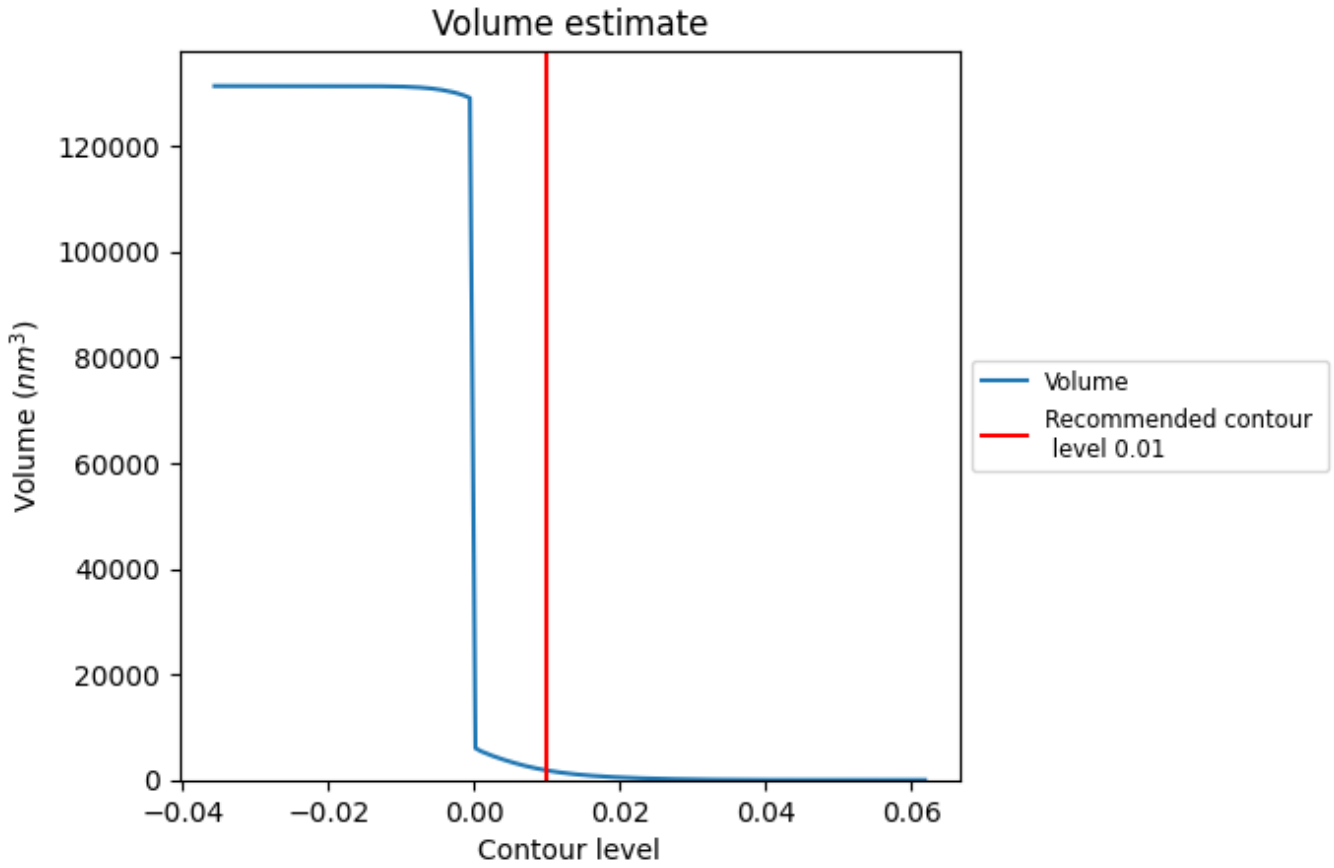
This section contains the results of statistical analysis of the map.

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.

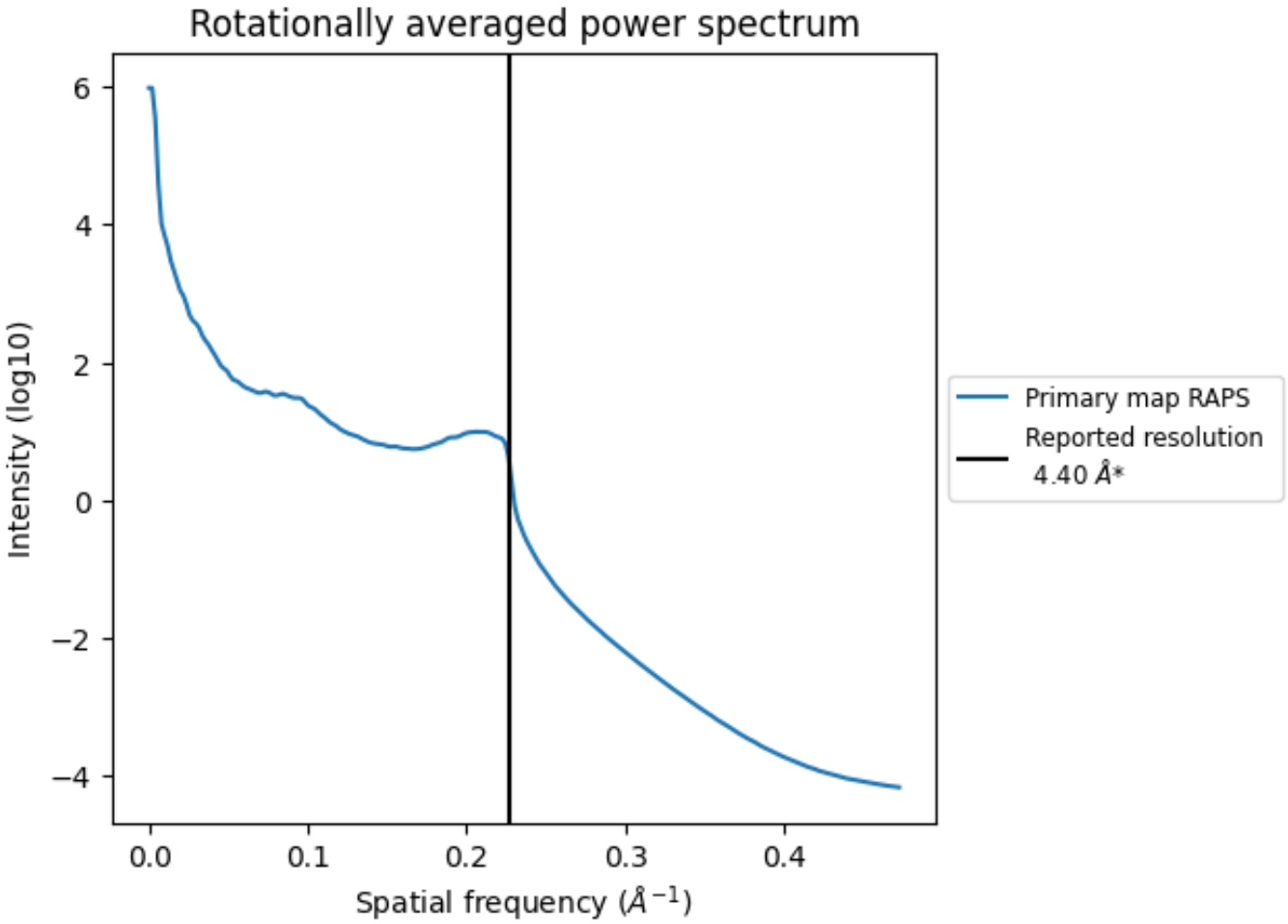
7.2 Volume estimate



The volume at the recommended contour level is 1809 nm^3; this corresponds to an approximate mass of 1634 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)

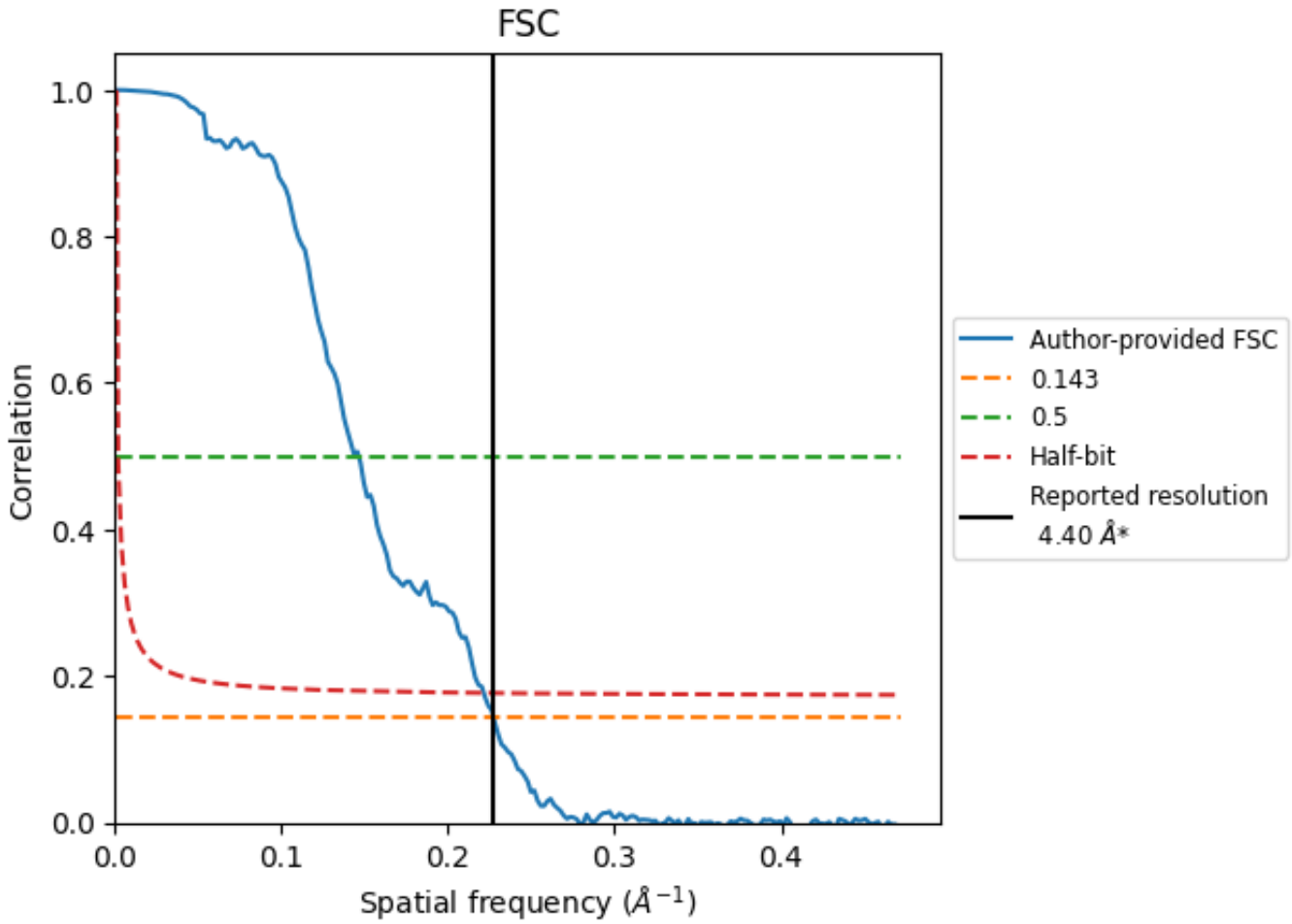


*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

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 0.227 Å^{-1}

8.2 Resolution estimates (i)

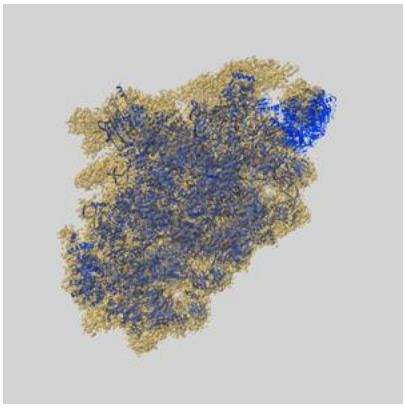
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.40	6.83	4.51
Unmasked-calculated*	-	-	-

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

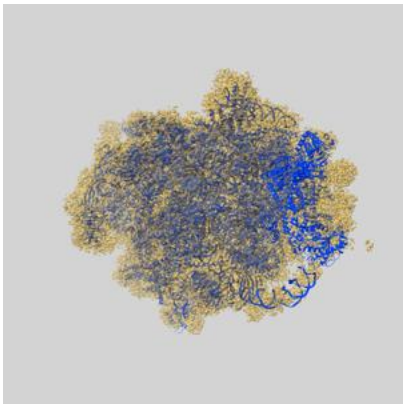
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11357 and PDB model 6ZQA. Per-residue inclusion information can be found in section 3 on page 16.

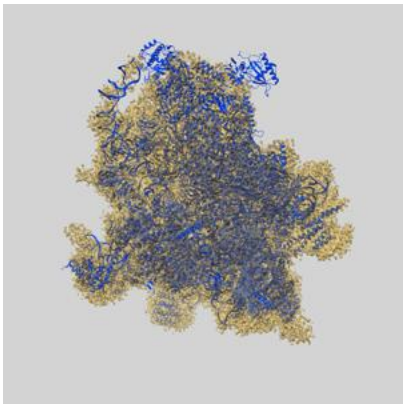
9.1 Map-model overlay



X



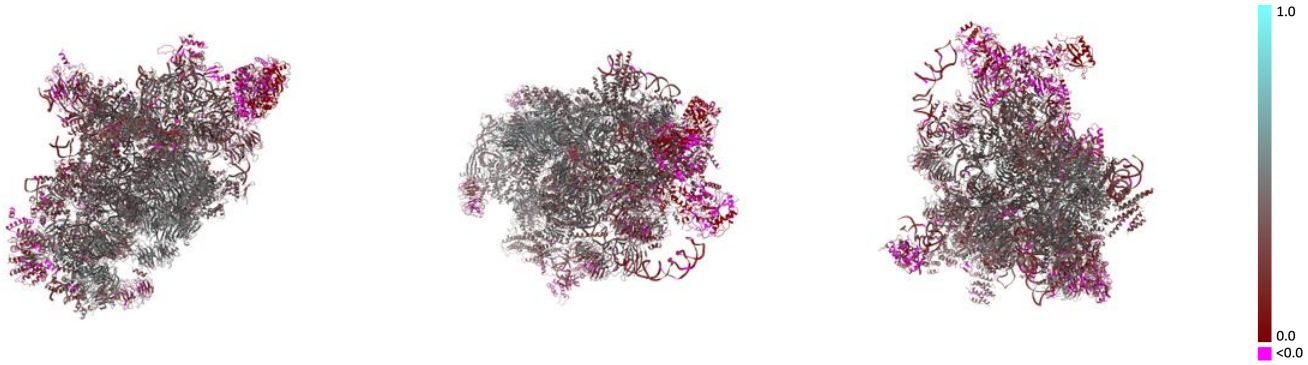
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

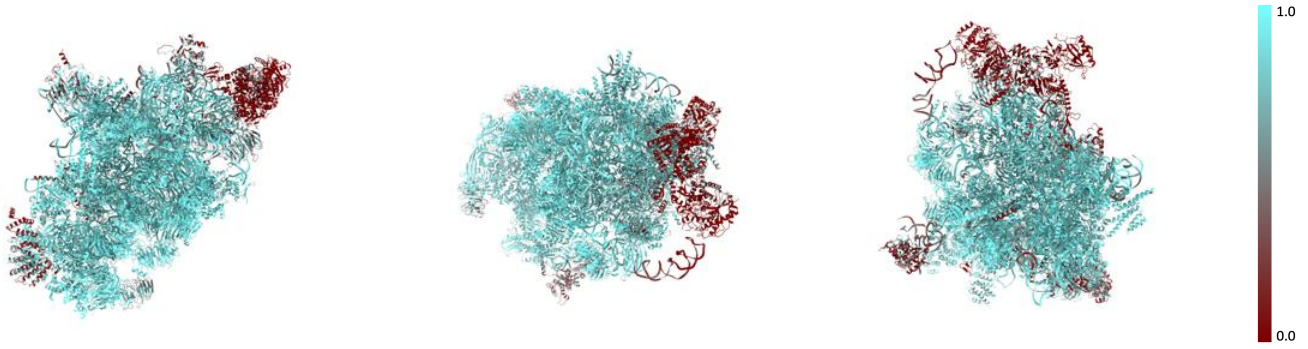
9.2 Q-score mapped to coordinate model (i)



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.

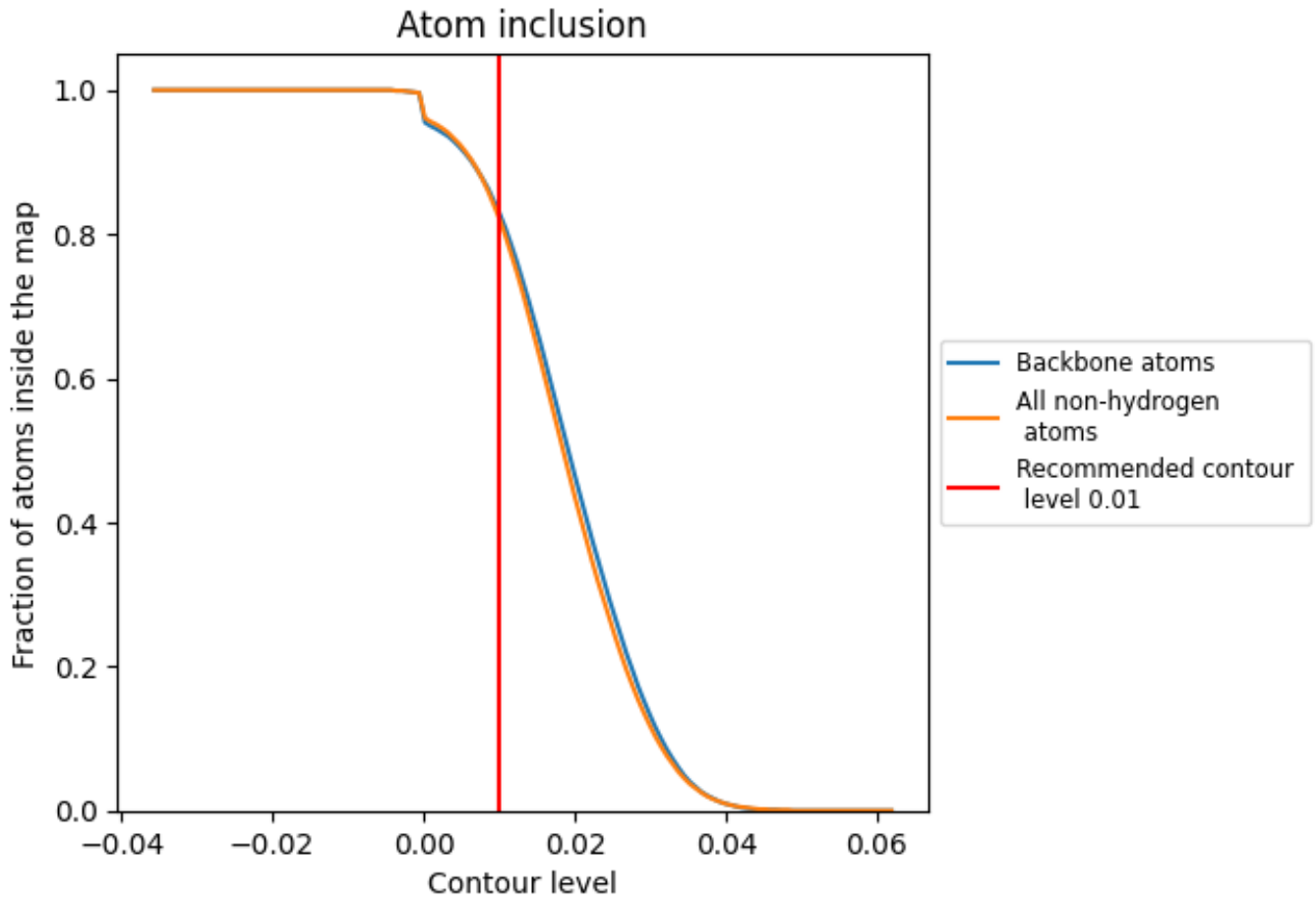
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 82% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8230	0.3460
CA	0.9450	0.4470
CB	0.9440	0.4010
CD	0.9190	0.3530
CE	0.9010	0.3480
CF	0.9640	0.4440
CG	0.9200	0.3700
CH	0.6660	0.2100
CI	0.9620	0.4390
CJ	0.9360	0.4310
CK	0.9340	0.4060
CL	0.8940	0.3820
CM	0.9280	0.3770
CN	0.0720	0.0340
D2	0.9090	0.3450
D3	0.8030	0.3160
D4	0.9050	0.3430
DA	0.6710	0.3100
DF	0.9370	0.4280
DH	0.4830	0.2050
DJ	0.8720	0.3550
DN	0.5860	0.2760
DO	0.8420	0.3740
DQ	0.9500	0.4520
DS	0.4030	0.2190
DW	0.8500	0.3970
DX	0.9080	0.4270
Db	0.1220	0.1760
Dc	0.9770	0.4680
JF	0.9140	0.3620
JG	0.9330	0.4250
JH	0.2780	0.0800
JJ	0.8550	0.3440
JM	0.9060	0.3970
JN	0.8380	0.3820

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Chain	Atom inclusion	Q-score
JO	0.8950	0.3890
JP	0.9470	0.4470
JQ	0.3910	0.2500
UA	0.9620	0.4620
UB	0.7940	0.2880
UC	0.9310	0.3950
UD	0.9530	0.4240
UE	0.9710	0.4420
UF	0.9460	0.3420
UG	0.9020	0.4350
UH	0.7550	0.2660
UI	0.9500	0.3370
UJ	0.6940	0.2990
UK	0.9550	0.4010
UL	0.9280	0.3590
UM	0.7190	0.2860
UN	0.8350	0.3770
UO	0.9650	0.4470
UP	0.9190	0.3510
UQ	0.9520	0.4320
UR	0.9600	0.4600
US	0.8930	0.3210
UU	0.9670	0.4630
UV	0.0720	0.0420
UX	0.9700	0.4540
UZ	0.9330	0.3770