Full wwPDB EM Validation Report ⓘ

Oct 21, 2024 – 11:51 AM JST

PDB ID	:	6ID0
EMDB ID	:	EMD-9646
Title	:	Cryo-EM structure of a human intron lariat spliceosome prior to Prp43 loaded (ILS1 complex) at 2.9 angstrom resolution
Authors	:	Zhang, X.; Zhan, X.; Yan, C.; Shi, Y.
Deposited on	:	2018-09-07
Resolution	:	2.90 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:

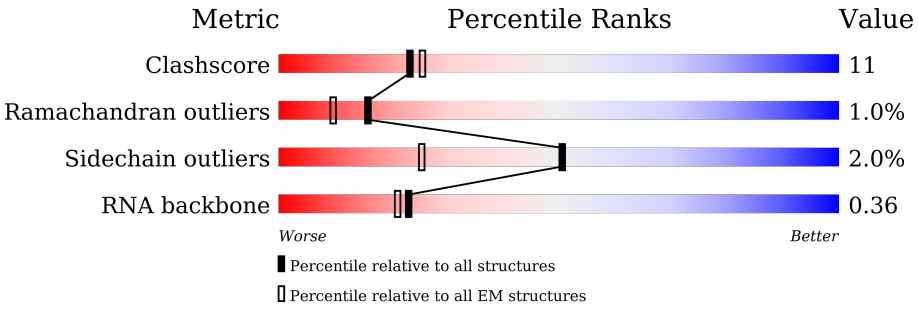
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	A	2335	70% 14% • 15%
2	B	117	9% 32% 31% 19% • 16%
3	C	972	70% 19% • 9%
4	E	357	61% 23% • 15%
5	F	107	44% 25% 20% • 9%
6	J	848	21% 58% 7% • 34%
7	L	802	24% 52% 6% 41%

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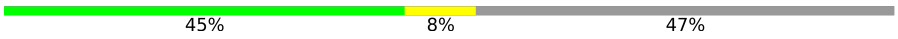
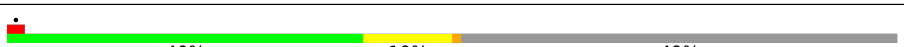
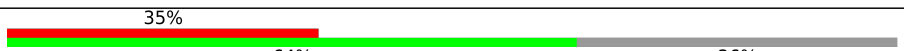
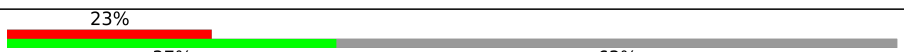
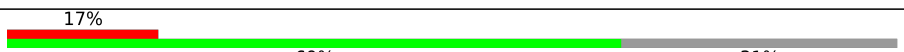
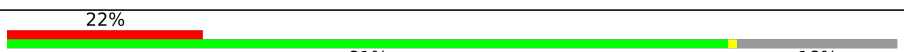
Mol	Chain	Length	Quality of chain
8	M	243	
9	N	144	
10	O	420	
11	P	229	
12	R	536	
13	S	166	
14	T	514	
15	W	579	
16	G	272	
17	H	188	
18	U	894	
19	I	855	
20	a	126	
20	h	126	
21	b	231	
21	i	231	
22	c	119	
22	j	119	
23	d	118	
23	k	118	
24	f	86	
24	m	86	
25	e	92	
25	l	92	
26	g	76	

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Mol	Chain	Length	Quality of chain
26	n	76	61% 88% 12%
27	q	504	25% 25% 74%
27	r	504	24% 25% 74%
27	s	504	12% 13% 87%
27	t	504	13% 13% 87%
28	K	225	56% 57% 9% 32%
29	o	255	57% 61% 36%
30	p	225	30% 42% 58%
31	Q	1485	87% 89% 11%
32	y	301	17% 26% 74%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	GTP	C	1500	-	-	X	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 78004 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 Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1981	16477	10621	2883	2902	71	0	0

- Molecule 2 is a RNA chain called U5snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	98	2060	923	341	698	98	0	0

- Molecule 3 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	888	7022	4494	1172	1322	34	0	0

- Molecule 4 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	303	2366	1487	415	451	13	0	0

- Molecule 5 is a RNA chain called U6snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	F	97	2075	928	381	669	97	0	0

- Molecule 6 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	J	556	3758	2344	705	703	6	0	0

- Molecule 7 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	475	Total	C	N	O	S	0	0
			3237	1985	627	619	6		

- Molecule 8 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	130	Total	C	N	O	S	0	0
			1098	684	204	208	2		

- Molecule 9 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	143	Total	C	N	O	S	0	0
			1184	746	217	209	12		

- Molecule 10 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	290	Total	C	N	O	S	0	0
			2340	1469	415	436	20		

- Molecule 11 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	118	Total	C	N	O	S	0	0
			985	601	194	188	2		

- Molecule 12 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	R	272	Total	C	N	O	P	S	0	0
			2165	1357	393	401	2	12		

- Molecule 13 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S	159	Total	C	N	O	S	0	0
			1236	787	215	227	7		

- Molecule 14 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	317	Total	C	N	O	S	0	0
			2496	1574	453	461	8		

- Molecule 15 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	509	Total	C	N	O	S	0	0
			3008	1833	568	603	4		

- Molecule 16 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	70	Total	C	N	O	P	0	0
			1246	549	158	469	70		

- Molecule 17 is a RNA chain called U2snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	140	Total	C	N	O	P	0	0
			2968	1327	511	990	140		

- Molecule 18 is a protein called CWF19-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	U	347	Total	C	N	O	S	0	0
			2864	1817	496	529	22		

- Molecule 19 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	I	568	Total	C	N	O	S	0	0
			2822	1683	569	569	1		

- Molecule 20 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	a	81	Total	C	N	O	0	0
			399	237	81	81		
20	h	81	Total	C	N	O	0	0
			398	236	81	81		

- Molecule 21 is a protein called Small nuclear ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	b	86	Total	C	N	O	0	0
			424	252	86	86		
21	i	86	Total	C	N	O	0	0
			424	252	86	86		

- Molecule 22 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	c	82	Total	C	N	O	0	0
			406	242	82	82		
22	j	82	Total	C	N	O	0	0
			406	242	82	82		

- Molecule 23 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	d	97	Total	C	N	O	0	0
			480	286	97	97		
23	k	85	Total	C	N	O	0	0
			422	252	85	85		

- Molecule 24 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	f	74	Total	C	N	O	0	0
			361	213	74	74		
24	m	74	Total	C	N	O	0	0
			361	213	74	74		

- Molecule 25 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	e	79	Total	C	N	O	0	0
			391	233	79	79		
25	l	79	Total	C	N	O	0	0
			391	233	79	79		

- Molecule 26 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	g	74	Total	C	N	O	0	0
			363	215	74	74		

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Mol	Chain	Residues	Atoms				AltConf	Trace
26	n	67	Total 329	C 195	N 67	O 67	0	0

- Molecule 27 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	q	132	Total 659	C 395	N 132	O 132	0	0
27	r	131	Total 654	C 392	N 131	O 131	0	0
27	s	67	Total 335	C 201	N 67	O 67	0	0
27	t	67	Total 335	C 201	N 67	O 67	0	0

- Molecule 28 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	K	152	Total 757	C 453	N 152	O 152	0	0

- Molecule 29 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	o	162	Total 804	C 480	N 162	O 162	0	0

- Molecule 30 is a protein called U2 small nuclear ribonucleoprotein B".

Mol	Chain	Residues	Atoms				AltConf	Trace
30	p	94	Total 464	C 276	N 94	O 94	0	0

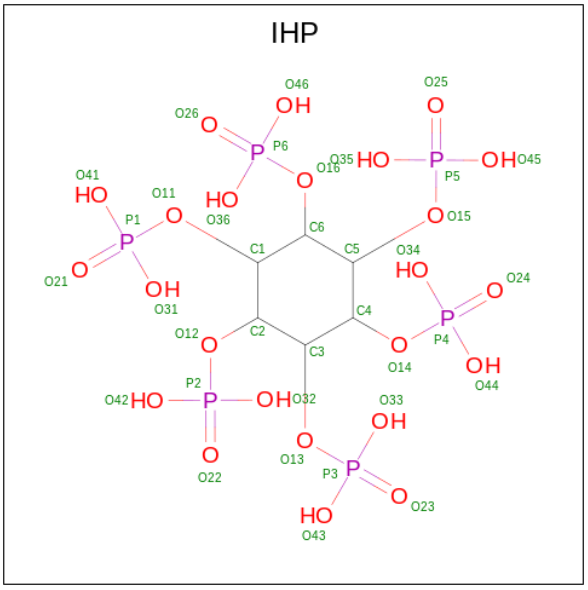
- Molecule 31 is a protein called RNA helicase aquarius.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	Q	1322	Total 6562	C 3918	N 1322	O 1322	4	0

- Molecule 32 is a protein called Peptidyl-prolyl cis-trans isomerase E.

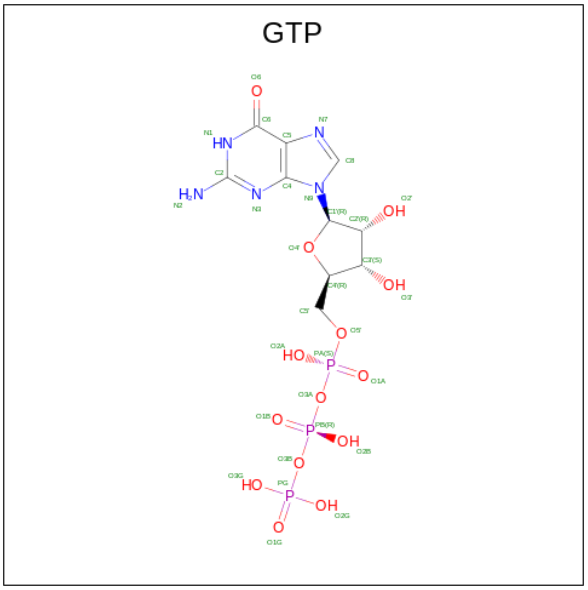
Mol	Chain	Residues	Atoms				AltConf	Trace
32	y	79	Total	C	N	O	0	0
			390	232	79	79		

- Molecule 33 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms				AltConf
33	A	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 34 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 35 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
35	C	1	Total	Mg	0
			1	1	
35	F	6	Total	Mg	0
			6	6	

- Molecule 36 is ZINC ION (three-letter code: ZN) (formula: Zn).

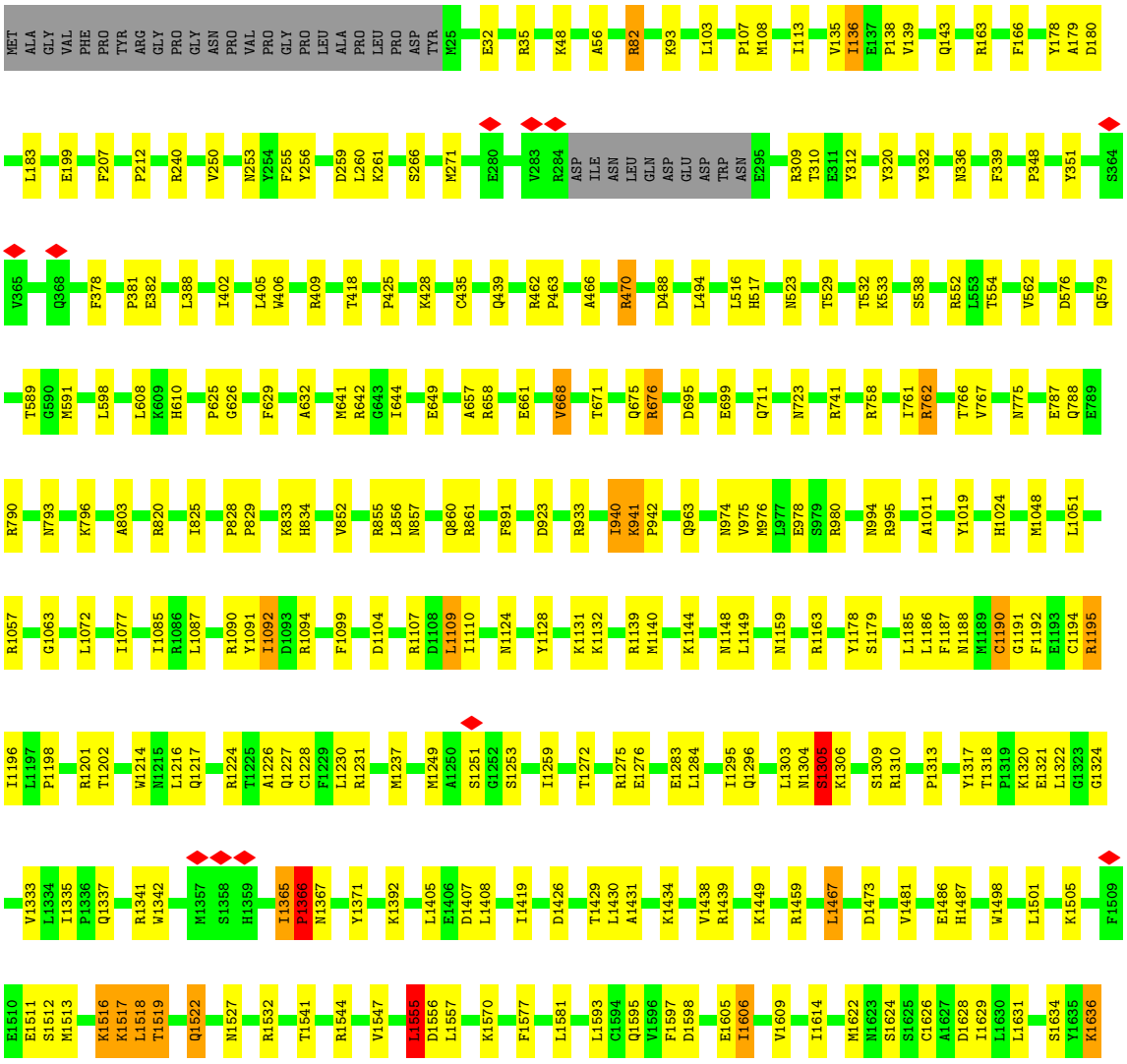
Mol	Chain	Residues	Atoms		AltConf
36	N	3	Total	Zn	0
			3	3	
36	O	3	Total	Zn	0
			3	3	
36	U	1	Total	Zn	0
			1	1	

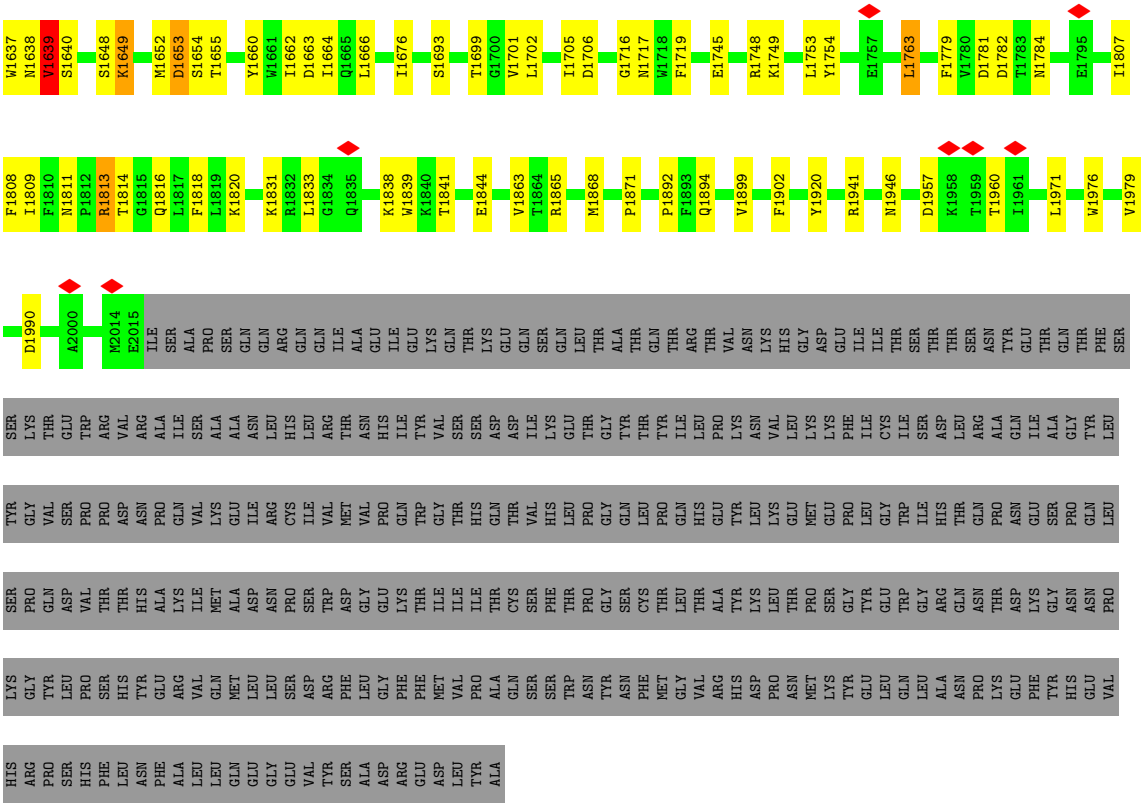
3 Residue-property plots (i)

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: Pre-mRNA-processing-splicing factor 8

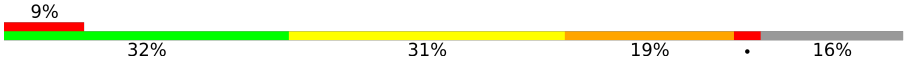
Chain A:

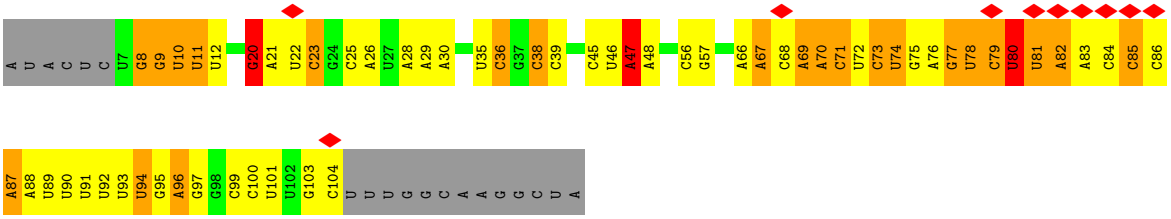




• Molecule 2: U5snRNA

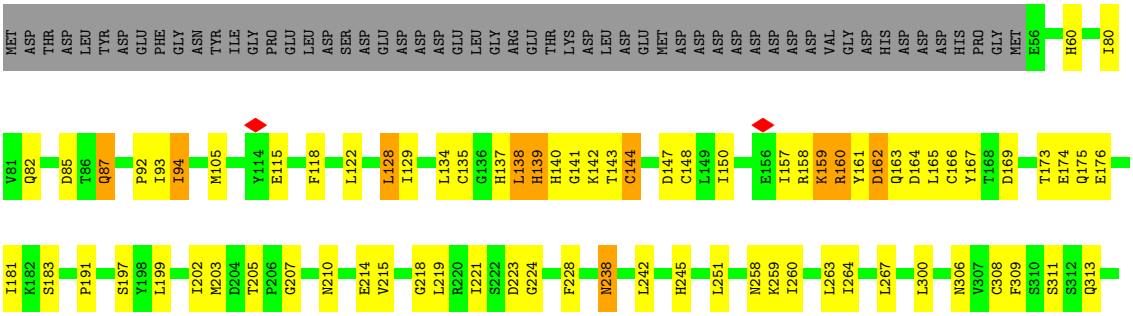
Chain B:

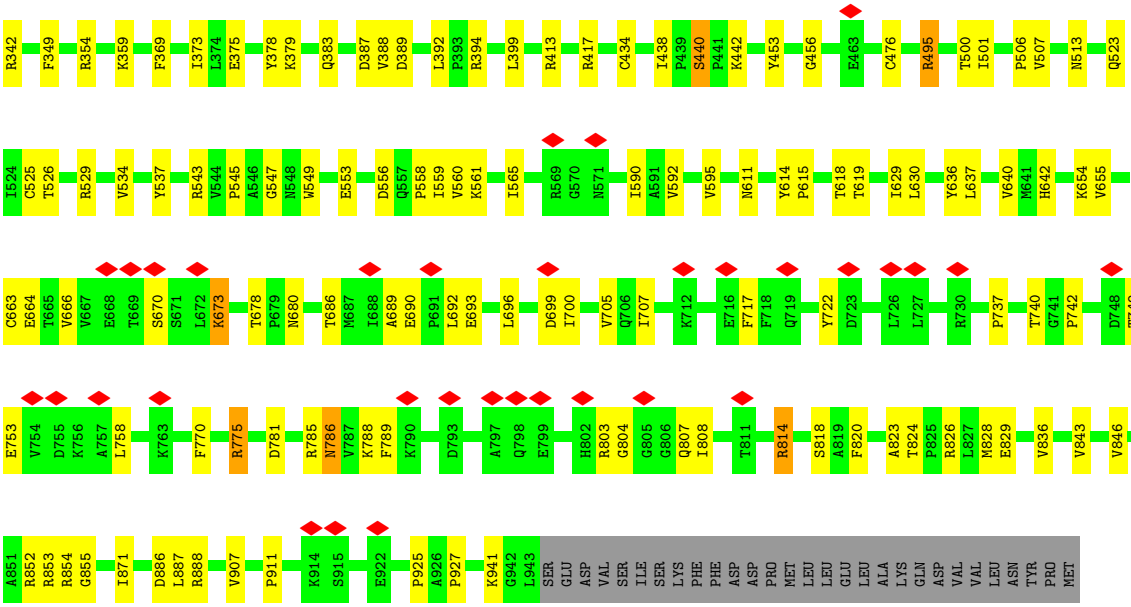




• Molecule 3: 116 kDa U5 small nuclear ribonucleoprotein component

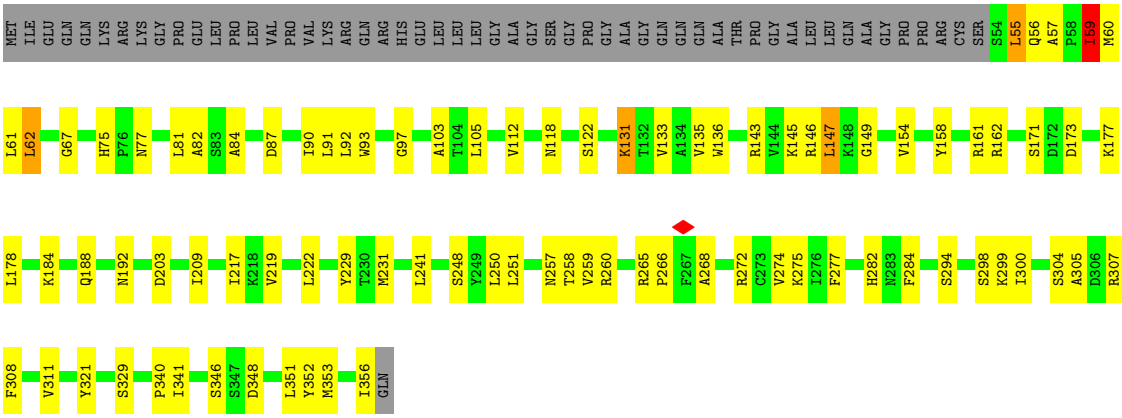
Chain C:





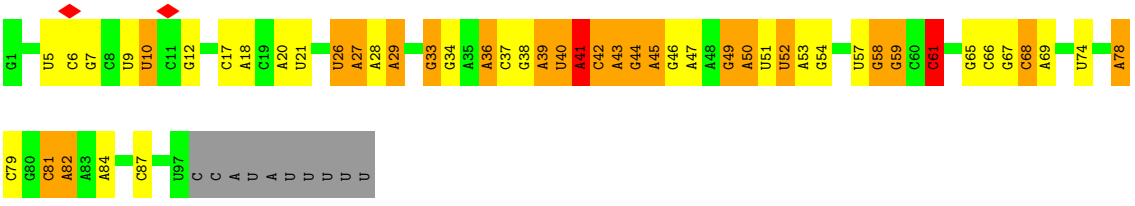
• Molecule 4: U5 small nuclear ribonucleoprotein 40 kDa protein

Chain E:



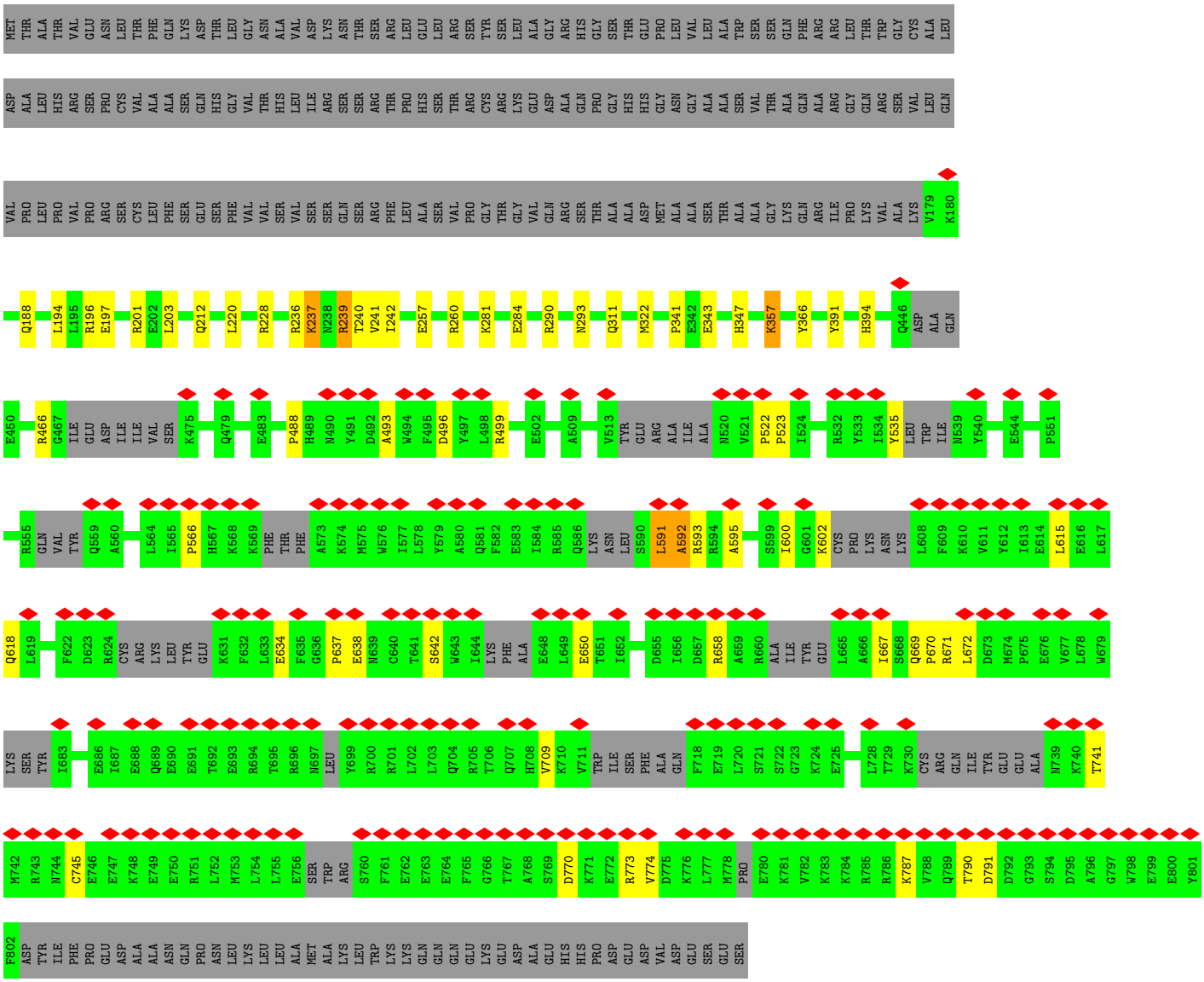
• Molecule 5: U6snRNA

Chain F:



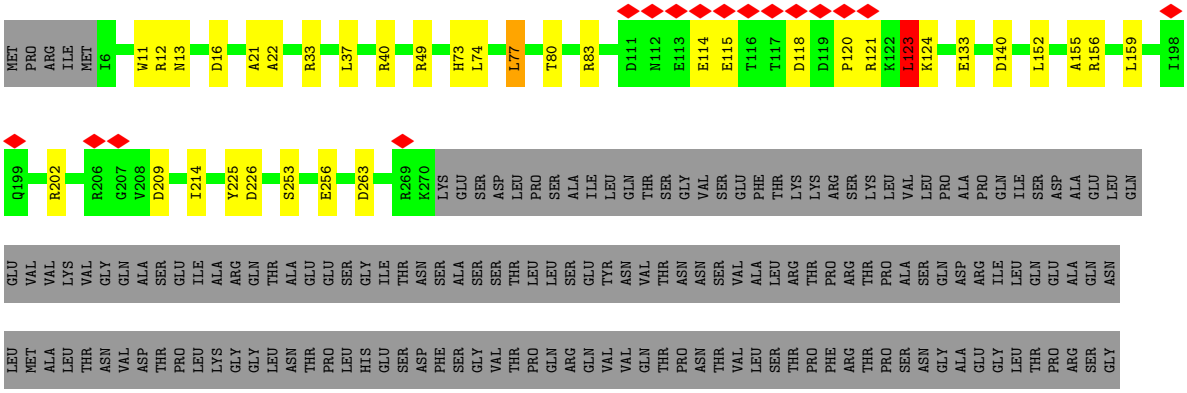
• Molecule 6: Crooked neck-like protein 1

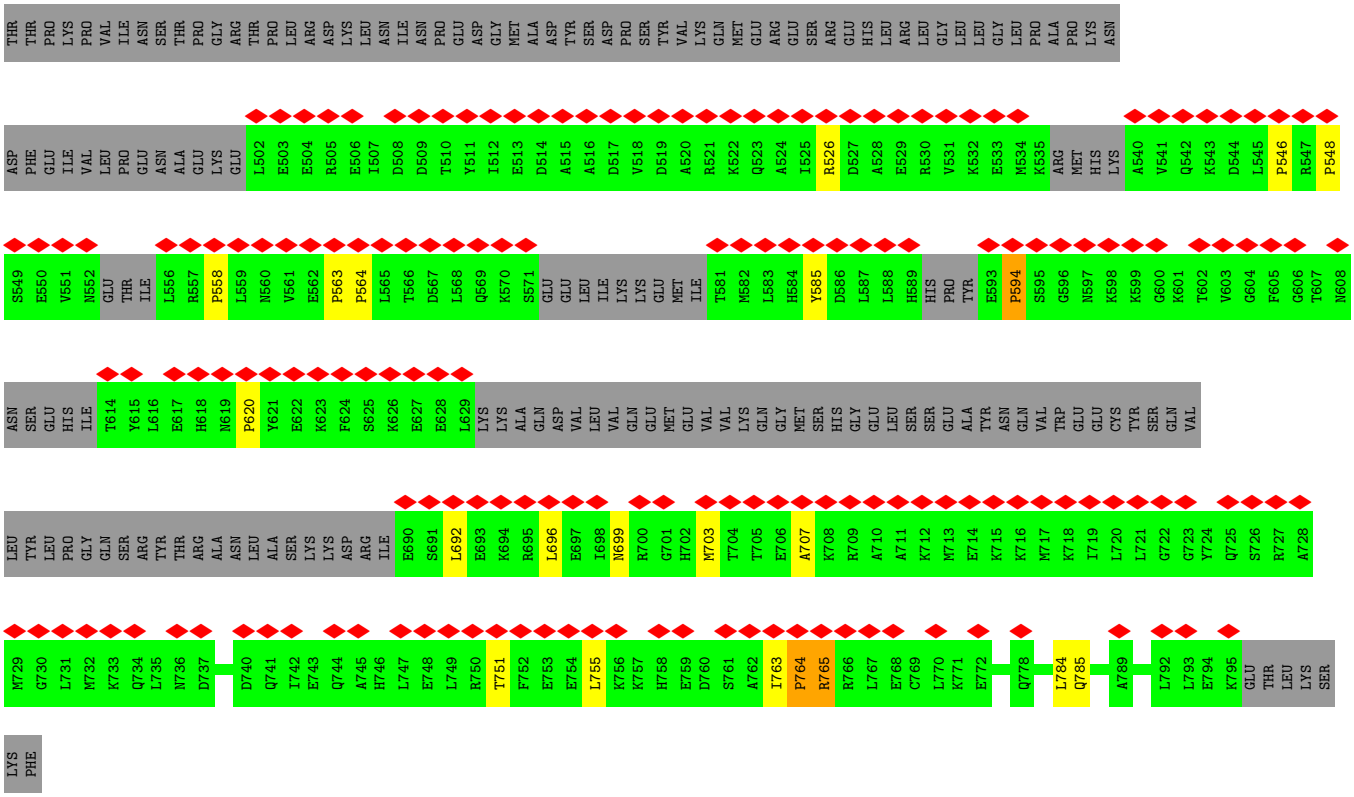
Chain J:



• Molecule 7: Cell division cycle 5-like protein

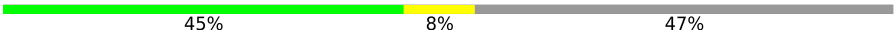
Chain L:

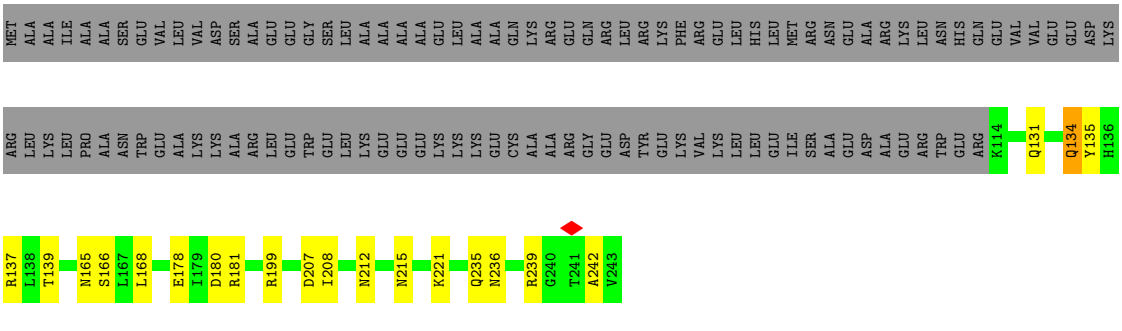




• Molecule 8: Pre-mRNA-splicing factor SYF2

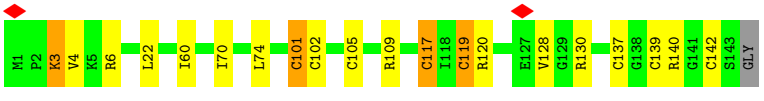
Chain M:





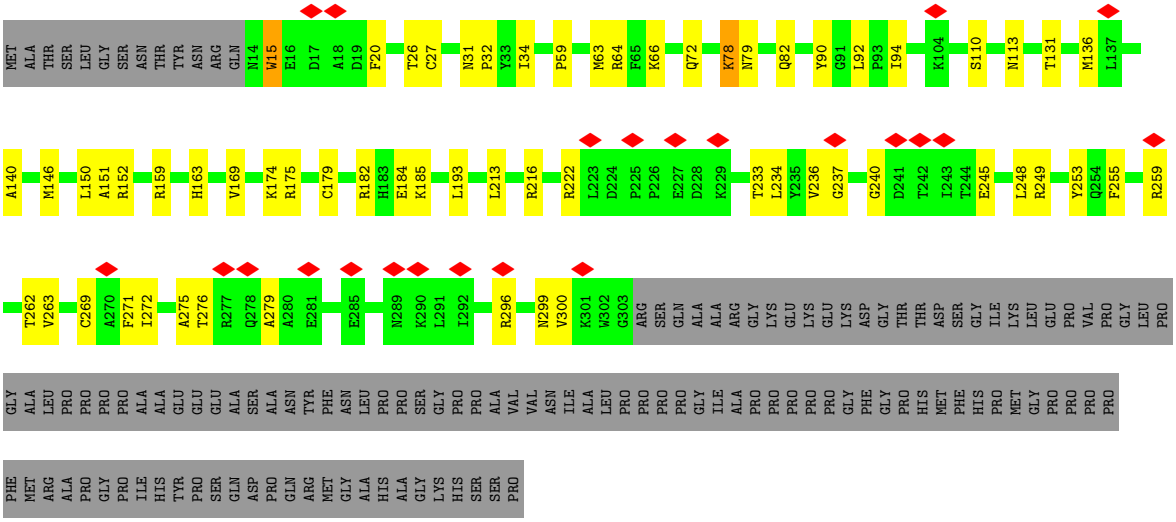
• Molecule 9: Protein BUD31 homolog

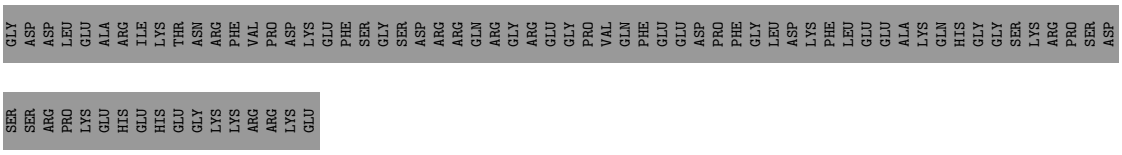
Chain N:



• Molecule 10: Pre-mRNA-splicing factor RBM22

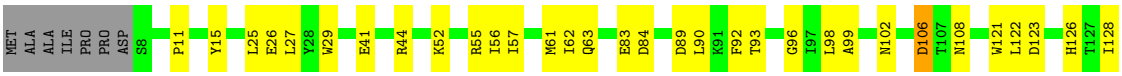
Chain O:

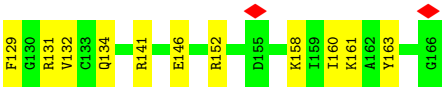




• Molecule 13: Peptidyl-prolyl cis-trans isomerase-like 1

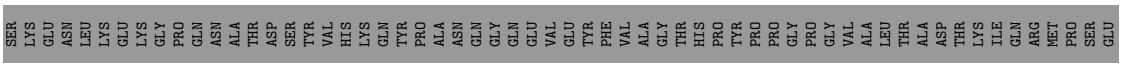
Chain S:

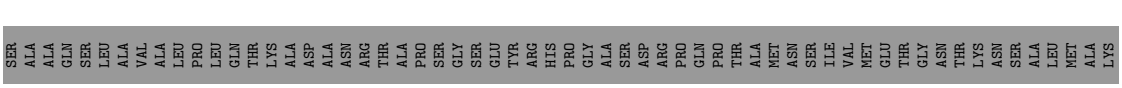


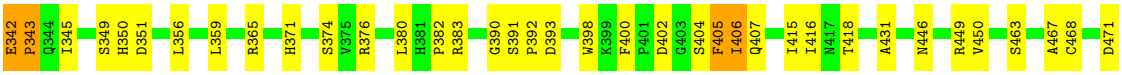


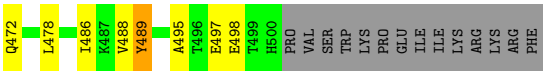
• Molecule 14: Pleiotropic regulator 1

Chain T:



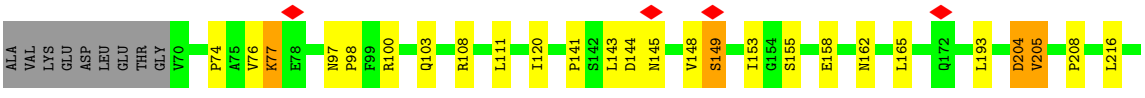


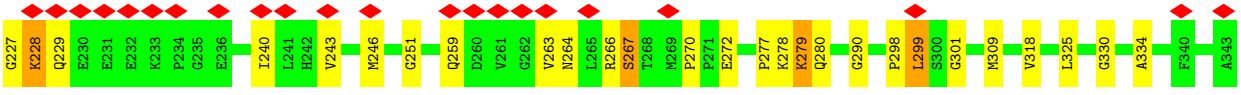


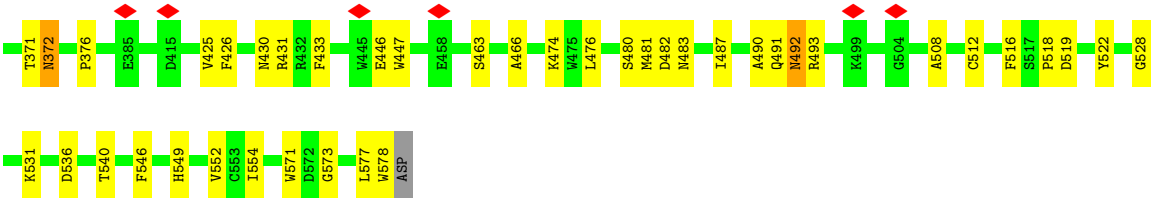


• Molecule 15: Pre-mRNA-processing factor 17

Chain W:

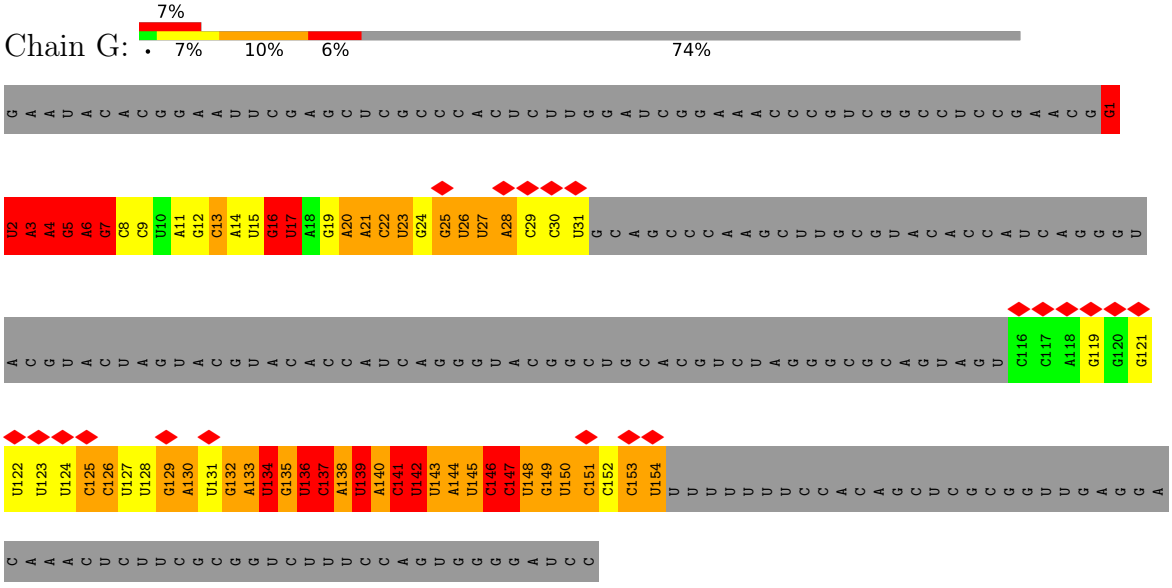






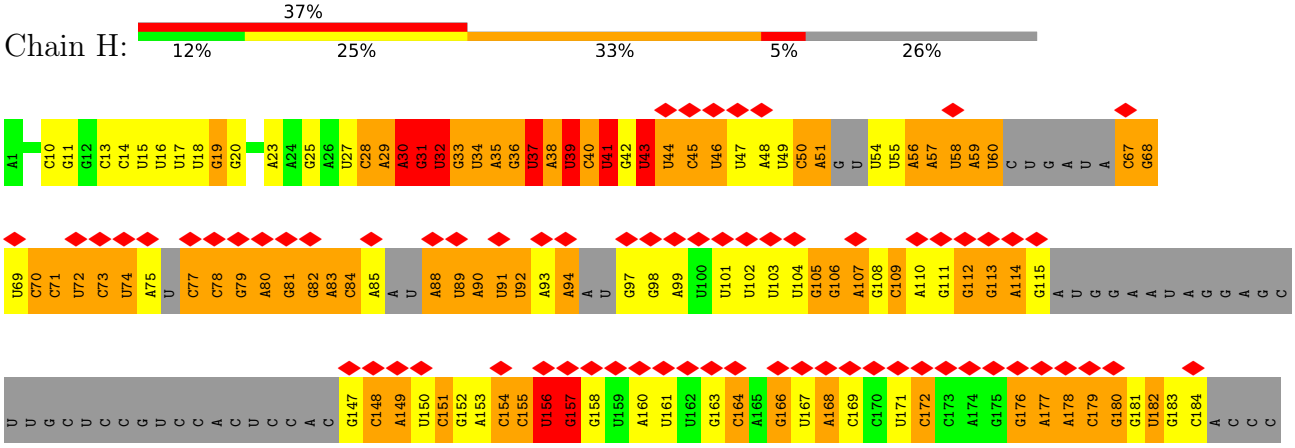
• Molecule 16: pre-mRNA

Chain G:



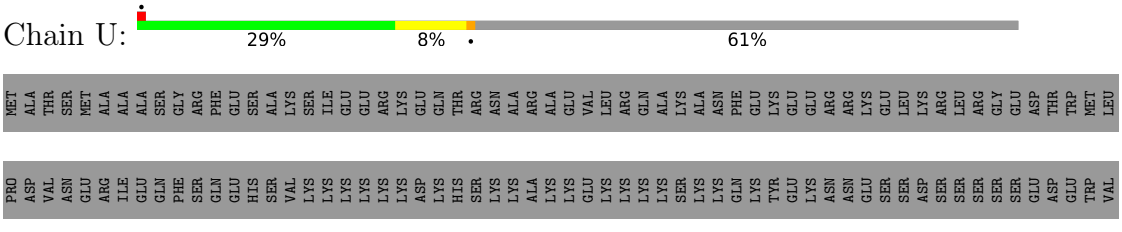
• Molecule 17: U2snRNA

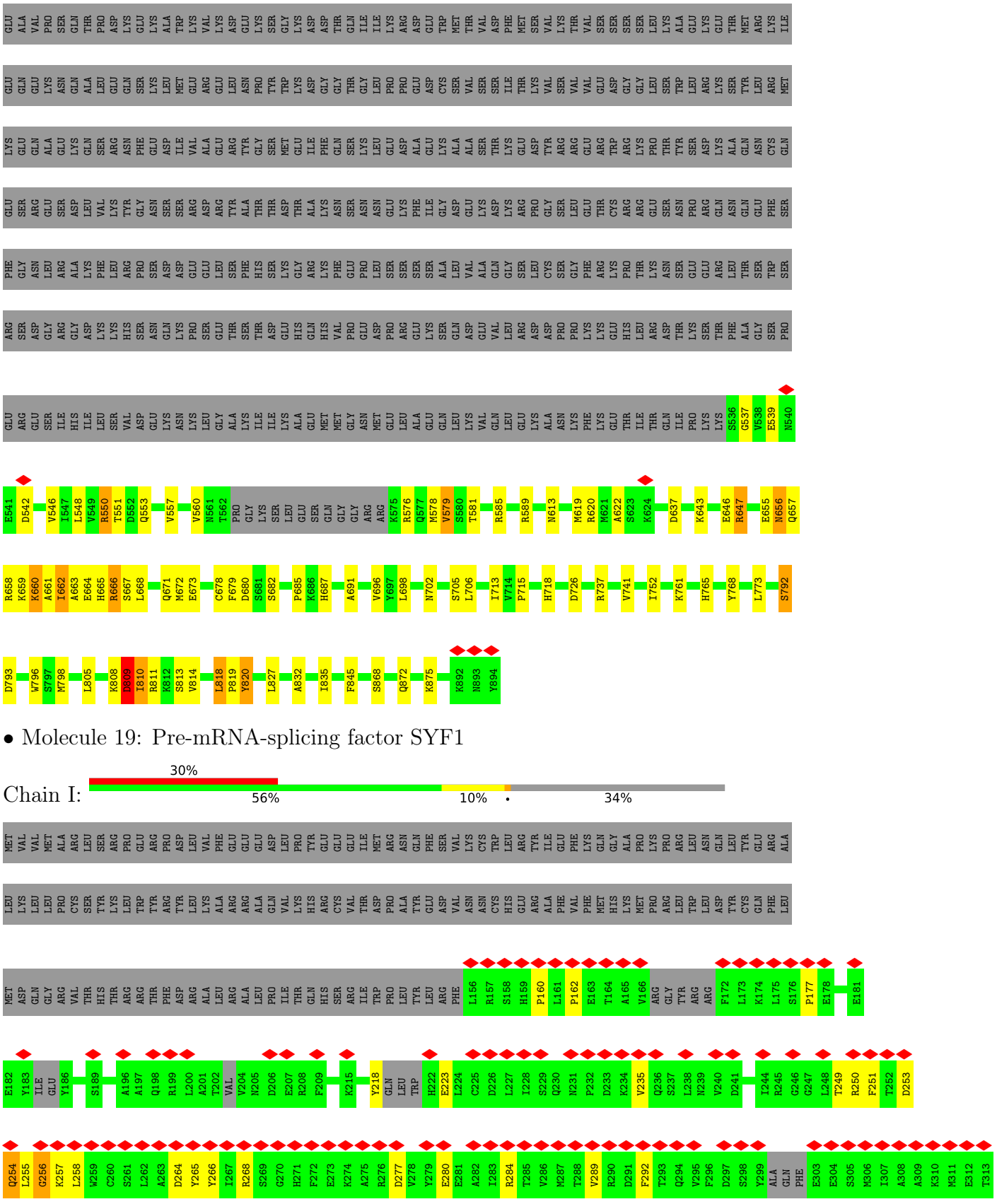
Chain H:



• Molecule 18: CWF19-like protein 2

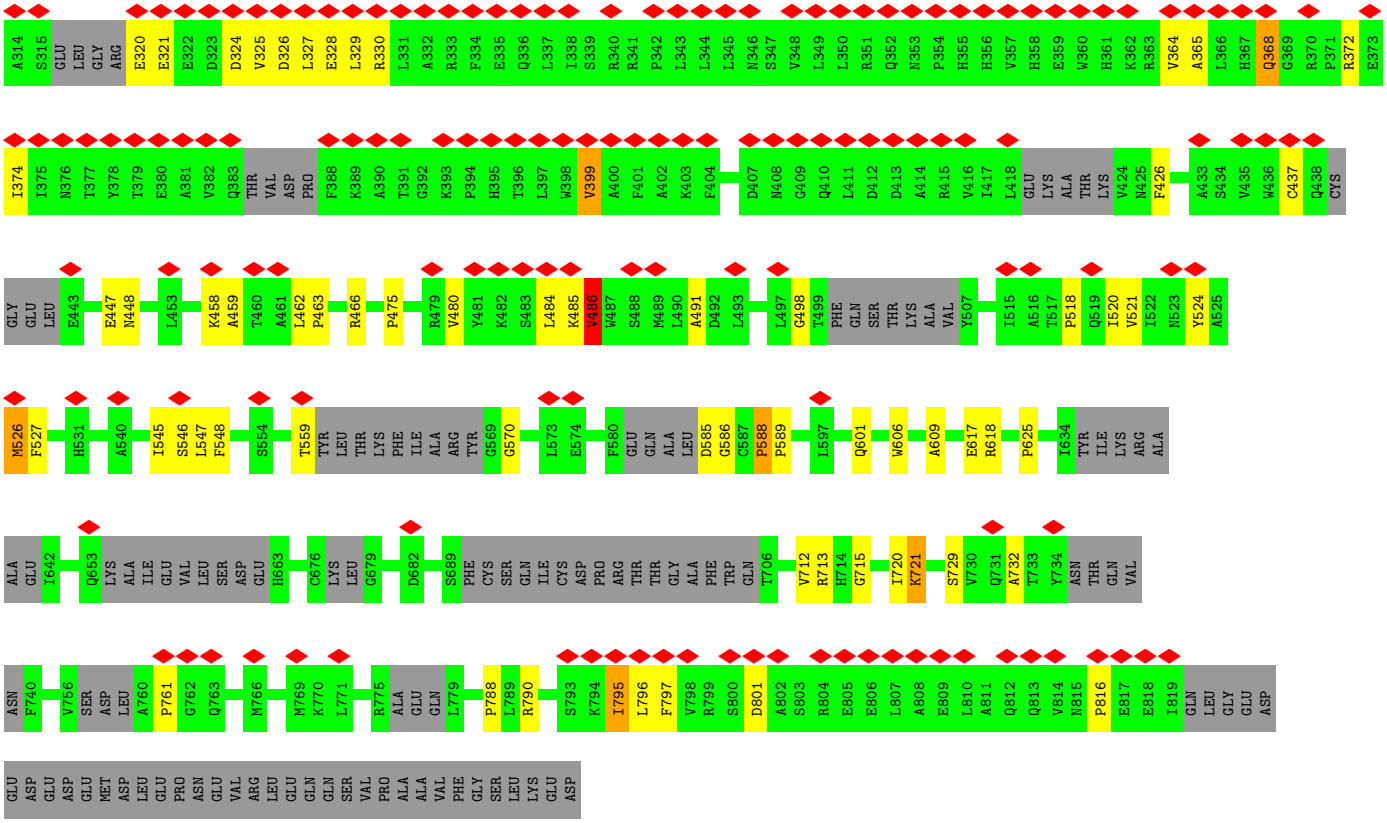
Chain U:



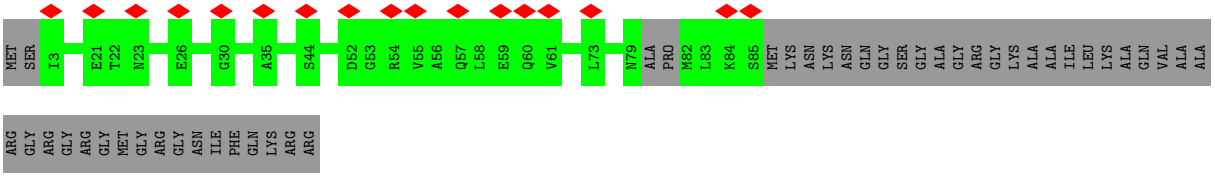


• Molecule 19: Pre-mRNA-splicing factor SYF1

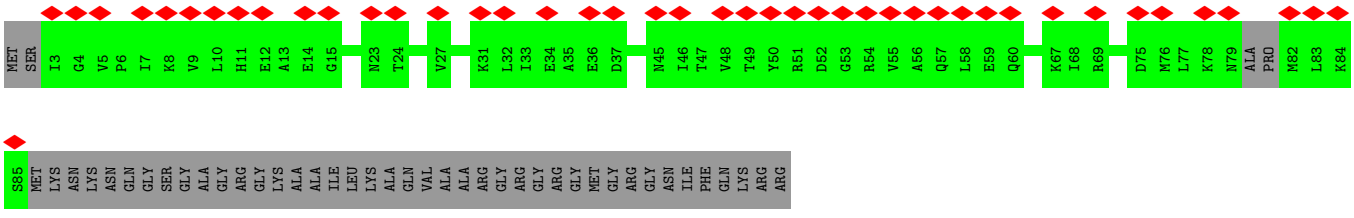
Chain I:



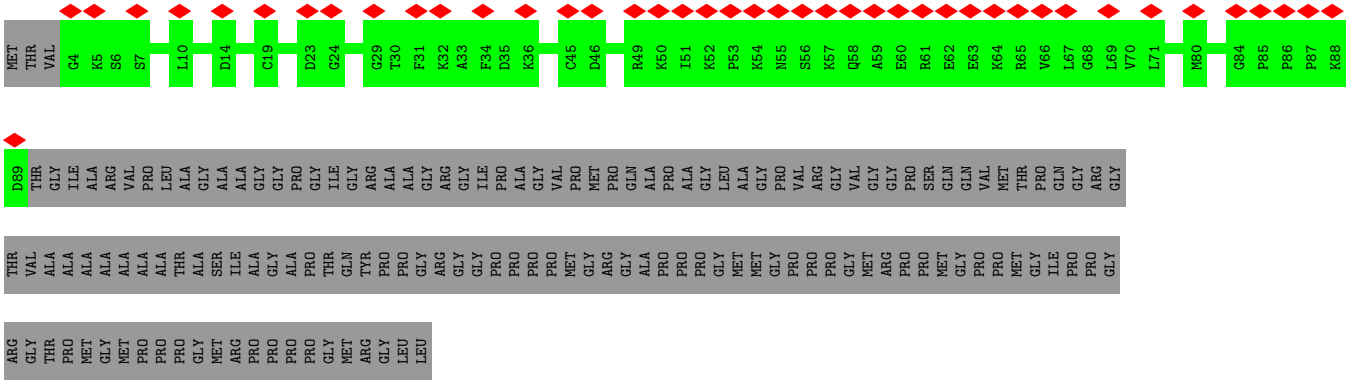
• Molecule 20: Small nuclear ribonucleoprotein Sm D3



• Molecule 20: Small nuclear ribonucleoprotein Sm D3

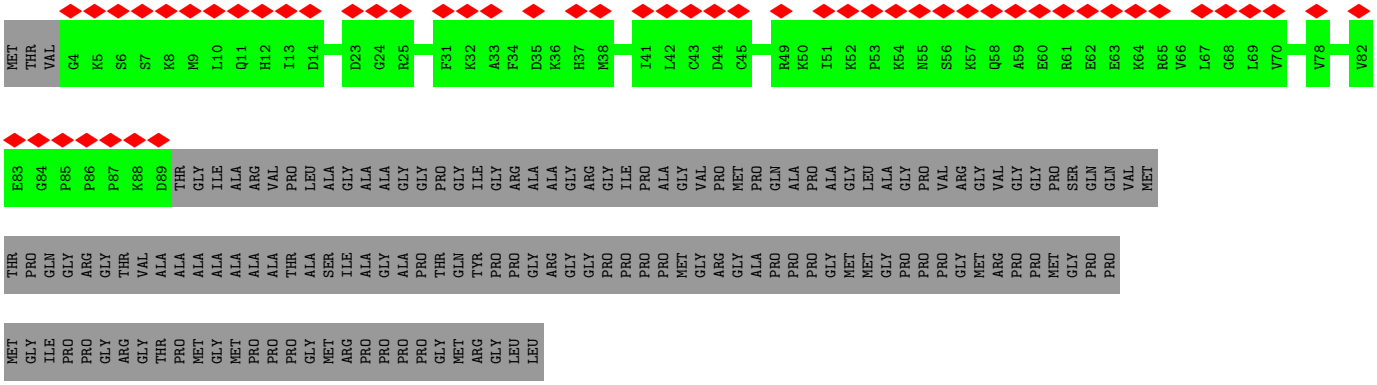


• Molecule 21: Small nuclear ribonucleoprotein-associated protein



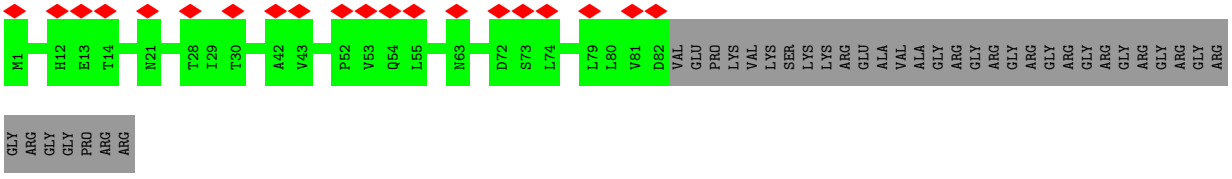
• Molecule 21: Small nuclear ribonucleoprotein-associated protein

Chain i:



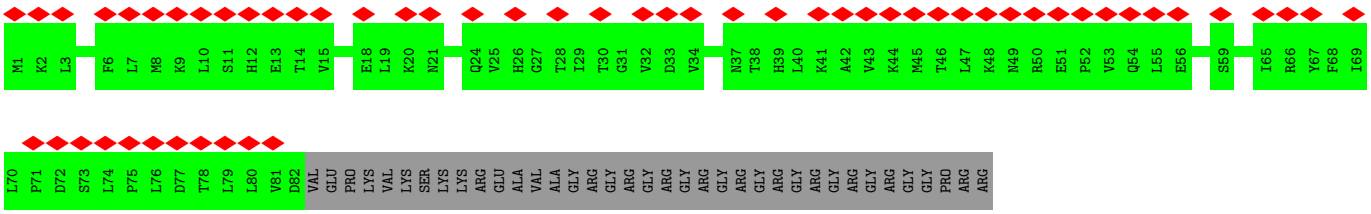
• Molecule 22: Small nuclear ribonucleoprotein Sm D1

Chain c:



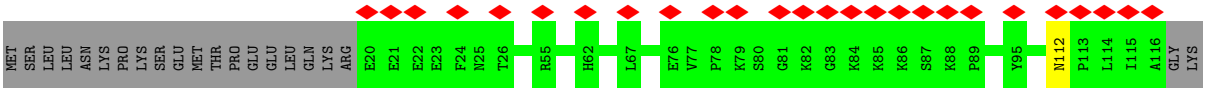
• Molecule 22: Small nuclear ribonucleoprotein Sm D1

Chain j:



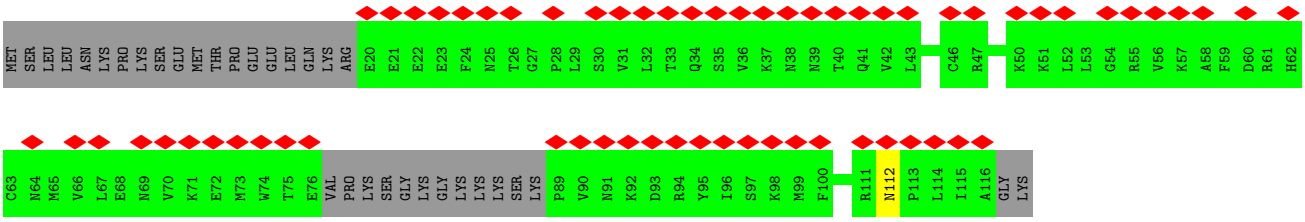
• Molecule 23: Small nuclear ribonucleoprotein Sm D2

Chain d:



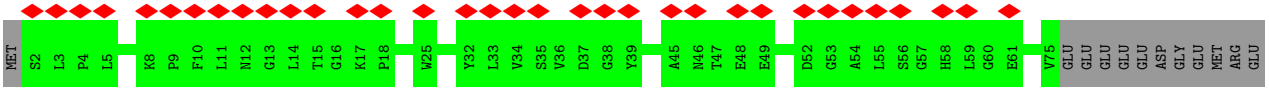
• Molecule 23: Small nuclear ribonucleoprotein Sm D2

Chain k:



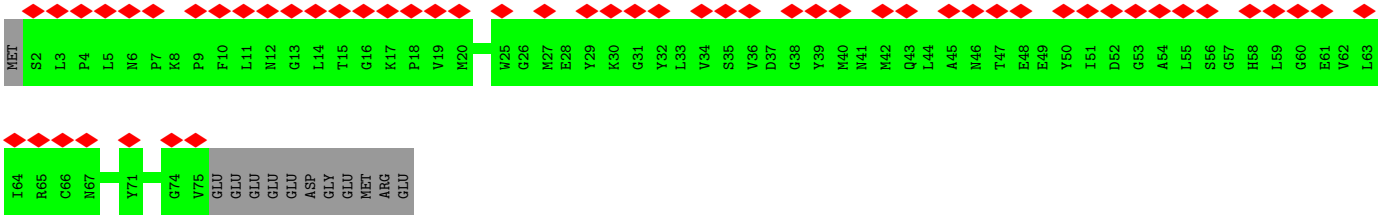
• Molecule 24: Small nuclear ribonucleoprotein F

Chain f:



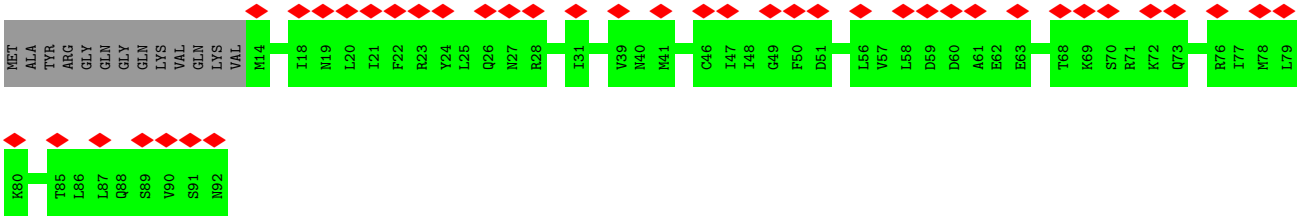
• Molecule 24: Small nuclear ribonucleoprotein F

Chain m:



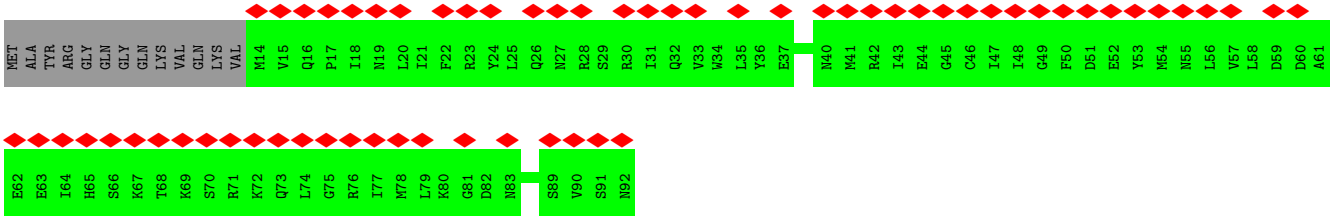
• Molecule 25: Small nuclear ribonucleoprotein E

Chain e:



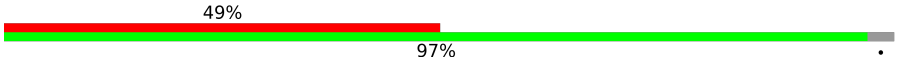
• Molecule 25: Small nuclear ribonucleoprotein E

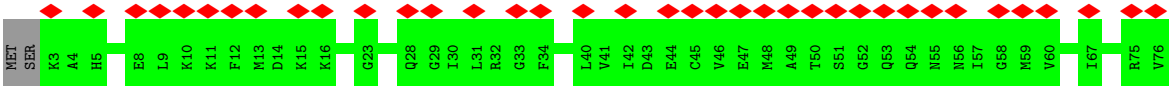
Chain l:



• Molecule 26: Small nuclear ribonucleoprotein G

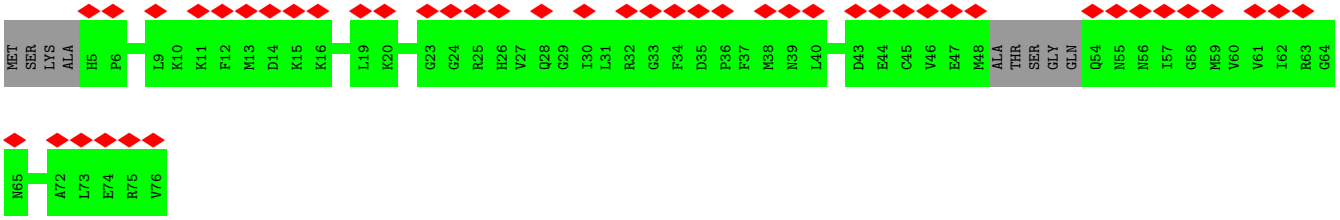
Chain g:





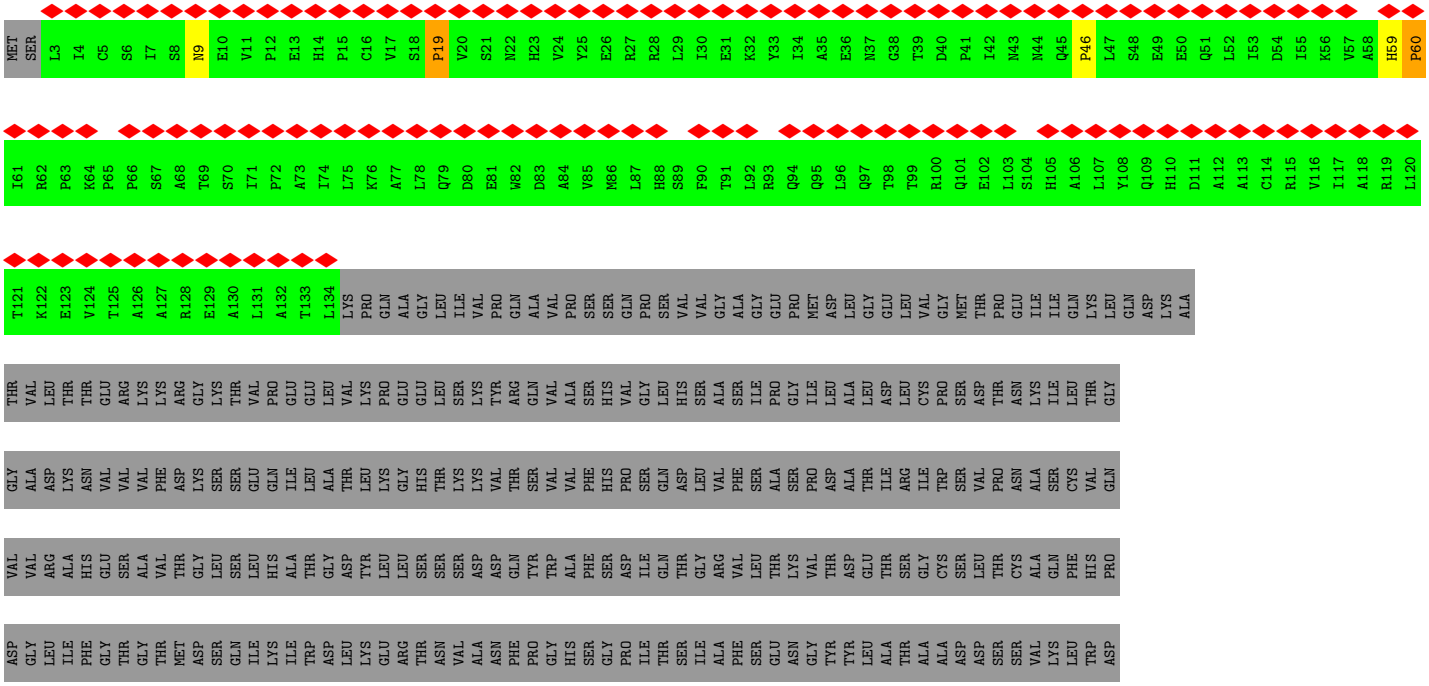
• Molecule 26: Small nuclear ribonucleoprotein G

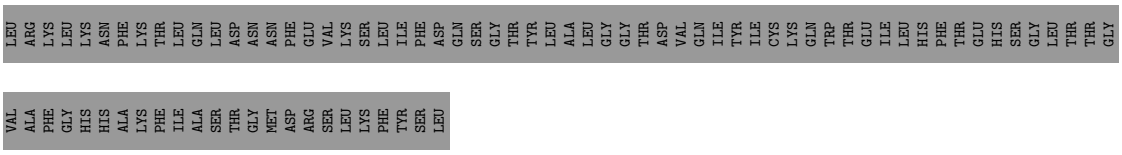
Chain n:



• Molecule 27: Pre-mRNA-processing factor 19

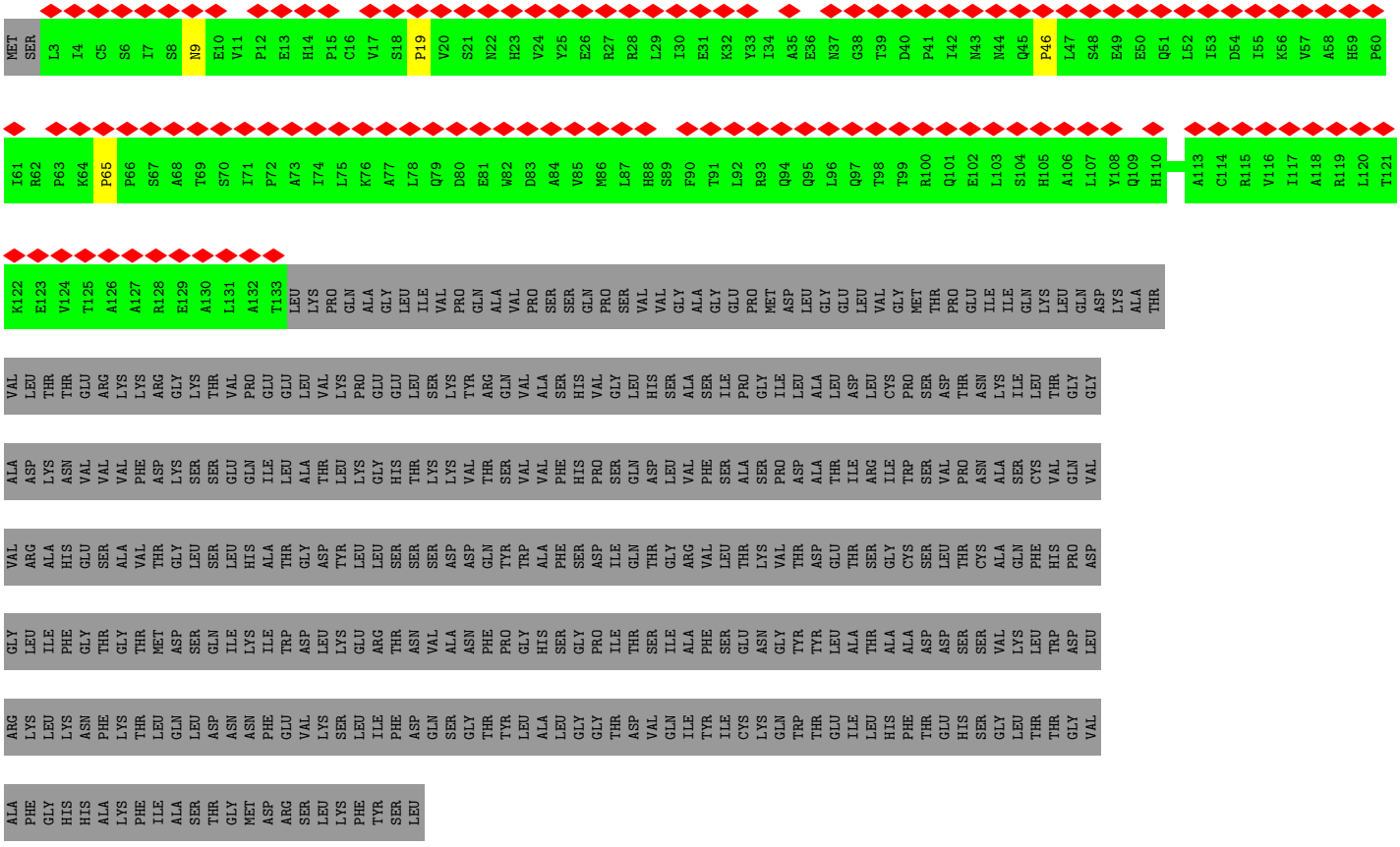
Chain q:





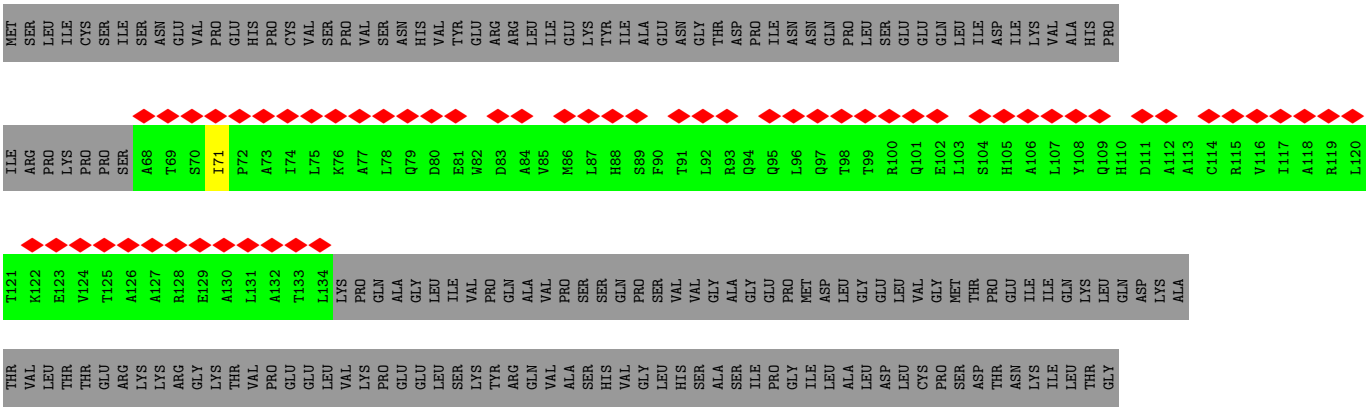
• Molecule 27: Pre-mRNA-processing factor 19

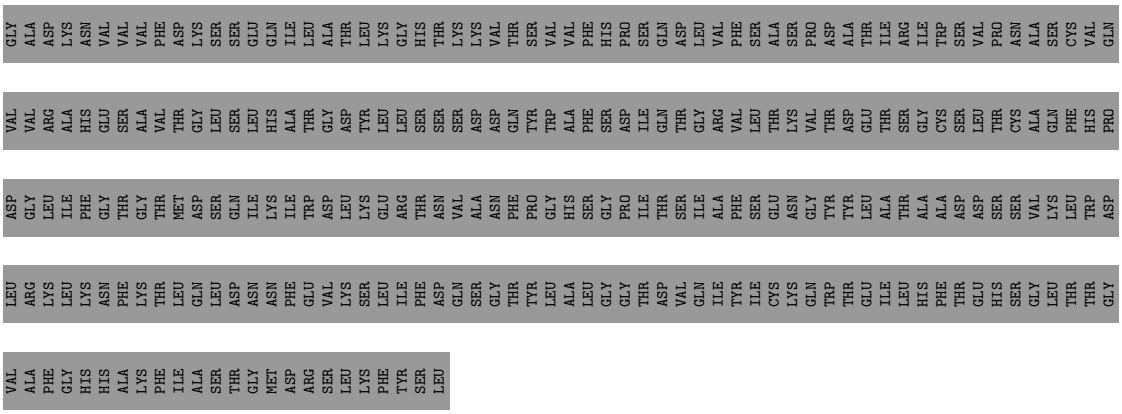
Chain r:



• Molecule 27: Pre-mRNA-processing factor 19

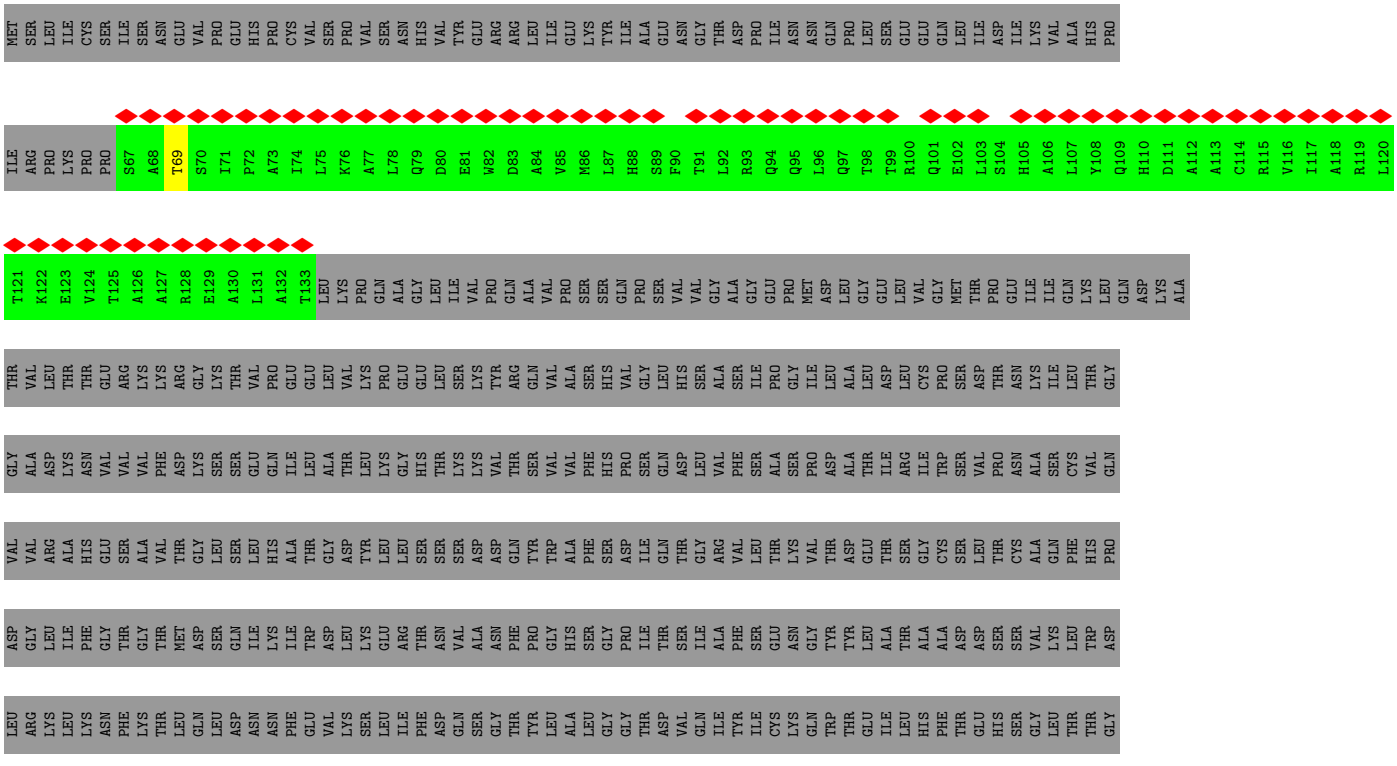
Chain s:





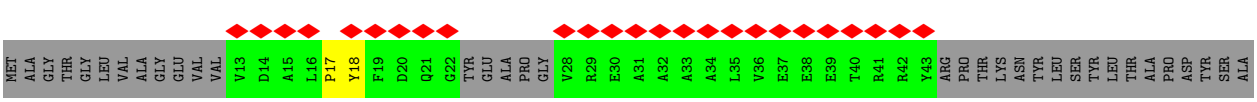
• Molecule 27: Pre-mRNA-processing factor 19

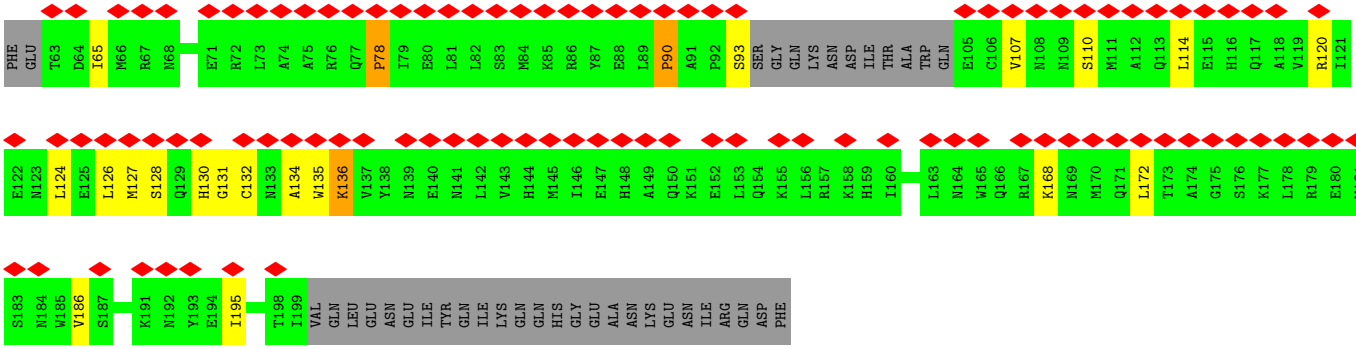
Chain t:



• Molecule 28: Pre-mRNA-splicing factor SPF27

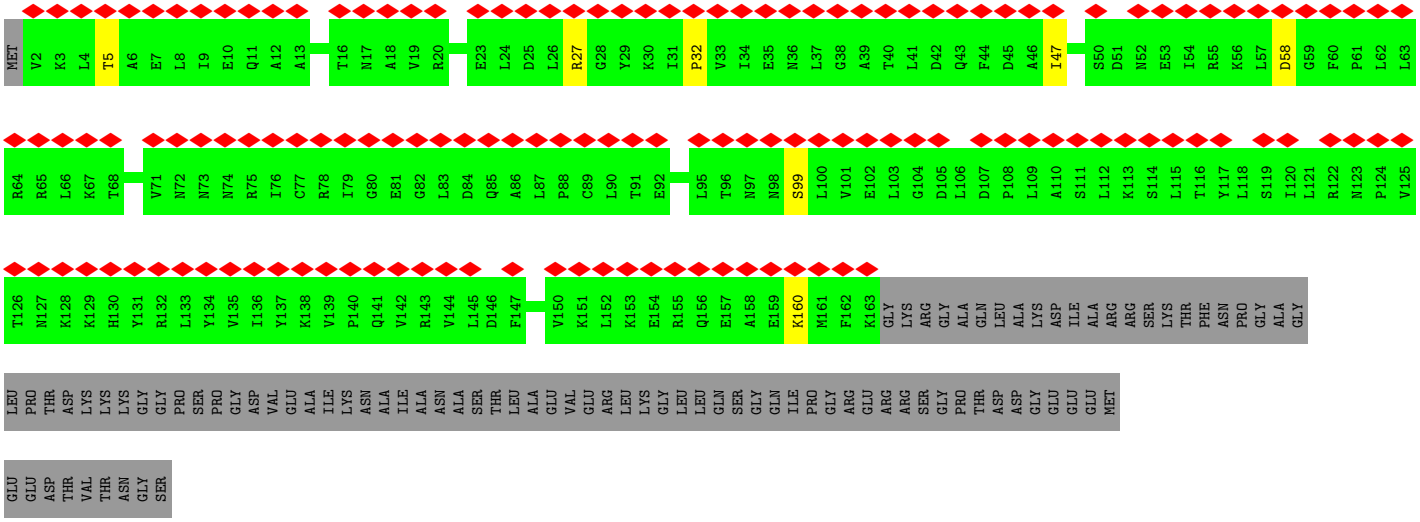
Chain K:





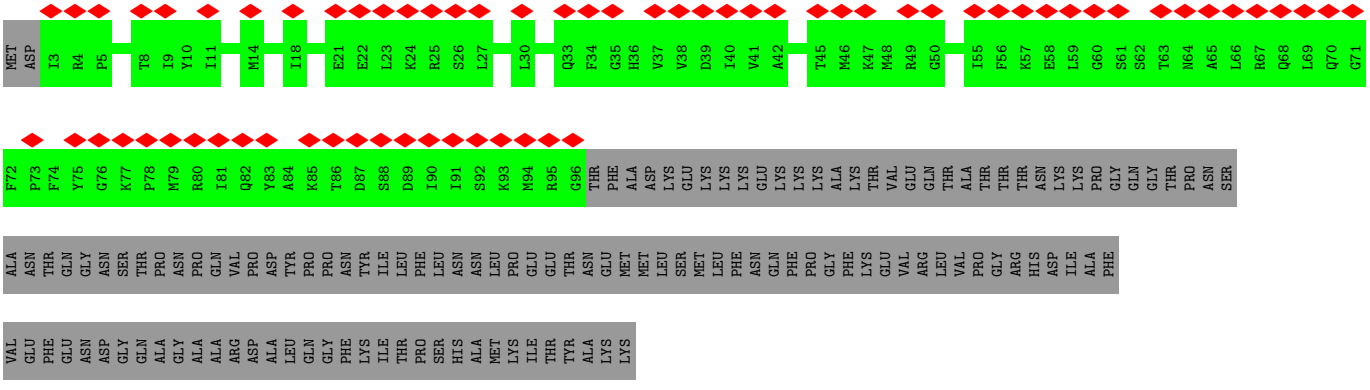
• Molecule 29: U2 small nuclear ribonucleoprotein A'

Chain o:



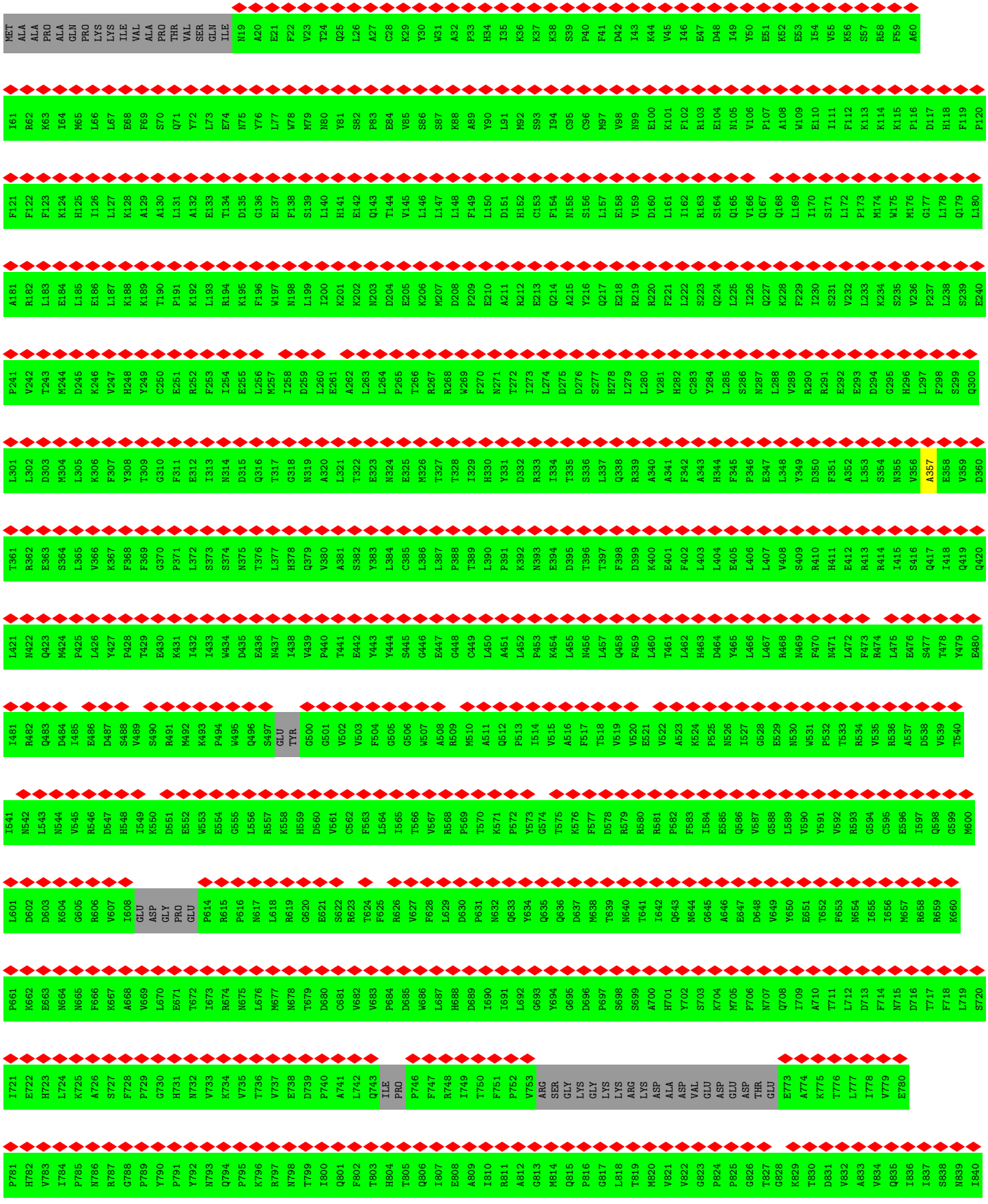
• Molecule 30: U2 small nuclear ribonucleoprotein B"

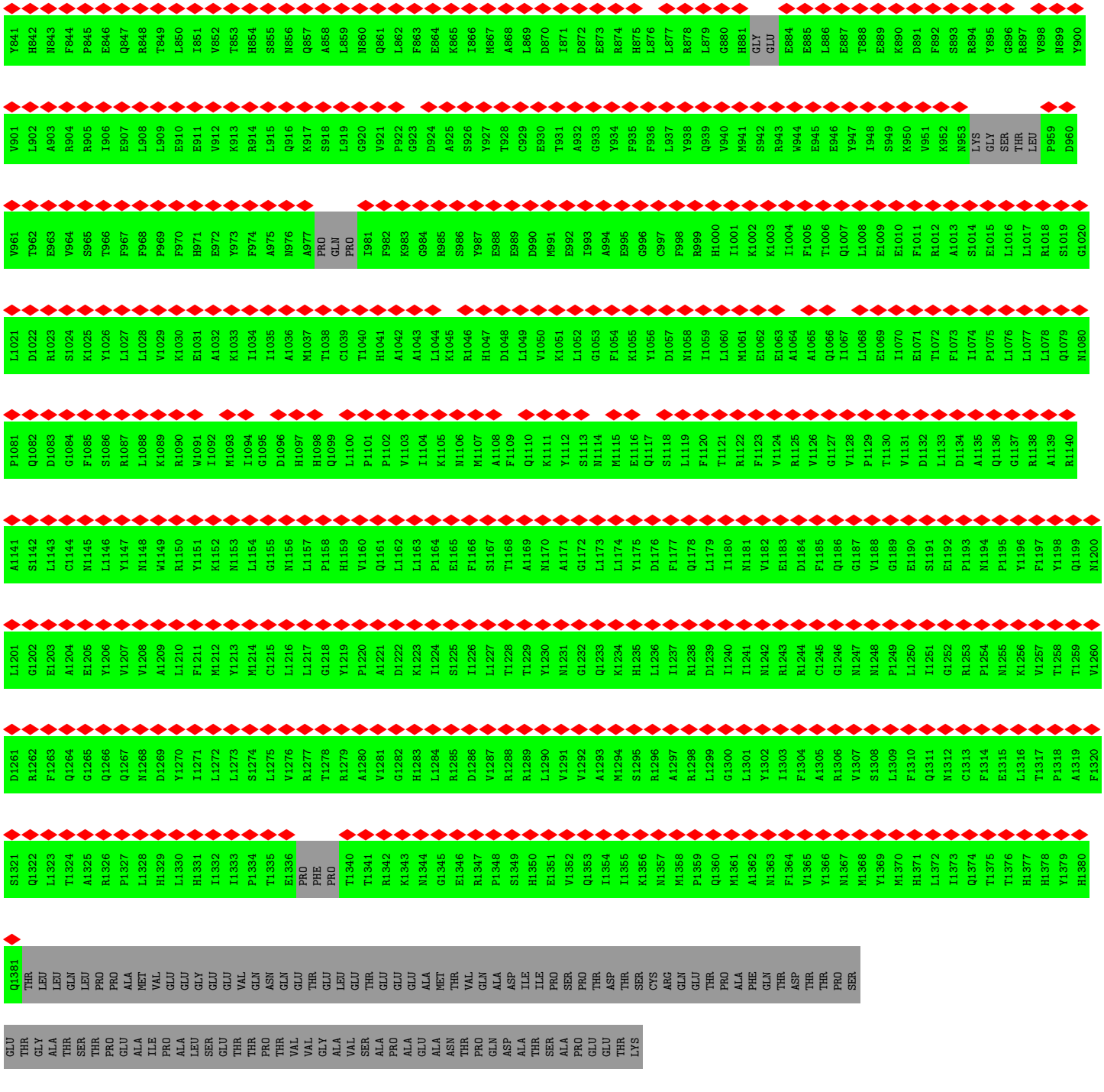
Chain p:



• Molecule 31: RNA helicase aquarius

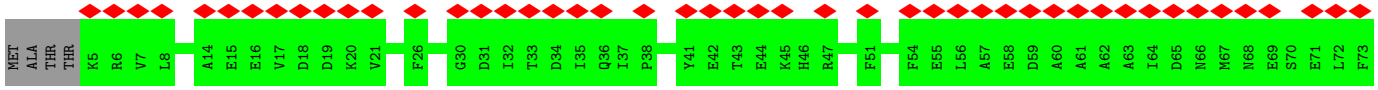
Chain Q:

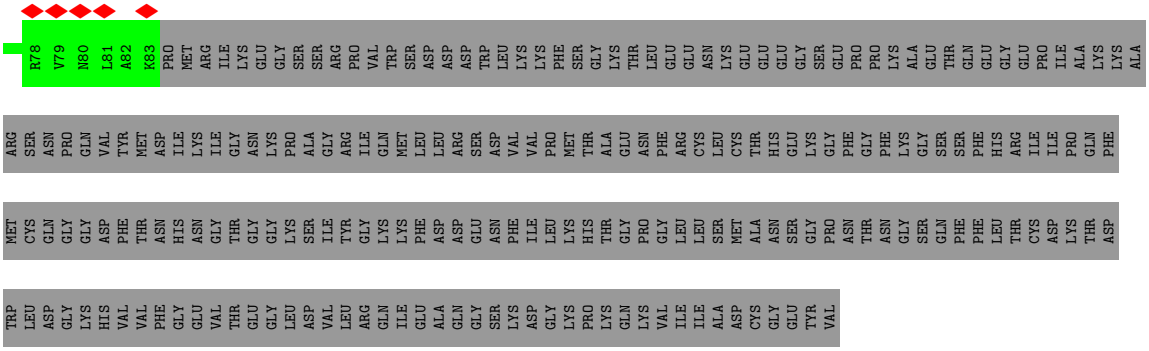

MET ALA ALA PRO ALA GLN PRO LYS LYS ILE VAL ALA PRO THR VAL SER GLN ILE N19 A20 E21 F22 V23 T24 Q25 L26 A27 C28 K29 Y30 W31 A32 P33 H34 I35 K36 K37 K38 S39 P40 F41 D42 I43 K44 V45 I46 E47 D48 I49 Y50 E51 K52 E53 I54 V55 K56 S57 R58 F59 A60
I61 R62 K63 I64 M65 L66 L67 E68 F69 S70 Q71 Y72 L73 E74 N75 Y76 L77 W78 M79 N80 Y81 S82 P83 E84 V85 S86 S87 K88 A89 Y90 L91 M92 S93 I94 C95 C96 M97 V98 N99 E100 K101 F102 R103 E104 N105 V106 P107 A108 W109 E110 I111 F112 K113 K114 K115 P116 D117 H118 F119 P120
F121 F122 F123 K124 H125 I126 L127 K128 A129 A130 L131 A132 E133 T134 D135 G136 E137 F138 S139 L140 H141 E142 Q143 T144 V145 L146 L147 L148 F149 L150 D151 H152 C153 F154 N155 S156 L157 E158 V159 D160 L161 I162 R163 S164 Q165 V166 Q167 Q168 L169 I170 S171 L172 P173 M174 W175 M176 G177 L178 Q179 L180
A181 R182 L183 E184 L185 E186 L187 K188 K189 T190 P191 K192 L193 R194 K195 F196 W197 N198 L199 I200 K201 K202 N203 D204 E205 K206 M207 D208 P209 E210 A211 R212 E213 Q214 A215 Y216 Q217 E218 R219 R220 F221 L222 S223 Q224 L225 I226 Q227 K228 F229 I230 S231 V232 L233 K234 S235 V236 P237 L238 S239 E240
P241 V242 T243 M244 D245 K246 V247 H248 Y249 C250 E251 R252 F253 I254 E255 L256 M257 I258 D259 L260 E261 A262 L263 L264 P265 T266 R267 R268 W269 F270 N271 T272 I273 L274 D275 D276 S277 H278 L279 L280 V281 H282 C283 Y284 L285 S286 N287 L288 V289 R290 R291 E292 E293 D294 G295 H296 L297 F298 S299 Q300
L301 L302 D303 M304 L305 K306 F307 Y308 T309 G310 F311 E312 I313 N314 D315 Q316 T317 G318 N319 A320 L321 T322 E323 N324 E325 M326 T327 T328 I329 H330 Y331 D332 R333 I334 T335 S336 L337 Q338 R339 A340 A341 F342 A343 H344 F345 P346 E347 L348 Y349 D350 F351 A352 L353 S354 N355 V356 A357 E358 V359 D360
T361 R362 E363 S364 L365 V366 K367 F368 F369 G370 P371 L372 S373 S374 N375 T376 L377 H378 Q379 V380 A381 S382 Y383 L384 C385 L386 L387 P388 T389 L390 P391 K392 N393 E394 D395 T396 T397 F398 D399 K400 E401 F402 L403 L404 E405 L406 L407 V408 S409 R410 H411 E412 R413 R414 I415 S416 Q417 I418 Q419 Q420
L421 N422 Q423 M424 P425 L426 Y427 P428 T429 E430 K431 I432 I433 W434 D435 E436 N437 I438 V439 P440 T441 E442 Y443 Y444 S445 G446 E447 G448 C449 L450 A451 L452 P453 K454 L455 N456 L457 Q458 F459 L460 T461 L462 H463 D464 Y465 L466 L467 R468 N469 F470 N471 L472 F473 R474 L475 E476 S477 T478 Y479 E480
I481 R482 Q483 D484 I485 E486 D487 S488 V489 S490 R491 M492 K493 P494 W495 Q496 S497 GLU TYR G500 G501 V502 V503 F504 G505 G506 W507 A508 R509 M510 A511 Q512 P513 I514 V515 A516 F517 T518 V519 V520 E521 V522 A523 K524 P525 N526 I527 G528 E529 N530 W531 P532 T533 R534 V535 R536 A537 D538 V539 T540
I541 N542 L543 N544 V545 R546 D547 H548 I549 K550 D551 E552 W553 E554 G555 L556 R557 K558 H559 D560 V561 C562 F563 L564 I565 T566 V567 R568 P569 T570 K571 P572 Y573 G574 T575 K576 F577 D578 R579 R580 R581 P582 F583 I584 E585 Q586 V587 G588 L589 V590 Y591 V592 R593 G594 C595 E596 I597 Q598 G599 M600
L601 D602 D603 K604 G605 R606 V607 I608 GLU ASP GLY PRO GLU P614 R615 P616 N617 L618 R619 G620 E621 S622 R623 T624 F625 R626 V627 F628 L629 D630 P631 N632 Q633 Y634 Q635 Q636 D637 M638 T639 N640 T641 I642 Q643 N644 G645 A646 E647 D648 V649 Y650 E651 T652 F653 N654 I655 I656 M657 R658 K659 K660
P661 K662 E663 N664 N665 F666 K667 A668 V669 L670 E671 T672 I673 R674 N675 L676 M677 N678 T679 D680 C681 V682 V683 P684 D685 W686 L687 H688 D689 I690 I691 L692 G693 Y694 G695 D696 P697 S698 S699 A700 H701 Y702 S703 K704 M705 P706 N707 Q708 I709 A710 T711 L712 D713 F714 N715 D716 T717 F718 L719 S720
I721 E722 H723 L724 K725 A726 S727 F728 P729 G730 H731 N732 V733 K734 V735 T736 V737 E738 D739 P740 A741 L742 Q743 ILE PRO P746 F747 R748 I749 T750 F751 P752 V753 ARG SER GLY LYS GLY LYS LYS ARG LYS ASP ALA ASP VAL GLU ASP GLU ASP THR GLU E773 A774 K775 T776 L777 I778 V779 E780
P781 H782 V783 I784 P785 N786 R787 G788 P789 Y790 P791 Y792 N793 Q794 P795 K796 R797 N798 T799 I800 Q801 F802 T803 H804 T805 Q806 I807 E808 A809 I810 R811 A812 G813 M814 Q815 P816 G817 L818 T819 M820 V821 V822 G823 P824 P825 G826 T827 G828 K829 T830 D831 V832 A833 V834 Q835 I836 I837 S838 N839 I840



• Molecule 32: Peptidyl-prolyl cis-trans isomerase E

Chain y:




R78 V79 N80 L81 A82 K83 PRO MET ARG ILE LYS GLU GLY SER SER ARG PRO VAL TRP SER ASP ASP ASP TRP LEU LYS LYS PHE SER GLY LYS THR LEU GLU GLU GLU ASN LYS GLU GLU GLU GLY SER GLU PRO PRO LYS ALA GLU THR GLN GLU GLY GLU PRO ILE ALA LYS LYS ALA
ARG SER ASN PRO GLN VAL TYR MET ASP ILE LYS ILE GLY ASN LYS PRO ALA GLY ARG ILE GLN MET LEU LEU ARG SER ASP VAL VAL PRO MET THR ALA GLU ASN PHE ARG CYS LEU CYS THR HIS GLU LYS GLY PHE GLY PHE LYS GLY SER SER PHE HIS ARG ILE ILE PRO GLN PHE
MET CYS GLN GLY GLY ASP PHE THR ASN HIS ASN GLY THR GLY GLY LYS SER ILE TYR GLY LYS LYS PHE ASP ASP GLU ASN PHE ILE LEU LYS HIS THR GLY PRO GLY LEU LEU SER MET ALA ASN SER GLY PRO ASN THR ASN GLY SER GLN PHE PHE LEU THR CYS ASP LYS THR ASP
TRP LEU ASP GLY LYS HIS VAL VAL PHE GLY GLU VAL THR GLU GLY LEU ASP VAL LEU ARG GLN ILE GLU ALA GLN GLY SER LYS ASP GLY LYS PRO LYS GLN LYS VAL ILE ILE ALA ASP CYS GLY GLU TYR VAL

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	390072	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.543	Depositor
Minimum map value	-0.239	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	535.2, 535.2, 535.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.338, 1.338, 1.338	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.41	0/16926	0.64	9/22947 (0.0%)
2	B	0.54	1/2296 (0.0%)	1.09	15/3569 (0.4%)
3	C	0.33	0/7181	0.65	3/9758 (0.0%)
4	E	0.32	0/2420	0.64	1/3281 (0.0%)
5	F	0.64	0/2323	1.14	11/3619 (0.3%)
6	J	0.43	0/3802	0.59	6/5162 (0.1%)
7	L	0.35	0/3267	0.61	9/4418 (0.2%)
8	M	0.33	0/1119	0.59	1/1497 (0.1%)
9	N	0.99	6/1210 (0.5%)	0.74	0/1622
10	O	0.39	0/2390	0.62	3/3227 (0.1%)
11	P	0.36	0/1000	0.58	0/1330
12	R	0.38	0/2186	0.71	4/2937 (0.1%)
13	S	0.33	0/1268	0.61	2/1714 (0.1%)
14	T	0.55	1/2562 (0.0%)	0.74	0/3492
15	W	0.47	0/3038	0.72	3/4171 (0.1%)
16	G	0.74	5/1378 (0.4%)	1.46	31/2133 (1.5%)
17	H	0.81	20/3308 (0.6%)	1.37	64/5135 (1.2%)
18	U	0.37	0/2928	0.71	4/3928 (0.1%)
19	I	0.34	0/2803	0.58	11/3870 (0.3%)
20	a	0.47	0/397	0.62	0/549
20	h	0.47	0/396	0.61	0/547
21	b	0.51	0/423	0.72	0/587
21	i	0.50	0/423	0.73	0/587
22	c	0.57	0/405	0.73	0/563
22	j	0.57	0/405	0.73	0/563
23	d	0.69	0/479	0.85	0/666
23	k	0.70	0/420	0.85	0/583
24	f	0.75	0/360	0.81	0/497
24	m	0.75	0/360	0.81	0/497
25	e	0.65	0/390	0.80	0/542
25	l	0.64	0/390	0.80	0/542
26	g	0.54	0/362	0.71	0/501

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
26	n	0.53	0/327	0.72	0/451
27	q	0.35	0/658	0.58	3/919 (0.3%)
27	r	0.33	0/653	0.56	2/912 (0.2%)
27	s	0.26	0/334	0.37	0/466
27	t	0.31	0/334	0.38	0/466
28	K	0.39	1/753 (0.1%)	0.53	3/1046 (0.3%)
29	o	0.64	0/803	1.49	5/1119 (0.4%)
30	p	0.62	0/463	1.27	0/643
31	Q	0.21	0/6565	0.42	0/9143
32	y	0.25	0/389	0.62	0/540
All	All	0.46	34/79894 (0.0%)	0.76	190/110739 (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	A	0	16
3	C	0	6
4	E	0	1
5	F	0	1
6	J	0	1
9	N	0	1
12	R	0	8
14	T	0	5
15	W	0	3
16	G	0	5
17	H	0	1
18	U	0	6
23	d	0	1
23	k	0	1
All	All	0	56

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	N	137	CYS	CB-SG	-11.04	1.63	1.82
9	N	119	CYS	CB-SG	-8.86	1.67	1.82
9	N	142	CYS	CB-SG	-8.41	1.68	1.82
9	N	101	CYS	CB-SG	-8.37	1.68	1.82
17	H	77	C	C1'-N1	7.34	1.59	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	306	CYS	CB-SG	-7.20	1.70	1.82
17	H	74	U	C1'-N1	6.92	1.59	1.48
17	H	91	U	C1'-N1	6.90	1.59	1.48
17	H	92	U	C1'-N1	6.88	1.59	1.48
16	G	5	G	N3-C4	6.87	1.40	1.35
2	B	103	G	C1'-N9	-6.87	1.37	1.46
17	H	60	U	C1'-N1	6.87	1.59	1.48
17	H	72	U	C1'-N1	6.86	1.59	1.48
17	H	58	U	C1'-N1	6.84	1.59	1.48
17	H	89	U	C1'-N1	6.77	1.58	1.48
9	N	102	CYS	CB-SG	-6.64	1.71	1.82
17	H	35	A	O3'-P	-6.51	1.53	1.61
17	H	97	G	C1'-N9	-6.44	1.37	1.46
17	H	84	C	C1'-N1	6.32	1.58	1.48
17	H	73	C	C1'-N1	6.32	1.58	1.48
17	H	78	C	C1'-N1	6.29	1.58	1.48
17	H	71	C	C1'-N1	6.20	1.58	1.48
17	H	148	C	C1'-N1	6.20	1.58	1.48
17	H	67	C	C1'-N1	6.12	1.57	1.48
16	G	137	C	C1'-N1	5.96	1.57	1.48
9	N	117	CYS	CB-SG	-5.47	1.73	1.81
16	G	139	U	C1'-N1	5.41	1.56	1.48
17	H	41	U	C1'-N1	5.40	1.56	1.48
17	H	37	U	C1'-N1	5.38	1.56	1.48
16	G	134	U	C1'-N1	5.37	1.56	1.48
16	G	136	U	C1'-N1	5.37	1.56	1.48
17	H	39	U	C1'-N1	5.37	1.56	1.48
17	H	43	U	C1'-N1	5.34	1.56	1.48
28	K	186	VAL	CA-CB	-5.12	1.44	1.54

All (190) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	G	147	C	O5'-P-OP1	-13.09	93.92	105.70
16	G	5	G	N3-C4-C5	-12.87	122.16	128.60
16	G	17	U	N1-C2-O2	9.52	129.47	122.80
16	G	2	U	N1-C1'-C2'	9.23	126.00	114.00
16	G	17	U	N3-C2-O2	-8.73	116.09	122.20
2	B	38	C	N1-C2-O2	8.71	124.12	118.90
18	U	809	ASP	CB-CG-OD1	8.45	125.90	118.30
16	G	17	U	C2-N1-C1'	8.36	127.73	117.70
16	G	1	G	N3-C4-C5	-8.32	124.44	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	G	4	A	N1-C6-N6	-8.15	113.71	118.60
16	G	142	U	O4'-C1'-N1	7.76	114.41	108.20
16	G	7	G	C6-C5-N7	-7.74	125.76	130.40
2	B	38	C	C2-N1-C1'	7.63	127.19	118.80
1	A	1109	LEU	CA-CB-CG	7.46	132.46	115.30
2	B	38	C	N3-C2-O2	-7.38	116.73	121.90
16	G	7	G	C4-C5-C6	-7.36	114.39	118.80
12	R	132	LEU	CA-CB-CG	7.34	132.18	115.30
5	F	26	U	N3-C2-O2	-7.31	117.08	122.20
15	W	278	LYS	CB-CA-C	-7.31	95.78	110.40
17	H	77	C	OP2-P-O3'	7.28	121.21	105.20
18	U	792	SER	C-N-CA	7.28	139.89	121.70
17	H	113	G	OP2-P-O3'	7.26	121.17	105.20
17	H	114	A	OP2-P-O3'	7.25	121.15	105.20
17	H	81	G	OP2-P-O3'	7.24	121.12	105.20
17	H	58	U	OP2-P-O3'	7.23	121.11	105.20
17	H	88	A	OP2-P-O3'	7.23	121.11	105.20
17	H	59	A	OP2-P-O3'	7.22	121.08	105.20
17	H	84	C	OP2-P-O3'	7.21	121.07	105.20
17	H	90	A	OP2-P-O3'	7.21	121.07	105.20
17	H	91	U	OP2-P-O3'	7.21	121.07	105.20
17	H	57	A	OP2-P-O3'	7.21	121.07	105.20
17	H	89	U	OP2-P-O3'	7.21	121.05	105.20
17	H	72	U	OP2-P-O3'	7.20	121.05	105.20
17	H	78	C	OP2-P-O3'	7.20	121.05	105.20
17	H	80	A	OP2-P-O3'	7.19	121.03	105.20
17	H	73	C	OP2-P-O3'	7.18	121.01	105.20
17	H	79	G	OP2-P-O3'	7.16	120.94	105.20
17	H	83	A	OP2-P-O3'	7.16	120.94	105.20
17	H	71	C	OP2-P-O3'	7.15	120.94	105.20
17	H	74	U	OP2-P-O3'	7.15	120.93	105.20
17	H	56	A	OP2-P-O3'	7.14	120.92	105.20
16	G	147	C	C2'-C3'-O3'	7.12	125.17	109.50
5	F	61	C	C5-C6-N1	7.12	124.56	121.00
2	B	36	C	N1-C2-O2	7.09	123.15	118.90
16	G	1	G	N3-C4-N9	7.08	130.25	126.00
17	H	82	G	OP2-P-O3'	7.07	120.76	105.20
5	F	52	U	N3-C2-O2	-6.91	117.36	122.20
12	R	268	LEU	CA-CB-CG	6.88	131.12	115.30
2	B	104	C	C2'-C3'-O3'	-6.84	94.44	109.50
17	H	88	A	O3'-P-O5'	-6.84	91.00	104.00
17	H	82	G	O3'-P-O5'	-6.84	91.01	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	36	C	C2-N1-C1'	6.83	126.31	118.80
17	H	73	C	O3'-P-O5'	-6.82	91.03	104.00
17	H	78	C	O3'-P-O5'	-6.82	91.04	104.00
17	H	72	U	O3'-P-O5'	-6.81	91.05	104.00
17	H	71	C	O3'-P-O5'	-6.80	91.08	104.00
17	H	80	A	O3'-P-O5'	-6.80	91.08	104.00
17	H	84	C	O3'-P-O5'	-6.80	91.08	104.00
17	H	83	A	O3'-P-O5'	-6.80	91.09	104.00
17	H	113	G	O3'-P-O5'	-6.79	91.09	104.00
1	A	1763	LEU	CA-CB-CG	6.79	130.91	115.30
17	H	57	A	O3'-P-O5'	-6.79	91.10	104.00
17	H	79	G	O3'-P-O5'	-6.79	91.11	104.00
17	H	77	C	O3'-P-O5'	-6.78	91.12	104.00
17	H	59	A	O3'-P-O5'	-6.77	91.13	104.00
17	H	89	U	O3'-P-O5'	-6.77	91.14	104.00
17	H	74	U	O3'-P-O5'	-6.76	91.15	104.00
17	H	81	G	O3'-P-O5'	-6.76	91.16	104.00
17	H	114	A	O3'-P-O5'	-6.75	91.18	104.00
17	H	90	A	O3'-P-O5'	-6.75	91.18	104.00
17	H	56	A	O3'-P-O5'	-6.74	91.20	104.00
17	H	91	U	O3'-P-O5'	-6.73	91.21	104.00
17	H	58	U	O3'-P-O5'	-6.71	91.25	104.00
17	H	155	C	P-O3'-C3'	6.69	127.73	119.70
2	B	20	G	C4-N9-C1'	6.65	135.15	126.50
27	q	46	PRO	N-CA-CB	6.63	111.26	103.30
15	W	279	LYS	N-CA-C	-6.60	93.19	111.00
16	G	1	G	C2-N3-C4	6.58	115.19	111.90
28	K	90	PRO	N-CA-CB	6.58	111.19	103.30
5	F	52	U	N1-C2-O2	6.50	127.35	122.80
27	r	46	PRO	N-CA-CB	6.46	111.05	103.30
17	H	13	C	N1-C2-O2	6.46	122.77	118.90
3	C	758	LEU	CA-CB-CG	6.45	130.14	115.30
16	G	4	A	C6-C5-N7	6.45	136.81	132.30
12	R	171	LEU	CA-CB-CG	6.44	130.12	115.30
27	q	60	PRO	N-CA-CB	6.40	110.98	103.30
16	G	7	G	C4-C5-N7	-6.34	108.26	110.80
28	K	78	PRO	N-CA-CB	6.34	110.91	103.30
19	I	589	PRO	N-CA-CB	6.33	110.90	103.30
16	G	3	A	N9-C1'-C2'	6.32	122.22	114.00
29	o	5	THR	N-CA-CB	-6.29	98.34	110.30
19	I	475	PRO	N-CA-CB	6.23	110.78	103.30
19	I	162	PRO	N-CA-CB	6.19	110.73	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	H	30	A	C4'-C3'-O3'	-6.18	96.41	109.40
7	L	558	PRO	N-CA-CB	6.15	110.68	103.30
19	I	177	PRO	N-CA-CB	6.14	110.67	103.30
18	U	818	LEU	CA-CB-CG	6.09	129.30	115.30
7	L	77	LEU	CA-CB-CG	6.07	129.25	115.30
7	L	546	PRO	N-CA-CB	6.06	110.57	103.30
16	G	16	G	P-O3'-C3'	6.03	126.93	119.70
19	I	788	PRO	N-CA-CB	6.03	110.53	103.30
3	C	87	GLN	CA-CB-CG	6.02	126.64	113.40
17	H	32	U	C1'-C2'-O2'	6.01	128.62	110.60
3	C	105	MET	CA-CB-CG	6.00	123.50	113.30
19	I	160	PRO	N-CA-CB	6.00	110.50	103.30
6	J	523	PRO	N-CA-CB	6.00	110.50	103.30
6	J	637	PRO	N-CA-CB	5.96	110.45	103.30
1	A	1467	LEU	CA-CB-CG	5.93	128.93	115.30
7	L	563	PRO	N-CA-CB	5.92	110.40	103.30
17	H	172	C	P-O3'-C3'	5.92	126.80	119.70
27	r	19	PRO	N-CA-CB	5.92	110.40	103.30
7	L	594	PRO	N-CA-CB	5.91	110.39	103.30
27	q	19	PRO	N-CA-CB	5.88	110.36	103.30
17	H	13	C	C2-N1-C1'	5.87	125.25	118.80
19	I	816	PRO	N-CA-CB	5.86	110.33	103.30
6	J	488	PRO	N-CA-CB	5.85	110.32	103.30
29	o	27	ARG	CB-CA-C	-5.83	98.73	110.40
7	L	548	PRO	N-CA-CB	5.83	110.29	103.30
5	F	26	U	C2-N1-C1'	5.82	124.69	117.70
19	I	518	PRO	N-CA-CB	5.81	110.27	103.30
1	A	941	LYS	N-CA-C	5.81	126.68	111.00
10	O	150	LEU	CA-CB-CG	5.81	128.66	115.30
7	L	564	PRO	N-CA-CB	5.79	110.25	103.30
6	J	566	PRO	N-CA-CB	5.77	110.22	103.30
2	B	20	G	C8-N9-C1'	-5.76	119.51	127.00
6	J	522	PRO	N-CA-CB	5.75	110.20	103.30
17	H	35	A	O4'-C1'-N9	5.75	112.80	108.20
17	H	156	U	P-O3'-C3'	-5.73	112.82	119.70
2	B	36	C	N3-C2-O2	-5.73	117.89	121.90
7	L	620	PRO	N-CA-CB	5.71	110.15	103.30
18	U	820	TYR	CA-CB-CG	5.70	124.23	113.40
8	M	168	LEU	CA-CB-CG	5.68	128.38	115.30
17	H	13	C	C6-N1-C2	-5.68	118.03	120.30
2	B	20	G	O4'-C1'-N9	5.68	112.75	108.20
16	G	142	U	C4'-C3'-O3'	5.67	124.35	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	R	86	LEU	CA-CB-CG	5.67	128.33	115.30
2	B	47	A	O4'-C1'-N9	5.62	112.70	108.20
16	G	147	C	C5'-C4'-O4'	5.61	115.83	109.10
5	F	52	U	C2-N1-C1'	5.58	124.39	117.70
19	I	588	PRO	N-CA-CB	5.58	109.99	103.30
16	G	4	A	C5-C6-N6	5.57	128.16	123.70
29	o	58	ASP	N-CA-CB	-5.56	100.59	110.60
16	G	17	U	C5-C6-N1	5.55	125.48	122.70
19	I	761	PRO	N-CA-CB	5.53	109.93	103.30
17	H	14	C	N1-C2-O2	5.52	122.21	118.90
5	F	26	U	N1-C2-O2	5.49	126.65	122.80
28	K	93	SER	N-CA-CB	-5.49	102.27	110.50
7	L	123	LEU	CA-CB-CG	5.47	127.89	115.30
19	I	625	PRO	N-CA-CB	5.45	109.84	103.30
17	H	31	G	C3'-C2'-C1'	-5.43	97.15	101.50
16	G	9	C	C5-C6-N1	5.41	123.71	121.00
13	S	27	LEU	CA-CB-CG	5.41	127.73	115.30
16	G	146	C	P-O3'-C3'	-5.41	113.21	119.70
16	G	147	C	OP1-P-OP2	5.41	127.71	119.60
1	A	260	LEU	CA-CB-CG	5.39	127.71	115.30
2	B	38	C	C6-N1-C1'	-5.37	114.36	120.80
13	S	106	ASP	CB-CG-OD1	5.37	123.13	118.30
16	G	6	A	N9-C1'-C2'	5.34	120.95	114.00
2	B	38	C	C6-N1-C2	-5.32	118.17	120.30
29	o	47	ILE	N-CA-CB	5.32	123.03	110.80
17	H	156	U	OP2-P-O3'	5.31	116.87	105.20
16	G	3	A	C2'-C3'-O3'	5.30	122.17	113.70
5	F	50	A	P-O3'-C3'	5.27	126.02	119.70
16	G	146	C	O3'-P-O5'	5.25	113.98	104.00
17	H	13	C	N3-C2-O2	-5.25	118.22	121.90
5	F	45	A	N3-C4-N9	5.24	131.59	127.40
1	A	1305	SER	C-N-CA	5.23	134.77	121.70
2	B	23	C	N1-C2-O2	5.22	122.03	118.90
1	A	1640	SER	C-N-CA	5.21	134.73	121.70
16	G	9	C	C6-N1-C2	-5.21	118.22	120.30
17	H	157	G	P-O5'-C5'	-5.19	112.60	120.90
17	H	156	U	C4'-C3'-C2'	5.18	107.78	102.60
17	H	160	A	P-O5'-C5'	-5.18	112.61	120.90
17	H	157	G	O4'-C1'-N9	-5.18	104.06	108.20
5	F	33	G	P-O3'-C3'	5.14	125.87	119.70
10	O	193	LEU	CA-CB-CG	5.14	127.13	115.30
17	H	176	G	OP1-P-OP2	-5.14	111.89	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1304	ASN	C-N-CA	5.11	134.47	121.70
4	E	81	LEU	CA-CB-CG	5.11	127.04	115.30
17	H	160	A	C4'-C3'-C2'	-5.08	97.52	102.60
16	G	17	U	C6-N1-C1'	-5.08	114.09	121.20
2	B	80	U	C2'-C3'-O3'	5.07	121.81	113.70
16	G	141	C	N1-C1'-C2'	5.06	120.58	114.00
6	J	220	LEU	CA-CB-CG	5.06	126.94	115.30
5	F	45	A	C4-N9-C1'	5.04	135.37	126.30
10	O	15	TRP	CA-CB-CG	5.01	123.21	113.70
17	H	13	C	C5-C6-N1	5.01	123.50	121.00
1	A	1303	LEU	C-N-CA	5.00	134.21	121.70
15	W	279	LYS	N-CA-CB	5.00	119.61	110.60
29	o	99	SER	N-CA-CB	-5.00	103.00	110.50

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1019	TYR	Peptide
1	A	107	PRO	Peptide
1	A	1091	TYR	Peptide
1	A	1190	CYS	Peptide
1	A	1305	SER	Peptide
1	A	135	VAL	Peptide
1	A	1366	PRO	Peptide
1	A	1555	LEU	Peptide
1	A	1606	ILE	Peptide
1	A	1638	ASN	Peptide
1	A	1639	VAL	Peptide
1	A	1653	ASP	Peptide
1	A	1763	LEU	Peptide
1	A	1920	TYR	Peptide
1	A	320	TYR	Peptide
1	A	940	ILE	Peptide
3	C	359	LYS	Peptide
3	C	440	SER	Peptide
3	C	559	ILE	Peptide
3	C	560	VAL	Peptide
3	C	823	ALA	Peptide
3	C	93	ILE	Peptide
4	E	192	ASN	Peptide
5	F	41	A	Sidechain

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Mol	Chain	Res	Type	Group
16	G	142	U	Sidechain
16	G	2	U	Sidechain
16	G	5	G	Sidechain
16	G	6	A	Sidechain
16	G	7	G	Sidechain
17	H	33	G	Sidechain
6	J	357	LYS	Peptide
9	N	3	LYS	Peptide
12	R	125	MET	Peptide
12	R	167	ALA	Peptide
12	R	168	ALA	Peptide
12	R	184	GLN	Peptide
12	R	185	GLY	Peptide
12	R	186	VAL	Peptide
12	R	189	ASN	Peptide
12	R	316	GLU	Peptide
14	T	342	GLU	Peptide
14	T	404	SER	Peptide
14	T	405	PHE	Peptide
14	T	495	ALA	Peptide
14	T	497	GLU	Peptide
18	U	542	ASP	Peptide
18	U	578	MET	Peptide
18	U	647	ARG	Peptide
18	U	792	SER	Peptide
18	U	809	ASP	Peptide
18	U	818	LEU	Peptide
15	W	148	VAL	Peptide
15	W	204	ASP	Peptide
15	W	76	VAL	Peptide
23	d	112	ASN	Peptide
23	k	112	ASN	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	A	16477	0	16462	234	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2060	0	1044	79	0
3	C	7022	0	7047	163	0
4	E	2366	0	2303	70	0
5	F	2075	0	1048	43	0
6	J	3758	0	2888	46	0
7	L	3237	0	2680	38	0
8	M	1098	0	1082	16	0
9	N	1184	0	1189	11	0
10	O	2340	0	2316	45	0
11	P	985	0	965	14	0
12	R	2165	0	2214	36	0
13	S	1236	0	1210	28	0
14	T	2496	0	2446	46	0
15	W	3008	0	1977	60	0
16	G	1246	0	631	212	0
17	H	2968	0	1504	256	0
18	U	2864	0	2814	80	0
19	I	2822	0	1319	64	0
20	a	399	0	173	0	0
20	h	398	0	172	0	0
21	b	424	0	179	0	0
21	i	424	0	179	0	0
22	c	406	0	170	0	0
22	j	406	0	170	0	0
23	d	480	0	200	0	0
23	k	422	0	175	0	0
24	f	361	0	158	0	0
24	m	361	0	158	0	0
25	e	391	0	163	0	0
25	l	391	0	163	0	0
26	g	363	0	160	0	0
26	n	329	0	138	0	0
27	q	659	0	296	0	0
27	r	654	0	294	0	0
27	s	335	0	168	0	0
27	t	335	0	168	0	0
28	K	757	0	338	18	0
29	o	804	0	350	0	0
30	p	464	0	205	0	0
31	Q	6562	0	2836	2	0
32	y	390	0	190	0	0
33	A	36	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	C	32	0	12	22	0
35	C	1	0	0	0	0
35	F	6	0	0	0	0
36	N	3	0	0	0	0
36	O	3	0	0	0	0
36	U	1	0	0	0	0
All	All	78004	0	60360	1359	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 11.

All (1359) 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)
19:I:437:CYS:CB	19:I:447:GLU:CB	1.98	1.42
5:F:44:G:N2	16:G:3:A:C2	1.84	1.38
18:U:546:VAL:HG21	18:U:665:HIS:CE1	1.56	1.38
5:F:44:G:N2	16:G:3:A:H2	1.14	1.36
5:F:41:A:N6	16:G:6:A:H61	1.17	1.34
17:H:34:U:H2'	17:H:35:A:C8	1.66	1.28
4:E:55:LEU:HD11	4:E:341:ILE:CD1	1.62	1.27
16:G:148:U:N3	17:H:30:A:N1	1.79	1.27
5:F:41:A:H61	16:G:6:A:N6	1.31	1.26
1:A:532:THR:OG1	16:G:3:A:C5'	1.84	1.25
17:H:153:A:H2'	17:H:154:C:C5'	1.70	1.21
16:G:151:C:H2'	16:G:152:C:C6	1.74	1.21
16:G:133:A:O2'	16:G:134:U:C6	1.86	1.21
17:H:179:C:O2'	17:H:180:G:H5'	1.44	1.18
19:I:462:LEU:CB	19:I:466:ARG:CB	2.21	1.17
19:I:790:ARG:CB	19:I:801:ASP:CB	2.23	1.16
16:G:143:U:O4	17:H:34:U:N3	1.77	1.15
1:A:861:ARG:NH1	17:H:29:A:H5'	1.59	1.15
19:I:364:VAL:C	19:I:372:ARG:CB	2.16	1.14
1:A:532:THR:HB	16:G:3:A:H3'	1.14	1.13
6:J:773:ARG:CB	6:J:790:THR:CB	2.26	1.13
3:C:139:HIS:HA	34:C:1500:GTP:O3B	1.45	1.13
4:E:61:LEU:HD13	4:E:352:TYR:CZ	1.83	1.13
1:A:532:THR:OG1	16:G:3:A:H5'	1.41	1.12
1:A:532:THR:HB	16:G:3:A:C3'	1.78	1.12
17:H:156:U:H6	17:H:156:U:H5"	1.10	1.12
17:H:179:C:C2'	17:H:180:G:H5'	1.80	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1512:SER:OG	16:G:148:U:OP2	1.68	1.11
5:F:44:G:N1	16:G:3:A:N1	1.99	1.10
16:G:151:C:C2	16:G:152:C:C5	2.38	1.10
2:B:74:U:H5	2:B:76:A:N6	1.49	1.10
17:H:179:C:H2'	17:H:180:G:H8	1.13	1.10
3:C:142:LYS:HG3	3:C:228:PHE:CD2	1.86	1.10
17:H:153:A:H2'	17:H:154:C:H5'	1.15	1.09
17:H:35:A:O2'	17:H:36:G:C8	2.04	1.08
5:F:43:A:H2	16:G:4:A:N1	1.48	1.08
16:G:132:G:P	16:G:133:A:OP1	2.12	1.08
18:U:550:ARG:HB3	18:U:660:LYS:HD3	1.29	1.08
17:H:153:A:C2'	17:H:154:C:H5'	1.83	1.07
1:A:855:ARG:HH22	1:A:1518:LEU:CD1	1.66	1.07
6:J:658:ARG:HA	6:J:667:ILE:CB	1.85	1.05
16:G:129:G:H4'	16:G:130:A:OP1	1.52	1.05
16:G:145:U:H3	17:H:33:G:N2	1.55	1.05
2:B:11:U:H6	2:B:11:U:H5'	1.18	1.05
4:E:55:LEU:CD1	4:E:341:ILE:CD1	2.35	1.04
1:A:533:LYS:NZ	16:G:5:G:OP2	1.90	1.04
16:G:148:U:O4	17:H:30:A:N6	1.92	1.03
1:A:532:THR:OG1	16:G:3:A:H5"	1.56	1.02
4:E:55:LEU:CD1	4:E:341:ILE:HD13	1.90	1.01
1:A:1517:LYS:HE2	1:A:1517:LYS:HA	1.44	1.00
17:H:54:U:H2'	17:H:55:U:H6	1.24	0.99
19:I:374:ILE:CB	31:Q:357:ALA:HB3	1.91	0.99
18:U:546:VAL:CG2	18:U:665:HIS:CE1	2.45	0.99
6:J:773:ARG:CB	6:J:787:LYS:HA	1.93	0.99
10:O:236:VAL:O	10:O:269:CYS:HA	1.62	0.99
17:H:92:U:H2'	17:H:93:A:C8	1.98	0.98
2:B:74:U:C5	2:B:76:A:N6	2.31	0.98
2:B:66:A:H5"	2:B:67:A:OP2	1.62	0.98
1:A:1522:GLN:HE22	18:U:622:ALA:HB1	1.27	0.97
16:G:151:C:H3'	16:G:152:C:C5	2.00	0.97
17:H:34:U:C2'	17:H:35:A:C8	2.47	0.96
17:H:54:U:O2'	17:H:55:U:H5'	1.66	0.96
16:G:151:C:C2'	16:G:152:C:C5	2.49	0.96
3:C:158:ARG:C	3:C:159:LYS:HD2	1.85	0.96
4:E:55:LEU:HD11	4:E:341:ILE:HD13	0.97	0.95
3:C:139:HIS:HB2	34:C:1500:GTP:H5"	1.48	0.95
6:J:212:GLN:HG2	15:W:508:ALA:HB1	1.49	0.95
17:H:156:U:H5"	17:H:156:U:C6	2.02	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:G:151:C:C4	16:G:152:C:N4	2.34	0.95
5:F:43:A:C2	16:G:4:A:N1	2.35	0.94
17:H:56:A:N6	17:H:92:U:C4	2.35	0.94
11:P:13:ARG:HH21	11:P:13:ARG:HG3	1.32	0.94
16:G:27:U:O2'	16:G:28:A:O5'	1.86	0.94
3:C:143:THR:CG2	34:C:1500:GTP:O1A	2.16	0.94
3:C:143:THR:HG22	34:C:1500:GTP:O1B	1.68	0.93
5:F:41:A:N6	16:G:6:A:N6	1.98	0.93
16:G:151:C:C5	16:G:152:C:N4	2.37	0.93
17:H:70:C:H2'	17:H:71:C:H6	1.33	0.93
16:G:151:C:H2'	16:G:152:C:C5	2.03	0.92
17:H:30:A:O2'	17:H:31:G:OP2	1.86	0.92
16:G:145:U:H3	17:H:33:G:H22	1.09	0.92
1:A:532:THR:CB	16:G:3:A:H3'	1.99	0.92
16:G:132:G:O2'	16:G:133:A:C8	2.22	0.91
17:H:27:U:O2'	17:H:28:C:H5'	1.70	0.91
17:H:34:U:O2'	17:H:35:A:O4'	1.89	0.91
3:C:139:HIS:HB2	34:C:1500:GTP:C5'	2.00	0.91
17:H:179:C:H2'	17:H:180:G:C8	2.05	0.90
3:C:142:LYS:HG3	3:C:228:PHE:HD2	1.31	0.90
17:H:33:G:OP1	18:U:666:ARG:NE	2.04	0.90
16:G:5:G:C2	16:G:6:A:N7	2.40	0.90
17:H:54:U:H2'	17:H:55:U:C6	2.06	0.90
3:C:143:THR:HG22	34:C:1500:GTP:O1A	1.71	0.90
1:A:855:ARG:HH22	1:A:1518:LEU:HD11	1.35	0.90
16:G:27:U:C2'	16:G:28:A:O5'	2.19	0.90
28:K:127:MET:O	28:K:131:GLY:N	2.03	0.90
16:G:151:C:H2'	16:G:152:C:H6	1.32	0.89
19:I:485:LYS:O	19:I:486:VAL:HG13	1.73	0.89
17:H:35:A:O2'	17:H:36:G:H8	1.52	0.89
1:A:861:ARG:HH11	17:H:29:A:H5'	1.38	0.89
1:A:855:ARG:NH2	1:A:1518:LEU:HD11	1.87	0.88
16:G:143:U:O4	17:H:34:U:C4	2.25	0.88
17:H:33:G:P	18:U:666:ARG:HE	1.96	0.88
19:I:448:ASN:CB	19:I:491:ALA:HB1	2.04	0.88
12:R:232:SEP:HB2	12:R:233:PRO:CD	2.02	0.88
16:G:151:C:C2'	16:G:152:C:C6	2.55	0.88
19:I:364:VAL:O	19:I:372:ARG:CB	2.22	0.88
3:C:158:ARG:O	3:C:159:LYS:HD2	1.73	0.88
17:H:109:C:O2'	17:H:110:A:H5'	1.74	0.88
19:I:325:VAL:O	19:I:328:GLU:CB	2.22	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11:U:H5'	2:B:11:U:C6	2.07	0.87
19:I:459:ALA:HB1	19:I:498:GLY:O	1.73	0.87
17:H:179:C:C2	17:H:180:G:N7	2.43	0.87
12:R:232:SEP:HB2	12:R:233:PRO:HD2	1.56	0.87
16:G:147:C:N3	17:H:31:G:N1	2.20	0.87
17:H:154:C:O2	17:H:176:G:N2	2.07	0.87
3:C:143:THR:CG2	34:C:1500:GTP:PA	2.63	0.87
19:I:520:ILE:O	19:I:524:TYR:CB	2.23	0.87
1:A:1517:LYS:HA	1:A:1517:LYS:CE	2.00	0.86
19:I:520:ILE:O	19:I:524:TYR:N	2.06	0.86
4:E:62:LEU:HB3	4:E:93:TRP:HZ3	1.41	0.86
16:G:151:C:C2	16:G:152:C:C4	2.63	0.85
16:G:5:G:C5	16:G:6:A:C8	2.64	0.85
1:A:533:LYS:HD2	16:G:4:A:H5"	1.57	0.85
16:G:5:G:C4	16:G:6:A:C8	2.64	0.85
16:G:151:C:C3'	16:G:152:C:C5	2.58	0.85
17:H:156:U:H6	17:H:156:U:C5'	1.88	0.85
16:G:140:A:O2'	16:G:141:C:OP2	1.94	0.85
16:G:151:C:C3'	16:G:152:C:H5	1.89	0.85
16:G:146:C:HO2'	16:G:147:C:P	2.00	0.85
3:C:144:CYS:SG	3:C:165:LEU:HD12	2.17	0.84
18:U:550:ARG:CB	18:U:660:LYS:HD3	2.07	0.84
2:B:80:U:H2'	2:B:80:U:OP1	1.77	0.84
19:I:365:ALA:N	19:I:372:ARG:CB	2.40	0.84
18:U:551:THR:HG22	18:U:664:GLU:OE1	1.78	0.83
19:I:448:ASN:CB	19:I:491:ALA:CB	2.55	0.83
16:G:129:G:C4'	16:G:130:A:OP1	2.25	0.83
3:C:144:CYS:CB	3:C:165:LEU:HD12	2.08	0.83
16:G:133:A:N6	17:H:43:U:O4	2.12	0.83
5:F:41:A:N1	16:G:6:A:N1	2.27	0.83
2:B:66:A:H2'	2:B:67:A:O4'	1.78	0.83
4:E:55:LEU:CD1	4:E:341:ILE:HD11	2.06	0.83
5:F:44:G:C2	16:G:3:A:N1	2.46	0.83
17:H:42:G:H2'	17:H:43:U:C6	2.14	0.82
17:H:153:A:C2'	17:H:154:C:C5'	2.51	0.82
17:H:56:A:N6	17:H:91:U:H3	1.77	0.82
19:I:255:LEU:O	19:I:258:LEU:N	2.12	0.82
1:A:855:ARG:HH22	1:A:1518:LEU:HD12	1.44	0.82
1:A:861:ARG:NH1	17:H:29:A:C5'	2.42	0.82
17:H:179:C:O2'	17:H:180:G:C5'	2.26	0.82
17:H:153:A:H2'	17:H:154:C:H5"	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:I:521:VAL:O	19:I:527:PHE:CB	2.27	0.82
1:A:861:ARG:HH11	17:H:29:A:C5'	1.93	0.82
3:C:137:HIS:HA	3:C:238:ASN:HB3	1.61	0.82
18:U:546:VAL:HG21	18:U:665:HIS:NE2	1.93	0.82
16:G:133:A:O2'	16:G:134:U:H6	1.59	0.81
1:A:1513:MET:CE	1:A:1517:LYS:HD2	2.11	0.81
3:C:139:HIS:HA	34:C:1500:GTP:PB	2.19	0.81
17:H:70:C:H2'	17:H:71:C:C6	2.15	0.81
16:G:151:C:N1	16:G:152:C:C5	2.49	0.80
1:A:855:ARG:NH2	1:A:1518:LEU:CD1	2.44	0.80
17:H:179:C:C2	17:H:180:G:C8	2.69	0.79
3:C:160:ARG:O	3:C:160:ARG:NH1	2.15	0.79
15:W:277:PRO:CB	15:W:578:TRP:C	2.51	0.79
17:H:27:U:C2'	17:H:28:C:H5'	2.12	0.79
16:G:147:C:O2	17:H:31:G:N2	2.15	0.79
18:U:560:VAL:HG11	18:U:660:LYS:HZ3	1.47	0.79
17:H:50:C:H5"	17:H:50:C:H6	1.48	0.78
1:A:532:THR:CB	16:G:3:A:C5'	2.61	0.78
16:G:5:G:N3	16:G:6:A:C8	2.50	0.78
16:G:132:G:OP2	16:G:133:A:OP1	2.00	0.78
16:G:147:C:N4	17:H:31:G:O6	2.15	0.78
16:G:151:C:H3'	16:G:152:C:H5	1.41	0.78
18:U:550:ARG:HB3	18:U:660:LYS:CD	2.12	0.78
2:B:11:U:H6	2:B:11:U:C5'	1.96	0.78
4:E:61:LEU:CD1	4:E:352:TYR:CE2	2.66	0.78
10:O:159:ARG:HD3	16:G:20:A:OP1	1.84	0.78
4:E:62:LEU:HB3	4:E:93:TRP:CZ3	2.19	0.77
17:H:179:C:O2	17:H:180:G:C8	2.37	0.77
16:G:6:A:N6	16:G:7:G:C6	2.53	0.77
17:H:34:U:H2'	17:H:35:A:N7	2.00	0.77
28:K:126:LEU:O	28:K:130:HIS:N	2.16	0.77
4:E:61:LEU:CD1	4:E:352:TYR:CZ	2.67	0.77
18:U:546:VAL:HG11	18:U:665:HIS:CE1	2.20	0.77
17:H:177:A:H5"	17:H:178:A:OP1	1.84	0.76
2:B:66:A:H3'	2:B:67:A:H5"	1.66	0.76
16:G:145:U:H3	17:H:33:G:H1	1.18	0.76
16:G:132:G:OP1	16:G:133:A:OP1	2.02	0.76
17:H:56:A:H61	17:H:91:U:H3	1.33	0.76
6:J:669:GLN:O	6:J:670:PRO:C	2.21	0.76
16:G:132:G:O2'	16:G:133:A:N7	2.19	0.75
12:R:235:ARG:HG2	12:R:235:ARG:HH11	1.48	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:H:56:A:N6	17:H:92:U:N3	2.35	0.75
1:A:532:THR:CB	16:G:3:A:H5'	2.16	0.75
2:B:8:G:N3	2:B:8:G:H2'	2.00	0.75
2:B:66:A:C5'	2:B:67:A:OP2	2.34	0.75
5:F:20:A:O2'	9:N:120:ARG:NH2	2.21	0.74
1:A:1513:MET:HE2	1:A:1517:LYS:HD2	1.67	0.74
3:C:143:THR:HG23	34:C:1500:GTP:O1A	1.86	0.74
28:K:131:GLY:O	28:K:135:TRP:N	2.21	0.74
16:G:150:U:O2'	16:G:151:C:H5"	1.87	0.74
5:F:41:A:H61	16:G:6:A:H61	0.75	0.74
19:I:720:ILE:O	19:I:721:LYS:CB	2.34	0.74
16:G:145:U:C2	17:H:33:G:N2	2.54	0.74
19:I:545:ILE:O	19:I:547:LEU:N	2.20	0.74
6:J:493:ALA:HB1	6:J:499:ARG:CB	2.18	0.74
17:H:179:C:H2'	17:H:180:G:H5'	1.66	0.74
1:A:1833:LEU:HD13	18:U:668:LEU:HD21	1.70	0.74
4:E:55:LEU:N	4:E:55:LEU:HD13	2.03	0.73
16:G:132:G:OP1	16:G:132:G:H4'	1.88	0.73
6:J:642:SER:CB	6:J:650:GLU:HA	2.17	0.73
1:A:179:ALA:O	1:A:183:LEU:HB2	1.89	0.73
16:G:151:C:N3	16:G:152:C:C4	2.57	0.73
28:K:126:LEU:O	28:K:130:HIS:CB	2.36	0.73
17:H:92:U:H2'	17:H:93:A:H8	1.52	0.73
5:F:41:A:H62	16:G:6:A:H61	1.35	0.73
19:I:545:ILE:C	19:I:547:LEU:H	1.91	0.73
4:E:55:LEU:HD13	4:E:55:LEU:H	1.54	0.72
3:C:137:HIS:O	3:C:207:GLY:O	2.05	0.72
5:F:44:G:C2	16:G:3:A:C2	2.76	0.72
3:C:690:GLU:O	3:C:788:LYS:HB3	1.88	0.72
15:W:491:GLN:O	15:W:493:ARG:N	2.21	0.72
10:O:26:THR:HG21	10:O:159:ARG:HH21	1.55	0.71
2:B:74:U:C5	2:B:76:A:C6	2.77	0.71
17:H:43:U:O2'	17:H:44:U:C6	2.43	0.71
2:B:87:A:N3	2:B:87:A:H3'	2.06	0.71
2:B:96:A:C6	2:B:97:G:C5	2.78	0.71
16:G:145:U:N3	17:H:33:G:N1	2.29	0.71
15:W:277:PRO:CB	15:W:578:TRP:O	2.39	0.71
28:K:120:ARG:O	28:K:124:LEU:N	2.21	0.71
16:G:145:U:O2	17:H:33:G:N2	2.23	0.71
3:C:143:THR:HG22	34:C:1500:GTP:PA	2.27	0.70
17:H:154:C:H2'	17:H:155:C:C6	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:K:135:TRP:O	28:K:136:LYS:CB	2.38	0.70
3:C:141:GLY:N	34:C:1500:GTP:O2B	2.24	0.70
16:G:27:U:H2'	16:G:28:A:O5'	1.91	0.70
10:O:159:ARG:CG	16:G:20:A:OP1	2.39	0.70
16:G:143:U:C6	16:G:143:U:H5"	2.27	0.70
16:G:147:C:C2	17:H:31:G:N2	2.56	0.70
19:I:585:ASP:O	19:I:588:PRO:N	2.25	0.70
4:E:61:LEU:HD13	4:E:352:TYR:CE2	2.24	0.70
1:A:1811:ASN:HD22	1:A:1816:GLN:HB3	1.55	0.70
4:E:162:ARG:HH21	4:E:203:ASP:HB3	1.56	0.70
6:J:496:ASP:CB	6:J:535:TYR:HA	2.21	0.70
1:A:1522:GLN:NE2	18:U:622:ALA:HB1	2.04	0.70
3:C:139:HIS:CA	34:C:1500:GTP:O3B	2.33	0.70
4:E:259:VAL:HB	4:E:277:PHE:HB2	1.74	0.70
16:G:145:U:N3	17:H:33:G:N2	2.23	0.70
1:A:1570:LYS:HE2	18:U:637:ASP:HB3	1.74	0.69
4:E:266:PRO:HG2	7:L:785:GLN:CB	2.22	0.69
16:G:146:C:O2'	16:G:147:C:P	2.48	0.69
11:P:13:ARG:HG3	11:P:13:ARG:NH2	2.00	0.69
18:U:548:LEU:HD22	18:U:661:ALA:HB1	1.74	0.69
18:U:678:CYS:SG	18:U:765:HIS:HE1	2.15	0.69
1:A:980:ARG:HG2	1:A:1094:ARG:HG2	1.75	0.69
15:W:466:ALA:CB	15:W:512:CYS:O	2.41	0.69
28:K:127:MET:O	28:K:131:GLY:CA	2.41	0.69
10:O:159:ARG:CD	16:G:20:A:OP1	2.41	0.68
1:A:942:PRO:HB2	1:A:1438:VAL:HG22	1.74	0.68
2:B:81:U:O2'	2:B:82:A:OP2	2.11	0.68
16:G:5:G:H4'	16:G:5:G:OP1	1.94	0.68
4:E:55:LEU:O	4:E:55:LEU:HD22	1.94	0.68
6:J:669:GLN:O	6:J:672:LEU:N	2.26	0.68
17:H:55:U:C4	17:H:93:A:N1	2.62	0.68
2:B:10:U:OP2	2:B:10:U:H6	1.78	0.67
5:F:40:U:H3	16:G:7:G:H22	1.42	0.67
10:O:262:THR:HB	10:O:271:PHE:HB2	1.76	0.67
16:G:6:A:C4	16:G:7:G:C8	2.83	0.67
16:G:147:C:N4	17:H:31:G:N1	2.42	0.67
19:I:484:LEU:O	19:I:486:VAL:HG22	1.93	0.67
16:G:147:C:N4	17:H:31:G:H1	1.92	0.67
17:H:166:G:H2'	17:H:166:G:N3	2.09	0.67
19:I:790:ARG:CB	19:I:797:PHE:O	2.42	0.67
15:W:474:LYS:HA	15:W:490:ALA:HB3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:U:673:GLU:OE2	18:U:682:SER:HB3	1.95	0.67
3:C:140:HIS:N	34:C:1500:GTP:O2B	2.27	0.67
17:H:34:U:HO2'	17:H:35:A:C1'	2.09	0.67
1:A:1662:ILE:HA	1:A:1701:VAL:O	1.94	0.66
17:H:156:U:C6	17:H:156:U:C5'	2.72	0.66
19:I:790:ARG:CB	19:I:801:ASP:CA	2.74	0.66
18:U:673:GLU:OE1	18:U:673:GLU:HA	1.93	0.66
3:C:144:CYS:SG	3:C:165:LEU:CD1	2.83	0.66
2:B:96:A:O2'	2:B:97:G:H5'	1.95	0.66
3:C:159:LYS:HD2	3:C:159:LYS:N	1.96	0.66
17:H:75:A:H61	17:H:77:C:H42	1.43	0.66
18:U:656:ASN:O	18:U:660:LYS:HE3	1.96	0.66
4:E:90:ILE:HB	4:E:105:LEU:HB2	1.78	0.66
2:B:96:A:C6	2:B:97:G:C6	2.84	0.66
17:H:153:A:C3'	17:H:154:C:H5'	2.24	0.66
17:H:150:U:H6	17:H:150:U:O5'	1.77	0.65
18:U:868:SER:HB2	18:U:872:GLN:H	1.61	0.65
16:G:147:C:N3	17:H:31:G:C2	2.63	0.65
17:H:34:U:O2'	17:H:35:A:C5'	2.44	0.65
18:U:656:ASN:O	18:U:660:LYS:HB3	1.95	0.65
17:H:151:C:H2'	17:H:152:G:C8	2.31	0.65
13:S:56:ILE:HG12	13:S:62:ILE:HG23	1.79	0.65
17:H:57:A:N6	17:H:91:U:N3	2.45	0.65
19:I:448:ASN:CB	19:I:491:ALA:HB2	2.26	0.65
1:A:761:ILE:HD12	1:A:775:ASN:HD22	1.61	0.65
17:H:43:U:O2'	17:H:44:U:C5	2.48	0.65
17:H:67:C:H42	17:H:85:A:H61	1.44	0.65
1:A:1214:TRP:HB2	1:A:1228:CYS:HB3	1.78	0.64
16:G:145:U:O4	17:H:33:G:O6	2.16	0.64
1:A:1629:ILE:HG22	1:A:1662:ILE:HG12	1.79	0.64
15:W:97:ASN:HD21	15:W:100:ARG:HH21	1.45	0.64
19:I:485:LYS:C	19:I:486:VAL:HG22	2.18	0.64
16:G:19:G:O2'	16:G:20:A:H5'	1.98	0.64
2:B:74:U:H5	2:B:76:A:H61	1.45	0.64
19:I:545:ILE:C	19:I:547:LEU:N	2.51	0.64
2:B:76:A:O2'	2:B:77:G:H5"	1.97	0.64
3:C:144:CYS:CA	3:C:165:LEU:HD12	2.27	0.64
16:G:125:C:O2'	16:G:126:C:H2'	1.98	0.64
3:C:678:THR:HG21	3:C:807:GLN:HB3	1.80	0.64
1:A:533:LYS:HD2	16:G:4:A:C5'	2.27	0.63
1:A:855:ARG:CZ	1:A:1518:LEU:HD11	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:165:ASN:HD22	12:R:95:LYS:HA	1.63	0.63
14:T:216:ASN:HD21	14:T:472:GLN:H	1.46	0.63
2:B:9:G:H4'	2:B:9:G:OP1	1.97	0.63
17:H:33:G:OP1	18:U:666:ARG:NH2	2.31	0.63
18:U:560:VAL:HG11	18:U:660:LYS:NZ	2.13	0.63
28:K:127:MET:O	28:K:131:GLY:HA3	1.97	0.63
15:W:264:ASN:O	15:W:267:SER:CB	2.46	0.63
17:H:33:G:P	18:U:666:ARG:NE	2.68	0.63
3:C:160:ARG:HH11	3:C:160:ARG:CG	2.11	0.63
1:A:1839:TRP:NE1	18:U:557:VAL:O	2.31	0.63
3:C:210:ASN:HB3	3:C:636:TYR:HB2	1.80	0.63
14:T:314:ILE:HD12	14:T:324:HIS:HB2	1.80	0.63
17:H:50:C:H5"	17:H:50:C:C6	2.33	0.63
17:H:67:C:H2'	17:H:68:G:H8	1.63	0.63
17:H:154:C:H2'	17:H:155:C:H6	1.62	0.63
1:A:1313:PRO:HG2	1:A:1335:ILE:HG22	1.81	0.63
10:O:15:TRP:HE1	11:P:26:LEU:HB2	1.64	0.63
4:E:219:VAL:HB	4:E:229:TYR:HB2	1.81	0.62
13:S:15:TYR:HB2	13:S:163:TYR:HB2	1.79	0.62
16:G:151:C:C4	16:G:152:C:C4	2.86	0.62
17:H:55:U:H2'	17:H:56:A:H8	1.63	0.62
18:U:539:GLU:OE2	18:U:662:ILE:CG1	2.47	0.62
4:E:158:TYR:OH	4:E:161:ARG:NH1	2.32	0.62
6:J:239:ARG:CG	6:J:239:ARG:HH11	2.12	0.62
12:R:235:ARG:HH11	12:R:235:ARG:CG	2.12	0.62
15:W:463:SER:O	15:W:480:SER:HA	1.98	0.62
1:A:1144:LYS:HE2	1:A:1148:ASN:HD21	1.64	0.62
4:E:274:VAL:HG12	4:E:275:LYS:HG3	1.81	0.62
10:O:233:THR:HA	10:O:272:ILE:O	1.99	0.62
16:G:151:C:C2'	16:G:152:C:H5	2.00	0.62
18:U:620:ARG:NH2	18:U:643:LYS:O	2.33	0.62
6:J:741:THR:O	6:J:745:CYS:CB	2.47	0.62
6:J:228:ARG:NH2	6:J:257:GLU:OE1	2.32	0.62
7:L:764:PRO:O	7:L:765:ARG:CB	2.48	0.62
16:G:143:U:C4	17:H:34:U:N3	2.49	0.62
19:I:559:THR:CB	19:I:570:GLY:HA3	2.30	0.62
1:A:610:HIS:NE2	33:A:3000:IHP:O33	2.31	0.62
3:C:523:GLN:NE2	3:C:525:CYS:SG	2.73	0.62
1:A:1809:ILE:HB	1:A:1818:PHE:HB2	1.80	0.62
1:A:1838:LYS:HG2	1:A:1871:PRO:HG2	1.82	0.62
16:G:145:U:O4	17:H:33:G:C6	2.53	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:U:663:ALA:HA	18:U:666:ARG:NH1	2.14	0.62
10:O:240:GLY:HA3	10:O:296:ARG:HH12	1.63	0.62
10:O:34:ILE:HB	12:R:197:ILE:HG12	1.81	0.61
18:U:576:ARG:HH22	18:U:647:ARG:HD3	1.65	0.61
18:U:658:ARG:O	18:U:662:ILE:HB	1.99	0.61
16:G:144:A:H4'	16:G:145:U:H3'	1.82	0.61
17:H:112:G:H2'	17:H:113:G:H8	1.65	0.61
6:J:658:ARG:CA	6:J:667:ILE:CB	2.71	0.61
16:G:4:A:H8	16:G:4:A:OP1	1.84	0.61
16:G:6:A:C5	16:G:7:G:N7	2.69	0.61
19:I:399:VAL:HG13	19:I:399:VAL:O	2.00	0.61
19:I:795:ILE:HG22	19:I:795:ILE:O	1.99	0.61
17:H:54:U:C4	17:H:93:A:N1	2.69	0.61
3:C:157:ILE:HG23	3:C:158:ARG:HG2	1.83	0.61
17:H:148:C:C2'	17:H:149:A:H5'	2.30	0.61
19:I:365:ALA:HA	19:I:372:ARG:CB	2.31	0.61
1:A:113:ILE:HG21	9:N:6:ARG:HE	1.66	0.61
1:A:199:GLU:O	1:A:240:ARG:NH2	2.33	0.61
1:A:532:THR:HB	16:G:3:A:C4'	2.30	0.61
10:O:92:LEU:HD11	10:O:151:ALA:HA	1.82	0.61
10:O:182:ARG:NH1	10:O:184:GLU:OE2	2.34	0.61
15:W:280:GLN:HA	15:W:577:LEU:O	2.00	0.61
15:W:290:GLY:CA	15:W:571:TRP:O	2.49	0.61
6:J:241:VAL:HG12	6:J:241:VAL:O	2.00	0.61
13:S:83:GLU:HA	13:S:106:ASP:HB2	1.82	0.61
16:G:6:A:C6	16:G:7:G:C4	2.89	0.61
16:G:147:C:N4	17:H:31:G:C6	2.56	0.61
19:I:365:ALA:CA	19:I:372:ARG:CB	2.79	0.61
1:A:382:GLU:HA	3:C:354:ARG:HH12	1.65	0.60
6:J:293:ASN:ND2	7:L:226:ASP:O	2.34	0.60
8:M:166:SER:O	13:S:141:ARG:NH2	2.34	0.60
15:W:491:GLN:CB	16:G:136:U:OP2	2.49	0.60
16:G:143:U:O4	17:H:34:U:O4	2.19	0.60
17:H:179:C:N3	17:H:180:G:N7	2.49	0.60
3:C:160:ARG:HH11	3:C:160:ARG:CB	2.14	0.60
3:C:160:ARG:HB3	3:C:164:ASP:HB2	1.83	0.60
3:C:618:THR:HB	3:C:630:LEU:HB2	1.82	0.60
1:A:1513:MET:HE3	1:A:1517:LYS:HD2	1.82	0.60
5:F:49:G:OP1	7:L:33:ARG:NH2	2.34	0.60
10:O:72:GLN:OE1	10:O:82:GLN:NE2	2.34	0.60
14:T:393:ASP:OD1	14:T:393:ASP:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:W:531:LYS:CB	15:W:546:PHE:O	2.50	0.60
17:H:157:G:H8	17:H:157:G:H5"	1.65	0.60
3:C:165:LEU:O	3:C:165:LEU:HD23	2.01	0.60
4:E:340:PRO:HB2	4:E:356:ILE:HB	1.84	0.60
17:H:34:U:O2'	17:H:35:A:C1'	2.48	0.60
19:I:374:ILE:CB	31:Q:357:ALA:CB	2.75	0.60
1:A:1371:TYR:OH	1:A:1473:ASP:OD2	2.17	0.60
18:U:551:THR:HG22	18:U:664:GLU:CD	2.21	0.60
2:B:11:U:H2'	2:B:12:U:O4'	2.02	0.60
16:G:26:U:H2'	16:G:27:U:H5"	1.82	0.60
6:J:669:GLN:O	6:J:671:ARG:N	2.34	0.60
1:A:82:ARG:NH2	16:G:14:A:OP2	2.35	0.59
1:A:695:ASP:OD2	14:T:376:ARG:NH2	2.35	0.59
7:L:123:LEU:HD13	7:L:124:LYS:H	1.67	0.59
15:W:290:GLY:HA3	15:W:571:TRP:HA	1.84	0.59
2:B:10:U:OP2	2:B:10:U:H2'	2.03	0.59
3:C:147:ASP:OD1	3:C:158:ARG:NH1	2.35	0.59
10:O:253:TYR:OH	13:S:123:ASP:OD2	2.19	0.59
10:O:234:LEU:HB2	10:O:272:ILE:HB	1.85	0.59
16:G:4:A:C6	16:G:5:G:N2	2.71	0.59
17:H:34:U:O2'	17:H:35:A:N9	2.35	0.59
11:P:20:GLU:OE2	14:T:313:ARG:NH2	2.36	0.59
16:G:1:G:H1'	16:G:2:U:OP1	2.03	0.59
17:H:55:U:O4	17:H:93:A:N6	2.36	0.59
1:A:1631:LEU:HB2	1:A:1660:TYR:HB3	1.83	0.59
3:C:139:HIS:HB2	34:C:1500:GTP:H5'	1.82	0.59
3:C:678:THR:OG1	3:C:680:ASN:O	2.21	0.59
12:R:101:ILE:O	12:R:104:GLN:NE2	2.36	0.59
12:R:196:VAL:HG11	15:W:120:ILE:HD12	1.85	0.59
1:A:163:ARG:NE	1:A:576:ASP:OD2	2.34	0.59
3:C:308:CYS:SG	3:C:309:PHE:N	2.76	0.59
2:B:96:A:N6	2:B:97:G:C6	2.71	0.58
4:E:143:ARG:HD3	4:E:146:ARG:HB2	1.85	0.58
18:U:678:CYS:SG	18:U:718:HIS:HD2	2.26	0.58
2:B:9:G:O6	2:B:69:A:C2	2.56	0.58
8:M:236:ASN:ND2	8:M:242:ALA:O	2.35	0.58
1:A:1813:ARG:HD3	1:A:1814:THR:HG23	1.83	0.58
4:E:178:LEU:HD12	4:E:188:GLN:HB2	1.84	0.58
17:H:107:A:O2'	17:H:108:G:H5'	2.03	0.58
16:G:145:U:C4	17:H:33:G:N1	2.58	0.58
1:A:48:LYS:NZ	5:F:21:U:OP2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:H:50:C:H6	17:H:50:C:C5'	2.17	0.58
1:A:255:PHE:HB3	1:A:259:ASP:HB3	1.86	0.58
11:P:13:ARG:NH1	14:T:330:THR:O	2.37	0.58
1:A:1194:CYS:HB3	1:A:1230:LEU:HD23	1.85	0.58
14:T:342:GLU:OE1	14:T:365:ARG:NH1	2.37	0.58
14:T:350:HIS:HA	14:T:374:SER:HB2	1.86	0.58
17:H:33:G:OP1	18:U:666:ARG:CZ	2.50	0.58
18:U:671:GLN:OE1	18:U:671:GLN:HA	2.02	0.58
1:A:163:ARG:HD2	1:A:166:PHE:HZ	1.69	0.58
4:E:67:GLY:N	4:E:87:ASP:OD1	2.37	0.58
4:E:268:ALA:HB2	4:E:272:ARG:HH21	1.67	0.58
16:G:143:U:C6	16:G:143:U:C5'	2.87	0.58
17:H:54:U:HO2'	17:H:55:U:H5'	1.65	0.58
18:U:657:GLN:HA	18:U:660:LYS:HZ1	1.69	0.58
1:A:1321:GLU:HG3	1:A:1322:LEU:HD22	1.85	0.57
1:A:1833:LEU:CD1	18:U:668:LEU:HD21	2.33	0.57
2:B:69:A:H2'	2:B:69:A:N3	2.18	0.57
2:B:74:U:O4	2:B:76:A:N1	2.37	0.57
3:C:663:CYS:HB2	3:C:828:MET:HB2	1.85	0.57
3:C:742:PRO:HG3	3:C:785:ARG:HD2	1.85	0.57
2:B:96:A:C5	2:B:97:G:N7	2.73	0.57
19:I:327:LEU:O	19:I:330:ARG:N	2.37	0.57
12:R:64:PHE:O	12:R:71:GLN:NE2	2.38	0.57
13:S:57:ILE:HD13	15:W:97:ASN:HB3	1.87	0.57
1:A:523:ASN:OD1	1:A:552:ARG:NH2	2.38	0.57
3:C:166:CYS:HA	3:C:169:ASP:HB3	1.86	0.57
5:F:41:A:C6	16:G:7:G:N2	2.73	0.57
5:F:59:G:O2'	5:F:61:C:OP1	2.22	0.57
16:G:26:U:H2'	16:G:27:U:C5'	2.34	0.57
17:H:154:C:O2'	17:H:155:C:H5'	2.04	0.57
1:A:466:ALA:HA	2:B:20:G:H21	1.69	0.57
1:A:1606:ILE:O	1:A:1634:SER:OG	2.23	0.57
3:C:224:GLY:HA3	3:C:438:ILE:HD12	1.84	0.57
16:G:5:G:N3	16:G:6:A:N7	2.48	0.57
16:G:141:C:OP2	16:G:141:C:H6	1.88	0.57
1:A:1555:LEU:HD21	1:A:1570:LYS:HG3	1.87	0.57
3:C:174:GLU:HG3	3:C:181:ILE:H	1.69	0.57
5:F:41:A:N6	16:G:7:G:C2	2.73	0.57
10:O:159:ARG:NH1	16:G:20:A:OP1	2.30	0.57
17:H:57:A:N6	17:H:90:A:C2	2.72	0.57
1:A:975:VAL:HB	1:A:1099:PHE:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:A:C2'	2:B:97:G:H5'	2.34	0.57
17:H:109:C:O2'	17:H:110:A:C5'	2.51	0.57
1:A:1624:SER:HB2	1:A:1693:SER:HB2	1.87	0.56
2:B:9:G:O6	2:B:69:A:H2	1.88	0.56
2:B:66:A:C2'	2:B:67:A:O4'	2.50	0.56
7:L:37:LEU:HD11	7:L:155:ALA:HA	1.87	0.56
12:R:148:ARG:NH2	14:T:299:THR:O	2.36	0.56
14:T:294:LEU:HD12	14:T:303:LEU:HD11	1.86	0.56
19:I:364:VAL:CB	19:I:372:ARG:CB	2.83	0.56
1:A:1186:LEU:HD23	1:A:1195:ARG:HB3	1.87	0.56
15:W:103:GLN:NE2	15:W:111:LEU:O	2.38	0.56
16:G:22:C:O2'	16:G:23:U:P	2.63	0.56
1:A:608:LEU:HD13	1:A:632:ALA:HB1	1.87	0.56
2:B:9:G:C5	2:B:70:A:C8	2.94	0.56
16:G:5:G:C2	16:G:6:A:C8	2.93	0.56
17:H:77:C:C2	17:H:78:C:C5	2.93	0.56
17:H:147:G:C2	17:H:148:C:C5	2.92	0.56
17:H:148:C:H2'	17:H:149:A:H8	1.70	0.56
4:E:346:SER:OG	4:E:348:ASP:OD1	2.23	0.56
13:S:52:LYS:HA	13:S:158:LYS:HA	1.88	0.56
16:G:136:U:O2'	16:G:137:C:C6	2.58	0.56
17:H:71:C:H2'	17:H:72:U:H6	1.70	0.56
17:H:73:C:H2'	17:H:74:U:H6	1.70	0.56
17:H:77:C:H2'	17:H:78:C:H6	1.70	0.56
1:A:143:GLN:NE2	1:A:207:PHE:O	2.32	0.56
1:A:855:ARG:NH1	1:A:1518:LEU:HD11	2.21	0.56
12:R:106:GLN:HG2	12:R:110:LYS:HG2	1.87	0.56
14:T:349:SER:OG	14:T:351:ASP:OD1	2.23	0.56
16:G:154:U:H2'	16:G:154:U:O2	2.05	0.56
17:H:72:U:C2	17:H:73:C:C5	2.94	0.56
17:H:90:A:H2'	17:H:91:U:H6	1.71	0.56
17:H:91:U:H2'	17:H:92:U:H6	1.71	0.56
1:A:405:LEU:HD22	3:C:413:ARG:HE	1.68	0.56
1:A:891:PHE:O	7:L:83:ARG:NH1	2.38	0.56
2:B:96:A:C4	2:B:97:G:C8	2.93	0.56
16:G:149:G:H8	16:G:149:G:OP2	1.89	0.56
17:H:71:C:C2	17:H:72:U:C5	2.94	0.56
17:H:88:A:H2'	17:H:89:U:H6	1.70	0.56
4:E:178:LEU:HD11	4:E:222:LEU:HD22	1.86	0.56
10:O:185:LYS:HZ3	15:W:216:LEU:HG	1.71	0.56
16:G:138:A:O2'	16:G:139:U:C6	2.59	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:H:73:C:C2	17:H:74:U:C5	2.94	0.56
14:T:190:TRP:HE1	14:T:498:GLU:HB3	1.71	0.56
17:H:38:A:O2'	17:H:39:U:C6	2.59	0.56
1:A:1342:TRP:HB2	1:A:1486:GLU:HG3	1.88	0.56
3:C:375:GLU:OE2	3:C:379:LYS:NZ	2.33	0.56
4:E:62:LEU:HB2	4:E:351:LEU:HB2	1.88	0.56
14:T:312:ALA:HB3	14:T:326:LEU:HB2	1.88	0.56
17:H:39:U:O2'	17:H:40:C:C6	2.59	0.56
17:H:151:C:H2'	17:H:152:G:H8	1.68	0.56
3:C:173:THR:OG1	3:C:642:HIS:NE2	2.36	0.56
3:C:205:THR:HB	3:C:215:VAL:HG22	1.87	0.56
4:E:257:ASN:HD22	15:W:149:SER:HA	1.71	0.56
13:S:25:LEU:HD22	13:S:98:LEU:HD22	1.88	0.56
17:H:59:A:H2'	17:H:60:U:H6	1.70	0.56
17:H:72:U:H2'	17:H:73:C:H6	1.71	0.56
3:C:135:CYS:HB2	3:C:242:LEU:HD13	1.87	0.55
17:H:33:G:O5'	18:U:666:ARG:NE	2.39	0.55
18:U:678:CYS:SG	18:U:718:HIS:CD2	2.98	0.55
1:A:1865:ARG:NH1	18:U:726:ASP:OD2	2.39	0.55
2:B:9:G:H5"	2:B:10:U:C5	2.41	0.55
12:R:78:ARG:HG3	12:R:79:LYS:HG2	1.86	0.55
17:H:161:U:O2'	17:H:163:G:N2	2.39	0.55
1:A:1392:LYS:HD3	1:A:1407:ASP:HB3	1.87	0.55
13:S:26:GLU:OE1	13:S:131:ARG:NH1	2.40	0.55
18:U:666:ARG:CZ	18:U:666:ARG:HB3	2.36	0.55
3:C:139:HIS:CA	34:C:1500:GTP:PB	2.93	0.55
6:J:618:GLN:O	6:J:634:GLU:CB	2.55	0.55
8:M:178:GLU:OE1	8:M:181:ARG:NH1	2.37	0.55
14:T:261:LEU:HB3	14:T:273:TRP:HB2	1.86	0.55
17:H:55:U:O2	17:H:56:A:C8	2.59	0.55
17:H:57:A:H2'	17:H:58:U:H6	1.71	0.55
17:H:83:A:H2'	17:H:84:C:H6	1.71	0.55
3:C:803:ARG:O	3:C:807:GLN:HB2	2.07	0.55
4:E:266:PRO:HG2	7:L:785:GLN:CA	2.37	0.55
10:O:236:VAL:HG22	10:O:300:VAL:HG22	1.87	0.55
12:R:232:SEP:CB	12:R:233:PRO:CD	2.77	0.55
16:G:6:A:C6	16:G:7:G:C6	2.94	0.55
16:G:148:U:C4	17:H:30:A:N1	2.70	0.55
14:T:418:THR:HG21	14:T:467:ALA:HA	1.88	0.55
18:U:546:VAL:CB	18:U:665:HIS:CE1	2.88	0.55
1:A:425:PRO:HB2	1:A:428:LYS:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:846:VAL:HG22	3:C:887:LEU:HD11	1.88	0.55
17:H:108:G:H2'	17:H:109:C:C6	2.41	0.55
2:B:71:C:H3'	2:B:71:C:H6	1.72	0.55
3:C:523:GLN:HE21	3:C:558:PRO:HG3	1.72	0.55
5:F:82:A:N6	17:H:19:G:OP1	2.34	0.55
6:J:770:ASP:CB	6:J:791:ASP:CB	2.85	0.55
17:H:88:A:C4	17:H:89:U:C5	2.95	0.55
3:C:692:LEU:O	3:C:786:ASN:ND2	2.39	0.55
4:E:90:ILE:HD11	4:E:112:VAL:HG11	1.87	0.55
6:J:260:ARG:HD3	7:L:214:ILE:HG12	1.88	0.55
3:C:637:LEU:HA	3:C:640:VAL:HG12	1.88	0.55
16:G:22:C:O2'	16:G:23:U:OP1	2.25	0.55
17:H:34:U:O2'	17:H:35:A:C8	2.60	0.55
18:U:546:VAL:CB	18:U:665:HIS:HE1	2.20	0.55
1:A:1132:LYS:HA	1:A:1139:ARG:HH12	1.72	0.54
1:A:1431:ALA:O	1:A:1434:LYS:NZ	2.40	0.54
4:E:118:ASN:ND2	4:E:122:SER:OG	2.37	0.54
15:W:531:LYS:HA	15:W:546:PHE:O	2.07	0.54
17:H:57:A:C4	17:H:58:U:C5	2.95	0.54
18:U:666:ARG:CZ	18:U:666:ARG:CB	2.85	0.54
1:A:1335:ILE:HG23	1:A:1365:ILE:HD11	1.88	0.54
1:A:1609:VAL:HG12	1:A:1631:LEU:HG	1.89	0.54
14:T:270:VAL:HB	14:T:284:TYR:HB2	1.89	0.54
17:H:91:U:C2	17:H:92:U:C5	2.94	0.54
17:H:148:C:H2'	17:H:149:A:C8	2.43	0.54
18:U:546:VAL:CG1	18:U:665:HIS:CE1	2.90	0.54
2:B:85:C:H3'	2:B:85:C:OP1	2.07	0.54
2:B:100:C:H2'	2:B:101:U:C6	2.42	0.54
3:C:219:LEU:HD13	3:C:245:HIS:HD2	1.72	0.54
17:H:50:C:H2'	17:H:51:A:C8	2.42	0.54
1:A:470:ARG:NH1	2:B:56:C:OP2	2.41	0.54
16:G:151:C:C2'	16:G:152:C:H6	2.09	0.54
17:H:83:A:C4	17:H:84:C:C5	2.95	0.54
1:A:657:ALA:O	1:A:661:GLU:HB2	2.08	0.54
5:F:43:A:O5'	5:F:43:A:H8	1.89	0.54
12:R:68:HIS:NE2	13:S:89:ASP:O	2.36	0.54
17:H:32:U:N3	17:H:33:G:C6	2.76	0.54
2:B:66:A:H3'	2:B:67:A:C5'	2.36	0.54
3:C:529:ARG:H	3:C:553:GLU:HB3	1.71	0.54
10:O:27:CYS:SG	10:O:66:LYS:NZ	2.71	0.54
16:G:135:G:O2'	16:G:136:U:C6	2.59	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:H:90:A:C4	17:H:91:U:C5	2.95	0.54
13:S:11:PRO:O	13:S:29:TRP:NE1	2.40	0.54
14:T:392:PRO:HG3	14:T:415:ILE:HA	1.90	0.54
17:H:59:A:C4	17:H:60:U:C5	2.95	0.54
17:H:153:A:C3'	17:H:154:C:C5'	2.85	0.54
1:A:1072:LEU:HD22	1:A:1087:LEU:HD22	1.90	0.54
2:B:10:U:O2'	2:B:11:U:OP2	2.17	0.54
5:F:29:A:N6	16:G:17:U:OP2	2.39	0.54
6:J:311:GLN:HG3	8:M:131:GLN:HG2	1.90	0.54
16:G:151:C:O2	16:G:152:C:C6	2.61	0.54
18:U:539:GLU:OE2	18:U:662:ILE:HG13	2.07	0.54
1:A:1614:ILE:HD13	1:A:1626:CYS:HB2	1.89	0.54
16:G:147:C:H6	16:G:147:C:OP1	1.90	0.54
19:I:797:PHE:O	19:I:801:ASP:CB	2.56	0.54
3:C:693:GLU:H	3:C:696:LEU:HD12	1.73	0.54
6:J:466:ARG:CB	19:I:606:TRP:CB	2.86	0.54
6:J:600:ILE:C	6:J:602:LYS:H	2.10	0.54
17:H:54:U:C2'	17:H:55:U:H5'	2.38	0.54
28:K:131:GLY:O	28:K:135:TRP:CB	2.56	0.54
1:A:658:ARG:NH2	5:F:65:G:OP2	2.41	0.53
2:B:79:C:H2'	2:B:79:C:O2	2.07	0.53
17:H:30:A:C2'	17:H:31:G:OP2	2.56	0.53
16:G:151:C:C3'	16:G:152:C:C6	2.89	0.53
17:H:36:G:O2'	17:H:37:U:C6	2.59	0.53
1:A:761:ILE:HG12	1:A:767:VAL:HG21	1.90	0.53
1:A:1104:ASP:OD1	1:A:1107:ARG:NH2	2.42	0.53
3:C:139:HIS:CD2	3:C:139:HIS:H	2.26	0.53
6:J:239:ARG:HG3	6:J:239:ARG:NH1	2.22	0.53
10:O:78:LYS:HD3	10:O:94:ILE:HG21	1.91	0.53
15:W:474:LYS:CA	15:W:490:ALA:HB3	2.37	0.53
16:G:6:A:C6	16:G:7:G:C5	2.97	0.53
1:A:766:THR:OG1	2:B:39:C:N4	2.41	0.53
9:N:139:CYS:SG	9:N:140:ARG:N	2.81	0.53
15:W:481:MET:O	15:W:483:ASN:N	2.41	0.53
16:G:22:C:H2'	16:G:22:C:O2	2.08	0.53
17:H:182:U:H2'	17:H:183:G:C8	2.44	0.53
18:U:814:VAL:HG11	18:U:820:TYR:HB3	1.90	0.53
1:A:253:ASN:ND2	1:A:336:ASN:OD1	2.42	0.53
1:A:1090:ARG:NH1	1:A:1092:ILE:O	2.41	0.53
1:A:1544:ARG:HB2	1:A:1547:VAL:HG12	1.91	0.53
14:T:371:HIS:ND1	14:T:391:SER:OG	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:W:227:GLY:O	15:W:228:LYS:O	2.25	0.53
18:U:539:GLU:OE2	18:U:662:ILE:HG12	2.07	0.53
13:S:84:ASP:OD1	13:S:108:ASN:ND2	2.41	0.53
17:H:107:A:H8	17:H:107:A:H5"	1.72	0.53
3:C:148:CYS:SG	3:C:417:ARG:NH2	2.82	0.53
14:T:390:GLY:HA3	14:T:416:ILE:HD11	1.89	0.53
18:U:809:ASP:O	18:U:811:ARG:N	2.42	0.53
2:B:9:G:H5"	2:B:10:U:H5	1.73	0.53
3:C:92:PRO:HA	14:T:278:ASN:HD21	1.74	0.53
3:C:139:HIS:CB	34:C:1500:GTP:O3A	2.57	0.53
3:C:534:VAL:HB	3:C:537:TYR:HB2	1.90	0.53
13:S:41:GLU:OE2	13:S:44:ARG:NH2	2.38	0.53
19:I:249:THR:O	19:I:250:ARG:CB	2.57	0.53
2:B:68:C:O2	2:B:68:C:H2'	2.09	0.52
3:C:134:LEU:HD13	3:C:202:ILE:HG23	1.89	0.52
4:E:75:HIS:ND1	4:E:77:ASN:OD1	2.42	0.52
5:F:29:A:H62	16:G:16:G:H1'	1.74	0.52
10:O:32:PRO:HG2	15:W:153:ILE:HD12	1.91	0.52
12:R:70:ALA:HA	13:S:93:THR:HG21	1.91	0.52
16:G:151:C:C6	16:G:152:C:N4	2.74	0.52
19:I:264:ASP:O	19:I:268:ARG:CB	2.58	0.52
1:A:261:LYS:NZ	3:C:176:GLU:OE2	2.42	0.52
2:B:96:A:N6	2:B:97:G:O6	2.42	0.52
4:E:84:ALA:HB2	4:E:90:ILE:HD13	1.91	0.52
10:O:110:SER:OG	10:O:113:ASN:ND2	2.42	0.52
15:W:536:ASP:O	15:W:540:THR:N	2.41	0.52
1:A:963:GLN:HG3	1:A:1077:ILE:HG23	1.91	0.52
10:O:31:ASN:O	12:R:195:ARG:NH1	2.40	0.52
16:G:7:G:H2'	16:G:8:C:C6	2.44	0.52
16:G:22:C:HO2'	16:G:23:U:P	2.31	0.52
16:G:151:C:C2	16:G:152:C:C6	2.96	0.52
17:H:147:G:C2	17:H:148:C:C6	2.97	0.52
1:A:1820:LYS:NZ	1:A:1844:GLU:OE1	2.42	0.52
2:B:9:G:C6	2:B:70:A:N7	2.77	0.52
17:H:40:C:O2'	17:H:41:U:C6	2.59	0.52
17:H:182:U:H2'	17:H:183:G:H8	1.74	0.52
3:C:143:THR:HG23	34:C:1500:GTP:PA	2.48	0.52
7:L:263:ASP:OD2	8:M:199:ARG:NH1	2.37	0.52
17:H:67:C:H2'	17:H:68:G:C8	2.42	0.52
16:G:2:U:H2'	16:G:3:A:C4	2.45	0.52
16:G:143:U:N3	17:H:34:U:N3	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:THR:CB	16:G:3:A:C3'	2.69	0.52
1:A:1320:LYS:HG2	18:U:798:MET:HG2	1.90	0.52
3:C:369:PHE:O	3:C:373:ILE:HB	2.10	0.52
4:E:171:SER:OG	4:E:173:ASP:OD1	2.25	0.52
6:J:774:VAL:CA	6:J:787:LYS:CB	2.86	0.52
7:L:526:ARG:CB	7:L:594:PRO:CB	2.88	0.52
16:G:147:C:N4	16:G:148:U:O4	2.42	0.52
1:A:378:PHE:HB3	3:C:342:ARG:HH11	1.75	0.52
16:G:143:U:N3	17:H:34:U:C2	2.70	0.52
1:A:1555:LEU:HD13	1:A:1556:ASP:H	1.74	0.52
2:B:70:A:N3	2:B:70:A:C5'	2.73	0.52
16:G:140:A:O2'	16:G:141:C:C6	2.61	0.52
17:H:54:U:N3	17:H:93:A:C2	2.77	0.52
17:H:183:G:H2'	17:H:184:C:C6	2.45	0.52
2:B:99:C:H2'	2:B:100:C:C6	2.45	0.52
10:O:276:THR:HG23	10:O:279:ALA:H	1.75	0.52
15:W:531:LYS:CA	15:W:546:PHE:O	2.57	0.52
16:G:146:C:O2'	16:G:147:C:OP2	2.27	0.52
3:C:203:MET:HG2	3:C:218:GLY:HA3	1.91	0.51
15:W:518:PRO:O	15:W:519:ASP:CB	2.57	0.51
1:A:1249:MET:O	1:A:1253:SER:OG	2.22	0.51
3:C:160:ARG:NH1	3:C:160:ARG:CG	2.73	0.51
3:C:507:VAL:HG13	3:C:565:ILE:HG23	1.92	0.51
7:L:21:ALA:HB1	7:L:159:LEU:HD21	1.92	0.51
10:O:169:VAL:HA	15:W:216:LEU:HD13	1.92	0.51
19:I:795:ILE:CD1	19:I:795:ILE:N	2.73	0.51
1:A:82:ARG:HH22	16:G:14:A:H5"	1.74	0.51
3:C:434:CYS:O	3:C:438:ILE:N	2.43	0.51
6:J:201:ARG:HB3	6:J:203:LEU:HD23	1.91	0.51
16:G:151:C:O2	16:G:152:C:C5	2.63	0.51
17:H:50:C:C6	17:H:50:C:C5'	2.94	0.51
17:H:70:C:C2	17:H:71:C:C5	2.98	0.51
28:K:128:SER:O	28:K:132:CYS:N	2.37	0.51
3:C:476:CYS:HB2	3:C:565:ILE:HB	1.92	0.51
15:W:425:VAL:O	15:W:433:PHE:CB	2.59	0.51
1:A:1190:CYS:O	1:A:1192:PHE:N	2.41	0.51
1:A:1605:GLU:HB3	1:A:1637:TRP:HE1	1.75	0.51
3:C:137:HIS:ND1	3:C:138:LEU:HB2	2.25	0.51
5:F:36:A:N6	5:F:38:G:O6	2.44	0.51
12:R:235:ARG:CG	12:R:235:ARG:NH1	2.73	0.51
16:G:148:U:C2	17:H:30:A:N1	2.70	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LEU:HD11	1:A:554:THR:HG22	1.92	0.51
2:B:87:A:N3	2:B:87:A:C3'	2.73	0.51
17:H:67:C:C2'	17:H:68:G:H5'	2.41	0.51
2:B:78:U:H4'	2:B:79:C:OP2	2.10	0.51
4:E:60:MET:HB2	4:E:353:MET:HB2	1.91	0.51
16:G:147:C:P	16:G:147:C:O4'	2.69	0.51
16:G:151:C:H2'	16:G:151:C:O2	2.10	0.51
3:C:115:GLU:HB2	3:C:118:PHE:HB3	1.93	0.51
3:C:849:VAL:HG22	3:C:852:ARG:HH21	1.75	0.51
1:A:976:MET:HG2	1:A:1187:PHE:HB3	1.93	0.51
3:C:666:VAL:HG13	3:C:824:THR:HG23	1.92	0.51
12:R:241:GLU:HA	12:R:244:GLU:HG2	1.93	0.51
16:G:133:A:C2'	16:G:134:U:C6	2.92	0.51
16:G:151:C:C1'	16:G:152:C:C5	2.93	0.51
19:I:729:SER:O	19:I:732:ALA:HB3	2.09	0.51
17:H:68:G:H2'	17:H:69:U:C6	2.46	0.51
1:A:711:GLN:HE22	17:H:18:U:H3'	1.77	0.50
1:A:1217:GLN:HA	1:A:1224:ARG:HA	1.92	0.50
6:J:188:GLN:NE2	7:L:140:ASP:OD1	2.44	0.50
18:U:819:PRO:HB2	18:U:835:ILE:HB	1.93	0.50
1:A:381:PRO:O	3:C:354:ARG:NH2	2.45	0.50
1:A:1628:ASP:OD2	1:A:1664:ILE:N	2.44	0.50
14:T:468:CYS:HA	14:T:478:LEU:O	2.12	0.50
17:H:180:G:H2'	17:H:181:G:C8	2.45	0.50
16:G:5:G:C6	16:G:6:A:C4	2.99	0.50
17:H:34:U:O2'	17:H:35:A:C4'	2.59	0.50
19:I:265:TYR:O	19:I:266:TYR:C	2.50	0.50
1:A:388:LEU:HD11	3:C:399:LEU:HD11	1.94	0.50
1:A:857:ASN:OD1	1:A:860:GLN:NE2	2.44	0.50
1:A:1309:SER:OG	1:A:1310:ARG:N	2.40	0.50
3:C:160:ARG:NH1	3:C:160:ARG:HG3	2.26	0.50
3:C:749:THR:HG23	3:C:753:GLU:HB3	1.93	0.50
7:L:696:LEU:HA	28:K:110:SER:CB	2.40	0.50
14:T:200:ILE:HB	14:T:486:ILE:HB	1.93	0.50
15:W:474:LYS:C	15:W:490:ALA:CB	2.80	0.50
19:I:795:ILE:N	19:I:795:ILE:HD12	2.26	0.50
12:R:235:ARG:HB2	12:R:235:ARG:CZ	2.40	0.50
17:H:111:G:O3'	17:H:112:G:O4'	2.28	0.50
1:A:136:ILE:HG22	1:A:138:PRO:HD2	1.93	0.50
1:A:1467:LEU:HD11	18:U:796:TRP:HH2	1.77	0.50
6:J:615:LEU:CB	6:J:638:GLU:CB	2.89	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:751:THR:O	7:L:755:LEU:N	2.38	0.50
10:O:259:ARG:HE	10:O:275:ALA:HA	1.77	0.50
15:W:430:ASN:O	15:W:447:TRP:CB	2.60	0.50
16:G:148:U:O2	17:H:30:A:C2	2.64	0.50
17:H:32:U:C2	17:H:33:G:C5	2.99	0.50
3:C:165:LEU:HD21	34:C:1500:GTP:O2A	2.12	0.50
3:C:260:ILE:HG13	3:C:311:SER:HB2	1.93	0.50
4:E:136:TRP:CD1	4:E:143:ARG:HA	2.46	0.50
1:A:1405:LEU:HD12	1:A:1408:LEU:HD23	1.94	0.50
3:C:699:ASP:OD2	3:C:722:TYR:OH	2.30	0.50
4:E:55:LEU:CD1	4:E:55:LEU:N	2.73	0.50
16:G:5:G:N1	16:G:6:A:C5	2.80	0.50
16:G:151:C:N1	16:G:152:C:H5	2.05	0.50
17:H:93:A:C2'	17:H:94:A:H5'	2.42	0.50
19:I:218:TYR:CB	19:I:223:GLU:CB	2.90	0.50
3:C:143:THR:HG22	34:C:1500:GTP:PB	2.52	0.50
3:C:673:LYS:HG3	3:C:686:THR:HG23	1.93	0.50
4:E:311:VAL:HB	4:E:321:TYR:HB2	1.93	0.49
6:J:239:ARG:HH11	6:J:239:ARG:HG3	1.77	0.49
17:H:106:G:H1'	17:H:107:A:C8	2.47	0.49
1:A:309:ARG:HE	1:A:310:THR:H	1.60	0.49
1:A:1782:ASP:HB3	1:A:1841:THR:HG21	1.93	0.49
1:A:641:MET:HA	1:A:644:ILE:HG22	1.93	0.49
1:A:825:ILE:HA	1:A:933:ARG:HH12	1.78	0.49
1:A:1663:ASP:HB3	1:A:1702:LEU:HB2	1.93	0.49
1:A:1863:VAL:HG11	1:A:1868:MET:HB2	1.93	0.49
6:J:290:ARG:NH1	8:M:180:ASP:OD1	2.40	0.49
17:H:93:A:H2'	17:H:94:A:H5'	1.94	0.49
17:H:149:A:H2'	17:H:150:U:C6	2.47	0.49
1:A:552:ARG:NH1	1:A:589:THR:O	2.45	0.49
1:A:1430:LEU:HD21	1:A:1459:ARG:HE	1.78	0.49
1:A:1518:LEU:HD13	1:A:1518:LEU:N	2.27	0.49
12:R:252:SER:OG	12:R:255:LYS:O	2.30	0.49
18:U:691:ALA:HB3	18:U:698:LEU:H	1.78	0.49
19:I:585:ASP:O	19:I:586:GLY:C	2.50	0.49
1:A:1131:LYS:O	1:A:1139:ARG:NH1	2.45	0.49
1:A:1231:ARG:NH2	1:A:1283:GLU:OE1	2.45	0.49
2:B:79:C:C6	2:B:79:C:C5'	2.95	0.49
15:W:474:LYS:C	15:W:490:ALA:HB3	2.33	0.49
16:G:144:A:H4'	16:G:145:U:H2'	1.95	0.49
19:I:320:GLU:O	19:I:324:ASP:CB	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:THR:OG1	18:U:581:THR:OG1	2.22	0.49
1:A:820:ARG:NH1	1:A:1063:GLY:O	2.43	0.49
1:A:1781:ASP:HB3	1:A:1808:PHE:HB3	1.94	0.49
14:T:287:HIS:NE2	14:T:305:THR:OG1	2.40	0.49
15:W:155:SER:OG	15:W:158:GLU:OE1	2.29	0.49
15:W:290:GLY:HA2	15:W:573:GLY:HA2	1.94	0.49
16:G:125:C:O2'	16:G:126:C:C2'	2.61	0.49
1:A:974:ASN:HB2	1:A:1178:TYR:HB3	1.94	0.49
1:A:1337:GLN:O	1:A:1341:ARG:NH2	2.46	0.49
5:F:41:A:C6	16:G:7:G:C2	2.99	0.49
17:H:168:A:H3'	17:H:169:C:H6	1.77	0.49
6:J:591:LEU:O	6:J:593:ARG:N	2.44	0.49
7:L:784:LEU:CB	28:K:195:ILE:CB	2.90	0.49
1:A:978:GLU:OE2	1:A:1188:ASN:N	2.45	0.49
15:W:144:ASP:N	15:W:144:ASP:OD1	2.44	0.49
1:A:1511:GLU:OE2	18:U:761:LYS:NZ	2.36	0.49
2:B:87:A:N3	2:B:87:A:C2'	2.75	0.49
9:N:70:ILE:HG12	9:N:74:LEU:HD23	1.95	0.49
17:H:93:A:O2'	17:H:94:A:H5'	2.13	0.49
1:A:1124:ASN:ND2	1:A:1148:ASN:OD1	2.46	0.48
4:E:61:LEU:HD13	4:E:352:TYR:CE1	2.43	0.48
19:I:326:ASP:O	19:I:329:LEU:CB	2.60	0.48
16:G:148:U:O2	17:H:30:A:H2	1.95	0.48
16:G:151:C:C1'	16:G:152:C:H5	2.25	0.48
18:U:579:VAL:HG22	18:U:646:GLU:HB2	1.94	0.48
3:C:139:HIS:HB2	34:C:1500:GTP:O3A	2.13	0.48
3:C:183:SER:HB2	3:C:214:GLU:HB3	1.94	0.48
18:U:663:ALA:HA	18:U:666:ARG:HH12	1.76	0.48
18:U:666:ARG:NH1	18:U:666:ARG:HB2	2.28	0.48
19:I:485:LYS:O	19:I:486:VAL:CG1	2.53	0.48
1:A:741:ARG:NH2	14:T:463:SER:O	2.47	0.48
1:A:1639:VAL:HG12	1:A:1719:PHE:HB3	1.94	0.48
2:B:70:A:H2	2:B:70:A:OP2	1.97	0.48
2:B:96:A:C2	2:B:97:G:C4	3.02	0.48
17:H:104:U:H4'	17:H:105:G:H5"	1.95	0.48
3:C:159:LYS:N	3:C:159:LYS:CD	2.74	0.48
3:C:814:ARG:NH1	3:C:818:SER:OG	2.46	0.48
17:H:51:A:H8	17:H:51:A:OP2	1.96	0.48
18:U:752:ILE:HD12	18:U:773:LEU:HD21	1.94	0.48
1:A:940:ILE:HD12	1:A:1090:ARG:HH21	1.78	0.48
1:A:1501:LEU:HD13	1:A:1753:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1522:GLN:NE2	18:U:622:ALA:O	2.47	0.48
1:A:1957:ASP:HB3	1:A:1960:THR:HG23	1.96	0.48
3:C:700:ILE:O	3:C:740:THR:OG1	2.32	0.48
15:W:528:GLY:O	15:W:552:VAL:CB	2.62	0.48
17:H:181:G:H2'	17:H:182:U:C6	2.49	0.48
18:U:713:ILE:HB	18:U:768:TYR:HB3	1.95	0.48
3:C:737:PRO:HB3	3:C:775:ARG:HB3	1.95	0.48
5:F:41:A:C6	16:G:6:A:N1	2.81	0.48
10:O:136:MET:O	10:O:140:ALA:HB2	2.13	0.48
10:O:245:GLU:HG2	10:O:248:LEU:HD12	1.95	0.48
14:T:223:SER:OG	14:T:224:ALA:N	2.47	0.48
3:C:501:ILE:O	3:C:543:ARG:HA	2.14	0.48
14:T:343:PRO:HG2	14:T:356:LEU:HD23	1.95	0.48
17:H:34:U:C2'	17:H:35:A:N9	2.76	0.48
1:A:855:ARG:HH12	1:A:1518:LEU:HD11	1.78	0.48
7:L:73:HIS:O	7:L:77:LEU:HB2	2.13	0.48
17:H:77:C:H2'	17:H:78:C:C6	2.49	0.48
1:A:1597:PHE:HB3	1:A:1609:VAL:HG11	1.96	0.48
1:A:1784:ASN:HD21	1:A:1894:GLN:HG2	1.78	0.48
3:C:826:ARG:HA	3:C:911:PRO:HG3	1.96	0.48
15:W:491:GLN:O	15:W:492:ASN:C	2.50	0.48
18:U:657:GLN:O	18:U:661:ALA:HB3	2.14	0.48
3:C:150:ILE:HD13	3:C:167:TYR:HD2	1.79	0.47
16:G:141:C:OP2	16:G:141:C:H2'	2.14	0.47
17:H:34:U:O2'	17:H:35:A:H5'	2.14	0.47
17:H:54:U:O4	17:H:93:A:N1	2.46	0.47
19:I:520:ILE:O	19:I:524:TYR:CA	2.61	0.47
1:A:136:ILE:HG12	1:A:418:THR:HG22	1.97	0.47
1:A:579:GLN:HG3	1:A:629:PHE:H	1.79	0.47
1:A:1214:TRP:NE1	1:A:1276:GLU:OE2	2.34	0.47
1:A:1577:PHE:HD1	1:A:1581:LEU:HB3	1.79	0.47
3:C:258:ASN:OD1	3:C:259:LYS:N	2.44	0.47
14:T:224:ALA:HA	14:T:248:THR:HG23	1.94	0.47
17:H:67:C:O2'	17:H:68:G:H5'	2.13	0.47
2:B:72:U:H3'	2:B:72:U:H6	1.78	0.47
12:R:52:PRO:HG3	12:R:67:ILE:HG21	1.97	0.47
17:H:104:U:H4'	17:H:105:G:C5'	2.44	0.47
18:U:741:VAL:HG11	18:U:827:LEU:HG	1.96	0.47
10:O:245:GLU:HG3	10:O:263:VAL:HG21	1.95	0.47
1:A:995:ARG:HG3	12:R:291:LEU:HD13	1.97	0.47
1:A:1636:LYS:HB2	1:A:1655:THR:HB	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:160:ARG:HH11	3:C:160:ARG:C	2.18	0.47
17:H:148:C:O2'	17:H:149:A:H5'	2.13	0.47
1:A:516:LEU:HD11	1:A:538:SER:HB2	1.97	0.47
6:J:197:GLU:OE1	7:L:156:ARG:NE	2.46	0.47
8:M:235:GLN:HB3	8:M:239:ARG:HH21	1.79	0.47
12:R:238:THR:HB	12:R:241:GLU:HG2	1.96	0.47
14:T:216:ASN:HD21	14:T:471:ASP:HB2	1.79	0.47
16:G:6:A:C5	16:G:7:G:C8	3.02	0.47
2:B:11:U:C6	2:B:11:U:C4'	2.97	0.47
3:C:829:GLU:HB2	3:C:907:VAL:HG22	1.97	0.47
17:H:50:C:C6	17:H:50:C:C3'	2.97	0.47
1:A:1237:MET:HG2	1:A:1284:LEU:HD23	1.95	0.47
1:A:1899:VAL:HB	1:A:1902:PHE:HD2	1.80	0.47
2:B:77:G:C6	2:B:80:U:C5	3.03	0.47
3:C:137:HIS:CE1	3:C:138:LEU:HB2	2.50	0.47
3:C:349:PHE:HZ	3:C:354:ARG:HE	1.63	0.47
7:L:12:ARG:HH12	7:L:40:ARG:HH11	1.63	0.47
8:M:134:GLN:HG2	8:M:137:ARG:HH21	1.79	0.47
10:O:131:THR:O	15:W:108:ARG:NH1	2.37	0.47
12:R:60:ASP:HB2	13:S:134:GLN:HA	1.96	0.47
16:G:1:G:H5'	16:G:144:A:H1'	1.95	0.47
17:H:71:C:H2'	17:H:72:U:C6	2.50	0.47
1:A:32:GLU:OE1	1:A:35:ARG:NH1	2.48	0.47
1:A:532:THR:CB	16:G:3:A:C4'	2.93	0.47
14:T:398:TRP:CD1	14:T:405:PHE:HA	2.50	0.47
16:G:147:C:OP1	16:G:147:C:C6	2.67	0.47
17:H:69:U:H6	17:H:69:U:O5'	1.97	0.47
19:I:289:VAL:O	19:I:292:PHE:CB	2.63	0.47
19:I:326:ASP:O	19:I:329:LEU:N	2.48	0.47
1:A:723:ASN:ND2	1:A:788:GLN:OE1	2.48	0.47
4:E:266:PRO:HG2	7:L:785:GLN:C	2.35	0.47
12:R:119:LEU:HD21	12:R:230:MET:HB3	1.97	0.47
13:S:55:ARG:HB3	13:S:63:GLN:HB3	1.96	0.47
13:S:90:LEU:HB3	13:S:128:ILE:HD12	1.97	0.47
17:H:10:C:H2'	17:H:11:G:H8	1.80	0.47
1:A:1745:GLU:O	1:A:1749:LYS:HB2	2.15	0.46
17:H:147:G:N3	17:H:148:C:C6	2.84	0.46
18:U:705:SER:OG	18:U:875:LYS:NZ	2.47	0.46
2:B:78:U:O2'	2:B:79:C:OP1	2.28	0.46
6:J:774:VAL:HA	6:J:787:LYS:CB	2.45	0.46
7:L:209:ASP:HB2	10:O:113:ASN:HD21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:207:ASP:N	8:M:207:ASP:OD1	2.48	0.46
14:T:213:GLU:HG3	14:T:218:TRP:CE2	2.50	0.46
17:H:51:A:N3	17:H:51:A:H2'	2.30	0.46
17:H:55:U:H2'	17:H:56:A:C8	2.48	0.46
18:U:659:LYS:O	18:U:663:ALA:CB	2.63	0.46
1:A:256:TYR:HE1	1:A:332:TYR:HB2	1.80	0.46
1:A:1518:LEU:O	1:A:1519:THR:C	2.52	0.46
3:C:80:ILE:HG22	3:C:82:GLN:HG2	1.97	0.46
6:J:391:TYR:HB3	6:J:394:HIS:HB2	1.96	0.46
17:H:90:A:H2'	17:H:91:U:C6	2.50	0.46
1:A:1676:ILE:HD13	1:A:1706:ASP:HB2	1.96	0.46
5:F:39:A:C2'	5:F:40:U:H5'	2.45	0.46
5:F:43:A:O5'	5:F:43:A:C8	2.69	0.46
14:T:416:ILE:HA	14:T:431:ALA:HA	1.97	0.46
16:G:148:U:C2	17:H:30:A:C2	3.04	0.46
17:H:81:G:H2'	17:H:82:G:H8	1.81	0.46
17:H:88:A:H2'	17:H:89:U:C6	2.50	0.46
17:H:164:C:OP2	17:H:164:C:H6	1.99	0.46
18:U:537:GLY:HA3	18:U:548:LEU:HD12	1.95	0.46
1:A:1481:VAL:HG11	1:A:1498:TRP:CD2	2.51	0.46
2:B:29:A:H2'	2:B:30:A:H8	1.80	0.46
4:E:217:ILE:HB	4:E:231:MET:HB2	1.97	0.46
4:E:257:ASN:OD1	4:E:282:HIS:N	2.48	0.46
16:G:4:A:C2	16:G:5:G:C2	3.04	0.46
17:H:80:A:H2'	17:H:81:G:H8	1.81	0.46
1:A:532:THR:HG1	16:G:3:A:H5'	1.66	0.46
1:A:1128:TYR:OH	1:A:1140:MET:SD	2.73	0.46
3:C:221:ILE:O	3:C:495:ARG:NH1	2.49	0.46
10:O:237:GLY:O	10:O:299:ASN:HB3	2.15	0.46
13:S:160:ILE:HG22	13:S:161:LYS:HG3	1.98	0.46
15:W:516:PHE:HA	15:W:522:TYR:O	2.16	0.46
19:I:521:VAL:O	19:I:527:PHE:N	2.48	0.46
4:E:56:GLN:HB3	4:E:57:ALA:H	1.47	0.46
4:E:266:PRO:HG2	7:L:785:GLN:O	2.16	0.46
10:O:255:PHE:O	12:R:78:ARG:NH1	2.48	0.46
12:R:151:LEU:HD22	14:T:323:VAL:HG11	1.96	0.46
16:G:5:G:C5	16:G:6:A:N9	2.84	0.46
17:H:78:C:H2'	17:H:79:G:H8	1.81	0.46
17:H:92:U:C2'	17:H:93:A:C8	2.85	0.46
17:H:114:A:H2'	17:H:115:G:H8	1.81	0.46
1:A:1163:ARG:HH12	11:P:201:VAL:HG11	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11:U:C6	2:B:11:U:C3'	2.99	0.46
3:C:191:PRO:HA	3:C:197:SER:HA	1.96	0.46
3:C:850:LEU:HD23	3:C:855:GLY:HA3	1.97	0.46
10:O:90:TYR:HB3	10:O:92:LEU:HD13	1.98	0.46
15:W:481:MET:C	15:W:483:ASN:H	2.18	0.46
17:H:108:G:O5'	17:H:108:G:H8	1.99	0.46
4:E:56:GLN:HG2	4:E:97:GLY:O	2.16	0.46
16:G:5:G:C2	16:G:6:A:C5	3.04	0.46
1:A:1198:PRO:HA	1:A:1226:ALA:HA	1.98	0.46
1:A:1699:THR:HA	1:A:1717:ASN:HD22	1.81	0.46
1:A:1946:ASN:ND2	1:A:1990:ASP:OD2	2.46	0.46
17:H:148:C:H2'	17:H:149:A:H5'	1.98	0.46
19:I:712:VAL:O	19:I:715:GLY:N	2.49	0.46
1:A:762:ARG:HH12	11:P:226:LYS:HZ1	1.63	0.45
1:A:941:LYS:HA	1:A:941:LYS:HD2	1.72	0.45
4:E:135:VAL:HB	4:E:145:LYS:HB3	1.97	0.45
5:F:41:A:C2'	5:F:42:C:H5'	2.46	0.45
8:M:135:TYR:O	8:M:139:THR:OG1	2.27	0.45
15:W:476:LEU:O	15:W:487:ILE:HA	2.17	0.45
16:G:23:U:C6	16:G:23:U:H5"	2.51	0.45
16:G:27:U:HO2'	16:G:28:A:C4'	2.29	0.45
16:G:133:A:N6	17:H:43:U:C4	2.79	0.45
17:H:82:G:H2'	17:H:83:A:H8	1.81	0.45
2:B:74:U:C4	2:B:76:A:C6	3.04	0.45
3:C:85:ASP:OD1	3:C:85:ASP:N	2.47	0.45
4:E:251:LEU:HD21	4:E:300:ILE:HG23	1.97	0.45
7:L:74:LEU:HA	7:L:77:LEU:HB3	1.97	0.45
10:O:175:ARG:HB2	10:O:179:CYS:HB2	1.98	0.45
17:H:74:U:H2'	17:H:75:A:H8	1.81	0.45
1:A:787:GLU:OE2	1:A:790:ARG:NH2	2.44	0.45
1:A:1426:ASP:OD1	1:A:1426:ASP:N	2.49	0.45
3:C:82:GLN:HE21	14:T:238:LEU:H	1.64	0.45
16:G:145:U:C5	16:G:146:C:C5	3.04	0.45
1:A:339:PHE:HE1	1:A:402:ILE:HG22	1.82	0.45
2:B:66:A:H2'	2:B:67:A:C1'	2.46	0.45
3:C:160:ARG:HH11	3:C:160:ARG:HB2	1.81	0.45
3:C:162:ASP:OD1	3:C:162:ASP:N	2.48	0.45
3:C:440:SER:O	3:C:442:LYS:N	2.46	0.45
7:L:16:ASP:OD2	7:L:49:ARG:NH2	2.39	0.45
17:H:73:C:H2'	17:H:74:U:C6	2.50	0.45
1:A:1201:ARG:HG3	1:A:1202:THR:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:142:LYS:HE2	3:C:142:LYS:HB2	1.67	0.45
3:C:383:GLN:HA	3:C:387:ASP:HB2	1.98	0.45
3:C:670:SER:HB2	3:C:689:ALA:H	1.82	0.45
17:H:89:U:H2'	17:H:90:A:H8	1.82	0.45
17:H:107:A:H5"	17:H:107:A:C8	2.50	0.45
1:A:668:VAL:HB	5:F:68:C:H5"	1.99	0.45
1:A:1807:ILE:HB	1:A:1820:LYS:HB3	1.98	0.45
2:B:93:U:H4'	2:B:94:U:H5"	1.99	0.45
2:B:96:A:N1	2:B:97:G:C5	2.84	0.45
3:C:595:VAL:HG22	3:C:654:LYS:HG3	1.99	0.45
16:G:7:G:H2'	16:G:8:C:H6	1.80	0.45
18:U:546:VAL:HG11	18:U:665:HIS:ND1	2.31	0.45
19:I:277:ASP:O	19:I:280:GLU:CB	2.64	0.45
1:A:1296:GLN:NE2	1:A:1317:TYR:OH	2.50	0.45
10:O:152:ARG:HH12	16:G:22:C:H41	1.65	0.45
11:P:3:THR:O	11:P:6:ARG:NE	2.43	0.45
17:H:58:U:O4	17:H:90:A:N1	2.50	0.45
17:H:113:G:H2'	17:H:114:A:H8	1.82	0.45
1:A:1011:ALA:HB2	7:L:80:THR:HB	1.98	0.45
1:A:1701:VAL:HA	1:A:1716:GLY:HA3	1.99	0.45
2:B:70:A:OP2	2:B:70:A:C2	2.70	0.45
3:C:94:ILE:H	3:C:94:ILE:HG13	1.44	0.45
3:C:157:ILE:O	3:C:159:LYS:HD3	2.17	0.45
3:C:556:ASP:OD1	3:C:556:ASP:N	2.49	0.45
6:J:322:MET:O	8:M:181:ARG:NH1	2.48	0.45
12:R:62:GLY:HA2	13:S:96:GLY:HA3	1.99	0.45
13:S:99:ALA:HA	13:S:129:PHE:H	1.81	0.45
1:A:1892:PRO:HD3	1:A:1941:ARG:HH21	1.81	0.45
3:C:139:HIS:CB	34:C:1500:GTP:H5"	2.33	0.45
5:F:9:U:O2	5:F:10:U:N3	2.50	0.45
7:L:699:ASN:CB	28:K:114:LEU:CB	2.95	0.45
8:M:221:LYS:NZ	17:H:18:U:OP2	2.38	0.45
15:W:466:ALA:HB2	15:W:512:CYS:O	2.17	0.45
16:G:2:U:H2'	16:G:3:A:N3	2.32	0.45
19:I:253:ASP:O	19:I:254:GLN:CB	2.64	0.45
2:B:66:A:C3'	2:B:67:A:O4'	2.65	0.45
3:C:770:PHE:HE1	3:C:789:PHE:HD2	1.64	0.45
16:G:144:A:H4'	16:G:145:U:C3'	2.46	0.45
1:A:435:CYS:SG	1:A:439:GLN:NE2	2.67	0.44
2:B:11:U:C6	2:B:11:U:C5'	2.85	0.44
3:C:144:CYS:HA	3:C:165:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:619:THR:HG22	3:C:629:ILE:HG13	1.99	0.44
4:E:149:GLY:O	4:E:177:LYS:NZ	2.50	0.44
9:N:119:CYS:SG	9:N:139:CYS:HB3	2.57	0.44
17:H:83:A:H2'	17:H:84:C:C6	2.49	0.44
18:U:655:GLU:O	18:U:659:LYS:HB3	2.16	0.44
18:U:805:LEU:HD11	18:U:832:ALA:HB2	1.99	0.44
2:B:8:G:N3	2:B:8:G:C2'	2.73	0.44
4:E:300:ILE:O	4:E:311:VAL:HA	2.18	0.44
17:H:34:U:C6	17:H:34:U:OP2	2.70	0.44
8:M:165:ASN:HB3	12:R:96:ILE:H	1.82	0.44
15:W:266:ARG:O	15:W:267:SER:O	2.35	0.44
17:H:50:C:H2'	17:H:51:A:C1'	2.48	0.44
17:H:51:A:C8	17:H:51:A:OP2	2.70	0.44
1:A:675:GLN:HG3	1:A:676:ARG:HD3	1.99	0.44
1:A:1831:LYS:HD2	1:A:1831:LYS:HA	1.76	0.44
4:E:61:LEU:HD13	4:E:352:TYR:OH	2.15	0.44
4:E:307:ARG:HH11	15:W:143:LEU:HD12	1.83	0.44
5:F:58:G:H2'	5:F:59:G:C8	2.52	0.44
9:N:70:ILE:HG23	9:N:74:LEU:HB3	1.98	0.44
10:O:174:LYS:HA	15:W:205:VAL:HG22	2.00	0.44
16:G:149:G:OP2	16:G:149:G:C8	2.70	0.44
17:H:79:G:H2'	17:H:80:A:H8	1.81	0.44
19:I:368:GLN:OE1	19:I:368:GLN:HA	2.18	0.44
4:E:92:LEU:HB2	4:E:103:ALA:HB3	1.99	0.44
5:F:44:G:OP2	5:F:44:G:C8	2.70	0.44
17:H:58:U:H2'	17:H:59:A:H8	1.82	0.44
17:H:84:C:H2'	17:H:85:A:H8	1.82	0.44
17:H:109:C:C5	17:H:109:C:OP2	2.71	0.44
1:A:139:VAL:HG11	1:A:212:PRO:HG2	1.99	0.44
1:A:671:THR:O	1:A:676:ARG:NH2	2.50	0.44
1:A:1426:ASP:HB2	1:A:1429:THR:HG22	1.98	0.44
3:C:614:TYR:HA	3:C:615:PRO:HD3	1.87	0.44
8:M:221:LYS:HE3	12:R:249:PRO:HB3	1.98	0.44
16:G:141:C:H2'	16:G:141:C:O5'	2.18	0.44
1:A:179:ALA:HA	1:A:183:LEU:HD13	2.00	0.44
1:A:1754:TYR:OH	18:U:553:GLN:OE1	2.35	0.44
3:C:144:CYS:CB	3:C:165:LEU:CD1	2.89	0.44
4:E:90:ILE:HG13	4:E:136:TRP:CZ3	2.53	0.44
10:O:64:ARG:HD2	10:O:163:HIS:CE1	2.53	0.44
17:H:56:A:H2'	17:H:57:A:H8	1.82	0.44
17:H:57:A:H2'	17:H:58:U:C6	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:H:154:C:O2'	17:H:155:C:C5'	2.66	0.44
18:U:546:VAL:HG11	18:U:665:HIS:HE1	1.75	0.44
19:I:251:PHE:CB	19:I:254:GLN:CB	2.95	0.44
1:A:1110:ILE:HD11	1:A:1149:LEU:HB2	2.00	0.44
3:C:122:LEU:HD22	3:C:128:LEU:HD12	1.98	0.44
3:C:300:LEU:HA	3:C:306:ASN:HD21	1.83	0.44
4:E:241:LEU:HD22	4:E:250:LEU:HD21	2.00	0.44
11:P:23:LEU:HD23	11:P:26:LEU:HD13	2.00	0.44
16:G:5:G:C4	16:G:6:A:H8	2.31	0.44
17:H:168:A:N3	17:H:168:A:H2'	2.33	0.44
1:A:348:PRO:HG2	1:A:351:TYR:HB3	1.99	0.44
1:A:517:HIS:CD2	18:U:585:ARG:HD3	2.53	0.44
1:A:1779:PHE:O	1:A:1809:ILE:HA	2.18	0.44
2:B:77:G:O6	2:B:80:U:C5	2.71	0.44
3:C:705:VAL:HG22	3:C:717:PHE:HE2	1.83	0.44
4:E:294:SER:HB3	4:E:299:LYS:HB2	2.00	0.44
7:L:703:MET:O	7:L:707:ALA:HB3	2.18	0.44
14:T:406:ILE:HG22	14:T:407:GLN:HB2	2.00	0.44
15:W:309:MET:HA	15:W:334:ALA:HB1	1.99	0.44
16:G:153:C:O5'	16:G:153:C:C6	2.70	0.44
1:A:266:SER:OG	1:A:271:MET:O	2.32	0.43
2:B:11:U:O2'	2:B:12:U:H5'	2.18	0.43
2:B:77:G:C6	2:B:80:U:H5	2.35	0.43
10:O:59:PRO:HB2	10:O:63:MET:HG3	1.99	0.43
12:R:97:LYS:NZ	13:S:146:GLU:OE1	2.50	0.43
16:G:146:C:C2'	16:G:147:C:OP1	2.66	0.43
1:A:1365:ILE:HA	1:A:1366:PRO:HD3	1.82	0.43
3:C:561:LYS:NZ	3:C:611:ASN:OD1	2.36	0.43
3:C:692:LEU:HD12	3:C:696:LEU:HB3	1.99	0.43
4:E:82:ALA:HA	4:E:91:LEU:O	2.19	0.43
9:N:128:VAL:HG13	9:N:130:ARG:H	1.82	0.43
10:O:213:LEU:CD1	16:G:21:A:H2'	2.48	0.43
15:W:162:ASN:HB3	15:W:165:LEU:HD22	2.00	0.43
17:H:59:A:H2'	17:H:60:U:C6	2.50	0.43
17:H:72:U:H2'	17:H:73:C:C6	2.50	0.43
1:A:1196:ILE:HA	1:A:1227:GLN:O	2.18	0.43
1:A:1595:GLN:HA	1:A:1598:ASP:HB2	2.01	0.43
3:C:925:PRO:HB2	3:C:927:PRO:HD2	1.99	0.43
4:E:284:PHE:HZ	15:W:120:ILE:HD13	1.83	0.43
4:E:294:SER:OG	4:E:298:SER:N	2.51	0.43
15:W:426:PHE:HA	15:W:433:PHE:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:G:134:U:O2'	16:G:135:G:C8	2.66	0.43
16:G:153:C:H3'	16:G:153:C:H6	1.83	0.43
1:A:178:TYR:OH	1:A:488:ASP:OD2	2.32	0.43
1:A:923:ASP:OD2	1:A:1439:ARG:NE	2.49	0.43
3:C:223:ASP:HA	3:C:251:LEU:HD22	2.00	0.43
6:J:196:ARG:HA	8:M:208:ILE:HD11	2.00	0.43
6:J:496:ASP:CB	6:J:535:TYR:CA	2.95	0.43
14:T:306:CYS:SG	14:T:336:VAL:HB	2.58	0.43
17:H:157:G:H5"	17:H:157:G:C8	2.50	0.43
1:A:793:ASN:HD22	3:C:60:HIS:CE1	2.37	0.43
16:G:27:U:HO2'	16:G:28:A:C5'	2.28	0.43
17:H:178:A:N3	17:H:178:A:H2'	2.33	0.43
1:A:494:LEU:HD21	1:A:562:VAL:HG21	2.00	0.43
1:A:856:LEU:HD23	1:A:860:GLN:HB3	2.00	0.43
1:A:1745:GLU:OE2	1:A:1748:ARG:NH1	2.51	0.43
2:B:71:C:C3'	2:B:71:C:C6	3.01	0.43
16:G:141:C:OP2	16:G:141:C:C6	2.70	0.43
17:H:45:C:O2'	17:H:46:U:O5'	2.33	0.43
17:H:50:C:C6	17:H:50:C:C4'	3.02	0.43
18:U:680:ASP:OD1	18:U:680:ASP:N	2.44	0.43
1:A:591:MET:HE2	1:A:598:LEU:HD21	2.01	0.43
3:C:590:ILE:HG22	3:C:592:VAL:HG23	2.01	0.43
3:C:707:ILE:H	3:C:707:ILE:HG13	1.67	0.43
13:S:122:LEU:O	13:S:126:HIS:N	2.52	0.43
17:H:157:G:H2'	17:H:158:G:O4'	2.19	0.43
28:K:134:ALA:O	28:K:136:LYS:N	2.52	0.43
1:A:180:ASP:OD1	1:A:180:ASP:N	2.49	0.43
1:A:828:PRO:HA	1:A:829:PRO:HD3	1.82	0.43
3:C:495:ARG:HB3	3:C:549:TRP:CD1	2.54	0.43
3:C:843:VAL:HG13	3:C:871:ILE:HD11	2.00	0.43
11:P:17:GLY:N	11:P:20:GLU:OE1	2.48	0.43
17:H:91:U:H2'	17:H:92:U:C6	2.50	0.43
2:B:11:U:H6	2:B:11:U:C4'	2.32	0.43
3:C:259:LYS:HG2	34:C:1500:GTP:C2	2.54	0.43
3:C:592:VAL:HG22	3:C:655:VAL:HG22	2.00	0.43
5:F:41:A:N6	5:F:42:C:N4	2.66	0.43
10:O:234:LEU:O	10:O:271:PHE:HA	2.19	0.43
12:R:178:ARG:NH1	15:W:141:PRO:O	2.52	0.43
13:S:25:LEU:HD23	13:S:132:VAL:HG12	2.00	0.43
16:G:22:C:C2'	16:G:23:U:O5'	2.66	0.43
17:H:37:U:O2'	17:H:38:A:C8	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:H:168:A:H3'	17:H:169:C:C6	2.53	0.43
2:B:46:U:O4	2:B:47:A:N6	2.46	0.43
3:C:453:TYR:HD2	3:C:456:GLY:H	1.67	0.43
3:C:829:GLU:OE2	3:C:854:ARG:NH2	2.52	0.43
6:J:194:LEU:HD21	7:L:152:LEU:HD22	2.01	0.43
16:G:21:A:H3'	16:G:21:A:H8	1.84	0.43
16:G:25:G:HO2'	16:G:26:U:P	2.41	0.43
17:H:98:G:H5'	17:H:104:U:OP2	2.19	0.43
1:A:1516:LYS:HB3	1:A:1516:LYS:HE2	1.57	0.42
3:C:160:ARG:NH1	3:C:160:ARG:C	2.73	0.42
4:E:75:HIS:HD1	4:E:77:ASN:H	1.66	0.42
4:E:258:THR:HG21	4:E:260:ARG:HH21	1.84	0.42
6:J:343:GLU:HG2	6:J:347:HIS:CD2	2.54	0.42
13:S:152:ARG:HH22	15:W:74:PRO:HG2	1.84	0.42
15:W:571:TRP:O	15:W:573:GLY:N	2.52	0.42
16:G:6:A:N1	16:G:7:G:C4	2.87	0.42
18:U:673:GLU:O	18:U:682:SER:OG	2.26	0.42
19:I:545:ILE:O	19:I:548:PHE:N	2.51	0.42
1:A:1272:THR:HA	1:A:1275:ARG:HD3	2.00	0.42
16:G:137:C:O2'	16:G:138:A:C8	2.67	0.42
16:G:140:A:O2'	16:G:141:C:C5	2.72	0.42
19:I:790:ARG:CB	19:I:801:ASP:HA	2.48	0.42
1:A:833:LYS:HG3	1:A:834:HIS:CD2	2.54	0.42
9:N:105:CYS:HB3	9:N:117:CYS:SG	2.59	0.42
10:O:159:ARG:HG2	16:G:20:A:P	2.59	0.42
16:G:125:C:O2'	16:G:126:C:C1'	2.67	0.42
18:U:685:PRO:O	18:U:687:HIS:ND1	2.50	0.42
4:E:305:ALA:HA	4:E:329:SER:HB2	2.01	0.42
13:S:26:GLU:N	13:S:131:ARG:O	2.50	0.42
17:H:32:U:H6	17:H:32:U:H2'	1.57	0.42
17:H:42:G:C2	17:H:43:U:O4	2.72	0.42
1:A:1259:ILE:HD13	1:A:1259:ILE:HA	1.89	0.42
3:C:388:VAL:HA	3:C:392:LEU:HB2	2.00	0.42
5:F:17:C:H2'	5:F:18:A:C8	2.54	0.42
14:T:478:LEU:HD13	14:T:488:VAL:HG22	2.02	0.42
15:W:431:ARG:O	15:W:446:GLU:HA	2.19	0.42
15:W:528:GLY:HA2	15:W:552:VAL:CB	2.49	0.42
16:G:6:A:N6	16:G:7:G:N1	2.68	0.42
17:H:69:U:C2'	17:H:70:C:H5'	2.49	0.42
28:K:18:TYR:CB	28:K:168:LYS:HA	2.50	0.42
1:A:462:ARG:HA	1:A:463:PRO:HD3	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:38:G:H2'	5:F:39:A:C8	2.55	0.42
16:G:1:G:C1'	16:G:2:U:OP1	2.67	0.42
16:G:6:A:C5	16:G:7:G:C5	3.07	0.42
1:A:1333:VAL:HG13	1:A:1365:ILE:HD13	2.02	0.42
1:A:1666:LEU:HD23	1:A:1705:ILE:HB	2.00	0.42
3:C:369:PHE:CD1	3:C:373:ILE:HG13	2.54	0.42
15:W:290:GLY:HA2	15:W:571:TRP:O	2.19	0.42
16:G:4:A:OP1	16:G:4:A:C8	2.70	0.42
16:G:12:G:H2'	16:G:13:C:C6	2.55	0.42
19:I:712:VAL:O	19:I:713:ARG:C	2.57	0.42
1:A:1057:ARG:NH2	1:A:1085:ILE:O	2.50	0.42
3:C:500:THR:HG22	3:C:545:PRO:HA	2.02	0.42
14:T:382:PRO:HB2	14:T:383:ARG:HD2	2.02	0.42
17:H:155:C:H2'	17:H:156:U:H5"	2.01	0.42
17:H:180:G:H2'	17:H:181:G:H8	1.83	0.42
3:C:129:ILE:HG22	3:C:199:LEU:HB3	2.02	0.42
3:C:853:ARG:NH2	3:C:886:ASP:OD2	2.52	0.42
5:F:57:U:H2'	5:F:58:G:C8	2.55	0.42
16:G:152:C:O2	16:G:152:C:H2'	2.19	0.42
1:A:1318:THR:HB	1:A:1324:GLY:HA3	2.01	0.42
3:C:781:ASP:HB2	3:C:941:LYS:HZ1	1.84	0.42
4:E:131:LYS:HA	4:E:154:VAL:HG23	2.01	0.42
4:E:209:ILE:HG12	4:E:219:VAL:HG22	2.02	0.42
7:L:11:TRP:HE1	7:L:133:GLU:HG3	1.84	0.42
7:L:253:SER:HA	7:L:256:GLU:HG2	2.02	0.42
17:H:147:G:N1	17:H:148:C:C4	2.88	0.42
1:A:758:ARG:HD2	1:A:758:ARG:HA	1.69	0.41
3:C:144:CYS:HB2	3:C:165:LEU:HD12	1.98	0.41
4:E:133:VAL:HB	4:E:147:LEU:HG	2.02	0.41
4:E:145:LYS:HE2	4:E:184:LYS:HG2	2.02	0.41
7:L:120:PRO:O	7:L:121:ARG:NE	2.53	0.41
17:H:112:G:H2'	17:H:113:G:C8	2.50	0.41
1:A:93:LYS:O	1:A:649:GLU:HG2	2.20	0.41
1:A:312:TYR:OH	3:C:886:ASP:OD2	2.37	0.41
3:C:506:PRO:HA	3:C:526:THR:HA	2.01	0.41
3:C:664:GLU:HB3	3:C:820:PHE:HZ	1.85	0.41
6:J:669:GLN:C	6:J:671:ARG:N	2.74	0.41
1:A:788:GLN:HG2	1:A:1024:HIS:HB3	2.02	0.41
3:C:263:LEU:HD23	3:C:267:LEU:HD12	2.02	0.41
3:C:389:ASP:OD1	3:C:389:ASP:N	2.54	0.41
4:E:59:ILE:HD12	4:E:59:ILE:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:248:SER:HB3	4:E:265:ARG:HH21	1.85	0.41
11:P:19:GLY:HA2	11:P:23:LEU:HD12	2.02	0.41
13:S:92:PHE:CD2	13:S:122:LEU:HB3	2.55	0.41
16:G:21:A:H3'	16:G:21:A:C8	2.55	0.41
17:H:103:U:C3'	17:H:104:U:H5'	2.51	0.41
17:H:150:U:C2'	17:H:151:C:H5'	2.50	0.41
28:K:128:SER:O	28:K:132:CYS:CB	2.68	0.41
1:A:1159:ASN:HB3	11:P:196:ASN:HA	2.02	0.41
2:B:70:A:N3	2:B:70:A:H5"	2.34	0.41
7:L:209:ASP:OD1	7:L:209:ASP:N	2.52	0.41
7:L:699:ASN:HA	28:K:114:LEU:CB	2.50	0.41
10:O:213:LEU:HD12	16:G:21:A:H2'	2.02	0.41
14:T:380:LEU:HG	14:T:400:PHE:HZ	1.85	0.41
15:W:371:THR:O	15:W:372:ASN:CB	2.68	0.41
16:G:21:A:C8	16:G:21:A:C3'	3.03	0.41
18:U:810:ILE:HA	18:U:813:SER:HB2	2.01	0.41
19:I:255:LEU:O	19:I:256:GLY:C	2.59	0.41
1:A:1048:MET:HG2	1:A:1051:LEU:HD12	2.03	0.41
3:C:163:GLN:HB3	3:C:164:ASP:H	1.60	0.41
3:C:375:GLU:O	3:C:379:LYS:HG2	2.21	0.41
18:U:560:VAL:CG1	18:U:660:LYS:HZ3	2.26	0.41
18:U:696:VAL:HG12	18:U:715:PRO:HA	2.02	0.41
19:I:255:LEU:O	19:I:257:LYS:N	2.53	0.41
1:A:250:VAL:HG13	1:A:406:TRP:HB3	2.02	0.41
1:A:796:LYS:HG3	12:R:279:HIS:HE1	1.84	0.41
1:A:1513:MET:SD	18:U:619:MET:HG2	2.60	0.41
3:C:836:VAL:HG11	3:C:846:VAL:HG21	2.03	0.41
5:F:27:A:OP1	10:O:175:ARG:NH1	2.46	0.41
10:O:216:ARG:HD2	16:G:22:C:H5"	2.03	0.41
11:P:32:SER:HA	11:P:35:LEU:HD13	2.02	0.41
11:P:204:GLN:O	11:P:206:LYS:N	2.53	0.41
14:T:380:LEU:HG	14:T:400:PHE:CZ	2.55	0.41
15:W:491:GLN:CB	16:G:136:U:P	3.09	0.41
17:H:168:A:H5"	17:H:169:C:H5	1.86	0.41
19:I:526:MET:O	19:I:526:MET:SD	2.78	0.41
1:A:332:TYR:O	3:C:888:ARG:NH2	2.48	0.41
17:H:153:A:H3'	17:H:154:C:H5'	2.00	0.41
18:U:620:ARG:NH1	18:U:647:ARG:HE	2.19	0.41
9:N:22:LEU:HD21	9:N:60:ILE:HD11	2.02	0.41
14:T:450:VAL:HG11	14:T:489:TYR:HE2	1.86	0.41
17:H:171:U:H2'	17:H:172:C:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:GLU:OE2	1:A:240:ARG:NH1	2.51	0.41
1:A:699:GLU:OE2	12:R:235:ARG:HB3	2.21	0.41
1:A:1178:TYR:HB2	1:A:1185:LEU:HB3	2.02	0.41
1:A:1487:HIS:HD2	1:A:1541:THR:HG21	1.85	0.41
1:A:1556:ASP:OD1	1:A:1557:LEU:N	2.50	0.41
1:A:1648:SER:HB2	1:A:1649:LYS:HD2	2.03	0.41
1:A:1971:LEU:HB2	1:A:1976:TRP:CE2	2.55	0.41
3:C:92:PRO:HA	14:T:278:ASN:ND2	2.36	0.41
3:C:804:GLY:O	3:C:808:ILE:HB	2.21	0.41
12:R:113:TYR:OH	14:T:402:ASP:O	2.25	0.41
13:S:121:TRP:CZ2	15:W:98:PRO:HG3	2.56	0.41
13:S:123:ASP:N	13:S:123:ASP:OD1	2.51	0.41
14:T:345:ILE:HD11	14:T:359:LEU:HD13	2.03	0.41
16:G:6:A:N9	16:G:7:G:C8	2.89	0.41
16:G:147:C:C4	17:H:31:G:N1	2.69	0.41
17:H:35:A:H8	17:H:35:A:OP2	2.03	0.41
17:H:51:A:H5’	17:H:99:A:O2’	2.21	0.41
17:H:112:G:H8	17:H:112:G:O5’	2.04	0.41
17:H:147:G:C4	17:H:148:C:C5	3.09	0.41
1:A:852:VAL:HG11	1:A:1449:LYS:HZ2	1.85	0.41
1:A:1971:LEU:O	1:A:1976:TRP:NE1	2.53	0.41
2:B:72:U:C3’	2:B:72:U:C6	3.04	0.41
6:J:600:ILE:C	6:J:602:LYS:N	2.74	0.41
17:H:88:A:C6	17:H:89:U:C4	3.09	0.41
17:H:92:U:C2’	17:H:93:A:H8	2.28	0.41
1:A:56:ALA:O	9:N:109:ARG:NH1	2.35	0.40
2:B:73:C:O2	2:B:73:C:O2’	2.35	0.40
3:C:158:ARG:C	3:C:159:LYS:CD	2.73	0.40
3:C:637:LEU:HA	3:C:637:LEU:HD23	1.90	0.40
5:F:17:C:H2’	5:F:18:A:H8	1.87	0.40
6:J:281:LYS:HA	6:J:284:GLU:HG2	2.02	0.40
6:J:774:VAL:CB	6:J:787:LYS:CB	2.99	0.40
7:L:114:GLU:HG2	7:L:115:GLU:H	1.86	0.40
14:T:213:GLU:HG3	14:T:218:TRP:CZ2	2.57	0.40
3:C:134:LEU:O	3:C:205:THR:OG1	2.29	0.40
6:J:293:ASN:OD1	7:L:225:TYR:HB3	2.21	0.40
7:L:22:ALA:HB2	7:L:37:LEU:HD23	2.04	0.40
15:W:298:PRO:O	15:W:299:LEU:CB	2.68	0.40
16:G:22:C:O2	16:G:22:C:C2’	2.69	0.40
16:G:141:C:O5’	16:G:141:C:C2’	2.70	0.40
17:H:59:A:C6	17:H:60:U:C4	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1179:SER:O	1:A:1201:ARG:NH2	2.37	0.40
3:C:495:ARG:HH21	3:C:547:GLY:HA2	1.86	0.40
5:F:78:A:H4'	6:J:237:LYS:HE2	2.03	0.40
7:L:140:ASP:OD1	7:L:140:ASP:N	2.55	0.40
15:W:77:LYS:HA	15:W:77:LYS:HD3	1.86	0.40
19:I:426:PHE:CB	19:I:458:LYS:CB	2.99	0.40
1:A:1976:TRP:HA	1:A:1979:VAL:HG22	2.04	0.40
2:B:85:C:H3'	2:B:85:C:P	2.61	0.40
5:F:81:C:H5"	5:F:82:A:H5"	2.03	0.40
6:J:493:ALA:CB	6:J:499:ARG:CB	2.96	0.40
6:J:592:ALA:N	6:J:595:ALA:HB3	2.37	0.40
9:N:3:LYS:HA	9:N:3:LYS:HD2	1.91	0.40
12:R:281:ASN:ND2	12:R:282:GLU:OE1	2.54	0.40
14:T:216:ASN:ND2	14:T:471:ASP:HB2	2.37	0.40
17:H:181:G:C4	17:H:182:U:C5	3.10	0.40
3:C:264:ILE:HG12	3:C:378:TYR:CE1	2.57	0.40
4:E:304:SER:OG	4:E:308:PHE:O	2.39	0.40
7:L:692:LEU:CB	28:K:107:VAL:CB	3.00	0.40
14:T:446:ASN:ND2	14:T:449:ARG:HE	2.19	0.40
19:I:606:TRP:O	19:I:609:ALA:HB3	2.21	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	A	1977/2335 (85%)	1793 (91%)	165 (8%)	19 (1%)	13	40
3	C	886/972 (91%)	788 (89%)	96 (11%)	2 (0%)	44	73
4	E	301/357 (84%)	280 (93%)	20 (7%)	1 (0%)	37	66
6	J	520/848 (61%)	473 (91%)	42 (8%)	5 (1%)	13	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	L	459/802 (57%)	423 (92%)	31 (7%)	5 (1%)	12 37
8	M	128/243 (53%)	116 (91%)	12 (9%)	0	100 100
9	N	141/144 (98%)	128 (91%)	12 (8%)	1 (1%)	19 49
10	O	288/420 (69%)	262 (91%)	25 (9%)	1 (0%)	37 66
11	P	114/229 (50%)	98 (86%)	15 (13%)	1 (1%)	14 43
12	R	268/536 (50%)	227 (85%)	38 (14%)	3 (1%)	12 37
13	S	157/166 (95%)	141 (90%)	16 (10%)	0	100 100
14	T	315/514 (61%)	292 (93%)	21 (7%)	2 (1%)	22 52
15	W	507/579 (88%)	433 (85%)	46 (9%)	28 (6%)	1 5
18	U	343/894 (38%)	277 (81%)	58 (17%)	8 (2%)	5 20
19	I	528/855 (62%)	491 (93%)	23 (4%)	14 (3%)	4 17
20	a	77/126 (61%)	76 (99%)	1 (1%)	0	100 100
20	h	77/126 (61%)	76 (99%)	1 (1%)	0	100 100
21	b	84/231 (36%)	82 (98%)	2 (2%)	0	100 100
21	i	84/231 (36%)	82 (98%)	2 (2%)	0	100 100
22	c	80/119 (67%)	77 (96%)	3 (4%)	0	100 100
22	j	80/119 (67%)	77 (96%)	3 (4%)	0	100 100
23	d	95/118 (80%)	91 (96%)	4 (4%)	0	100 100
23	k	81/118 (69%)	78 (96%)	3 (4%)	0	100 100
24	f	72/86 (84%)	69 (96%)	3 (4%)	0	100 100
24	m	72/86 (84%)	68 (94%)	4 (6%)	0	100 100
25	e	77/92 (84%)	76 (99%)	1 (1%)	0	100 100
25	l	77/92 (84%)	76 (99%)	1 (1%)	0	100 100
26	g	72/76 (95%)	70 (97%)	2 (3%)	0	100 100
26	n	63/76 (83%)	61 (97%)	2 (3%)	0	100 100
27	q	130/504 (26%)	119 (92%)	7 (5%)	4 (3%)	3 14
27	r	129/504 (26%)	119 (92%)	8 (6%)	2 (2%)	8 28
27	s	65/504 (13%)	62 (95%)	2 (3%)	1 (2%)	8 29
27	t	65/504 (13%)	64 (98%)	0	1 (2%)	8 29
28	K	144/225 (64%)	130 (90%)	8 (6%)	6 (4%)	2 9
29	o	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	10 33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	p	92/225 (41%)	90 (98%)	2 (2%)	0	100	100
31	Q	1308/1485 (88%)	1283 (98%)	25 (2%)	0	100	100
32	y	77/301 (26%)	75 (97%)	2 (3%)	0	100	100
All	All	10193/16097 (63%)	9369 (92%)	718 (7%)	106 (1%)	16	40

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1306	LYS
1	A	1367	ASN
1	A	1639	VAL
1	A	1653	ASP
1	A	1654	SER
4	E	59	ILE
6	J	592	ALA
15	W	228	LYS
15	W	240	ILE
15	W	259	GLN
15	W	263	VAL
15	W	267	SER
15	W	279	LYS
15	W	299	LEU
15	W	372	ASN
15	W	492	ASN
18	U	579	VAL
18	U	613	ASN
18	U	706	LEU
18	U	793	ASP
18	U	810	ILE
19	I	463	PRO
19	I	486	VAL
19	I	721	LYS
27	q	59	HIS
27	q	60	PRO
27	s	71	ILE
27	t	69	THR
28	K	78	PRO
28	K	90	PRO
1	A	136	ILE
1	A	626	GLY
1	A	1191	GLY

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Mol	Chain	Res	Type
1	A	1305	SER
1	A	1366	PRO
1	A	1419	ILE
6	J	709	VAL
7	L	765	ARG
9	N	4	VAL
11	P	205	LYS
12	R	52	PRO
12	R	234	SER
14	T	406	ILE
15	W	318	VAL
15	W	325	LEU
15	W	482	ASP
19	I	368	GLN
19	I	546	SER
19	I	618	ARG
27	q	9	ASN
28	K	136	LYS
28	K	172	LEU
29	o	160	LYS
1	A	625	PRO
1	A	803	ALA
1	A	1092	ILE
3	C	94	ILE
7	L	118	ASP
12	R	53	ARG
14	T	343	PRO
15	W	77	LYS
15	W	149	SER
15	W	243	VAL
15	W	246	MET
18	U	679	PHE
18	U	809	ASP
19	I	284	ARG
19	I	480	VAL
19	I	601	GLN
27	q	19	PRO
27	r	9	ASN
1	A	1519	THR
6	J	341	PRO
6	J	591	LEU
7	L	585	TYR

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Mol	Chain	Res	Type
15	W	204	ASP
15	W	272	GLU
15	W	554	ILE
18	U	845	PHE
19	I	617	GLU
28	K	65	ILE
29	o	32	PRO
1	A	108	MET
1	A	1365	ILE
1	A	1652	MET
6	J	357	LYS
15	W	301	GLY
15	W	330	GLY
19	I	254	GLN
19	I	256	GLY
19	I	321	GLU
19	I	796	LEU
1	A	1251	SER
7	L	763	ILE
10	O	20	PHE
15	W	229	GLN
15	W	376	PRO
15	W	549	HIS
7	L	764	PRO
15	W	205	VAL
15	W	208	PRO
3	C	87	GLN
15	W	251	GLY
27	r	65	PRO
28	K	17	PRO
15	W	270	PRO

5.3.2 Protein sidechains (i)

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1792/2108 (85%)	1767 (99%)	25 (1%)	62 86
3	C	787/866 (91%)	769 (98%)	18 (2%)	45 77
4	E	259/300 (86%)	254 (98%)	5 (2%)	52 81
6	J	242/751 (32%)	236 (98%)	6 (2%)	42 75
7	L	228/709 (32%)	225 (99%)	3 (1%)	65 88
8	M	117/209 (56%)	114 (97%)	3 (3%)	41 74
9	N	130/130 (100%)	129 (99%)	1 (1%)	79 93
10	O	259/361 (72%)	254 (98%)	5 (2%)	52 81
11	P	104/203 (51%)	101 (97%)	3 (3%)	37 72
12	R	227/457 (50%)	218 (96%)	9 (4%)	27 61
13	S	129/134 (96%)	127 (98%)	2 (2%)	58 84
14	T	273/441 (62%)	270 (99%)	3 (1%)	70 90
15	W	135/502 (27%)	133 (98%)	2 (2%)	60 85
18	U	313/806 (39%)	302 (96%)	11 (4%)	31 66
19	I	7/749 (1%)	2 (29%)	5 (71%)	0 0
All	All	5002/8726 (57%)	4901 (98%)	101 (2%)	50 79

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ARG
1	A	409	ARG
1	A	470	ARG
1	A	642	ARG
1	A	668	VAL
1	A	676	ARG
1	A	762	ARG
1	A	994	ASN
1	A	1109	LEU
1	A	1195	ARG
1	A	1216	LEU
1	A	1295	ILE
1	A	1505	LYS
1	A	1516	LYS
1	A	1517	LYS

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Mol	Chain	Res	Type
1	A	1518	LEU
1	A	1522	GLN
1	A	1527	ASN
1	A	1532	ARG
1	A	1555	LEU
1	A	1593	LEU
1	A	1622	MET
1	A	1636	LYS
1	A	1649	LYS
1	A	1813	ARG
3	C	128	LEU
3	C	138	LEU
3	C	139	HIS
3	C	144	CYS
3	C	159	LYS
3	C	160	ARG
3	C	161	TYR
3	C	162	ASP
3	C	175	GLN
3	C	238	ASN
3	C	313	GLN
3	C	394	ARG
3	C	495	ARG
3	C	513	ASN
3	C	673	LYS
3	C	775	ARG
3	C	786	ASN
3	C	814	ARG
4	E	55	LEU
4	E	59	ILE
4	E	62	LEU
4	E	131	LYS
4	E	147	LEU
6	J	236	ARG
6	J	237	LYS
6	J	239	ARG
6	J	240	THR
6	J	242	ILE
6	J	366	TYR
7	L	13	ASN
7	L	123	LEU
7	L	202	ARG

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Mol	Chain	Res	Type
8	M	134	GLN
8	M	212	ASN
8	M	215	ASN
9	N	101	CYS
10	O	78	LYS
10	O	79	ASN
10	O	146	MET
10	O	222	ARG
10	O	249	ARG
11	P	13	ARG
11	P	75	ASN
11	P	212	ASN
12	R	95	LYS
12	R	163	MET
12	R	165	VAL
12	R	166	ARG
12	R	234	SER
12	R	235	ARG
12	R	276	GLN
12	R	281	ASN
12	R	305	ARG
13	S	61	MET
13	S	102	ASN
14	T	220	VAL
14	T	308	ARG
14	T	489	TYR
15	W	145	ASN
15	W	193	LEU
18	U	550	ARG
18	U	589	ARG
18	U	656	ASN
18	U	660	LYS
18	U	662	ILE
18	U	666	ARG
18	U	667	SER
18	U	672	MET
18	U	702	ASN
18	U	737	ARG
18	U	808	LYS
19	I	235	VAL
19	I	399	VAL
19	I	486	VAL

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Mol	Chain	Res	Type
19	I	526	MET
19	I	795	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	328	HIS
1	A	361	HIS
1	A	711	GLN
1	A	723	ASN
1	A	775	ASN
1	A	793	ASN
1	A	860	GLN
1	A	1215	ASN
1	A	1296	GLN
1	A	1373	GLN
1	A	1487	HIS
1	A	1522	GLN
1	A	1580	HIS
1	A	1811	ASN
3	C	60	HIS
3	C	82	GLN
3	C	139	HIS
3	C	238	ASN
3	C	245	HIS
3	C	513	ASN
3	C	523	GLN
3	C	903	HIS
4	E	191	GLN
4	E	253	ASN
6	J	188	GLN
6	J	311	GLN
6	J	347	HIS
6	J	410	HIS
8	M	212	ASN
9	N	37	HIS
10	O	14	ASN
10	O	79	ASN
10	O	113	ASN
11	P	75	ASN
11	P	212	ASN
12	R	189	ASN

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Mol	Chain	Res	Type
12	R	231	HIS
12	R	242	GLN
12	R	279	HIS
13	S	102	ASN
14	T	191	HIS
14	T	216	ASN
14	T	283	HIS
14	T	324	HIS
14	T	446	ASN
15	W	145	ASN
18	U	656	ASN
18	U	665	HIS
18	U	702	ASN
18	U	718	HIS
18	U	765	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	G	69/272 (25%)	55 (79%)	12 (17%)
17	H	133/188 (70%)	52 (39%)	8 (6%)
2	B	97/117 (82%)	44 (45%)	5 (5%)
5	F	96/107 (89%)	41 (42%)	6 (6%)
All	All	395/684 (57%)	192 (48%)	31 (7%)

All (192) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	8	G
2	B	9	G
2	B	10	U
2	B	11	U
2	B	20	G
2	B	21	A
2	B	22	U
2	B	23	C
2	B	25	C
2	B	26	A
2	B	28	A
2	B	35	U
2	B	36	C

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Mol	Chain	Res	Type
2	B	38	C
2	B	45	C
2	B	47	A
2	B	48	A
2	B	57	G
2	B	67	A
2	B	69	A
2	B	70	A
2	B	71	C
2	B	73	C
2	B	74	U
2	B	75	G
2	B	77	G
2	B	78	U
2	B	79	C
2	B	80	U
2	B	81	U
2	B	82	A
2	B	83	A
2	B	84	C
2	B	85	C
2	B	86	C
2	B	87	A
2	B	88	A
2	B	89	U
2	B	90	U
2	B	91	U
2	B	92	U
2	B	94	U
2	B	95	G
2	B	96	A
5	F	5	U
5	F	6	C
5	F	7	G
5	F	10	U
5	F	12	G
5	F	26	U
5	F	27	A
5	F	28	A
5	F	29	A
5	F	33	G
5	F	34	G

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Mol	Chain	Res	Type
5	F	36	A
5	F	37	C
5	F	39	A
5	F	40	U
5	F	41	A
5	F	42	C
5	F	43	A
5	F	44	G
5	F	45	A
5	F	46	G
5	F	47	A
5	F	49	G
5	F	51	U
5	F	52	U
5	F	53	A
5	F	54	G
5	F	58	G
5	F	59	G
5	F	61	C
5	F	66	C
5	F	67	G
5	F	68	C
5	F	69	A
5	F	74	U
5	F	78	A
5	F	79	C
5	F	81	C
5	F	82	A
5	F	84	A
5	F	87	C
16	G	2	U
16	G	3	A
16	G	4	A
16	G	5	G
16	G	7	G
16	G	11	A
16	G	13	C
16	G	15	U
16	G	17	U
16	G	20	A
16	G	21	A
16	G	22	C

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Mol	Chain	Res	Type
16	G	23	U
16	G	24	G
16	G	25	G
16	G	26	U
16	G	27	U
16	G	28	A
16	G	29	C
16	G	30	C
16	G	31	U
16	G	119	G
16	G	121	G
16	G	122	U
16	G	123	U
16	G	124	U
16	G	125	C
16	G	126	C
16	G	127	U
16	G	128	U
16	G	129	G
16	G	130	A
16	G	131	U
16	G	132	G
16	G	133	A
16	G	134	U
16	G	135	G
16	G	136	U
16	G	137	C
16	G	138	A
16	G	139	U
16	G	140	A
16	G	141	C
16	G	142	U
16	G	143	U
16	G	144	A
16	G	145	U
16	G	146	C
16	G	147	C
16	G	148	U
16	G	149	G
16	G	150	U
16	G	151	C
16	G	153	C

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Mol	Chain	Res	Type
16	G	154	U
17	H	15	U
17	H	16	U
17	H	17	U
17	H	19	G
17	H	20	G
17	H	23	A
17	H	25	G
17	H	28	C
17	H	29	A
17	H	30	A
17	H	31	G
17	H	32	U
17	H	34	U
17	H	36	G
17	H	37	U
17	H	38	A
17	H	39	U
17	H	40	C
17	H	41	U
17	H	43	U
17	H	44	U
17	H	45	C
17	H	46	U
17	H	47	U
17	H	48	A
17	H	49	U
17	H	50	C
17	H	51	A
17	H	68	G
17	H	70	C
17	H	94	A
17	H	101	U
17	H	102	U
17	H	105	G
17	H	106	G
17	H	107	A
17	H	109	C
17	H	112	G
17	H	149	A
17	H	151	C
17	H	154	C

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Mol	Chain	Res	Type
17	H	156	U
17	H	157	G
17	H	164	C
17	H	166	G
17	H	167	U
17	H	168	A
17	H	177	A
17	H	178	A
17	H	179	C
17	H	180	G
17	H	182	U

All (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	78	U
2	B	79	C
2	B	80	U
2	B	92	U
2	B	95	G
5	F	5	U
5	F	33	G
5	F	43	A
5	F	45	A
5	F	50	A
5	F	58	G
16	G	1	G
16	G	2	U
16	G	3	A
16	G	16	G
16	G	21	A
16	G	22	C
16	G	133	A
16	G	141	C
16	G	143	U
16	G	145	U
16	G	147	C
16	G	148	U
17	H	29	A
17	H	30	A
17	H	31	G
17	H	34	U

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Mol	Chain	Res	Type
17	H	46	U
17	H	49	U
17	H	50	C
17	H	156	U

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	SEP	R	224	12	8,9,10	0.85	0	8,12,14	2.02	1 (12%)
12	SEP	R	232	12	8,9,10	0.91	0	8,12,14	2.06	1 (12%)

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
12	SEP	R	224	12	-	1/5/8/10	-
12	SEP	R	232	12	-	3/5/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	R	232	SEP	OG-CB-CA	5.17	113.17	108.14
12	R	224	SEP	OG-CB-CA	4.66	112.67	108.14

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	R	224	SEP	N-CA-CB-OG
12	R	232	SEP	CB-OG-P-O1P
12	R	232	SEP	CB-OG-P-O2P
12	R	232	SEP	CB-OG-P-O3P

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	R	232	SEP	3	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 14 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
33	IHP	A	3000	-	36,36,36	0.70	0	54,60,60	0.97	0
34	GTP	C	1500	35	26,34,34	0.96	1 (3%)	32,54,54	1.46	4 (12%)

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
33	IHP	A	3000	-	-	8/30/54/54	0/1/1/1
34	GTP	C	1500	35	-	4/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	C	1500	GTP	C6-N1	-2.74	1.33	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	C	1500	GTP	PA-O3A-PB	-3.98	119.17	132.83
34	C	1500	GTP	PB-O3B-PG	-3.53	120.71	132.83
34	C	1500	GTP	C5-C6-N1	2.44	118.26	113.95
34	C	1500	GTP	C8-N7-C5	2.43	107.61	102.99

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	A	3000	IHP	C6-C1-O11-P1
33	A	3000	IHP	C4-O14-P4-O44
33	A	3000	IHP	C6-O16-P6-O26
34	C	1500	GTP	C5'-O5'-PA-O3A
33	A	3000	IHP	C2-C1-O11-P1
33	A	3000	IHP	C1-C2-O12-P2
33	A	3000	IHP	C3-C2-O12-P2
33	A	3000	IHP	C6-O16-P6-O36
34	C	1500	GTP	C5'-O5'-PA-O1A
34	C	1500	GTP	C5'-O5'-PA-O2A
33	A	3000	IHP	C1-O11-P1-O31
34	C	1500	GTP	PB-O3A-PA-O2A

There are no ring outliers.

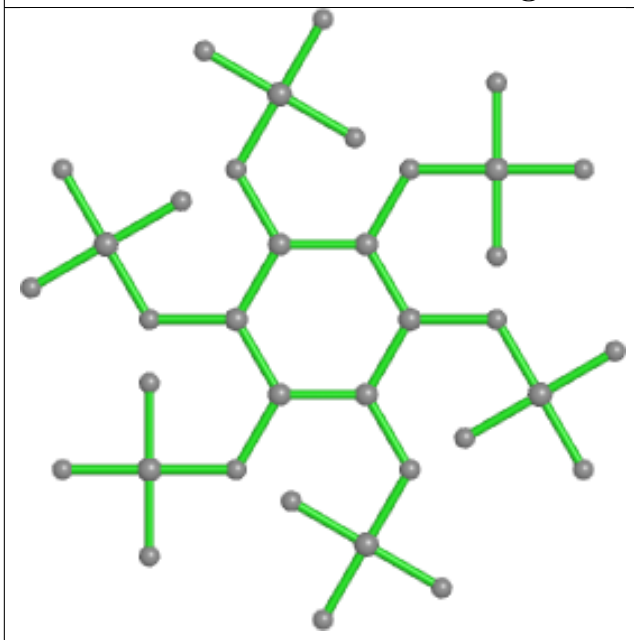
2 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	A	3000	IHP	1	0
34	C	1500	GTP	22	0

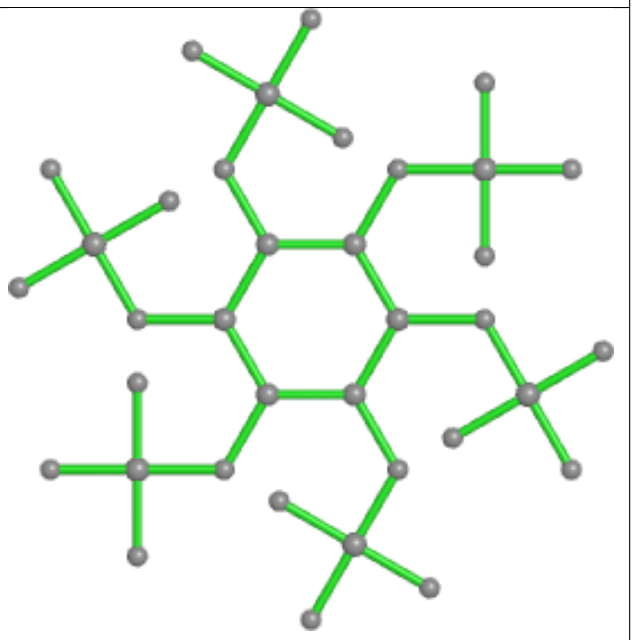
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

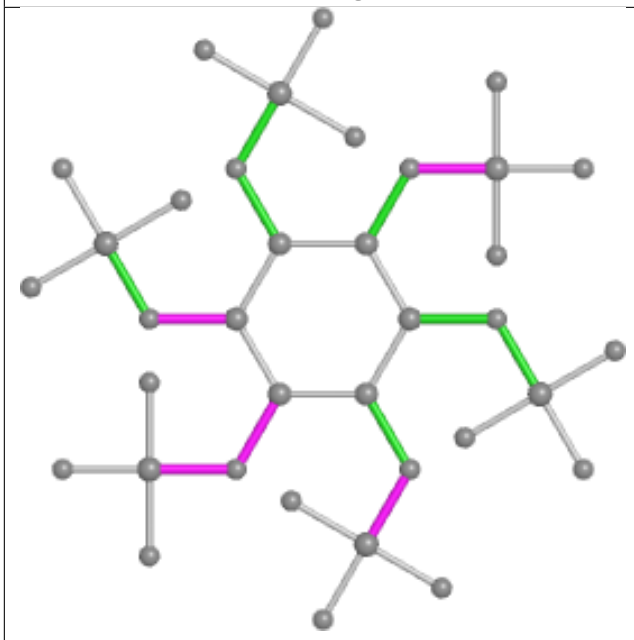
Ligand IHP A 3000



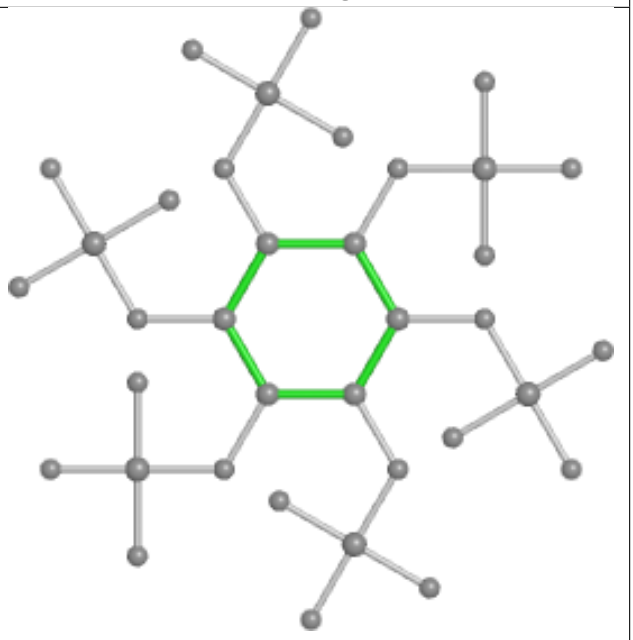
Bond lengths



Bond angles

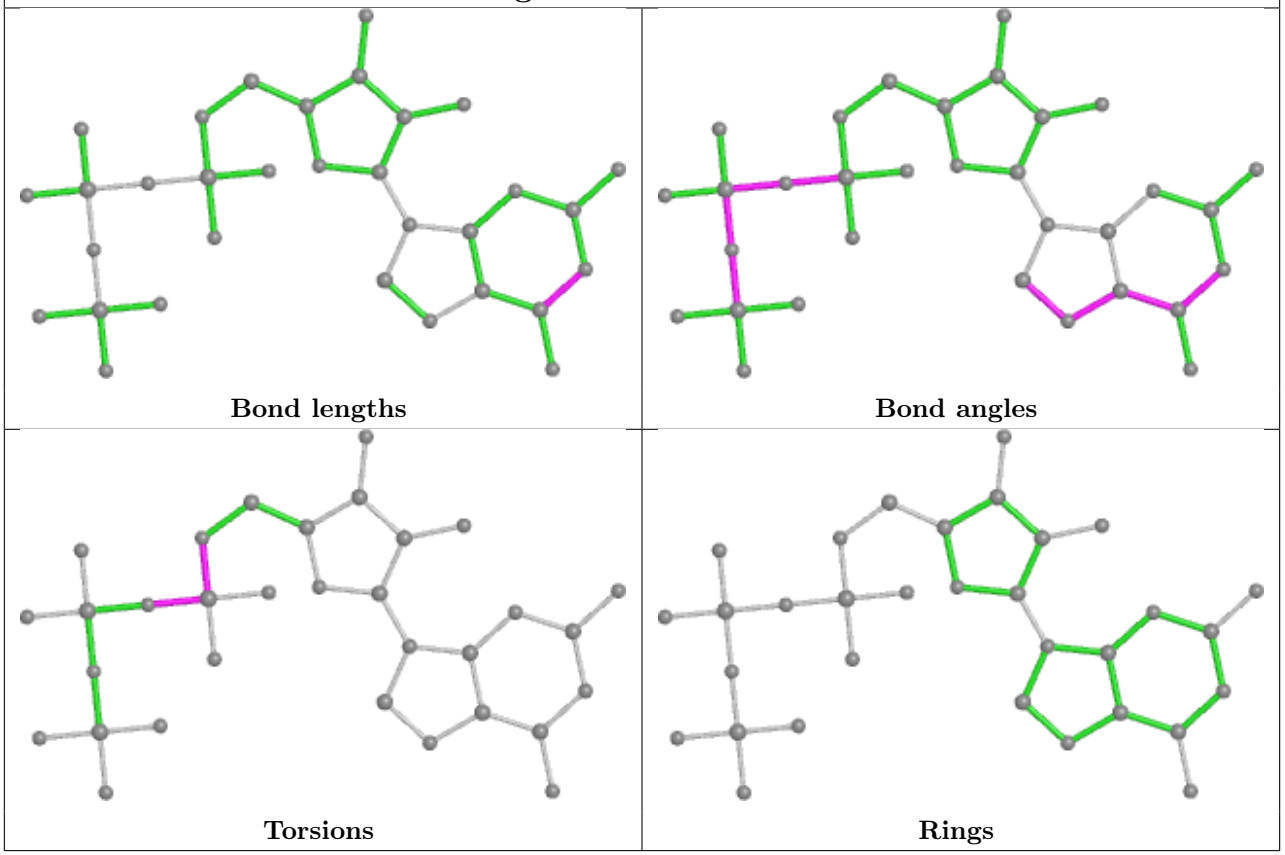


Torsions



Rings

Ligand GTP C 1500



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

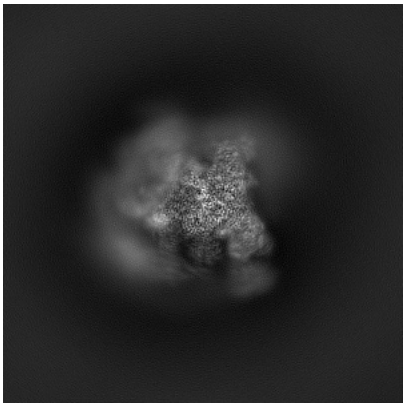
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9646. These allow visual inspection of the internal detail of the map and identification of artifacts.

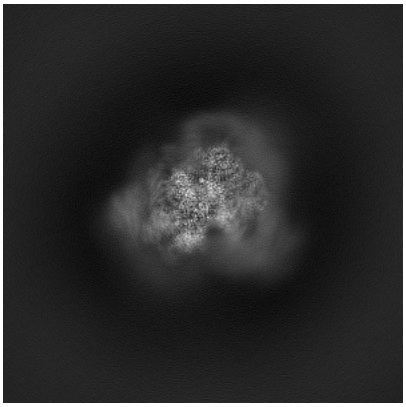
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

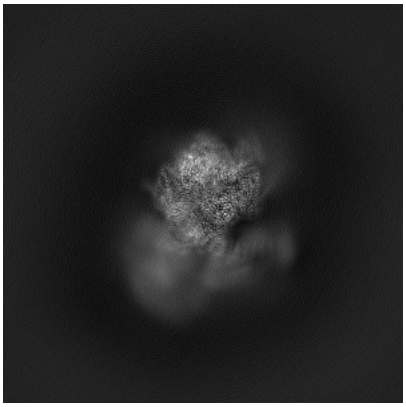
6.1.1 Primary map



X



Y

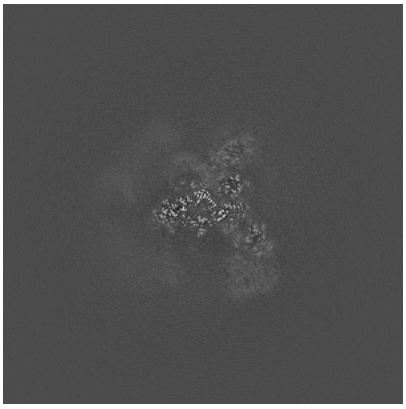


Z

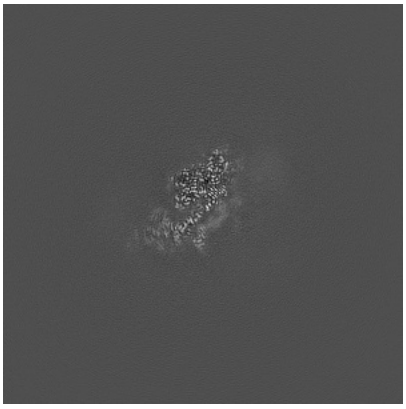
The images above show the map projected in three orthogonal directions.

6.2 Central slices

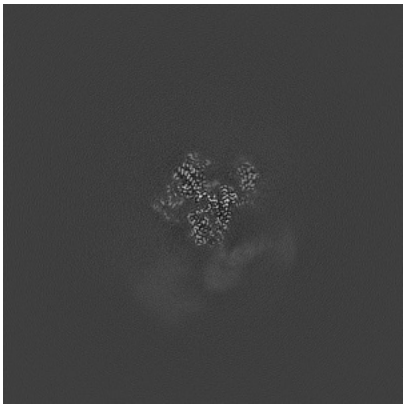
6.2.1 Primary map



X Index: 200



Y Index: 200



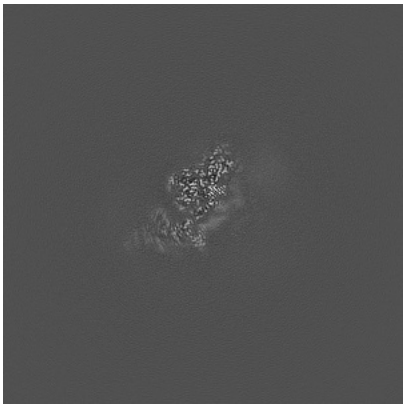
Z Index: 200

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

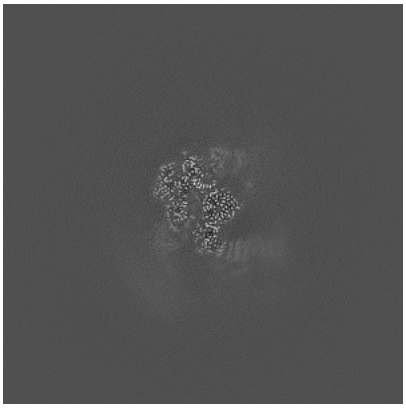
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 210



Y Index: 201

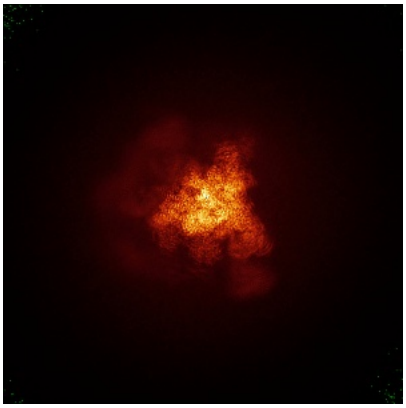


Z Index: 185

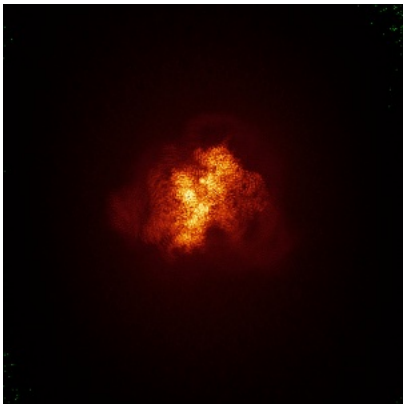
The images above show the largest variance slices of the map in three orthogonal directions.

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

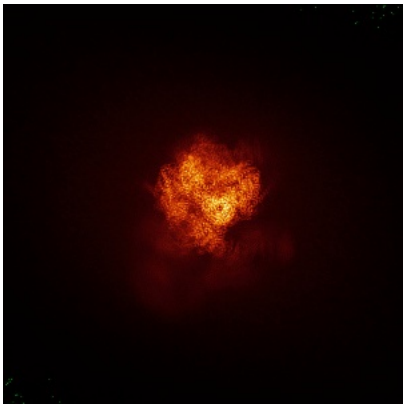
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

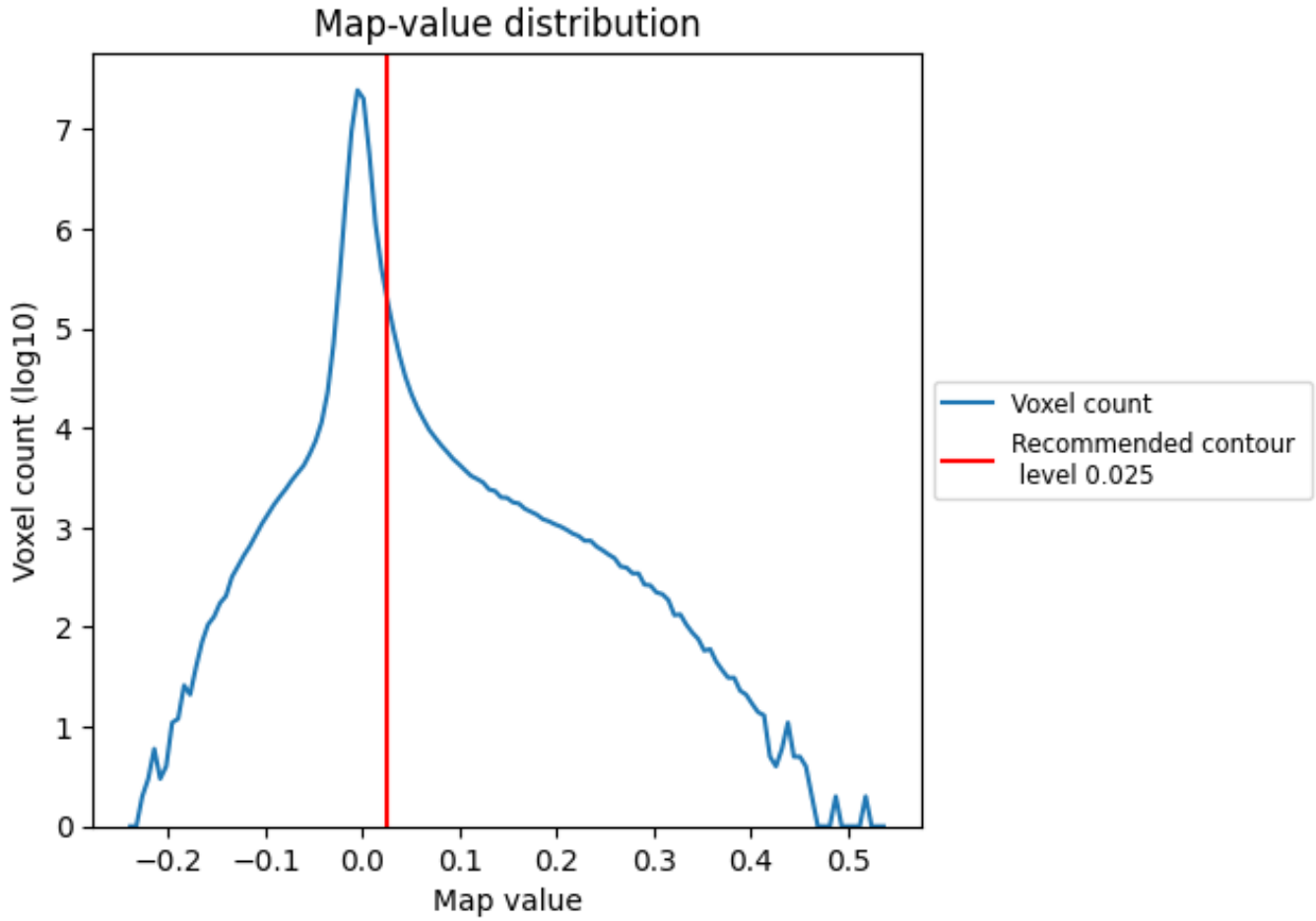
6.6 Mask visualisation (i)

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

7 Map analysis

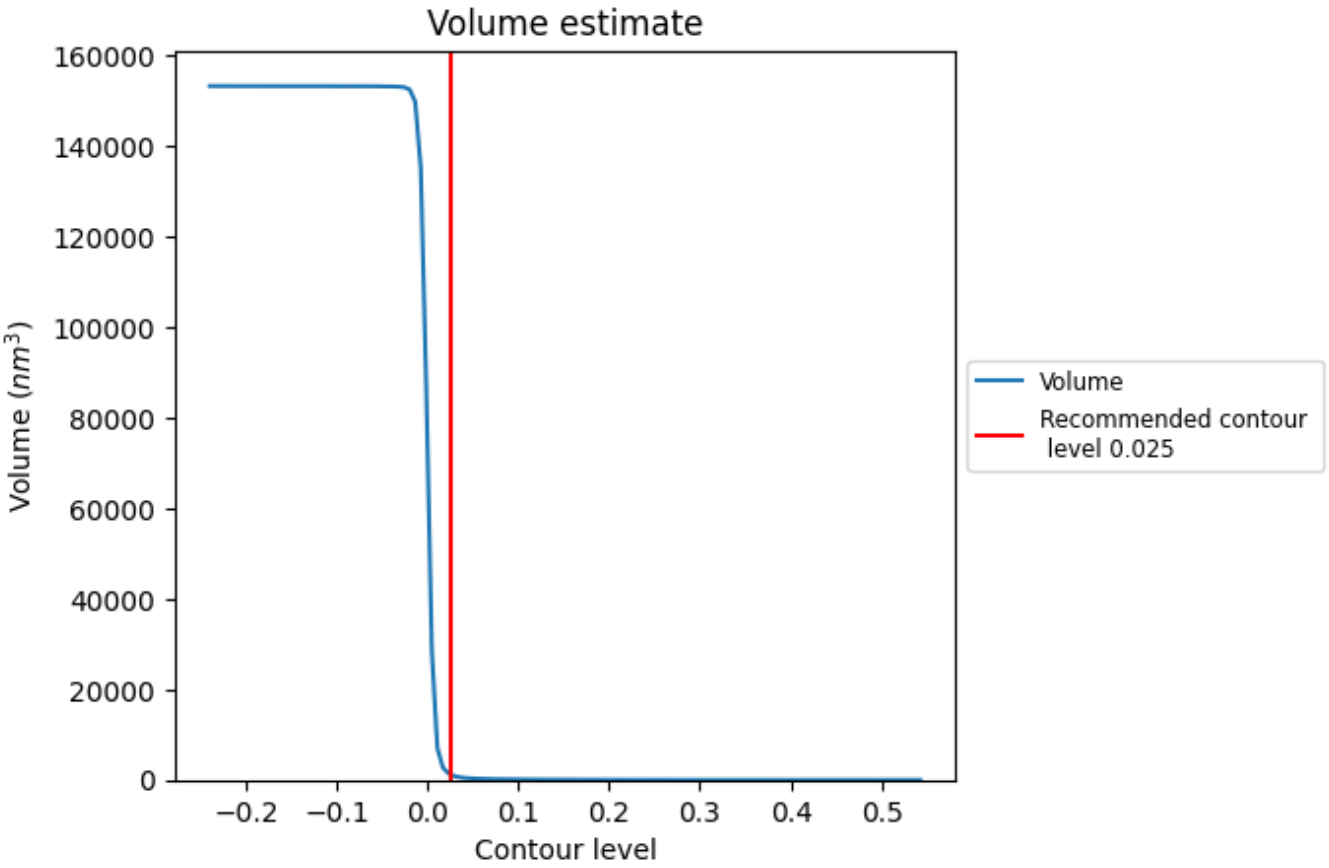
This section contains the results of statistical analysis of the map.

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.

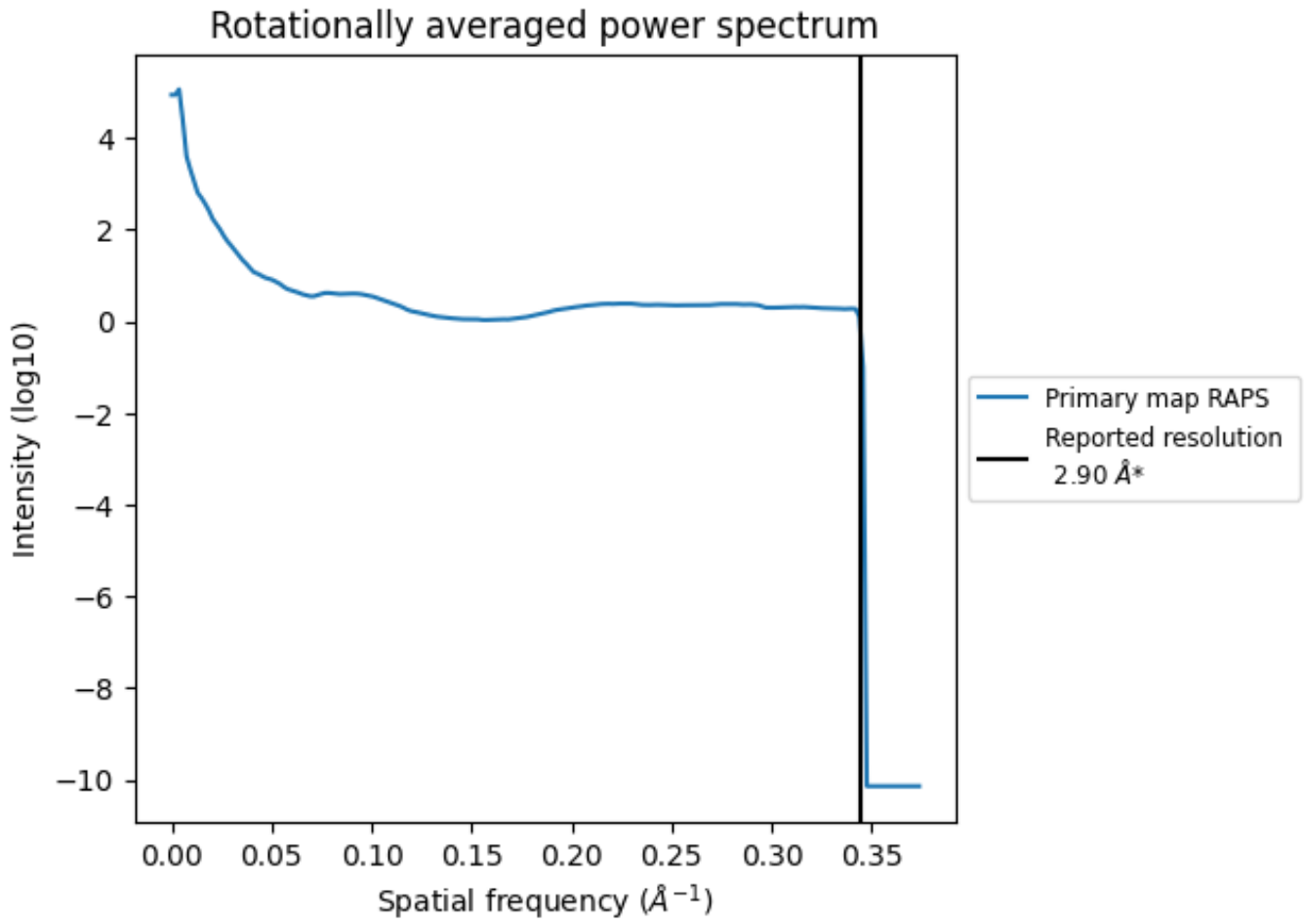
7.2 Volume estimate



The volume at the recommended contour level is 1297 nm^3; this corresponds to an approximate mass of 1172 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 0.345 Å^{-1}

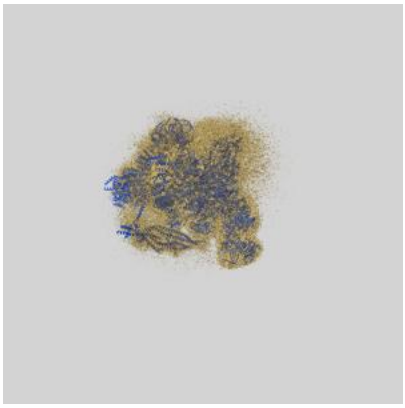
8 Fourier-Shell correlation (i)

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

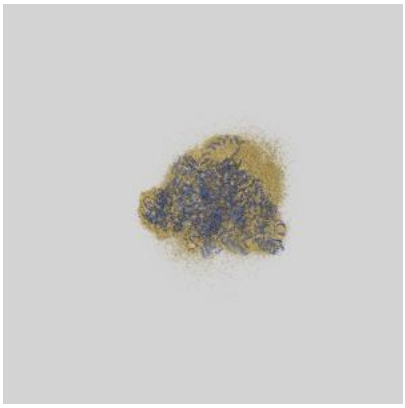
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9646 and PDB model 6ID0. Per-residue inclusion information can be found in section 3 on page 12.

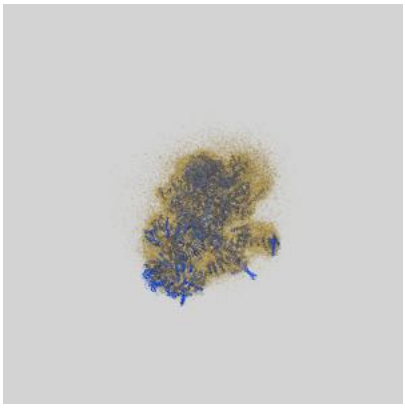
9.1 Map-model overlay



X



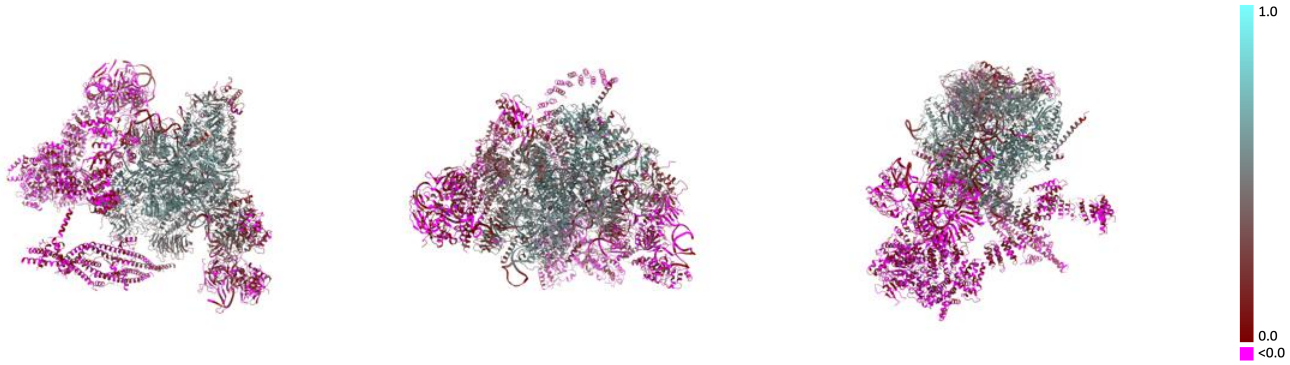
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 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.

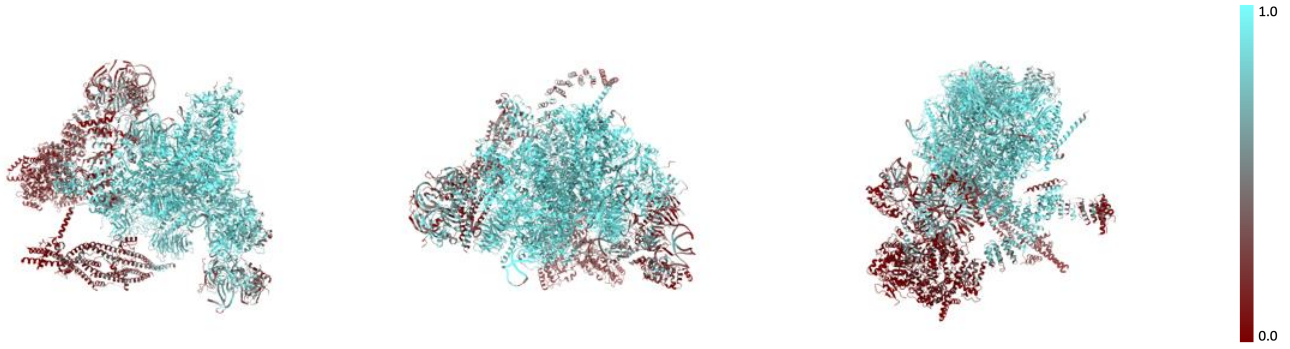
9.2 Q-score mapped to coordinate model (i)



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.

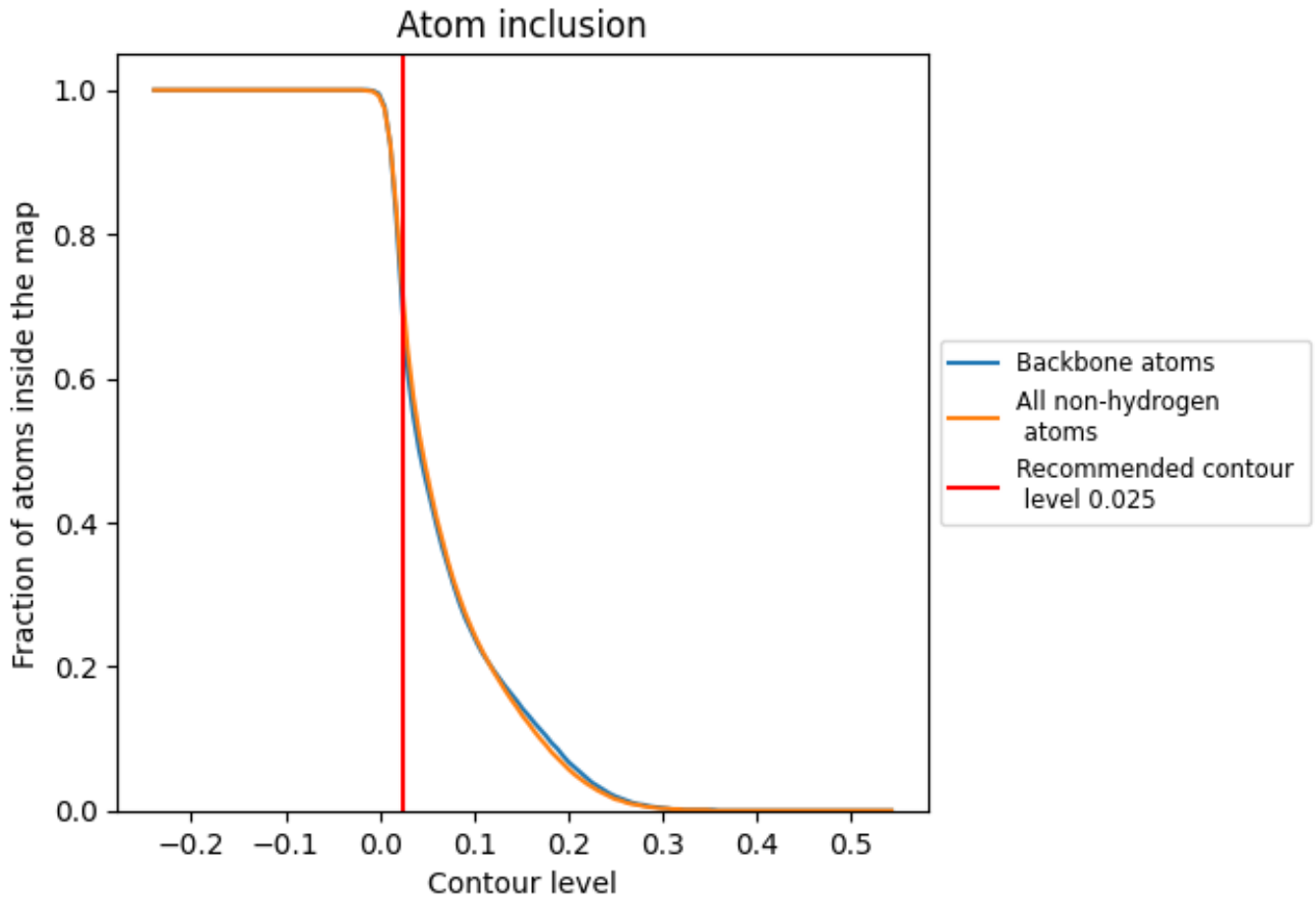
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 70% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7050	0.3140
A	0.9230	0.5020
B	0.8300	0.3370
C	0.8520	0.3270
E	0.8910	0.4110
F	0.9420	0.4650
G	0.6680	0.1420
H	0.5130	0.1100
I	0.5350	0.0560
J	0.7370	0.3250
K	0.2560	0.0580
L	0.6480	0.3380
M	0.8870	0.4960
N	0.9570	0.5500
O	0.8310	0.3930
P	0.8380	0.4610
Q	0.0690	-0.0050
R	0.8700	0.4660
S	0.9190	0.4670
T	0.9760	0.5980
U	0.8780	0.4540
W	0.8620	0.3360
a	0.6670	0.1900
b	0.4910	0.0340
c	0.6480	0.0540
d	0.6400	0.0330
e	0.4810	0.0550
f	0.4930	-0.0020
g	0.4850	0.0500
h	0.4700	0.0160
i	0.3660	0.0240
j	0.3520	-0.0110
k	0.3010	-0.0100
l	0.2530	-0.0090
m	0.3130	0.0350

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
n	0.3830	0.0330
o	0.1870	-0.0010
p	0.3730	0.0250
q	0.1150	0.0380
r	0.1850	0.0200
s	0.2330	0.0550
t	0.1400	0.0050
y	0.3920	0.0170