Full wwPDB EM Validation Report

Dec 17, 2024 – 04:33 pm GMT

PDB ID	:	9ESH
EMDB ID	:	EMD-19941
Title	:	Structure of a B-state intermediate committed to discard (Bd-I state)
Authors	:	Soni, K.; Wild, K.; Sinning, I.
Deposited on	:	2024-03-26
Resolution	:	3.20 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:

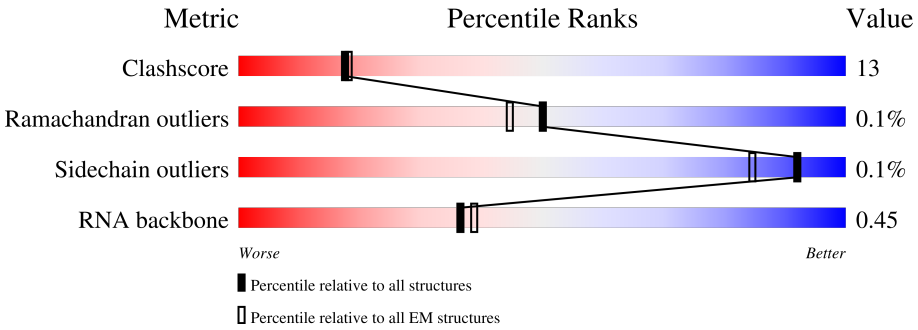
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	1	29	62% 31% 45% 24%
2	2	186	8% 5% 6% 87%
3	5	120	53% 22% 9% 15%
4	6	99	37% 26% 39% 27% 7%
5	A	2363	56% 18% 26%
6	B	984	69% 25% 7%
7	C	340	9% 57% 32% 11%

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Mol	Chain	Length	Quality of chain
8	D	97	64% 35%
9	E	147	6% 48% 18% 34%
10	F	117	5% 32% 37% 31%
11	G	115	8% 49% 40% 11%
12	H	84	74% 21% 5%
13	I	78	54% 38% 6%
14	J	77	73% 22% 5%
15	K	473	59% 24% 17%
16	L	557	8% 34% 8% 58%
17	M	354	40% 45% 21% 34%
18	N	1284	100% 78% 22%
19	O	146	74% 25%
20	P	388	33% 42% 27% 30%
21	Q	265	29% 5% 66%
22	R	674	53% 59% 30% 11%
23	S	488	27% 18% 9% 73%
23	T	488	26% 15% 12% 73%
23	U	488	86% 71% 17% 12%
23	V	488	27% 20% 7% 73%
24	W	757	38% 47% 22% 31%
25	X	790	81% 56% 27% 17%
26	Y	229	43% 32% 20% 48%
27	Z	187	67% 52% 31% 17%
28	a	558	12% 27% 73%
29	b	293	26% 35% 65%

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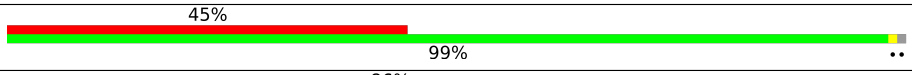
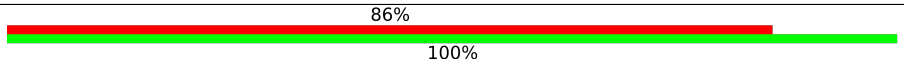
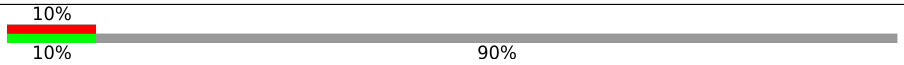
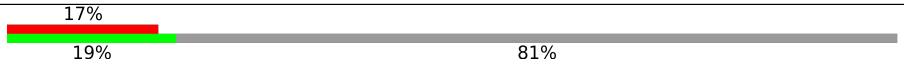
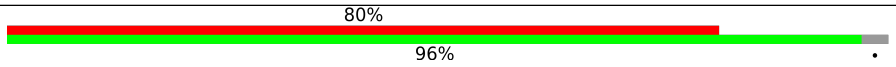
Mol	Chain	Length	Quality of chain
30	c	887	
31	d	155	
32	f	22	
33	m	797	
34	r	346	
35	y	534	
36	z	647	

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 90868 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	29	605	272	91	213	29	0	0

- Molecule 2 is a RNA chain called U2snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	24	500	224	79	173	24	0	0

- Molecule 3 is a RNA chain called U5snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	5	102	2149	963	358	726	102	0	0

- Molecule 4 is a RNA chain called U6snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	6	92	1970	882	365	631	92	0	0

- Molecule 5 is a protein called Pre-mRNA-splicing factor spp42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	A	1737	14402	9229	2543	2565	65	0	0

- Molecule 6 is a protein called Pre-mRNA-splicing factor cwf10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	B	918	7298	4650	1251	1362	35	0	0

- Molecule 7 is a protein called Pre-mRNA-splicing factor cwf17.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	301	Total	C	N	O	S	0	0
			2328	1460	415	442	11		

- Molecule 8 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	96	Total	C	N	O	S	0	0
			760	470	147	136	7		

- Molecule 9 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	97	Total	C	N	O	S	0	0
			726	462	129	130	5		

- Molecule 10 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	81	Total	C	N	O	S	0	0
			638	407	109	118	4		

- Molecule 11 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	102	Total	C	N	O	S	0	0
			819	516	150	149	4		

- Molecule 12 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	80	Total	C	N	O	S	0	0
			652	422	113	115	2		

- Molecule 13 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	73	Total	C	N	O	S	0	0
			574	373	95	104	2		

- Molecule 14 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	73	Total	C	N	O	S	0	0
			573	366	98	108	1		

- Molecule 15 is a protein called Pre-mRNA-splicing factor prp5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	391	Total	C	N	O	S	0	0
			3053	1925	551	563	14		

- Molecule 16 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	234	Total	C	N	O	S	0	0
			1849	1154	345	345	5		

- Molecule 17 is a protein called Pre-mRNA-splicing factor cwf5.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	234	Total	C	N	O	S	0	0
			1818	1131	329	343	15		

- Molecule 18 is a protein called Pre-mRNA-splicing factor cwf11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	1284	Total	C	N	O	S	0	0
			10461	6715	1732	1969	45		

- Molecule 19 is a protein called Pre-mRNA-splicing factor cwf14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	144	Total	C	N	O	S	0	0
			1176	733	216	214	13		

- Molecule 20 is a protein called Pre-mRNA-splicing factor cwf2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	271	Total	C	N	O	S	0	0
			2178	1354	397	416	11		

- Molecule 21 is a protein called Pre-mRNA-splicing factor cwf15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	90	Total	C	N	O	S	0	0
			752	467	146	138	1		

- Molecule 22 is a protein called Pre-mRNA-splicing factor cwf4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	603	Total	C	N	O	S	0	0
			5108	3280	892	913	23		

- Molecule 23 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	132	Total	C	N	O	S	0	0
			1055	664	181	207	3		
23	T	134	Total	C	N	O	S	0	0
			1069	671	183	212	3		
23	U	430	Total	C	N	O	S	0	0
			2870	1806	492	563	9		
23	V	131	Total	C	N	O	S	0	0
			1044	655	180	206	3		

- Molecule 24 is a protein called Pre-mRNA-splicing factor cdc5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	526	Total	C	N	O	S	0	0
			4346	2710	792	832	12		

- Molecule 25 is a protein called Pre-mRNA-splicing factor cwf3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	654	Total	C	N	O	S	0	0
			5467	3534	918	996	19		

- Molecule 26 is a protein called Pre-mRNA-splicing factor syf2.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	Y	120	Total	C	N	O	0	0
			1049	656	195	198		

- Molecule 27 is a protein called Pre-mRNA-splicing factor cwf7.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	155	Total	C	N	O	S	0	0
			1232	766	220	243	3		

- Molecule 28 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	152	Total	C	N	O	S	0	0
			1035	644	185	205	1		

- Molecule 29 is a protein called Pre-mRNA-splicing factor cwf21.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	104	Total	C	N	O	S	0	0
			822	503	148	169	2		

- Molecule 30 is a protein called Pre-mRNA-splicing factor cwf22.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	204	Total	C	N	O	S	0	0
			1678	1071	280	315	12		

- Molecule 31 is a protein called Peptidyl-prolyl cis-trans isomerase ppi1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	154	Total	C	N	O	S	0	0
			1179	750	202	223	4		

- Molecule 32 is a protein called UNK1.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	f	22	Total	C	N	O	0	0
			110	66	22	22		

- Molecule 33 is a protein called G-patch domain-containing protein C1486.03.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	m	81	Total	C	N	O	S	0	0
			649	413	112	122	2		

- Molecule 34 is a protein called UNK2.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	r	67	Total	C	N	O	0	0
			335	201	67	67		

- Molecule 35 is a protein called Uncharacterized protein C20H4.06c.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	y	185	Total	C	N	O	S	0	0
			1480	921	257	298	4		

- Molecule 36 is a protein called Putative pre-mRNA-splicing factor ATP-dependent RNA helicase C20H4.09.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	z	626	Total	C	N	O	S	0	0
			4980	3193	835	933	19		

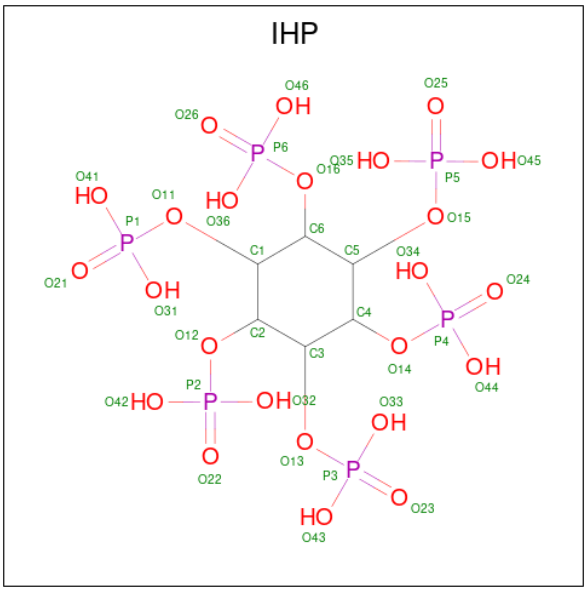
- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
37	6	3	Total	Mg	0
			3	3	
37	B	1	Total	Mg	0
			1	1	

- Molecule 38 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

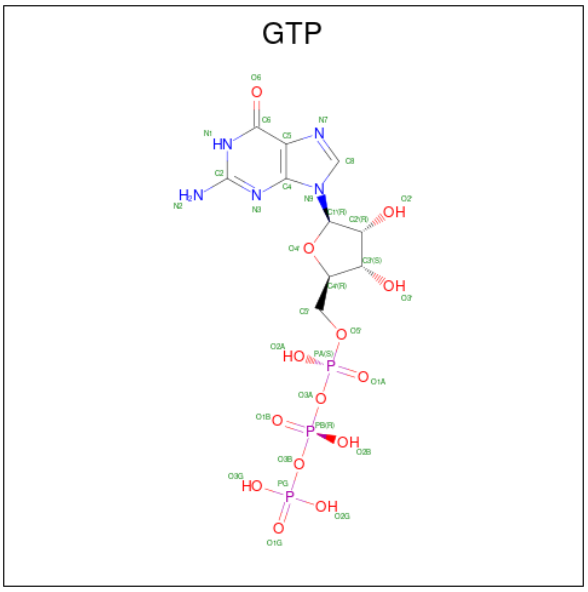
Mol	Chain	Residues	Atoms		AltConf
38	6	1	Total	K	0
			1	1	

- Molecule 39 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 40 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



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

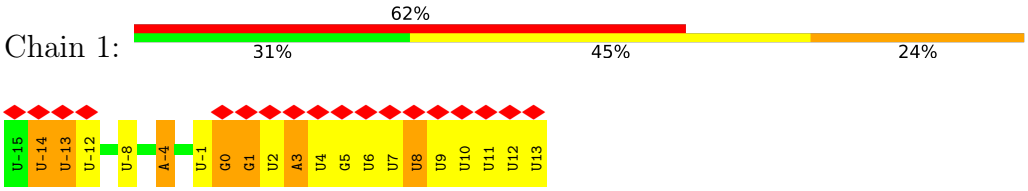
- Molecule 41 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
41	M	2	Total Zn 2 2	0
41	O	3	Total Zn 3 3	0
41	P	1	Total Zn 1 1	0

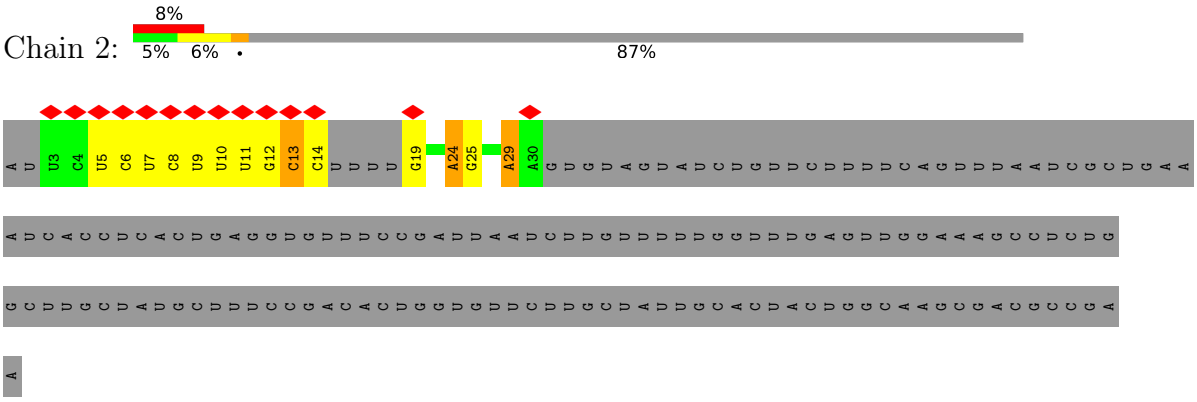
3 Residue-property plots (i)

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

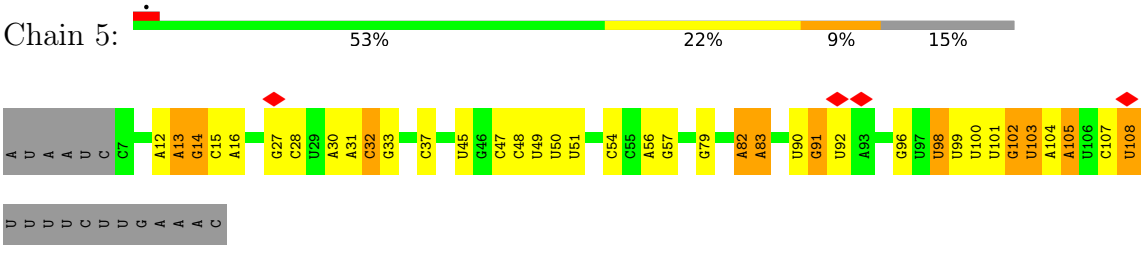
• Molecule 1: pre-mRNA



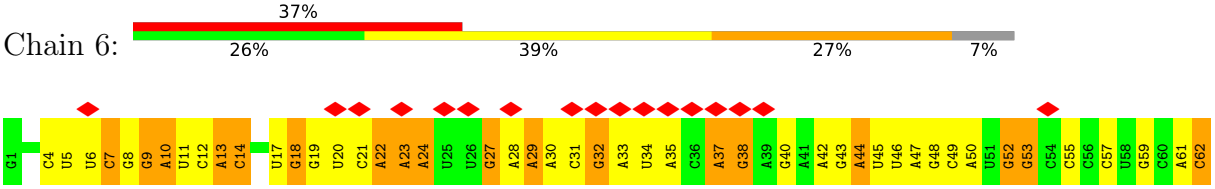
• Molecule 2: U2snRNA

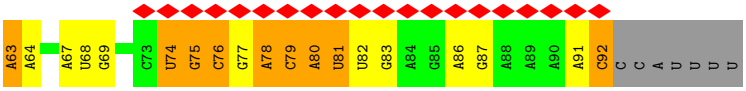


• Molecule 3: U5snRNA



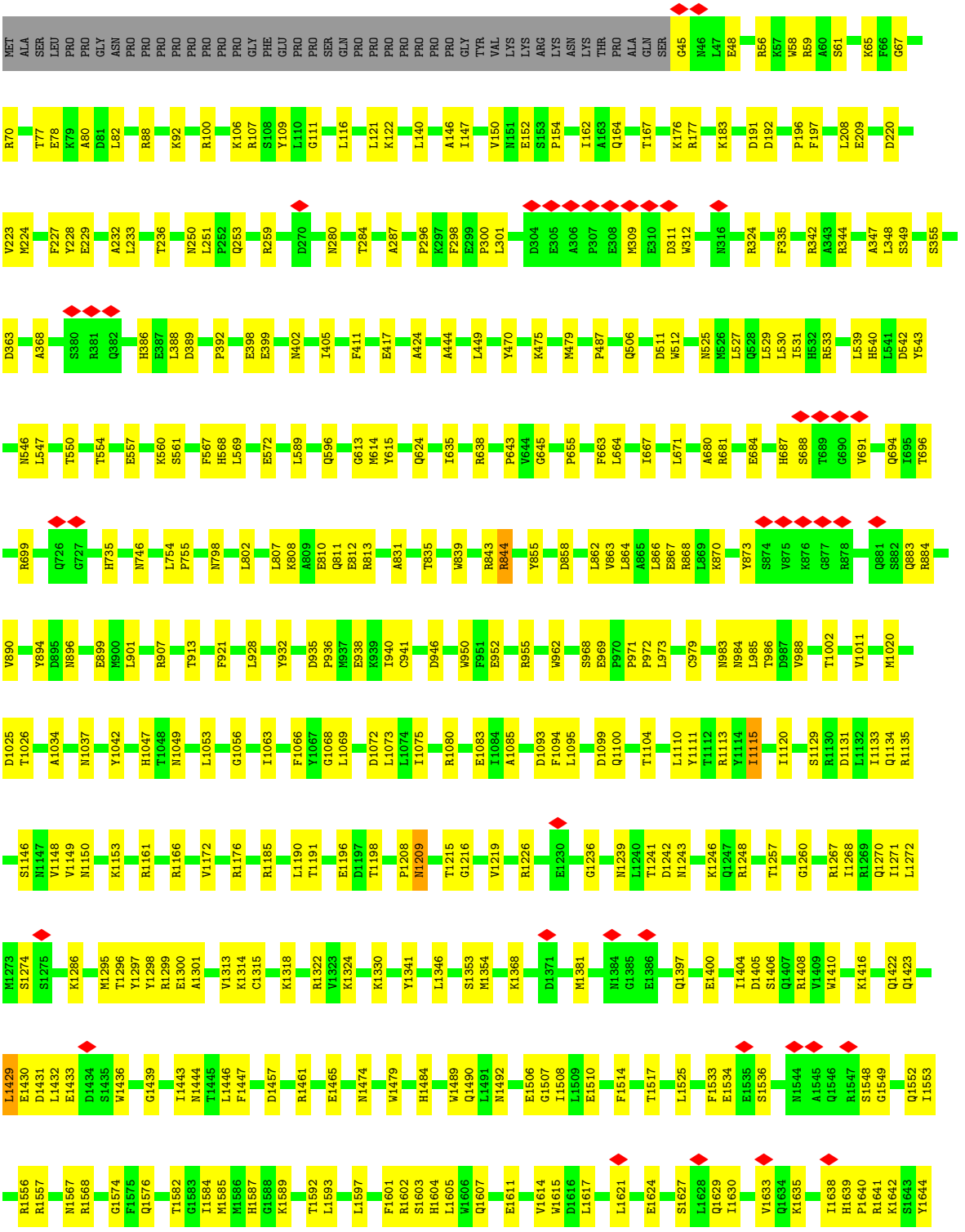
• Molecule 4: U6snRNA

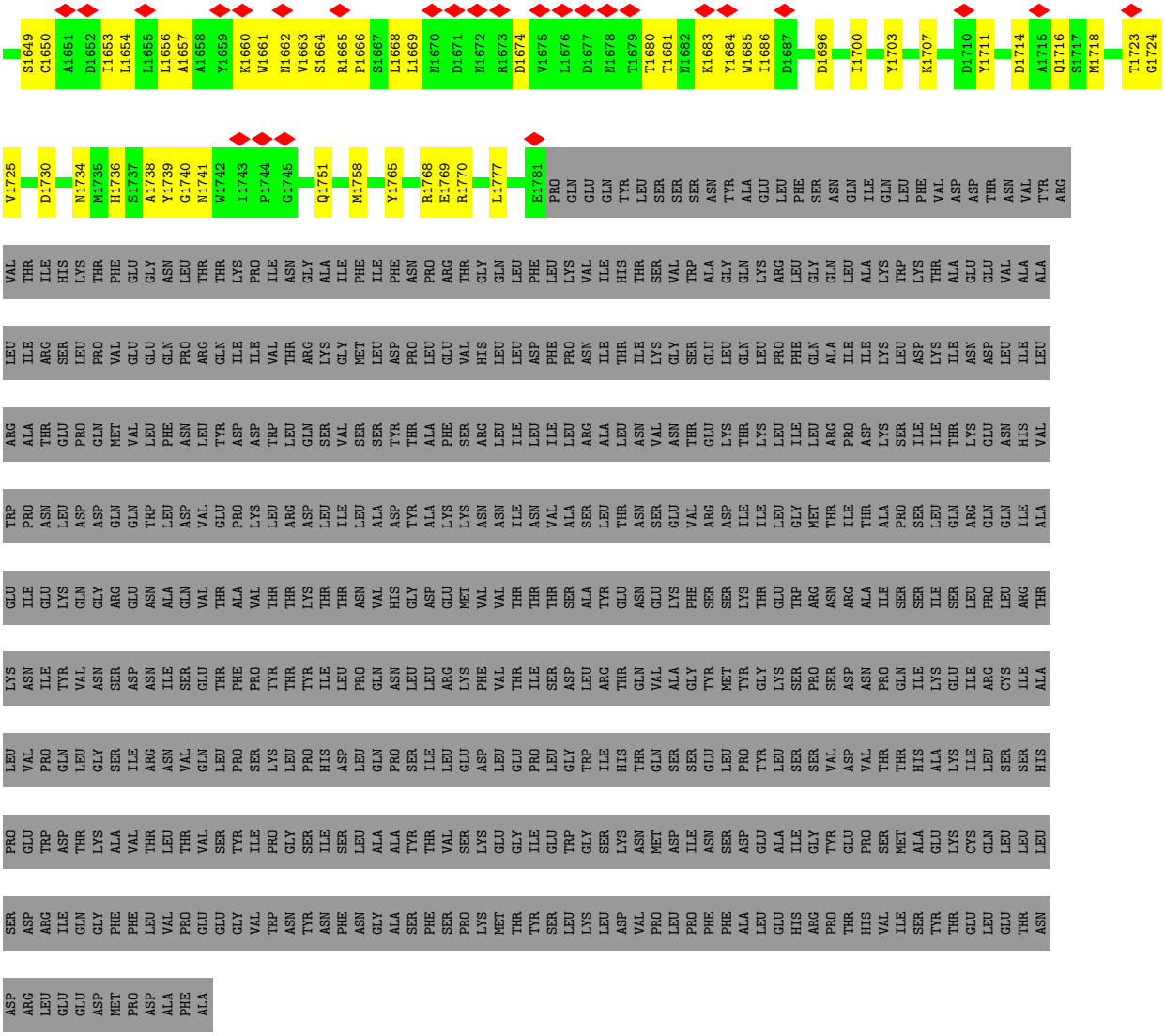




• Molecule 5: Pre-mRNA-splicing factor spp42

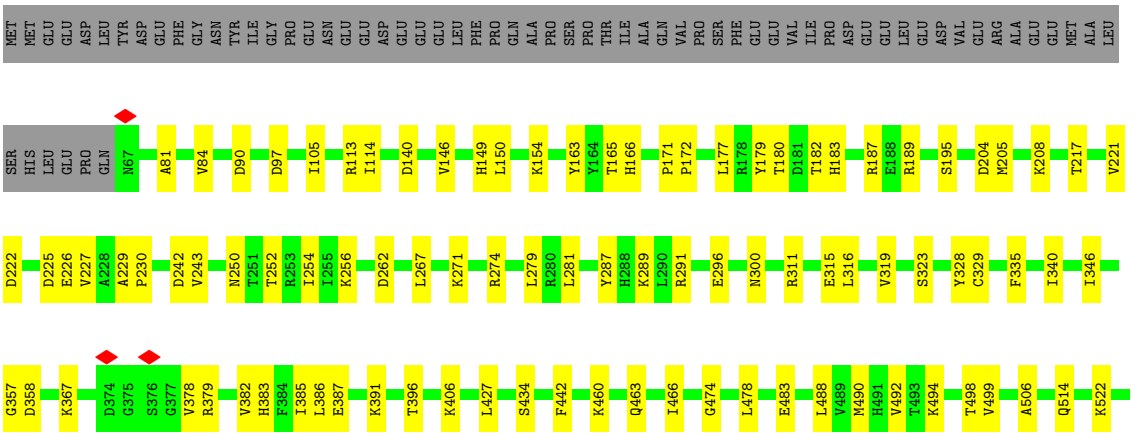
Chain A:

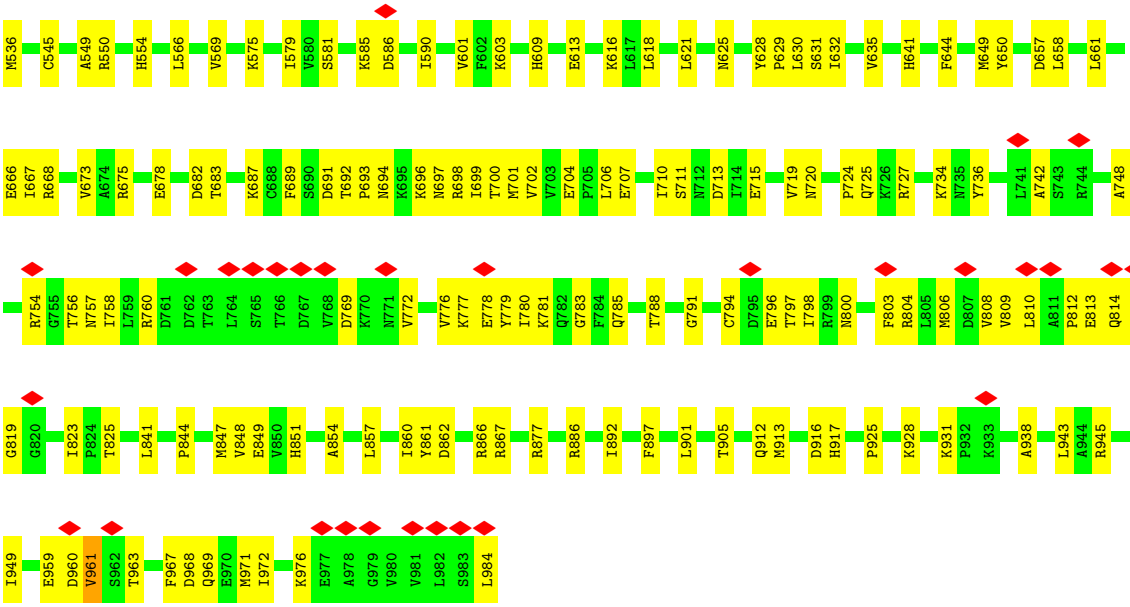




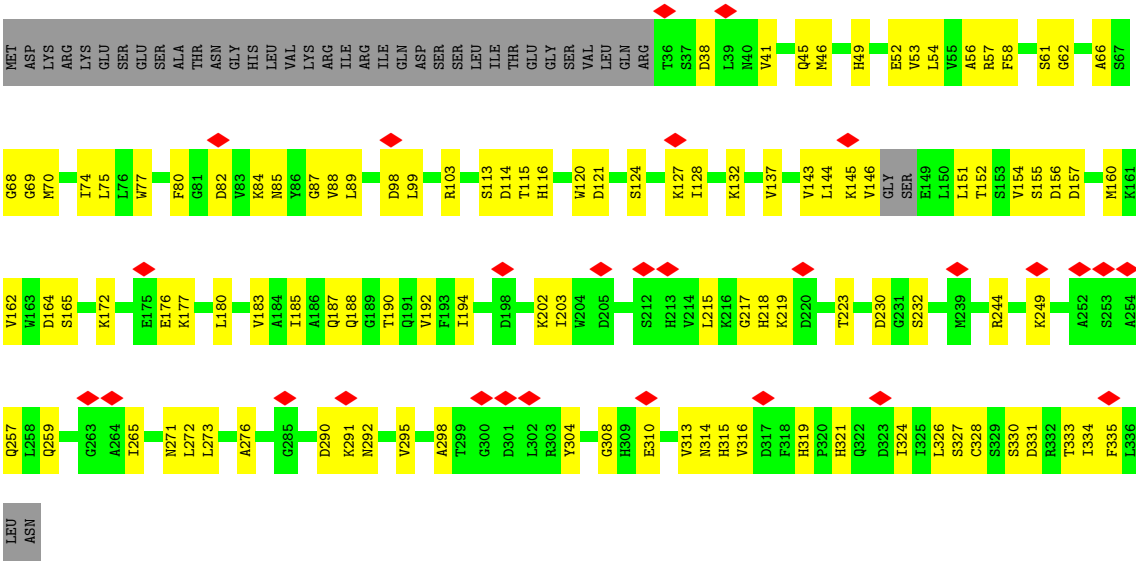
• Molecule 6: Pre-mRNA-splicing factor cwf10

Chain B:

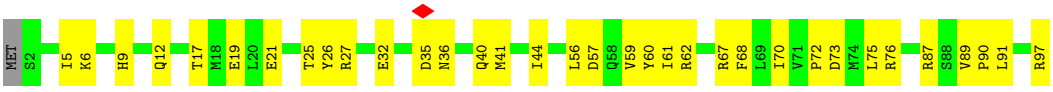




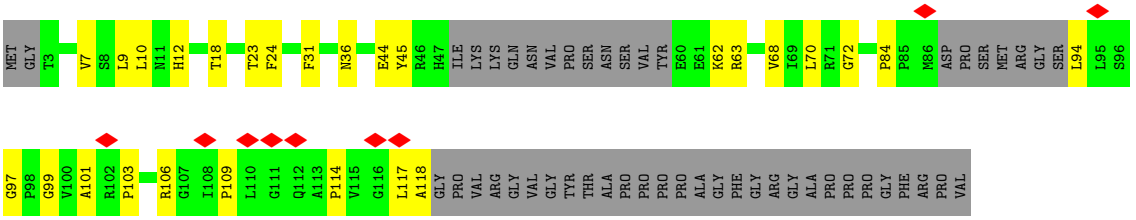
• Molecule 7: Pre-mRNA-splicing factor cwf17



• Molecule 8: Small nuclear ribonucleoprotein Sm D3

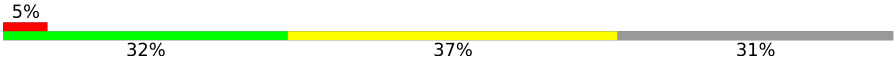


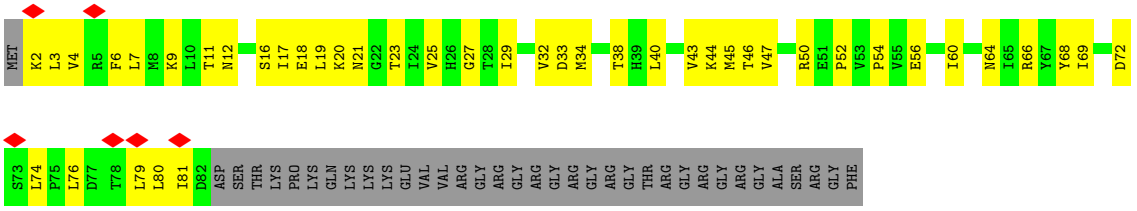
• Molecule 9: Small nuclear ribonucleoprotein-associated protein B



• Molecule 10: Small nuclear ribonucleoprotein Sm D1

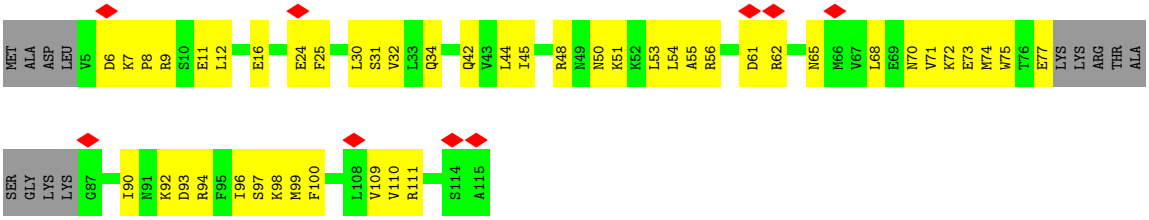
Chain F:





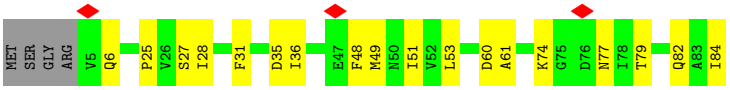
• Molecule 11: Small nuclear ribonucleoprotein Sm D2

Chain G:



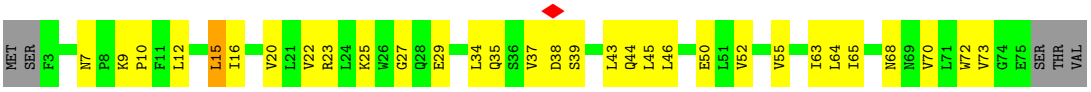
• Molecule 12: Small nuclear ribonucleoprotein E

Chain H:



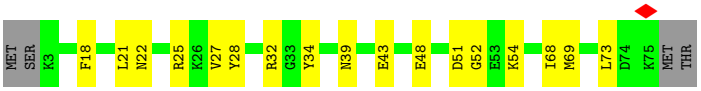
• Molecule 13: Small nuclear ribonucleoprotein F

Chain I:



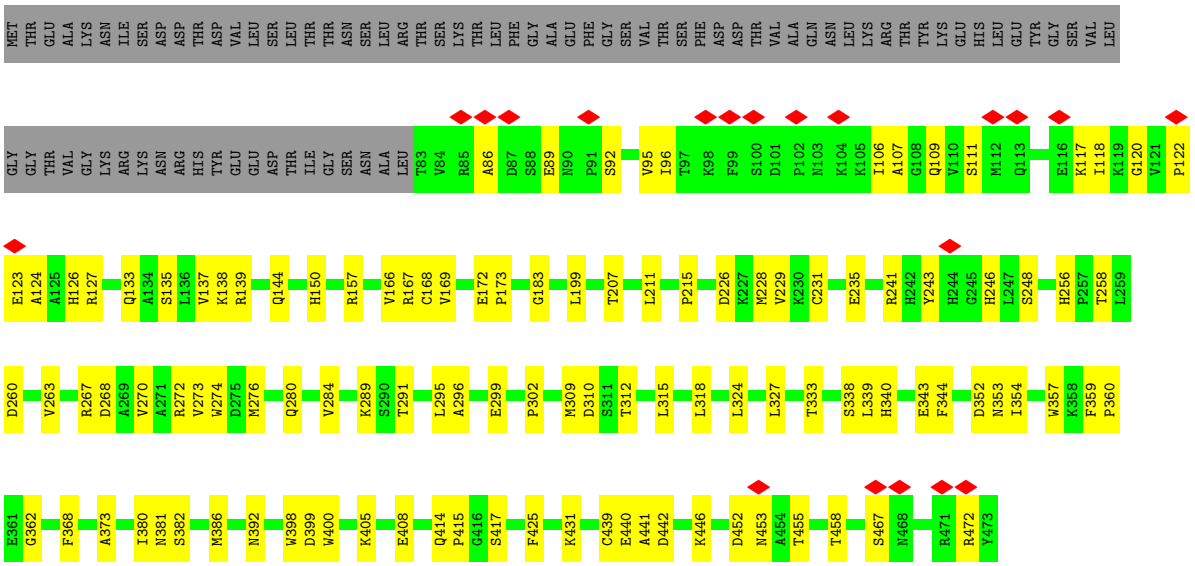
• Molecule 14: Small nuclear ribonucleoprotein G

Chain J:



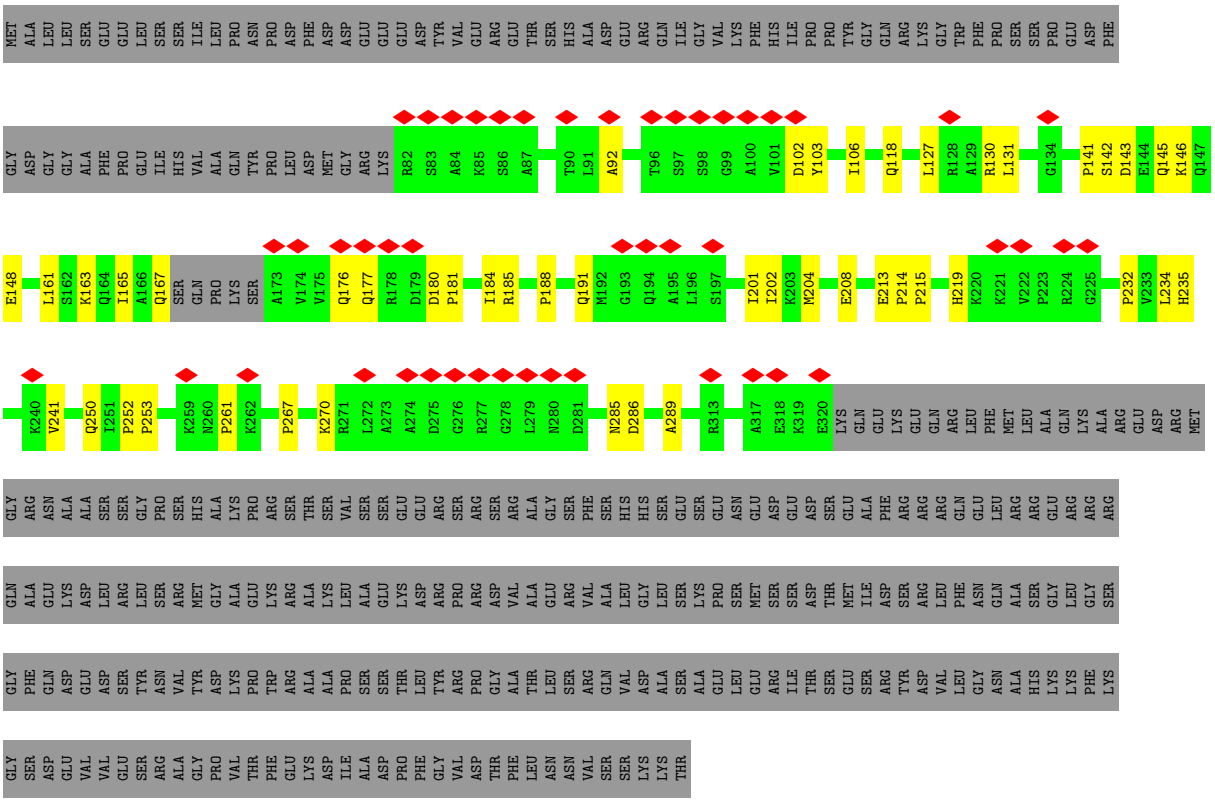
• Molecule 15: Pre-mRNA-splicing factor prp5

Chain K:



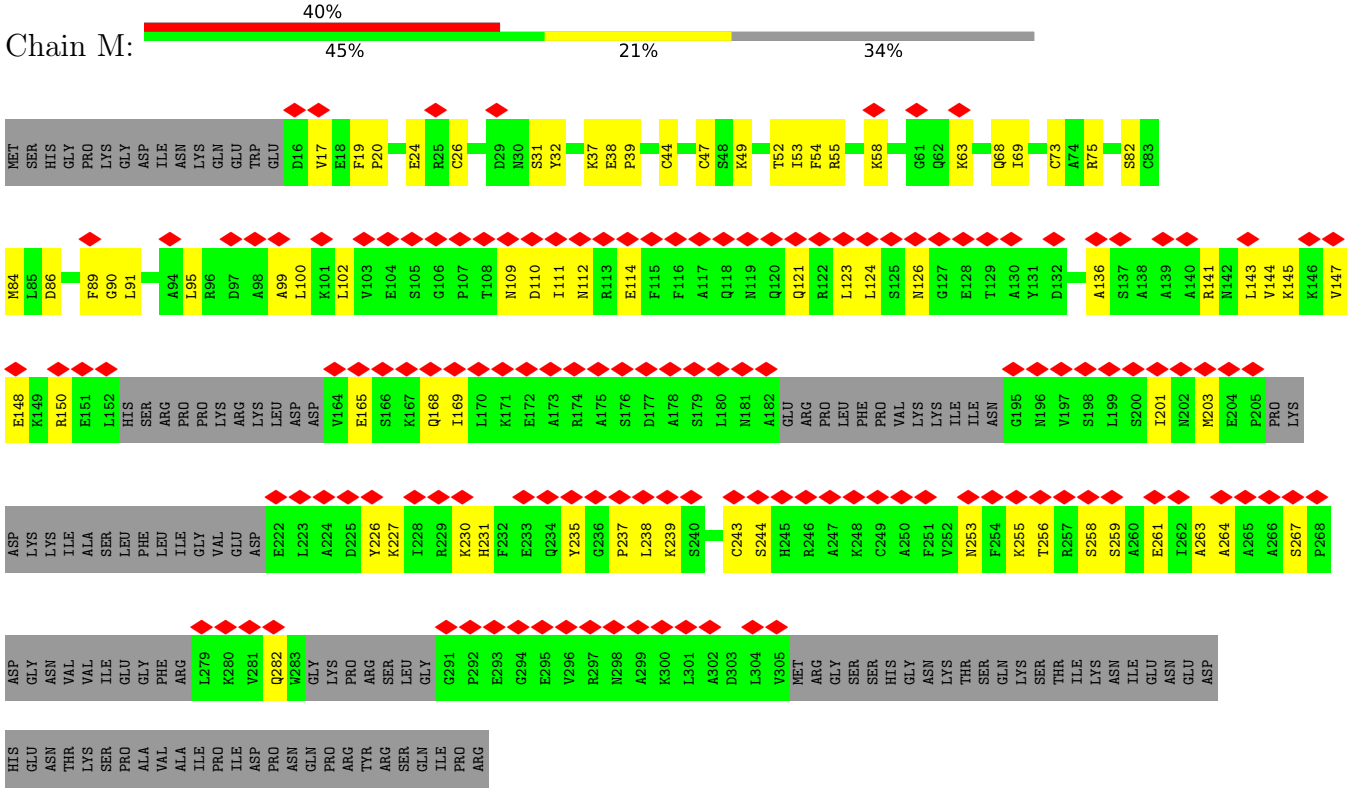
• Molecule 16: Pre-mRNA-processing protein 45

Chain L:



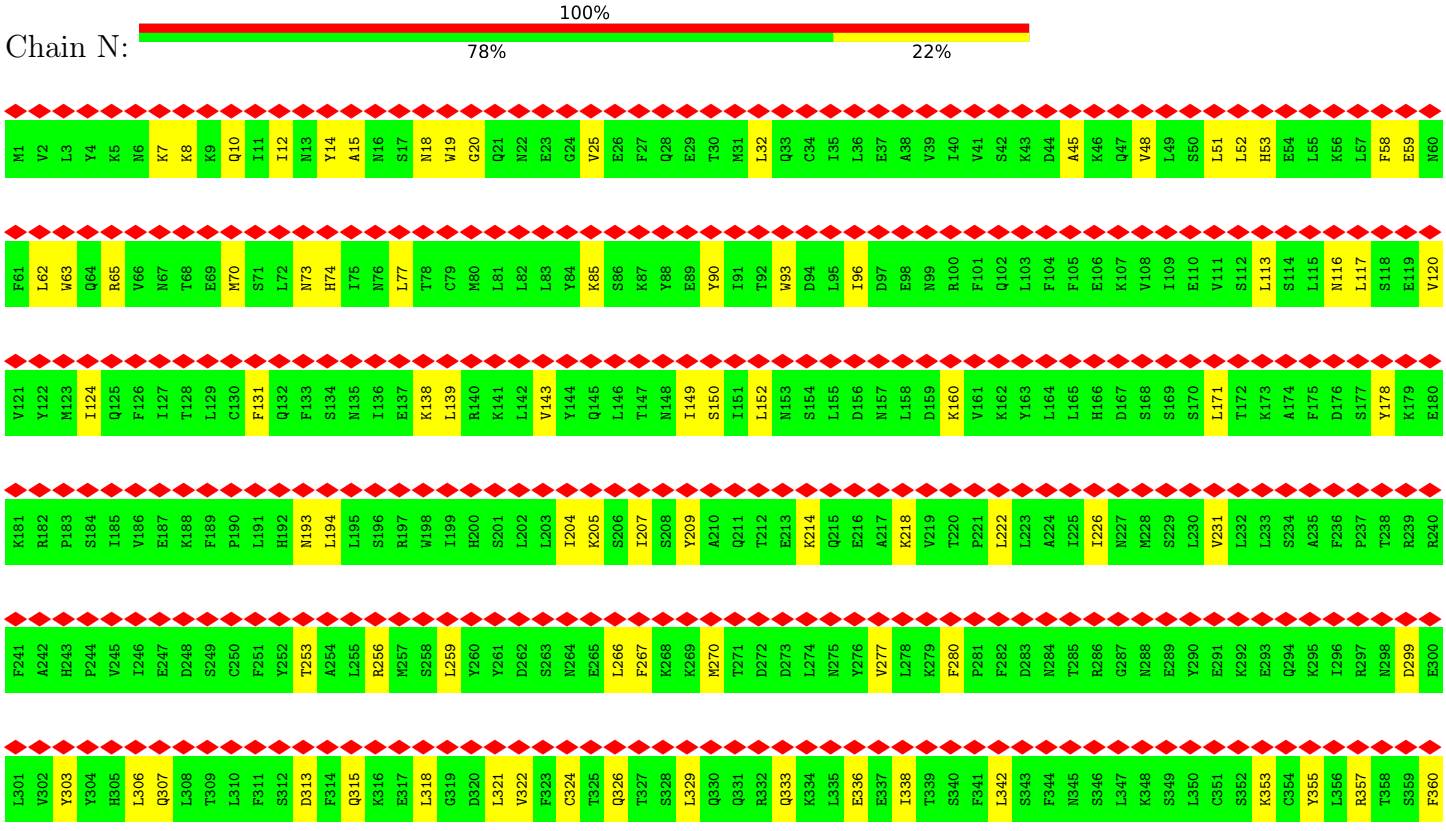
• Molecule 17: Pre-mRNA-splicing factor cwf5

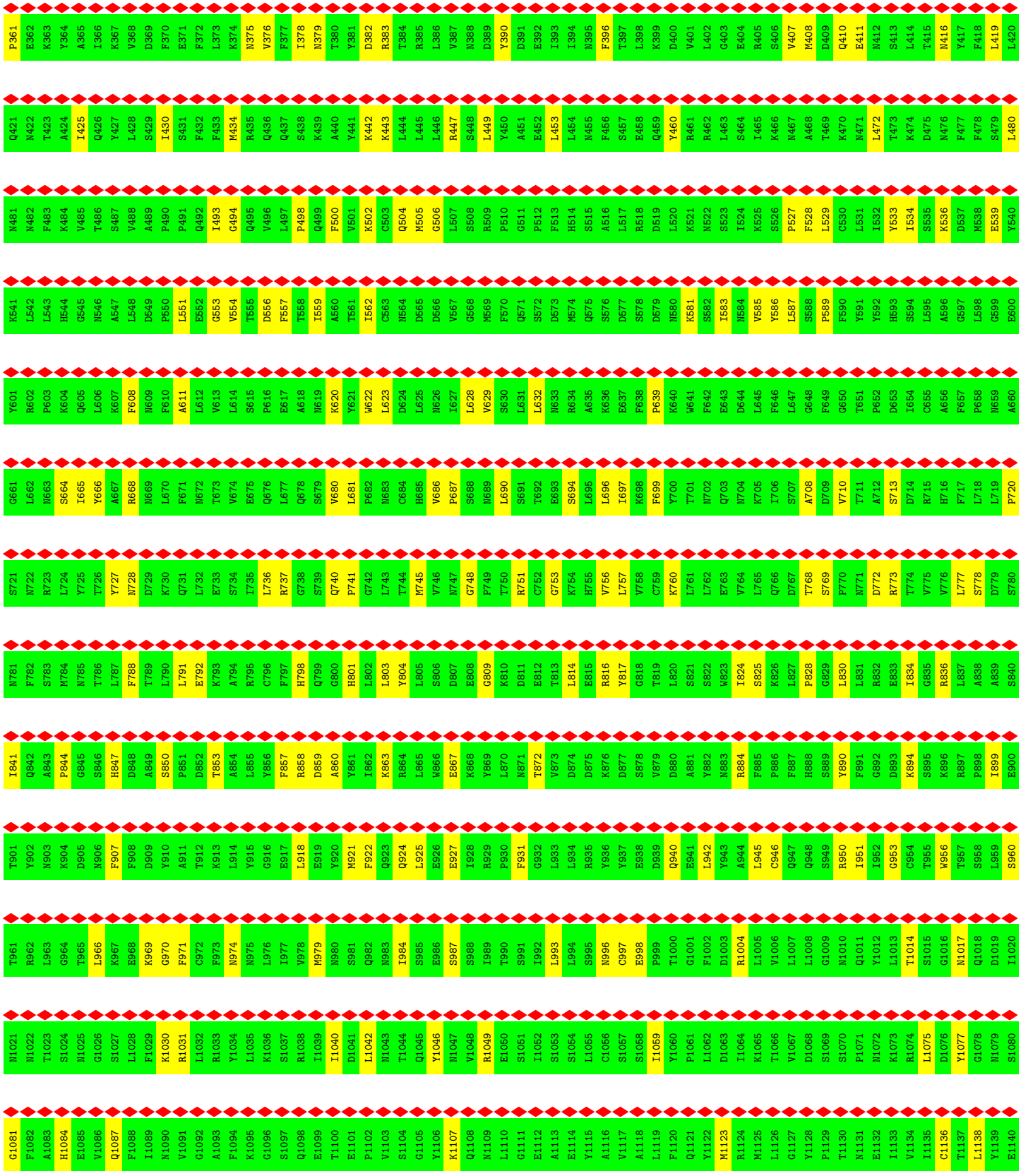
Chain M:



• Molecule 18: Pre-mRNA-splicing factor cwf11

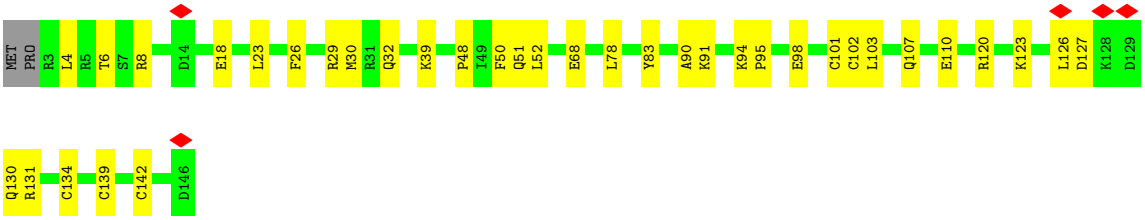
Chain N:




P361 E362 K363 Y364 A365 I366 K367 V368 D369 F370 E371 F372 L373 K374 N375 V376 F377 I378 N379 T380 Y381 D382 R383 T384 R385 L386 V387 N388 D389 Y390 D391 E392 I393 I394 N395 F396 T397 L398 K399 D400 V401 L402 G403 E404 R405 S406 V407 M408 D409 Q410 E411 N412 S413 L414 T415 N416 Y417 F418 L419 L420
Q421 N422 T423 A424 I425 Q426 Y427 L428 S429 T430 S431 F432 F433 M434 R435 Q436 Q437 S438 K439 A440 Y441 K442 K443 L444 L445 L446 R447 S448 L449 Y450 A451 E452 L453 L454 N455 F456 S457 E458 Q459 Y460 R461 R462 L463 S464 I465 K466 N467 A468 T469 K470 N471 L472 T473 K474 D475 N476 F477 F478 S479 L480
N481 N482 F483 K484 V485 T486 S487 V488 A489 P490 P491 Q492 I493 G494 Q495 V496 L497 P498 Q499 F500 V501 K502 C503 Q504 M505 G506 L507 S508 R509 P510 G511 P512 F513 H514 S515 A516 L517 R518 D519 L520 K521 N522 S523 I524 K525 S526 P527 F528 L529 C530 L531 I532 Y533 I534 S535 K536 D537 N538 E539 Y540
K541 L542 L543 H544 G545 N546 A547 L548 D549 P550 L551 E552 G553 V554 T555 D556 F557 T558 I559 A560 T561 I562 C563 N564 D565 D566 V567 G568 M569 F570 Q571 S572 D573 M574 Q575 S576 D577 S578 D579 N580 K581 S582 I583 N584 V585 Y586 L587 S588 P589 F590 Y591 Y592 H593 S594 L595 A596 G597 L598 G599 E600
Y601 R602 P603 K604 Q605 L606 K607 F608 N609 F610 A611 L612 V613 L614 S615 P616 E617 A618 N619 K620 Y621 W622 L623 D624 L625 N626 I627 L628 V629 S630 L631 L632 N633 R634 A635 K636 E637 F638 P639 K640 W641 F642 E643 D644 L645 F646 L647 G648 F649 G650 T651 P652 D653 I654 C655 A656 F657 P658 N659 A660
G661 L662 N663 S664 I665 Y666 A667 R668 N669 L670 F671 N672 T673 V674 E675 Q676 L677 Q678 S679 V680 L681 P682 N683 C684 H685 V686 P687 S688 N689 L690 S691 T692 E693 S694 L695 L696 I697 K698 F699 Y700 T701 N702 Q703 N704 K705 I706 S707 A708 D709 V710 T711 A712 S713 D714 R715 H716 F717 L718 L719 P720
S721 N722 R723 L724 Y725 T726 Y727 N728 D729 K730 Q731 L732 E733 S734 L735 L736 R737 G738 S739 Q740 P741 G742 L743 T744 M745 V746 N747 G748 P749 T750 R751 C752 G753 K754 H755 V756 L757 V758 C759 K760 L761 L762 E763 V764 L765 Q766 D767 T768 S769 P770 N771 D772 R773 T774 V775 V776 L777 S778 D779 S780
N781 F782 S783 M784 N785 T786 L787 F788 T789 L790 L791 E792 K793 A794 R795 C796 F797 H798 Q799 G800 H801 L802 L803 Y804 L805 S806 D807 E808 G809 K810 D811 E812 T813 L814 E815 R816 Y817 G818 T819 L820 S821 S822 W823 I824 S825 K826 L827 P828 G829 L830 L831 R832 E833 I834 G835 R836 L837 A838 A839 S840
I841 Q842 A843 P844 G845 S846 H847 D848 A849 S850 P851 D852 T853 A854 L855 Y856 F857 R858 D859 A860 Y861 I862 K863 R864 L865 W866 E867 K868 Y869 L870 N871 T872 V873 D874 D875 K876 D877 S878 V879 D880 A881 Y882 N883 R884 F885 P886 F887 H888 S889 Y890 F891 G892 D893 K894 S895 K896 R897 P898 I899 E900
T901 Y902 N903 K904 D905 N906 F907 F908 D909 Y910 A911 T912 K913 L914 Y915 G916 E917 L918 E919 Y920 M921 F922 Q923 Q924 L925 E926 E927 I928 R929 P930 F931 G932 L933 L934 R935 Y936 Y937 E938 D939 Q940 E941 L942 Y943 A944 L945 C946 Q947 Q948 S949 R950 I951 Y952 G953 C954 T955 W956 T957 S958 L959 S960
T961 R962 L963 G964 T965 L966 K967 E968 K969 G970 F971 C972 F973 N974 N975 L976 I977 V978 M979 N980 S981 Q982 N983 I984 S985 E986 S987 S988 I989 T990 S991 I992 L993 L994 S995 N996 C997 E998 P999 T1000 G1001 F1002 D1003 R1004 L1005 V1006 L1007 L1008 G1009 N1010 Q1011 Y1012 L1013 T1014 S1015 G1016 N1017 Q1018 D1019 I1020
N1021 N1022 T1023 S1024 N1025 G1026 S1027 L1028 F1029 K1030 R1031 L1032 R1033 Y1034 L1035 K1036 S1037 R1038 I1039 I1040 D1041 L1042 N1043 T1044 Q1045 Y1046 N1047 V1048 R1049 E1050 S1051 I1052 S1053 S1054 L1055 C1056 S1057 S1058 I1059 Y1060 P1061 L1062 D1063 I1064 K1065 T1066 V1067 D1068 S1069 S1070 P1071 N1072 K1073 R1074 L1075 D1076 Y1077 G1078 N1079 S1080
G1081 F1082 A1083 H1084 E1085 V1086 Q1087 F1088 I1089 N1090 V1091 G1092 A1093 F1094 K1095 G1096 S1097 Q1098 E1099 T1100 E1101 P1102 V1103 S1104 G1105 Y1106 K1107 Q1108 N1109 L1110 G1111 E1112 A1113 E1114 Y1115 A1116 V1117 A1118 L1119 F1120 Q1121 Y1122 M1123 R1124 M1125 L1126 G1127 Y1128 P1129 T1130 N1131 E1132 I1133 V1134 I1135 C1136 T1137 L1138 Y1139 E1140

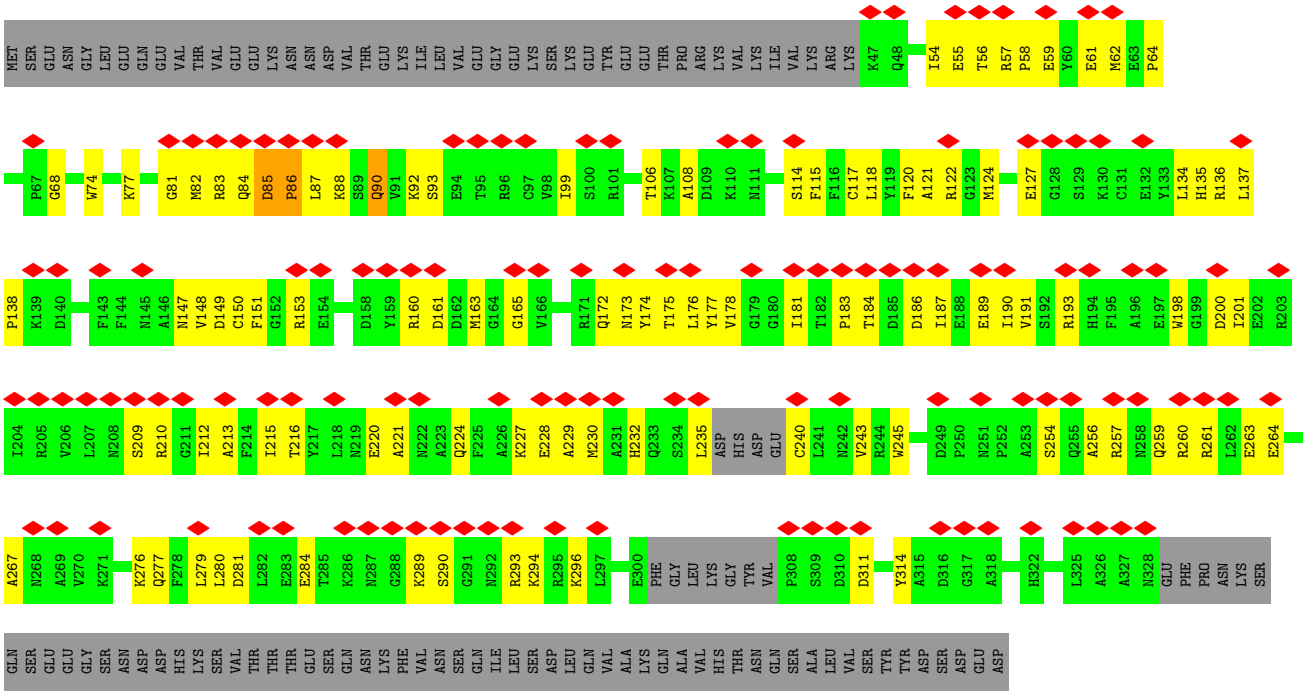
• Molecule 19: Pre-mRNA-splicing factor cwf14

Chain O:



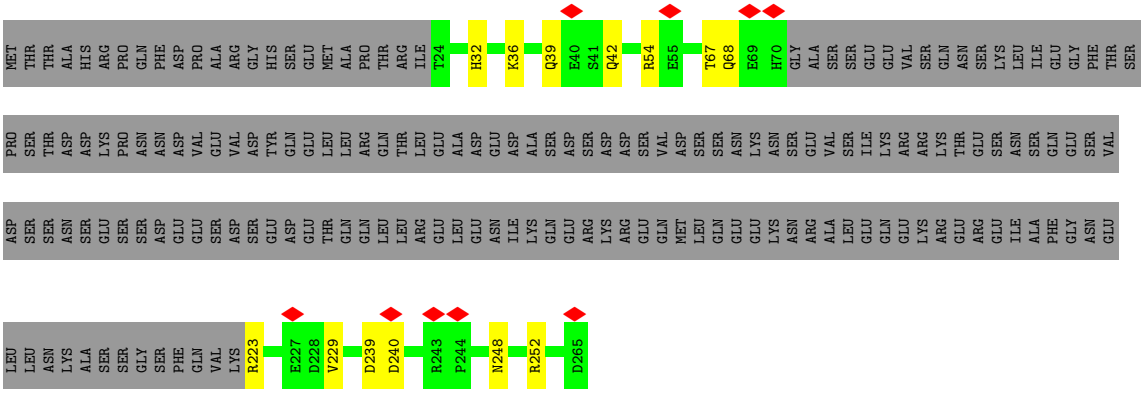
• Molecule 20: Pre-mRNA-splicing factor cwf2

Chain P:



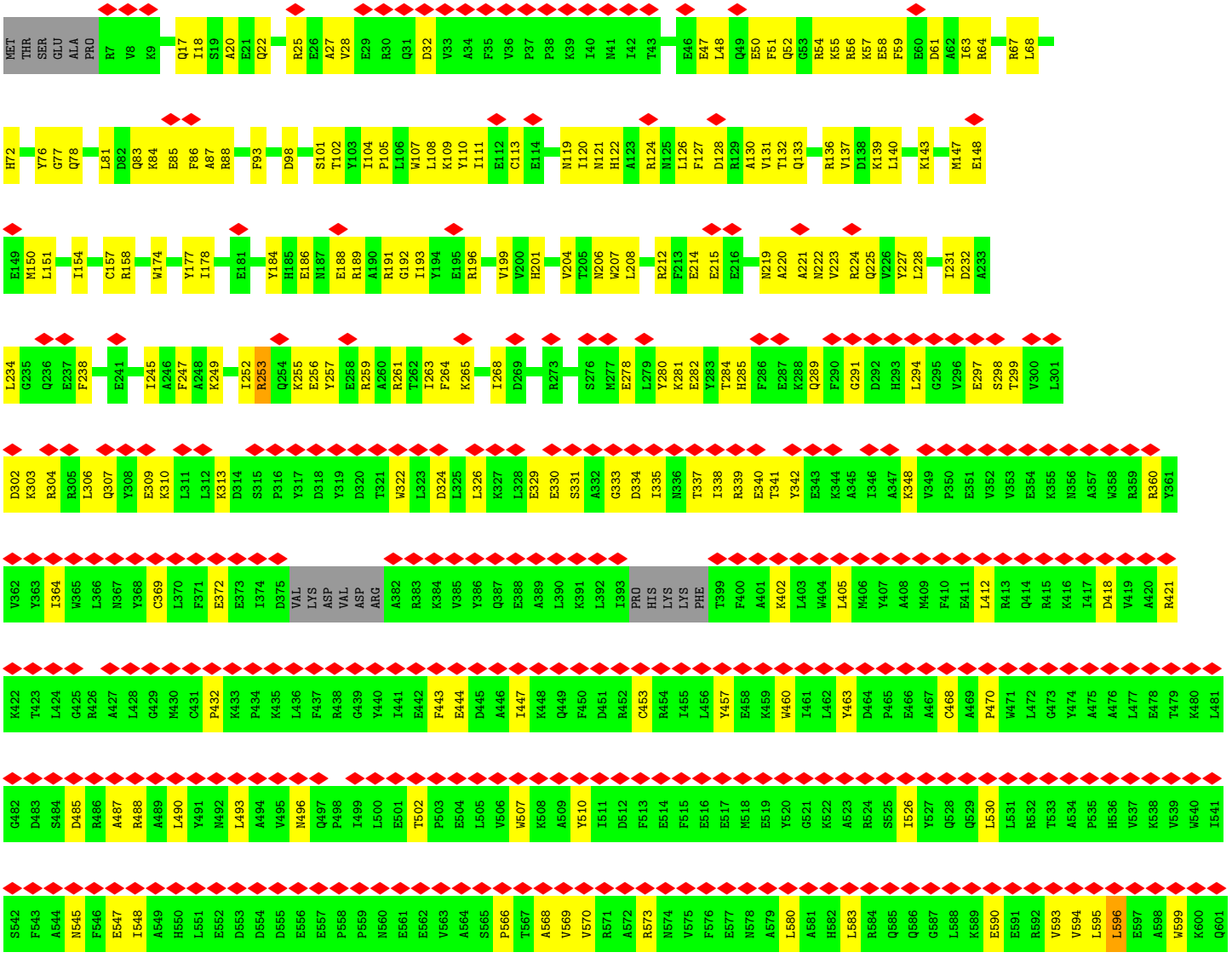
• Molecule 21: Pre-mRNA-splicing factor cwf15

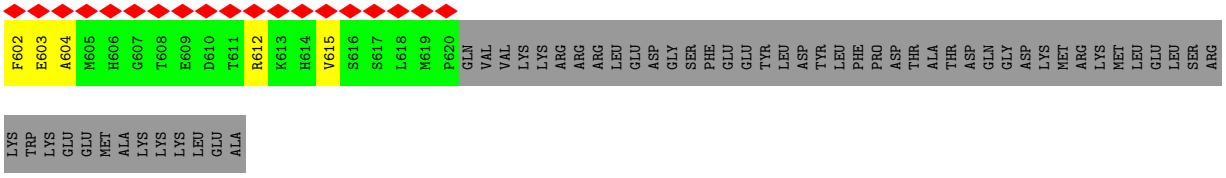
Chain Q:



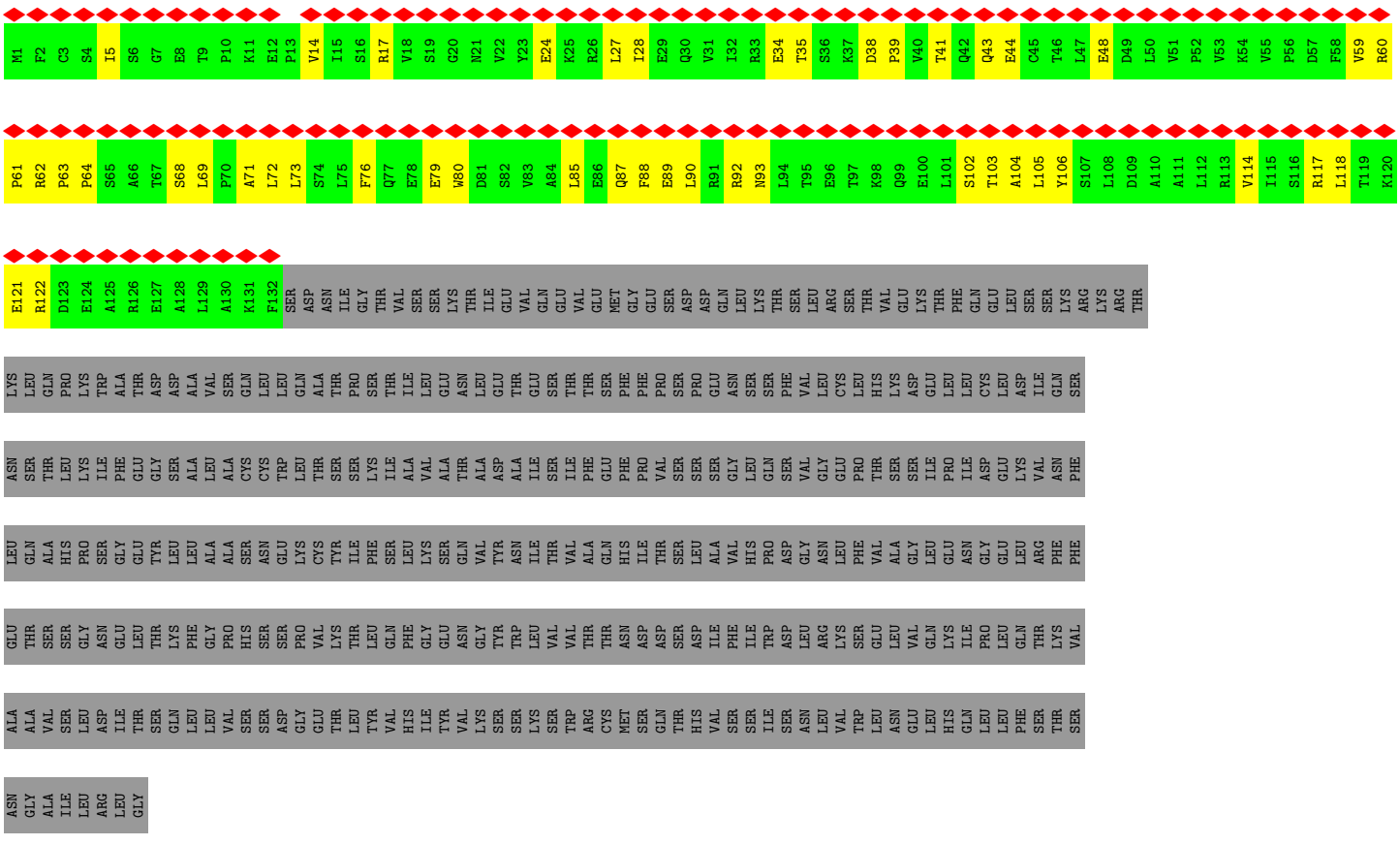
• Molecule 22: Pre-mRNA-splicing factor cwf4

Chain R:

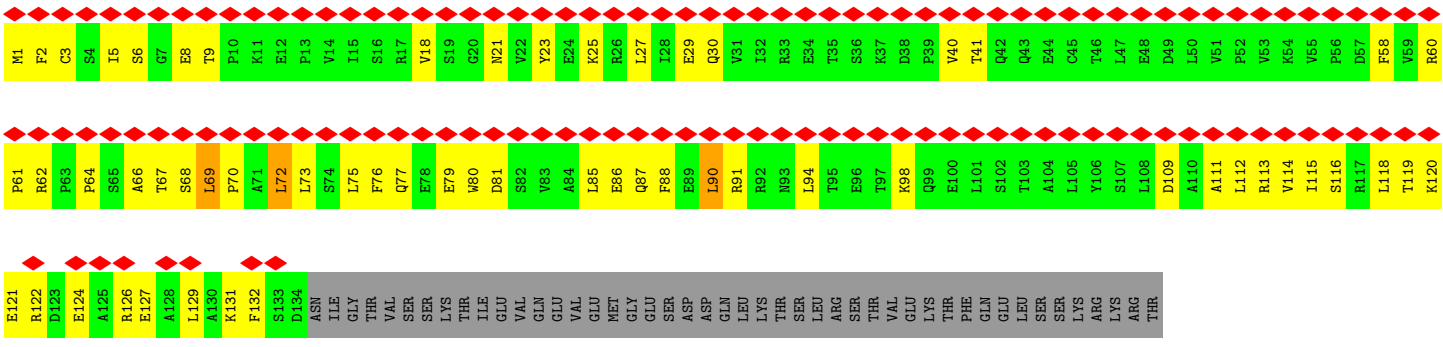


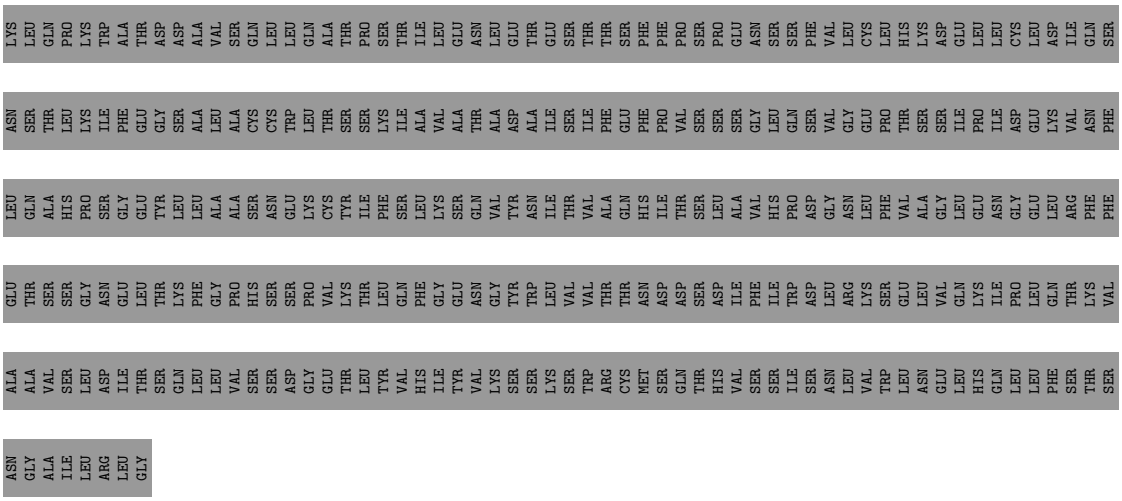


• Molecule 23: Pre-mRNA-processing factor 19



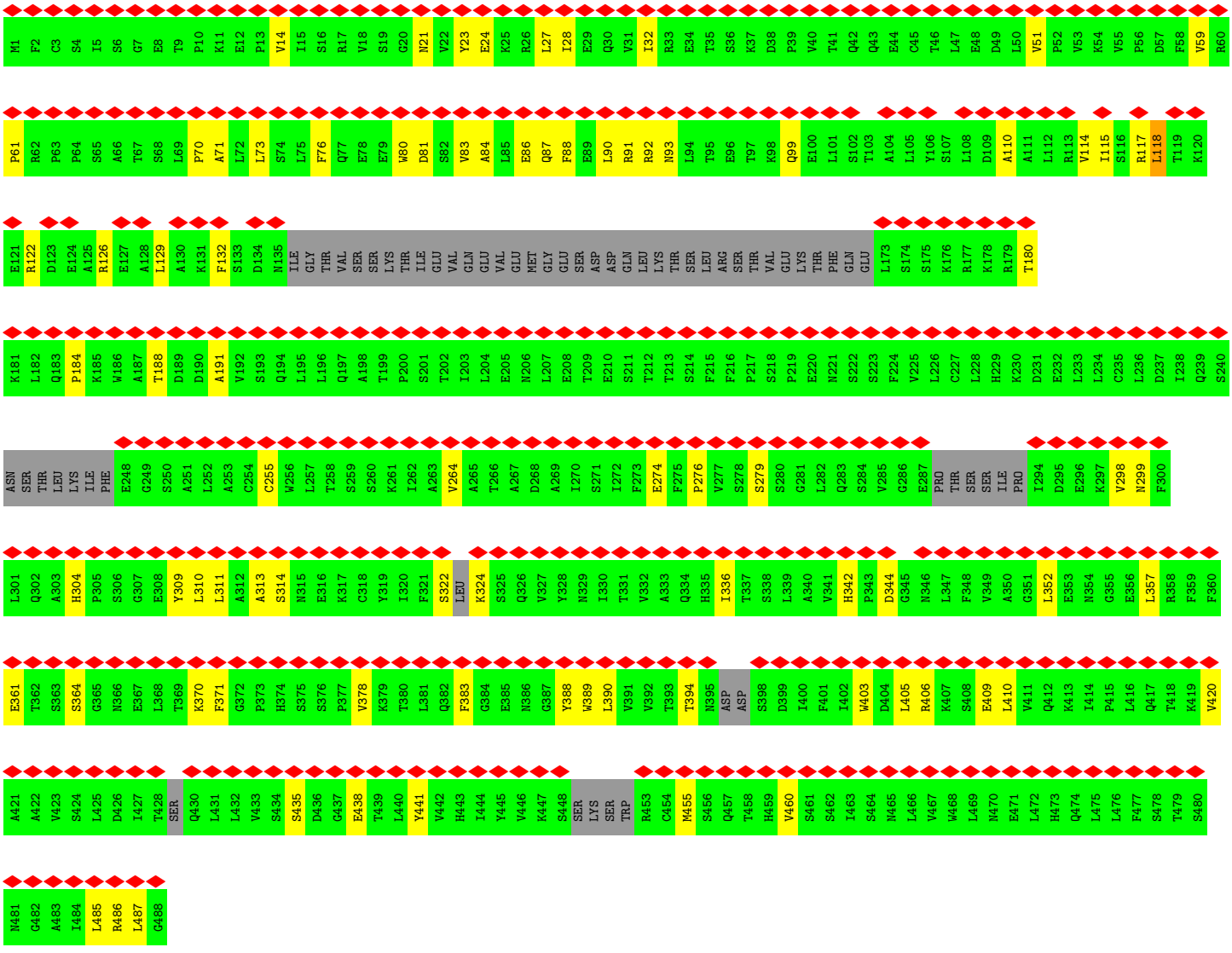
• Molecule 23: Pre-mRNA-processing factor 19





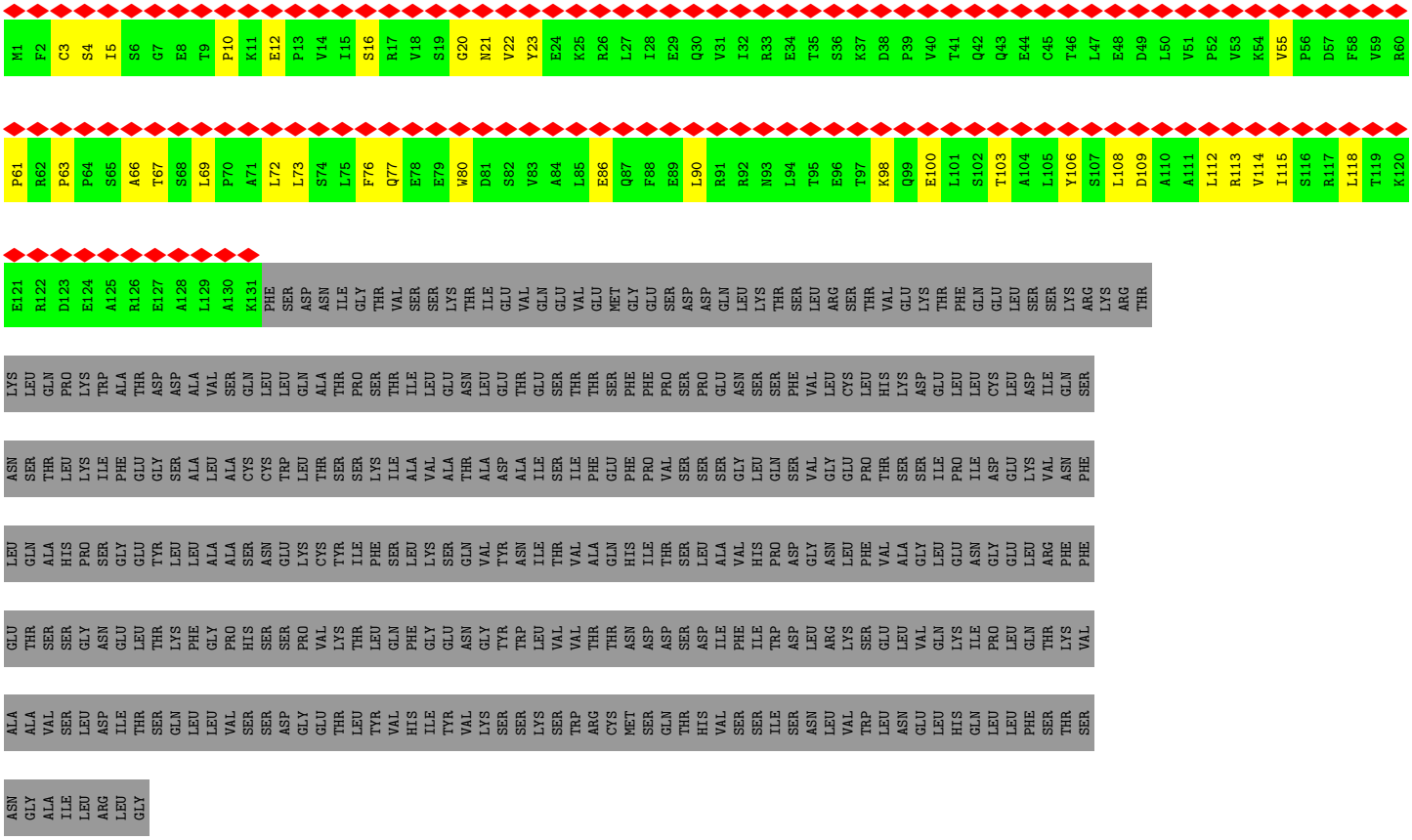
• Molecule 23: Pre-mRNA-processing factor 19

Chain U:



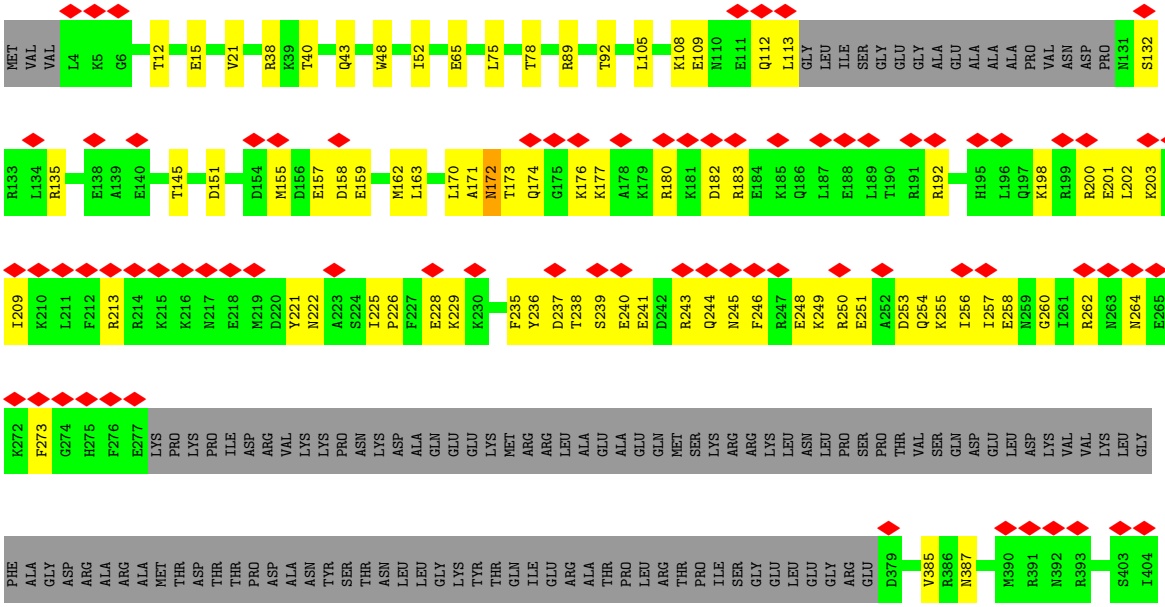
• Molecule 23: Pre-mRNA-processing factor 19

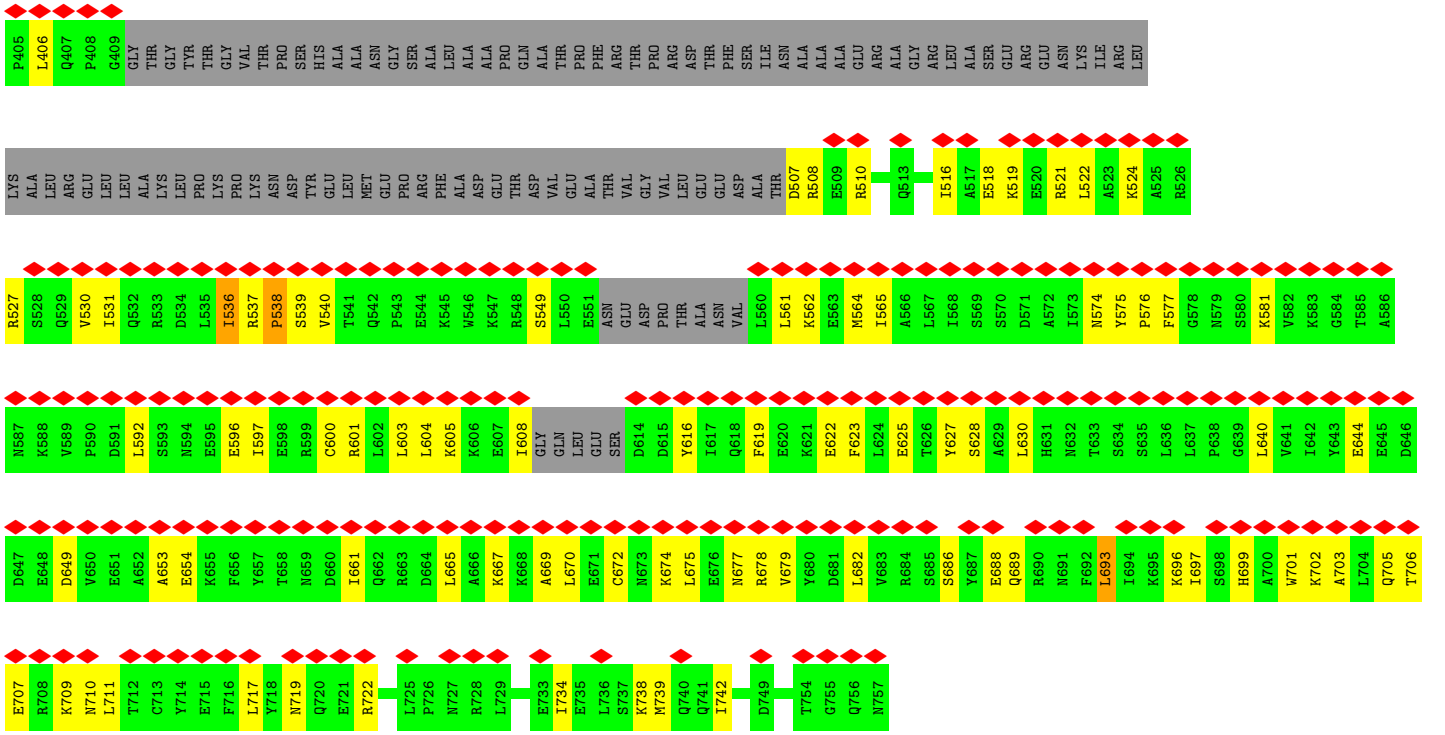
Chain V:



• Molecule 24: Pre-mRNA-splicing factor cdc5

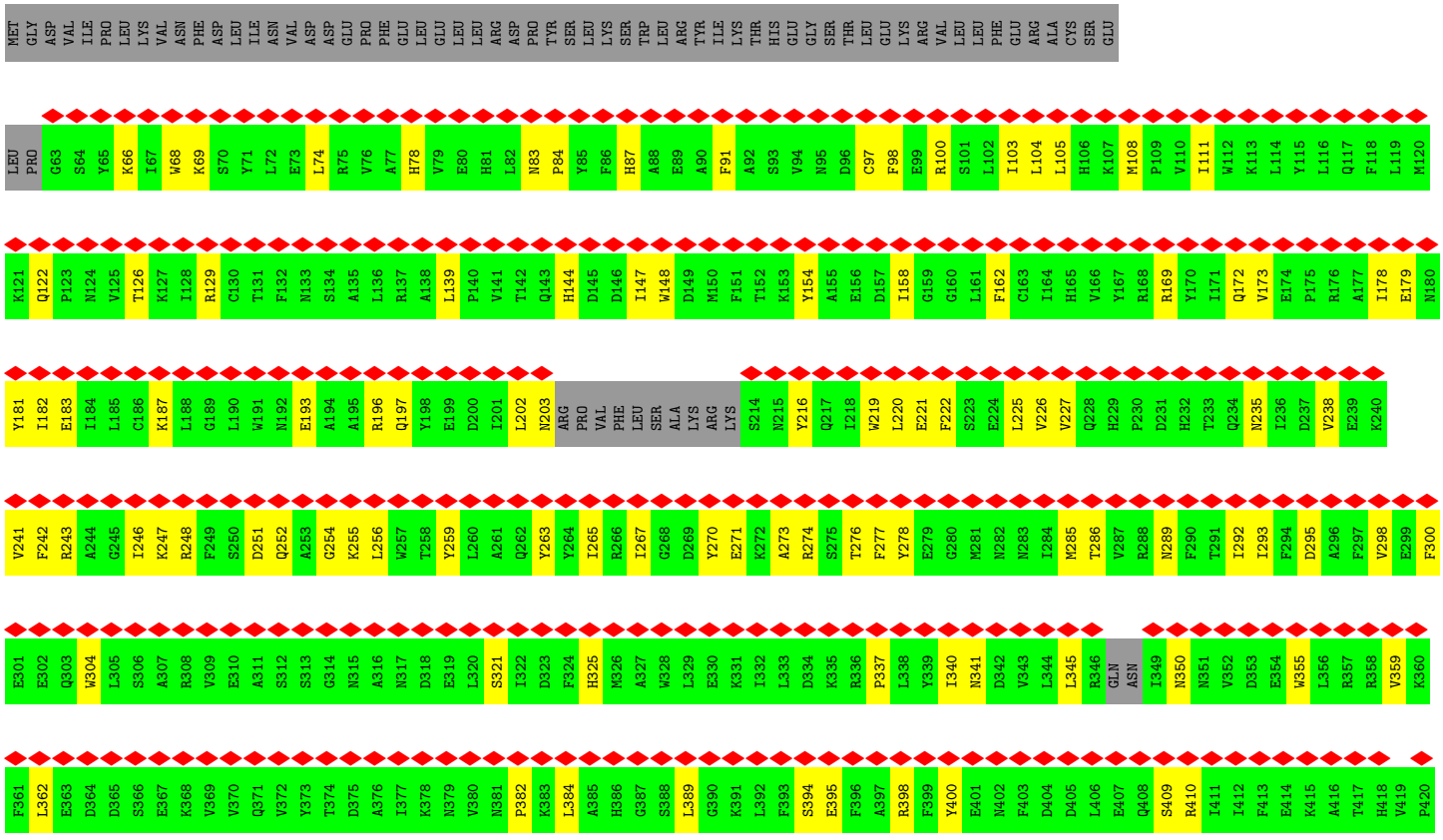
Chain W:

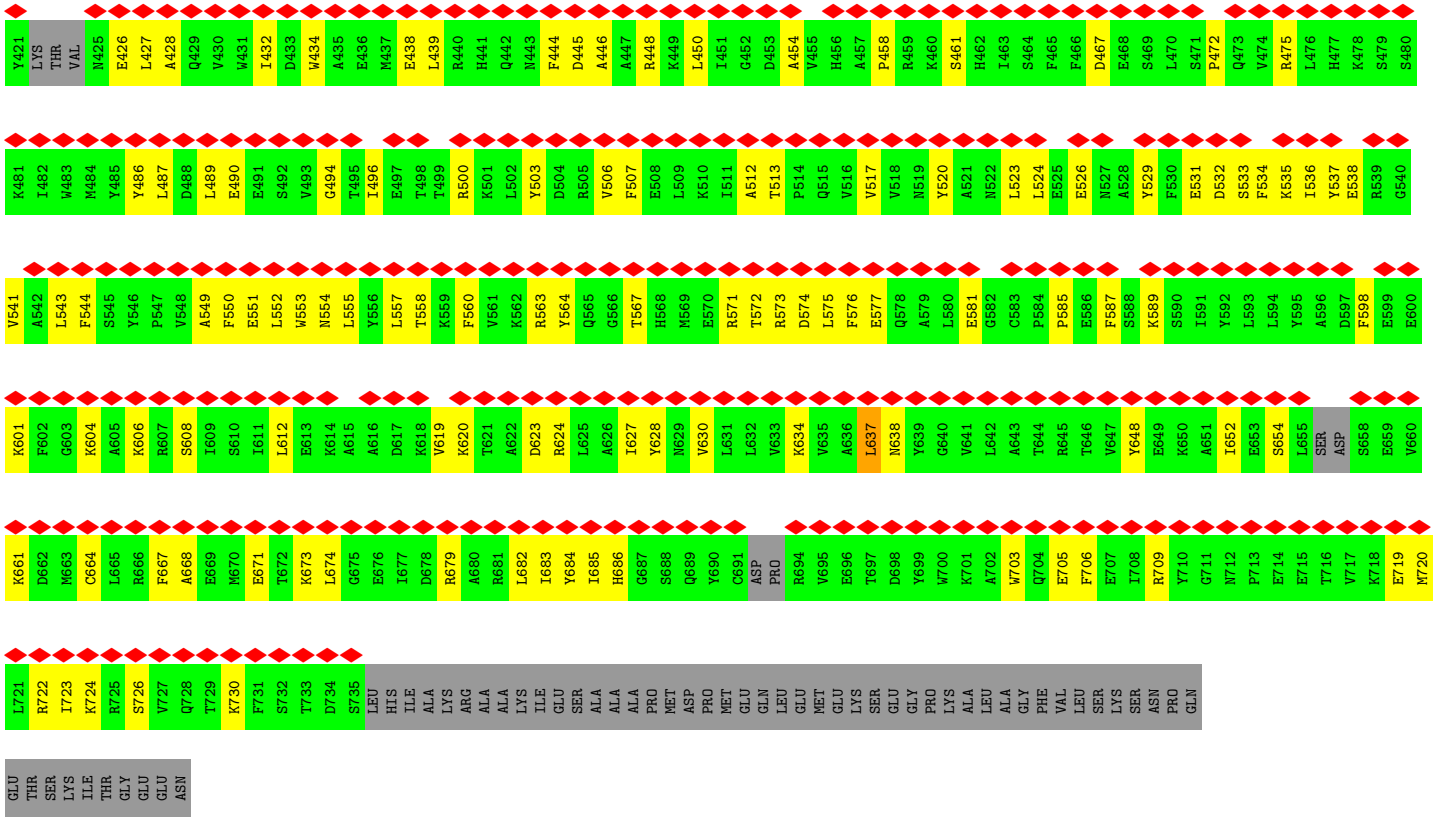




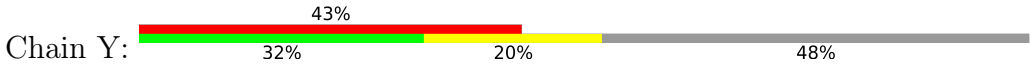
• Molecule 25: Pre-mRNA-splicing factor cwf3

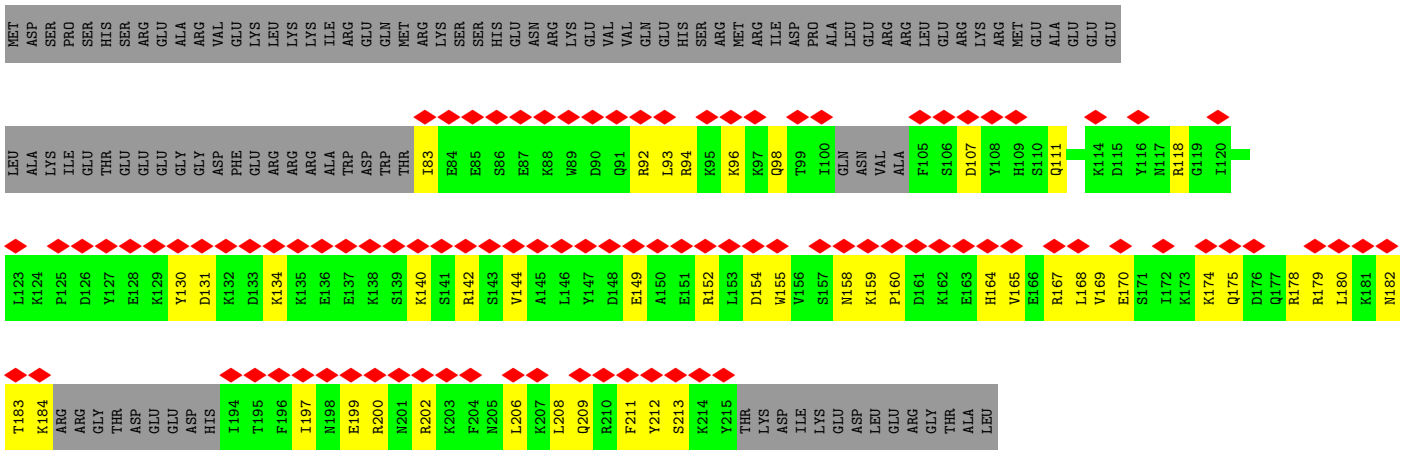
Chain X:



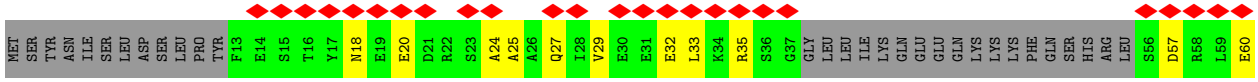


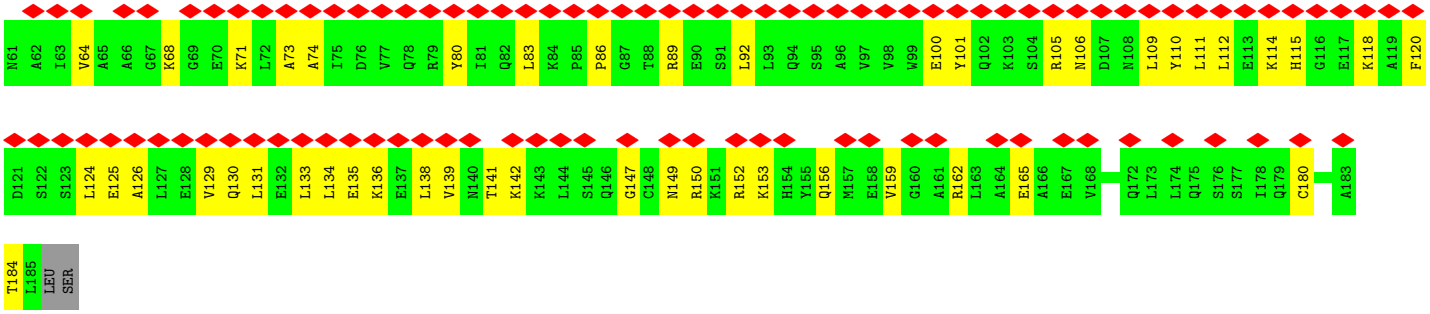
• Molecule 26: Pre-mRNA-splicing factor syf2





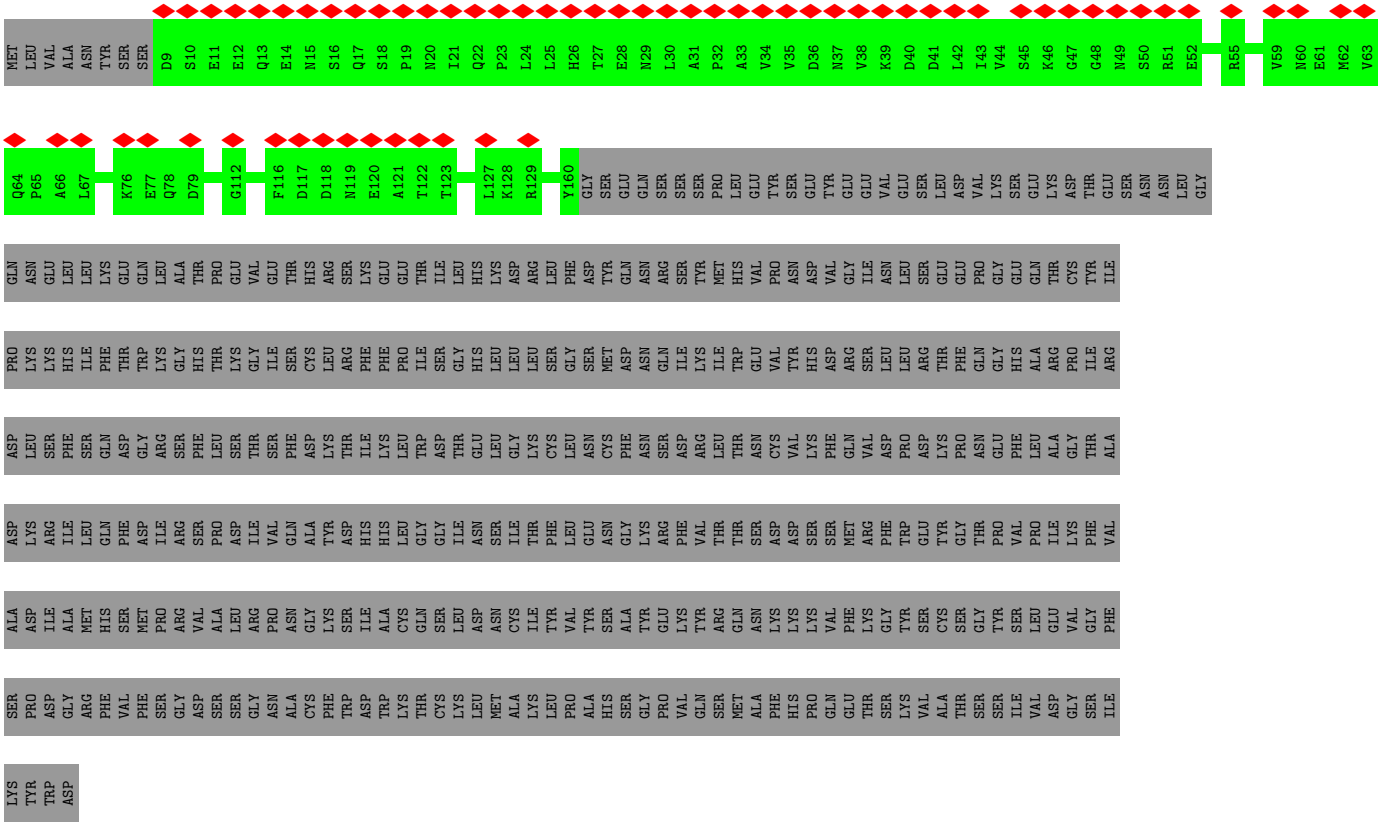
• Molecule 27: Pre-mRNA-splicing factor cwf7





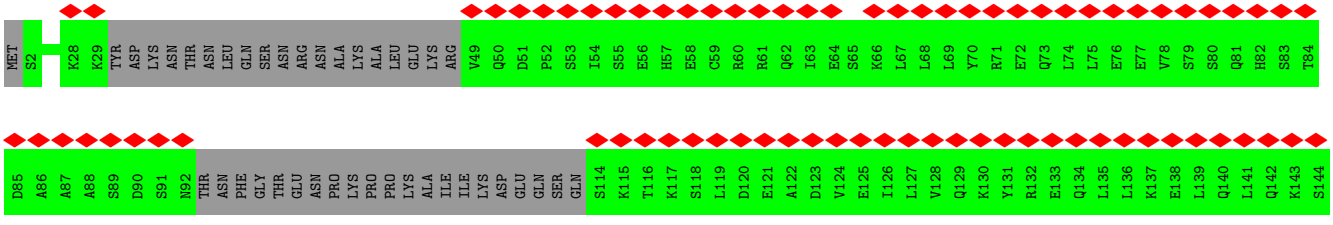
• Molecule 28: Pre-mRNA-processing factor 17

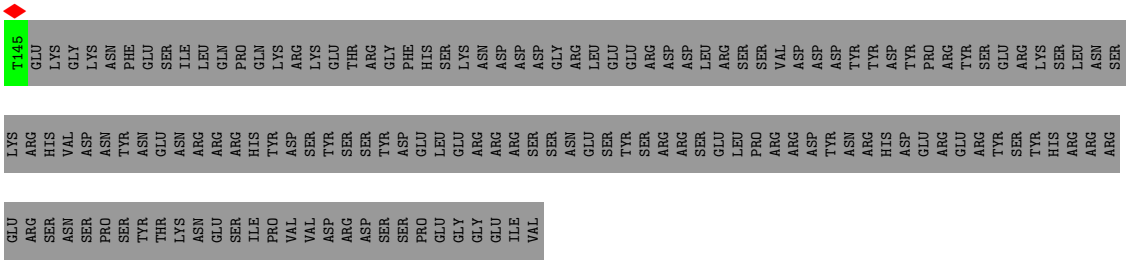
Chain a:



• Molecule 29: Pre-mRNA-splicing factor cwf21

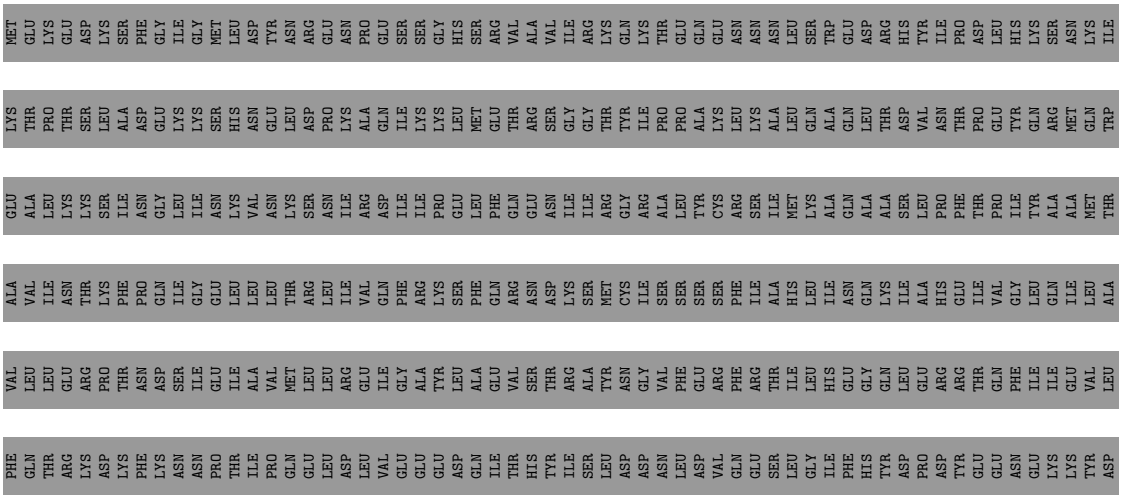
Chain b:

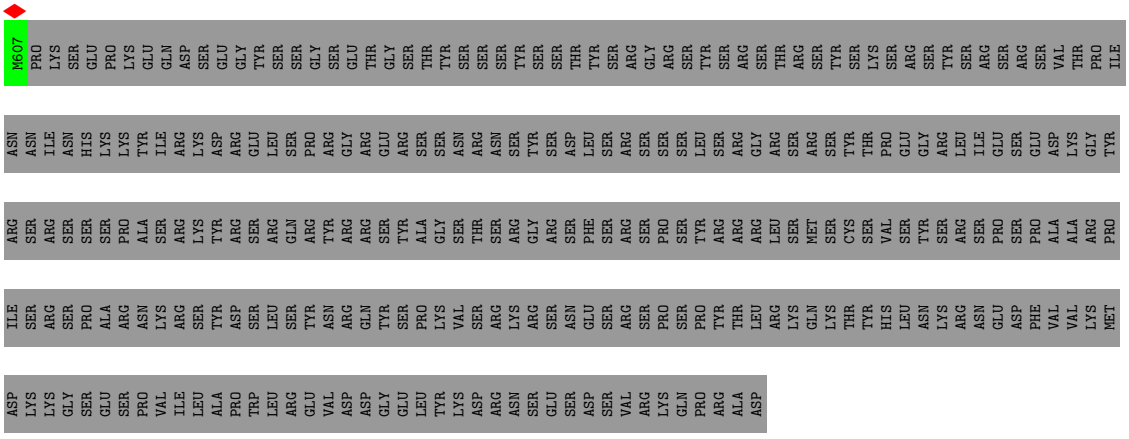




• Molecule 30: Pre-mRNA-splicing factor cwf22

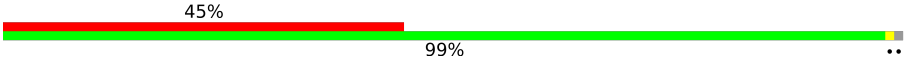
Chain c:

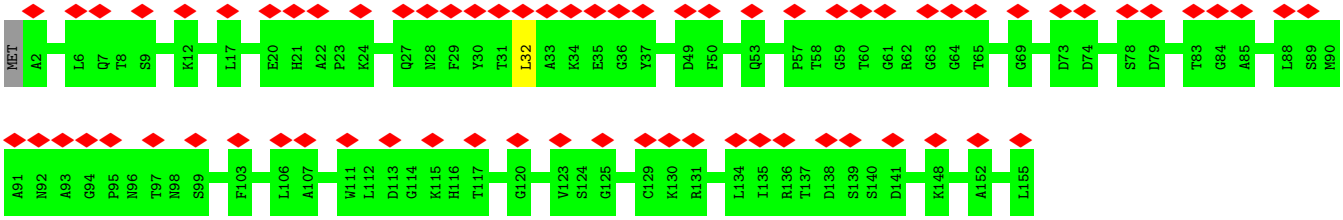




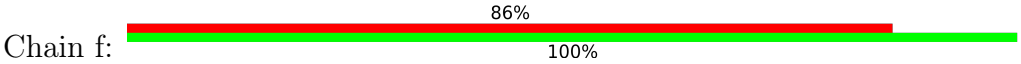
• Molecule 31: Peptidyl-prolyl cis-trans isomerase ppi1

Chain d:

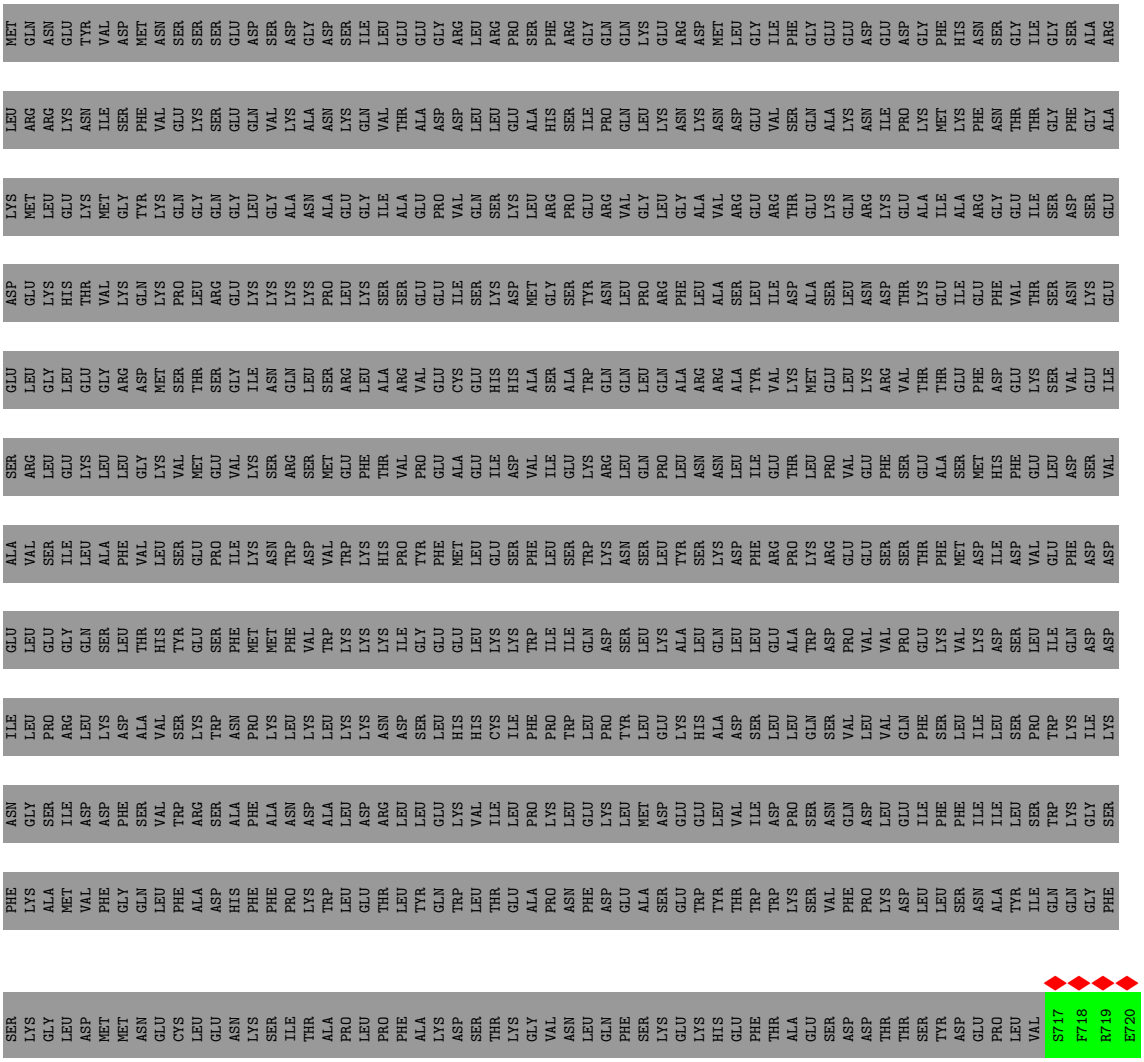




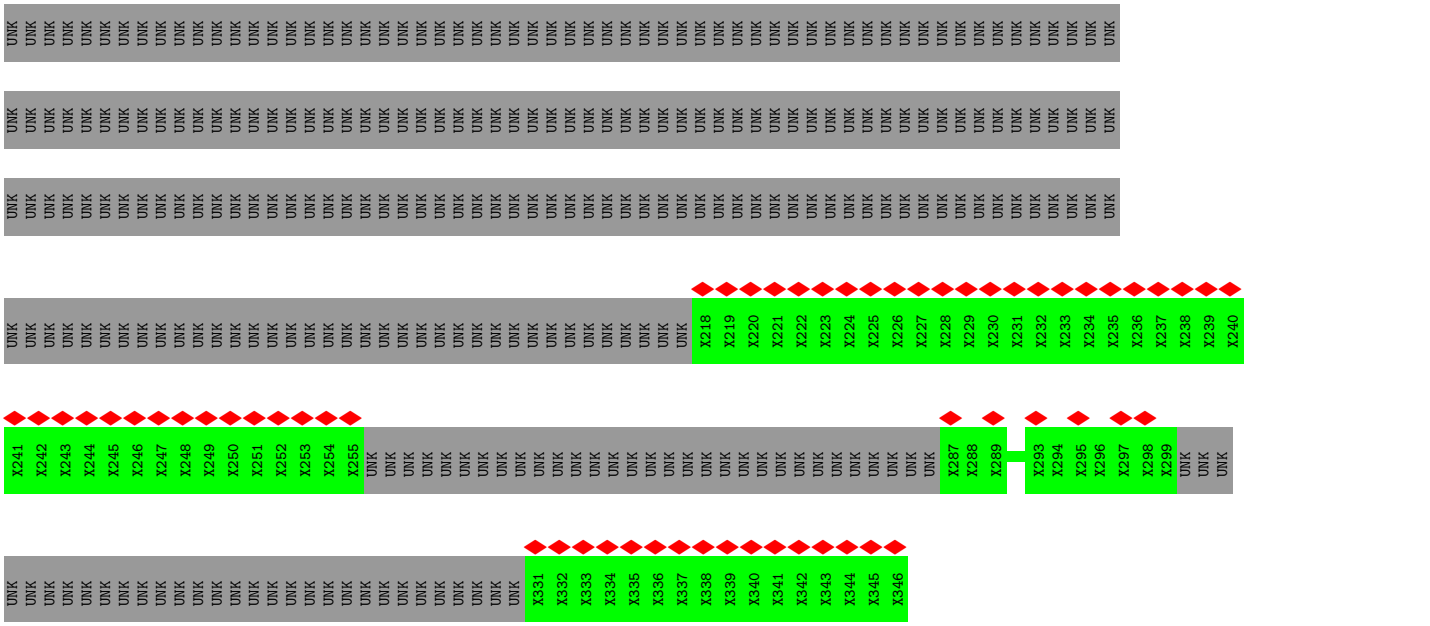
• Molecule 32: UNK1



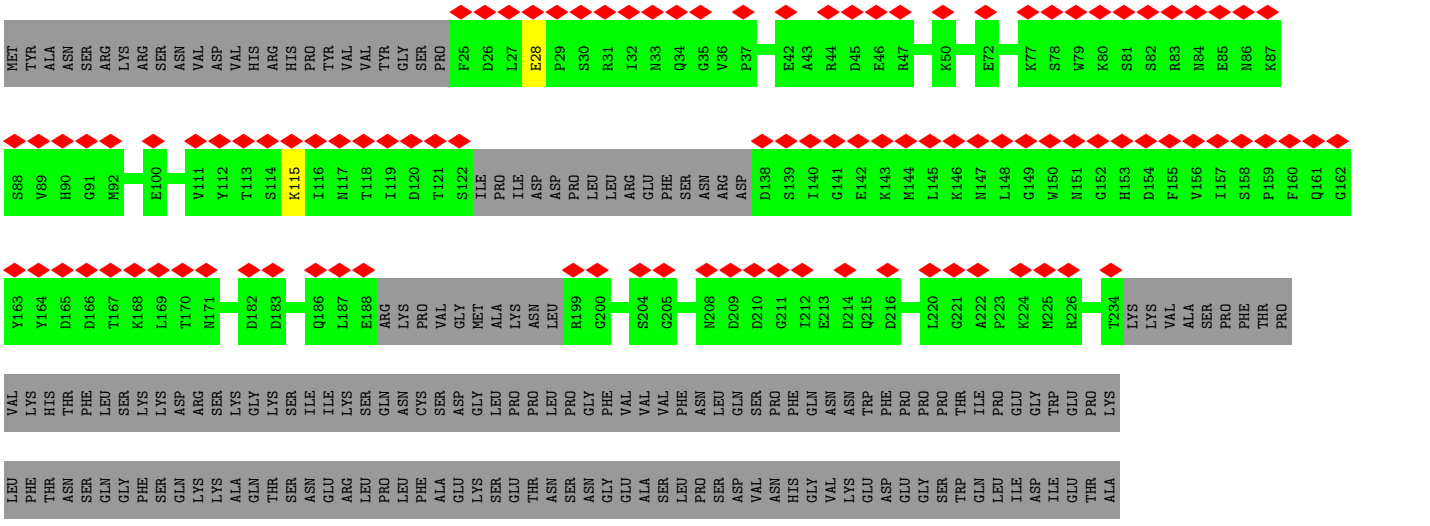
• Molecule 33: G-patch domain-containing protein C1486.03

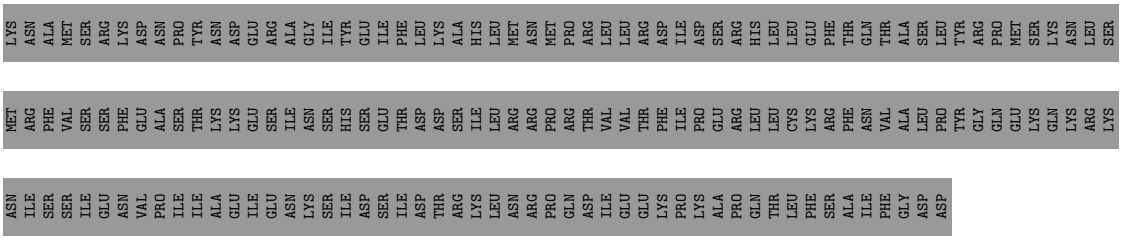


• Molecule 34: UNK2



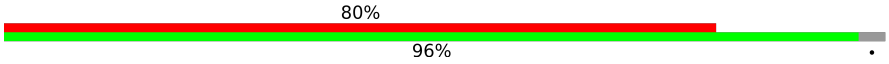
• Molecule 35: Uncharacterized protein C20H4.06c

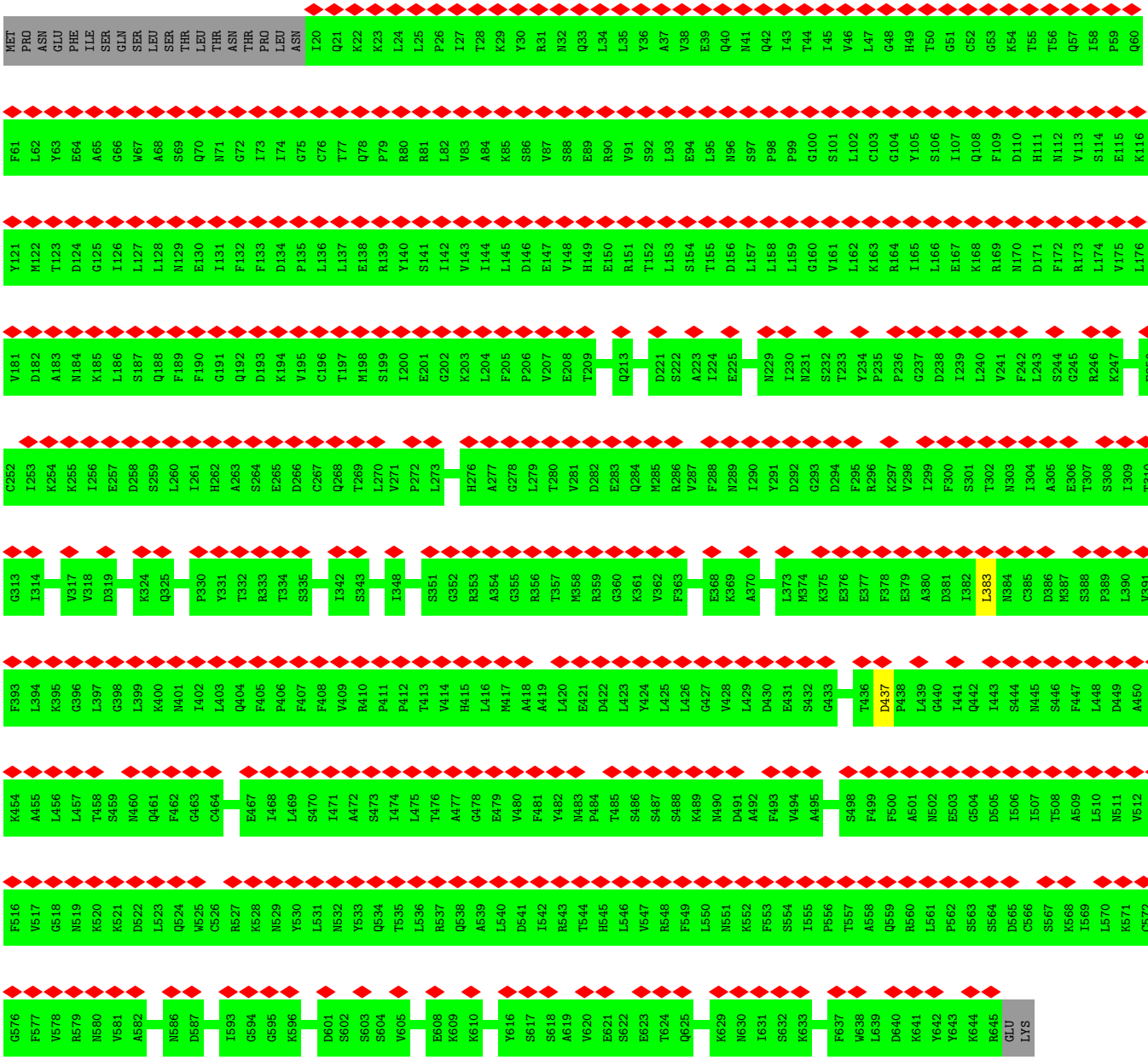




• Molecule 36: Putative pre-mRNA-splicing factor ATP-dependent RNA helicase C20H4.09

Chain z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61423	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	49.4	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	37.729	Depositor
Minimum map value	-20.085	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.902	Depositor
Recommended contour level	3.55	Depositor
Map size (Å)	460.32, 460.32, 460.32	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	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: IHP, ZN, K, GTP, MG

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	1	0.30	0/673	0.78	0/1043
2	2	0.23	0/554	0.74	0/856
3	5	0.36	0/2397	0.76	4/3727 (0.1%)
4	6	0.26	0/2207	0.78	0/3438
5	A	0.32	0/14793	0.56	1/20040 (0.0%)
6	B	0.31	0/7459	0.56	0/10117
7	C	0.28	0/2376	0.59	0/3216
8	D	0.30	0/772	0.63	0/1038
9	E	0.29	0/737	0.62	0/993
10	F	0.33	0/646	0.69	0/875
11	G	0.30	0/829	0.72	0/1111
12	H	0.26	0/662	0.57	0/894
13	I	0.28	0/585	0.59	1/794 (0.1%)
14	J	0.31	0/578	0.56	0/774
15	K	0.32	0/3130	0.58	0/4251
16	L	0.29	0/1885	0.57	0/2545
17	M	0.30	0/1841	0.61	0/2468
18	N	0.25	0/10690	0.47	1/14463 (0.0%)
19	O	0.33	0/1199	0.63	0/1609
20	P	0.33	0/2222	0.65	1/2991 (0.0%)
21	Q	0.28	0/767	0.57	0/1028
22	R	0.30	0/5235	0.60	1/7067 (0.0%)
23	S	0.29	0/1072	0.59	0/1453
23	T	0.31	0/1086	0.71	3/1472 (0.2%)
23	U	0.25	0/2897	0.56	1/3914 (0.0%)
23	V	0.27	0/1060	0.60	0/1437
24	W	0.28	0/4407	0.59	1/5907 (0.0%)
25	X	0.27	0/5599	0.54	2/7566 (0.0%)
26	Y	0.26	0/1065	0.60	0/1413
27	Z	0.27	0/1244	0.56	0/1667
28	a	0.31	0/1055	0.54	0/1443
29	b	0.30	0/829	0.51	0/1111

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
30	c	0.31	0/1711	0.56	0/2312
31	d	0.29	0/1206	0.62	1/1636 (0.1%)
33	m	0.27	0/663	0.55	0/895
35	y	0.29	0/1511	0.61	0/2032
36	z	0.27	0/5079	0.53	1/6875 (0.0%)
All	All	0.29	0/92721	0.58	18/126471 (0.0%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	U	118	LEU	CA-CB-CG	9.08	136.19	115.30
22	R	596	LEU	CA-CB-CG	8.87	135.71	115.30
3	5	32	C	C2-N1-C1'	7.93	127.52	118.80
3	5	32	C	N1-C2-O2	7.66	123.50	118.90
23	T	72	LEU	CA-CB-CG	6.72	130.76	115.30
31	d	32	LEU	CA-CB-CG	6.21	129.58	115.30
3	5	32	C	N3-C2-O2	-6.14	117.61	121.90
23	T	90	LEU	CA-CB-CG	6.10	129.34	115.30
25	X	487	LEU	CA-CB-CG	6.03	129.17	115.30
24	W	693	LEU	CA-CB-CG	5.79	128.61	115.30
3	5	32	C	C6-N1-C1'	-5.71	113.94	120.80
25	X	637	LEU	CA-CB-CG	5.57	128.12	115.30
36	z	383	LEU	CA-CB-CG	5.55	128.06	115.30
23	T	69	LEU	CA-CB-CG	5.53	128.02	115.30
13	I	15	LEU	CA-CB-CG	5.47	127.88	115.30
5	A	1429	LEU	CA-CB-CG	5.40	127.72	115.30
18	N	1123	MET	CA-CB-CG	5.10	121.97	113.30
20	P	85	ASP	CB-CA-C	-5.05	100.30	110.40

There are no chirality outliers.

There are no planarity outliers.

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	1	605	0	302	10	0
2	2	500	0	257	12	0
3	5	2149	0	1085	23	0
4	6	1970	0	994	52	0
5	A	14402	0	14306	312	0
6	B	7298	0	7336	178	0
7	C	2328	0	2276	84	0
8	D	760	0	776	26	0
9	E	726	0	750	23	0
10	F	638	0	682	37	0
11	G	819	0	845	46	0
12	H	652	0	680	13	0
13	I	574	0	591	27	0
14	J	573	0	602	12	0
15	K	3053	0	3011	88	0
16	L	1849	0	1879	47	0
17	M	1818	0	1822	67	0
18	N	10461	0	10412	189	0
19	O	1176	0	1167	31	0
20	P	2178	0	2101	105	0
21	Q	752	0	729	15	0
22	R	5108	0	5024	179	0
23	S	1055	0	1075	61	0
23	T	1069	0	1084	72	0
23	U	2870	0	2403	82	0
23	V	1044	0	1066	44	0
24	W	4346	0	4375	176	0
25	X	5467	0	5372	160	0
26	Y	1049	0	1052	46	0
27	Z	1232	0	1242	56	0
28	a	1035	0	837	0	0
29	b	822	0	820	0	0
30	c	1678	0	1659	0	0
31	d	1179	0	1169	0	0
32	f	110	0	29	0	0
33	m	649	0	641	0	0
34	r	335	0	77	0	0
35	y	1480	0	1379	0	0
36	z	4980	0	5047	0	0
37	6	3	0	0	0	0
37	B	1	0	0	0	0
38	6	1	0	0	0	0
39	A	36	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	B	32	0	12	3	0
41	M	2	0	0	0	0
41	O	3	0	0	0	0
41	P	1	0	0	0	0
All	All	90868	0	86972	1981	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 13.

All (1981) 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)
5:A:1642:LYS:HD3	5:A:1650:CYS:SG	1.36	1.62
5:A:1642:LYS:CD	5:A:1650:CYS:SG	2.14	1.34
5:A:1638:ILE:CD1	5:A:1642:LYS:HE3	1.73	1.18
4:6:32:G:N2	20:P:82:MET:HG2	1.57	1.17
4:6:32:G:N2	20:P:82:MET:CG	2.07	1.16
4:6:32:G:H21	20:P:82:MET:CG	1.57	1.15
5:A:1638:ILE:HD12	5:A:1642:LYS:HE3	1.14	1.13
4:6:32:G:H21	20:P:82:MET:HG2	0.91	1.08
15:K:117:LYS:HG3	22:R:225:GLN:HE21	1.22	1.01
5:A:1638:ILE:HG21	5:A:1642:LYS:HE2	1.44	0.96
15:K:86:ALA:O	22:R:259:ARG:NH2	2.01	0.92
4:6:32:G:N2	20:P:82:MET:SD	2.47	0.87
23:V:98:LYS:HE3	24:W:537:ARG:HA	1.58	0.85
20:P:149:ASP:OD1	20:P:224:GLN:NE2	2.08	0.85
22:R:78:GLN:NE2	22:R:113:CYS:SG	2.49	0.85
10:F:27:GLY:HA3	10:F:43:VAL:HG12	1.58	0.84
26:Y:94:ARG:O	26:Y:98:GLN:NE2	2.10	0.84
22:R:191:ARG:NH1	22:R:214:GLU:OE2	2.10	0.84
11:G:94:ARG:HE	11:G:96:ILE:HD11	1.41	0.83
5:A:866:LEU:HD12	5:A:890:VAL:HG13	1.60	0.83
6:B:195:SER:HB3	6:B:226:GLU:HB3	1.59	0.83
7:C:271:ASN:ND2	7:C:314:ASN:OD1	2.12	0.83
5:A:1601:PHE:HA	5:A:1605:LEU:HD12	1.60	0.83
23:S:73:LEU:HD23	23:S:76:PHE:HD2	1.44	0.82
20:P:281:ASP:HA	20:P:284:GLU:HG2	1.61	0.82
20:P:160:ARG:HH12	20:P:165:GLY:H	1.28	0.82
5:A:1642:LYS:HD2	5:A:1650:CYS:SG	2.19	0.81
7:C:87:GLY:HA3	9:E:94:LEU:HD23	1.62	0.81
15:K:343:GLU:OE1	15:K:400:TRP:NE1	2.12	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:653:ALA:HB1	27:Z:92:LEU:HD11	1.63	0.81
7:C:45:GLN:NE2	7:C:333:THR:HB	1.95	0.81
4:6:55:C:OP2	22:R:64:ARG:NH2	2.14	0.81
11:G:45:ILE:HB	11:G:53:LEU:HB2	1.63	0.81
27:Z:153:LYS:HE3	27:Z:156:GLN:HE22	1.45	0.81
5:A:1638:ILE:CD1	5:A:1642:LYS:CE	2.58	0.80
24:W:507:ASP:OD2	25:X:563:ARG:NH1	2.14	0.80
25:X:490:GLU:HG2	25:X:494:GLY:HA3	1.63	0.80
11:G:42:GLN:HG2	11:G:56:ARG:HH22	1.47	0.80
10:F:16:SER:HB3	10:F:69:ILE:HB	1.64	0.80
5:A:1429:LEU:HD12	5:A:1430:GLU:H	1.47	0.79
11:G:32:VAL:O	11:G:111:ARG:NH2	2.16	0.79
3:5:91:G:N7	8:D:97:ARG:NH1	2.31	0.79
23:T:94:LEU:HD12	23:U:90:LEU:HD11	1.64	0.79
23:T:122:ARG:NH1	23:U:118:LEU:O	2.16	0.79
27:Z:153:LYS:HE3	27:Z:156:GLN:NE2	1.98	0.78
24:W:672:CYS:HA	24:W:675:LEU:HG	1.65	0.78
17:M:239:LYS:HD2	17:M:253:ASN:HD22	1.49	0.78
20:P:293:ARG:HB2	20:P:296:LYS:HE2	1.64	0.78
23:V:12:GLU:HA	23:V:55:VAL:HG11	1.66	0.78
18:N:1188:SER:OG	18:N:1216:ASN:ND2	2.16	0.78
24:W:258:GLU:HB3	24:W:262:ARG:HH12	1.49	0.77
22:R:280:TYR:HB3	22:R:306:LEU:HD11	1.65	0.77
15:K:263:VAL:HG12	15:K:295:LEU:HD21	1.66	0.77
16:L:191:GLN:NE2	17:M:24:GLU:OE1	2.15	0.77
25:X:585:PRO:HG2	25:X:620:LYS:HE2	1.66	0.77
23:S:72:LEU:HG	23:S:76:PHE:CZ	2.19	0.77
8:D:17:THR:HG22	8:D:27:ARG:HD2	1.67	0.76
18:N:737:ARG:HD3	18:N:1040:ILE:HD11	1.67	0.76
18:N:798:HIS:HE1	18:N:924:GLN:HG2	1.50	0.76
7:C:203:ILE:HD11	7:C:215:LEU:HG	1.68	0.75
4:6:42:A:H5"	24:W:176:LYS:HG3	1.69	0.75
4:6:22:A:OP2	17:M:63:LYS:NZ	2.19	0.75
18:N:306:LEU:HD23	18:N:329:LEU:HD21	1.68	0.75
25:X:719:GLU:O	25:X:722:ARG:HG2	1.87	0.75
4:6:81:U:H5"	26:Y:178:ARG:HH21	1.52	0.75
23:S:62:ARG:HH21	23:S:64:PRO:HA	1.52	0.75
23:T:86:GLU:OE2	23:U:91:ARG:NH2	2.20	0.75
18:N:1136:CYS:HA	18:N:1167:GLY:O	1.87	0.74
23:U:383:PHE:HD1	23:U:390:LEU:HD22	1.52	0.74
17:M:38:GLU:OE2	17:M:55:ARG:NH1	2.19	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:47:CYS:SG	17:M:121:GLN:NE2	2.60	0.74
27:Z:126:ALA:O	27:Z:130:GLN:NE2	2.20	0.74
20:P:165:GLY:O	20:P:227:LYS:NZ	2.21	0.74
15:K:440:GLU:OE1	15:K:446:LYS:NZ	2.20	0.74
20:P:150:CYS:SG	20:P:224:GLN:NE2	2.61	0.74
20:P:198:TRP:NE1	20:P:230:MET:SD	2.59	0.74
23:S:63:PRO:HB3	24:W:693:LEU:HD21	1.67	0.74
23:V:108:LEU:HD11	24:W:604:LEU:HB2	1.69	0.74
5:A:1665:ARG:HE	5:A:1666:PRO:HD2	1.53	0.74
7:C:145:LYS:HE2	7:C:187:GLN:HE21	1.53	0.74
10:F:40:LEU:HB3	10:F:43:VAL:HG11	1.70	0.74
24:W:537:ARG:HD2	24:W:577:PHE:CG	2.23	0.74
3:5:105:A:O2'	11:G:50:ASN:OD1	2.06	0.74
22:R:151:LEU:HD22	26:Y:168:LEU:HD11	1.69	0.74
5:A:1185:ARG:HD2	21:Q:229:VAL:HG11	1.70	0.73
22:R:78:GLN:NE2	22:R:109:LYS:HE2	2.03	0.73
22:R:121:ASN:ND2	24:W:237:ASP:O	2.22	0.73
4:6:80:A:O5'	26:Y:111:GLN:NE2	2.22	0.73
4:6:75:G:N7	26:Y:200:ARG:NH1	2.35	0.73
23:T:90:LEU:HD21	23:U:90:LEU:HB3	1.70	0.73
23:T:122:ARG:NH1	23:U:122:ARG:HB2	2.02	0.73
22:R:264:PHE:O	22:R:268:ILE:HG12	1.89	0.73
15:K:107:ALA:HB1	22:R:238:PHE:HE2	1.52	0.72
23:S:90:LEU:HB2	23:V:90:LEU:HD11	1.69	0.72
7:C:217:GLY:O	7:C:219:LYS:NZ	2.21	0.72
11:G:25:PHE:HB3	11:G:34:GLN:HE21	1.54	0.72
24:W:575:TYR:CG	24:W:576:PRO:HD2	2.25	0.72
18:N:830:LEU:O	18:N:834:ILE:HG13	1.88	0.72
7:C:46:MET:HB3	7:C:334:ILE:HG13	1.71	0.72
5:A:1635:LYS:HB2	5:A:1653:ILE:HG22	1.71	0.72
5:A:1723:THR:OG1	5:A:1741:ASN:OD1	2.05	0.72
15:K:117:LYS:HG3	22:R:225:GLN:NE2	2.03	0.72
9:E:45:TYR:HE1	9:E:62:LYS:HE2	1.54	0.72
22:R:84:LYS:NZ	22:R:87:ALA:HB3	2.04	0.71
23:U:59:VAL:HG23	23:U:61:PRO:HD3	1.72	0.71
23:U:76:PHE:HE2	23:V:72:LEU:HD22	1.55	0.71
13:I:25:LYS:NZ	13:I:68:ASN:O	2.22	0.71
5:A:59:ARG:HH12	7:C:156:ASP:HB3	1.54	0.71
19:O:30:MET:HG2	19:O:52:LEU:HD23	1.73	0.71
24:W:387:ASN:HD22	24:W:406:LEU:HD22	1.55	0.71
20:P:90:GLN:HB3	20:P:240:CYS:SG	2.31	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1582:THR:HG22	5:A:1584:ILE:H	1.54	0.71
24:W:112:GLN:HG2	24:W:113:LEU:HD12	1.73	0.71
26:Y:93:LEU:HA	26:Y:96:LYS:HE2	1.71	0.71
24:W:516:ILE:HA	24:W:519:LYS:HE2	1.73	0.71
10:F:9:LYS:NZ	10:F:81:ILE:O	2.24	0.71
23:U:71:ALA:HB1	23:V:63:PRO:HD3	1.72	0.71
23:T:62:ARG:HH21	23:T:66:ALA:H	1.38	0.70
6:B:585:LYS:NZ	6:B:586:ASP:O	2.24	0.70
17:M:39:PRO:HA	17:M:52:THR:HG22	1.73	0.70
22:R:17:GLN:NE2	24:W:151:ASP:OD1	2.23	0.70
15:K:120:GLY:HA2	22:R:191:ARG:HD2	1.72	0.70
15:K:455:THR:OG1	15:K:458:THR:OG1	2.08	0.70
6:B:713:ASP:OD2	6:B:736:TYR:OH	2.09	0.70
17:M:38:GLU:HG2	17:M:53:ILE:HB	1.74	0.70
20:P:232:HIS:HA	20:P:240:CYS:HB2	1.74	0.70
6:B:114:ILE:HG21	6:B:661:LEU:HD11	1.74	0.69
13:I:15:LEU:HD21	13:I:20:VAL:HG11	1.74	0.69
18:N:209:TYR:HB3	18:N:222:LEU:HD21	1.73	0.69
24:W:507:ASP:N	25:X:529:TYR:O	2.25	0.69
23:S:73:LEU:HA	23:S:76:PHE:CD2	2.27	0.69
23:T:118:LEU:HA	23:T:121:GLU:HG2	1.74	0.69
7:C:74:ILE:HB	7:C:89:LEU:HB2	1.75	0.69
23:V:112:LEU:HD13	24:W:596:GLU:HG2	1.74	0.69
23:T:119:THR:HA	23:T:122:ARG:HG2	1.75	0.69
5:A:1209:ASN:HD22	5:A:1209:ASN:C	1.96	0.69
22:R:294:LEU:HD23	22:R:297:GLU:HB2	1.74	0.69
22:R:418:ASP:OD1	22:R:421:ARG:NH1	2.25	0.69
18:N:93:TRP:O	18:N:138:LYS:NZ	2.25	0.69
15:K:310:ASP:HB2	15:K:312:THR:HG22	1.74	0.69
25:X:668:ALA:HB2	25:X:683:ILE:HD11	1.74	0.69
6:B:848:VAL:HG12	6:B:913:MET:HG2	1.76	0.68
6:B:492:VAL:HG21	6:B:506:ALA:HB1	1.75	0.68
19:O:120:ARG:HH11	19:O:142:CYS:HB3	1.57	0.68
23:S:69:LEU:HD23	23:U:80:TRP:HB2	1.74	0.68
23:S:43:GLN:NE2	23:S:44:GLU:OE1	2.25	0.68
25:X:105:LEU:HD12	25:X:108:MET:HB2	1.76	0.68
11:G:6:ASP:OD1	11:G:7:LYS:NZ	2.25	0.68
18:N:1183:PHE:HB3	18:N:1213:VAL:HG22	1.74	0.68
11:G:61:ASP:OD1	11:G:62:ARG:N	2.26	0.68
23:T:69:LEU:HD12	23:T:70:PRO:HD2	1.74	0.68
23:U:191:ALA:HB3	23:U:485:LEU:HB3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:155:SER:OG	7:C:157:ASP:OD1	2.12	0.68
20:P:160:ARG:NH1	20:P:165:GLY:H	1.91	0.68
25:X:472:PRO:HA	25:X:475:ARG:HB2	1.76	0.68
5:A:1638:ILE:HD13	5:A:1642:LYS:HE3	1.74	0.67
11:G:93:ASP:OD1	11:G:94:ARG:N	2.27	0.67
22:R:485:ASP:OD1	22:R:488:ARG:NH1	2.27	0.67
24:W:105:LEU:HD22	24:W:385:VAL:HG12	1.76	0.67
5:A:1429:LEU:O	5:A:1430:GLU:HG3	1.94	0.67
3:5:101:U:H3	11:G:65:ASN:HD21	1.41	0.67
24:W:203:LYS:HA	24:W:207:ILE:HB	1.76	0.67
6:B:812:PRO:HG2	6:B:817:ARG:HH12	1.57	0.67
5:A:1602:ARG:HE	5:A:1770:ARG:HH11	1.42	0.67
23:V:3:CYS:HB2	23:V:10:PRO:HD3	1.77	0.67
4:6:32:G:N2	20:P:82:MET:CB	2.58	0.67
17:M:141:ARG:NH2	20:P:314:TYR:O	2.28	0.67
23:S:118:LEU:O	23:S:122:ARG:HD3	1.95	0.67
24:W:132:SER:OG	24:W:135:ARG:NH2	2.28	0.67
7:C:41:VAL:HG21	9:E:103:PRO:HB3	1.76	0.67
13:I:22:VAL:HG12	13:I:73:VAL:HG12	1.75	0.67
24:W:518:GLU:HA	24:W:521:ARG:HE	1.58	0.67
5:A:107:ARG:NH1	16:L:213:GLU:OE2	2.27	0.67
18:N:529:LEU:HD11	18:N:611:ALA:HB1	1.76	0.67
24:W:172:ASN:O	24:W:173:THR:HG22	1.94	0.67
10:F:17:ILE:HD12	10:F:40:LEU:HD11	1.76	0.66
18:N:207:ILE:HG21	18:N:360:PHE:HE2	1.60	0.66
17:M:24:GLU:OE1	17:M:24:GLU:N	2.28	0.66
22:R:603:GLU:HG3	22:R:615:VAL:HG21	1.77	0.66
23:T:94:LEU:O	23:T:98:LYS:HD3	1.96	0.66
5:A:694:GLN:O	5:A:699:ARG:NH2	2.25	0.66
18:N:697:ILE:HD11	18:N:708:ALA:HB1	1.78	0.66
19:O:127:ASP:O	19:O:131:ARG:NE	2.28	0.66
4:6:47:A:H5"	4:6:47:A:H8	1.59	0.66
5:A:1267:ARG:HH11	5:A:1270:GLN:HE21	1.43	0.66
5:A:1663:VAL:HG11	5:A:1741:ASN:HB3	1.77	0.66
6:B:227:VAL:HG11	6:B:254:ILE:HD12	1.77	0.66
6:B:267:LEU:HB3	6:B:319:VAL:HG22	1.78	0.66
22:R:545:ASN:HA	22:R:548:ILE:HD12	1.77	0.66
11:G:55:ALA:HB2	11:G:71:VAL:HA	1.78	0.66
22:R:289:GLN:HE22	25:X:538:GLU:HB2	1.61	0.66
23:T:73:LEU:HA	23:T:76:PHE:HD2	1.60	0.66
4:6:32:G:C2	20:P:82:MET:HG2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:952:GLU:OE2	5:A:955:ARG:NH2	2.29	0.66
18:N:922:PHE:HA	18:N:925:LEU:HD12	1.77	0.66
22:R:48:LEU:HD11	22:R:52:GLN:HE22	1.61	0.66
23:U:336:ILE:HA	23:U:352:LEU:HA	1.78	0.66
17:M:86:ASP:OD1	17:M:90:GLY:N	2.29	0.65
24:W:510:ARG:HH21	25:X:531:GLU:HG2	1.62	0.65
5:A:250:ASN:HB2	5:A:253:GLN:HG3	1.78	0.65
23:V:76:PHE:HB3	23:V:80:TRP:HZ3	1.59	0.65
24:W:246:PHE:HA	24:W:249:LYS:HG2	1.78	0.65
24:W:696:LYS:HG3	27:Z:131:LEU:HD12	1.77	0.65
17:M:237:PRO:HB2	17:M:255:LYS:HD3	1.77	0.65
22:R:593:VAL:HA	22:R:596:LEU:HD22	1.77	0.65
5:A:1602:ARG:HH21	5:A:1770:ARG:HD3	1.62	0.65
6:B:628:TYR:OH	6:B:657:ASP:OD2	2.13	0.65
22:R:285:HIS:O	22:R:289:GLN:HG2	1.97	0.65
23:T:62:ARG:NH2	23:T:66:ALA:H	1.95	0.65
25:X:139:LEU:HD13	25:X:147:ILE:HG23	1.79	0.65
5:A:810:GLU:OE2	5:A:813:ARG:NH2	2.29	0.65
18:N:694:SER:HB3	18:N:713:SER:HB3	1.78	0.65
20:P:160:ARG:HH22	20:P:165:GLY:N	1.94	0.65
22:R:256:GLU:HB3	22:R:259:ARG:HH11	1.61	0.65
25:X:439:LEU:HD11	25:X:489:LEU:HD11	1.79	0.65
5:A:1020:MET:HG2	5:A:1066:PHE:HZ	1.62	0.65
5:A:1025:ASP:OD1	5:A:1026:THR:N	2.30	0.65
7:C:217:GLY:O	7:C:244:ARG:NH1	2.29	0.65
15:K:109:GLN:HA	15:K:133:GLN:NE2	2.12	0.65
23:S:69:LEU:N	23:T:79:GLU:OE2	2.30	0.65
7:C:188:GLN:HE22	7:C:190:THR:H	1.45	0.65
23:U:180:THR:O	23:U:184:PRO:CG	2.45	0.65
26:Y:167:ARG:HA	26:Y:170:GLU:HG2	1.78	0.65
5:A:1115:ILE:HD11	5:A:1465:GLU:HG2	1.79	0.64
18:N:803:LEU:HD21	18:N:945:LEU:HD23	1.79	0.64
20:P:134:LEU:HD23	20:P:136:ARG:HE	1.61	0.64
23:T:6:SER:HB3	23:U:84:ALA:HB1	1.78	0.64
24:W:105:LEU:O	24:W:109:GLU:HG2	1.97	0.64
25:X:87:HIS:HB2	25:X:91:PHE:HE1	1.63	0.64
5:A:873:TYR:CE1	5:A:883:GLN:NE2	2.65	0.64
5:A:899:GLU:OE1	5:A:899:GLU:N	2.29	0.64
18:N:378:ILE:O	18:N:382:ASP:N	2.28	0.64
5:A:58:TRP:HH2	7:C:272:LEU:HD11	1.63	0.64
17:M:227:LYS:O	17:M:231:HIS:ND1	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:164:GLN:NE2	5:A:227:PHE:O	2.23	0.64
20:P:190:ILE:HG22	20:P:193:ARG:HH22	1.62	0.64
25:X:243:ARG:HA	25:X:246:ILE:HG12	1.78	0.64
27:Z:18:ASN:ND2	27:Z:20:GLU:HG3	2.12	0.64
5:A:1298:TYR:HB3	5:A:1301:ALA:HB3	1.78	0.64
18:N:390:TYR:HE1	18:N:632:LEU:HD11	1.61	0.64
25:X:500:ARG:NH1	25:X:532:ASP:OD2	2.28	0.64
5:A:45:GLY:N	5:A:48:GLU:OE2	2.31	0.64
16:L:163:LYS:O	16:L:167:GLN:NE2	2.30	0.64
20:P:118:LEU:HA	20:P:151:PHE:CZ	2.32	0.64
23:V:98:LYS:HD2	24:W:536:ILE:HG13	1.79	0.64
5:A:1185:ARG:HH11	21:Q:229:VAL:HG11	1.63	0.64
10:F:46:THR:HG22	10:F:52:PRO:HB3	1.80	0.64
6:B:644:PHE:CE2	6:B:675:ARG:HD2	2.32	0.64
7:C:45:GLN:HE22	7:C:333:THR:HB	1.60	0.64
18:N:1179:ASN:HA	18:N:1208:SER:HB2	1.79	0.64
24:W:597:ILE:O	24:W:601:ARG:HG2	1.98	0.64
4:6:34:U:H2'	4:6:35:A:H8	1.62	0.63
5:A:1432:LEU:HD12	5:A:1447:PHE:HZ	1.63	0.63
6:B:90:ASP:OD2	15:K:157:ARG:NH1	2.31	0.63
17:M:267:SER:HB2	17:M:282:GLN:HE21	1.63	0.63
5:A:1430:GLU:HA	5:A:1433:GLU:HG2	1.81	0.63
7:C:244:ARG:HB3	7:C:257:GLN:HE22	1.64	0.63
18:N:460:TYR:HD1	18:N:472:LEU:HD21	1.61	0.63
19:O:101:CYS:SG	19:O:102:CYS:N	2.71	0.63
15:K:122:PRO:HA	15:K:126:HIS:HB2	1.79	0.63
17:M:243:CYS:SG	17:M:244:SER:N	2.72	0.63
25:X:458:PRO:HG2	25:X:461:SER:HB3	1.80	0.63
2:2:19:G:H22	4:6:50:A:H2	1.47	0.63
5:A:251:LEU:HD21	5:A:424:ALA:HB2	1.79	0.63
5:A:839:TRP:CZ2	5:A:843:ARG:HD2	2.33	0.63
23:T:122:ARG:HD3	23:U:122:ARG:HH21	1.64	0.63
25:X:84:PRO:HG2	25:X:122:GLN:HG2	1.79	0.63
25:X:538:GLU:HA	25:X:541:VAL:HG22	1.79	0.63
6:B:692:THR:HA	6:B:825:THR:HG21	1.80	0.63
7:C:327:SER:HB2	7:C:335:PHE:HB2	1.81	0.63
19:O:98:GLU:OE1	19:O:98:GLU:N	2.30	0.63
24:W:207:ILE:HG12	24:W:209:ILE:H	1.61	0.63
5:A:1296:THR:HG21	5:A:1489:TRP:CE3	2.34	0.63
7:C:183:VAL:HG12	7:C:194:ILE:HG22	1.81	0.63
24:W:250:ARG:HH11	24:W:254:GLN:HG3	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:986:THR:HG21	5:A:1100:GLN:HG2	1.80	0.63
5:A:1669:LEU:HD23	5:A:1751:GLN:HG2	1.80	0.63
7:C:185:ILE:HG13	7:C:192:VAL:HG12	1.81	0.63
23:S:88:PHE:O	23:S:92:ARG:HG2	1.98	0.63
24:W:251:GLU:HB2	24:W:255:LYS:HZ3	1.63	0.63
25:X:554:ASN:O	25:X:558:THR:HG23	1.98	0.63
5:A:1153:LYS:HE3	5:A:1196:GLU:HA	1.81	0.62
5:A:1765:TYR:O	5:A:1769:GLU:HG2	1.98	0.62
7:C:145:LYS:HE2	7:C:187:GLN:NE2	2.13	0.62
23:T:118:LEU:HD12	23:U:122:ARG:NH2	2.14	0.62
4:6:42:A:OP1	24:W:176:LYS:NZ	2.27	0.62
5:A:140:LEU:HD12	5:A:506:GLN:O	1.99	0.62
16:L:127:LEU:HA	16:L:130:ARG:HG3	1.82	0.62
16:L:127:LEU:HD23	16:L:130:ARG:HG3	1.80	0.62
19:O:123:LYS:HD2	19:O:131:ARG:HD2	1.81	0.62
6:B:777:LYS:HA	6:B:780:ILE:HG22	1.81	0.62
17:M:82:SER:O	20:P:147:ASN:ND2	2.32	0.62
18:N:533:TYR:HB3	18:N:556:ASP:HB2	1.82	0.62
5:A:1639:HIS:CE1	5:A:1650:CYS:HB3	2.34	0.62
23:S:62:ARG:HD3	23:T:8:GLU:HA	1.82	0.62
23:U:118:LEU:HG	23:U:122:ARG:NH2	2.15	0.62
24:W:200:ARG:HA	24:W:203:LYS:HG2	1.80	0.62
26:Y:199:GLU:HG3	26:Y:202:ARG:HH12	1.64	0.62
19:O:127:ASP:OD2	19:O:130:GLN:NE2	2.32	0.62
22:R:48:LEU:HD22	24:W:257:ILE:HG23	1.80	0.62
23:U:115:ILE:HD13	23:U:118:LEU:HD23	1.80	0.62
27:Z:89:ARG:HA	27:Z:92:LEU:HD13	1.79	0.62
5:A:1405:ASP:OD1	5:A:1408:ARG:NH2	2.31	0.62
15:K:150:HIS:CE1	15:K:399:ASP:OD2	2.53	0.62
15:K:172:GLU:HG2	15:K:173:PRO:HD2	1.81	0.62
17:M:109:ASN:OD1	17:M:112:ASN:HB2	1.98	0.62
18:N:7:LYS:HA	18:N:10:GLN:HG2	1.81	0.62
23:U:90:LEU:HD12	23:U:93:ASN:HB2	1.81	0.62
23:V:77:GLN:NE2	27:Z:101:TYR:OH	2.32	0.62
5:A:1629:GLN:HA	5:A:1657:ALA:HA	1.80	0.62
6:B:715:GLU:O	6:B:754:ARG:NH1	2.32	0.62
20:P:209:SER:OG	20:P:210:ARG:NH1	2.32	0.62
22:R:329:GLU:HG3	22:R:330:GLU:OE2	1.99	0.62
26:Y:178:ARG:O	26:Y:182:ASN:ND2	2.33	0.62
2:2:29:A:OP1	5:A:884:ARG:NH2	2.33	0.62
23:V:76:PHE:HB3	23:V:80:TRP:CZ3	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:10:A:OP1	5:A:56:ARG:NH1	2.27	0.62
5:A:1638:ILE:HD13	5:A:1642:LYS:CE	2.29	0.62
6:B:204:ASP:OD1	6:B:205:MET:N	2.31	0.62
23:S:88:PHE:HB3	23:S:92:ARG:NH2	2.15	0.62
24:W:689:GLN:O	24:W:693:LEU:HB2	2.00	0.62
7:C:62:GLY:O	7:C:319:HIS:NE2	2.32	0.61
18:N:357:ARG:HH21	18:N:361:PRO:HD3	1.65	0.61
18:N:741:PRO:HA	18:N:1004:ARG:HG2	1.81	0.61
18:N:772:ASP:OD1	18:N:950:ARG:NH1	2.33	0.61
22:R:61:ASP:HA	22:R:64:ARG:HG2	1.82	0.61
3:5:103:U:OP2	13:I:68:ASN:ND2	2.33	0.61
7:C:77:TRP:CZ3	7:C:85:ASN:HB3	2.35	0.61
27:Z:111:LEU:HA	27:Z:114:LYS:HG3	1.82	0.61
7:C:58:PHE:CE1	7:C:326:LEU:HD22	2.35	0.61
24:W:157:GLU:OE1	24:W:157:GLU:N	2.33	0.61
5:A:1209:ASN:O	5:A:1209:ASN:ND2	2.24	0.61
5:A:1660:LYS:NZ	5:A:1661:TRP:O	2.33	0.61
6:B:769:ASP:HB2	6:B:772:VAL:HB	1.81	0.61
22:R:67:ARG:HG3	22:R:68:LEU:HD22	1.82	0.61
5:A:921:PHE:HD2	5:A:928:LEU:HB3	1.65	0.61
15:K:268:ASP:OD2	15:K:272:ARG:NH1	2.33	0.61
23:U:299:ASN:N	23:U:313:ALA:O	2.30	0.61
25:X:286:THR:HG21	25:X:289:ASN:HB2	1.83	0.61
5:A:287:ALA:HA	5:A:301:LEU:HD23	1.82	0.61
25:X:295:ASP:HA	25:X:298:VAL:HG12	1.83	0.61
5:A:1020:MET:HG2	5:A:1066:PHE:CZ	2.36	0.61
6:B:154:LYS:NZ	40:B:1001:GTP:O2G	2.34	0.61
6:B:860:ILE:HG12	6:B:901:LEU:HD11	1.81	0.61
8:D:21:GLU:HA	8:D:67:ARG:HE	1.65	0.61
15:K:302:PRO:HG3	15:K:315:LEU:HD23	1.83	0.61
18:N:778:SER:HB2	18:N:979:MET:HG3	1.82	0.61
23:T:129:LEU:HD22	23:U:129:LEU:HD12	1.81	0.61
5:A:1534:GLU:OE2	5:A:1557:ARG:NH2	2.34	0.61
6:B:706:LEU:HD12	6:B:710:ILE:HD13	1.83	0.61
7:C:188:GLN:NE2	7:C:190:THR:H	1.98	0.61
18:N:113:LEU:O	18:N:205:LYS:NZ	2.34	0.61
24:W:198:LYS:HE3	24:W:198:LYS:HA	1.83	0.61
18:N:307:GLN:NE2	18:N:324:CYS:O	2.33	0.60
5:A:1215:THR:OG1	5:A:1216:GLY:N	2.33	0.60
6:B:488:LEU:HD12	6:B:514:GLN:O	2.02	0.60
6:B:678:GLU:OE2	6:B:791:GLY:HA3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:146:VAL:O	6:B:217:THR:OG1	2.18	0.60
15:K:231:CYS:HB3	15:K:241:ARG:HB2	1.84	0.60
20:P:160:ARG:HH22	20:P:165:GLY:H	1.49	0.60
5:A:870:LYS:NZ	5:A:894:TYR:OH	2.34	0.60
5:A:1190:LEU:HD12	5:A:1191:THR:HG22	1.84	0.60
5:A:1633:VAL:HA	5:A:1654:LEU:O	2.00	0.60
18:N:18:ASN:HA	18:N:25:VAL:HG21	1.84	0.60
18:N:836:ARG:NH2	18:N:890:TYR:O	2.33	0.60
22:R:326:LEU:HD23	22:R:329:GLU:OE2	2.01	0.60
23:U:357:LEU:O	23:U:370:LYS:HA	2.02	0.60
5:A:1239:ASN:HB3	5:A:1248:ARG:HD3	1.83	0.60
6:B:140:ASP:OD2	6:B:208:LYS:NZ	2.28	0.60
22:R:214:GLU:HB3	22:R:223:VAL:HG22	1.83	0.60
23:S:73:LEU:HD23	23:S:76:PHE:CD2	2.32	0.60
22:R:219:ASN:ND2	22:R:222:ASN:HB2	2.16	0.60
22:R:593:VAL:HA	22:R:596:LEU:CD2	2.31	0.60
23:T:90:LEU:HD23	23:U:90:LEU:HD23	1.83	0.60
4:6:18:G:N1	16:L:208:GLU:O	2.30	0.60
5:A:533:ARG:HG2	5:A:533:ARG:O	2.02	0.60
5:A:746:ASN:OD1	5:A:808:LYS:NZ	2.35	0.60
5:A:1685:TRP:O	5:A:1725:VAL:N	2.31	0.60
25:X:139:LEU:HD22	25:X:147:ILE:HG12	1.83	0.60
5:A:1700:ILE:HD12	5:A:1730:ASP:HB2	1.82	0.60
4:6:52:G:H2'	4:6:53:G:C8	2.37	0.59
6:B:229:ALA:HB3	6:B:494:LYS:NZ	2.16	0.59
18:N:628:LEU:HD11	18:N:987:SER:HB3	1.83	0.59
15:K:92:SER:HA	15:K:95:VAL:HG12	1.83	0.59
15:K:417:SER:OG	21:Q:248:ASN:ND2	2.35	0.59
25:X:400:TYR:HD2	25:X:409:SER:HB2	1.67	0.59
13:I:45:LEU:HB2	13:I:63:ILE:HB	1.83	0.59
15:K:235:GLU:OE2	21:Q:42:GLN:NE2	2.35	0.59
17:M:44:CYS:SG	17:M:47:CYS:HB2	2.42	0.59
24:W:270:GLY:HA2	24:W:273:PHE:HB3	1.84	0.59
25:X:129:ARG:HD2	25:X:169:ARG:HH22	1.66	0.59
9:E:12:HIS:CE1	9:E:84:PRO:HD3	2.38	0.59
10:F:23:THR:HG22	10:F:47:VAL:HA	1.83	0.59
9:E:44:GLU:OE1	9:E:63:ARG:NE	2.31	0.59
18:N:824:ILE:HD11	18:N:940:GLN:HE22	1.68	0.59
22:R:110:TYR:CE2	22:R:126:LEU:HD13	2.37	0.59
15:K:168:CYS:SG	15:K:211:LEU:HG	2.42	0.59
16:L:188:PRO:HB3	17:M:24:GLU:OE2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:383:PHE:CD1	23:U:390:LEU:HD22	2.36	0.59
24:W:258:GLU:HB3	24:W:262:ARG:NH1	2.18	0.59
25:X:337:PRO:HA	25:X:340:ILE:HG12	1.84	0.59
5:A:635:ILE:HD11	5:A:655:PRO:HG2	1.84	0.59
5:A:1295:MET:HG3	5:A:1354:MET:SD	2.42	0.59
10:F:33:ASP:OD1	10:F:34:MET:N	2.36	0.59
23:T:40:VAL:HG22	23:U:92:ARG:HH22	1.68	0.59
23:U:342:HIS:HD2	23:U:344:ASP:HB2	1.68	0.59
24:W:203:LYS:HB3	24:W:207:ILE:HD12	1.85	0.59
25:X:512:ALA:HB2	26:Y:83:ILE:HG13	1.85	0.59
25:X:671:GLU:HA	25:X:674:LEU:HD12	1.85	0.59
5:A:664:LEU:HA	5:A:667:ILE:HG22	1.84	0.59
6:B:704:GLU:OE2	6:B:804:ARG:NH2	2.35	0.59
10:F:6:PHE:CE1	10:F:80:LEU:HD22	2.37	0.59
17:M:235:TYR:HB3	17:M:263:ALA:HB2	1.83	0.59
22:R:20:ALA:N	24:W:15:GLU:OE1	2.35	0.59
22:R:487:ALA:HA	22:R:490:LEU:HD12	1.82	0.59
23:S:103:THR:HA	23:S:106:TYR:CE2	2.38	0.59
11:G:44:LEU:HB3	11:G:110:VAL:HG23	1.85	0.59
1:1:3:A:N6	4:6:38:G:O2'	2.36	0.59
6:B:250:ASN:O	6:B:254:ILE:HG12	2.02	0.59
7:C:328:CYS:HA	7:C:334:ILE:HG22	1.84	0.59
19:O:18:GLU:OE1	19:O:18:GLU:N	2.32	0.59
22:R:84:LYS:HZ1	22:R:87:ALA:HB3	1.66	0.59
23:T:132:PHE:CZ	23:U:132:PHE:HB3	2.38	0.59
25:X:679:ARG:HA	25:X:682:LEU:HD12	1.85	0.59
6:B:242:ASP:OD1	6:B:271:LYS:HD2	2.03	0.58
6:B:631:SER:HA	6:B:644:PHE:O	2.03	0.58
24:W:705:GLN:O	24:W:709:LYS:HG2	2.03	0.58
5:A:177:ARG:HD3	5:A:643:PRO:HB2	1.85	0.58
5:A:539:LEU:HD11	5:A:561:SER:HB2	1.83	0.58
6:B:601:VAL:HB	6:B:844:PRO:HG3	1.85	0.58
7:C:57:ARG:HG2	7:C:57:ARG:HH11	1.68	0.58
10:F:32:VAL:HG23	10:F:38:THR:HG22	1.84	0.58
15:K:229:VAL:HB	15:K:243:TYR:HB2	1.86	0.58
22:R:121:ASN:HA	22:R:124:ARG:HD3	1.84	0.58
23:T:121:GLU:HA	23:T:124:GLU:CD	2.24	0.58
24:W:521:ARG:HA	24:W:524:LYS:HD3	1.86	0.58
6:B:916:ASP:OD2	6:B:917:HIS:ND1	2.32	0.58
16:L:250:GLN:HG2	26:Y:211:PHE:HE1	1.68	0.58
23:S:122:ARG:HE	23:V:114:VAL:HG22	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:T:1:MET:SD	27:Z:130:GLN:HG2	2.44	0.58
5:A:1638:ILE:CG2	5:A:1642:LYS:HE2	2.27	0.58
9:E:45:TYR:CE1	9:E:62:LYS:HE2	2.38	0.58
10:F:7:LEU:HB3	10:F:32:VAL:HG11	1.83	0.58
16:L:184:ILE:HG21	17:M:19:PHE:CE1	2.38	0.58
18:N:25:VAL:O	18:N:65:ARG:NH2	2.37	0.58
18:N:945:LEU:HD13	18:N:966:LEU:HD21	1.86	0.58
23:T:62:ARG:HH11	27:Z:112:LEU:HD22	1.67	0.58
25:X:624:ARG:NH1	25:X:654:SER:O	2.36	0.58
15:K:352:ASP:OD1	15:K:353:ASN:N	2.36	0.58
18:N:70:MET:HG3	18:N:74:HIS:ND1	2.19	0.58
23:U:71:ALA:HB2	23:V:61:PRO:HG2	1.84	0.58
25:X:637:LEU:HD23	25:X:638:ASN:H	1.69	0.58
5:A:1576:GLN:HG2	5:A:1587:HIS:CE1	2.38	0.58
25:X:252:GLN:OE1	25:X:255:LYS:NZ	2.37	0.58
1:1:-4:A:H5'	5:A:1589:LYS:HG3	1.86	0.58
18:N:664:SER:HB2	18:N:696:LEU:HD11	1.86	0.58
5:A:1063:ILE:HA	5:A:1066:PHE:CE1	2.38	0.58
6:B:146:VAL:HG12	6:B:154:LYS:HB2	1.85	0.58
7:C:308:GLY:HA3	9:E:106:ARG:HG2	1.85	0.58
20:P:121:ALA:HB1	20:P:229:ALA:HB2	1.86	0.58
22:R:333:GLY:O	22:R:337:THR:OG1	2.21	0.58
25:X:685:ILE:HD11	25:X:723:ILE:HG21	1.85	0.58
5:A:1111:TYR:HD1	5:A:1120:ILE:HG12	1.69	0.57
6:B:221:VAL:HG21	6:B:912:GLN:HB3	1.86	0.57
18:N:117:LEU:HD11	18:N:205:LYS:HB3	1.85	0.57
18:N:872:THR:O	18:N:884:ARG:NH1	2.37	0.57
22:R:86:PHE:HE1	22:R:119:ASN:HD21	1.50	0.57
23:S:71:ALA:HB2	23:T:60:ARG:HH21	1.69	0.57
23:V:106:TYR:CE2	24:W:564:MET:HB3	2.39	0.57
25:X:337:PRO:O	25:X:341:ASN:ND2	2.36	0.57
25:X:394:SER:O	25:X:398:ARG:HG3	2.03	0.57
1:1:-1:U:H5'	1:1:0:G:H5"	1.86	0.57
5:A:1642:LYS:HG2	5:A:1642:LYS:O	2.04	0.57
6:B:378:VAL:HG13	6:B:383:HIS:HB2	1.86	0.57
18:N:809:GLY:HA2	18:N:814:LEU:HD12	1.86	0.57
5:A:1236:GLY:HA2	5:A:1300:GLU:HG3	1.86	0.57
6:B:658:LEU:HD22	6:B:667:ILE:HD13	1.84	0.57
5:A:863:VAL:O	5:A:867:GLU:HG3	2.03	0.57
20:P:201:ILE:HD13	20:P:215:ILE:HD11	1.85	0.57
25:X:560:PHE:HZ	25:X:571:ARG:HD2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1638:ILE:HG21	5:A:1642:LYS:CE	2.28	0.57
7:C:121:ASP:HB2	7:C:128:ILE:HD11	1.87	0.57
7:C:259:GLN:NE2	7:C:298:ALA:O	2.36	0.57
19:O:126:LEU:O	19:O:131:ARG:NH2	2.37	0.57
23:U:118:LEU:HG	23:U:122:ARG:HH22	1.67	0.57
25:X:524:LEU:HD21	25:X:532:ASP:HB2	1.86	0.57
25:X:552:LEU:HD23	25:X:555:LEU:HD21	1.87	0.57
5:A:154:PRO:O	5:A:444:ALA:N	2.37	0.57
5:A:1568:ARG:NH2	5:A:1696:ASP:OD1	2.32	0.57
24:W:510:ARG:NH2	25:X:531:GLU:HG2	2.20	0.57
25:X:543:LEU:HD13	26:Y:83:ILE:HD11	1.86	0.57
15:K:344:PHE:CE2	15:K:360:PRO:HG3	2.40	0.57
23:U:83:VAL:HG22	23:U:87:GLN:HE21	1.70	0.57
5:A:968:SER:HB2	5:A:969:GLU:OE1	2.03	0.57
9:E:23:THR:HB	9:E:45:TYR:HB2	1.86	0.57
19:O:29:ARG:O	19:O:32:GLN:HG2	2.05	0.57
25:X:532:ASP:HA	25:X:535:LYS:HB2	1.85	0.57
5:A:1669:LEU:HD13	5:A:1738:ALA:HB3	1.86	0.57
15:K:118:ILE:HG13	22:R:225:GLN:NE2	2.19	0.57
18:N:149:ILE:HG13	18:N:152:LEU:HD12	1.87	0.57
18:N:527:PRO:O	18:N:562:ILE:N	2.25	0.57
18:N:562:ILE:HA	18:N:585:VAL:HG22	1.87	0.57
22:R:104:ILE:HD13	22:R:137:VAL:HG21	1.86	0.57
23:T:118:LEU:HD12	23:U:122:ARG:CZ	2.35	0.57
5:A:983:ASN:ND2	5:A:1241:THR:O	2.38	0.57
5:A:1660:LYS:HZ1	5:A:1680:THR:C	2.08	0.57
15:K:386:MET:HB3	15:K:398:TRP:HB2	1.85	0.57
20:P:289:LYS:O	20:P:293:ARG:NH1	2.37	0.57
23:T:21:ASN:HB2	23:T:23:TYR:CE2	2.39	0.57
25:X:321:SER:O	25:X:325:HIS:ND1	2.35	0.57
15:K:381:ASN:OD1	15:K:382:SER:N	2.38	0.56
3:5:102:G:N7	11:G:48:ARG:HD3	2.19	0.56
5:A:811:GLN:HG2	5:A:1047:HIS:HB3	1.87	0.56
5:A:1268:ILE:HG21	5:A:1315:CYS:HB2	1.86	0.56
5:A:1736:HIS:ND1	5:A:1758:MET:SD	2.78	0.56
6:B:886:ARG:HG3	6:B:886:ARG:HH11	1.70	0.56
5:A:402:ASN:HA	6:B:367:LYS:HE3	1.88	0.56
7:C:265:ILE:HD11	7:C:290:ASP:HB3	1.86	0.56
11:G:12:LEU:HB3	11:G:16:GLU:HG2	1.87	0.56
15:K:256:HIS:HD1	15:K:258:THR:H	1.53	0.56
23:T:25:LYS:O	23:T:29:GLU:HG2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:405:LEU:HG	23:U:406:ARG:HD2	1.87	0.56
24:W:38:ARG:NH2	24:W:158:ASP:OD2	2.38	0.56
24:W:244:GLN:HG2	24:W:245:ASN:HD22	1.71	0.56
5:A:1641:ARG:HB3	5:A:1644:TYR:CZ	2.41	0.56
24:W:678:ARG:HD2	27:Z:109:LEU:HD22	1.86	0.56
25:X:400:TYR:CD2	25:X:409:SER:HB2	2.41	0.56
25:X:551:GLU:HA	25:X:554:ASN:HD22	1.70	0.56
3:5:103:U:O5’	11:G:48:ARG:NH2	2.38	0.56
5:A:312:TRP:H	5:A:312:TRP:HE3	1.53	0.56
17:M:102:LEU:HD11	17:M:136:ALA:HA	1.88	0.56
18:N:299:ASP:HB3	18:N:383:ARG:HH12	1.71	0.56
18:N:1049:ARG:HE	18:N:1075:LEU:HA	1.70	0.56
22:R:261:ARG:O	22:R:265:LYS:HG2	2.05	0.56
23:T:85:LEU:HA	23:T:88:PHE:HD2	1.70	0.56
25:X:684:TYR:HB3	25:X:703:TRP:CZ3	2.41	0.56
3:5:12:A:HO2’	3:5:13:A:H8	1.51	0.56
7:C:82:ASP:OD2	7:C:84:LYS:HD3	2.06	0.56
8:D:19:GLU:HB3	8:D:25:THR:HG22	1.88	0.56
25:X:661:LYS:HA	25:X:664:CYS:HB2	1.87	0.56
5:A:1639:HIS:HE1	5:A:1650:CYS:HB3	1.71	0.56
20:P:93:SER:N	20:P:232:HIS:O	2.39	0.56
20:P:176:LEU:HD22	20:P:227:LYS:HB2	1.87	0.56
23:U:388:TYR:HA	23:U:405:LEU:HD22	1.87	0.56
25:X:581:GLU:OE1	25:X:581:GLU:N	2.39	0.56
26:Y:140:LYS:HB3	26:Y:142:ARG:HH11	1.71	0.56
1:1:8:U:OP1	24:W:213:ARG:NH2	2.39	0.56
5:A:1069:LEU:O	5:A:1073:LEU:HD13	2.06	0.56
7:C:103:ARG:HD3	7:C:145:LYS:HA	1.88	0.56
18:N:396:PHE:HE1	18:N:442:LYS:HG3	1.70	0.56
18:N:460:TYR:CD1	18:N:472:LEU:HD21	2.40	0.56
22:R:604:ALA:O	22:R:612:ARG:NH2	2.39	0.56
23:S:61:PRO:HB3	23:T:2:PHE:HB3	1.87	0.56
6:B:711:SER:HG	6:B:800:ASN:HD22	1.53	0.56
18:N:1223:THR:HB	18:N:1226:LEU:HD12	1.87	0.56
22:R:83:GLN:HG2	22:R:84:LYS:N	2.21	0.56
5:A:309:MET:HG2	5:A:311:ASP:H	1.70	0.55
23:T:87:GLN:OE1	23:U:87:GLN:NE2	2.32	0.55
24:W:202:LEU:HG	24:W:207:ILE:HA	1.86	0.55
25:X:395:GLU:OE1	25:X:398:ARG:NH1	2.38	0.55
26:Y:174:LYS:HD2	26:Y:174:LYS:O	2.06	0.55
4:6:74:U:H4’	4:6:75:G:OP1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:542:ASP:OD2	5:A:546:ASN:ND2	2.30	0.55
6:B:396:THR:HG23	6:B:427:LEU:HG	1.87	0.55
6:B:862:ASP:OD1	6:B:866:ARG:NH2	2.40	0.55
7:C:113:SER:HA	7:C:137:VAL:HG13	1.88	0.55
7:C:218:HIS:CE1	7:C:244:ARG:HG3	2.40	0.55
12:H:35:ASP:OD1	12:H:36:ILE:N	2.40	0.55
15:K:344:PHE:HE2	15:K:360:PRO:HG3	1.71	0.55
22:R:63:ILE:HG22	22:R:72:HIS:HB3	1.89	0.55
23:V:98:LYS:NZ	24:W:530:VAL:HG13	2.21	0.55
24:W:238:THR:HG23	24:W:241:GLU:HB3	1.86	0.55
25:X:103:ILE:HG22	25:X:104:LEU:HD22	1.88	0.55
5:A:812:GLU:OE2	21:Q:252:ARG:NH2	2.39	0.55
10:F:44:LYS:NZ	10:F:54:PRO:HB3	2.20	0.55
11:G:44:LEU:HA	11:G:53:LEU:O	2.06	0.55
18:N:860:ALA:HA	25:X:103:ILE:HG12	1.86	0.55
23:V:98:LYS:HE3	24:W:537:ARG:CA	2.33	0.55
24:W:575:TYR:CD1	24:W:576:PRO:HD2	2.41	0.55
5:A:220:ASP:O	5:A:224:MET:HG2	2.07	0.55
5:A:1684:TYR:HB2	5:A:1724:GLY:HA2	1.87	0.55
22:R:110:TYR:HE2	22:R:126:LEU:HD22	1.71	0.55
23:T:73:LEU:HD22	23:V:73:LEU:HD22	1.89	0.55
5:A:80:ALA:HB2	19:O:103:LEU:HD23	1.88	0.55
18:N:680:VAL:HG12	18:N:681:LEU:HG	1.88	0.55
18:N:1151:SER:HA	18:N:1155:SER:HB3	1.87	0.55
22:R:547:GLU:O	22:R:568:ALA:HB1	2.07	0.55
24:W:717:LEU:HB3	27:Z:152:ARG:HH22	1.71	0.55
8:D:21:GLU:HA	8:D:67:ARG:NE	2.22	0.55
18:N:267:PHE:HA	18:N:270:MET:HG3	1.87	0.55
24:W:173:THR:HG23	24:W:174:GLN:N	2.22	0.55
5:A:1507:GLY:O	5:A:1510:GLU:HG2	2.06	0.55
24:W:686:SER:HB2	27:Z:120:PHE:HE2	1.72	0.55
25:X:274:ARG:HG2	25:X:278:TYR:CE2	2.42	0.55
4:6:78:A:C8	22:R:105:PRO:HG3	2.42	0.55
6:B:230:PRO:HD3	6:B:494:LYS:HZ1	1.71	0.55
15:K:373:ALA:HB1	15:K:392:ASN:HD21	1.72	0.55
19:O:68:GLU:N	19:O:68:GLU:OE1	2.40	0.55
25:X:560:PHE:CZ	25:X:571:ARG:HD2	2.41	0.55
27:Z:180:CYS:O	27:Z:184:THR:HG23	2.07	0.55
5:A:67:GLY:HA3	5:A:70:ARG:HD2	1.89	0.55
5:A:109:TYR:CE1	5:A:146:ALA:HA	2.42	0.55
5:A:1461:ARG:NH1	5:A:1479:TRP:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:241:VAL:HG22	26:Y:107:ASP:OD1	2.06	0.55
22:R:460:TRP:CE2	22:R:470:PRO:HG3	2.41	0.55
25:X:637:LEU:HD23	25:X:638:ASN:N	2.22	0.55
5:A:176:LYS:NZ	5:A:645:GLY:O	2.40	0.55
22:R:120:ILE:HG22	22:R:124:ARG:HD2	1.89	0.55
24:W:654:GLU:HG2	27:Z:86:PRO:HB3	1.88	0.55
26:Y:159:LYS:NZ	26:Y:160:PRO:O	2.30	0.55
5:A:935:ASP:HB3	5:A:938:GLU:HG3	1.89	0.54
6:B:358:ASP:H	6:B:379:ARG:NH1	2.04	0.54
20:P:99:ILE:HG12	20:P:137:LEU:HB2	1.87	0.54
25:X:243:ARG:HD2	25:X:246:ILE:HD11	1.88	0.54
25:X:503:TYR:HD1	25:X:507:PHE:HE2	1.54	0.54
18:N:253:THR:HG21	18:N:376:VAL:HA	1.89	0.54
23:V:67:THR:C	23:V:69:LEU:H	2.10	0.54
25:X:238:VAL:O	25:X:242:PHE:HB2	2.08	0.54
25:X:273:ALA:O	25:X:276:THR:OG1	2.22	0.54
18:N:950:ARG:HG2	18:N:951:ILE:HG13	1.89	0.54
20:P:160:ARG:HH12	20:P:165:GLY:N	2.01	0.54
24:W:561:LEU:HA	24:W:564:MET:HE2	1.87	0.54
26:Y:199:GLU:HG3	26:Y:202:ARG:NH1	2.21	0.54
4:6:53:G:O2'	4:6:55:C:OP1	2.22	0.54
6:B:725:GLN:N	6:B:725:GLN:OE1	2.36	0.54
14:J:21:LEU:HB2	14:J:25:ARG:HB2	1.87	0.54
17:M:75:ARG:HG2	17:M:75:ARG:HH11	1.73	0.54
22:R:177:TYR:CE2	22:R:193:ILE:HD13	2.41	0.54
22:R:204:VAL:O	22:R:208:LEU:HG	2.07	0.54
5:A:1714:ASP:OD2	5:A:1716:GLN:NE2	2.40	0.54
18:N:32:LEU:HD22	18:N:77:LEU:HD11	1.89	0.54
22:R:337:THR:OG1	22:R:342:TYR:OH	2.15	0.54
23:T:9:THR:HB	23:T:58:PHE:CD2	2.42	0.54
5:A:1605:LEU:HD11	5:A:1770:ARG:NH2	2.23	0.54
5:A:1725:VAL:HA	5:A:1740:GLY:HA3	1.89	0.54
7:C:244:ARG:HD3	7:C:257:GLN:NE2	2.23	0.54
24:W:239:SER:OG	24:W:240:GLU:N	2.38	0.54
25:X:68:TRP:HE1	25:X:104:LEU:HD23	1.72	0.54
6:B:434:SER:O	8:D:87:ARG:NH2	2.40	0.54
18:N:736:LEU:O	18:N:740:GLN:HG3	2.07	0.54
20:P:160:ARG:NH2	20:P:165:GLY:H	2.06	0.54
24:W:703:ALA:O	24:W:707:GLU:HG2	2.08	0.54
5:A:862:LEU:HD12	5:A:901:LEU:HG	1.89	0.54
5:A:971:PRO:HB3	5:A:1215:THR:HG21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1267:ARG:CZ	5:A:1474:ASN:HD21	2.20	0.54
5:A:1629:GLN:HG3	5:A:1657:ALA:HB2	1.90	0.54
5:A:1641:ARG:HG2	5:A:1644:TYR:OH	2.08	0.54
10:F:11:THR:HA	10:F:29:ILE:HD11	1.90	0.54
3:5:98:U:C2	8:D:36:ASN:HB3	2.43	0.54
5:A:932:TYR:HB2	5:A:1056:GLY:HA3	1.90	0.54
7:C:75:LEU:HD13	7:C:88:VAL:HG12	1.90	0.54
12:H:25:PRO:HG2	12:H:84:ILE:HG12	1.90	0.54
15:K:414:GLN:HB2	15:K:415:PRO:HD2	1.88	0.54
17:M:227:LYS:HD3	17:M:230:LYS:HZ3	1.73	0.54
21:Q:68:GLN:N	21:Q:68:GLN:OE1	2.41	0.54
23:U:310:LEU:H	23:U:322:SER:HB3	1.71	0.54
6:B:609:HIS:O	6:B:668:ARG:NH2	2.40	0.54
6:B:819:GLY:O	6:B:823:ILE:HG13	2.08	0.54
7:C:265:ILE:HD12	9:E:114:PRO:HG3	1.90	0.54
8:D:17:THR:HA	8:D:26:TYR:O	2.08	0.54
22:R:219:ASN:OD1	22:R:220:ALA:N	2.40	0.54
27:Z:149:ASN:O	27:Z:153:LYS:HG2	2.08	0.54
27:Z:162:ARG:O	27:Z:165:GLU:HG3	2.08	0.54
1:1:0:G:H1'	1:1:1:G:OP2	2.08	0.53
10:F:2:LYS:NZ	11:G:62:ARG:HH22	2.06	0.53
23:U:371:PHE:HE1	27:Z:35:ARG:HA	1.73	0.53
5:A:1639:HIS:CE1	5:A:1718:MET:HE1	2.42	0.53
16:L:145:GLN:HA	16:L:148:GLU:HG2	1.90	0.53
17:M:123:LEU:HA	17:M:126:ASN:OD1	2.08	0.53
23:S:122:ARG:HD2	23:V:118:LEU:HB2	1.90	0.53
25:X:572:THR:O	25:X:575:LEU:HG	2.08	0.53
6:B:315:GLU:HG2	6:B:316:LEU:HD12	1.90	0.53
20:P:150:CYS:SG	20:P:221:ALA:HA	2.49	0.53
5:A:1422:GLN:NE2	5:A:1423:GLN:HE21	2.07	0.53
5:A:1666:PRO:HD3	5:A:1741:ASN:HD21	1.72	0.53
7:C:98:ASP:OD1	7:C:99:LEU:N	2.41	0.53
20:P:163:MET:HB3	20:P:245:TRP:HB2	1.90	0.53
22:R:121:ASN:HB3	24:W:241:GLU:OE1	2.08	0.53
22:R:306:LEU:O	22:R:310:LYS:HG2	2.08	0.53
5:A:969:GLU:HB2	5:A:973:LEU:HB3	1.90	0.53
6:B:696:LYS:HZ1	6:B:816:TYR:HB3	1.72	0.53
6:B:854:ALA:HA	6:B:857:LEU:HD23	1.89	0.53
15:K:340:HIS:CD2	15:K:380:ILE:HG21	2.44	0.53
24:W:540:VAL:HG11	24:W:581:LYS:HB3	1.89	0.53
24:W:688:GLU:OE1	24:W:688:GLU:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:706:THR:O	24:W:710:ASN:ND2	2.42	0.53
7:C:249:LYS:O	7:C:256:ARG:NH2	2.37	0.53
15:K:144:GLN:HE22	15:K:467:SER:H	1.57	0.53
20:P:172:GLN:OE1	20:P:172:GLN:N	2.40	0.53
23:U:114:VAL:HG13	23:U:117:ARG:NH2	2.24	0.53
23:V:108:LEU:HD12	24:W:600:CYS:SG	2.49	0.53
5:A:1129:SER:O	5:A:1133:ILE:HG13	2.09	0.53
5:A:1341:TYR:CE1	5:A:1353:SER:HB2	2.43	0.53
17:M:264:ALA:O	17:M:282:GLN:NE2	2.42	0.53
20:P:293:ARG:O	20:P:296:LYS:HG2	2.09	0.53
22:R:333:GLY:O	22:R:342:TYR:OH	2.27	0.53
23:U:255:CYS:HB3	23:U:264:VAL:HG23	1.90	0.53
24:W:531:ILE:HG12	24:W:537:ARG:NH2	2.23	0.53
24:W:686:SER:HB2	27:Z:120:PHE:CE2	2.44	0.53
25:X:178:ILE:HA	25:X:181:TYR:CE1	2.43	0.53
4:6:27:G:C2	20:P:160:ARG:HG3	2.43	0.53
6:B:222:ASP:HB3	6:B:650:TYR:HB2	1.90	0.53
6:B:575:LYS:NZ	6:B:625:ASN:O	2.42	0.53
15:K:280:GLN:HG3	16:L:165:ILE:HD11	1.90	0.53
17:M:26:CYS:HA	17:M:58:LYS:NZ	2.24	0.53
20:P:186:ASP:O	20:P:189:GLU:HG3	2.09	0.53
25:X:98:PHE:HD1	25:X:111:ILE:HG23	1.74	0.53
5:A:121:LEU:HD13	5:A:664:LEU:HB3	1.91	0.53
5:A:530:LEU:HG	5:A:530:LEU:O	2.07	0.53
5:A:681:ARG:HH11	5:A:681:ARG:HG2	1.74	0.53
15:K:183:GLY:HA2	15:K:207:THR:HG23	1.91	0.53
18:N:430:ILE:HG22	18:N:434:MET:HE2	1.91	0.53
18:N:966:LEU:HD22	18:N:971:PHE:HB2	1.91	0.53
20:P:68:GLY:O	20:P:81:GLY:HA3	2.09	0.53
22:R:154:ILE:HA	22:R:157:CYS:SG	2.49	0.53
22:R:322:TRP:HH2	22:R:348:LYS:HG3	1.74	0.53
22:R:326:LEU:HA	22:R:329:GLU:HG2	1.91	0.53
23:S:90:LEU:HD13	23:V:86:GLU:HG2	1.90	0.53
24:W:640:LEU:O	24:W:644:GLU:N	2.40	0.53
24:W:678:ARG:CZ	27:Z:109:LEU:HB3	2.38	0.53
5:A:1267:ARG:NH1	5:A:1474:ASN:HD21	2.07	0.53
17:M:201:ILE:HG22	17:M:203:MET:CE	2.39	0.53
27:Z:71:LYS:HE3	27:Z:73:ALA:HB2	1.89	0.53
5:A:1649:SER:H	5:A:1711:TYR:HE2	1.57	0.52
7:C:89:LEU:HD12	7:C:120:TRP:CD2	2.45	0.52
5:A:913:THR:HG21	24:W:92:THR:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1514:PHE:O	5:A:1517:THR:OG1	2.27	0.52
5:A:1584:ILE:HD13	5:A:1597:LEU:HD13	1.91	0.52
5:A:1668:LEU:HD23	5:A:1739:TYR:HD1	1.74	0.52
7:C:54:LEU:HD11	7:C:70:MET:HE1	1.90	0.52
22:R:98:ASP:OD2	24:W:229:LYS:NZ	2.40	0.52
22:R:338:ILE:O	22:R:341:THR:HG22	2.08	0.52
23:T:122:ARG:HD2	23:U:122:ARG:HE	1.74	0.52
25:X:445:ASP:OD1	25:X:446:ALA:N	2.42	0.52
5:A:896:ASN:ND2	5:A:899:GLU:OE2	2.42	0.52
10:F:29:ILE:HA	10:F:40:LEU:HD23	1.90	0.52
17:M:91:LEU:HD12	17:M:95:LEU:HD22	1.91	0.52
18:N:777:LEU:HD23	18:N:984:ILE:HD13	1.91	0.52
20:P:177:TYR:HE1	20:P:212:ILE:HG23	1.73	0.52
22:R:221:ALA:O	22:R:225:GLN:HB2	2.09	0.52
3:5:104:A:O2'	11:G:48:ARG:HG2	2.09	0.52
6:B:757:ASN:OD1	6:B:788:THR:OG1	2.24	0.52
16:L:184:ILE:HG21	17:M:19:PHE:HE1	1.74	0.52
23:S:118:LEU:HD22	23:S:122:ARG:HH22	1.74	0.52
24:W:719:ASN:O	24:W:722:ARG:HG3	2.09	0.52
6:B:335:PHE:CD2	6:B:385:ILE:HG12	2.45	0.52
6:B:692:THR:HG22	6:B:693:PRO:HD2	1.92	0.52
24:W:40:THR:OG1	24:W:43:GLN:OE1	2.23	0.52
24:W:245:ASN:HB2	24:W:248:GLU:HG2	1.91	0.52
5:A:368:ALA:H	5:A:417:GLU:CD	2.12	0.52
5:A:962:TRP:HZ3	5:A:1085:ALA:HB2	1.75	0.52
9:E:117:LEU:O	16:L:185:ARG:NH2	2.27	0.52
15:K:302:PRO:HD2	15:K:359:PHE:CE2	2.45	0.52
23:T:27:LEU:O	23:T:30:GLN:HG2	2.09	0.52
26:Y:131:ASP:HA	26:Y:134:LYS:HG2	1.92	0.52
13:I:23:ARG:HH12	13:I:27:GLY:HA2	1.72	0.52
18:N:226:ILE:HG21	18:N:270:MET:HE1	1.92	0.52
18:N:1014:THR:HG21	18:N:1030:LYS:HE3	1.90	0.52
23:T:18:VAL:HG11	23:T:41:THR:HG21	1.91	0.52
5:A:363:ASP:N	5:A:363:ASP:OD1	2.42	0.52
6:B:960:ASP:OD1	6:B:961:VAL:N	2.43	0.52
7:C:162:VAL:HG12	7:C:172:LYS:HB3	1.91	0.52
18:N:318:LEU:HD21	18:N:342:LEU:HG	1.92	0.52
20:P:87:LEU:O	20:P:88:LYS:C	2.47	0.52
25:X:557:LEU:HD22	25:X:576:PHE:HE1	1.75	0.52
1:1:8:U:H5"	24:W:213:ARG:NH2	2.24	0.52
5:A:1072:ASP:OD1	5:A:1111:TYR:OH	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:20:PRO:HG3	17:M:54:PHE:CG	2.45	0.52
19:O:23:LEU:HD23	19:O:83:TYR:CD1	2.45	0.52
23:T:116:SER:O	23:T:120:LYS:HG2	2.10	0.52
23:V:16:SER:H	23:V:20:GLY:HA2	1.75	0.52
25:X:251:ASP:OD1	25:X:251:ASP:N	2.43	0.52
4:6:29:A:H2	20:P:77:LYS:HZ3	1.55	0.52
5:A:1324:LYS:HB3	5:A:1330:LYS:HA	1.92	0.52
6:B:928:LYS:O	6:B:931:LYS:NZ	2.32	0.52
13:I:16:ILE:HG23	13:I:35:GLN:HA	1.91	0.52
19:O:90:ALA:O	19:O:94:LYS:NZ	2.42	0.52
20:P:149:ASP:N	20:P:153:ARG:O	2.38	0.52
21:Q:239:ASP:N	21:Q:239:ASP:OD1	2.43	0.52
23:S:122:ARG:NE	23:V:114:VAL:HG22	2.25	0.52
23:T:122:ARG:HH11	23:U:122:ARG:CZ	2.22	0.52
24:W:627:TYR:O	24:W:630:LEU:N	2.43	0.52
6:B:781:LYS:O	6:B:785:GLN:HG2	2.10	0.51
8:D:57:ASP:OD1	8:D:57:ASP:N	2.41	0.51
17:M:238:LEU:O	17:M:255:LYS:NZ	2.42	0.51
18:N:699:PHE:CZ	18:N:736:LEU:HD21	2.46	0.51
20:P:174:TYR:CE1	20:P:220:GLU:HG2	2.46	0.51
22:R:47:GLU:HA	22:R:50:GLU:HG3	1.92	0.51
24:W:251:GLU:CB	24:W:255:LYS:HZ3	2.22	0.51
24:W:623:PHE:CE1	24:W:627:TYR:CE1	2.98	0.51
27:Z:64:VAL:O	27:Z:68:LYS:HG2	2.10	0.51
5:A:985:LEU:HB2	5:A:988:VAL:HB	1.91	0.51
8:D:73:ASP:OD1	8:D:76:ARG:NH2	2.43	0.51
17:M:141:ARG:NH1	20:P:311:ASP:OD1	2.43	0.51
18:N:498:PRO:HG2	18:N:589:PRO:HB3	1.92	0.51
24:W:537:ARG:NH1	24:W:577:PHE:HB2	2.25	0.51
5:A:61:SER:OG	5:A:65:LYS:NZ	2.42	0.51
5:A:296:PRO:HB3	5:A:475:LYS:HB2	1.91	0.51
5:A:1111:TYR:CD1	5:A:1120:ILE:HG12	2.44	0.51
13:I:43:LEU:HD11	13:I:65:ILE:HD12	1.91	0.51
18:N:1059:ILE:HG21	18:N:1201:TYR:HB2	1.92	0.51
18:N:1107:LYS:NZ	18:N:1187:GLU:OE2	2.35	0.51
24:W:158:ASP:OD1	24:W:159:GLU:N	2.43	0.51
25:X:444:PHE:O	25:X:448:ARG:HG2	2.10	0.51
26:Y:155:TRP:HA	26:Y:158:ASN:OD1	2.10	0.51
27:Z:29:VAL:O	27:Z:32:GLU:HG2	2.10	0.51
5:A:569:LEU:HD23	5:A:671:LEU:HD21	1.93	0.51
17:M:100:LEU:HD22	17:M:143:LEU:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:P:54:ILE:HD13	20:P:124:MET:HB2	1.92	0.51
23:S:76:PHE:CE1	23:T:72:LEU:HG	2.45	0.51
23:S:89:GLU:OE2	23:S:93:ASN:ND2	2.44	0.51
23:U:276:PRO:HG2	23:U:279:SER:HB2	1.92	0.51
15:K:169:VAL:HB	15:K:439:CYS:SG	2.50	0.51
15:K:296:ALA:HB1	15:K:339:LEU:HD11	1.93	0.51
21:Q:240:ASP:N	21:Q:240:ASP:OD1	2.44	0.51
25:X:179:GLU:HA	25:X:182:ILE:HG22	1.93	0.51
4:6:37:A:O2'	4:6:38:G:OP1	2.29	0.51
5:A:280:ASN:HB2	5:A:349:SER:HB3	1.93	0.51
6:B:113:ARG:HE	6:B:499:VAL:HG11	1.74	0.51
6:B:225:ASP:OD1	6:B:630:LEU:HG	2.11	0.51
18:N:396:PHE:CE1	18:N:442:LYS:HG3	2.46	0.51
23:V:73:LEU:HD11	23:V:77:GLN:HE21	1.76	0.51
24:W:248:GLU:HA	24:W:251:GLU:HG2	1.91	0.51
4:6:92:C:H5'	26:Y:92:ARG:HH22	1.74	0.51
5:A:1274:SER:OG	5:A:1286:LYS:NZ	2.44	0.51
10:F:18:GLU:HG3	10:F:66:ARG:HB3	1.93	0.51
15:K:109:GLN:HA	15:K:133:GLN:HE22	1.74	0.51
15:K:327:LEU:HD23	15:K:357:TRP:CE2	2.46	0.51
17:M:47:CYS:HB3	17:M:49:LYS:HB2	1.93	0.51
18:N:687:PRO:HD2	18:N:690:LEU:HD12	1.93	0.51
18:N:751:ARG:NH1	18:N:1207:CYS:O	2.44	0.51
20:P:254:SER:HA	20:P:257:ARG:HG2	1.92	0.51
23:U:99:GLN:HA	24:W:709:LYS:HZ1	1.75	0.51
25:X:667:PHE:CE2	25:X:683:ILE:HD13	2.46	0.51
4:6:47:A:H5"	4:6:47:A:C8	2.43	0.51
5:A:972:PRO:HD3	5:A:1297:TYR:HE1	1.75	0.51
11:G:68:LEU:HB2	11:G:99:MET:HB2	1.93	0.51
15:K:135:SER:O	15:K:139:ARG:HG3	2.11	0.51
22:R:150:MET:SD	26:Y:168:LEU:HD12	2.50	0.51
23:T:67:THR:HB	27:Z:105:ARG:HA	1.93	0.51
26:Y:159:LYS:HD2	26:Y:160:PRO:HD2	1.92	0.51
27:Z:159:VAL:HG12	27:Z:162:ARG:HH22	1.75	0.51
3:5:96:G:N2	13:I:39:SER:O	2.39	0.51
5:A:936:PRO:O	5:A:940:ILE:HG12	2.11	0.51
7:C:164:ASP:OD1	7:C:165:SER:N	2.43	0.51
15:K:106:ILE:HG21	15:K:137:VAL:HA	1.91	0.51
18:N:62:LEU:HB2	18:N:74:HIS:HE2	1.73	0.51
18:N:536:LYS:HA	18:N:539:GLU:HG3	1.93	0.51
22:R:83:GLN:HA	24:W:256:ILE:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:84:LYS:HZ3	22:R:87:ALA:HB3	1.76	0.51
22:R:147:MET:O	22:R:151:LEU:HD23	2.11	0.51
5:A:1533:PHE:O	5:A:1536:SER:OG	2.23	0.50
20:P:173:ASN:OD1	20:P:175:THR:HG22	2.11	0.50
23:T:3:CYS:N	23:T:8:GLU:O	2.28	0.50
6:B:711:SER:OG	6:B:800:ASN:ND2	2.39	0.50
11:G:42:GLN:HE21	11:G:56:ARG:HH12	1.60	0.50
16:L:184:ILE:HB	16:L:202:ILE:HG22	1.93	0.50
18:N:494:GLY:HA2	25:X:241:VAL:HA	1.91	0.50
18:N:844:PRO:O	18:N:847:HIS:NE2	2.45	0.50
22:R:490:LEU:HA	22:R:493:LEU:HD12	1.93	0.50
5:A:1272:LEU:O	5:A:1322:ARG:NH2	2.44	0.50
7:C:194:ILE:HG13	7:C:202:LYS:HB2	1.93	0.50
13:I:7:ASN:HB2	13:I:10:PRO:HD2	1.92	0.50
20:P:59:GLU:OE2	20:P:61:GLU:HG3	2.11	0.50
22:R:107:TRP:O	22:R:111:ILE:HG12	2.12	0.50
23:T:90:LEU:HD11	23:U:91:ARG:HG3	1.93	0.50
5:A:1567:ASN:HB2	5:A:1593:LEU:HD21	1.94	0.50
6:B:252:THR:O	6:B:256:LYS:HG2	2.10	0.50
6:B:804:ARG:O	6:B:806:MET:HE2	2.11	0.50
18:N:139:LEU:O	18:N:143:VAL:HG23	2.12	0.50
18:N:407:VAL:HG13	18:N:419:LEU:HD13	1.94	0.50
18:N:443:LYS:HE2	18:N:447:ARG:HH21	1.76	0.50
22:R:261:ARG:NH2	22:R:291:GLY:O	2.43	0.50
23:S:90:LEU:CD1	23:V:86:GLU:HG2	2.41	0.50
24:W:177:LYS:HB3	24:W:180:ARG:HH12	1.77	0.50
27:Z:134:LEU:O	27:Z:138:LEU:HD23	2.11	0.50
5:A:1611:GLU:O	5:A:1615:TRP:HB2	2.11	0.50
15:K:166:VAL:HG12	15:K:439:CYS:HB3	1.93	0.50
18:N:666:TYR:HB2	18:N:768:THR:HA	1.93	0.50
22:R:83:GLN:HG2	22:R:84:LYS:H	1.75	0.50
23:T:61:PRO:HB2	27:Z:120:PHE:CZ	2.46	0.50
5:A:1657:ALA:O	5:A:1683:LYS:NZ	2.45	0.50
14:J:32:ARG:HG3	14:J:43:GLU:HG3	1.92	0.50
18:N:772:ASP:HB2	18:N:974:ASN:HB2	1.94	0.50
18:N:1049:ARG:NH2	18:N:1077:TYR:O	2.44	0.50
23:U:389:TRP:O	23:U:390:LEU:HD23	2.12	0.50
6:B:632:ILE:O	6:B:644:PHE:HD1	1.94	0.50
6:B:796:GLU:HG3	6:B:797:THR:N	2.27	0.50
22:R:186:GLU:HG3	22:R:189:ARG:HG2	1.93	0.50
22:R:212:ARG:O	22:R:215:GLU:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:T:94:LEU:HD12	23:U:90:LEU:CD1	2.39	0.50
23:U:99:GLN:HA	24:W:709:LYS:NZ	2.27	0.50
25:X:550:PHE:CE1	25:X:587:PHE:HB3	2.47	0.50
5:A:109:TYR:OH	5:A:525:ASN:HB2	2.12	0.50
15:K:302:PRO:O	15:K:359:PHE:HZ	1.94	0.50
17:M:69:ILE:HD11	17:M:84:MET:SD	2.51	0.50
18:N:12:ILE:HG13	18:N:51:LEU:HD21	1.94	0.50
18:N:15:ALA:O	18:N:20:GLY:N	2.45	0.50
18:N:528:PHE:HE2	18:N:623:LEU:HD21	1.77	0.50
18:N:753:GLY:O	18:N:757:LEU:HD23	2.12	0.50
22:R:59:PHE:HD2	22:R:76:TYR:HD1	1.59	0.50
22:R:84:LYS:NZ	22:R:88:ARG:HG2	2.27	0.50
23:U:126:ARG:HG2	23:U:126:ARG:HH11	1.77	0.50
24:W:600:CYS:HA	24:W:603:LEU:HB2	1.93	0.50
4:6:49:C:H2'	4:6:50:A:O4'	2.12	0.50
17:M:75:ARG:HH12	17:M:124:LEU:CD2	2.24	0.50
5:A:197:PHE:CE2	5:A:589:LEU:HD21	2.46	0.49
5:A:1313:VAL:HG13	5:A:1381:MET:HG3	1.94	0.49
5:A:1410:TRP:CH2	5:A:1446:LEU:HD21	2.47	0.49
17:M:264:ALA:HA	17:M:282:GLN:HE22	1.76	0.49
22:R:151:LEU:HD21	26:Y:168:LEU:HD21	1.94	0.49
23:S:62:ARG:HH12	23:S:71:ALA:HB2	1.77	0.49
24:W:159:GLU:HA	24:W:162:MET:HG3	1.94	0.49
5:A:405:ILE:HG22	6:B:346:ILE:HD13	1.93	0.49
5:A:907:ARG:HD2	5:A:941:CYS:SG	2.52	0.49
9:E:9:LEU:HA	9:E:12:HIS:CD2	2.47	0.49
18:N:748:GLY:HA3	18:N:1042:LEU:HD12	1.93	0.49
22:R:278:GLU:HA	22:R:281:LYS:HG2	1.94	0.49
22:R:310:LYS:O	22:R:313:LYS:HG2	2.12	0.49
25:X:549:ALA:O	25:X:553:TRP:HD1	1.95	0.49
5:A:687:HIS:CE1	16:L:219:HIS:HD1	2.31	0.49
5:A:1649:SER:N	5:A:1711:TYR:HE2	2.10	0.49
6:B:701:MET:SD	6:B:803:PHE:HB3	2.53	0.49
6:B:972:ILE:HG22	6:B:976:LYS:HE3	1.94	0.49
15:K:138:LYS:HD3	16:L:131:LEU:HA	1.94	0.49
18:N:1185:THR:O	18:N:1187:GLU:N	2.43	0.49
20:P:290:SER:O	20:P:294:LYS:HG2	2.12	0.49
22:R:56:ARG:NH1	24:W:222:ASN:OD1	2.45	0.49
4:6:32:G:N2	20:P:82:MET:HB3	2.25	0.49
5:A:342:ARG:HD2	5:A:344:ARG:NH1	2.27	0.49
10:F:17:ILE:HG12	10:F:68:TYR:CE1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:7:LYS:N	11:G:8:PRO:HD3	2.28	0.49
12:H:60:ASP:OD1	12:H:61:ALA:N	2.39	0.49
23:S:87:GLN:HA	23:S:90:LEU:HG	1.95	0.49
23:U:24:GLU:HB3	23:U:27:LEU:HD12	1.94	0.49
2:2:12:G:H2'	2:2:13:C:H4'	1.94	0.49
5:A:1429:LEU:C	5:A:1431:ASP:H	2.16	0.49
12:H:27:SER:H	12:H:82:GLN:HB3	1.77	0.49
15:K:263:VAL:HG22	15:K:273:VAL:HG22	1.94	0.49
22:R:228:LEU:HA	22:R:231:ILE:HG12	1.94	0.49
23:S:73:LEU:HD22	23:U:73:LEU:HD12	1.95	0.49
25:X:216:TYR:CZ	25:X:220:LEU:HD21	2.47	0.49
27:Z:147:GLY:O	27:Z:150:ARG:HG2	2.12	0.49
5:A:107:ARG:NH2	16:L:215:PRO:O	2.37	0.49
5:A:613:GLY:HA2	5:A:615:TYR:CE2	2.48	0.49
5:A:1669:LEU:CD1	5:A:1738:ALA:HB3	2.41	0.49
6:B:742:ALA:HB1	6:B:760:ARG:HH11	1.77	0.49
18:N:751:ARG:NH2	18:N:1206:ALA:O	2.45	0.49
18:N:769:SER:OG	18:N:772:ASP:OD2	2.18	0.49
24:W:616:TYR:HA	24:W:619:PHE:HD2	1.78	0.49
27:Z:25:ALA:O	27:Z:29:VAL:HG23	2.12	0.49
5:A:527:LEU:O	5:A:531:ILE:HG13	2.12	0.49
7:C:49:HIS:HE1	7:C:68:GLY:HA2	1.78	0.49
18:N:453:LEU:HB3	18:N:551:LEU:HD11	1.95	0.49
18:N:788:PHE:CD1	18:N:791:LEU:HD12	2.48	0.49
24:W:738:LYS:HD3	24:W:738:LYS:N	2.27	0.49
25:X:246:ILE:HG13	25:X:247:LYS:N	2.27	0.49
25:X:289:ASN:HA	25:X:292:ILE:HG22	1.93	0.49
26:Y:175:GLN:HE21	26:Y:179:ARG:HG2	1.77	0.49
7:C:114:ASP:OD1	7:C:116:HIS:HD2	1.96	0.49
15:K:354:ILE:HB	15:K:368:PHE:HB2	1.95	0.49
16:L:267:PRO:HG2	16:L:270:LYS:HD2	1.93	0.49
18:N:411:GLU:HG3	18:N:419:LEU:HD12	1.95	0.49
19:O:39:LYS:HD2	19:O:39:LYS:O	2.13	0.49
22:R:22:GLN:HA	22:R:25:ARG:HG2	1.93	0.49
22:R:338:ILE:HG13	22:R:340:GLU:H	1.78	0.49
24:W:531:ILE:HG12	24:W:537:ARG:HH21	1.78	0.49
9:E:36:ASN:OD1	9:E:72:GLY:N	2.46	0.49
15:K:120:GLY:CA	22:R:191:ARG:HD2	2.42	0.49
18:N:533:TYR:HB2	18:N:608:PHE:HA	1.95	0.49
18:N:534:ILE:HG12	18:N:554:VAL:HA	1.95	0.49
22:R:108:LEU:HD11	22:R:139:LYS:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:294:LEU:O	22:R:298:SER:OG	2.24	0.49
22:R:78:GLN:HE21	22:R:109:LYS:HE2	1.78	0.49
5:A:572:GLU:HB3	5:A:614:MET:HB2	1.94	0.48
5:A:979:CYS:SG	5:A:1219:VAL:HG11	2.53	0.48
5:A:1131:ASP:O	5:A:1134:GLN:HG2	2.13	0.48
6:B:474:GLY:O	6:B:478:LEU:HD23	2.13	0.48
22:R:566:PRO:O	22:R:570:VAL:HG23	2.13	0.48
23:V:80:TRP:CD1	27:Z:100:GLU:HB3	2.47	0.48
5:A:862:LEU:HD23	5:A:866:LEU:HD23	1.95	0.48
5:A:1548:SER:O	5:A:1552:GLN:HG2	2.13	0.48
20:P:122:ARG:HG3	20:P:228:GLU:OE2	2.13	0.48
22:R:304:ARG:HE	22:R:335:ILE:HD13	1.78	0.48
22:R:583:LEU:HD12	22:R:595:LEU:HD22	1.96	0.48
25:X:534:PHE:HA	25:X:537:TYR:HD2	1.78	0.48
26:Y:152:ARG:O	26:Y:155:TRP:NE1	2.44	0.48
6:B:905:THR:O	6:B:905:THR:HG22	2.13	0.48
8:D:9:HIS:O	8:D:12:GLN:HG2	2.12	0.48
18:N:73:ASN:O	18:N:77:LEU:HG	2.12	0.48
18:N:504:GLN:HA	18:N:583:ILE:O	2.13	0.48
22:R:61:ASP:O	22:R:64:ARG:HG2	2.14	0.48
22:R:306:LEU:O	22:R:309:GLU:HG3	2.12	0.48
23:S:104:ALA:HB1	23:V:100:GLU:HG2	1.95	0.48
25:X:496:ILE:O	25:X:500:ARG:HG2	2.13	0.48
27:Z:139:VAL:HA	27:Z:142:LYS:HG2	1.94	0.48
3:5:82:A:HO2'	3:5:83:A:H8	1.58	0.48
6:B:699:ILE:HG13	6:B:808:VAL:HG22	1.96	0.48
6:B:849:GLU:OE2	6:B:851:HIS:NE2	2.43	0.48
11:G:61:ASP:HB3	11:G:65:ASN:HB2	1.96	0.48
23:V:112:LEU:O	23:V:115:ILE:HG22	2.12	0.48
4:6:59:G:N2	4:6:62:C:OP2	2.39	0.48
5:A:324:ARG:HG3	6:B:892:ILE:HG13	1.96	0.48
5:A:1148:VAL:HG12	5:A:1172:VAL:HG11	1.96	0.48
5:A:1654:LEU:HD21	5:A:1656:LEU:HG	1.95	0.48
10:F:72:ASP:HA	11:G:98:LYS:HZ1	1.78	0.48
18:N:14:TYR:O	18:N:18:ASN:ND2	2.47	0.48
18:N:58:PHE:HA	18:N:62:LEU:HG	1.96	0.48
18:N:209:TYR:OH	18:N:218:LYS:HD3	2.13	0.48
23:T:5:ILE:HA	23:U:88:PHE:CD1	2.48	0.48
4:6:23:A:N6	20:P:127:GLU:OE1	2.47	0.48
5:A:109:TYR:CD1	5:A:146:ALA:HA	2.49	0.48
5:A:1432:LEU:HD12	5:A:1447:PHE:CZ	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Q:39:GLN:OE1	21:Q:39:GLN:HA	2.14	0.48
24:W:251:GLU:HB2	24:W:255:LYS:NZ	2.29	0.48
24:W:706:THR:O	24:W:709:LYS:HB2	2.13	0.48
24:W:734:ILE:HG23	24:W:738:LYS:HE2	1.96	0.48
5:A:1490:GLN:NE2	5:A:1492:ASN:HD22	2.11	0.48
7:C:291:LYS:HD2	9:E:109:PRO:HG3	1.95	0.48
7:C:319:HIS:HB2	7:C:324:ILE:HB	1.95	0.48
14:J:51:ASP:OD1	14:J:52:GLY:N	2.47	0.48
17:M:110:ASP:N	17:M:110:ASP:OD1	2.44	0.48
23:T:109:ASP:O	23:T:113:ARG:HG3	2.13	0.48
24:W:674:LYS:O	24:W:678:ARG:HG3	2.14	0.48
5:A:1315:CYS:HA	5:A:1318:LYS:HG2	1.96	0.48
17:M:75:ARG:HH22	17:M:124:LEU:HD23	1.78	0.48
18:N:90:TYR:OH	18:N:1224:ARG:NH2	2.33	0.48
24:W:65:GLU:OE2	24:W:89:ARG:NH2	2.46	0.48
25:X:624:ARG:O	25:X:627:ILE:HG22	2.14	0.48
4:6:13:A:O2'	4:6:14:C:OP1	2.27	0.48
4:6:44:A:H2'	4:6:45:U:C6	2.49	0.48
5:A:80:ALA:CB	19:O:103:LEU:HD23	2.43	0.48
6:B:105:ILE:HD11	15:K:199:LEU:CD2	2.44	0.48
6:B:498:THR:HG22	6:B:499:VAL:H	1.79	0.48
11:G:73:GLU:OE2	11:G:94:ARG:HB3	2.14	0.48
16:L:185:ARG:HA	16:L:201:ILE:HG22	1.96	0.48
17:M:145:LYS:O	17:M:148:GLU:HG3	2.14	0.48
22:R:101:SER:OG	22:R:133:GLN:OE1	2.25	0.48
2:2:24:A:H5'	2:2:25:G:H5"	1.96	0.48
10:F:3:LEU:HD13	11:G:61:ASP:HB2	1.95	0.48
18:N:321:LEU:HD13	18:N:338:ILE:HA	1.96	0.48
18:N:830:LEU:HB3	18:N:925:LEU:HD21	1.95	0.48
18:N:850:SER:O	18:N:853:THR:OG1	2.29	0.48
24:W:207:ILE:HG12	24:W:209:ILE:N	2.29	0.48
25:X:503:TYR:HA	25:X:506:VAL:HG22	1.94	0.48
25:X:513:THR:H	25:X:544:PHE:HZ	1.61	0.48
25:X:703:TRP:NE1	25:X:724:LYS:HE2	2.28	0.48
6:B:498:THR:HG22	6:B:499:VAL:N	2.29	0.47
8:D:17:THR:CG2	8:D:27:ARG:HD2	2.40	0.47
17:M:68:GLN:CD	20:P:147:ASN:HD21	2.17	0.47
18:N:727:TYR:HE1	18:N:756:VAL:HG12	1.78	0.47
22:R:299:THR:O	22:R:303:LYS:HG2	2.14	0.47
23:U:361:GLU:HB3	23:U:364:SER:OG	2.14	0.47
23:V:66:ALA:HB1	27:Z:60:GLU:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:682:LEU:HD11	27:Z:120:PHE:CZ	2.49	0.47
25:X:178:ILE:HG22	25:X:181:TYR:HE1	1.79	0.47
5:A:1161:ARG:HD3	5:A:1368:LYS:NZ	2.30	0.47
6:B:229:ALA:HB3	6:B:494:LYS:HZ1	1.77	0.47
6:B:814:GLN:HA	6:B:817:ARG:HD3	1.96	0.47
6:B:963:THR:OG1	6:B:984:LEU:OXT	2.32	0.47
9:E:118:ALA:N	17:M:32:TYR:OH	2.44	0.47
17:M:75:ARG:HH12	17:M:124:LEU:HD21	1.79	0.47
18:N:788:PHE:HZ	18:N:953:GLY:HA3	1.79	0.47
23:U:264:VAL:HA	23:U:274:GLU:HA	1.95	0.47
24:W:682:LEU:HG	24:W:686:SER:HB3	1.96	0.47
5:A:1416:LYS:NZ	5:A:1431:ASP:O	2.43	0.47
6:B:165:THR:OG1	6:B:166:HIS:ND1	2.44	0.47
18:N:942:LEU:HB3	18:N:969:LYS:HD2	1.95	0.47
20:P:261:ARG:O	20:P:264:GLU:HG3	2.14	0.47
22:R:83:GLN:HA	24:W:256:ILE:HG21	1.95	0.47
22:R:259:ARG:O	22:R:263:ILE:HG23	2.13	0.47
22:R:281:LYS:O	22:R:284:THR:OG1	2.26	0.47
23:T:112:LEU:HA	23:T:115:ILE:HG12	1.96	0.47
23:U:188:THR:N	23:U:487:LEU:O	2.40	0.47
5:A:862:LEU:O	5:A:866:LEU:HD23	2.14	0.47
8:D:68:PHE:HB3	9:E:70:LEU:HD13	1.96	0.47
14:J:27:VAL:HG12	14:J:28:TYR:O	2.14	0.47
16:L:232:PRO:HB2	16:L:234:LEU:CD1	2.45	0.47
20:P:82:MET:C	20:P:84:GLN:N	2.66	0.47
25:X:608:SER:O	25:X:612:LEU:HD23	2.14	0.47
5:A:1406:SER:HA	5:A:1439:GLY:HA2	1.97	0.47
6:B:81:ALA:HA	6:B:84:VAL:HG12	1.96	0.47
7:C:45:GLN:OE1	7:C:335:PHE:CE1	2.68	0.47
13:I:29:GLU:OE1	13:I:29:GLU:N	2.47	0.47
18:N:480:LEU:HD23	18:N:608:PHE:O	2.15	0.47
23:S:122:ARG:CD	23:V:118:LEU:HB2	2.44	0.47
25:X:549:ALA:O	25:X:553:TRP:CD1	2.68	0.47
6:B:490:MET:CG	6:B:579:ILE:HB	2.44	0.47
7:C:58:PHE:CZ	7:C:326:LEU:HB2	2.50	0.47
20:P:177:TYR:CE1	20:P:212:ILE:HG23	2.50	0.47
23:S:122:ARG:NH1	23:V:118:LEU:HD22	2.29	0.47
24:W:675:LEU:O	24:W:679:VAL:HG22	2.15	0.47
3:5:56:A:O2'	3:5:57:G:H5"	2.15	0.47
5:A:191:ASP:OD1	5:A:192:ASP:N	2.48	0.47
5:A:1099:ASP:N	5:A:1099:ASP:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:644:PHE:CD2	6:B:675:ARG:HD2	2.49	0.47
6:B:867:ARG:HD2	6:B:897:PHE:HD1	1.80	0.47
10:F:20:LYS:HB2	10:F:64:ASN:HA	1.97	0.47
12:H:31:PHE:HA	12:H:79:THR:OG1	2.14	0.47
15:K:338:SER:OG	15:K:380:ILE:HD12	2.15	0.47
15:K:398:TRP:CZ3	15:K:405:LYS:HB2	2.49	0.47
20:P:92:LYS:O	20:P:93:SER:C	2.52	0.47
22:R:184:TYR:HB3	26:Y:130:TYR:CE2	2.49	0.47
22:R:278:GLU:O	22:R:282:GLU:HG2	2.14	0.47
23:U:110:ALA:O	23:U:114:VAL:HG23	2.15	0.47
23:V:80:TRP:HD1	27:Z:100:GLU:HB3	1.79	0.47
24:W:245:ASN:HB2	24:W:248:GLU:CG	2.45	0.47
24:W:537:ARG:C	24:W:539:SER:H	2.18	0.47
24:W:549:SER:OG	24:W:562:LYS:HB2	2.14	0.47
25:X:382:PRO:HA	25:X:389:LEU:HD21	1.96	0.47
17:M:165:GLU:O	17:M:168:GLN:NE2	2.48	0.47
18:N:737:ARG:HA	18:N:740:GLN:NE2	2.30	0.47
18:N:931:PHE:HD1	18:N:940:GLN:HG3	1.79	0.47
23:S:38:ASP:N	23:S:43:GLN:O	2.48	0.47
23:S:62:ARG:HD3	23:T:9:THR:H	1.80	0.47
24:W:518:GLU:O	24:W:522:LEU:HG	2.15	0.47
5:A:220:ASP:OD1	5:A:259:ARG:NH2	2.42	0.47
5:A:531:ILE:HG22	5:A:531:ILE:O	2.15	0.47
15:K:467:SER:O	15:K:467:SER:OG	2.32	0.47
18:N:534:ILE:HG23	18:N:553:GLY:O	2.15	0.47
22:R:57:LYS:HA	24:W:221:TYR:CE2	2.50	0.47
23:T:127:GLU:O	23:T:131:LYS:HG2	2.14	0.47
24:W:253:ASP:OD1	24:W:257:ILE:HD11	2.15	0.47
5:A:1703:TYR:O	5:A:1707:LYS:HG2	2.15	0.47
6:B:613:GLU:OE1	6:B:616:LYS:NZ	2.30	0.47
10:F:21:ASN:OD1	10:F:23:THR:HG23	2.15	0.47
10:F:50:ARG:NH1	10:F:50:ARG:HG2	2.30	0.47
11:G:9:ARG:O	11:G:9:ARG:HD3	2.15	0.47
17:M:73:CYS:C	17:M:75:ARG:H	2.18	0.47
18:N:8:LYS:HG3	18:N:51:LEU:HD22	1.97	0.47
19:O:107:GLN:HE21	19:O:110:GLU:HG3	1.79	0.47
22:R:444:GLU:HA	22:R:447:ILE:HG22	1.97	0.47
23:U:14:VAL:HG12	23:U:51:VAL:HB	1.97	0.47
4:6:6:U:O2'	4:6:7:C:O5'	2.30	0.46
5:A:688:SER:O	5:A:691:VAL:HG22	2.15	0.46
5:A:1400:GLU:O	5:A:1404:ILE:HG12	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:628:TYR:O	6:B:631:SER:OG	2.31	0.46
6:B:813:GLU:HG2	6:B:815:ILE:H	1.79	0.46
7:C:46:MET:SD	9:E:101:ALA:HB2	2.55	0.46
18:N:1184:THR:HG22	18:N:1214:LEU:HD12	1.97	0.46
22:R:143:LYS:HE2	22:R:143:LYS:HB2	1.79	0.46
24:W:524:LYS:O	24:W:527:ARG:NE	2.48	0.46
25:X:246:ILE:HA	25:X:256:LEU:HD12	1.96	0.46
5:A:88:ARG:HG2	5:A:92:LYS:HE3	1.97	0.46
6:B:460:LYS:HD2	6:B:460:LYS:HA	1.73	0.46
14:J:48:GLU:HG2	14:J:54:LYS:HE3	1.96	0.46
16:L:235:HIS:O	22:R:136:ARG:HG3	2.15	0.46
17:M:226:TYR:HB3	20:P:200:ASP:OD1	2.15	0.46
22:R:249:LYS:O	22:R:253:ARG:NE	2.46	0.46
23:S:79:GLU:OE2	23:T:68:SER:HB2	2.15	0.46
25:X:179:GLU:O	25:X:182:ILE:HG22	2.15	0.46
3:5:100:U:H4'	3:5:101:U:H5'	1.97	0.46
4:6:86:A:H2'	4:6:87:G:C8	2.50	0.46
5:A:122:LYS:NZ	5:A:152:GLU:O	2.40	0.46
5:A:1075:ILE:HA	5:A:1185:ARG:HG2	1.96	0.46
6:B:697:ASN:HA	6:B:809:VAL:O	2.15	0.46
7:C:144:LEU:HG	7:C:146:VAL:H	1.79	0.46
17:M:31:SER:O	17:M:32:TYR:CD1	2.68	0.46
21:Q:67:THR:OG1	21:Q:68:GLN:OE1	2.31	0.46
24:W:605:LYS:HA	24:W:608:ILE:HG22	1.97	0.46
25:X:604:LYS:HE2	25:X:606:LYS:HB2	1.97	0.46
5:A:162:ILE:HG12	5:A:449:LEU:HD23	1.95	0.46
6:B:113:ARG:HG3	6:B:113:ARG:HH11	1.81	0.46
8:D:72:PRO:HG2	8:D:75:LEU:HD13	1.98	0.46
15:K:173:PRO:HA	15:K:431:LYS:HE3	1.96	0.46
22:R:18:ILE:O	24:W:15:GLU:HG3	2.15	0.46
22:R:289:GLN:NE2	25:X:538:GLU:HB2	2.30	0.46
23:V:112:LEU:HG	24:W:600:CYS:HB2	1.97	0.46
24:W:198:LYS:O	24:W:201:GLU:HG3	2.16	0.46
24:W:682:LEU:HD12	24:W:682:LEU:HA	1.64	0.46
25:X:97:CYS:SG	25:X:100:ARG:NH2	2.88	0.46
25:X:624:ARG:HD3	25:X:628:TYR:OH	2.15	0.46
25:X:705:GLU:OE2	25:X:709:ARG:NH2	2.49	0.46
26:Y:209:GLN:OE1	26:Y:213:SER:HB3	2.15	0.46
4:6:64:A:OP1	5:A:696:THR:OG1	2.27	0.46
5:A:831:ALA:O	5:A:835:THR:HG23	2.16	0.46
20:P:160:ARG:CZ	20:P:165:GLY:H	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:121:ASN:OD1	24:W:236:TYR:HB3	2.15	0.46
23:T:70:PRO:HG2	27:Z:80:TYR:HD2	1.80	0.46
23:U:304:HIS:HB2	23:U:309:TYR:HD2	1.81	0.46
5:A:59:ARG:HG2	5:A:59:ARG:HH11	1.80	0.46
9:E:68:VAL:HG12	9:E:70:LEU:HD22	1.98	0.46
15:K:106:ILE:HG12	15:K:109:GLN:HG2	1.96	0.46
22:R:196:ARG:HA	22:R:199:VAL:HG12	1.98	0.46
23:S:62:ARG:NH1	23:S:68:SER:HB3	2.30	0.46
23:T:68:SER:OG	23:T:69:LEU:N	2.48	0.46
23:U:28:ILE:O	23:U:32:ILE:HG12	2.15	0.46
26:Y:131:ASP:N	26:Y:131:ASP:OD1	2.48	0.46
5:A:411:PHE:HB2	6:B:391:LYS:HD2	1.97	0.46
6:B:387:GLU:O	6:B:391:LYS:HG3	2.16	0.46
8:D:32:GLU:HB2	8:D:40:GLN:HG3	1.96	0.46
12:H:74:LYS:HG3	13:I:70:VAL:HG23	1.98	0.46
16:L:289:ALA:HA	24:W:75:LEU:HD22	1.98	0.46
22:R:302:ASP:O	22:R:306:LEU:HD23	2.16	0.46
23:S:69:LEU:HD23	23:U:80:TRP:CD1	2.51	0.46
25:X:289:ASN:O	25:X:292:ILE:HG22	2.15	0.46
25:X:573:ARG:O	25:X:577:GLU:OE1	2.34	0.46
5:A:298:PHE:HE1	5:A:479:MET:HG2	1.80	0.46
5:A:1135:ARG:HD2	21:Q:223:ARG:CZ	2.46	0.46
10:F:50:ARG:HG2	10:F:50:ARG:HH11	1.79	0.46
11:G:51:LYS:HD3	11:G:75:TRP:HB3	1.98	0.46
11:G:54:LEU:HD23	11:G:72:LYS:O	2.16	0.46
12:H:28:ILE:HD12	12:H:53:LEU:HD11	1.97	0.46
15:K:267:ARG:HG3	15:K:291:THR:HG22	1.97	0.46
20:P:117:CYS:HB2	20:P:120:PHE:HB2	1.97	0.46
23:S:105:LEU:HD13	24:W:625:GLU:CD	2.36	0.46
25:X:172:GLN:NE2	25:X:173:VAL:HG13	2.31	0.46
5:A:1660:LYS:HZ1	5:A:1681:THR:N	2.14	0.46
6:B:700:THR:HG23	6:B:806:MET:HB2	1.98	0.46
6:B:938:ALA:HB3	6:B:943:LEU:HD23	1.96	0.46
7:C:38:ASP:HB3	7:C:80:PHE:CE1	2.51	0.46
9:E:9:LEU:HA	9:E:12:HIS:HD2	1.80	0.46
15:K:96:ILE:HG21	22:R:228:LEU:HB3	1.97	0.46
20:P:117:CYS:SG	20:P:135:HIS:HD2	2.22	0.46
22:R:57:LYS:HA	24:W:221:TYR:HE2	1.80	0.46
22:R:510:TYR:CE2	22:R:526:ILE:HG21	2.50	0.46
23:U:378:VAL:HA	23:U:394:THR:HA	1.98	0.46
25:X:517:VAL:HG21	25:X:544:PHE:HE2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:523:LEU:O	25:X:526:GLU:HG2	2.16	0.46
7:C:121:ASP:OD2	7:C:124:SER:OG	2.34	0.46
15:K:270:VAL:HG11	15:K:284:VAL:HG13	1.97	0.46
17:M:111:ILE:O	17:M:114:GLU:HG3	2.16	0.46
17:M:143:LEU:HD21	20:P:263:GLU:O	2.16	0.46
24:W:697:ILE:HG23	24:W:701:TRP:CD1	2.51	0.46
26:Y:154:ASP:OD1	26:Y:154:ASP:N	2.94	0.46
2:2:14:C:H2'	4:6:76:C:C4	2.51	0.45
3:5:51:U:HO2'	4:6:63:A:H8	1.62	0.45
5:A:1556:ARG:HG2	5:A:1592:THR:HG23	1.98	0.45
6:B:382:VAL:HG22	6:B:386:LEU:HD12	1.98	0.45
7:C:77:TRP:HH2	9:E:99:GLY:HA3	1.81	0.45
8:D:17:THR:OG1	8:D:70:ILE:HB	2.15	0.45
11:G:77:GLU:OE2	11:G:92:LYS:NZ	2.40	0.45
15:K:309:MET:HA	15:K:333:THR:OG1	2.15	0.45
19:O:6:THR:HG21	19:O:8:ARG:NH1	2.32	0.45
20:P:183:PRO:HD2	20:P:187:ILE:HG22	1.97	0.45
21:Q:54:ARG:HE	21:Q:54:ARG:HB2	1.59	0.45
22:R:412:LEU:HD13	22:R:443:PHE:HE1	1.81	0.45
23:S:5:ILE:HD11	23:S:39:PRO:HG3	1.97	0.45
23:V:21:ASN:HB3	23:V:23:TYR:CE2	2.51	0.45
4:6:57:C:H4'	5:A:560:LYS:NZ	2.32	0.45
5:A:284:THR:OG1	5:A:347:ALA:O	2.34	0.45
6:B:490:MET:HG3	6:B:579:ILE:HB	1.98	0.45
7:C:188:GLN:OE1	7:C:190:THR:HG22	2.17	0.45
15:K:299:GLU:HG3	16:L:146:LYS:HZ2	1.81	0.45
18:N:45:ALA:O	18:N:48:VAL:HG12	2.16	0.45
23:T:73:LEU:HA	23:T:76:PHE:CD2	2.45	0.45
23:T:87:GLN:HE21	23:T:91:ARG:HG2	1.81	0.45
23:T:122:ARG:CZ	23:U:118:LEU:HD12	2.46	0.45
24:W:48:TRP:HA	24:W:52:ILE:HB	1.97	0.45
24:W:537:ARG:O	24:W:539:SER:N	2.49	0.45
25:X:183:GLU:O	25:X:187:LYS:HG2	2.16	0.45
2:2:12:G:H1	4:6:77:G:H21	1.65	0.45
5:A:1299:ARG:HD3	5:A:1397:GLN:O	2.16	0.45
15:K:235:GLU:OE1	21:Q:36:LYS:NZ	2.45	0.45
18:N:193:ASN:OD1	18:N:194:LEU:N	2.49	0.45
18:N:668:ARG:NH1	18:N:720:PRO:HA	2.32	0.45
23:T:73:LEU:O	23:T:76:PHE:HB2	2.17	0.45
5:A:969:GLU:HB3	5:A:973:LEU:HD22	1.98	0.45
11:G:90:ILE:HG13	11:G:92:LYS:NZ	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:97:SER:OG	11:G:98:LYS:N	2.49	0.45
13:I:12:LEU:HD22	13:I:37:VAL:HG21	1.96	0.45
15:K:405:LYS:HD3	15:K:408:GLU:HG3	1.97	0.45
18:N:665:ILE:HD11	18:N:740:GLN:HG2	1.98	0.45
20:P:68:GLY:O	20:P:81:GLY:CA	2.65	0.45
22:R:51:PHE:HA	22:R:54:ARG:HG2	1.98	0.45
23:S:85:LEU:HA	23:S:88:PHE:HD2	1.82	0.45
23:U:83:VAL:HG22	23:U:87:GLN:NE2	2.31	0.45
23:V:3:CYS:HA	23:V:22:VAL:HG11	1.98	0.45
5:A:109:TYR:HD2	5:A:529:LEU:HD12	1.82	0.45
5:A:312:TRP:HB3	5:A:1161:ARG:NH1	2.31	0.45
5:A:389:ASP:N	5:A:389:ASP:OD1	2.48	0.45
6:B:707:GLU:HB2	6:B:710:ILE:HD12	1.98	0.45
7:C:152:THR:OG1	7:C:160:MET:SD	2.75	0.45
18:N:798:HIS:NE2	18:N:927:GLU:OE1	2.49	0.45
23:S:117:ARG:O	23:S:121:GLU:HG2	2.17	0.45
24:W:240:GLU:HA	24:W:243:ARG:HG3	1.99	0.45
24:W:264:ASN:HA	24:W:267:GLU:HG2	1.97	0.45
24:W:507:ASP:HA	24:W:510:ARG:NE	2.32	0.45
24:W:507:ASP:HB3	24:W:508:ARG:HH21	1.82	0.45
25:X:219:TRP:HE1	25:X:256:LEU:HD22	1.82	0.45
5:A:386:HIS:CE1	6:B:311:ARG:HG3	2.52	0.45
5:A:1272:LEU:HA	5:A:1272:LEU:HD23	1.81	0.45
6:B:271:LYS:HG2	40:B:1001:GTP:C6	2.52	0.45
11:G:109:VAL:HG22	13:I:64:LEU:HB3	1.99	0.45
13:I:50:GLU:OE1	13:I:50:GLU:N	2.43	0.45
18:N:587:LEU:O	18:N:589:PRO:HD3	2.17	0.45
20:P:106:THR:HG23	20:P:108:ALA:H	1.82	0.45
23:S:102:SER:OG	24:W:622:GLU:OE2	2.27	0.45
3:5:101:U:H3	11:G:65:ASN:ND2	2.13	0.45
5:A:399:GLU:OE2	12:H:6:GLN:NE2	2.50	0.45
5:A:984:ASN:ND2	5:A:1243:ASN:OD1	2.50	0.45
6:B:183:HIS:O	6:B:187:ARG:HG2	2.17	0.45
18:N:48:VAL:O	18:N:52:LEU:HG	2.17	0.45
18:N:506:GLY:HA2	18:N:581:LYS:O	2.17	0.45
22:R:493:LEU:HA	22:R:496:ASN:ND2	2.32	0.45
23:U:21:ASN:HB3	23:U:23:TYR:CZ	2.52	0.45
24:W:649:ASP:OD1	24:W:649:ASP:N	2.50	0.45
25:X:277:PHE:HZ	25:X:300:PHE:CD2	2.35	0.45
25:X:524:LEU:HD11	25:X:529:TYR:HD2	1.82	0.45
25:X:673:LYS:HA	25:X:673:LYS:HD2	1.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:7:U:H2'	2:2:8:C:C6	2.51	0.45
3:5:15:C:H2'	3:5:16:A:C8	2.52	0.45
5:A:111:GLY:HA3	16:L:214:PRO:HD3	1.98	0.45
6:B:97:ASP:OD2	15:K:199:LEU:HA	2.17	0.45
6:B:490:MET:SD	6:B:566:LEU:HD11	2.57	0.45
6:B:689:PHE:HB2	6:B:698:ARG:HD2	1.99	0.45
7:C:53:VAL:HA	7:C:69:GLY:HA3	1.99	0.45
11:G:45:ILE:HD13	11:G:109:VAL:HG12	1.98	0.45
16:L:204:MET:CE	17:M:37:LYS:HD3	2.46	0.45
18:N:620:LYS:HE2	18:N:956:TRP:CD1	2.52	0.45
18:N:751:ARG:NH1	18:N:1208:SER:OG	2.50	0.45
18:N:859:ASP:OD1	18:N:860:ALA:N	2.50	0.45
22:R:507:TRP:CD2	22:R:530:LEU:HD13	2.52	0.45
23:S:17:ARG:NH2	23:S:48:GLU:O	2.42	0.45
23:S:38:ASP:OD2	23:S:41:THR:OG1	2.32	0.45
25:X:98:PHE:CD1	25:X:111:ILE:HG23	2.52	0.45
25:X:634:LYS:HA	25:X:634:LYS:HD2	1.85	0.45
5:A:855:TYR:HB3	5:A:858:ASP:OD2	2.17	0.45
5:A:1093:ASP:OD1	5:A:1094:PHE:N	2.46	0.45
10:F:76:LEU:HD11	11:G:98:LYS:HZ2	1.82	0.45
13:I:23:ARG:HD3	13:I:72:TRP:NE1	2.32	0.45
16:L:253:PRO:O	26:Y:212:TYR:OH	2.20	0.45
22:R:570:VAL:HA	22:R:573:ARG:HD2	1.99	0.45
23:S:76:PHE:HE1	23:T:72:LEU:HG	1.81	0.45
23:T:75:LEU:HD12	23:T:75:LEU:HA	1.72	0.45
24:W:92:THR:HG21	24:W:145:THR:HG21	1.98	0.45
24:W:260:GLY:O	24:W:264:ASN:ND2	2.50	0.45
27:Z:136:LYS:O	27:Z:139:VAL:HG12	2.17	0.45
5:A:1080:ARG:NH1	5:A:1083:GLU:OE1	2.40	0.45
6:B:857:LEU:O	6:B:861:TYR:HD1	2.00	0.45
13:I:34:LEU:H	13:I:34:LEU:HD23	1.82	0.45
20:P:172:GLN:O	20:P:172:GLN:HG2	2.17	0.45
22:R:28:VAL:HG23	26:Y:197:ILE:O	2.17	0.45
22:R:303:LYS:O	22:R:307:GLN:HG2	2.17	0.45
23:T:122:ARG:O	23:T:126:ARG:HG2	2.17	0.45
24:W:537:ARG:HG2	24:W:538:PRO:HD2	1.98	0.45
5:A:1257:THR:HG23	5:A:1260:GLY:H	1.82	0.44
6:B:179:TYR:O	6:B:180:THR:OG1	2.28	0.44
7:C:46:MET:HB3	7:C:334:ILE:CG1	2.43	0.44
8:D:41:MET:HB2	8:D:59:VAL:HG22	1.98	0.44
17:M:150:ARG:O	17:M:150:ARG:HD3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:378:ILE:HG13	18:N:379:ASN:N	2.33	0.44
18:N:825:SER:O	18:N:828:PRO:HD2	2.16	0.44
18:N:970:GLY:HA2	18:N:997:CYS:SG	2.58	0.44
22:R:54:ARG:NH2	24:W:192:ARG:NH2	2.65	0.44
22:R:58:GLU:HA	22:R:61:ASP:OD1	2.16	0.44
22:R:453:CYS:HB3	22:R:457:TYR:CE2	2.52	0.44
23:T:77:GLN:OE1	27:Z:74:ALA:HB3	2.17	0.44
23:T:114:VAL:O	23:T:118:LEU:HD23	2.17	0.44
25:X:277:PHE:HZ	25:X:300:PHE:HD2	1.65	0.44
3:5:15:C:H2'	3:5:16:A:H8	1.82	0.44
5:A:1666:PRO:HD3	5:A:1741:ASN:ND2	2.32	0.44
5:A:1686:ILE:HG12	5:A:1725:VAL:HB	1.98	0.44
6:B:632:ILE:HB	6:B:644:PHE:HB2	1.98	0.44
6:B:776:VAL:HA	6:B:779:TYR:CZ	2.52	0.44
6:B:959:GLU:O	6:B:961:VAL:HG23	2.17	0.44
7:C:61:SER:O	7:C:321:HIS:NE2	2.50	0.44
7:C:230:ASP:OD1	7:C:232:SER:N	2.50	0.44
22:R:249:LYS:HA	22:R:252:ILE:HG12	1.99	0.44
23:S:114:VAL:O	23:S:118:LEU:HG	2.18	0.44
23:T:72:LEU:HD23	23:T:76:PHE:HE2	1.82	0.44
24:W:241:GLU:C	24:W:245:ASN:HD21	2.20	0.44
25:X:285:MET:HG3	25:X:285:MET:O	2.17	0.44
25:X:589:LYS:NZ	25:X:623:ASP:O	2.48	0.44
25:X:703:TRP:HZ2	25:X:720:MET:CG	2.30	0.44
5:A:196:PRO:HD3	5:A:543:TYR:CE1	2.52	0.44
5:A:342:ARG:HD3	6:B:666:GLU:OE2	2.17	0.44
5:A:398:GLU:CD	12:H:6:GLN:HE22	2.21	0.44
6:B:689:PHE:HB3	6:B:700:THR:HB	1.98	0.44
6:B:724:PRO:HG2	6:B:727:ARG:HG3	1.98	0.44
8:D:6:LYS:HD2	8:D:90:PRO:HG2	1.99	0.44
18:N:773:ARG:HG2	18:N:950:ARG:HA	2.00	0.44
22:R:569:VAL:HG13	22:R:602:PHE:CZ	2.51	0.44
23:S:34:GLU:OE2	23:S:35:THR:HG22	2.17	0.44
23:S:118:LEU:HD22	23:S:122:ARG:NH2	2.32	0.44
25:X:222:PHE:O	25:X:226:VAL:HG23	2.18	0.44
25:X:270:TYR:CE2	25:X:304:TRP:HB2	2.53	0.44
25:X:537:TYR:O	25:X:541:VAL:HG13	2.17	0.44
25:X:554:ASN:O	25:X:557:LEU:HG	2.17	0.44
5:A:1095:LEU:HD22	5:A:1110:LEU:HD22	1.98	0.44
6:B:698:ARG:HB3	6:B:809:VAL:CG2	2.48	0.44
18:N:256:ARG:HD3	18:N:379:ASN:ND2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:697:ILE:HD13	18:N:710:VAL:HG22	2.00	0.44
18:N:918:LEU:O	18:N:921:MET:HG2	2.16	0.44
23:U:90:LEU:HD12	23:U:90:LEU:HA	1.71	0.44
26:Y:159:LYS:HZ3	26:Y:160:PRO:HG2	1.82	0.44
26:Y:202:ARG:O	26:Y:206:LEU:HD23	2.17	0.44
5:A:183:LYS:O	5:A:596:GLN:NE2	2.51	0.44
6:B:243:VAL:O	6:B:289:LYS:HE3	2.18	0.44
6:B:406:LYS:HE3	6:B:406:LYS:HB3	1.80	0.44
15:K:289:LYS:HB2	15:K:310:ASP:OD2	2.18	0.44
18:N:751:ARG:HH21	18:N:1178:VAL:H	1.66	0.44
20:P:99:ILE:HD11	20:P:137:LEU:HD13	1.99	0.44
22:R:127:PHE:O	22:R:131:VAL:HG22	2.18	0.44
27:Z:131:LEU:O	27:Z:135:GLU:HG2	2.17	0.44
5:A:754:LEU:HD12	5:A:755:PRO:HD2	1.99	0.44
6:B:748:ALA:HB2	6:B:781:LYS:HD3	2.00	0.44
6:B:810:LEU:HD12	6:B:817:ARG:NE	2.32	0.44
17:M:99:ALA:HB1	20:P:263:GLU:HA	1.99	0.44
19:O:134:CYS:HB3	19:O:139:CYS:H	1.83	0.44
20:P:57:ARG:HD3	20:P:58:PRO:HD2	1.99	0.44
20:P:62:MET:SD	20:P:64:PRO:HD3	2.58	0.44
22:R:207:TRP:CD1	22:R:234:LEU:HD11	2.53	0.44
22:R:360:ARG:O	22:R:364:ILE:HG12	2.17	0.44
25:X:154:TYR:O	25:X:158:ILE:HG22	2.17	0.44
25:X:216:TYR:O	25:X:220:LEU:HD23	2.17	0.44
25:X:427:LEU:HD11	25:X:472:PRO:HB2	2.00	0.44
25:X:439:LEU:HD21	25:X:489:LEU:CD2	2.47	0.44
27:Z:29:VAL:O	27:Z:33:LEU:HD23	2.17	0.44
4:6:32:G:C2	20:P:82:MET:CB	3.00	0.44
5:A:167:THR:HG21	5:A:228:TYR:OH	2.18	0.44
5:A:229:GLU:HB2	5:A:232:ALA:HA	1.99	0.44
5:A:300:PRO:O	5:A:301:LEU:HB3	2.16	0.44
6:B:603:LYS:HE2	6:B:644:PHE:CZ	2.52	0.44
6:B:778:GLU:OE2	6:B:779:TYR:HD2	2.01	0.44
7:C:116:HIS:ND1	7:C:132:LYS:HG2	2.32	0.44
13:I:23:ARG:HD3	13:I:72:TRP:CE2	2.52	0.44
20:P:114:SER:OG	20:P:134:LEU:HD11	2.18	0.44
22:R:324:ASP:OD1	22:R:324:ASP:N	2.46	0.44
23:U:298:VAL:HA	23:U:314:SER:HA	1.99	0.44
25:X:144:HIS:HB2	25:X:148:TRP:NE1	2.33	0.44
25:X:574:ASP:HA	25:X:577:GLU:CD	2.38	0.44
25:X:648:TYR:CE2	25:X:667:PHE:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:24:ALA:O	27:Z:27:GLN:HG2	2.17	0.44
6:B:182:THR:O	6:B:183:HIS:ND1	2.51	0.44
6:B:692:THR:OG1	6:B:697:ASN:HB2	2.17	0.44
11:G:70:ASN:N	11:G:97:SER:O	2.41	0.44
14:J:73:LEU:H	14:J:73:LEU:HD23	1.83	0.44
17:M:256:THR:HG23	17:M:259:SER:H	1.83	0.44
20:P:115:PHE:CZ	20:P:148:VAL:HG11	2.53	0.44
22:R:59:PHE:HD2	22:R:76:TYR:CD1	2.35	0.44
23:S:122:ARG:HG2	23:V:114:VAL:HG22	1.99	0.44
5:A:335:PHE:HE1	6:B:649:MET:HE2	1.82	0.44
5:A:470:TYR:OH	5:A:638:ARG:NH1	2.50	0.44
5:A:1346:LEU:HD23	5:A:1508:ILE:HG21	2.00	0.44
6:B:847:MET:HB2	6:B:916:ASP:HB2	2.00	0.44
7:C:176:GLU:HG3	7:C:177:LYS:H	1.83	0.44
8:D:26:TYR:HD2	8:D:44:ILE:HG21	1.81	0.44
10:F:19:LEU:HD21	10:F:60:ILE:HD12	1.99	0.44
15:K:167:ARG:HA	15:K:167:ARG:HD2	1.75	0.44
17:M:282:GLN:OE1	17:M:282:GLN:HA	2.17	0.44
18:N:686:VAL:HG13	18:N:690:LEU:HD13	2.00	0.44
18:N:804:TYR:HE2	18:N:816:ARG:HH11	1.65	0.44
19:O:30:MET:CG	19:O:52:LEU:HD23	2.44	0.44
20:P:85:ASP:OD2	20:P:88:LYS:N	2.51	0.44
20:P:181:ILE:HG13	20:P:183:PRO:HD3	1.99	0.44
22:R:84:LYS:HZ3	22:R:88:ARG:HG2	1.82	0.44
22:R:111:ILE:HG21	22:R:127:PHE:CZ	2.52	0.44
23:S:59:VAL:HG22	23:S:60:ARG:H	1.83	0.44
5:A:843:ARG:O	5:A:844:ARG:C	2.56	0.43
5:A:1686:ILE:HA	5:A:1725:VAL:O	2.18	0.43
6:B:657:ASP:O	6:B:661:LEU:HB2	2.18	0.43
6:B:689:PHE:H	6:B:971:MET:HE1	1.83	0.43
15:K:226:ASP:OD1	15:K:228:MET:HG2	2.18	0.43
16:L:184:ILE:HD13	17:M:19:PHE:HE1	1.83	0.43
17:M:17:VAL:O	17:M:17:VAL:HG12	2.18	0.43
18:N:798:HIS:HD2	18:N:801:HIS:H	1.65	0.43
20:P:175:THR:HB	20:P:216:THR:HG23	2.00	0.43
22:R:77:GLY:HA3	22:R:93:PHE:CZ	2.53	0.43
24:W:192:ARG:CZ	24:W:192:ARG:HB2	2.47	0.43
24:W:537:ARG:HH11	24:W:577:PHE:HB2	1.83	0.43
5:A:1603:SER:O	5:A:1605:LEU:N	2.51	0.43
6:B:967:PHE:HB2	6:B:971:MET:HG2	1.99	0.43
7:C:310:GLU:HB2	7:C:331:ASP:OD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:5:ILE:HG21	8:D:35:ASP:HA	2.00	0.43
16:L:252:PRO:HB2	26:Y:212:TYR:OH	2.18	0.43
18:N:204:ILE:HA	18:N:207:ILE:HD12	2.00	0.43
20:P:178:VAL:HG13	20:P:213:ALA:HB3	2.00	0.43
22:R:280:TYR:CD2	22:R:309:GLU:HG2	2.54	0.43
23:T:64:PRO:HG3	24:W:682:LEU:HD23	2.00	0.43
5:A:106:LYS:HB3	20:P:74:TRP:CZ3	2.53	0.43
5:A:969:GLU:CB	5:A:973:LEU:HD22	2.48	0.43
5:A:1068:GLY:O	5:A:1113:ARG:NE	2.51	0.43
9:E:10:LEU:HD21	9:E:31:PHE:CE1	2.53	0.43
11:G:45:ILE:CD1	11:G:109:VAL:HG12	2.48	0.43
16:L:252:PRO:HB2	26:Y:212:TYR:CZ	2.53	0.43
18:N:313:ASP:OD1	18:N:353:LYS:NZ	2.51	0.43
18:N:528:PHE:CE2	18:N:623:LEU:HD21	2.54	0.43
18:N:863:LYS:O	18:N:867:GLU:HG3	2.19	0.43
19:O:120:ARG:NH1	19:O:142:CYS:HB3	2.28	0.43
20:P:85:ASP:CG	20:P:88:LYS:HB3	2.38	0.43
20:P:86:PRO:CD	20:P:87:LEU:H	2.31	0.43
20:P:227:LYS:HE2	20:P:245:TRP:CE2	2.53	0.43
22:R:339:ARG:HA	22:R:342:TYR:HD2	1.83	0.43
2:2:9:U:H2'	2:2:10:U:H6	1.82	0.43
5:A:116:LEU:HA	5:A:147:ILE:HD11	1.99	0.43
5:A:624:GLN:HG2	5:A:663:PHE:HB2	1.99	0.43
5:A:1037:ASN:ND2	5:A:1049:ASN:O	2.45	0.43
6:B:687:LYS:NZ	6:B:806:MET:HG3	2.33	0.43
6:B:788:THR:HA	6:B:798:ILE:HD12	2.00	0.43
18:N:559:ILE:HG21	18:N:622:TRP:HE1	1.83	0.43
22:R:201:HIS:O	22:R:206:ASN:ND2	2.49	0.43
22:R:245:ILE:O	22:R:249:LYS:HG3	2.18	0.43
23:S:68:SER:O	23:S:72:LEU:N	2.36	0.43
23:T:80:TRP:HZ2	23:U:76:PHE:CD1	2.36	0.43
24:W:574:ASN:OD1	24:W:575:TYR:N	2.52	0.43
25:X:503:TYR:O	25:X:507:PHE:HD2	2.01	0.43
25:X:598:PHE:HA	25:X:601:LYS:HD3	2.00	0.43
27:Z:153:LYS:O	27:Z:156:GLN:HG2	2.18	0.43
4:6:24:A:C4	5:A:100:ARG:HD2	2.53	0.43
5:A:511:ASP:OD1	5:A:512:TRP:N	2.51	0.43
5:A:811:GLN:HG2	5:A:1047:HIS:CB	2.49	0.43
5:A:1657:ALA:HB1	5:A:1661:TRP:HE1	1.82	0.43
10:F:25:VAL:HG12	10:F:45:MET:HA	1.99	0.43
15:K:362:GLY:O	16:L:118:GLN:NE2	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:285:ASN:OD1	16:L:286:ASP:N	2.51	0.43
18:N:266:LEU:HD11	18:N:419:LEU:HD11	1.99	0.43
20:P:277:GLN:HA	20:P:280:LEU:HG	2.01	0.43
22:R:51:PHE:O	22:R:55:LYS:HG2	2.18	0.43
22:R:130:ALA:HB1	22:R:140:LEU:HD13	1.99	0.43
22:R:158:ARG:HB3	26:Y:149:GLU:OE1	2.18	0.43
22:R:225:GLN:HA	22:R:228:LEU:HD12	2.01	0.43
23:S:105:LEU:HA	23:V:100:GLU:OE2	2.17	0.43
23:T:111:ALA:HA	23:T:114:VAL:HG12	1.99	0.43
23:U:403:TRP:CD1	23:U:410:LEU:HA	2.53	0.43
25:X:221:GLU:O	25:X:225:LEU:HG	2.17	0.43
5:A:1549:GLY:O	5:A:1553:ILE:HG12	2.19	0.43
6:B:569:VAL:O	6:B:569:VAL:HG13	2.19	0.43
13:I:52:VAL:O	13:I:55:VAL:HG22	2.17	0.43
15:K:123:GLU:O	15:K:127:ARG:HD3	2.19	0.43
18:N:502:LYS:HE2	18:N:586:TYR:HE1	1.83	0.43
22:R:227:TYR:CD2	22:R:247:PHE:HD1	2.36	0.43
23:S:63:PRO:CB	24:W:693:LEU:HD21	2.44	0.43
23:T:91:ARG:NH2	23:U:86:GLU:OE2	2.50	0.43
23:U:59:VAL:HG12	23:V:4:SER:HA	1.99	0.43
24:W:12:THR:HB	24:W:163:LEU:HD21	2.01	0.43
24:W:536:ILE:O	24:W:537:ARG:HB2	2.18	0.43
25:X:683:ILE:HG13	25:X:684:TYR:N	2.32	0.43
25:X:726:SER:O	25:X:730:LYS:HG2	2.18	0.43
5:A:540:HIS:HB2	5:A:550:THR:HG23	2.01	0.43
5:A:1640:PRO:HD2	5:A:1641:ARG:HH12	1.83	0.43
10:F:17:ILE:HG12	10:F:68:TYR:CD1	2.53	0.43
11:G:74:MET:N	11:G:74:MET:SD	2.92	0.43
13:I:35:GLN:NE2	13:I:46:LEU:HD21	2.33	0.43
15:K:173:PRO:HG3	15:K:215:PRO:HA	2.00	0.43
16:L:103:TYR:HA	24:W:235:PHE:HE2	1.82	0.43
18:N:326:GLN:HG3	25:X:271:GLU:HG2	2.00	0.43
22:R:188:GLU:O	22:R:191:ARG:HG2	2.19	0.43
22:R:255:LYS:HG2	22:R:257:TYR:OH	2.18	0.43
24:W:170:LEU:O	26:Y:197:ILE:HD13	2.18	0.43
26:Y:165:VAL:O	26:Y:169:VAL:HG23	2.18	0.43
6:B:296:GLU:O	6:B:300:ASN:ND2	2.39	0.43
6:B:329:CYS:SG	6:B:442:PHE:HB2	2.58	0.43
6:B:466:ILE:HG12	6:B:590:ILE:O	2.19	0.43
6:B:702:VAL:HG13	6:B:804:ARG:HE	1.84	0.43
15:K:248:SER:HB2	15:K:267:ARG:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:1138:LEU:HG	18:N:1183:PHE:HZ	1.83	0.43
19:O:30:MET:SD	19:O:52:LEU:HD23	2.58	0.43
22:R:54:ARG:O	22:R:57:LYS:HG2	2.18	0.43
22:R:88:ARG:HB3	24:W:225:ILE:HG12	2.00	0.43
24:W:689:GLN:HB2	27:Z:124:LEU:HD11	1.99	0.43
24:W:702:LYS:O	24:W:706:THR:HG23	2.19	0.43
4:6:5:U:H1'	4:6:9:G:N2	2.34	0.43
4:6:75:G:C8	26:Y:200:ARG:NH1	2.87	0.43
5:A:82:LEU:HD22	19:O:50:PHE:HE1	1.84	0.43
5:A:1034:ALA:HB2	24:W:78:THR:HB	2.01	0.43
6:B:262:ASP:OD2	6:B:463:GLN:NE2	2.52	0.43
7:C:82:ASP:OD2	7:C:84:LYS:CD	2.67	0.43
7:C:154:VAL:HB	7:C:180:LEU:HB2	2.01	0.43
8:D:40:GLN:HG2	8:D:60:TYR:CD2	2.54	0.43
16:L:176:GLN:OE1	16:L:177:GLN:N	2.52	0.43
18:N:171:LEU:HD23	18:N:171:LEU:HA	1.85	0.43
20:P:259:GLN:O	20:P:263:GLU:OE1	2.35	0.43
22:R:18:ILE:H	22:R:18:ILE:HD12	1.84	0.43
22:R:32:ASP:OD1	22:R:32:ASP:N	2.52	0.43
22:R:56:ARG:NH1	24:W:221:TYR:O	2.51	0.43
23:U:420:VAL:HG23	23:U:438:GLU:HB2	2.00	0.43
23:U:460:VAL:HG12	23:U:486:ARG:HB2	2.00	0.43
25:X:254:GLY:CA	25:X:293:ILE:HD11	2.49	0.43
26:Y:118:ARG:NH2	26:Y:175:GLN:OE1	2.51	0.43
3:5:32:C:C5	5:A:487:PRO:HB2	2.54	0.43
5:A:554:THR:OG1	5:A:557:GLU:OE1	2.35	0.43
6:B:217:THR:HB	6:B:227:VAL:HG22	2.01	0.43
6:B:545:CYS:HG	6:B:554:HIS:HD1	1.66	0.43
10:F:18:GLU:HG3	10:F:66:ARG:HD2	2.00	0.43
14:J:18:PHE:HE2	14:J:73:LEU:HB3	1.84	0.43
15:K:302:PRO:CG	15:K:315:LEU:HD23	2.47	0.43
18:N:480:LEU:HD11	18:N:505:MET:HB3	2.00	0.43
18:N:668:ARG:HH12	18:N:720:PRO:HA	1.84	0.43
19:O:95:PRO:HA	19:O:98:GLU:OE2	2.17	0.43
22:R:590:GLU:O	22:R:594:VAL:HG23	2.18	0.43
24:W:711:LEU:HD11	27:Z:141:THR:HB	2.00	0.43
25:X:66:LYS:HA	25:X:69:LYS:HG2	2.00	0.43
4:6:13:A:HO2'	4:6:14:C:P	2.42	0.42
6:B:776:VAL:HA	6:B:779:TYR:CE1	2.53	0.42
16:L:141:PRO:O	16:L:145:GLN:HB2	2.19	0.42
17:M:267:SER:HB2	17:M:282:GLN:NE2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:375:ASN:HA	18:N:378:ILE:HG12	2.01	0.42
18:N:745:MET:N	18:N:745:MET:SD	2.92	0.42
18:N:931:PHE:CD1	18:N:940:GLN:HG3	2.54	0.42
22:R:227:TYR:CG	22:R:247:PHE:HD1	2.37	0.42
22:R:331:SER:HA	22:R:334:ASP:OD2	2.19	0.42
22:R:468:CYS:SG	22:R:502:THR:OG1	2.60	0.42
24:W:159:GLU:O	24:W:163:LEU:HD23	2.19	0.42
25:X:350:ASN:HD22	25:X:384:LEU:C	2.23	0.42
5:A:798:ASN:O	5:A:802:LEU:HD23	2.19	0.42
5:A:1630:ILE:HD12	5:A:1630:ILE:HA	1.91	0.42
5:A:1684:TYR:HA	5:A:1723:THR:O	2.19	0.42
6:B:618:LEU:HD21	6:B:641:HIS:CE1	2.54	0.42
6:B:841:LEU:HG	6:B:925:PRO:HG3	2.01	0.42
12:H:31:PHE:O	14:J:22:ASN:ND2	2.42	0.42
15:K:302:PRO:HB3	15:K:324:LEU:HD12	2.00	0.42
15:K:452:ASP:OD1	15:K:453:ASN:N	2.52	0.42
16:L:232:PRO:HB2	16:L:234:LEU:HD12	2.02	0.42
18:N:120:VAL:HG23	18:N:124:ILE:HD12	2.01	0.42
25:X:126:THR:HG22	25:X:162:PHE:HZ	1.83	0.42
25:X:652:ILE:HD13	25:X:686:HIS:CE1	2.54	0.42
27:Z:111:LEU:HD12	27:Z:114:LYS:HE2	2.02	0.42
27:Z:129:VAL:O	27:Z:133:LEU:HG	2.19	0.42
5:A:388:LEU:HD22	5:A:392:PRO:HD3	2.01	0.42
5:A:1604:HIS:HB3	5:A:1607:GLN:HE21	1.84	0.42
6:B:783:GLY:HA2	6:B:823:ILE:HG23	2.01	0.42
6:B:968:ASP:O	6:B:972:ILE:HG13	2.19	0.42
15:K:89:GLU:OE2	22:R:259:ARG:NE	2.50	0.42
16:L:131:LEU:HA	16:L:131:LEU:HD23	1.92	0.42
18:N:993:LEU:HD23	18:N:993:LEU:HA	1.91	0.42
18:N:1084:HIS:HB2	18:N:1087:GLN:HE21	1.84	0.42
20:P:83:ARG:CZ	20:P:83:ARG:HB3	2.47	0.42
22:R:432:PRO:HG2	22:R:463:TYR:CZ	2.53	0.42
23:S:63:PRO:HB3	24:W:693:LEU:CD2	2.45	0.42
24:W:627:TYR:O	24:W:628:SER:C	2.57	0.42
25:X:630:VAL:O	25:X:634:LYS:HG2	2.19	0.42
25:X:667:PHE:CD2	25:X:683:ILE:HD13	2.54	0.42
5:A:864:LEU:HD22	5:A:1457:ASP:HB2	2.02	0.42
5:A:1457:ASP:OD2	5:A:1484:HIS:NE2	2.46	0.42
5:A:1576:GLN:HB3	5:A:1585:MET:CE	2.49	0.42
5:A:1602:ARG:NE	5:A:1770:ARG:HH11	2.14	0.42
6:B:488:LEU:HB3	6:B:581:SER:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:44:ILE:HB	8:D:56:LEU:HB2	2.01	0.42
10:F:3:LEU:HD23	10:F:3:LEU:O	2.20	0.42
11:G:11:GLU:C	11:G:12:LEU:HD12	2.40	0.42
15:K:425:PHE:CE2	15:K:441:ALA:HB2	2.54	0.42
18:N:59:GLU:OE1	18:N:85:LYS:NZ	2.52	0.42
18:N:1240:LEU:HD23	18:N:1263:ILE:HG13	2.01	0.42
20:P:92:LYS:HE2	20:P:240:CYS:N	2.34	0.42
20:P:184:THR:O	20:P:187:ILE:HG23	2.19	0.42
20:P:227:LYS:HG2	20:P:243:VAL:HG12	2.00	0.42
23:U:309:TYR:CE2	23:U:311:LEU:HD11	2.54	0.42
25:X:434:TRP:O	25:X:438:GLU:HG2	2.18	0.42
27:Z:115:HIS:HB3	27:Z:118:LYS:HE3	2.02	0.42
3:5:47:C:H2'	3:5:48:C:O4'	2.19	0.42
5:A:1208:PRO:HB3	5:A:1226:ARG:CZ	2.50	0.42
7:C:53:VAL:O	7:C:314:ASN:ND2	2.51	0.42
7:C:85:ASN:OD1	9:E:97:GLY:N	2.53	0.42
11:G:30:LEU:HD23	13:I:64:LEU:HD11	2.01	0.42
13:I:12:LEU:HD21	13:I:37:VAL:HG11	2.01	0.42
13:I:15:LEU:O	13:I:15:LEU:HD23	2.20	0.42
15:K:414:GLN:HG2	15:K:442:ASP:OD1	2.20	0.42
16:L:161:LEU:O	16:L:165:ILE:HG12	2.20	0.42
18:N:946:CYS:SG	18:N:969:LYS:HD3	2.59	0.42
19:O:26:PHE:CD1	19:O:52:LEU:HD11	2.54	0.42
22:R:256:GLU:HB3	22:R:259:ARG:NH1	2.32	0.42
22:R:402:LYS:O	22:R:405:LEU:HG	2.19	0.42
23:U:114:VAL:O	23:U:118:LEU:HB2	2.19	0.42
24:W:739:MET:HA	24:W:742:ILE:HG12	2.00	0.42
25:X:507:PHE:CZ	25:X:536:ILE:HD11	2.55	0.42
25:X:550:PHE:CD1	25:X:587:PHE:HB3	2.55	0.42
5:A:946:ASP:OD1	5:A:950:TRP:HD1	2.02	0.42
5:A:1624:GLU:OE2	5:A:1627:SER:OG	2.37	0.42
6:B:945:ARG:O	6:B:949:ILE:HG12	2.20	0.42
11:G:53:LEU:HD23	11:G:73:GLU:HB3	2.01	0.42
15:K:111:SER:OG	22:R:232:ASP:OD1	2.27	0.42
15:K:472:ARG:HD2	15:K:472:ARG:HA	1.83	0.42
18:N:62:LEU:HB2	18:N:74:HIS:NE2	2.34	0.42
18:N:267:PHE:HA	18:N:270:MET:CG	2.48	0.42
18:N:728:ASN:OD1	18:N:1046:TYR:OH	2.13	0.42
20:P:85:ASP:CB	20:P:88:LYS:HB3	2.50	0.42
23:T:30:GLN:OE1	23:U:81:ASP:HB3	2.19	0.42
24:W:677:ASN:OD1	24:W:678:ARG:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:227:VAL:HG21	25:X:259:TYR:HD1	1.84	0.42
25:X:265:ILE:HG12	25:X:270:TYR:CE1	2.55	0.42
25:X:520:TYR:HD2	25:X:536:ILE:HG12	1.84	0.42
3:5:107:C:O2'	3:5:108:U:H5'	2.19	0.42
5:A:1011:VAL:HG11	5:A:1053:LEU:HD12	2.02	0.42
5:A:1268:ILE:HD13	5:A:1271:ILE:HD12	2.02	0.42
7:C:89:LEU:HD12	7:C:120:TRP:CE3	2.55	0.42
18:N:53:HIS:ND1	18:N:85:LYS:HE2	2.35	0.42
18:N:63:TRP:CZ2	18:N:96:ILE:HG23	2.55	0.42
18:N:277:VAL:HA	18:N:280:PHE:HD2	1.85	0.42
18:N:303:TYR:CD2	18:N:329:LEU:HD23	2.55	0.42
18:N:792:GLU:OE1	18:N:817:TYR:HB2	2.19	0.42
18:N:1017:ASN:ND2	18:N:1170:GLU:OE2	2.36	0.42
19:O:91:LYS:HD3	19:O:91:LYS:HA	1.81	0.42
20:P:115:PHE:CE2	20:P:148:VAL:HG11	2.54	0.42
22:R:249:LYS:O	22:R:252:ILE:HG12	2.19	0.42
22:R:299:THR:O	22:R:302:ASP:OD1	2.37	0.42
22:R:493:LEU:HA	22:R:496:ASN:HD21	1.84	0.42
24:W:254:GLN:HA	24:W:257:ILE:HD12	2.01	0.42
24:W:387:ASN:ND2	24:W:406:LEU:HD22	2.28	0.42
24:W:678:ARG:O	24:W:682:LEU:HB2	2.20	0.42
25:X:398:ARG:HG3	25:X:398:ARG:H	1.73	0.42
25:X:426:GLU:HG2	25:X:427:LEU:N	2.35	0.42
2:2:5:U:H2'	2:2:6:C:C6	2.55	0.42
4:6:67:A:OP1	4:6:69:G:O2'	2.38	0.42
5:A:1242:ASP:O	5:A:1246:LYS:N	2.51	0.42
5:A:1730:ASP:O	5:A:1734:ASN:N	2.53	0.42
6:B:812:PRO:HD2	6:B:817:ARG:HH22	1.85	0.42
7:C:120:TRP:HH2	7:C:127:LYS:HE3	1.85	0.42
10:F:74:LEU:HG	10:F:76:LEU:HG	2.01	0.42
14:J:68:ILE:HG22	14:J:69:MET:HG3	2.01	0.42
17:M:68:GLN:OE1	20:P:147:ASN:ND2	2.53	0.42
17:M:141:ARG:HA	17:M:144:VAL:HG12	2.02	0.42
18:N:150:SER:HA	18:N:178:TYR:CZ	2.55	0.42
18:N:410:GLN:HB3	18:N:416:ASN:ND2	2.33	0.42
18:N:500:PHE:HE2	18:N:502:LYS:HB2	1.85	0.42
22:R:148:GLU:HG2	22:R:157:CYS:HB3	2.02	0.42
22:R:192:GLY:O	22:R:196:ARG:HG3	2.20	0.42
23:S:71:ALA:CB	23:T:60:ARG:HH21	2.33	0.42
23:U:441:TYR:HA	23:U:455:MET:O	2.20	0.42
24:W:699:HIS:HA	24:W:702:LYS:HE2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:738:LYS:O	24:W:742:ILE:HG23	2.20	0.42
5:A:1436:TRP:CE2	5:A:1444:ASN:ND2	2.88	0.42
5:A:1506:GLU:CD	5:A:1506:GLU:H	2.23	0.42
6:B:635:VAL:HG22	6:B:641:HIS:ND1	2.34	0.42
7:C:290:ASP:OD1	7:C:292:ASN:HB2	2.20	0.42
9:E:18:THR:HG21	9:E:24:PHE:HE1	1.84	0.42
10:F:17:ILE:HB	10:F:25:VAL:HG23	2.02	0.42
14:J:22:ASN:O	14:J:25:ARG:HD3	2.20	0.42
15:K:414:GLN:NE2	21:Q:248:ASN:HB2	2.35	0.42
17:M:112:ASN:ND2	24:W:226:PRO:O	2.53	0.42
20:P:83:ARG:HH22	20:P:86:PRO:HA	1.85	0.42
25:X:448:ARG:HH22	25:X:489:LEU:HD23	1.85	0.42
25:X:585:PRO:HB2	25:X:620:LYS:HG3	2.02	0.42
2:2:8:C:H2'	2:2:9:U:C6	2.55	0.42
5:A:223:VAL:O	5:A:227:PHE:HB2	2.19	0.42
5:A:539:LEU:HB3	5:A:547:LEU:HD11	2.02	0.42
5:A:687:HIS:NE2	16:L:219:HIS:HB2	2.35	0.42
5:A:864:LEU:O	5:A:868:ARG:HG2	2.20	0.42
5:A:907:ARG:NH1	5:A:907:ARG:HB2	2.35	0.42
5:A:1443:ILE:HA	5:A:1446:LEU:HD23	2.02	0.42
6:B:163:TYR:CE1	6:B:177:LEU:HD22	2.55	0.42
6:B:279:LEU:HG	6:B:281:LEU:HG	2.01	0.42
7:C:58:PHE:HE1	7:C:326:LEU:HD22	1.81	0.42
7:C:313:VAL:HG13	7:C:313:VAL:O	2.20	0.42
11:G:25:PHE:O	11:G:31:SER:HB3	2.19	0.42
18:N:629:VAL:HA	18:N:632:LEU:HD23	2.02	0.42
20:P:55:GLU:HG3	20:P:56:THR:HG23	2.02	0.42
20:P:118:LEU:HA	20:P:151:PHE:HZ	1.83	0.42
22:R:81:LEU:HD12	22:R:85:GLU:HA	2.02	0.42
25:X:74:LEU:O	25:X:78:HIS:ND1	2.36	0.42
25:X:384:LEU:HD23	25:X:384:LEU:H	1.84	0.42
27:Z:83:LEU:HD23	27:Z:83:LEU:O	2.20	0.42
27:Z:125:GLU:O	27:Z:129:VAL:HG23	2.20	0.42
1:1:0:G:O2'	1:1:1:G:OP1	2.32	0.41
2:2:19:G:H5'	16:L:261:PRO:HG2	2.02	0.41
5:A:735:HIS:HE1	16:L:252:PRO:O	2.03	0.41
5:A:1166:ARG:HH11	5:A:1166:ARG:HG3	1.84	0.41
5:A:1490:GLN:NE2	5:A:1492:ASN:ND2	2.68	0.41
5:A:1525:LEU:HD13	5:A:1777:LEU:HD21	2.02	0.41
6:B:271:LYS:HG2	40:B:1001:GTP:C5	2.55	0.41
6:B:678:GLU:OE1	6:B:678:GLU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:734:LYS:O	6:B:734:LYS:HD3	2.20	0.41
10:F:4:VAL:HG11	10:F:34:MET:O	2.20	0.41
10:F:20:LYS:HA	10:F:20:LYS:HD2	1.86	0.41
13:I:9:LYS:HB3	13:I:10:PRO:HD3	2.02	0.41
15:K:246:HIS:CE1	15:K:274:TRP:HZ2	2.38	0.41
18:N:214:LYS:HE3	18:N:259:LEU:HD12	2.02	0.41
18:N:841:ILE:HD11	18:N:857:PHE:CE1	2.55	0.41
23:U:435:SER:OG	23:U:441:TYR:O	2.26	0.41
23:V:4:SER:H	23:V:22:VAL:CG1	2.32	0.41
24:W:661:ILE:O	24:W:665:LEU:HG	2.20	0.41
25:X:341:ASN:O	25:X:345:LEU:HG	2.20	0.41
25:X:467:ASP:O	25:X:475:ARG:NH2	2.53	0.41
1:1:-1:U:H6	1:1:-1:U:H5”	1.85	0.41
2:2:6:C:H2’	2:2:7:U:C6	2.55	0.41
5:A:1617:LEU:O	5:A:1621:LEU:HD23	2.20	0.41
6:B:180:THR:HG22	6:B:549:ALA:HB2	2.01	0.41
6:B:691:ASP:OD1	6:B:698:ARG:NE	2.36	0.41
15:K:124:ALA:HA	15:K:127:ARG:HD3	2.01	0.41
18:N:836:ARG:HH22	18:N:894:LYS:HB2	1.85	0.41
22:R:184:TYR:HB3	26:Y:130:TYR:HE2	1.85	0.41
24:W:182:ASP:OD1	24:W:183:ARG:N	2.53	0.41
26:Y:140:LYS:O	26:Y:142:ARG:HD3	2.19	0.41
5:A:807:LEU:HD11	5:A:1042:TYR:HB3	2.02	0.41
5:A:1422:GLN:HE21	5:A:1423:GLN:HE21	1.67	0.41
6:B:149:HIS:CG	6:B:150:LEU:H	2.38	0.41
6:B:969:GLN:HA	6:B:972:ILE:HD12	2.01	0.41
11:G:51:LYS:HD3	11:G:51:LYS:HA	1.93	0.41
12:H:49:MET:O	12:H:51:ILE:HG13	2.21	0.41
14:J:34:TYR:HA	14:J:39:ASN:O	2.20	0.41
15:K:89:GLU:OE1	22:R:259:ARG:HG2	2.20	0.41
17:M:147:VAL:HG21	20:P:267:ALA:HB2	2.03	0.41
18:N:18:ASN:HB2	18:N:19:TRP:HE3	1.85	0.41
18:N:690:LEU:HD11	18:N:710:VAL:CG1	2.51	0.41
23:S:103:THR:HA	23:S:106:TYR:CZ	2.54	0.41
25:X:564:TYR:O	25:X:567:THR:OG1	2.31	0.41
5:A:1080:ARG:HA	5:A:1080:ARG:HD2	1.78	0.41
5:A:1314:LYS:HE3	5:A:1314:LYS:HB2	1.81	0.41
5:A:1662:ASN:OD1	5:A:1680:THR:HG22	2.20	0.41
5:A:1758:MET:O	5:A:1768:ARG:NH2	2.51	0.41
6:B:179:TYR:CE1	6:B:550:ARG:HD2	2.55	0.41
6:B:603:LYS:HB3	6:B:673:VAL:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:689:PHE:N	6:B:971:MET:HE1	2.35	0.41
8:D:89:VAL:HG12	8:D:91:LEU:HG	2.03	0.41
10:F:68:TYR:HB2	11:G:100:PHE:HB3	2.02	0.41
15:K:453:ASN:O	15:K:455:THR:HG23	2.20	0.41
17:M:227:LYS:HD3	17:M:230:LYS:NZ	2.34	0.41
19:O:52:LEU:HD12	19:O:52:LEU:HA	1.79	0.41
20:P:137:LEU:HD12	20:P:138:PRO:HD2	2.02	0.41
20:P:224:GLN:HG2	20:P:245:TRP:CH2	2.55	0.41
22:R:102:THR:O	22:R:102:THR:HG22	2.20	0.41
22:R:593:VAL:O	22:R:596:LEU:HD23	2.20	0.41
23:S:69:LEU:HD23	23:U:80:TRP:CB	2.47	0.41
23:S:80:TRP:HH2	23:U:70:PRO:HG3	1.85	0.41
23:T:122:ARG:HH11	23:U:122:ARG:NH2	2.18	0.41
23:V:103:THR:HG23	24:W:565:ILE:HD11	2.02	0.41
23:V:106:TYR:OH	23:V:113:ARG:NH2	2.54	0.41
24:W:225:ILE:HG22	24:W:228:GLU:H	1.84	0.41
25:X:263:TYR:CZ	25:X:267:ILE:HD11	2.55	0.41
1:1:0:G:HO2'	1:1:1:G:P	2.44	0.41
3:5:14:G:H2'	3:5:15:C:C6	2.56	0.41
5:A:348:LEU:HD22	6:B:189:ARG:NH2	2.34	0.41
5:A:1641:ARG:H	5:A:1641:ARG:HG3	1.58	0.41
6:B:171:PRO:HA	6:B:172:PRO:HD3	1.94	0.41
6:B:628:TYR:HB3	6:B:650:TYR:OH	2.20	0.41
6:B:760:ARG:HH21	6:B:804:ARG:CD	2.34	0.41
6:B:794:CYS:O	6:B:796:GLU:N	2.54	0.41
7:C:115:THR:O	7:C:115:THR:HG22	2.20	0.41
8:D:56:LEU:HD13	8:D:59:VAL:HG11	2.02	0.41
11:G:24:GLU:HG2	13:I:38:ASP:HB2	2.03	0.41
16:L:204:MET:HE3	17:M:37:LYS:HD3	2.00	0.41
18:N:160:LYS:NZ	18:N:355:TYR:O	2.51	0.41
18:N:315:GLN:HA	18:N:322:VAL:HG21	2.02	0.41
18:N:798:HIS:CD2	18:N:801:HIS:H	2.37	0.41
18:N:841:ILE:HD11	18:N:857:PHE:CZ	2.55	0.41
20:P:276:LYS:HA	20:P:279:LEU:HD12	2.03	0.41
22:R:580:LEU:HD13	22:R:599:TRP:HZ3	1.85	0.41
23:T:70:PRO:O	23:T:73:LEU:HG	2.20	0.41
23:U:409:GLU:HB3	27:Z:35:ARG:HH21	1.85	0.41
23:V:3:CYS:SG	23:V:5:ILE:HG22	2.60	0.41
24:W:667:LYS:HA	24:W:670:LEU:HG	2.03	0.41
27:Z:57:ASP:OD1	27:Z:57:ASP:N	2.50	0.41
3:5:98:U:H5"	8:D:62:ARG:NH2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:79:C:C5	26:Y:183:THR:HA	2.56	0.41
5:A:355:SER:O	6:B:274:ARG:NH2	2.53	0.41
6:B:291:ARG:HH21	6:B:357:GLY:HA3	1.85	0.41
6:B:719:VAL:HG12	6:B:720:ASN:N	2.36	0.41
15:K:241:ARG:HE	21:Q:32:HIS:HB3	1.85	0.41
18:N:1081:GLY:HA2	18:N:1243:THR:HB	2.03	0.41
22:R:224:ARG:O	22:R:228:LEU:HG	2.19	0.41
23:V:109:ASP:OD2	24:W:592:LEU:HD21	2.20	0.41
25:X:551:GLU:HA	25:X:554:ASN:ND2	2.35	0.41
25:X:668:ALA:HA	25:X:671:GLU:HB2	2.02	0.41
27:Z:106:ASN:ND2	27:Z:110:TYR:OH	2.53	0.41
4:6:33:A:H2'	4:6:34:U:C6	2.56	0.41
6:B:279:LEU:HD12	6:B:279:LEU:HA	1.87	0.41
6:B:287:TYR:OH	6:B:357:GLY:HA2	2.21	0.41
6:B:682:ASP:OD1	6:B:683:THR:N	2.53	0.41
13:I:44:GLN:HA	13:I:63:ILE:O	2.20	0.41
15:K:260:ASP:O	15:K:276:MET:HB2	2.21	0.41
18:N:408:MET:HE2	18:N:447:ARG:HD3	2.03	0.41
18:N:639:PRO:HG2	18:N:993:LEU:HD13	2.03	0.41
20:P:256:ALA:HB1	20:P:260:ARG:HH12	1.84	0.41
24:W:21:VAL:HG11	24:W:48:TRP:CH2	2.56	0.41
24:W:537:ARG:CG	24:W:538:PRO:CD	2.99	0.41
25:X:193:GLU:O	25:X:197:GLN:HG2	2.20	0.41
25:X:196:ARG:HH12	25:X:235:ASN:HB2	1.85	0.41
25:X:448:ARG:HE	25:X:486:TYR:HE1	1.69	0.41
3:5:96:G:C5	12:H:48:PHE:HE2	2.38	0.41
5:A:122:LYS:HE3	5:A:150:VAL:O	2.21	0.41
5:A:208:LEU:HG	5:A:209:GLU:H	1.86	0.41
8:D:61:ILE:HG12	14:J:69:MET:HG2	2.02	0.41
10:F:56:GLU:OE1	10:F:56:GLU:N	2.30	0.41
16:L:180:ASP:HA	16:L:181:PRO:HD3	1.93	0.41
17:M:227:LYS:HA	17:M:230:LYS:HZ3	1.86	0.41
17:M:258:SER:O	17:M:261:GLU:HG2	2.21	0.41
18:N:117:LEU:HA	18:N:120:VAL:HG22	2.03	0.41
18:N:425:ILE:HA	18:N:1031:ARG:HD2	2.02	0.41
22:R:128:ASP:O	22:R:132:THR:HG22	2.21	0.41
5:A:807:LEU:HD23	5:A:807:LEU:HA	1.94	0.41
5:A:1146:SER:O	5:A:1149:VAL:HG12	2.21	0.41
5:A:1576:GLN:HB3	5:A:1585:MET:HE2	2.03	0.41
6:B:195:SER:O	6:B:195:SER:OG	2.33	0.41
6:B:323:SER:HB3	6:B:328:TYR:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:340:ILE:HD13	6:B:340:ILE:HA	1.84	0.41
6:B:483:GLU:OE1	6:B:483:GLU:N	2.40	0.41
6:B:522:LYS:CG	6:B:536:MET:HG2	2.50	0.41
10:F:11:THR:HG23	10:F:12:ASN:OD1	2.21	0.41
12:H:77:ASN:OD1	13:I:25:LYS:HE3	2.20	0.41
15:K:267:ARG:HG3	15:K:291:THR:CG2	2.51	0.41
16:L:142:SER:OG	16:L:143:ASP:N	2.54	0.41
18:N:131:PHE:HB3	18:N:231:VAL:HG11	2.03	0.41
18:N:996:ASN:ND2	18:N:998:GLU:O	2.54	0.41
19:O:78:LEU:HD23	19:O:78:LEU:HA	1.85	0.41
22:R:27:ALA:HB1	24:W:171:ALA:HB2	2.02	0.41
22:R:174:TRP:O	22:R:178:ILE:HG12	2.20	0.41
22:R:369:CYS:HA	22:R:372:GLU:HG2	2.02	0.41
22:R:569:VAL:HG12	22:R:573:ARG:NE	2.36	0.41
23:S:14:VAL:HG11	23:S:28:ILE:HG21	2.01	0.41
23:S:121:GLU:HB2	23:S:122:ARG:HH11	1.86	0.41
23:T:81:ASP:O	23:T:85:LEU:HG	2.21	0.41
24:W:158:ASP:OD1	24:W:159:GLU:HG3	2.21	0.41
25:X:355:TRP:O	25:X:359:VAL:HG23	2.20	0.41
25:X:684:TYR:HE2	25:X:706:PHE:CG	2.39	0.41
4:6:32:G:C2	20:P:82:MET:HB3	2.56	0.41
5:A:233:LEU:HB3	5:A:236:THR:OG1	2.21	0.41
5:A:680:ALA:O	5:A:684:GLU:HB2	2.21	0.41
5:A:1002:THR:HB	5:A:1198:THR:HG23	2.03	0.41
5:A:1104:THR:O	5:A:1104:THR:HG22	2.21	0.41
5:A:1605:LEU:HD11	5:A:1770:ARG:CZ	2.51	0.41
7:C:56:ALA:HA	7:C:66:ALA:O	2.21	0.41
10:F:6:PHE:CE1	10:F:79:LEU:HG	2.56	0.41
22:R:122:HIS:O	22:R:126:LEU:HG	2.20	0.41
23:S:24:GLU:OE2	23:S:27:LEU:N	2.46	0.41
24:W:162:MET:SD	24:W:163:LEU:HD22	2.60	0.41
24:W:669:ALA:HA	24:W:672:CYS:SG	2.61	0.41
26:Y:180:LEU:O	26:Y:184:LYS:NZ	2.43	0.41
6:B:706:LEU:HD11	6:B:758:ILE:HD12	2.02	0.40
6:B:851:HIS:HE1	6:B:877:ARG:NE	2.19	0.40
7:C:295:VAL:HB	7:C:304:TYR:HB2	2.03	0.40
18:N:449:LEU:HD13	18:N:557:PHE:HZ	1.85	0.40
18:N:493:ILE:HD13	25:X:248:ARG:NH1	2.36	0.40
18:N:899:ILE:HG21	18:N:907:PHE:HE1	1.86	0.40
20:P:160:ARG:HB3	20:P:161:ASP:H	1.77	0.40
22:R:284:THR:HG21	22:R:306:LEU:HG	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:322:SER:O	23:U:324:LYS:N	2.54	0.40
25:X:362:LEU:HD23	25:X:362:LEU:HA	1.89	0.40
4:6:32:G:N3	20:P:82:MET:HA	2.37	0.40
5:A:615:TYR:OH	5:A:1574:GLY:HA2	2.21	0.40
16:L:106:ILE:HD12	16:L:106:ILE:H	1.85	0.40
16:L:270:LYS:HD3	26:Y:208:LEU:HD13	2.03	0.40
18:N:333:GLN:O	18:N:336:GLU:HG2	2.21	0.40
18:N:668:ARG:O	18:N:760:LYS:NZ	2.52	0.40
18:N:1138:LEU:HG	18:N:1183:PHE:CZ	2.55	0.40
19:O:4:LEU:H	19:O:4:LEU:HD23	1.86	0.40
19:O:48:PRO:O	19:O:51:GLN:HB3	2.21	0.40
20:P:191:VAL:HG12	20:P:235:LEU:HD21	2.02	0.40
22:R:189:ARG:O	22:R:193:ILE:HG13	2.20	0.40
23:S:72:LEU:HG	23:S:76:PHE:CE1	2.57	0.40
23:U:80:TRP:HA	23:U:83:VAL:HG12	2.03	0.40
24:W:105:LEU:HA	24:W:108:LYS:HG2	2.03	0.40
24:W:251:GLU:OE1	24:W:255:LYS:NZ	2.54	0.40
1:1:-14:U:H3'	1:1:-13:U:H5"	2.03	0.40
5:A:527:LEU:HD22	5:A:567:PHE:CE1	2.56	0.40
5:A:1611:GLU:HA	5:A:1614:VAL:HG22	2.03	0.40
5:A:1656:LEU:HB3	5:A:1683:LYS:HZ2	1.86	0.40
5:A:1664:SER:O	5:A:1741:ASN:ND2	2.54	0.40
6:B:692:THR:HB	6:B:694:ASN:OD1	2.21	0.40
7:C:143:VAL:HG12	7:C:151:LEU:HD22	2.03	0.40
7:C:145:LYS:HB2	7:C:187:GLN:HG3	2.04	0.40
7:C:176:GLU:HG3	7:C:177:LYS:N	2.36	0.40
7:C:223:THR:OG1	7:C:273:LEU:O	2.32	0.40
9:E:7:VAL:O	9:E:10:LEU:HD23	2.20	0.40
15:K:299:GLU:OE1	15:K:299:GLU:N	2.51	0.40
18:N:956:TRP:O	18:N:960:SER:HB3	2.21	0.40
20:P:175:THR:HA	20:P:216:THR:HA	2.02	0.40
24:W:640:LEU:O	24:W:644:GLU:HG3	2.21	0.40
24:W:697:ILE:O	24:W:701:TRP:HB2	2.21	0.40
24:W:701:TRP:CH2	27:Z:134:LEU:HD21	2.57	0.40
25:X:202:LEU:O	25:X:203:ASN:ND2	2.54	0.40
25:X:428:ALA:O	25:X:432:ILE:HG23	2.21	0.40
25:X:450:LEU:O	25:X:454:ALA:HB2	2.20	0.40
25:X:589:LYS:HZ1	25:X:619:VAL:HG11	1.86	0.40
27:Z:139:VAL:HA	27:Z:142:LYS:CG	2.51	0.40
5:A:77:THR:HG22	5:A:78:GLU:N	2.37	0.40
5:A:1150:ASN:O	5:A:1176:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:225:ASP:HB3	6:B:629:PRO:HG2	2.04	0.40
6:B:621:LEU:HD23	6:B:621:LEU:HA	1.93	0.40
6:B:756:THR:HG22	6:B:756:THR:O	2.22	0.40
16:L:92:ALA:HB1	16:L:102:ASP:H	1.86	0.40
18:N:116:ASN:O	18:N:120:VAL:HG13	2.22	0.40
18:N:858:ARG:HB2	18:N:922:PHE:CZ	2.55	0.40
22:R:186:GLU:HG3	22:R:186:GLU:O	2.21	0.40
23:T:122:ARG:HH12	23:U:122:ARG:HB2	1.84	0.40
27:Z:159:VAL:HG12	27:Z:162:ARG:NH2	2.36	0.40
5:A:208:LEU:O	19:O:8:ARG:NH1	2.55	0.40
5:A:568:HIS:O	5:A:572:GLU:HG2	2.22	0.40
5:A:1639:HIS:CE1	5:A:1718:MET:CE	3.04	0.40
5:A:1674:ASP:OD1	5:A:1674:ASP:N	2.47	0.40
7:C:52:GLU:HB3	7:C:330:SER:HB2	2.04	0.40
7:C:57:ARG:HH21	7:C:315:HIS:CE1	2.39	0.40
7:C:162:VAL:CG1	7:C:172:LYS:HB3	2.51	0.40
7:C:276:ALA:HB2	7:C:316:VAL:O	2.22	0.40
11:G:71:VAL:HG12	11:G:96:ILE:O	2.21	0.40
15:K:318:LEU:HD23	15:K:318:LEU:HA	1.97	0.40
17:M:89:PHE:HZ	17:M:136:ALA:HB1	1.85	0.40
17:M:168:GLN:NE2	17:M:169:ILE:HG23	2.37	0.40
24:W:675:LEU:HD11	27:Z:105:ARG:HH21	1.86	0.40
25:X:533:SER:O	25:X:536:ILE:HG22	2.21	0.40
25:X:535:LYS:HA	25:X:538:GLU:OE2	2.22	0.40
26:Y:164:HIS:O	26:Y:167:ARG:HG2	2.22	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
5	A	1735/2363 (73%)	1635 (94%)	99 (6%)	1 (0%)	48 80

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	B	916/984 (93%)	866 (94%)	49 (5%)	1 (0%)	48 80
7	C	297/340 (87%)	274 (92%)	23 (8%)	0	100 100
8	D	94/97 (97%)	92 (98%)	2 (2%)	0	100 100
9	E	91/147 (62%)	85 (93%)	6 (7%)	0	100 100
10	F	79/117 (68%)	73 (92%)	6 (8%)	0	100 100
11	G	98/115 (85%)	93 (95%)	5 (5%)	0	100 100
12	H	78/84 (93%)	77 (99%)	1 (1%)	0	100 100
13	I	71/78 (91%)	70 (99%)	1 (1%)	0	100 100
14	J	71/77 (92%)	66 (93%)	5 (7%)	0	100 100
15	K	389/473 (82%)	357 (92%)	32 (8%)	0	100 100
16	L	230/557 (41%)	211 (92%)	19 (8%)	0	100 100
17	M	222/354 (63%)	214 (96%)	8 (4%)	0	100 100
18	N	1282/1284 (100%)	1260 (98%)	22 (2%)	0	100 100
19	O	142/146 (97%)	135 (95%)	7 (5%)	0	100 100
20	P	265/388 (68%)	244 (92%)	19 (7%)	2 (1%)	16 51
21	Q	86/265 (32%)	77 (90%)	9 (10%)	0	100 100
22	R	597/674 (89%)	588 (98%)	9 (2%)	0	100 100
23	S	130/488 (27%)	122 (94%)	8 (6%)	0	100 100
23	T	132/488 (27%)	123 (93%)	9 (7%)	0	100 100
23	U	414/488 (85%)	394 (95%)	20 (5%)	0	100 100
23	V	129/488 (26%)	118 (92%)	11 (8%)	0	100 100
24	W	514/757 (68%)	479 (93%)	32 (6%)	3 (1%)	22 57
25	X	642/790 (81%)	610 (95%)	31 (5%)	1 (0%)	44 75
26	Y	114/229 (50%)	108 (95%)	5 (4%)	1 (1%)	14 49
27	Z	151/187 (81%)	144 (95%)	7 (5%)	0	100 100
28	a	150/558 (27%)	140 (93%)	10 (7%)	0	100 100
29	b	98/293 (33%)	94 (96%)	4 (4%)	0	100 100
30	c	202/887 (23%)	192 (95%)	10 (5%)	0	100 100
31	d	152/155 (98%)	137 (90%)	15 (10%)	0	100 100
33	m	79/797 (10%)	78 (99%)	1 (1%)	0	100 100
35	y	179/534 (34%)	154 (86%)	23 (13%)	2 (1%)	12 44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
36	z	624/647 (96%)	611 (98%)	12 (2%)	1 (0%)	44 75
All	All	10453/16329 (64%)	9921 (95%)	520 (5%)	12 (0%)	50 80

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	P	90	GLN
24	W	536	ILE
35	y	115	LYS
5	A	1115	ILE
26	Y	144	VAL
20	P	86	PRO
36	z	437	ASP
24	W	172	ASN
24	W	538	PRO
6	B	961	VAL
25	X	83	ASN
35	y	28	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	A	1570/2138 (73%)	1568 (100%)	2 (0%)	92 98
6	B	821/881 (93%)	821 (100%)	0	100 100
7	C	257/292 (88%)	257 (100%)	0	100 100
8	D	85/86 (99%)	85 (100%)	0	100 100
9	E	80/118 (68%)	80 (100%)	0	100 100
10	F	76/102 (74%)	76 (100%)	0	100 100
11	G	91/101 (90%)	91 (100%)	0	100 100
12	H	73/76 (96%)	73 (100%)	0	100 100
13	I	64/69 (93%)	64 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	J	63/67 (94%)	63 (100%)	0	100 100
15	K	333/405 (82%)	333 (100%)	0	100 100
16	L	200/477 (42%)	200 (100%)	0	100 100
17	M	198/306 (65%)	198 (100%)	0	100 100
18	N	1188/1188 (100%)	1188 (100%)	0	100 100
19	O	130/132 (98%)	130 (100%)	0	100 100
20	P	231/340 (68%)	231 (100%)	0	100 100
21	Q	79/240 (33%)	79 (100%)	0	100 100
22	R	532/597 (89%)	531 (100%)	1 (0%)	92 97
23	S	121/443 (27%)	121 (100%)	0	100 100
23	T	123/443 (28%)	123 (100%)	0	100 100
23	U	223/443 (50%)	223 (100%)	0	100 100
23	V	120/443 (27%)	120 (100%)	0	100 100
24	W	469/656 (72%)	468 (100%)	1 (0%)	92 97
25	X	586/707 (83%)	585 (100%)	1 (0%)	92 97
26	Y	116/214 (54%)	116 (100%)	0	100 100
27	Z	132/163 (81%)	132 (100%)	0	100 100
28	a	79/496 (16%)	79 (100%)	0	100 100
29	b	95/275 (34%)	95 (100%)	0	100 100
30	c	188/816 (23%)	188 (100%)	0	100 100
31	d	128/129 (99%)	128 (100%)	0	100 100
33	m	72/719 (10%)	72 (100%)	0	100 100
35	y	158/478 (33%)	158 (100%)	0	100 100
36	z	564/585 (96%)	564 (100%)	0	100 100
All	All	9245/14625 (63%)	9240 (100%)	5 (0%)	92 98

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	844	ARG
5	A	1209	ASN
22	R	253	ARG
24	W	155	MET
25	X	410	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	896	ASN
5	A	984	ASN
5	A	1270	GLN
5	A	1423	GLN
5	A	1474	ASN
5	A	1490	GLN
5	A	1607	GLN
5	A	1639	HIS
7	C	45	GLN
7	C	116	HIS
7	C	188	GLN
9	E	12	HIS
11	G	34	GLN
15	K	150	HIS
15	K	303	GLN
17	M	253	ASN
17	M	282	GLN
18	N	740	GLN
18	N	1216	ASN
20	P	224	GLN
20	P	232	HIS
21	Q	248	ASN
22	R	225	GLN
22	R	497	GLN
23	S	43	GLN
23	U	342	HIS
23	V	77	GLN
23	V	87	GLN
24	W	245	ASN
24	W	387	ASN
24	W	710	ASN
25	X	289	ASN
26	Y	111	GLN
26	Y	182	ASN
27	Z	106	ASN
27	Z	130	GLN
27	Z	156	GLN
28	a	101	GLN
30	c	442	GLN
31	d	7	GLN
35	y	117	ASN

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Mol	Chain	Res	Type
35	y	147	ASN
36	z	231	ASN
36	z	268	GLN
36	z	323	ASN
36	z	534	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	28/29 (96%)	19 (67%)	2 (7%)
2	2	22/186 (11%)	4 (18%)	0
3	5	101/120 (84%)	23 (22%)	2 (1%)
4	6	91/99 (91%)	44 (48%)	7 (7%)
All	All	242/434 (55%)	90 (37%)	11 (4%)

All (90) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	-14	U
1	1	-13	U
1	1	-12	U
1	1	-8	U
1	1	-4	A
1	1	0	G
1	1	1	G
1	1	2	U
1	1	3	A
1	1	4	U
1	1	5	G
1	1	6	U
1	1	7	U
1	1	8	U
1	1	9	U
1	1	10	U
1	1	11	U
1	1	12	U
1	1	13	U
2	2	11	U
2	2	13	C
2	2	24	A
2	2	29	A

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Mol	Chain	Res	Type
3	5	13	A
3	5	14	G
3	5	27	G
3	5	28	C
3	5	30	A
3	5	31	A
3	5	33	G
3	5	37	C
3	5	45	U
3	5	50	U
3	5	54	C
3	5	79	G
3	5	82	A
3	5	83	A
3	5	90	U
3	5	91	G
3	5	92	U
3	5	98	U
3	5	99	U
3	5	102	G
3	5	103	U
3	5	105	A
3	5	108	U
4	6	4	C
4	6	7	C
4	6	8	G
4	6	9	G
4	6	10	A
4	6	11	U
4	6	12	C
4	6	14	C
4	6	18	G
4	6	19	G
4	6	20	U
4	6	21	C
4	6	22	A
4	6	23	A
4	6	24	A
4	6	27	G
4	6	28	A
4	6	29	A
4	6	30	A

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Mol	Chain	Res	Type
4	6	31	C
4	6	32	G
4	6	38	G
4	6	40	G
4	6	43	G
4	6	44	A
4	6	46	U
4	6	48	G
4	6	52	G
4	6	53	G
4	6	61	A
4	6	62	C
4	6	63	A
4	6	68	U
4	6	74	U
4	6	75	G
4	6	76	C
4	6	78	A
4	6	79	C
4	6	80	A
4	6	81	U
4	6	82	U
4	6	83	G
4	6	91	A
4	6	92	C

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	0	G
1	1	1	G
3	5	27	G
3	5	49	U
4	6	13	A
4	6	17	U
4	6	29	A
4	6	30	A
4	6	37	A
4	6	52	G
4	6	74	U

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 11 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	$\#\|Z\| > 2$
40	GTP	B	1001	37	26,34,34	1.22	2 (7%)	32,54,54	1.69	7 (21%)
39	IHP	A	2401	-	36,36,36	1.39	13 (36%)	54,60,60	1.47	9 (16%)

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
40	GTP	B	1001	37	-	0/18/38/38	0/3/3/3
39	IHP	A	2401	-	-	5/30/54/54	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	B	1001	GTP	C5-C6	-4.21	1.38	1.47
39	A	2401	IHP	P6-O46	-2.42	1.45	1.54
39	A	2401	IHP	P1-O31	-2.19	1.46	1.54
39	A	2401	IHP	P1-O11	2.18	1.63	1.59
39	A	2401	IHP	P5-O45	-2.11	1.46	1.54
39	A	2401	IHP	P6-O36	-2.10	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	A	2401	IHP	P4-O44	-2.09	1.46	1.54
39	A	2401	IHP	P3-O43	-2.09	1.46	1.54
39	A	2401	IHP	P3-O33	-2.07	1.46	1.54
39	A	2401	IHP	P4-O34	-2.05	1.46	1.54
39	A	2401	IHP	P2-O32	-2.05	1.46	1.54
40	B	1001	GTP	C2-N3	2.05	1.38	1.33
39	A	2401	IHP	P2-O42	-2.03	1.47	1.54
39	A	2401	IHP	P5-O35	-2.02	1.47	1.54
39	A	2401	IHP	P1-O41	-2.02	1.47	1.54

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	B	1001	GTP	PB-O3B-PG	-4.73	116.59	132.83
40	B	1001	GTP	C5-C6-N1	3.36	119.88	113.95
40	B	1001	GTP	O4'-C1'-C2'	-3.25	102.18	106.93
39	A	2401	IHP	O11-P1-O21	-3.17	97.15	109.39
39	A	2401	IHP	C5-C6-C1	3.15	117.30	110.41
40	B	1001	GTP	C8-N7-C5	3.06	108.83	102.99
40	B	1001	GTP	PA-O3A-PB	-3.06	122.32	132.83
40	B	1001	GTP	C2-N1-C6	-3.01	119.55	125.10
39	A	2401	IHP	C6-C1-C2	2.81	116.56	110.41
39	A	2401	IHP	O41-P1-O31	2.68	117.89	107.64
39	A	2401	IHP	C6-C5-C4	2.36	115.59	110.41
40	B	1001	GTP	O6-C6-C5	-2.25	119.97	124.37
39	A	2401	IHP	O12-P2-O22	-2.22	100.83	109.39
39	A	2401	IHP	O41-P1-O21	2.09	118.86	110.68
39	A	2401	IHP	O15-P5-O25	-2.05	101.48	109.39
39	A	2401	IHP	O42-P2-O32	2.02	115.36	107.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
39	A	2401	IHP	C6-O16-P6-O26
39	A	2401	IHP	C1-O11-P1-O41
39	A	2401	IHP	C6-O16-P6-O36
39	A	2401	IHP	C5-O15-P5-O35
39	A	2401	IHP	C5-O15-P5-O45

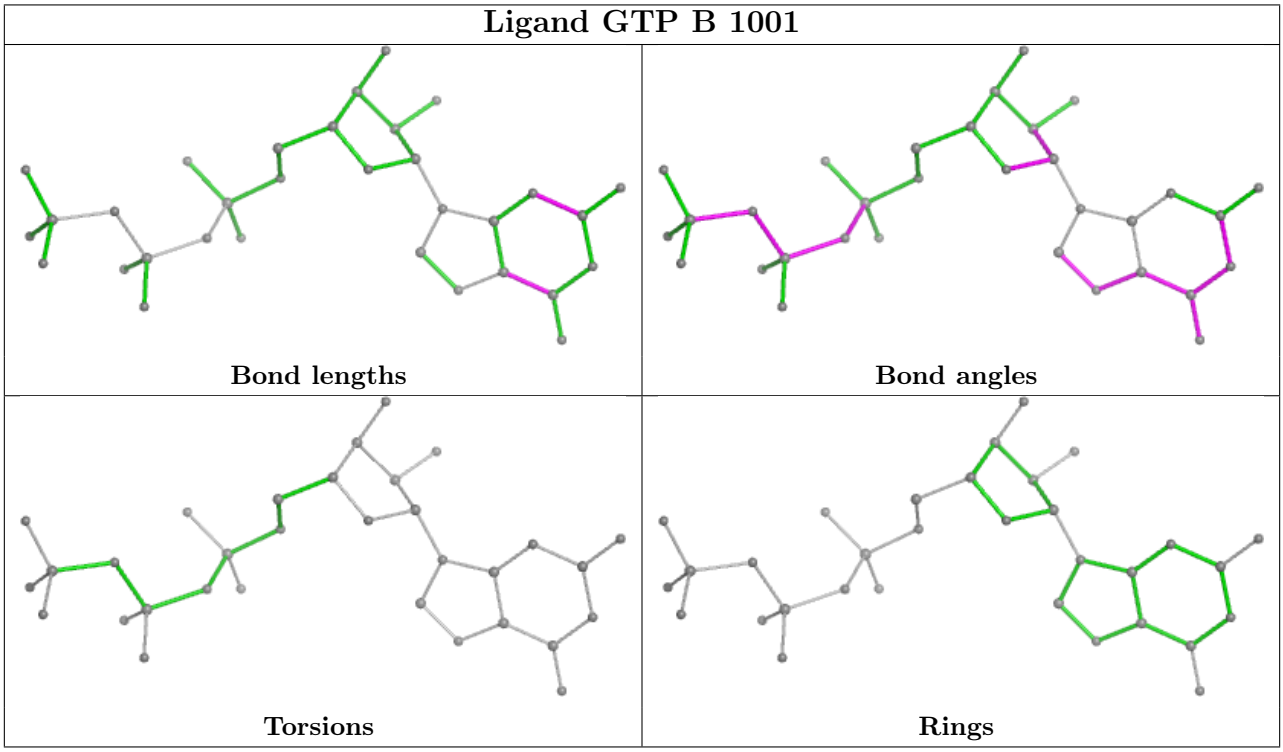
There are no ring outliers.

1 monomer is involved in 3 short contacts:

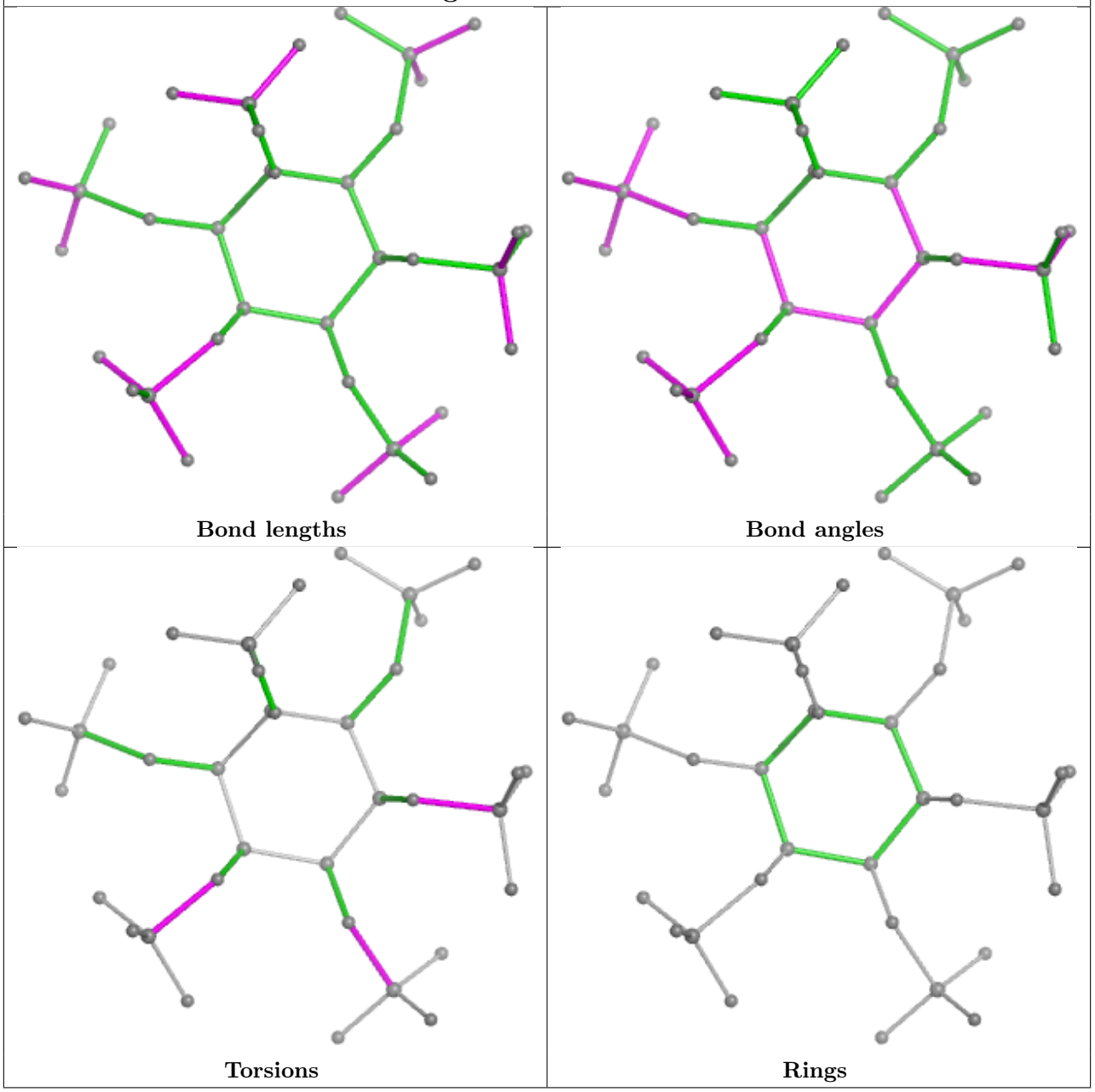
Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	B	1001	GTP	3	0

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 GTP B 1001



Ligand IHP A 2401



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.

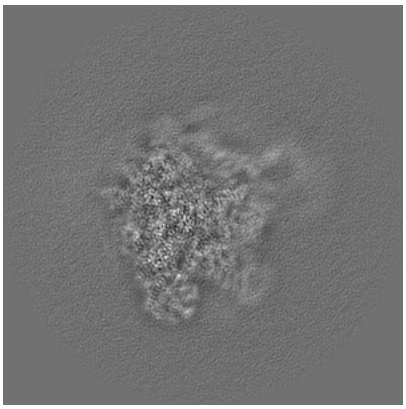
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19941. These allow visual inspection of the internal detail of the map and identification of artifacts.

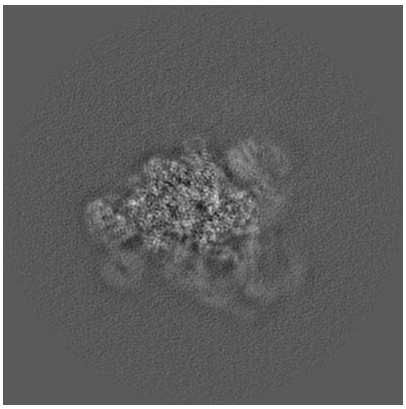
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

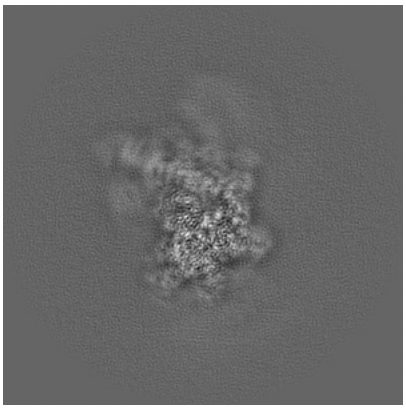
6.1.1 Primary map



X

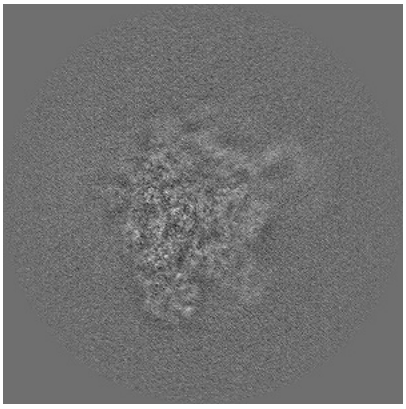


Y

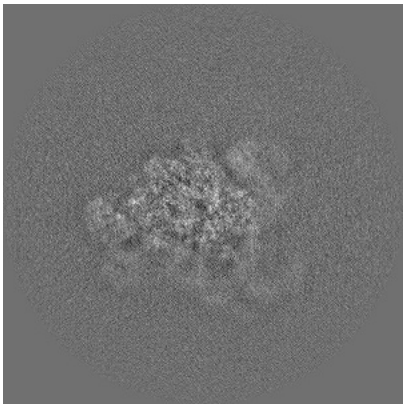


Z

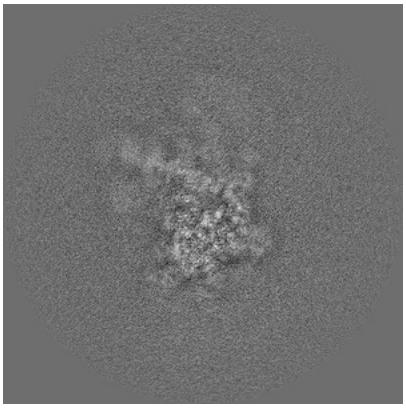
6.1.2 Raw map



X



Y

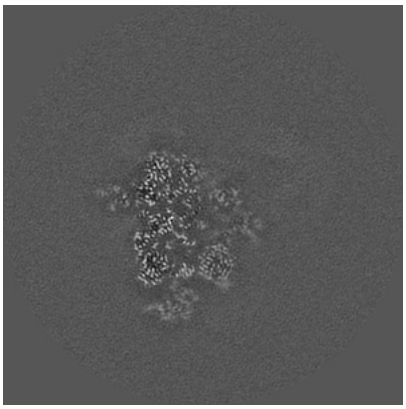


Z

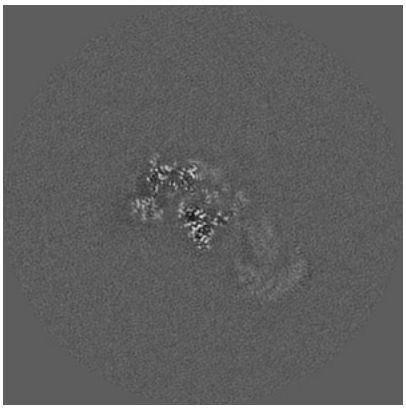
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

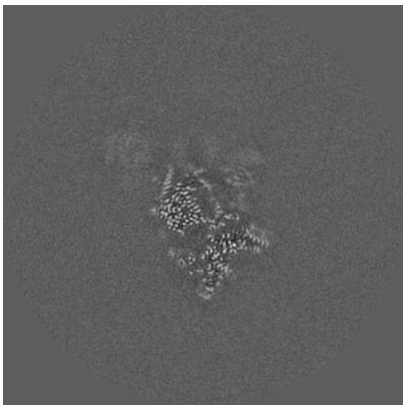
6.2.1 Primary map



X Index: 280

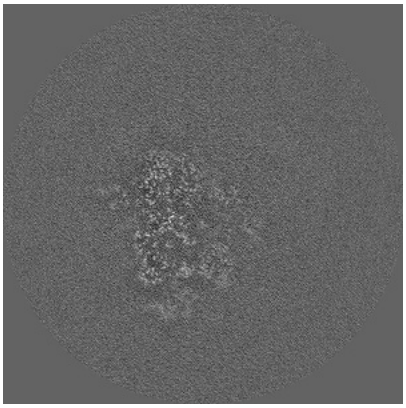


Y Index: 280

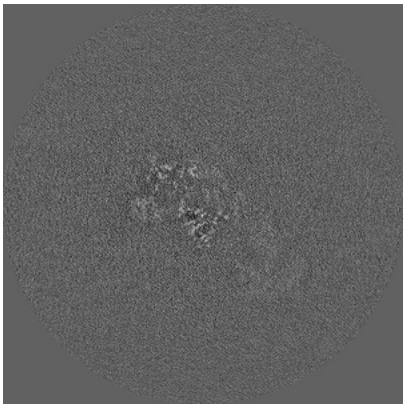


Z Index: 280

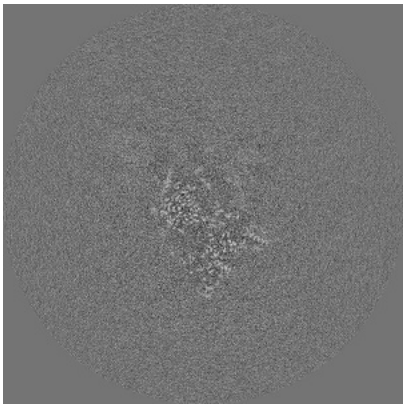
6.2.2 Raw map



X Index: 280



Y Index: 280

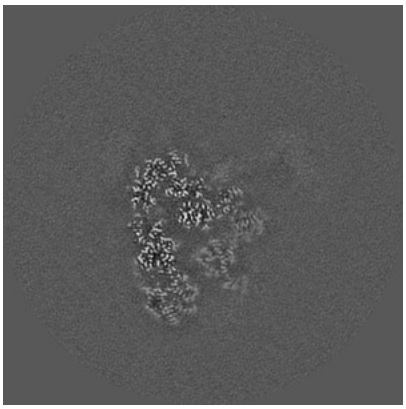


Z Index: 280

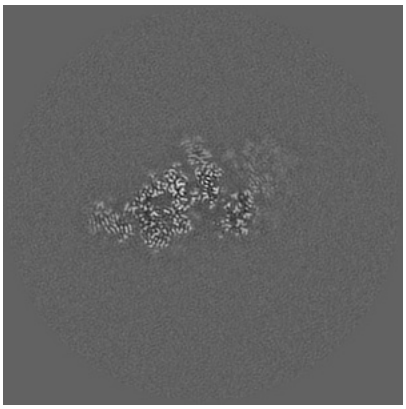
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

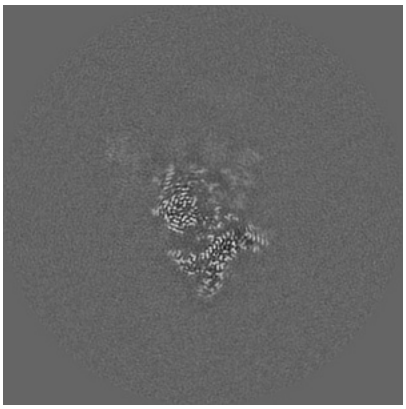
6.3.1 Primary map



X Index: 263

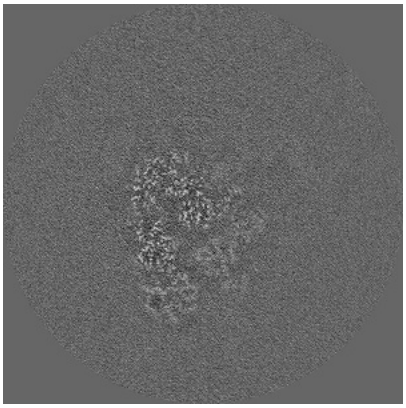


Y Index: 220

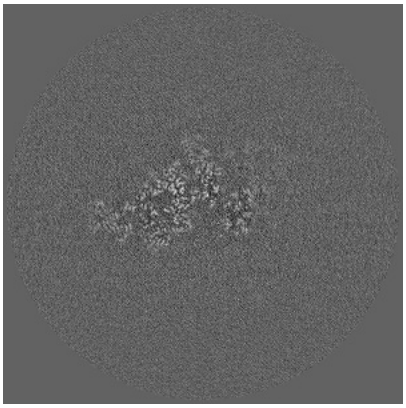


Z Index: 282

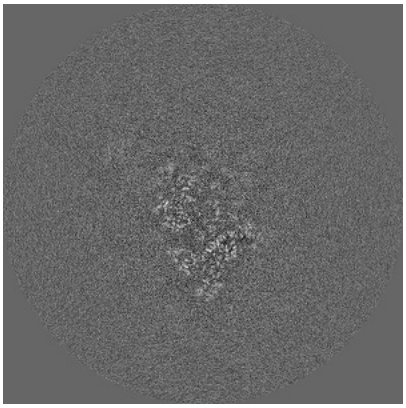
6.3.2 Raw map



X Index: 263



Y Index: 220

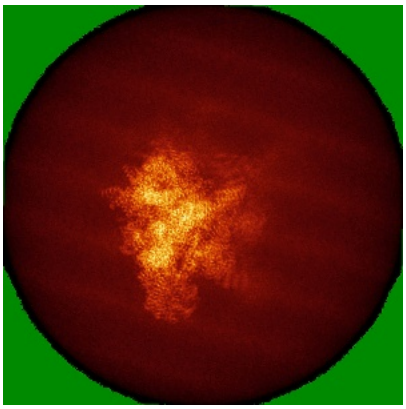


Z Index: 284

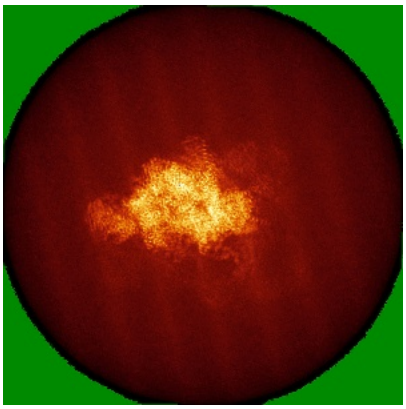
The images above show the largest variance slices of the map in three orthogonal directions.

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

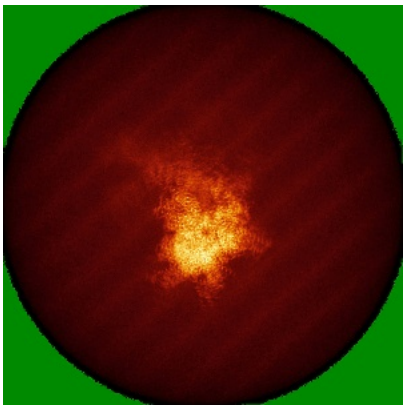
6.4.1 Primary map



X

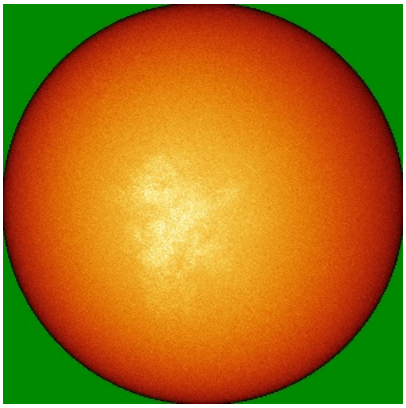


Y

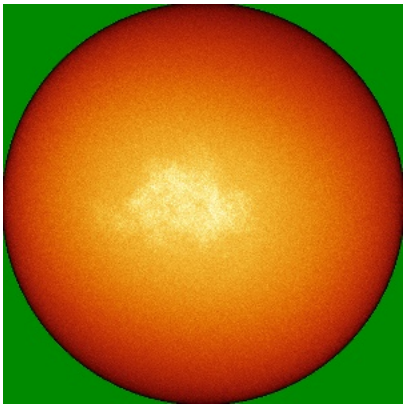


Z

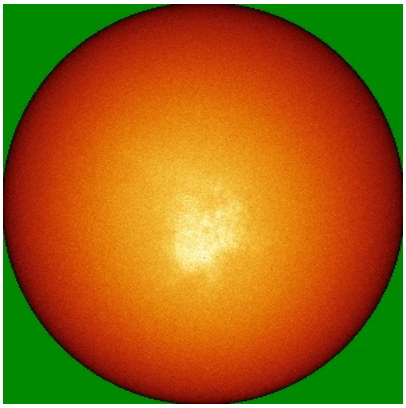
6.4.2 Raw map



X



Y



Z

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

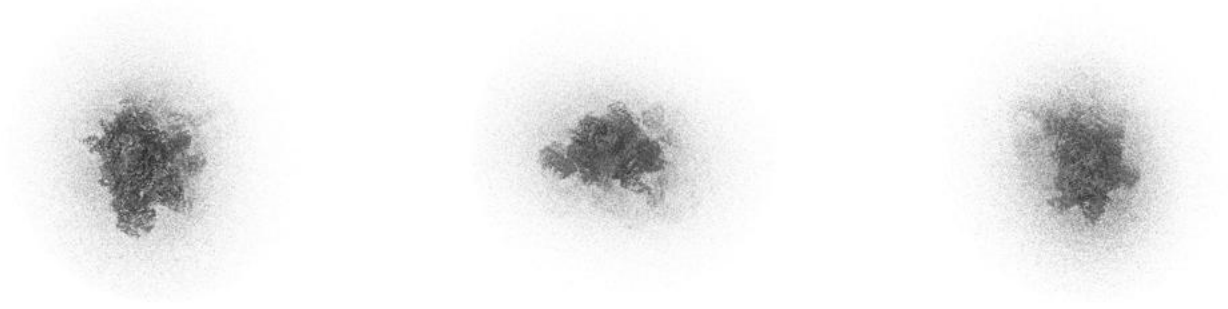
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

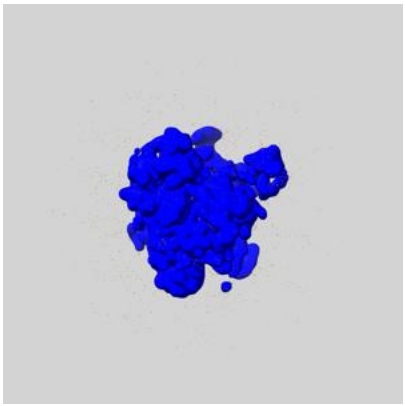
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

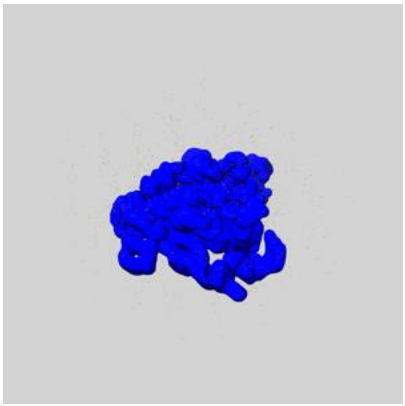
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

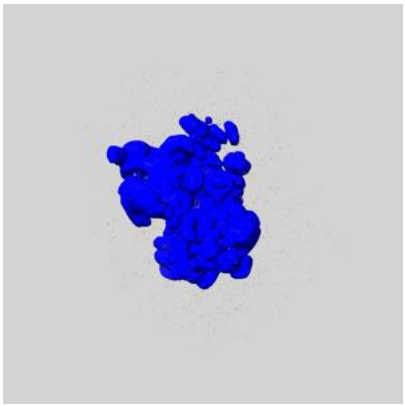
6.6.1 emd_19941_msk_1.map



X



Y

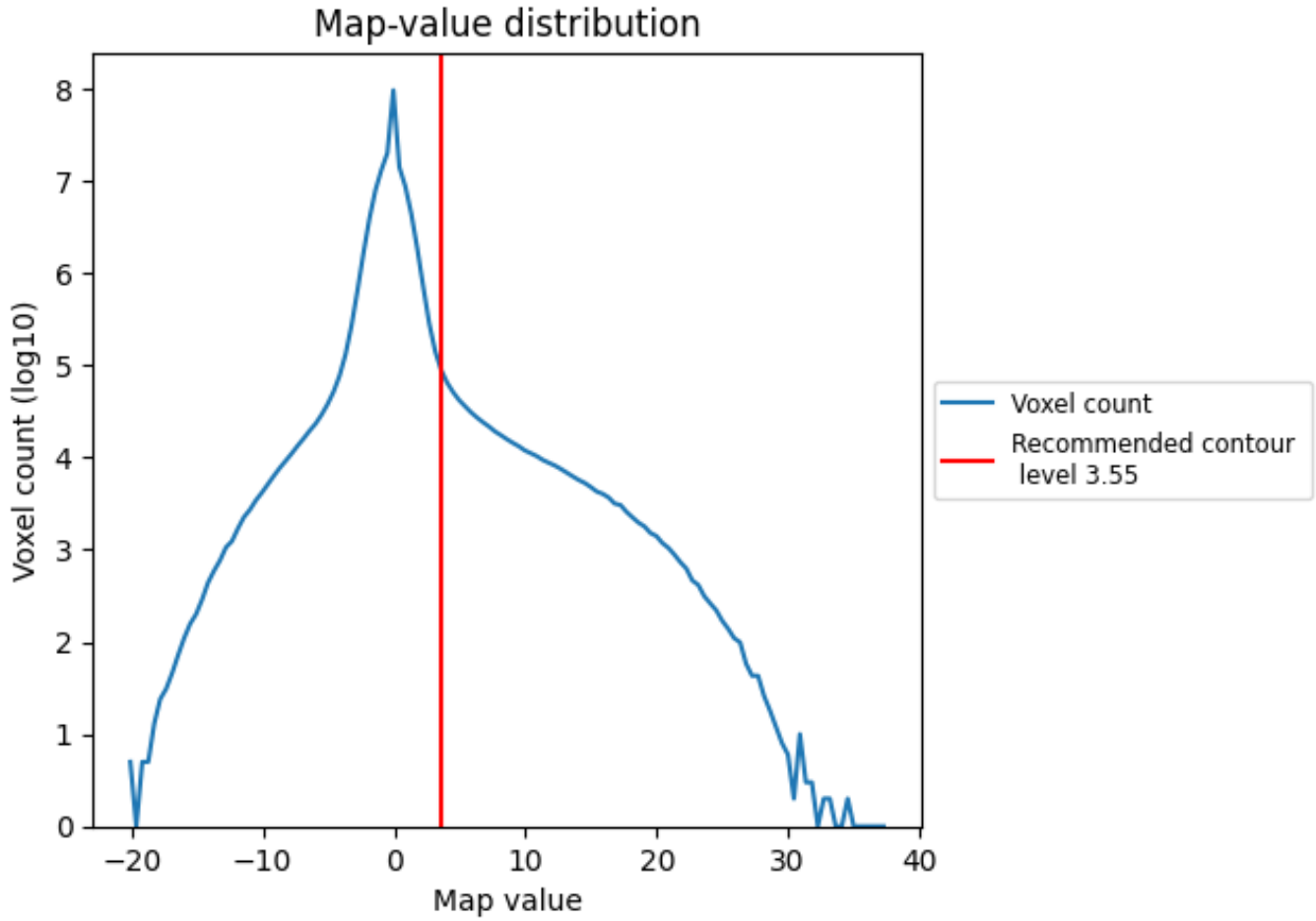


Z

7 Map analysis

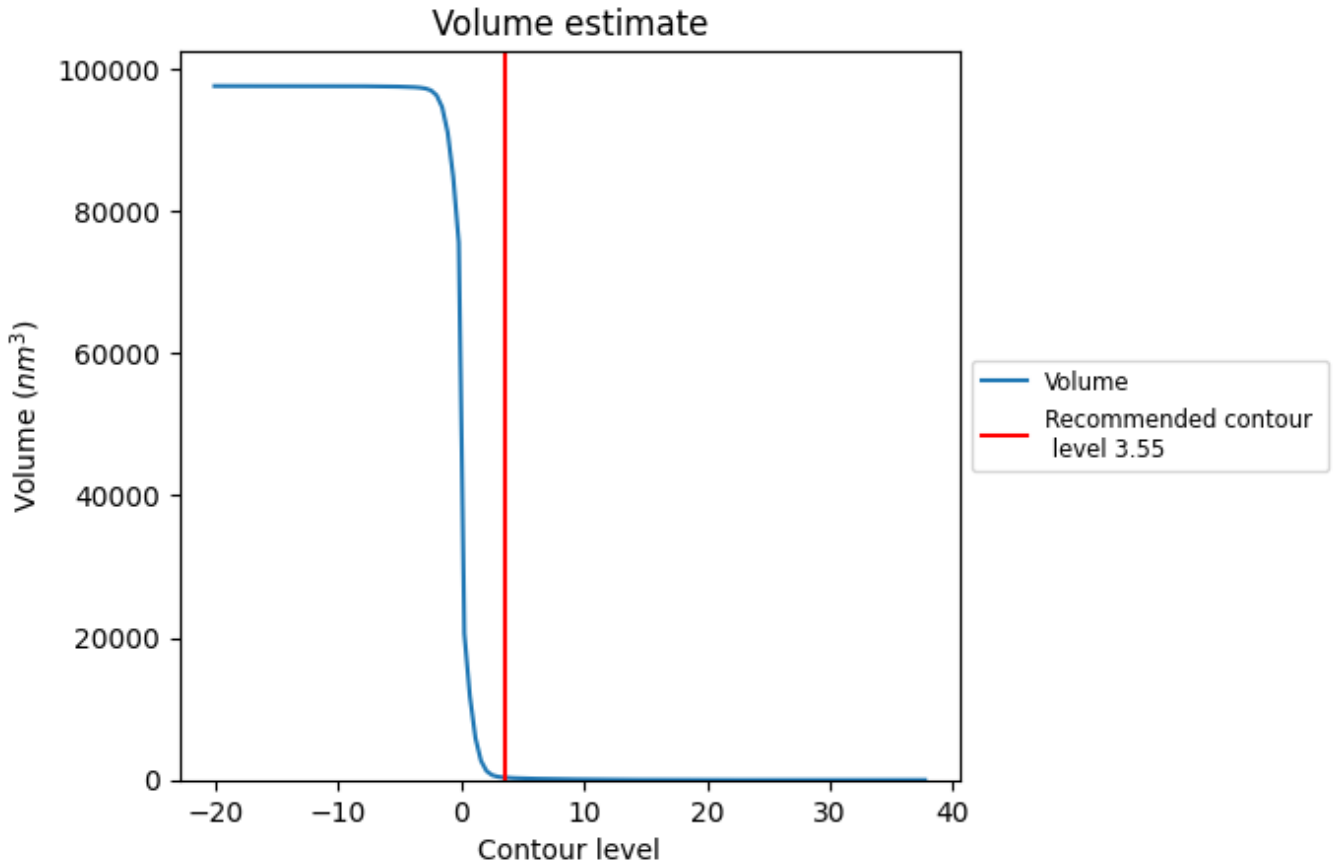
This section contains the results of statistical analysis of the map.

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.

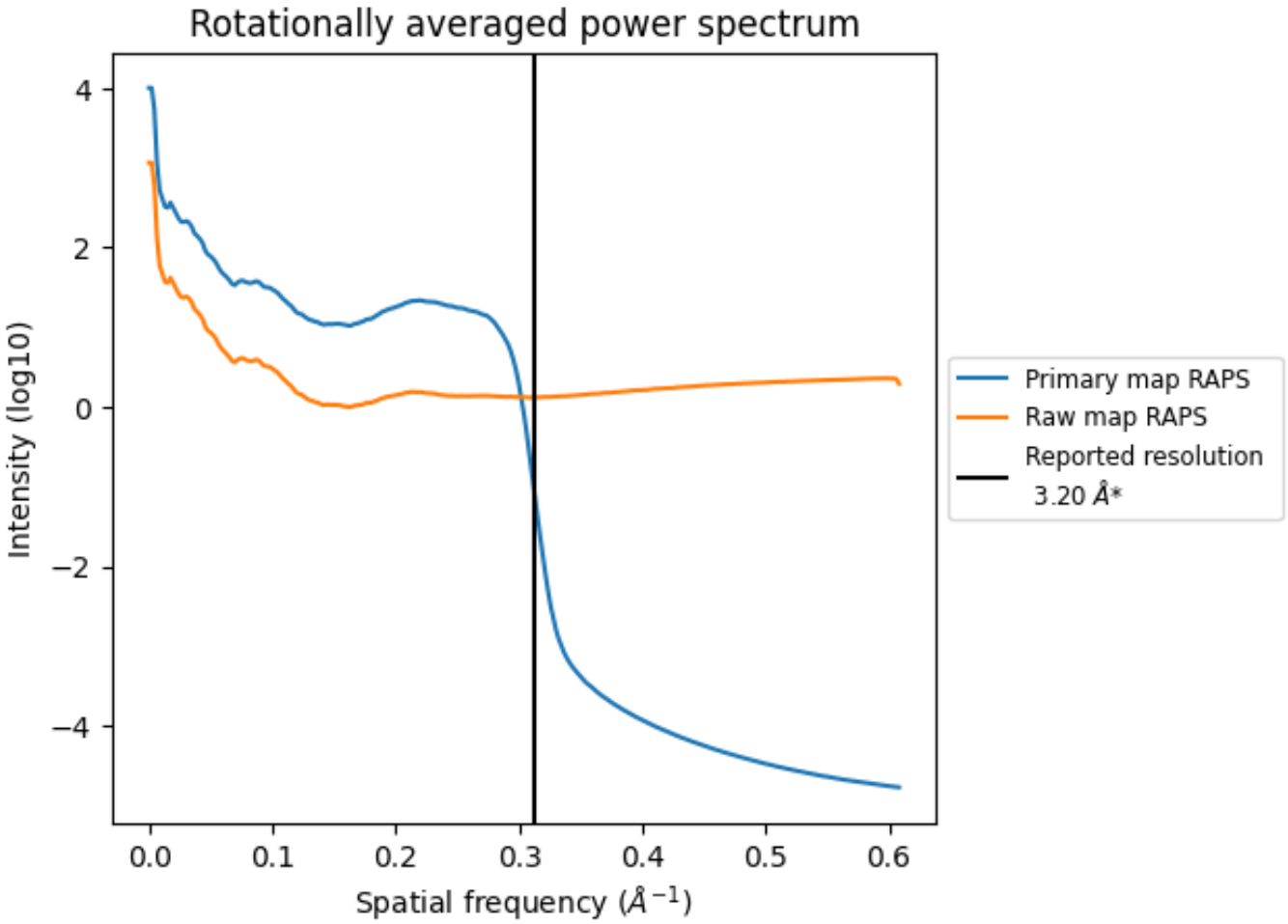
7.2 Volume estimate



The volume at the recommended contour level is 341 nm^3; this corresponds to an approximate mass of 308 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)

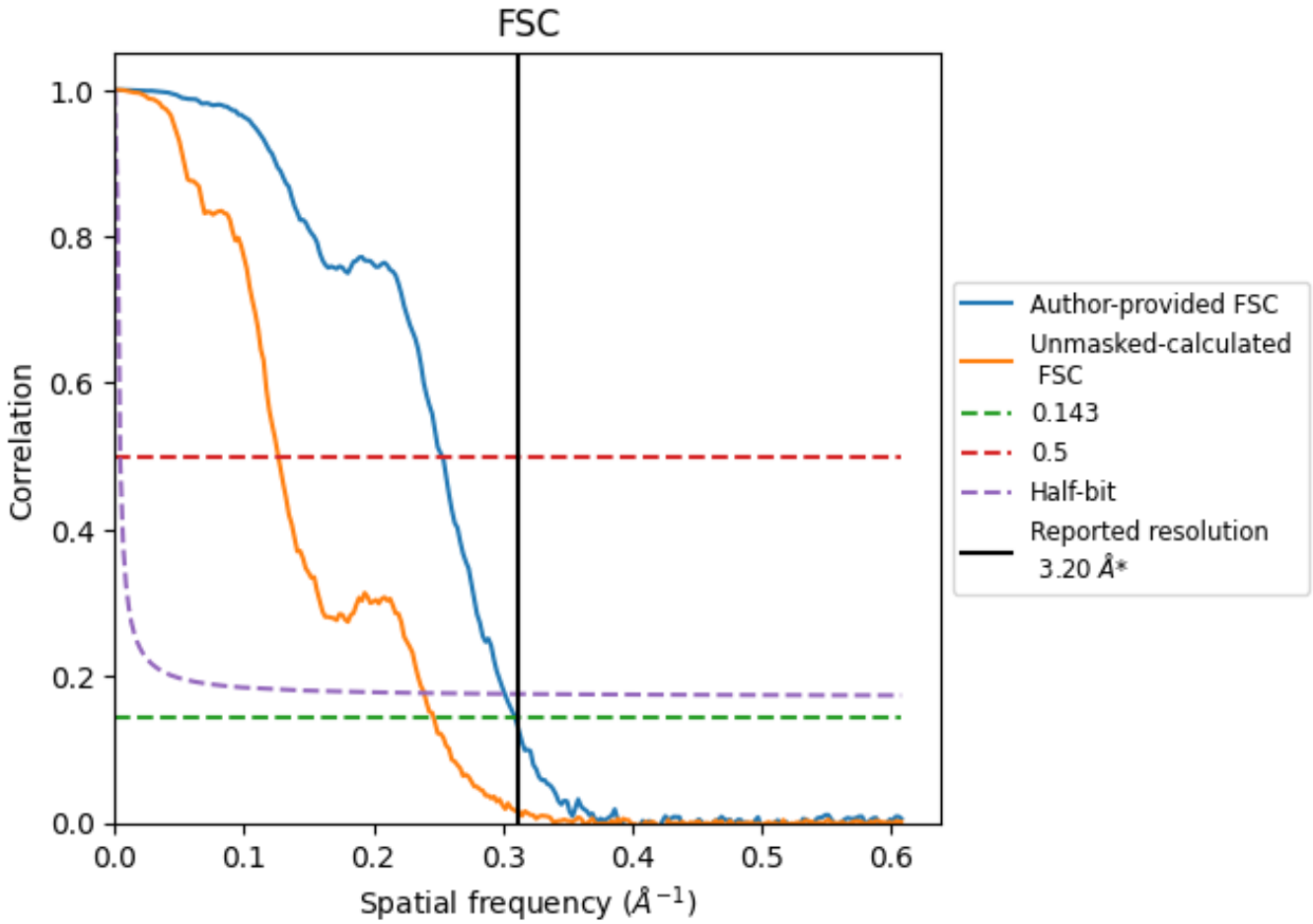


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

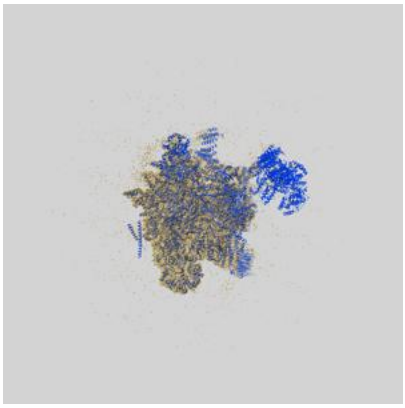
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.23	3.95	3.31
Unmasked-calculated*	4.06	7.91	4.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.06 differs from the reported value 3.2 by more than 10 %

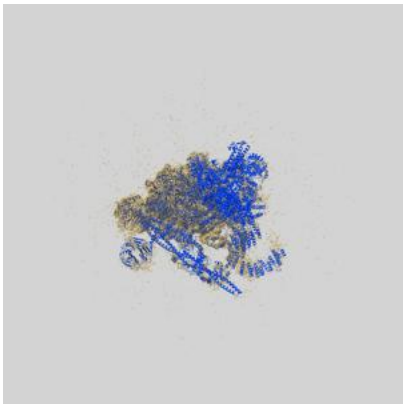
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19941 and PDB model 9ESH. Per-residue inclusion information can be found in section 3 on page 13.

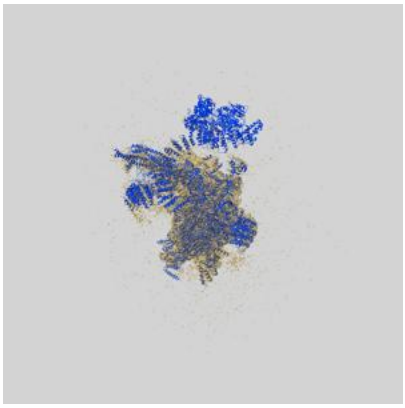
9.1 Map-model overlay



X



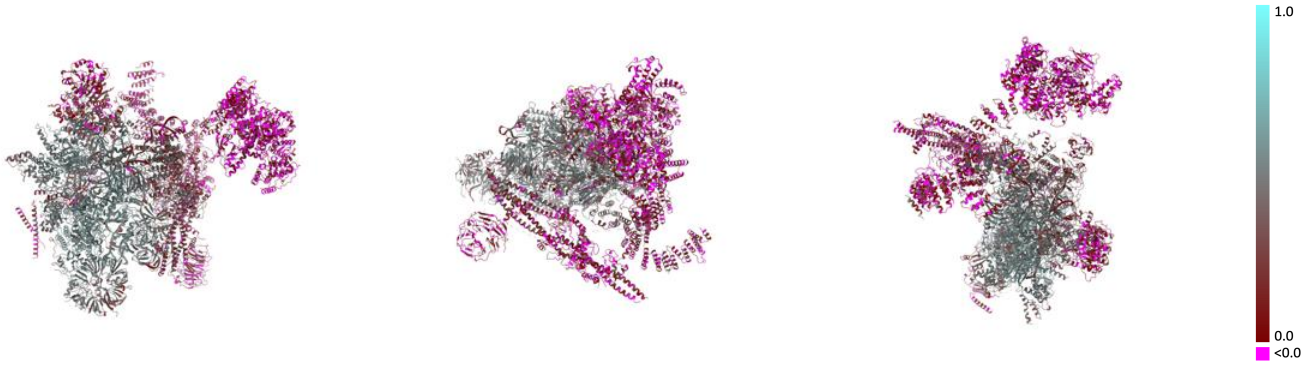
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.55 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.

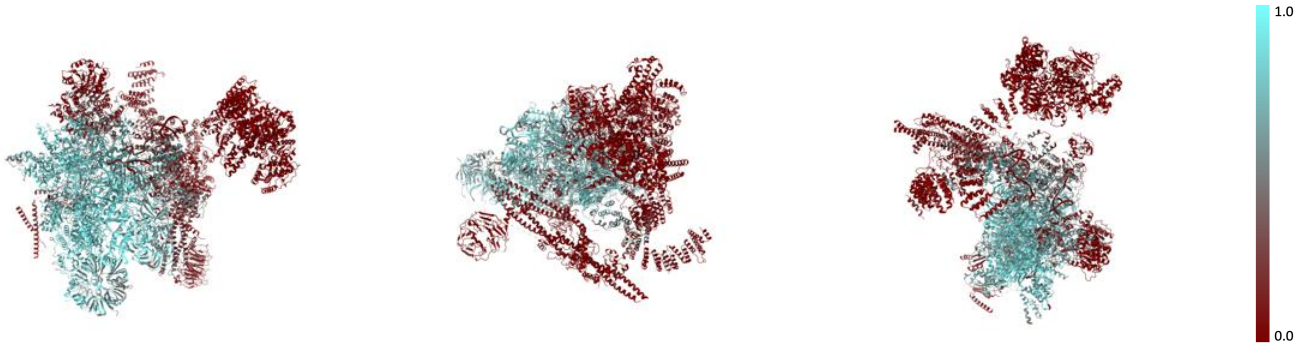
9.2 Q-score mapped to coordinate model (i)



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.

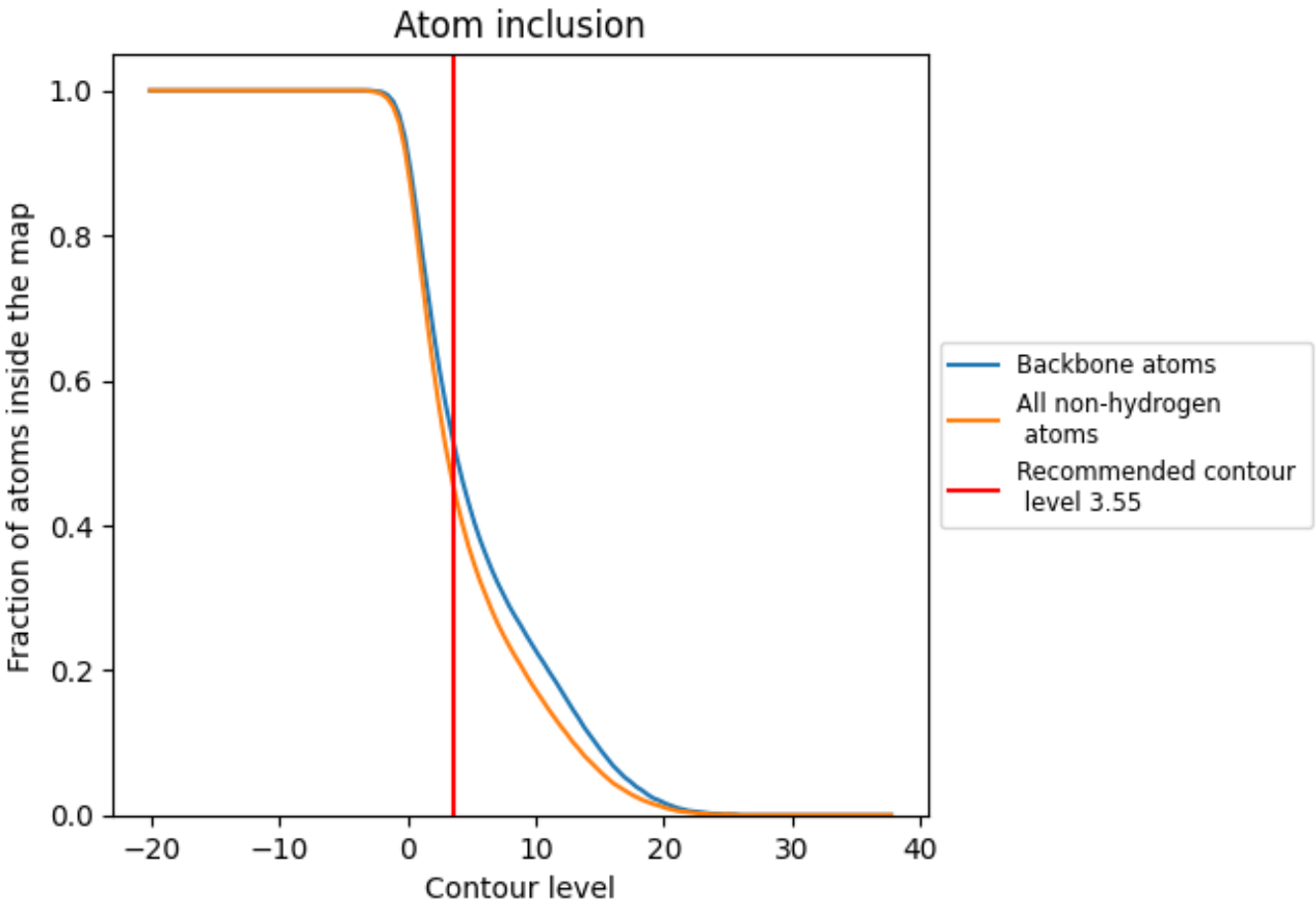
9.3 Atom inclusion mapped to coordinate model (i)



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 (3.55).

9.4 Atom inclusion (i)



At the recommended contour level, 52% of all backbone atoms, 46% 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 (3.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4560	0.3240
1	0.4260	0.3460
2	0.4240	0.3160
5	0.8960	0.5180
6	0.5250	0.3510
A	0.8180	0.5270
B	0.8010	0.5140
C	0.6820	0.4410
D	0.8140	0.5290
E	0.7040	0.4790
F	0.6540	0.4320
G	0.6130	0.3800
H	0.7050	0.4650
I	0.7230	0.4510
J	0.7460	0.5120
K	0.8210	0.5120
L	0.6500	0.4400
M	0.3530	0.3180
N	0.0010	0.0390
O	0.7960	0.5120
P	0.4460	0.3400
Q	0.7420	0.5080
R	0.3340	0.2400
S	0.0210	0.0950
T	0.0830	0.1130
U	0.0550	0.1060
V	0.0350	0.0900
W	0.3780	0.2880
X	0.0550	0.0880
Y	0.2010	0.2840
Z	0.1880	0.1880
a	0.5000	0.3400
b	0.2540	0.2530
c	0.7340	0.4730
d	0.4530	0.3460

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Chain	Atom inclusion	Q-score
f	0.2270	0.2320
m	0.1690	0.3020
r	0.1580	0.1660
y	0.3800	0.2950
z	0.1960	0.1910