Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 02:16 AM JST

PDB ID	:	6ICZ
EMDB ID	:	EMD-9645
Title	:	Cryo-EM structure of a human post-catalytic spliceosome (P complex) at 3.0 angstrom
Authors	:	Zhang, X.; Zhan, X.; Yan, C.; Shi, Y.
Deposited on	:	2018-09-07
Resolution	:	3.00 Å(reported)

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

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

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

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

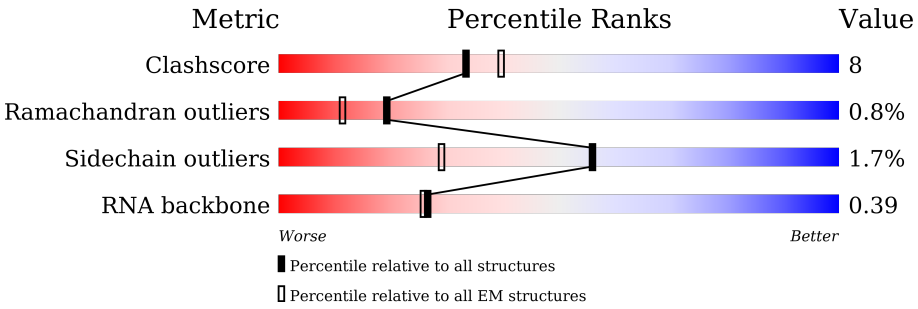
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 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	v	148	97% 97% ·
2	w	174	52% 51% ·· 48%
3	u	411	94% 93% · 6%
4	x	703	· · 96%
5	A	2335	12% 81% 15% ·
6	B	117	14% 26% 38% 17% · 17%
7	C	972	· 74% 17% · 8%

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Mol	Chain	Length	Quality of chain
8	E	357	62% 22% 15%
9	F	107	44% 34% 12% 9%
10	G	273	6% 12% 8% 9% 69%
11	H	188	37% 16% 16% 39% 26%
12	J	848	33% 62% 5% 33%
13	L	802	27% 50% 6% 43%
14	M	243	42% 9% 47%
15	N	144	76% 17% 6%
16	O	420	53% 15% 32%
17	P	229	43% 5% 52%
18	R	536	38% 10% 51%
19	S	166	78% 18%
20	T	514	43% 16% 39%
21	U	2752	99%
22	V	908	28% 47% 50%
23	W	579	69% 17% 12%
24	X	184	14% 43% 7% 50%
25	Z	586	34% 7% 59%
26	I	855	57% 60% 6% 34%
27	y	301	24% 26% 74%
28	Q	1485	89% 89% 11%
29	a	126	44% 64% 36%
29	h	126	56% 64% 36%
30	b	231	28% 37% 63%
30	i	231	33% 37% 63%

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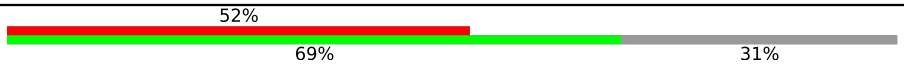
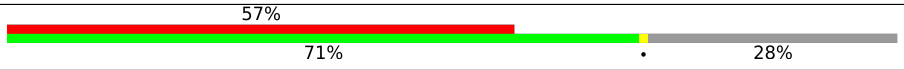
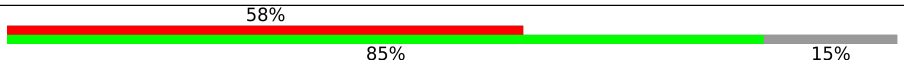
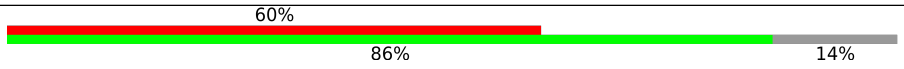
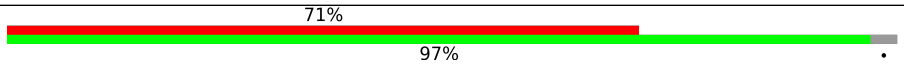
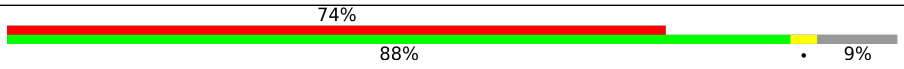
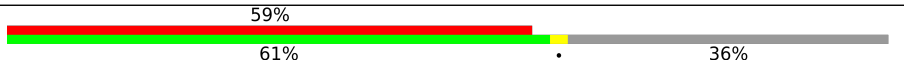
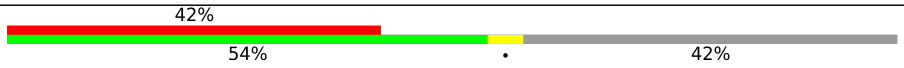
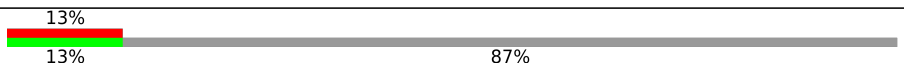
Mol	Chain	Length	Quality of chain
31	c	119	
31	j	119	
32	d	118	
32	k	118	
33	f	86	
33	m	86	
34	e	92	
34	l	92	
35	g	76	
35	n	76	
36	o	255	
37	p	225	
38	Y	1220	
39	K	225	
40	q	504	
40	r	504	
40	s	504	
40	t	504	
41	D	2136	

2 Entry composition

There are 46 unique types of molecules in this entry. The entry contains 97900 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Protein mago nashi homolog 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	v	144	711	423	144	144	0	0

- Molecule 2 is a protein called RNA-binding protein 8A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	w	91	445	263	91	91	0	0

- Molecule 3 is a protein called Eukaryotic initiation factor 4A-III.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	u	386	1907	1135	386	386	0	0

- Molecule 4 is a protein called Protein CASC3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	x	25	124	74	25	25	0	0

- Molecule 5 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	A	2253	17837	11432	3157	3177	71	0	0

- Molecule 6 is a RNA chain called U5snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	B	97	2040	914	339	690	97	0	0

- Molecule 7 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	894	Total	C	N	O	S	0	0
			7066	4520	1178	1334	34		

- Molecule 8 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

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

- Molecule 9 is a RNA chain called U6snRNA.

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

- Molecule 10 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	84	Total	C	N	O	P	0	0
			1549	684	218	563	84		

- Molecule 11 is a RNA chain called U2snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	140	Total	C	N	O	P	0	0
			2966	1326	510	990	140		

- Molecule 12 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	571	Total	C	N	O	S	0	0
			3829	2385	720	718	6		

- Molecule 13 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	454	Total	C	N	O	S	0	0
			3064	1884	596	578	6		

- Molecule 14 is a protein called Pre-mRNA-splicing factor SYF2.

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

- Molecule 15 is a protein called Protein BUD31 homolog.

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

- Molecule 16 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	285	Total	C	N	O	S	0	0
			2296	1442	408	426	20		

- Molecule 17 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	110	Total	C	N	O	S	0	0
			929	569	182	176	2		

- Molecule 18 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	261	Total	C	N	O	P	S	0	0
			2073	1300	373	386	2	12		

- Molecule 19 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

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

- Molecule 20 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	313	Total	C	N	O	S	0	0
			2461	1554	447	452	8		

- Molecule 21 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	26	Total	C	N	O	S	0	0
			193	120	36	36	1		

- Molecule 22 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	452	Total	C	N	O	S	0	0
			2765	1723	508	523	11		

- Molecule 23 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	508	Total	C	N	O	S	0	0
			4122	2623	714	761	24		

- Molecule 24 is a protein called PRKR-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	92	Total	C	N	O	S	0	0
			701	432	133	132	4		

- Molecule 25 is a protein called Pre-mRNA-splicing factor SLU7.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	242	Total	C	N	O	S	0	0
			1999	1260	357	374	8		

- Molecule 26 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	I	564	Total	C	N	O	0	0
			2782	1654	564	564		

- Molecule 27 is a protein called Peptidyl-prolyl cis-trans isomerase E.

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

- Molecule 28 is a protein called RNA helicase aquarius.

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

- Molecule 29 is a protein called Small nuclear ribonucleoprotein Sm D3.

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

- Molecule 30 is a protein called Small nuclear ribonucleoprotein-associated protein.

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

- Molecule 31 is a protein called Small nuclear ribonucleoprotein Sm D1.

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

- Molecule 32 is a protein called Small nuclear ribonucleoprotein Sm D2.

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

- Molecule 33 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	m	73	Total	C	N	O	0	0
			356	210	73	73		
33	f	74	Total	C	N	O	0	0
			361	213	74	74		

- Molecule 34 is a protein called Small nuclear ribonucleoprotein E.

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

- Molecule 35 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	n	69	Total 339	C 201	N 69	O 69	0	0
35	g	74	Total 363	C 215	N 74	O 74	0	0

- Molecule 36 is a protein called U2 small nuclear ribonucleoprotein A'.

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

- Molecule 37 is a protein called U2 small nuclear ribonucleoprotein B".

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

- Molecule 38 is a protein called ATP-dependent RNA helicase DHX8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Y	713	Total 2917	C 1486	N 716	O 714	S 1	0	0

- Molecule 39 is a protein called Pre-mRNA-splicing factor SPF27.

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

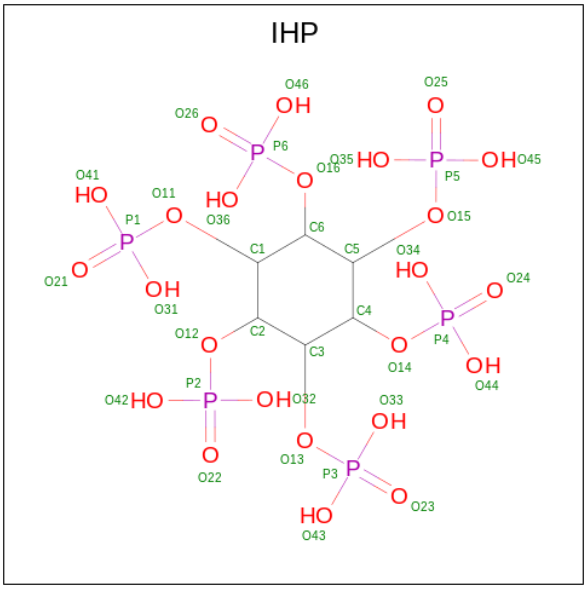
- Molecule 40 is a protein called Pre-mRNA-processing factor 19.

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

- Molecule 41 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

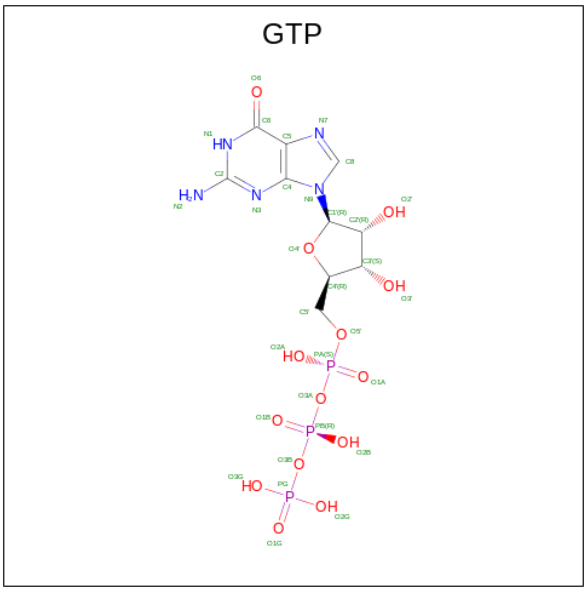
Mol	Chain	Residues	Atoms				AltConf	Trace
41	D	1722	Total	C	N	O	0	0
			8530	5086	1722	1722		

- Molecule 42 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- Molecule 43 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

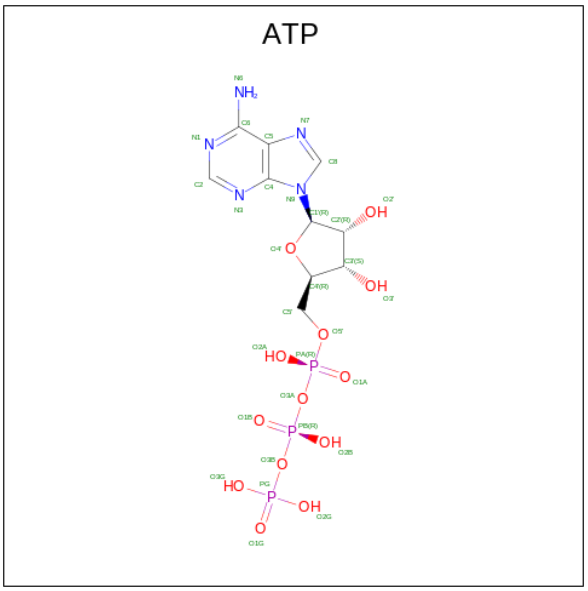
- Molecule 44 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
44	C	1	Total	Mg	0
			1	1	
44	F	6	Total	Mg	0
			6	6	
44	Q	2	Total	Mg	0
			2	2	

- Molecule 45 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
45	N	3	Total	Zn	0
			3	3	
45	O	3	Total	Zn	0
			3	3	
45	Z	1	Total	Zn	0
			1	1	

- Molecule 46 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



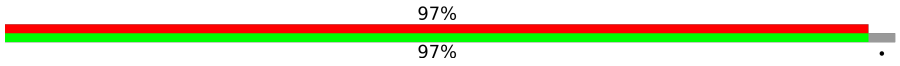
Mol	Chain	Residues	Atoms					AltConf
46	Q	1	Total	C	N	O	P	0
			31	10	5	13	3	

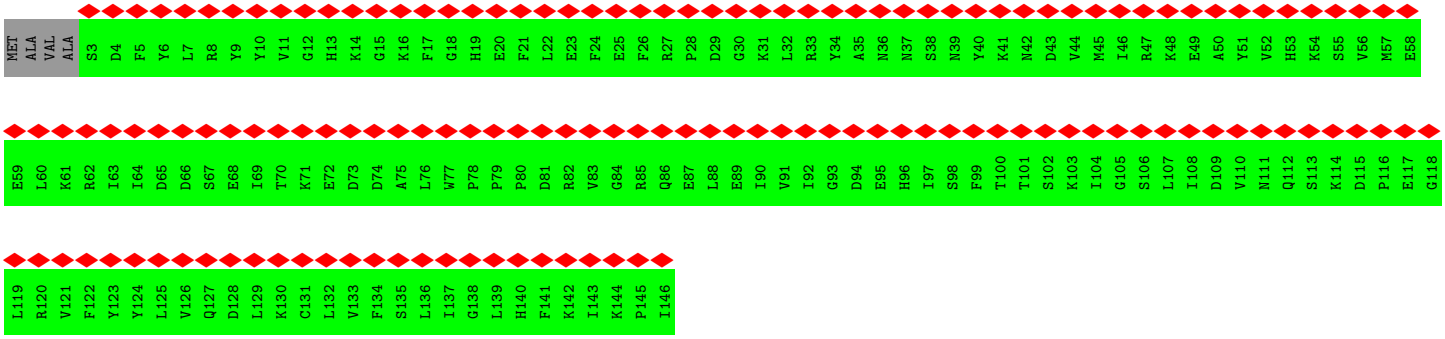
3 Residue-property plots (i)

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

• Molecule 1: Protein mago nashi homolog 2

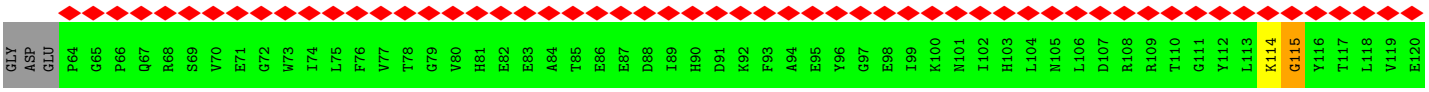
Chain v:





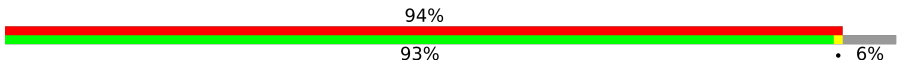
• Molecule 2: RNA-binding protein 8A

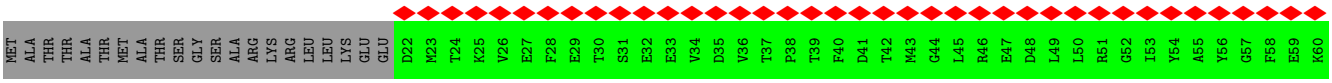
Chain w:

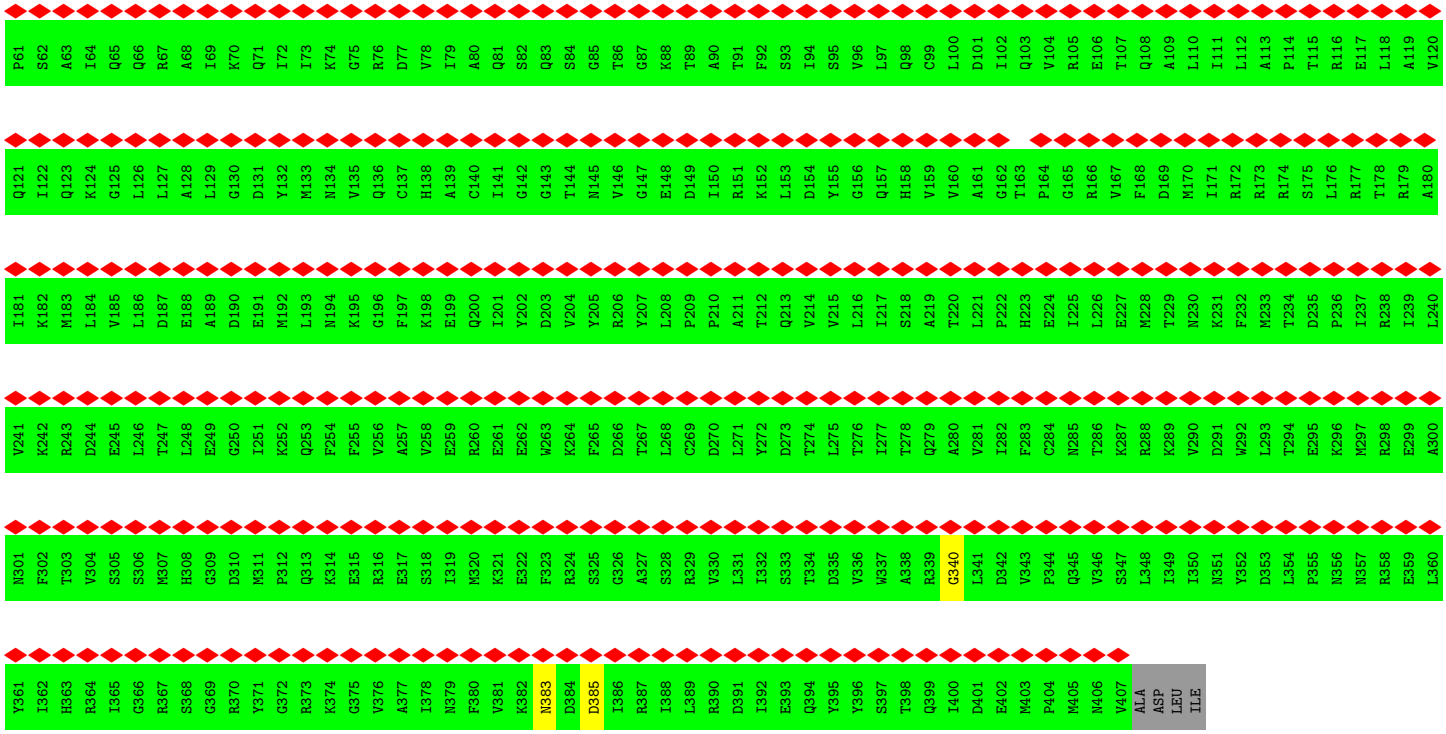


• Molecule 3: Eukaryotic initiation factor 4A-III

Chain u:

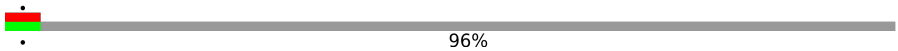


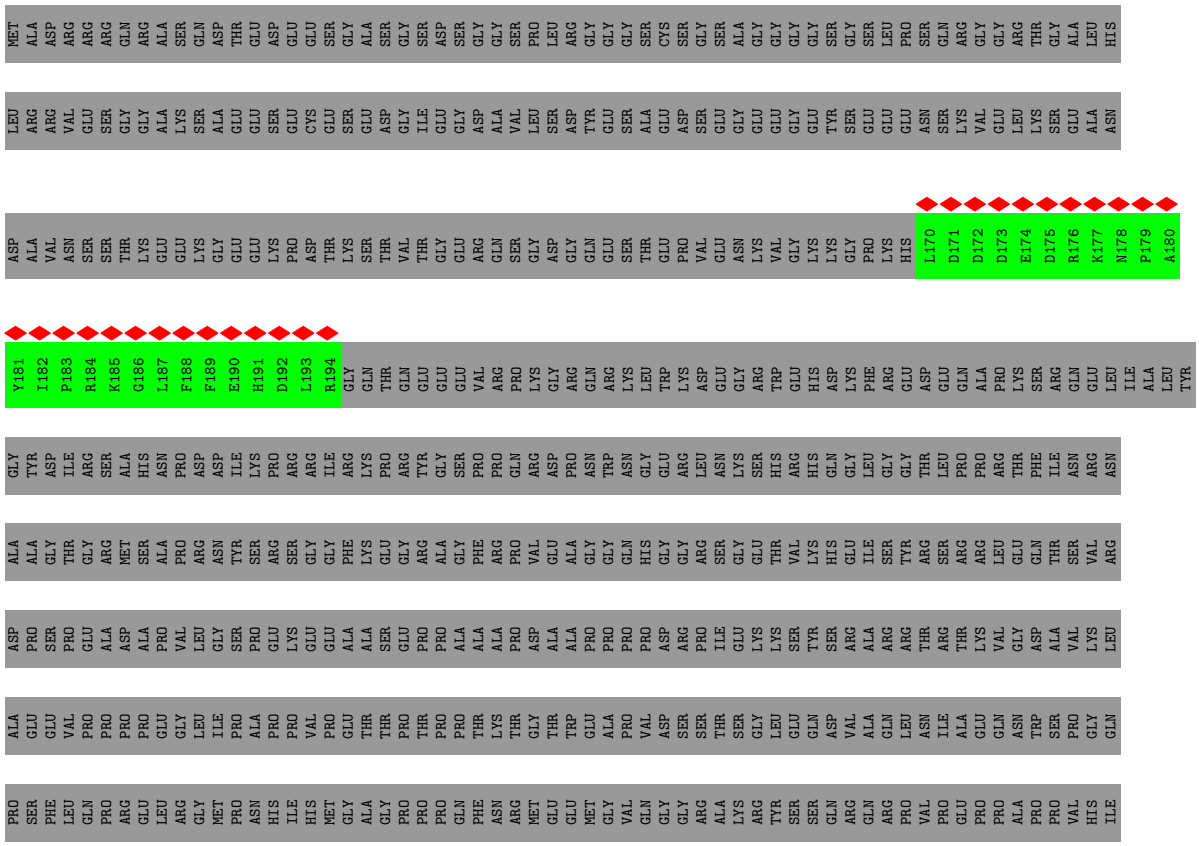


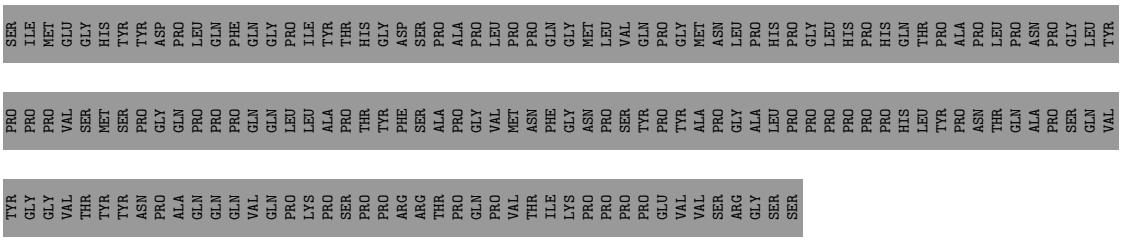


- Molecule 4: Protein CASC3

Chain x:

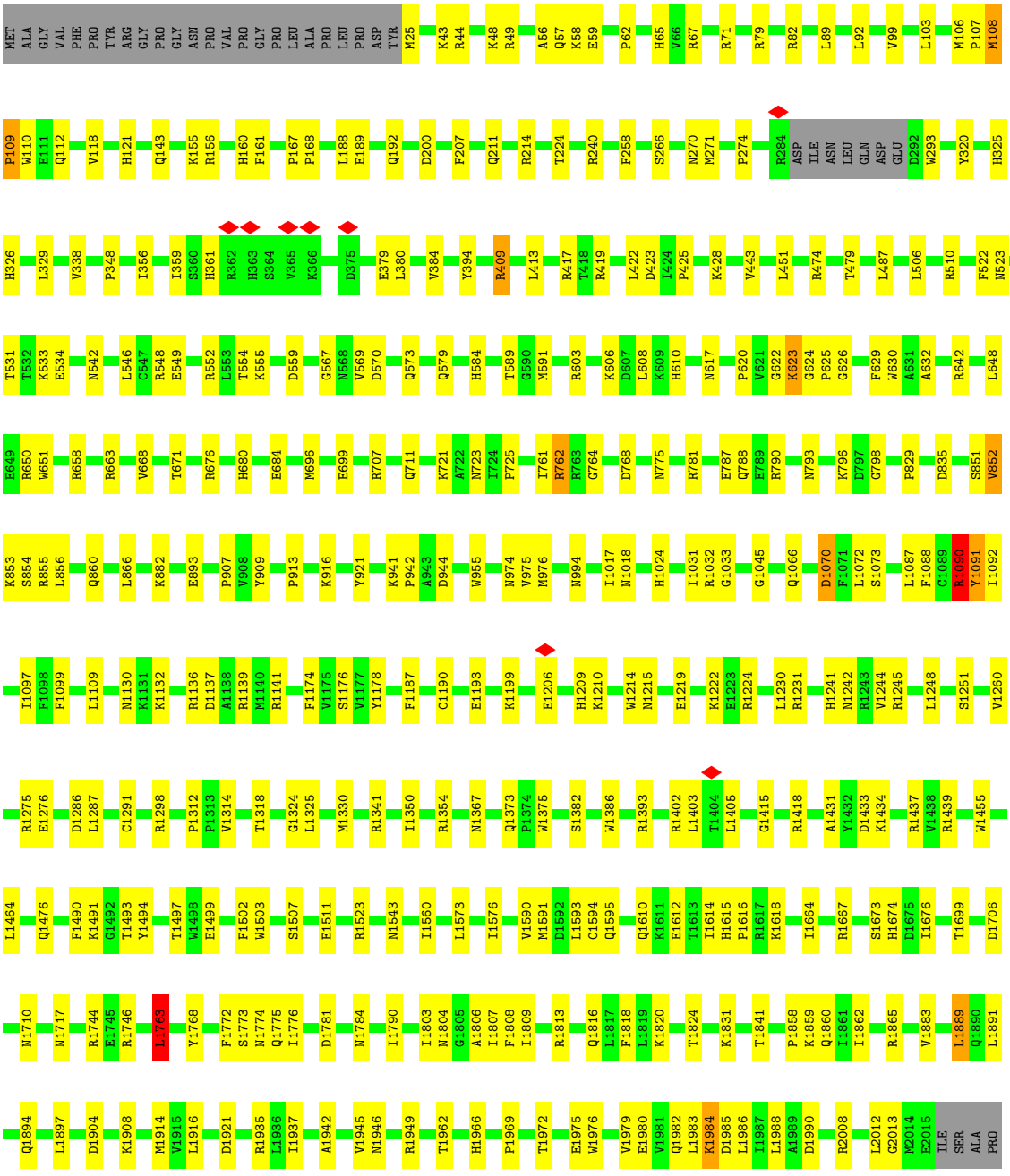


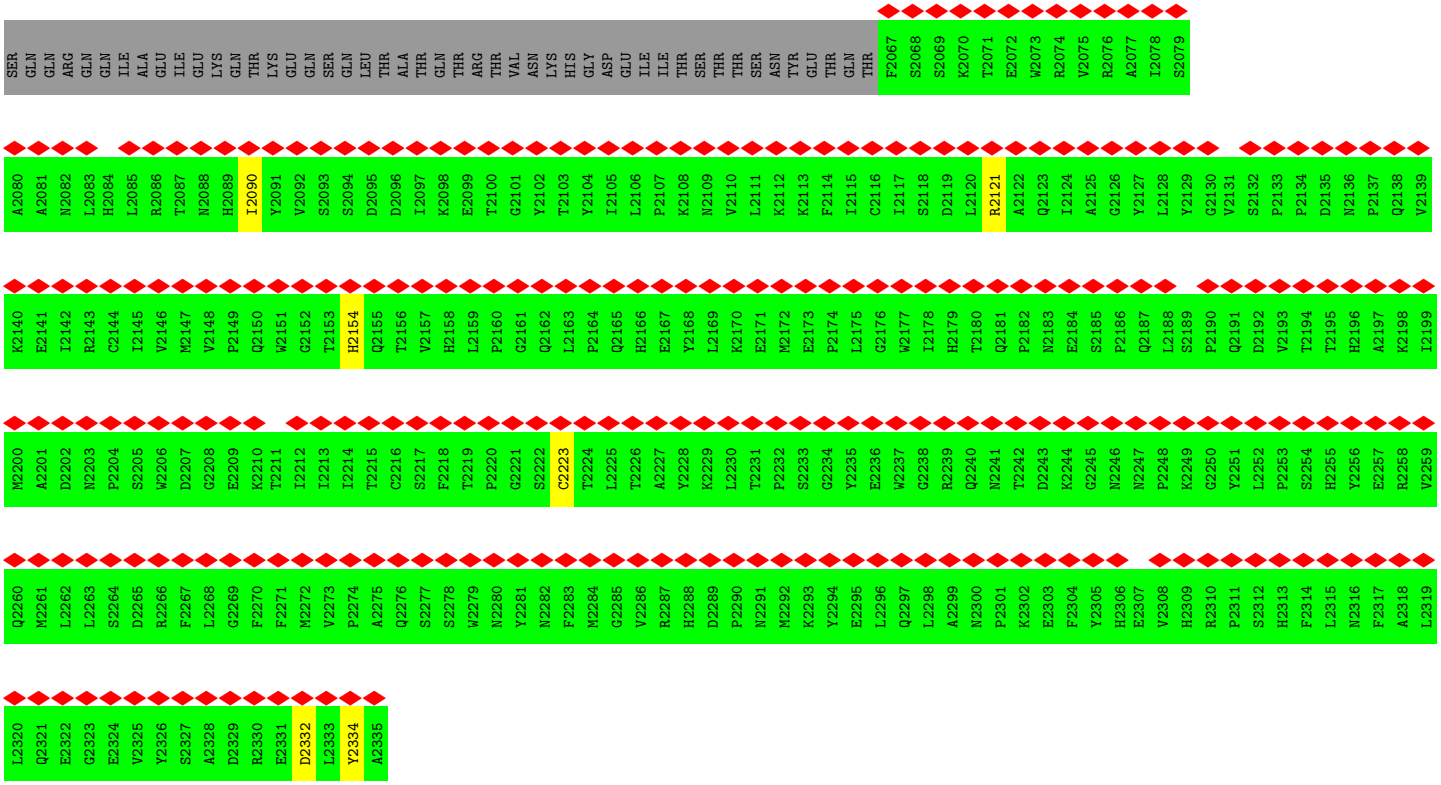




• Molecule 5: Pre-mRNA-processing-splicing factor 8

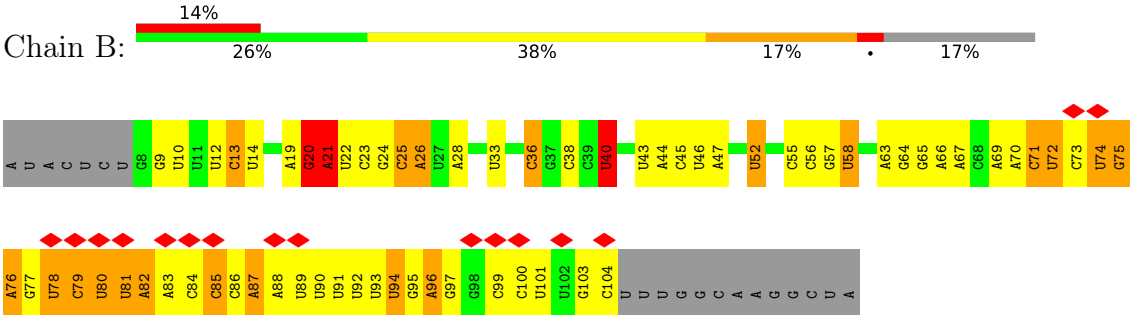
Chain A:





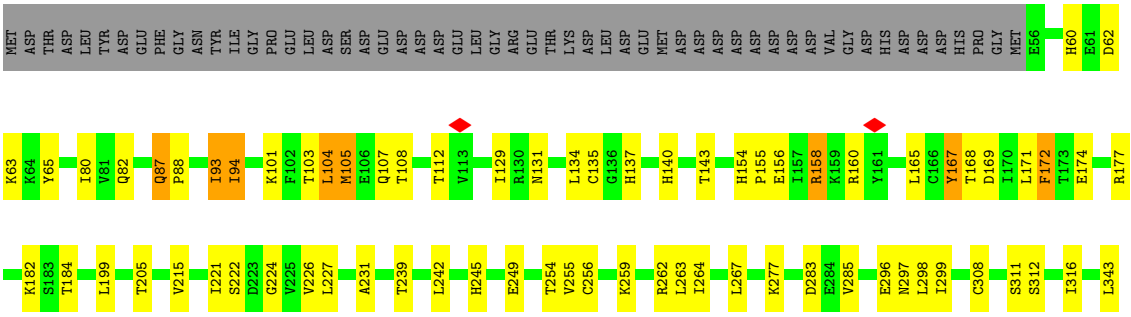
• Molecule 6: U5snRNA

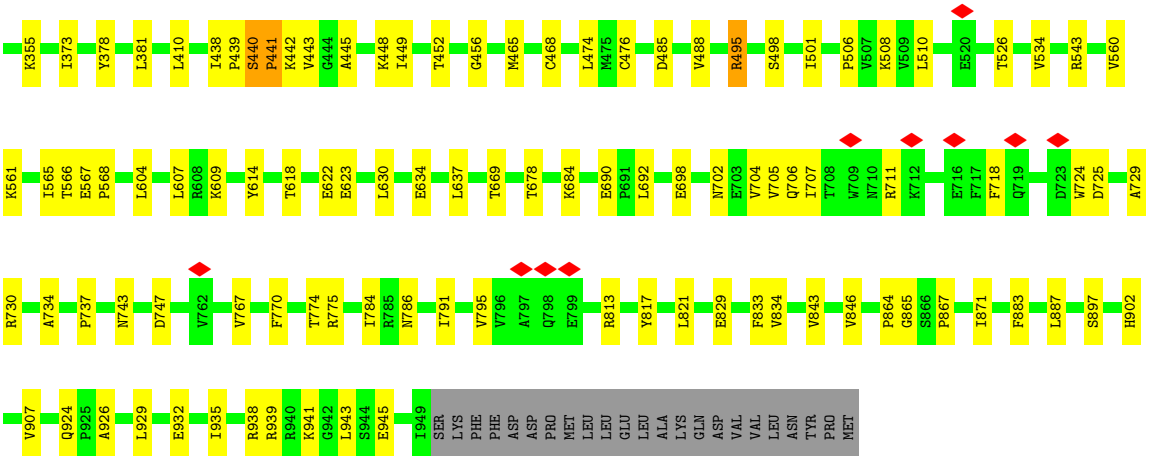
Chain B:



• Molecule 7: 116 kDa U5 small nuclear ribonucleoprotein component

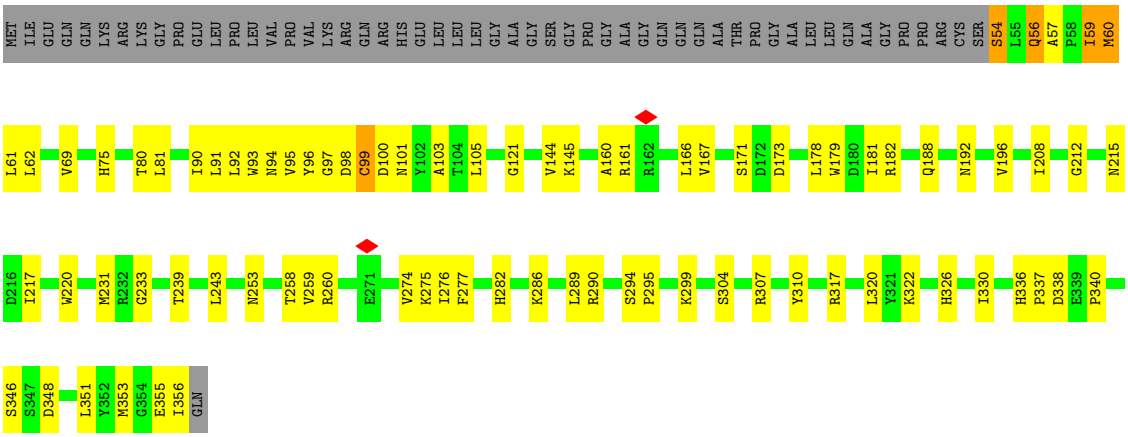
Chain C:





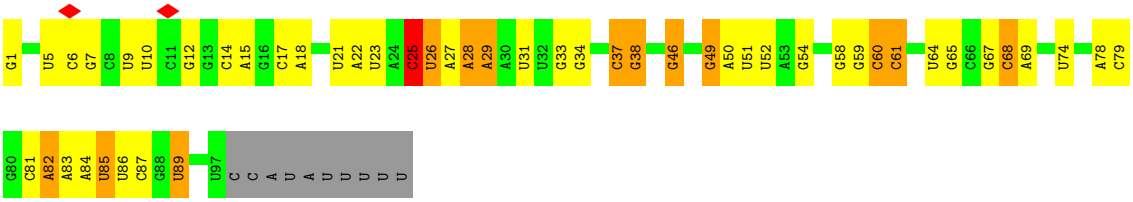
• Molecule 8: U5 small nuclear ribonucleoprotein 40 kDa protein

Chain E:



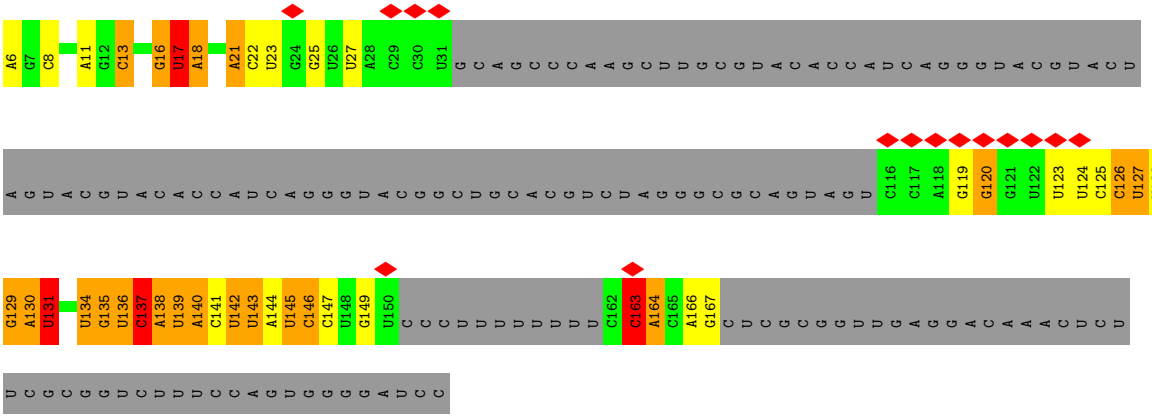
• Molecule 9: U6snRNA

Chain F:



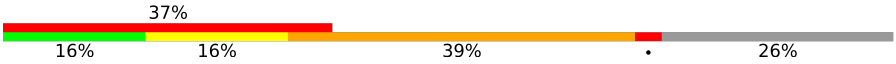
• Molecule 10: pre-mRNA

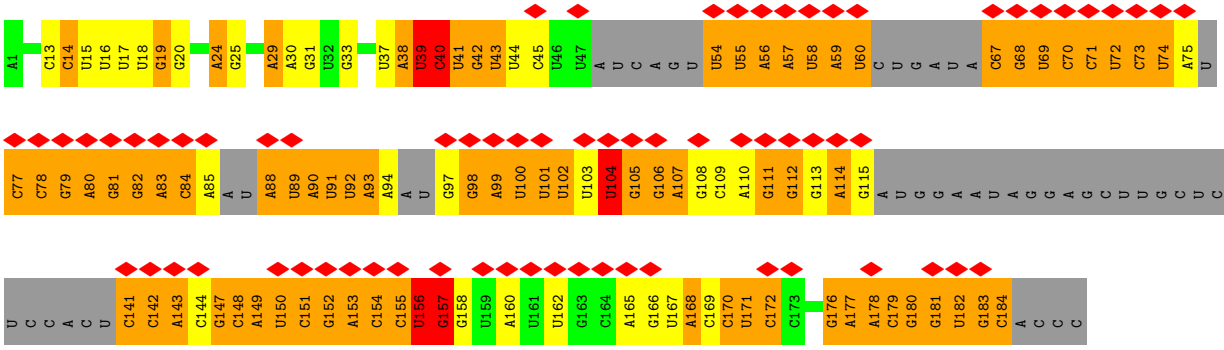
Chain G:



• Molecule 11: U2snRNA

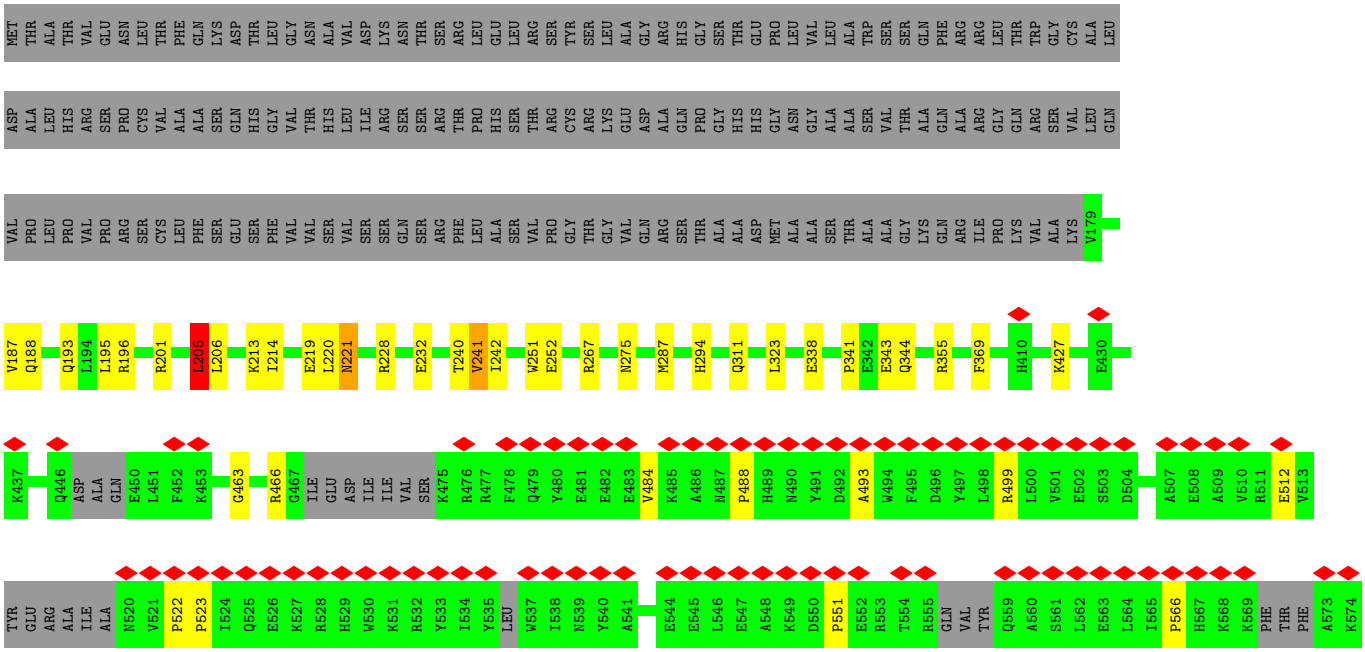
Chain H:

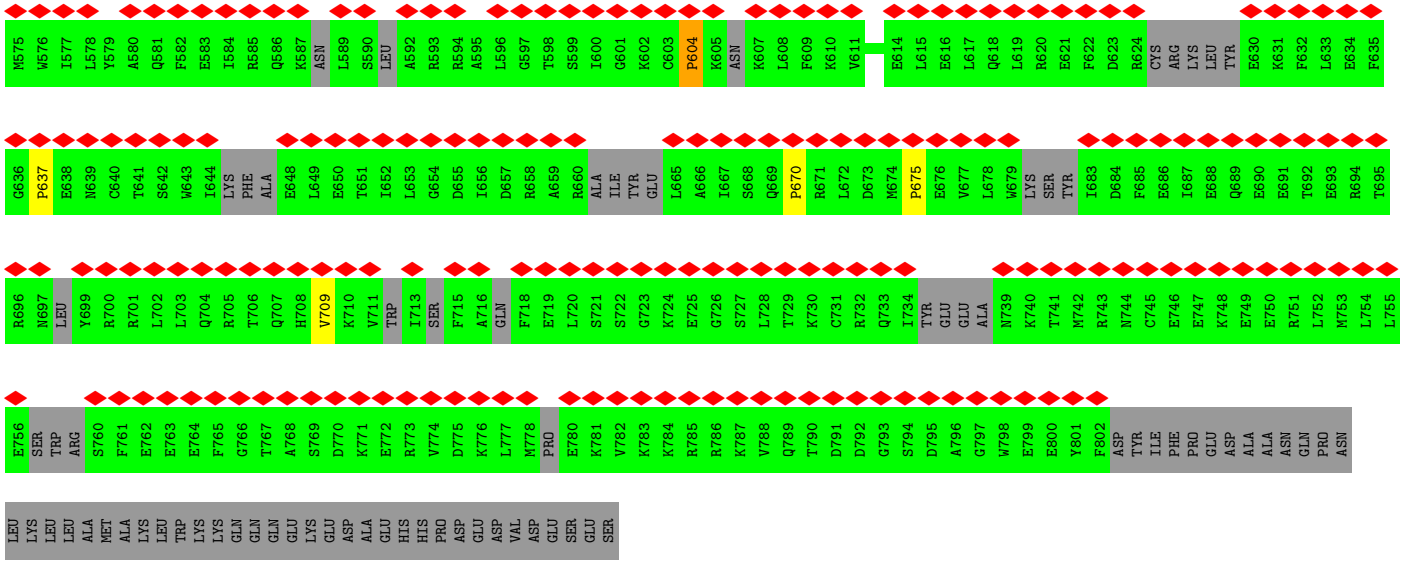




• Molecule 12: Crooked neck-like protein 1

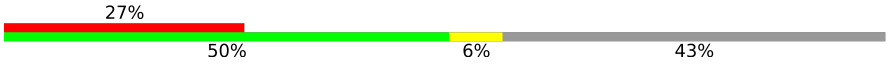
Chain J:

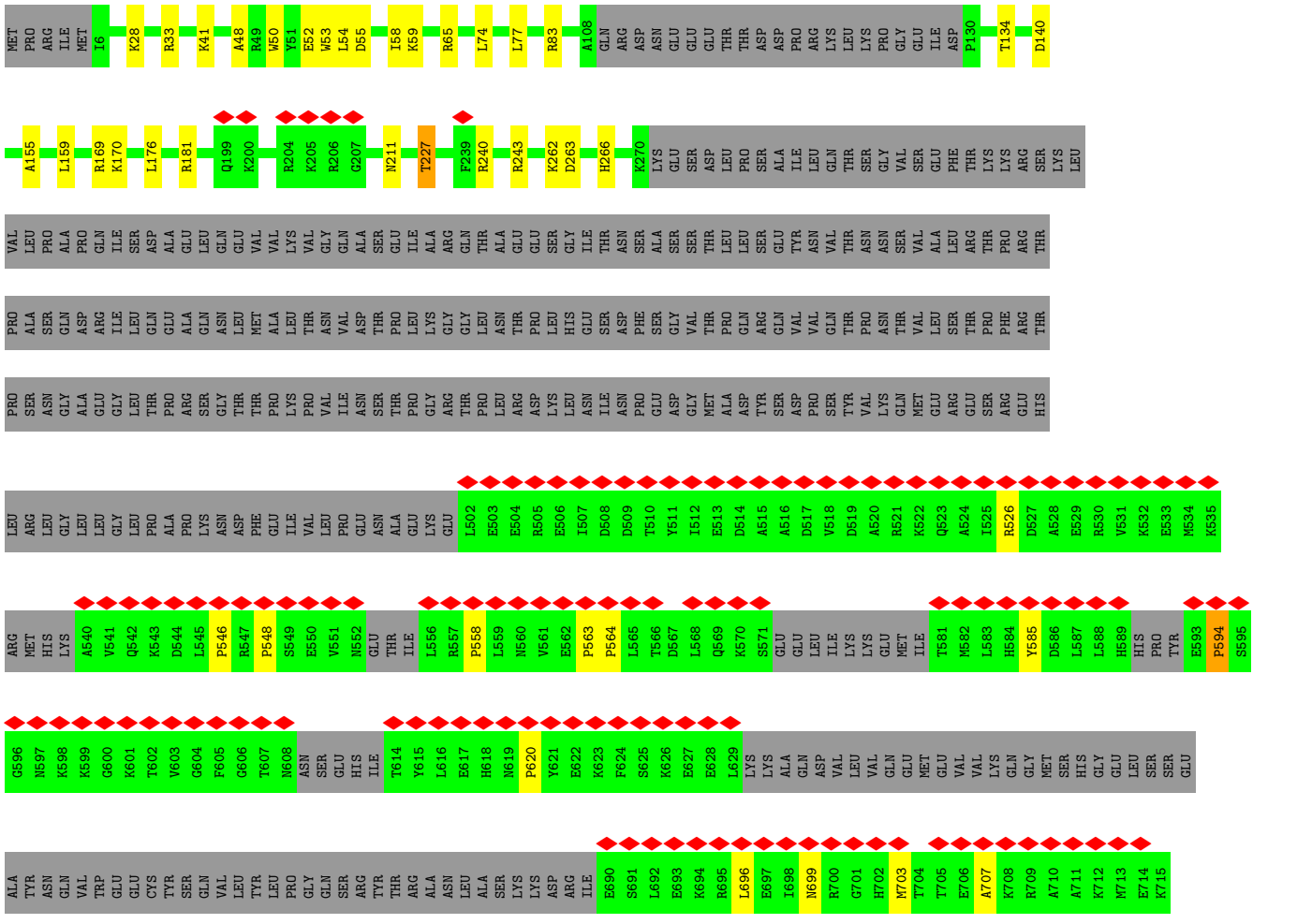


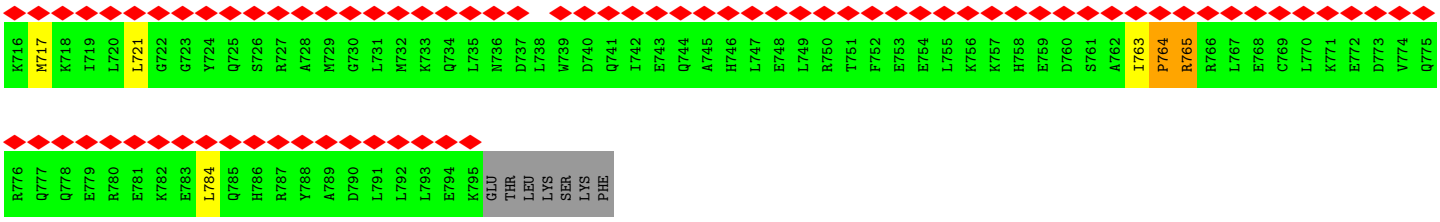


• Molecule 13: Cell division cycle 5-like protein

Chain L:

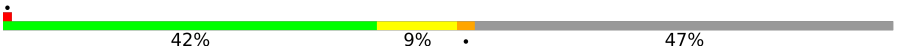


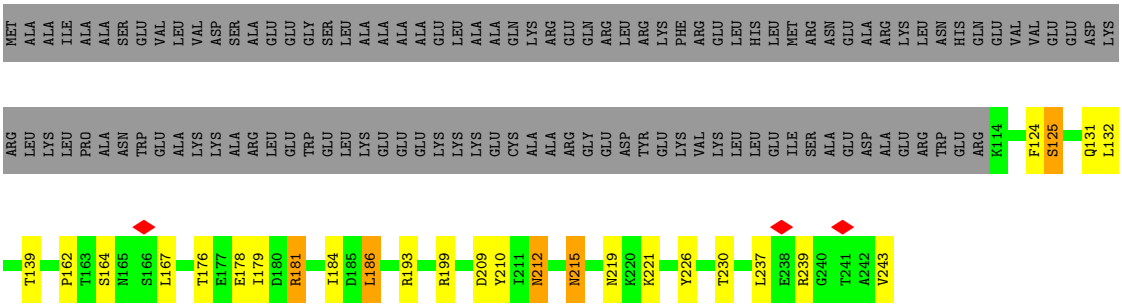




• Molecule 14: Pre-mRNA-splicing factor SYF2

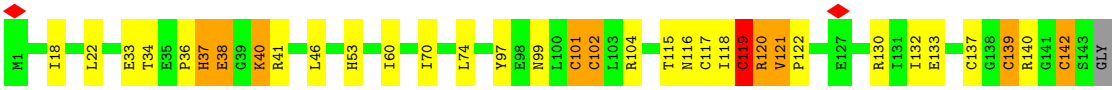
Chain M:





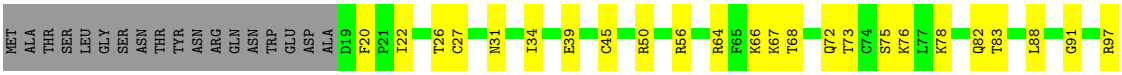
• Molecule 15: Protein BUD31 homolog

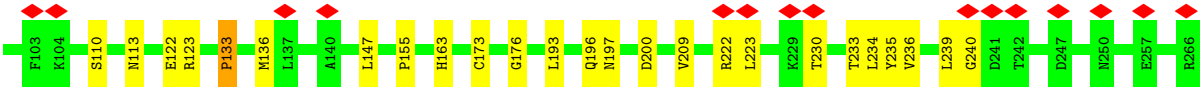
Chain N:

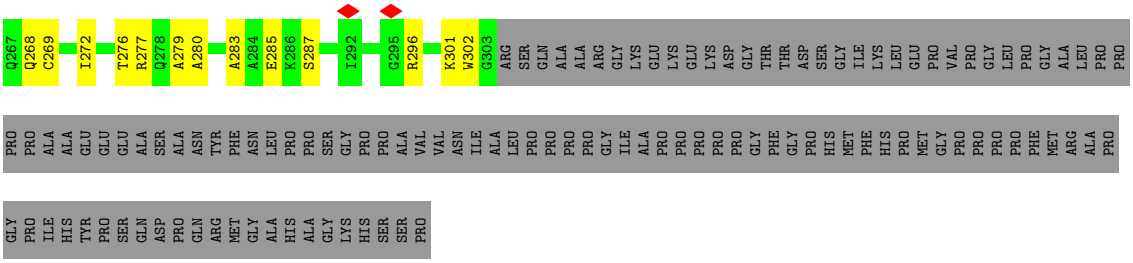


• Molecule 16: Pre-mRNA-splicing factor RBM22

Chain O:

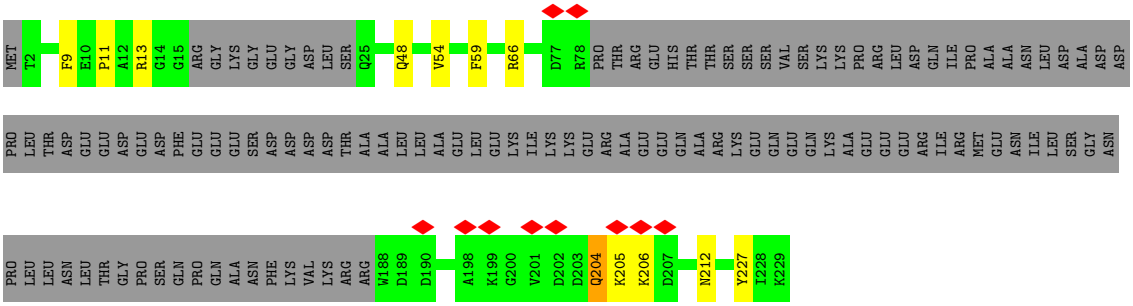






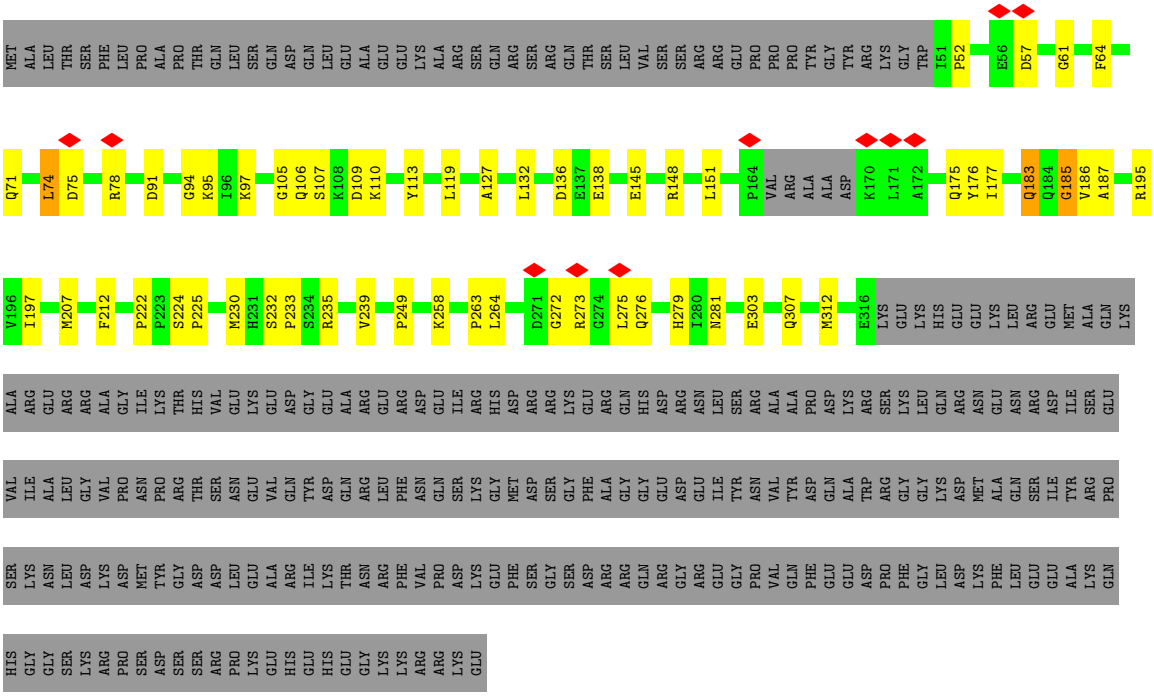
• Molecule 17: Spliceosome-associated protein CWC15 homolog

Chain P:



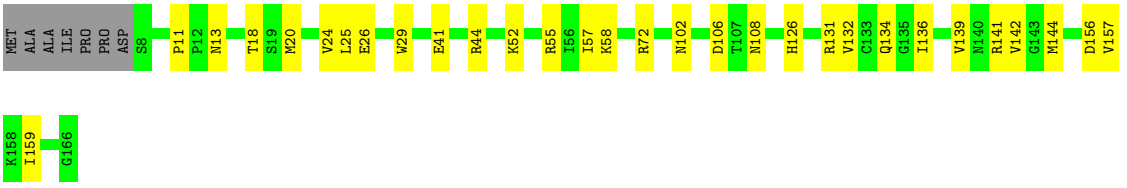
• Molecule 18: SNW domain-containing protein 1

Chain R:



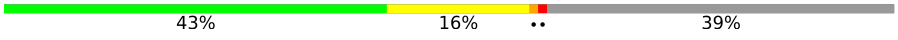
• Molecule 19: Peptidyl-prolyl cis-trans isomerase-like 1

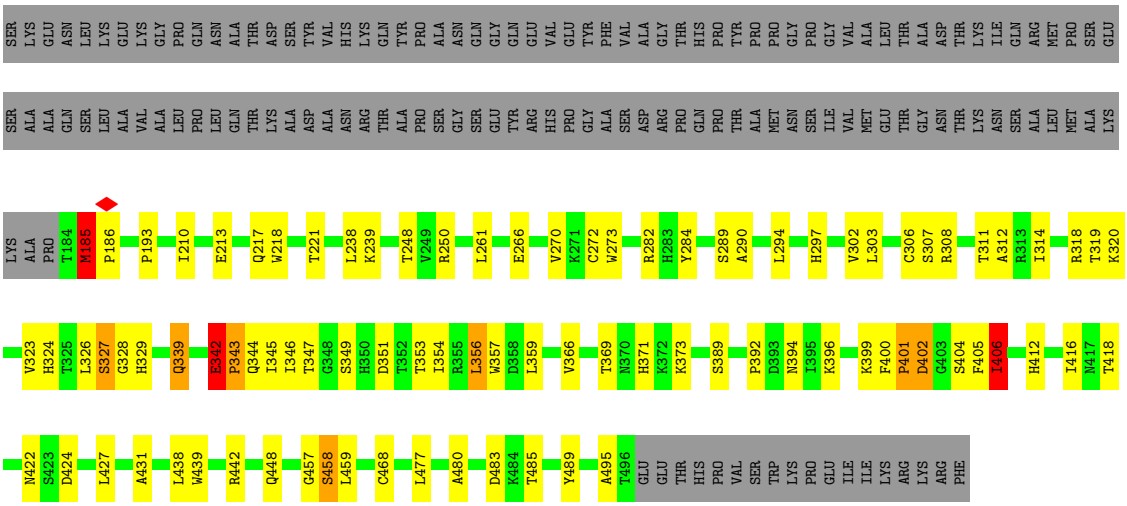
Chain S:



• Molecule 20: Pleiotropic regulator 1

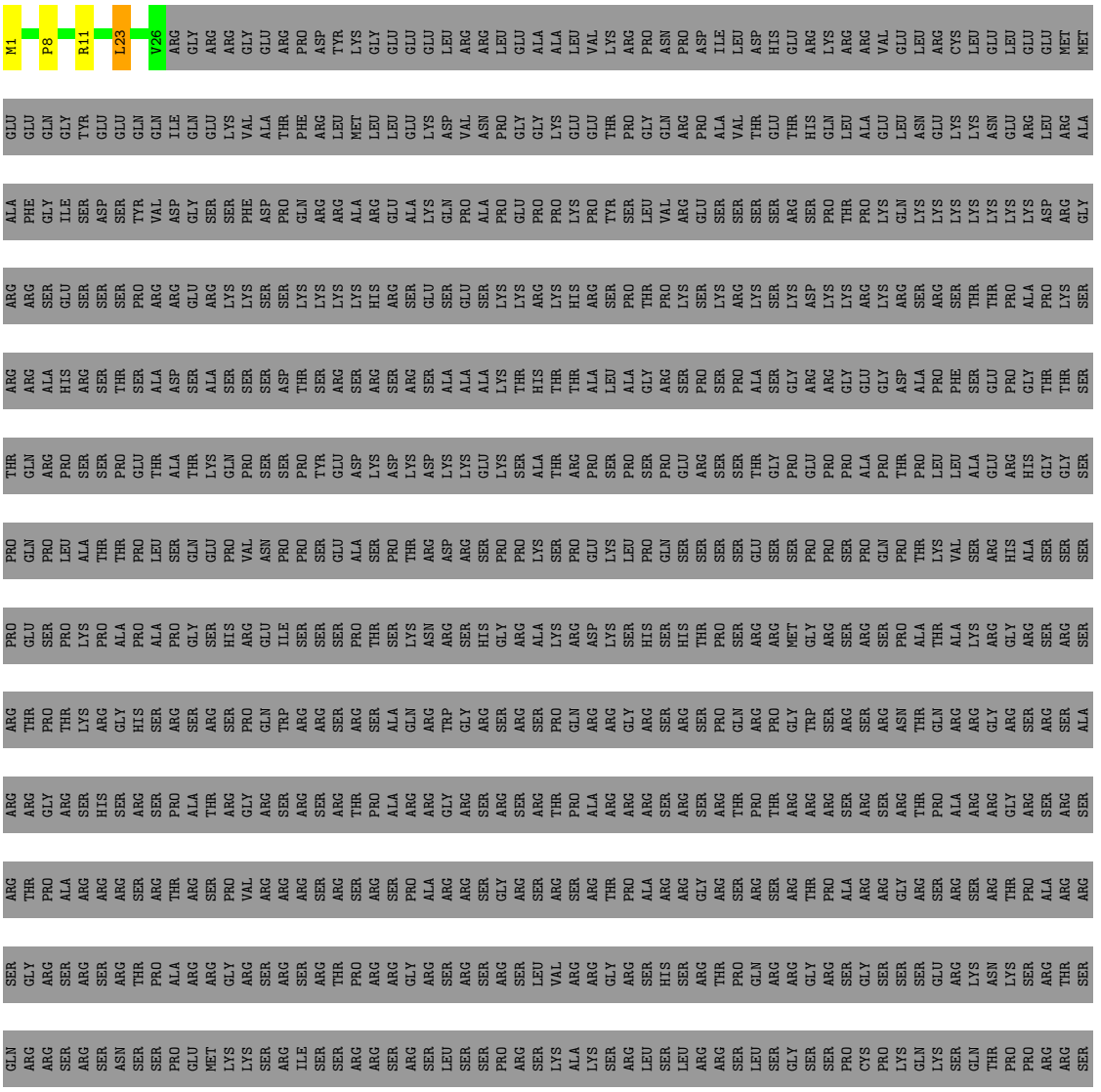
Chain T:

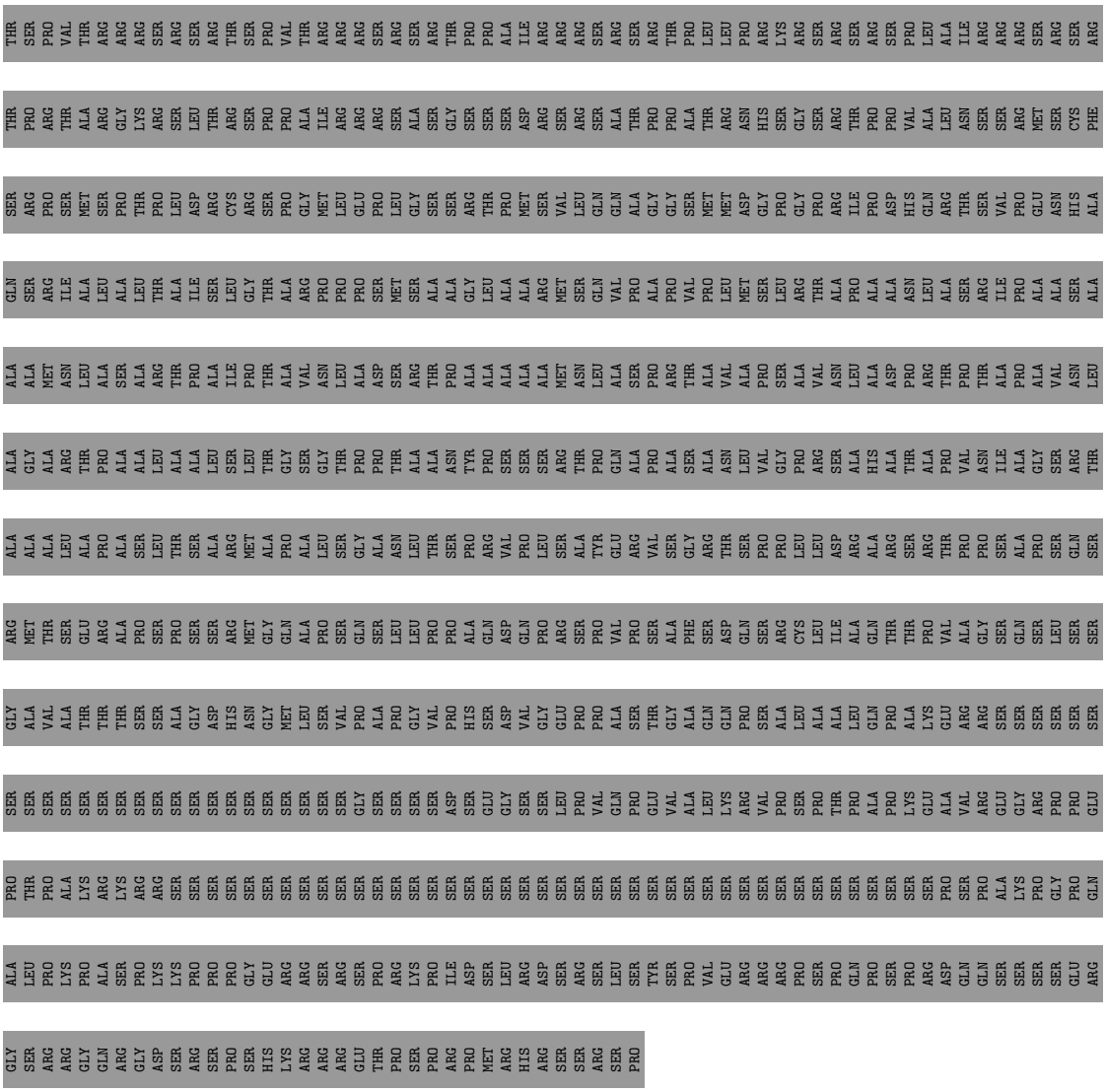




• Molecule 21: Serine/arginine repetitive matrix protein 2

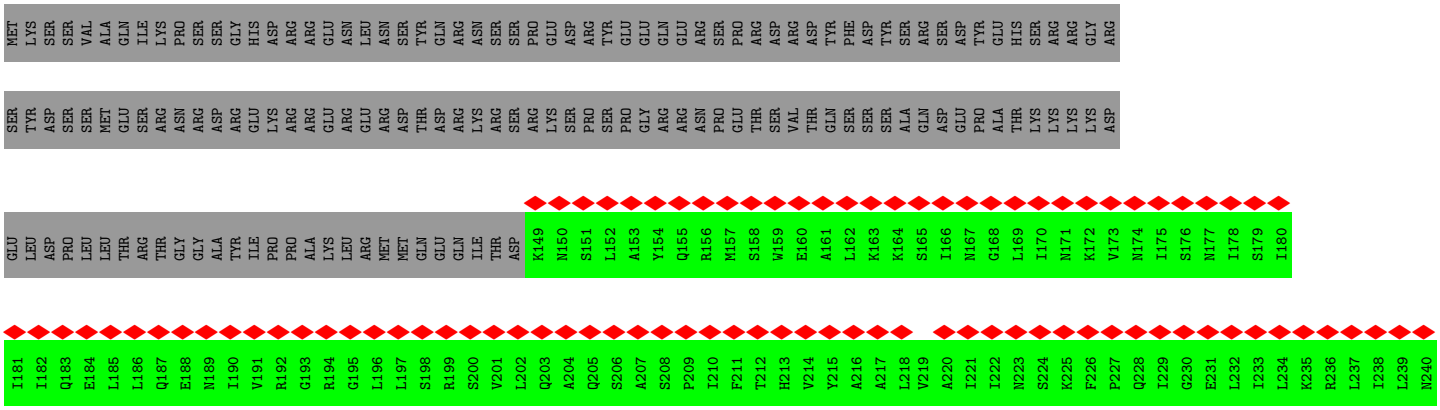
Chain U: 99%

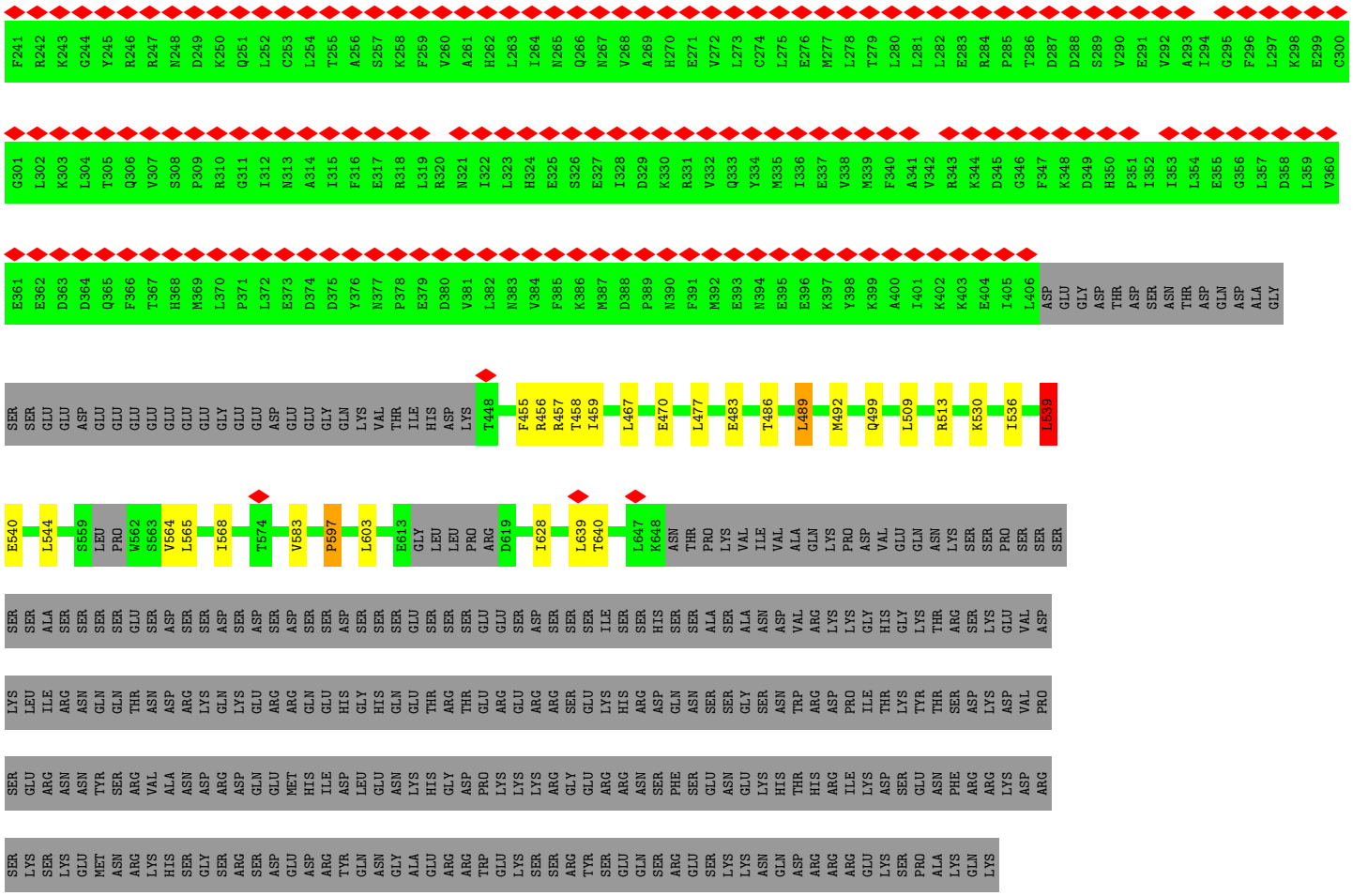




• Molecule 22: Pre-mRNA-splicing factor CWC22 homolog

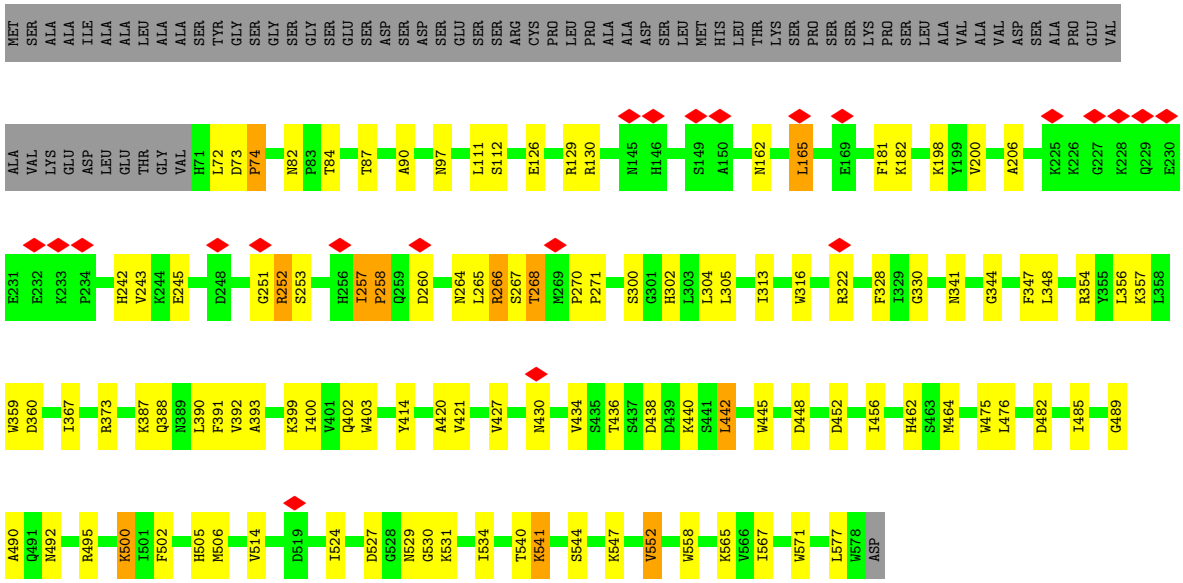
Chain V:





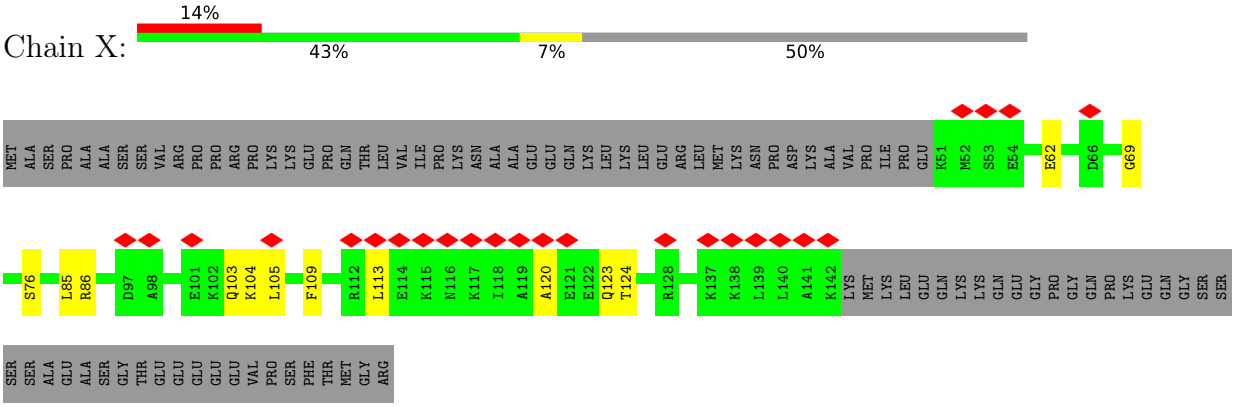
• Molecule 23: Pre-mRNA-processing factor 17

Chain W:



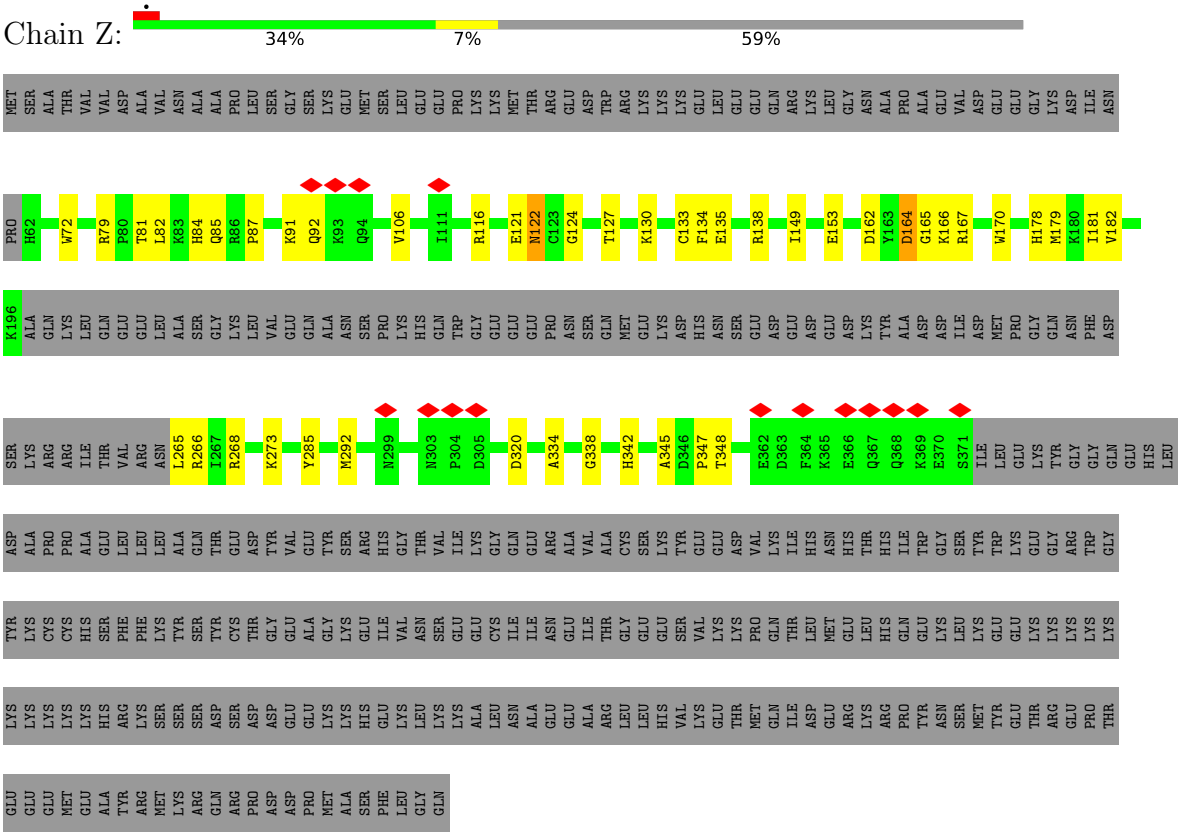
• Molecule 24: PRKR-interacting protein 1

Chain X:



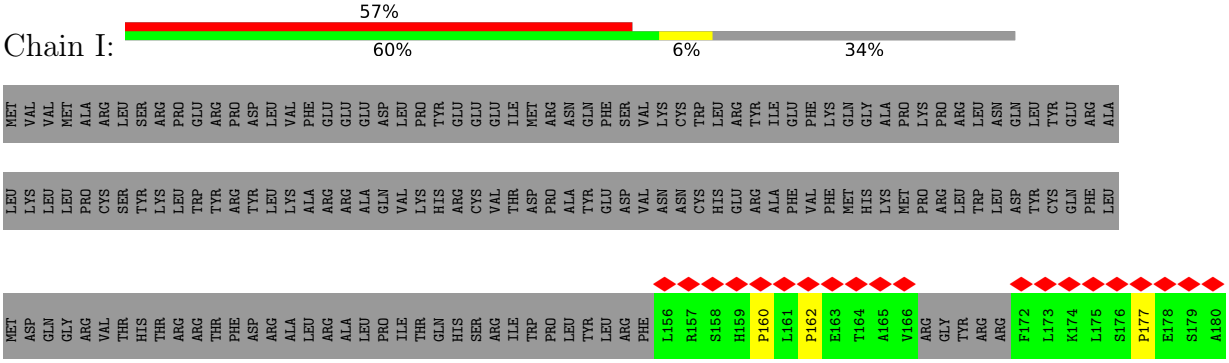
• Molecule 25: Pre-mRNA-splicing factor SLU7

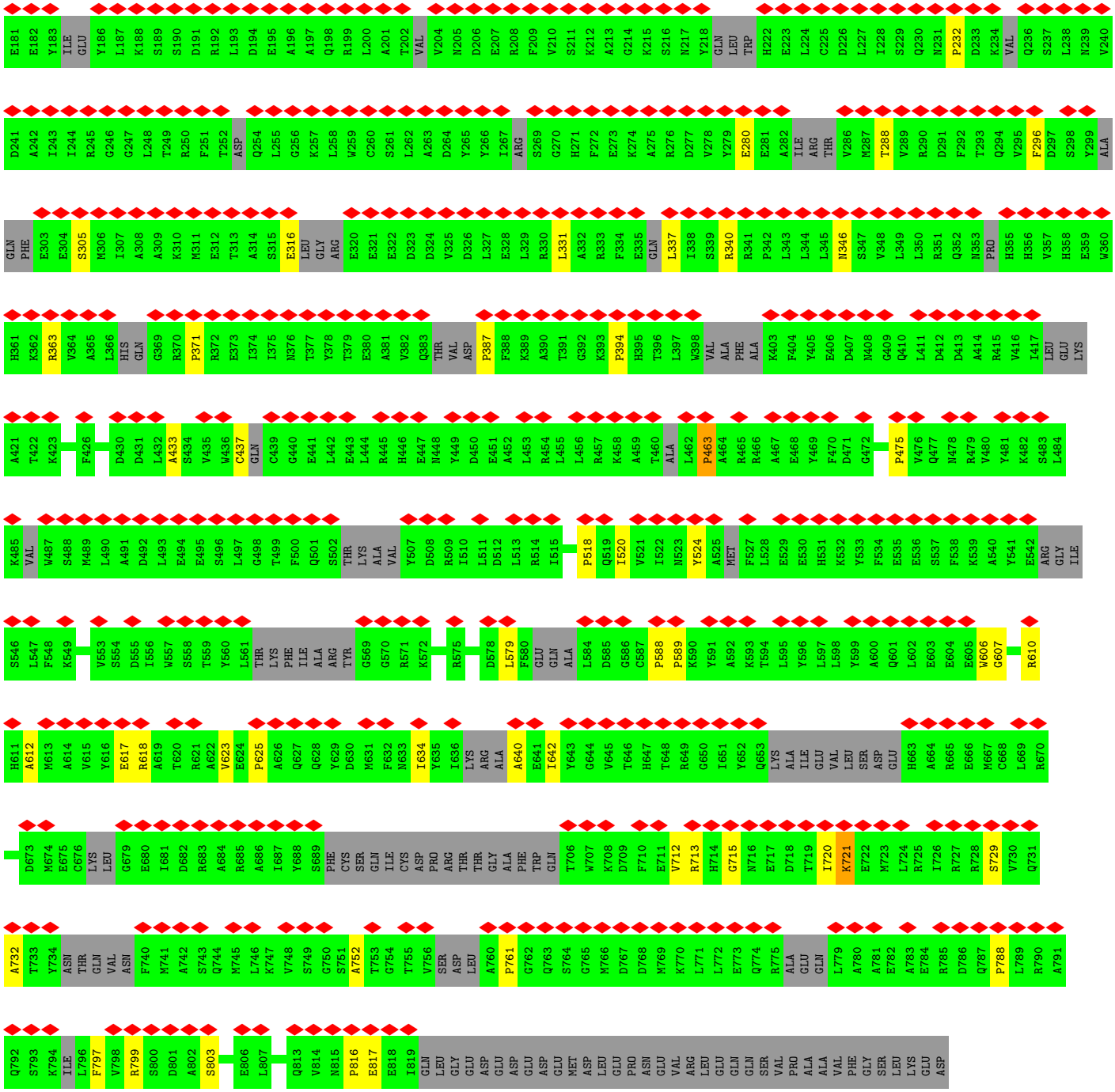
Chain Z:



• Molecule 26: Pre-mRNA-splicing factor SYF1

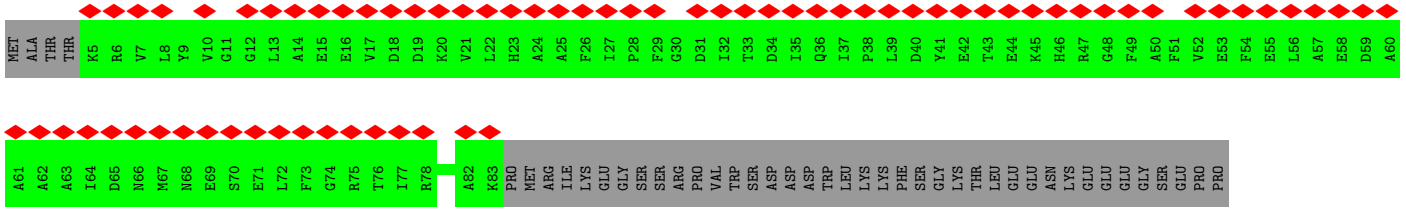
Chain I:

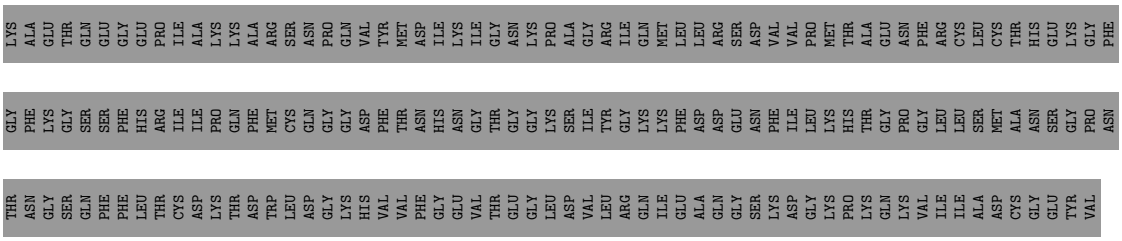




• Molecule 27: Peptidyl-prolyl cis-trans isomerase E

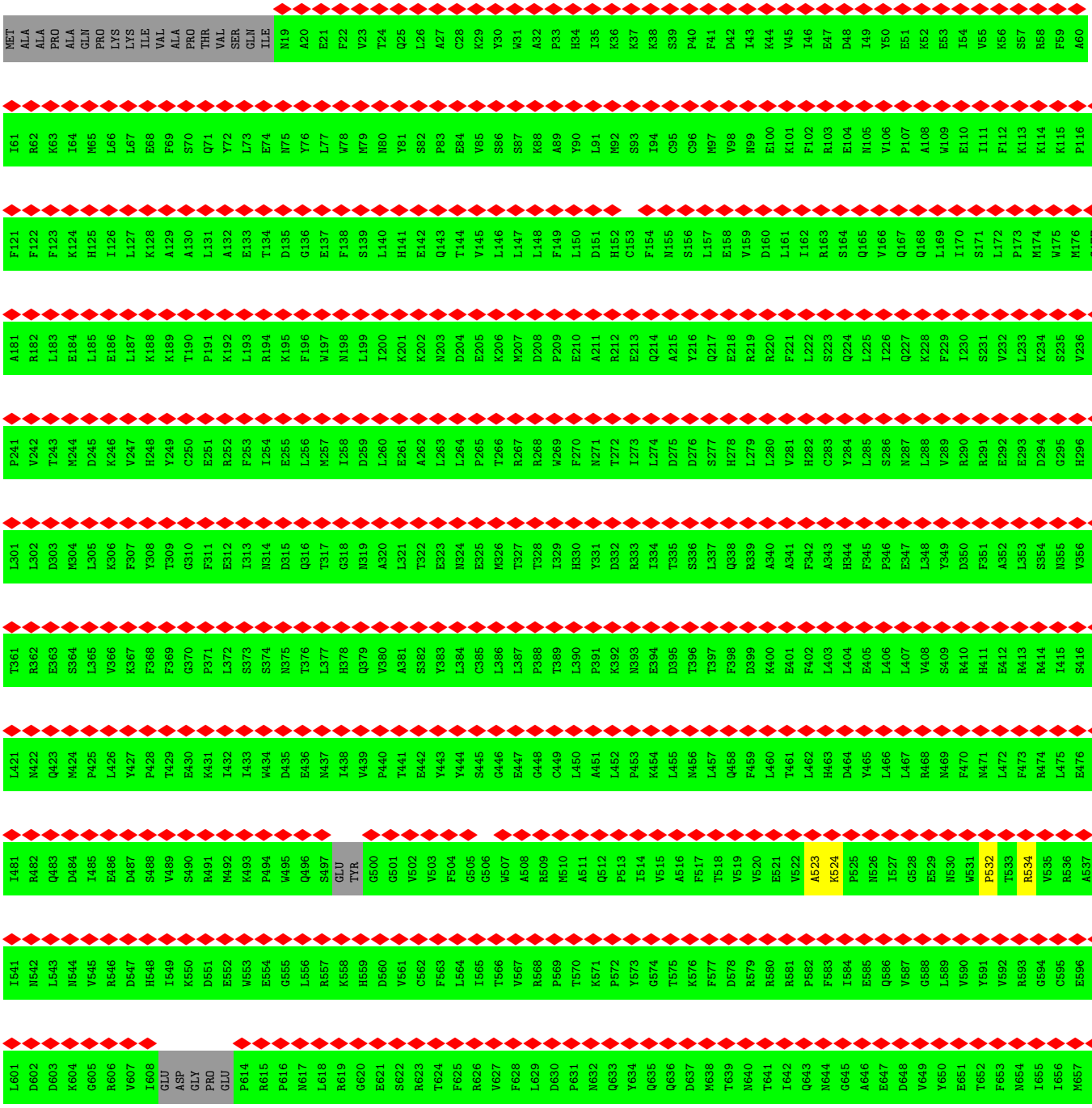
Chain y:

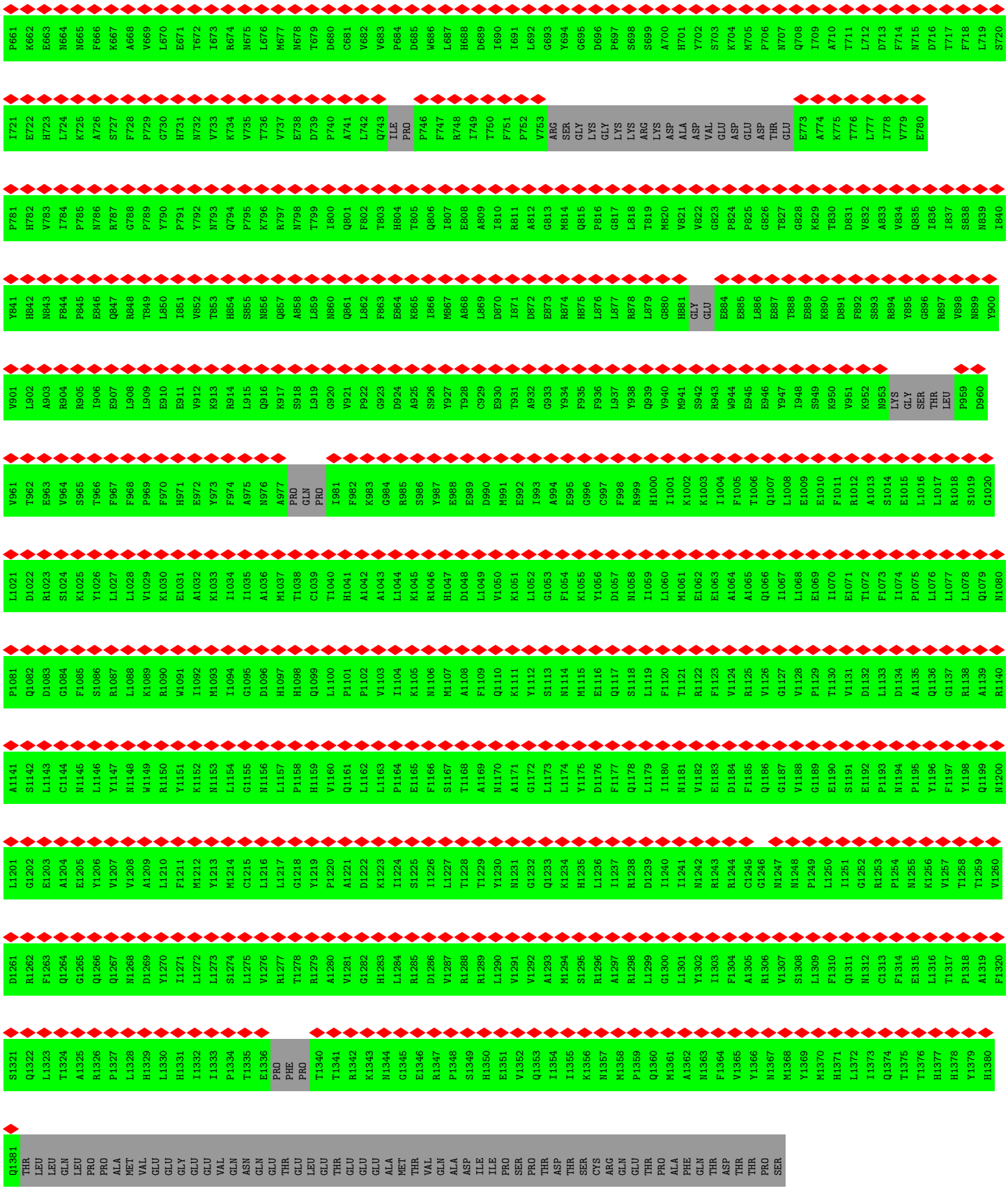




• Molecule 28: RNA helicase aquarius

Chain Q:

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I721 E722 H723 L724 K725 A726 S727 F728 P729 G730 H731 N732 V733 K734 V735 T736 V737 E738 D739 P740 A741 L742 Q743 ILE PRO P746 F747 R748 I749 T750 F751 P752 V753 ARG SER GLY LYS GLY LYS LYS ARG LYS ASP ALA ASP VAL GLU ASP GLU ASP THR GLU E773 A774 K775 T776 L777 I778 V779 E780
P781 H782 V783 I784 P785 N786 R787 G788 P789 Y790 P791 Y792 N793 Q794 P795 K796 R797 N798 T799 I800 Q801 F802 T803 H804 T805 Q806 I807 E808 A809 I810 R811 A812 G813 M814 Q815 P816 G817 L818 T819 M820 V821 V822 G823 P824 P825 G826 T827 G828 K829 T830 D831 V832 A833 V834 Q835 I836 I837 S838 N839 I840
Y841 H842 N843 F844 P845 E846 Q847 R848 T849 L850 I851 V852 T853 H854 S855 N856 Q857 A858 L859 N860 Q861 L862 F863 E864 K865 I866 M867 A868 L869 D870 I871 D872 E873 R874 H875 L876 L877 R878 L879 G880 H881 GLY GLU E884 E885 L886 E887 T888 E889 K890 D891 F892 S893 R894 Y895 G896 R897 V898 N899 Y900
V901 L902 A903 R904 R905 I906 E907 L908 L909 E910 E911 V912 K913 R914 L915 Q916 K917 S918 L919 G920 V921 P922 G923 D924 A925 S926 Y927 T928 C929 E930 T931 A932 G933 Y934 F935 F936 L937 Y938 Q939 V940 M941 S942 R943 W944 E945 E946 Y947 I948 S949 K950 V951 K952 N953 LYS GLY SER THR LEU P959 D960
V961 T962 E963 V964 S965 T966 F967 F968 P969 F970 H971 E972 Y973 F974 A975 N976 A977 PRO GLN PRO I981 P982 K983 G984 R985 S986 Y987 E988 E989 D990 M991 E992 I993 A994 E995 G996 C997 F998 R999 H1000 I1001 K1002 K1003 I1004 F1005 T1006 Q1007 L1008 E1009 E1010 F1011 R1012 A1013 S1014 E1015 L1016 L1017 R1018 S1019 G1020
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A1141 S1142 L1143 C1144 N1145 L1146 Y1147 N1148 W1149 R1150 Y1151 K1152 N1153 L1154 G1155 N1156 L1157 P1158 H1159 V1160 Q1161 L1162 L1163 P1164 E1165 F1166 S1167 T1168 A1169 N1170 A1171 G1172 L1173 L1174 Y1175 D1176 F1177 Q1178 L1179 I1180 N1181 V1182 E1183 D1184 F1185 Q1186 G1187 V1188 G1189 E1190 S1191 E1192 P1193 N1194 P1195 Y1196 F1197 Y1198 Q1199 N1200
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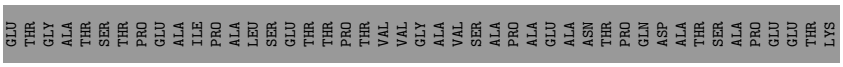
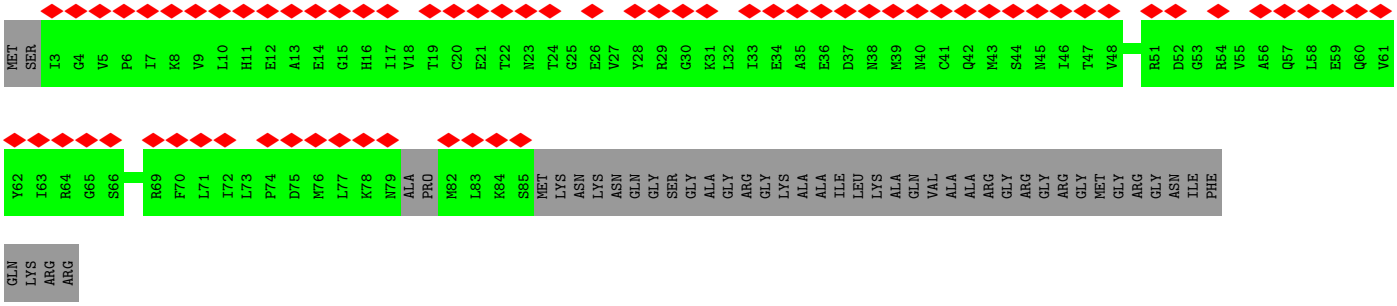


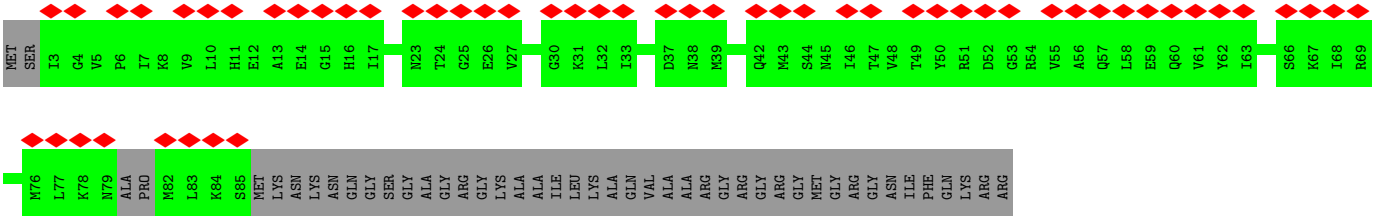
• Molecule 29: Small nuclear ribonucleoprotein Sm D3

Chain h:



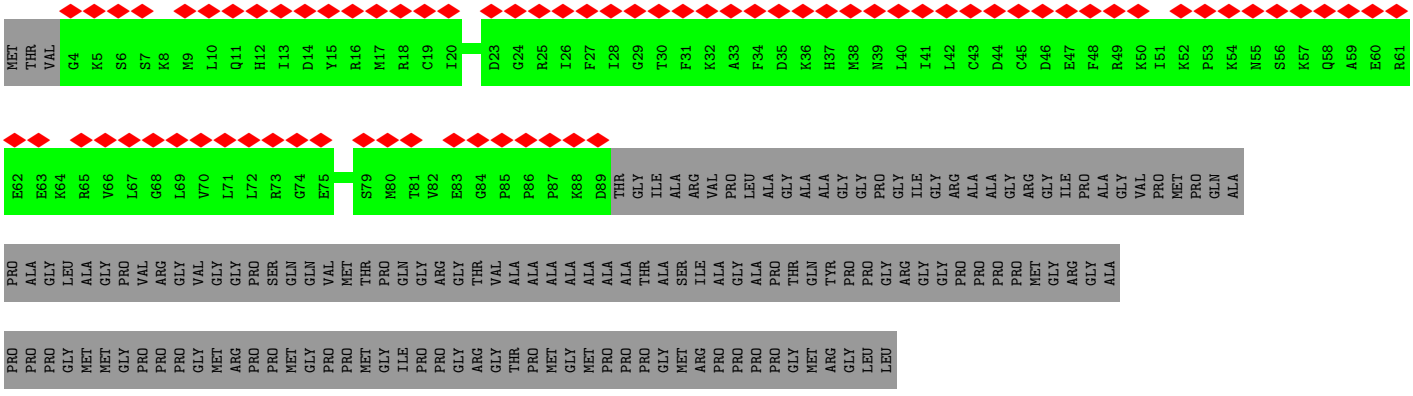
• Molecule 29: Small nuclear ribonucleoprotein Sm D3

Chain a:



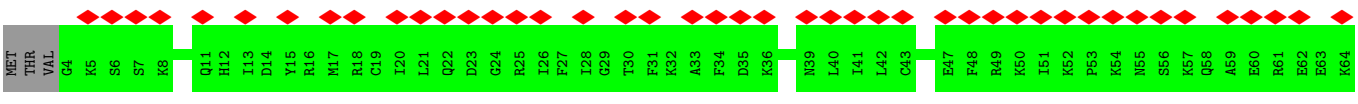
• Molecule 30: Small nuclear ribonucleoprotein-associated protein

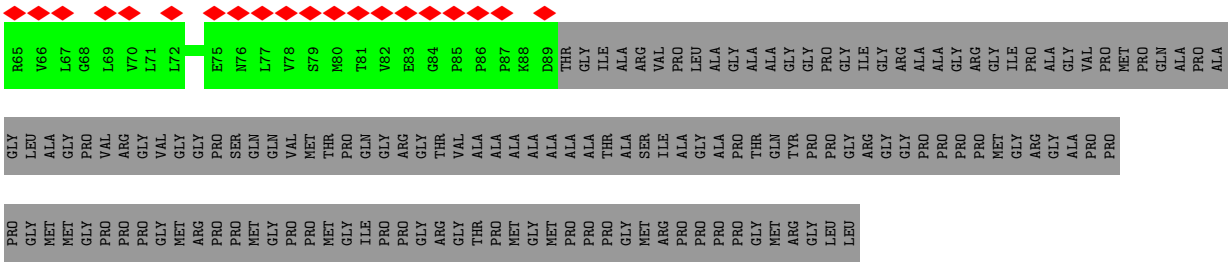
Chain i:



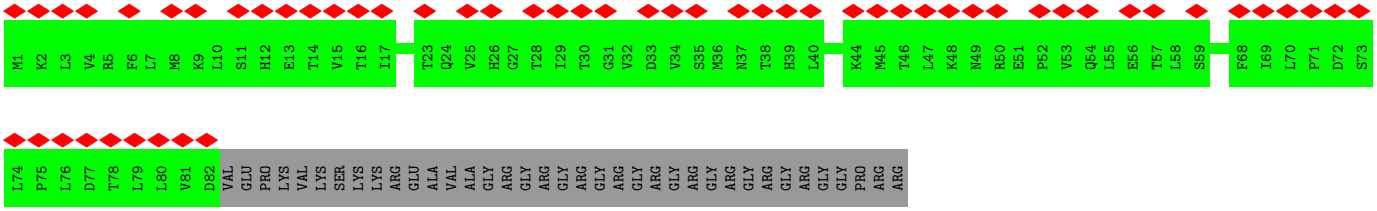
• Molecule 30: Small nuclear ribonucleoprotein-associated protein

Chain b:

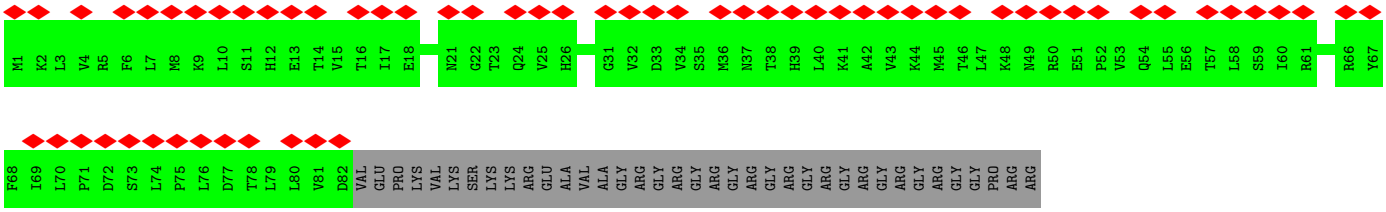




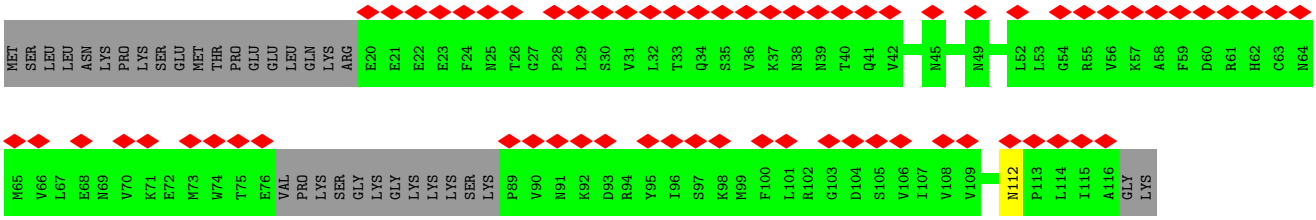
• Molecule 31: Small nuclear ribonucleoprotein Sm D1



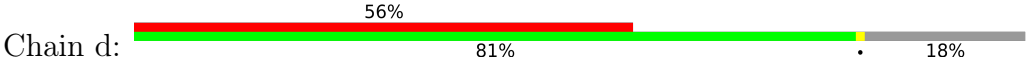
• Molecule 31: Small nuclear ribonucleoprotein Sm D1

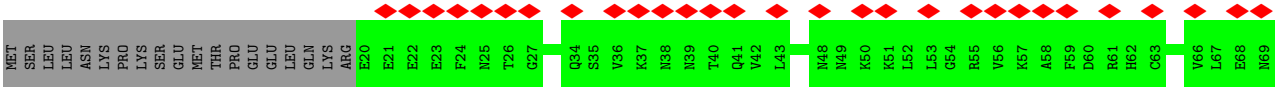


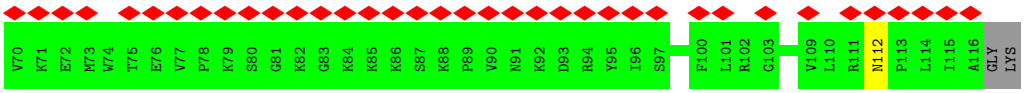
• Molecule 32: Small nuclear ribonucleoprotein Sm D2



• Molecule 32: Small nuclear ribonucleoprotein Sm D2

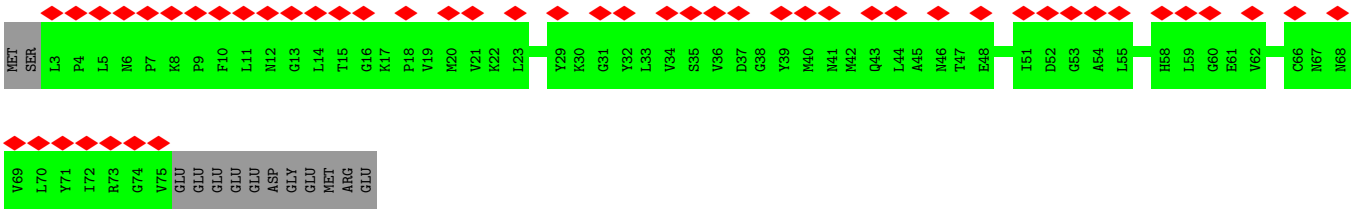






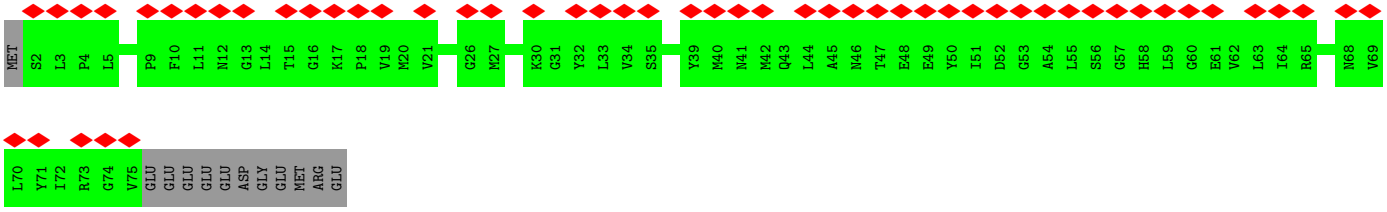
• Molecule 33: Small nuclear ribonucleoprotein F

Chain m:



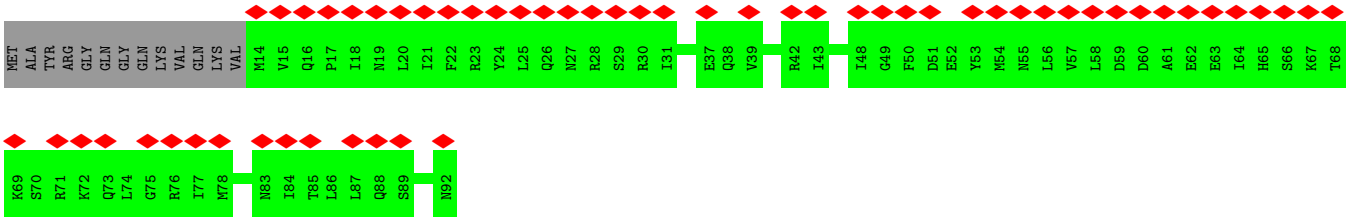
• Molecule 33: Small nuclear ribonucleoprotein F

Chain f:



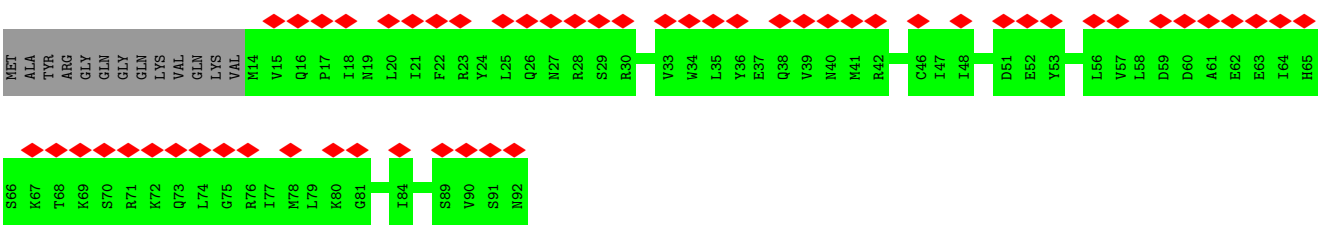
• Molecule 34: Small nuclear ribonucleoprotein E

Chain l:



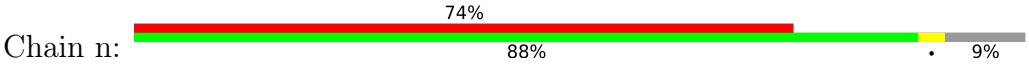
• Molecule 34: Small nuclear ribonucleoprotein E

Chain e:



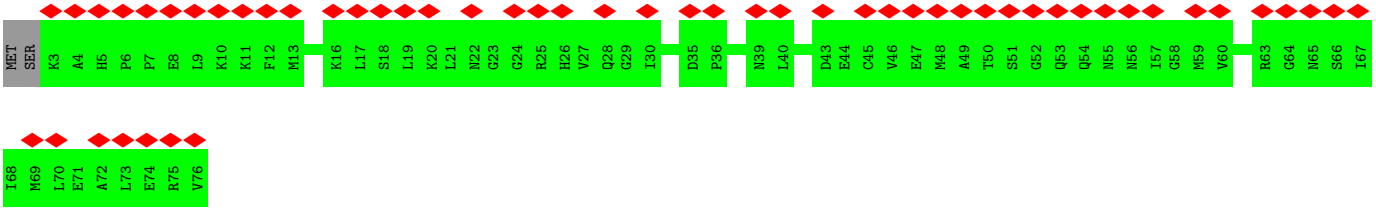
• Molecule 35: Small nuclear ribonucleoprotein G

Chain n:



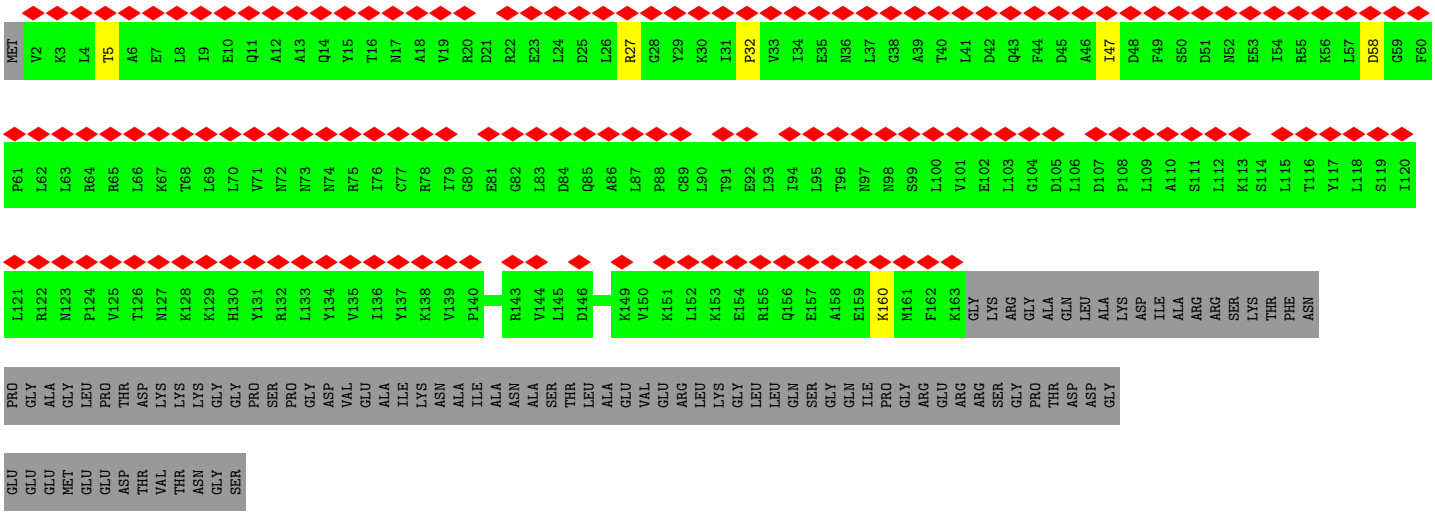
• Molecule 35: Small nuclear ribonucleoprotein G

Chain g:



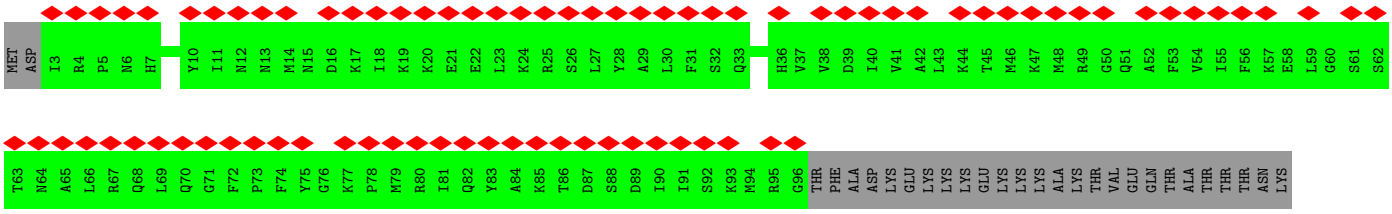
• Molecule 36: U2 small nuclear ribonucleoprotein A'

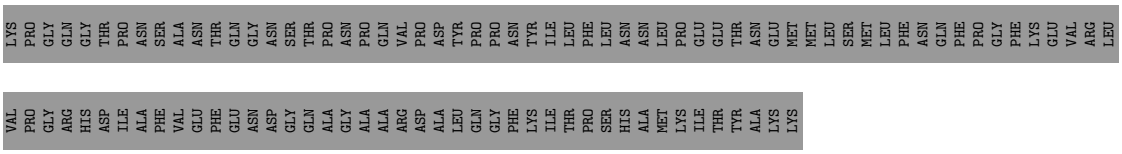
Chain o:



• Molecule 37: U2 small nuclear ribonucleoprotein B"

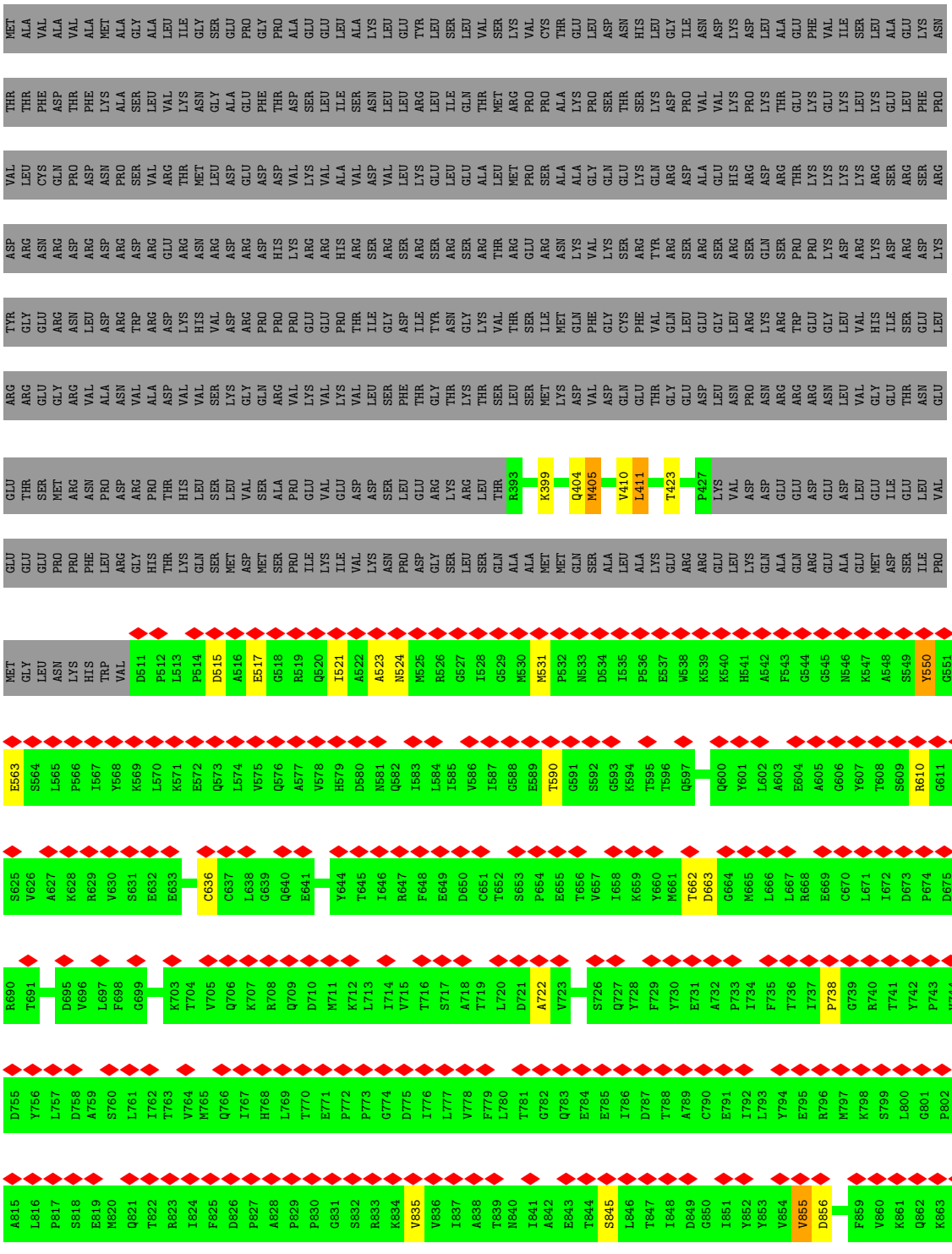
Chain p:

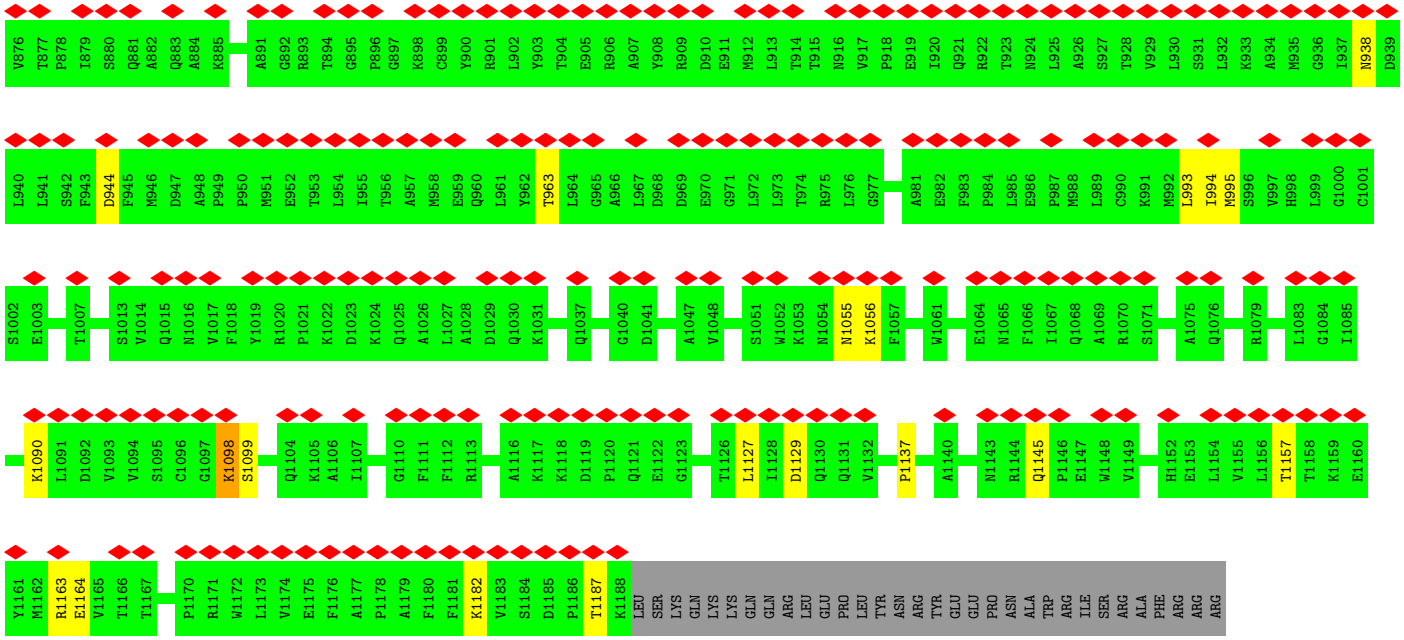




• Molecule 38: ATP-dependent RNA helicase DHX8

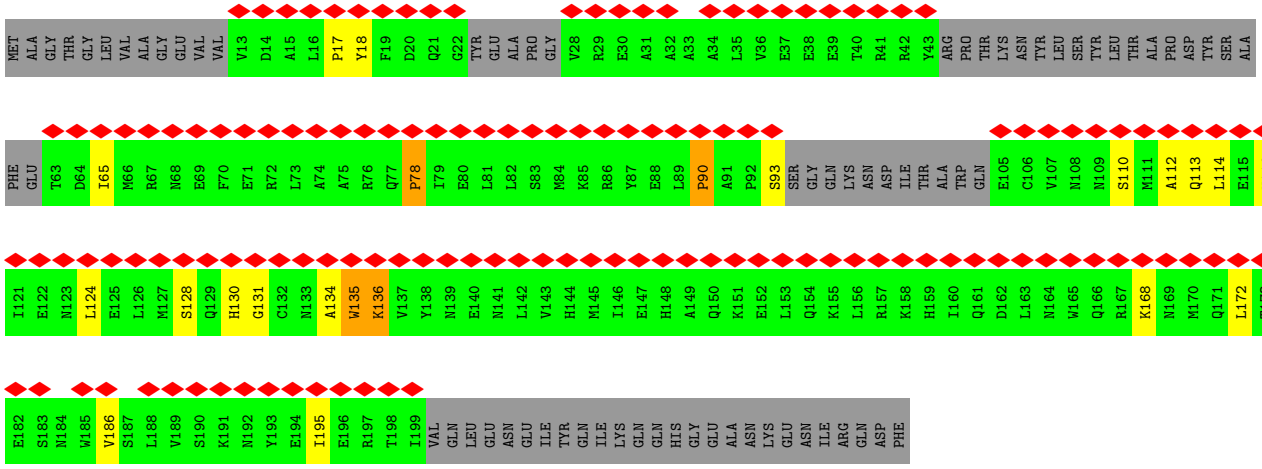
Chain Y:





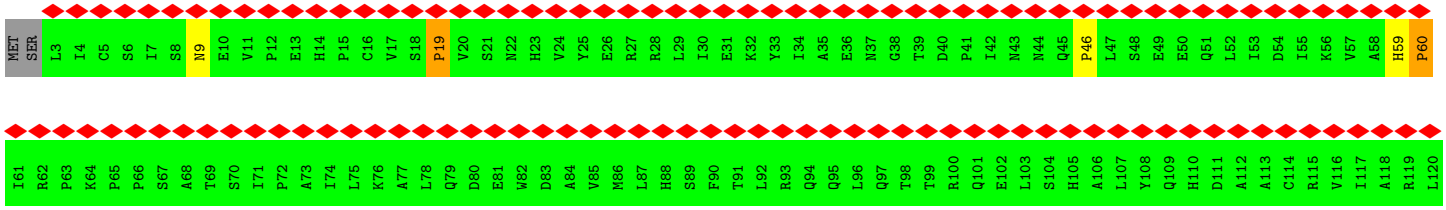
• Molecule 39: Pre-mRNA-splicing factor SPF27

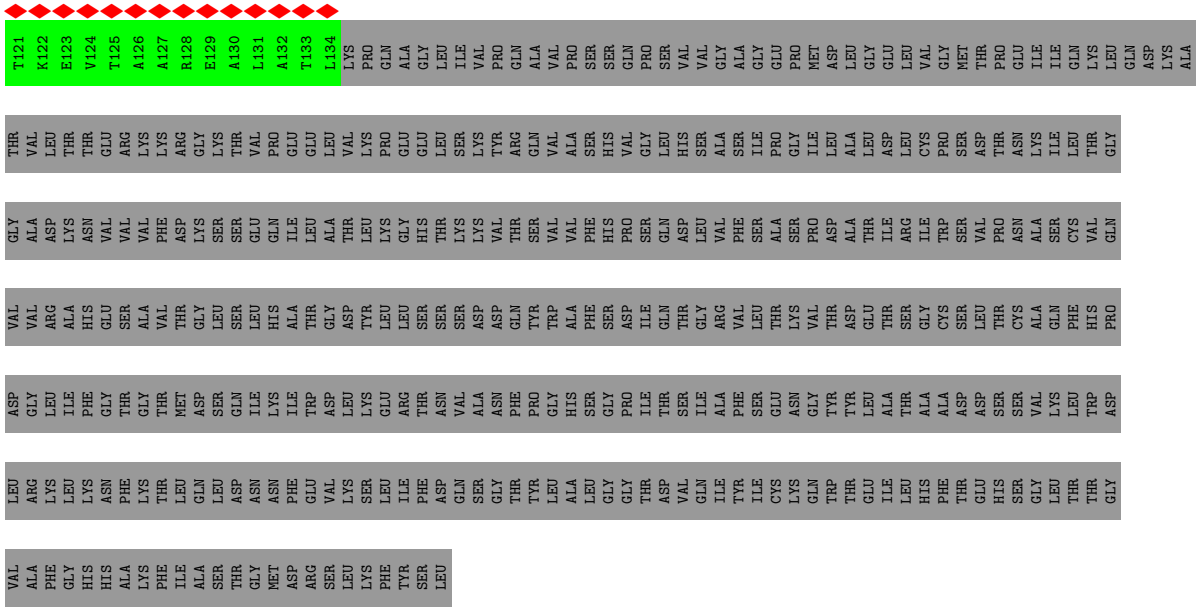
Chain K:



• Molecule 40: Pre-mRNA-processing factor 19

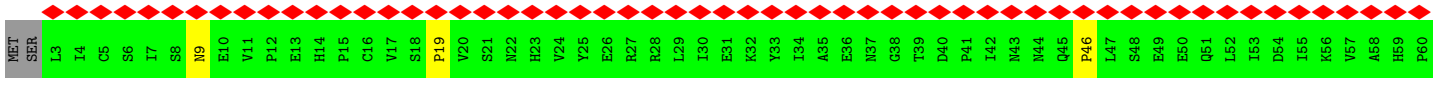
Chain q:

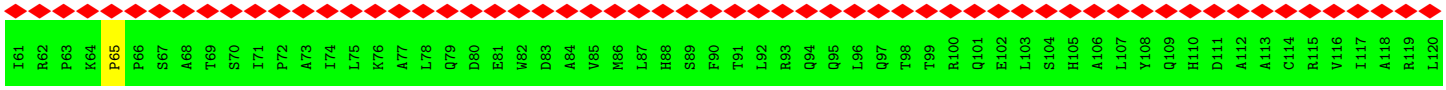


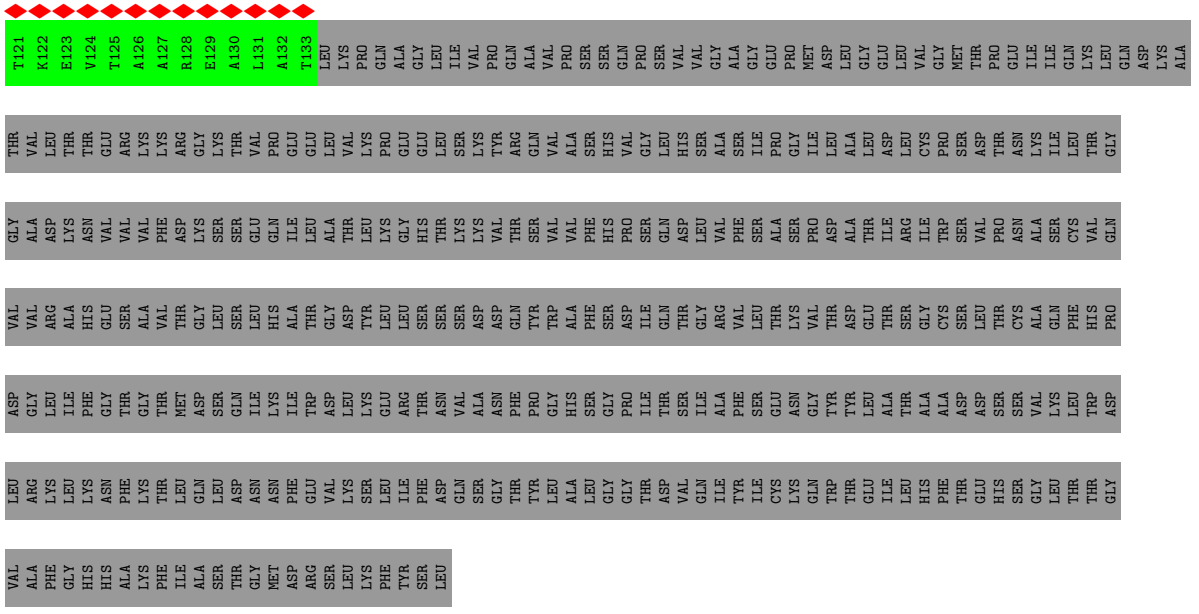


• Molecule 40: Pre-mRNA-processing factor 19

Chain r:







• Molecule 40: Pre-mRNA-processing factor 19

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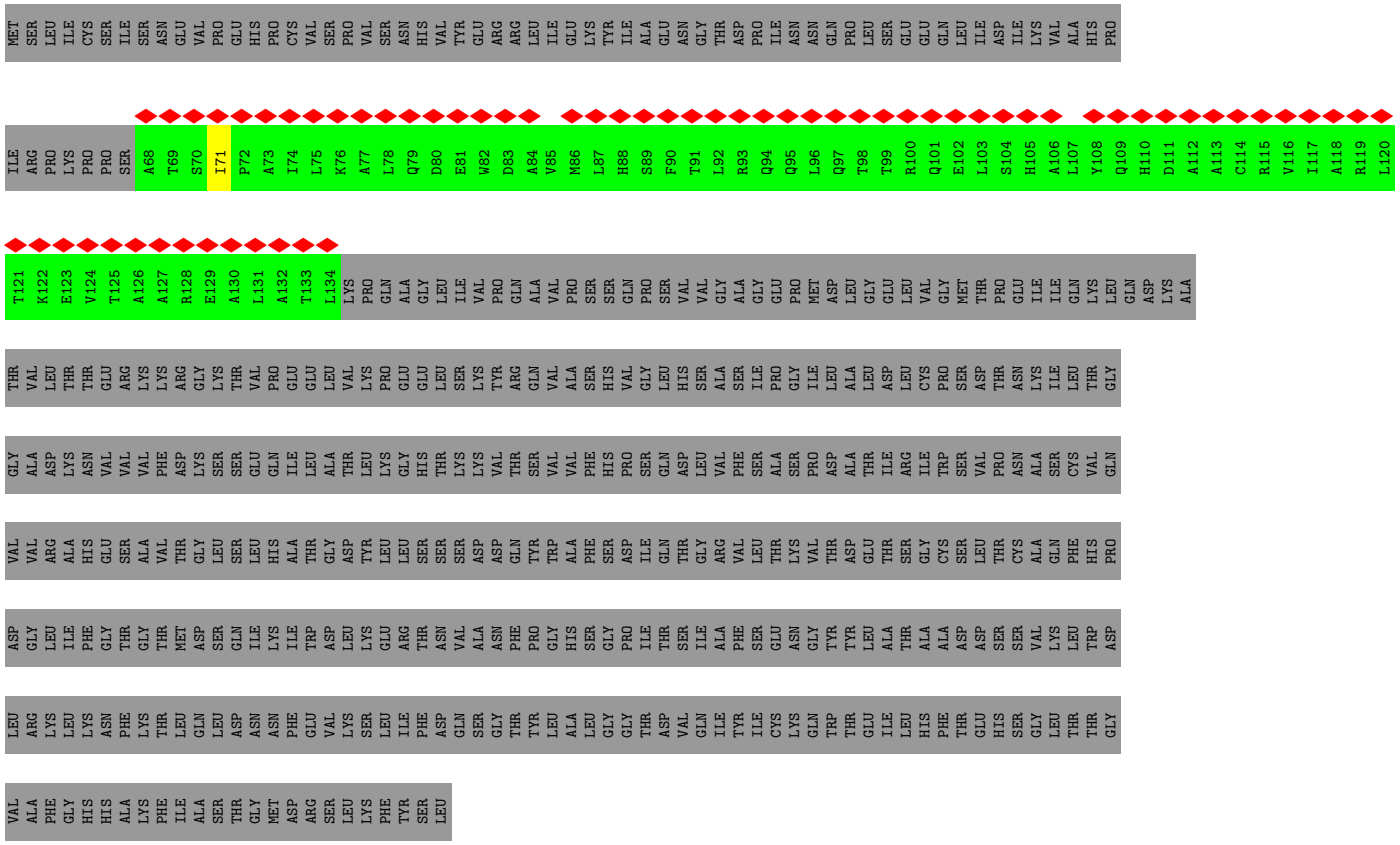
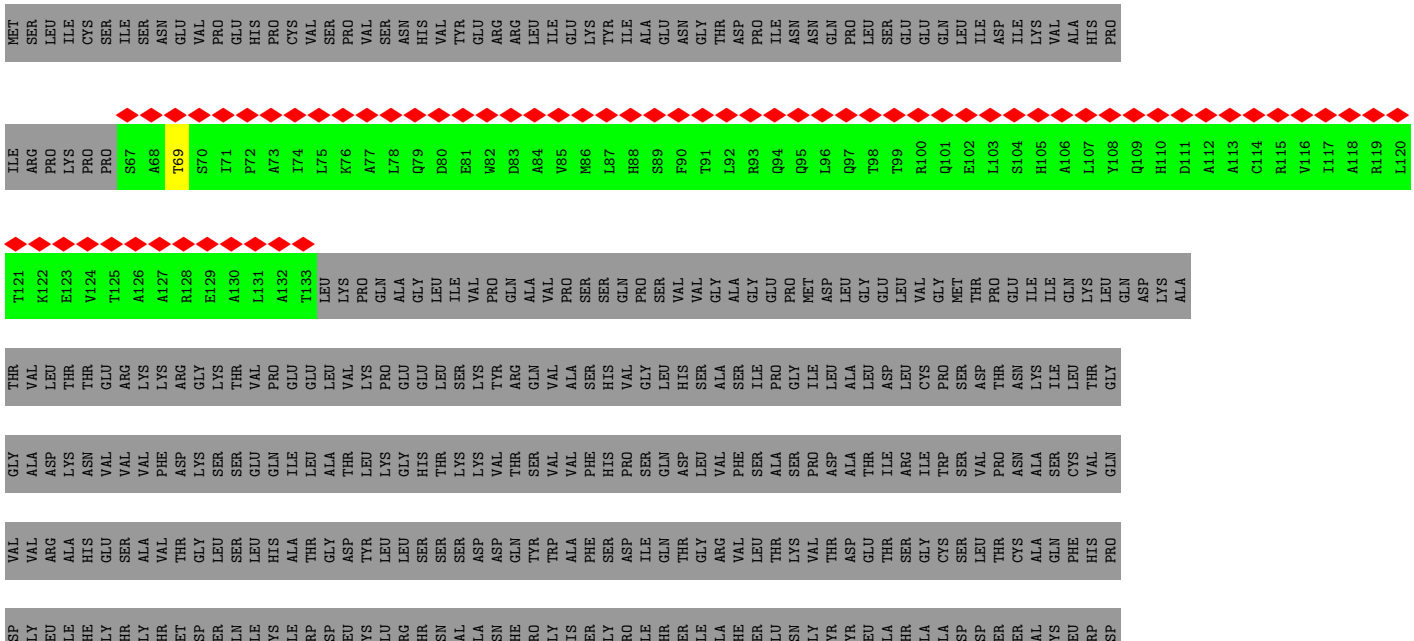
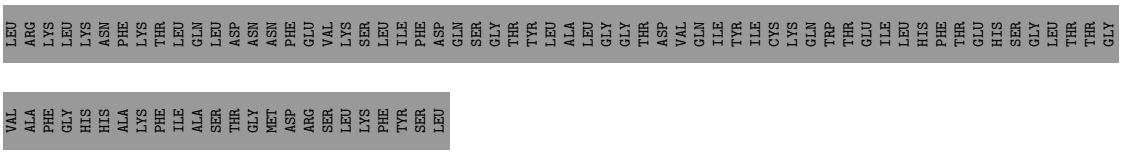


• Molecule 40: Pre-mRNA-processing factor 19

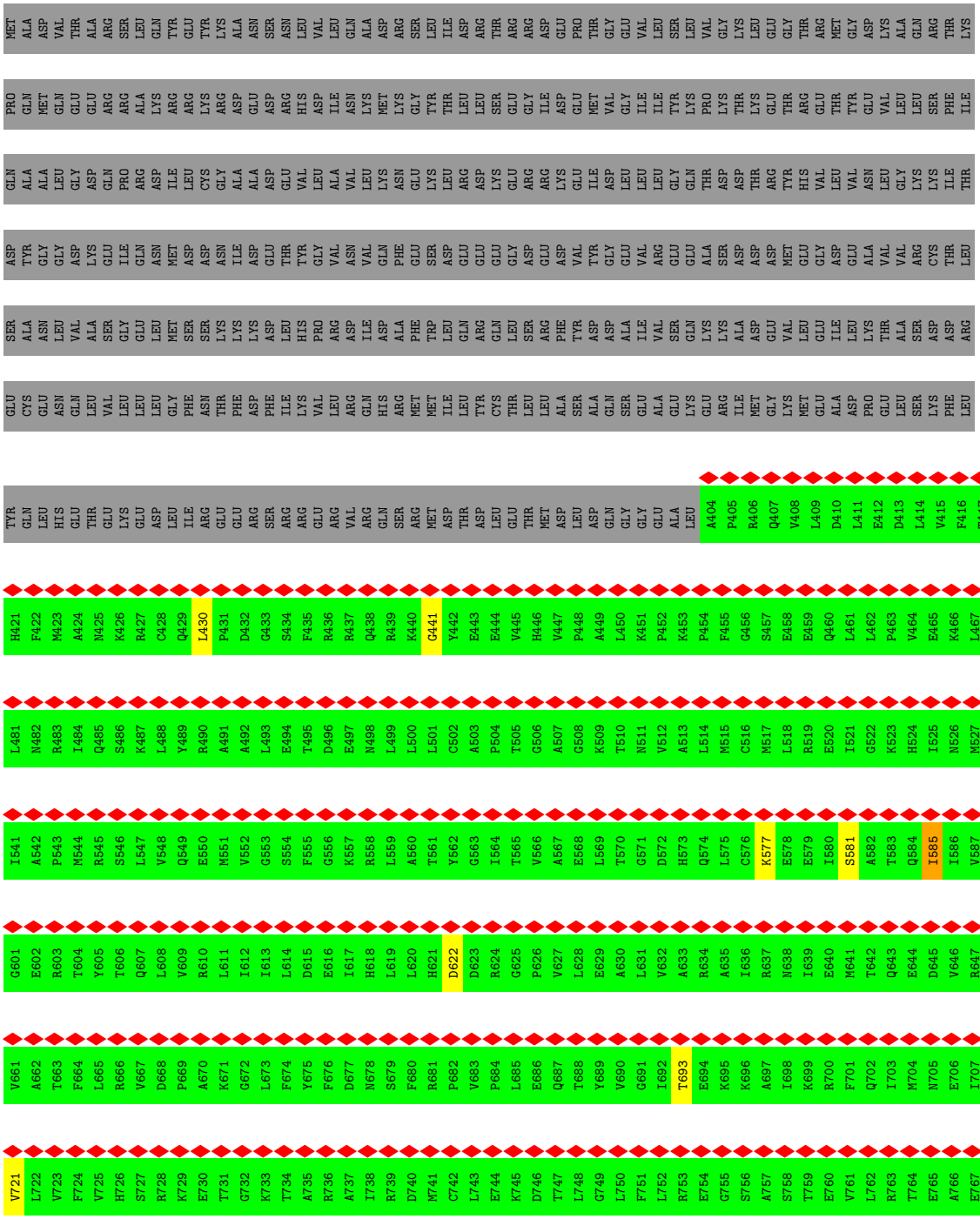
Chain t:





• Molecule 41: U5 small nuclear ribonucleoprotein 200 kDa helicase

Chain D:



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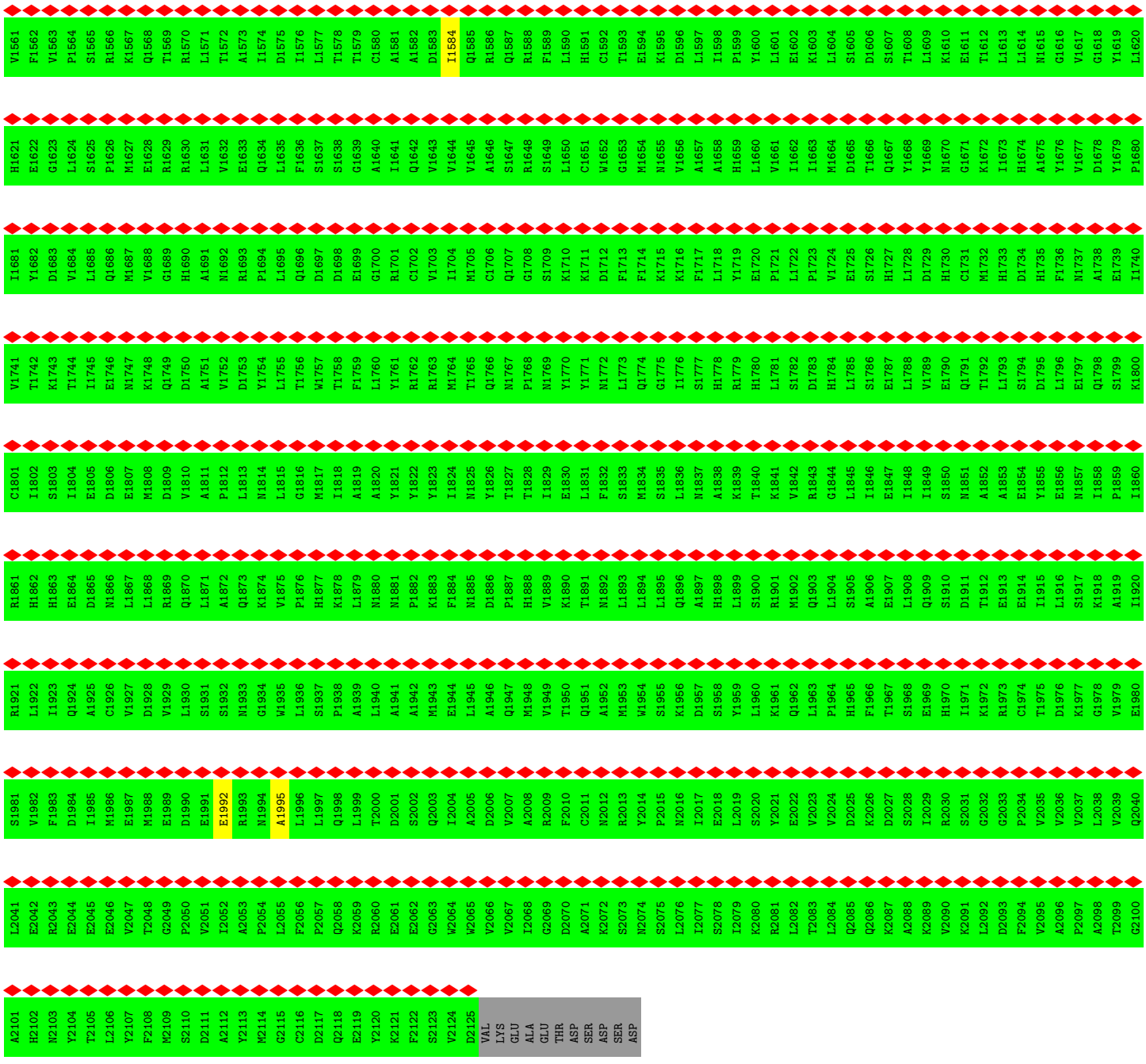
V1561 F1562 V1563 P1564 S1565 R1566 K1567 Q1568 T1569 R1570 L1571 T1572 A1573 I1574 D1575 I1576 L1577 T1578 T1579 C1580 A1581 A1582 D1583 I1584 Q1585 R1586 Q1587 R1588 F1589 L1590 H1591 C1592 T1593 E1594 K1595 D1596 L1597 I1598 P1599 Y1600 L1601 E1602 K1603 L1604 S1605 D1606 S1607 T1608 L1609 K1610 E1611 T1612 L1613 L1614 N1615 G1616 V1617 G1618 Y1619 L1620
H1621 E1622 G1623 L1624 S1625 P1626 M1627 E1628 R1629 R1630 L1631 V1632 E1633 Q1634 L1635 F1636 S1637 S1638 G1639 A1640 I1641 Q1642 V1643 V1644 V1645 A1646 S1647 R1648 S1649 L1650 C1651 W1652 G1653 M1654 N1655 V1656 A1657 A1658 H1659 L1660 V1661 I1662 I1663 M1664 D1665 T1666 Q1667 Y1668 Y1669 N1670 G1671 K1672 I1673 H1674 A1675 Y1676 V1677 D1678 Y1679 P1680
I1681 Y1682 D1683 V1684 L1685 Q1686 M1687 V1688 G1689 H1690 A1691 N1692 R1693 P1694 L1695 Q1696 D1697 D1698 E1699 G1700 R1701 C1702 V1703 I1704 M1705 C1706 Q1707 G1708 S1709 K1710 K1711 D1712 F1713 F1714 K1715 K1716 F1717 L1718 Y1719 E1720 P1721 L1722 P1723 V1724 E1725 S1726 H1727 L1728 D1729 H1730 C1731 M1732 H1733 D1734 H1735 F1736 N1737 A1738 E1739 I1740
V1741 T1742 K1743 T1744 I1745 E1746 N1747 K1748 Q1749 D1750 A1751 V1752 D1753 Y1754 L1755 T1756 W1757 T1758 F1759 L1760 Y1761 R1762 R1763 M1764 T1765 Q1766 N1767 P1768 N1769 Y1770 Y1771 N1772 L1773 Q1774 G1775 I1776 S1777 H1778 R1779 H1780 L1781 S1782 D1783 H1784 L1785 S1786 E1787 L1788 V1789 E1790 Q1791 T1792 L1793 S1794 D1795 L1796 E1797 Q1798 S1799 K1800
C1801 I1802 S1803 I1804 E1805 D1806 E1807 M1808 D1809 V1810 A1811 P1812 L1813 N1814 L1815 G1816 M1817 I1818 A1819 A1820 Y1821 Y1822 Y1823 I1824 N1825 Y1826 T1827 T1828 I1829 E1830 L1831 F1832 S1833 M1834 S1835 L1836 N1837 A1838 K1839 T1840 K1841 V1842 R1843 G1844 L1845 I1846 E1847 I1848 I1849 S1850 N1851 A1852 A1853 E1854 Y1855 E1856 N1857 I1858 P1859 I1860
R1861 H1862 H1863 E1864 D1865 N1866 L1867 L1868 R1869 Q1870 L1871 A1872 Q1873 K1874 V1875 P1876 H1877 K1878 L1879 N1880 N1881 P1882 K1883 F1884 N1885 D1886 P1887 H1888 V1889 K1890 T1691 N1892 L1893 L1894 L1895 Q1896 A1897 H1698 L1899 S1900 T1901 M1902 Q1903 L1904 S1905 A1906 E1907 L1908 Q1909 S1910 D1911 T1912 E1913 E1914 I1915 L1916 S1917 K1918 A1919 I1920
R1921 L1922 I1923 Q1924 A1925 C1926 V1927 D1928 V1929 L1930 S1931 S1932 N1933 G1934 W1935 L1936 S1937 P1938 A1939 L1940 A1941 A1942 M1943 E1944 L1945 A1946 Q1947 M1948 V1949 T1950 Q1951 A1952 M1953 W1954 S1955 K1956 D1957 S1958 Y1959 L1960 K1961 Q1962 L1963 P1964 H1965 F1966 T1967 S1968 E1969 H1970 I1971 K1972 R1973 C1974 T1975 D1976 K1977 G1978 V1979 E1980
S1981 V1982 F1983 D1984 I1985 M1986 E1987 M1988 E1989 D1990 E1991 E1992 R1993 N1994 A1995 L1996 L1997 Q1998 L1999 T2000 D2001 S2002 Q2003 I2004 A2005 D2006 V2007 A2008 R2009 F2010 C2011 N2012 R2013 Y2014 P2015 N2016 I2017 E2018 L2019 S2020 Y2021 E2022 V2023 V2024 D2025 K2026 D2027 S2028 I2029 R2030 S2031 G2032 G2033 P2034 V2035 V2036 V2037 L2038 V2039 Q2040
L2041 E2042 R2043 E2044 E2045 E2046 V2047 T2048 G2049 P2050 V2051 I2052 A2053 P2054 L2055 F2056 P2057 Q2058 K2059 R2060 E2061 E2062 G2063 W2064 W2065 V2066 V2067 I2068 G2069 D2070 A2071 K2072 S2073 N2074 S2075 L2076 I2077 S2078 I2079 K2080 R2081 L2082 T2083 L2084 Q2085 Q2086 K2087 A2088 K2089 V2090 K2091 L2092 D2093 F2094 V2095 A2096 P2097 A2098 T2099 G2100
A2101 H2102 N2103 Y2104 T2105 L2106 Y2107 F2108 M2109 S2110 D2111 A2112 Y2113 M2114 G2115 C2116 D2117 Q2118 E2119 Y2120 K2121 F2122 S2123 V2124 D2125 VAL LYS GLU ALA GLU THR ASP SER ASP SER ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	143320	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.552	Depositor
Minimum map value	-0.288	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	535.2, 535.2, 535.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.338, 1.338, 1.338	Depositor

5 Model quality

5.1 Standard geometry

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

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	v	0.30	0/710	0.65	0/987
2	w	0.30	0/444	0.78	2/614 (0.3%)
3	u	0.32	0/1906	0.69	0/2653
4	x	0.34	0/123	0.70	0/170
5	A	0.53	0/18287	0.65	7/24842 (0.0%)
6	B	0.77	1/2274 (0.0%)	1.17	25/3535 (0.7%)
7	C	2.14	9/7225 (0.1%)	0.78	12/9818 (0.1%)
8	E	0.34	0/2420	0.64	0/3281
9	F	0.95	0/2323	1.23	19/3619 (0.5%)
10	G	0.57	0/1716	1.23	21/2656 (0.8%)
11	H	0.95	24/3305 (0.7%)	1.55	96/5130 (1.9%)
12	J	0.46	0/3870	0.61	13/5252 (0.2%)
13	L	0.41	0/3091	0.59	7/4178 (0.2%)
14	M	0.41	0/1119	0.63	1/1497 (0.1%)
15	N	1.19	6/1210 (0.5%)	0.87	2/1622 (0.1%)
16	O	0.47	0/2344	0.62	1/3163 (0.0%)
17	P	0.46	0/943	0.61	0/1255
18	R	0.47	0/2091	0.66	1/2809 (0.0%)
19	S	0.35	0/1268	0.59	1/1714 (0.1%)
20	T	0.65	1/2526 (0.0%)	0.82	3/3443 (0.1%)
21	U	0.34	0/196	0.63	0/265
22	V	0.31	0/2784	0.54	3/3791 (0.1%)
23	W	0.40	0/4230	0.69	3/5713 (0.1%)
24	X	0.32	0/714	0.53	2/959 (0.2%)
25	Z	0.37	0/2049	0.61	1/2757 (0.0%)
26	I	0.38	0/2749	0.56	16/3773 (0.4%)
27	y	0.25	0/389	0.62	0/540
28	Q	0.22	0/6565	0.42	0/9143
29	a	0.48	0/397	0.62	0/549
29	h	0.47	0/396	0.61	0/547
30	b	0.51	0/423	0.72	0/587
30	i	0.50	0/423	0.73	0/587

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	c	0.57	0/405	0.73	0/563
31	j	0.57	0/405	0.73	0/563
32	d	0.68	0/479	0.85	0/666
32	k	0.70	0/420	0.85	0/583
33	f	0.75	0/360	0.81	0/497
33	m	0.76	0/355	0.81	0/490
34	e	0.65	0/390	0.80	0/542
34	l	0.62	0/390	0.80	0/542
35	g	0.54	0/362	0.71	0/501
35	n	0.50	0/337	0.70	0/465
36	o	0.64	0/803	1.49	4/1119 (0.4%)
37	p	0.61	0/463	1.25	0/643
38	Y	0.46	0/2917	0.92	0/3670
39	K	0.40	1/753 (0.1%)	0.55	3/1046 (0.3%)
40	q	0.35	0/658	0.58	3/919 (0.3%)
40	r	0.33	0/653	0.56	2/912 (0.2%)
40	s	0.27	0/334	0.37	0/466
40	t	0.31	0/334	0.38	0/466
41	D	0.33	0/8529	0.59	0/11891
All	All	0.76	42/99857 (0.0%)	0.77	248/137993 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	A	0	6
7	C	0	7
8	E	0	1
11	H	0	1
12	J	0	3
14	M	0	1
16	O	0	1
17	P	0	1
18	R	0	2
20	T	0	3
23	W	0	3
25	Z	0	2
32	d	0	1
32	k	0	1
38	Y	0	15

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Mol	Chain	#Chirality outliers	#Planarity outliers
41	D	0	1
All	All	0	49

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	172	PHE	CE1-CZ	84.80	2.98	1.37
7	C	172	PHE	CE2-CZ	79.82	2.89	1.37
7	C	172	PHE	CD1-CE1	78.14	2.95	1.39
7	C	172	PHE	CD2-CE2	76.95	2.93	1.39
7	C	172	PHE	CG-CD1	47.98	2.10	1.38
7	C	172	PHE	CG-CD2	47.86	2.10	1.38
7	C	104	LEU	CB-CG	38.63	2.64	1.52
15	N	137	CYS	CB-SG	-12.16	1.61	1.82
15	N	142	CYS	CB-SG	-8.15	1.68	1.82
15	N	102	CYS	CB-SG	-8.14	1.68	1.82
11	H	142	C	C1'-N1	7.52	1.60	1.48
11	H	77	C	C1'-N1	7.33	1.59	1.48
11	H	69	U	C1'-N1	7.03	1.59	1.48
11	H	54	U	C1'-N1	7.01	1.59	1.48
11	H	91	U	C1'-N1	6.99	1.59	1.48
11	H	60	U	C1'-N1	6.91	1.59	1.48
6	B	103	G	C1'-N9	-6.89	1.37	1.46
11	H	74	U	C1'-N1	6.88	1.59	1.48
11	H	89	U	C1'-N1	6.87	1.59	1.48
11	H	72	U	C1'-N1	6.86	1.59	1.48
11	H	150	U	C1'-N1	6.79	1.58	1.48
11	H	55	U	C1'-N1	6.79	1.58	1.48
11	H	92	U	C1'-N1	6.76	1.58	1.48
11	H	182	U	C1'-N1	6.75	1.58	1.48
11	H	58	U	C1'-N1	6.73	1.58	1.48
15	N	117	CYS	CB-SG	-6.55	1.71	1.82
11	H	73	C	C1'-N1	6.41	1.58	1.48
15	N	139	CYS	CB-SG	-6.37	1.71	1.82
11	H	78	C	C1'-N1	6.36	1.58	1.48
11	H	151	C	C1'-N1	6.35	1.58	1.48
11	H	141	C	C1'-N1	6.34	1.58	1.48
11	H	184	C	C1'-N1	6.29	1.58	1.48
11	H	84	C	C1'-N1	6.24	1.58	1.48
11	H	67	C	C1'-N1	6.24	1.58	1.48
11	H	148	C	C1'-N1	6.24	1.58	1.48
11	H	71	C	C1'-N1	6.22	1.58	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	70	C	C1'-N1	6.18	1.58	1.48
7	C	104	LEU	CG-CD1	6.12	1.74	1.51
7	C	104	LEU	CG-CD2	6.00	1.74	1.51
15	N	101	CYS	CB-SG	-5.92	1.72	1.81
20	T	306	CYS	CB-SG	-5.56	1.72	1.81
39	K	186	VAL	CA-CB	-5.14	1.44	1.54

All (248) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	104	LEU	CA-CB-CG	18.46	157.76	115.30
7	C	104	LEU	CB-CG-CD1	16.32	138.75	111.00
7	C	104	LEU	CB-CG-CD2	15.04	136.56	111.00
11	H	167	U	C5-C4-O4	11.93	133.06	125.90
7	C	172	PHE	CD1-CG-CD2	9.95	131.24	118.30
6	B	23	C	N1-C2-O2	9.93	124.86	118.90
7	C	172	PHE	CB-CG-CD2	-9.29	114.30	120.80
7	C	104	LEU	CD1-CG-CD2	-9.28	82.65	110.50
7	C	172	PHE	CB-CG-CD1	-9.20	114.36	120.80
20	T	342	GLU	C-N-CD	-9.10	100.57	120.60
10	G	163	C	N1-C2-O2	9.09	124.35	118.90
10	G	-6	C	N1-C2-O2	8.96	124.28	118.90
11	H	162	U	N3-C2-O2	-8.82	116.02	122.20
6	B	23	C	C2-N1-C1'	8.81	128.49	118.80
10	G	17	U	N1-C2-O2	8.68	128.87	122.80
10	G	-6	C	C2-N1-C1'	8.50	128.15	118.80
10	G	163	C	N3-C2-O2	-8.42	116.01	121.90
6	B	23	C	N3-C2-O2	-8.14	116.20	121.90
20	T	402	ASP	CB-CG-OD1	8.02	125.52	118.30
10	G	17	U	N3-C2-O2	-8.02	116.59	122.20
9	F	60	C	C6-N1-C2	-7.98	117.11	120.30
11	H	167	U	N3-C4-O4	-7.97	113.82	119.40
10	G	17	U	C2-N1-C1'	7.95	127.24	117.70
11	H	39	U	C2'-C3'-O3'	7.91	126.90	109.50
10	G	163	C	C2-N1-C1'	7.59	127.15	118.80
10	G	163	C	C6-N1-C2	-7.49	117.31	120.30
6	B	36	C	N1-C2-O2	7.42	123.35	118.90
6	B	55	C	C6-N1-C2	-7.41	117.33	120.30
11	H	69	U	OP2-P-O3'	7.34	121.34	105.20
11	H	167	U	N1-C2-O2	7.32	127.92	122.80
11	H	77	C	OP2-P-O3'	7.28	121.21	105.20
11	H	70	C	OP2-P-O3'	7.27	121.20	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	H	83	A	OP2-P-O3'	7.27	121.19	105.20
11	H	141	C	OP2-P-O3'	7.27	121.19	105.20
11	H	54	U	OP2-P-O3'	7.26	121.18	105.20
11	H	92	U	OP2-P-O3'	7.26	121.16	105.20
11	H	149	A	OP2-P-O3'	7.26	121.16	105.20
11	H	148	C	OP2-P-O3'	7.25	121.16	105.20
11	H	59	A	OP2-P-O3'	7.23	121.11	105.20
11	H	81	G	OP2-P-O3'	7.23	121.10	105.20
11	H	180	G	OP2-P-O3'	7.22	121.08	105.20
11	H	67	C	OP2-P-O3'	7.22	121.08	105.20
11	H	78	C	OP2-P-O3'	7.22	121.08	105.20
11	H	80	A	OP2-P-O3'	7.22	121.08	105.20
11	H	89	U	OP2-P-O3'	7.22	121.08	105.20
11	H	74	U	OP2-P-O3'	7.21	121.05	105.20
11	H	88	A	OP2-P-O3'	7.20	121.04	105.20
11	H	55	U	OP2-P-O3'	7.20	121.03	105.20
11	H	181	G	OP2-P-O3'	7.20	121.03	105.20
11	H	182	U	OP2-P-O3'	7.19	121.03	105.20
11	H	90	A	OP2-P-O3'	7.19	121.02	105.20
6	B	36	C	C2-N1-C1'	7.19	126.71	118.80
11	H	183	G	OP2-P-O3'	7.19	121.01	105.20
11	H	91	U	OP2-P-O3'	7.18	121.00	105.20
11	H	57	A	OP2-P-O3'	7.18	121.00	105.20
11	H	150	U	OP2-P-O3'	7.18	121.00	105.20
11	H	71	C	OP2-P-O3'	7.17	120.98	105.20
11	H	93	A	OP2-P-O3'	7.17	120.98	105.20
11	H	58	U	OP2-P-O3'	7.16	120.95	105.20
11	H	72	U	OP2-P-O3'	7.16	120.95	105.20
11	H	68	G	OP2-P-O3'	7.16	120.95	105.20
11	H	84	C	OP2-P-O3'	7.16	120.95	105.20
11	H	56	A	OP2-P-O3'	7.16	120.94	105.20
11	H	73	C	OP2-P-O3'	7.15	120.94	105.20
11	H	79	G	OP2-P-O3'	7.15	120.92	105.20
24	X	85	LEU	CA-CB-CG	7.13	131.69	115.30
11	H	82	G	OP2-P-O3'	7.07	120.76	105.20
11	H	167	U	N3-C2-O2	-7.05	117.27	122.20
11	H	54	U	O3'-P-O5'	-6.86	90.97	104.00
11	H	82	G	O3'-P-O5'	-6.86	90.97	104.00
6	B	104	C	C2'-C3'-O3'	-6.85	94.44	109.50
11	H	84	C	O3'-P-O5'	-6.84	91.00	104.00
11	H	150	U	O3'-P-O5'	-6.84	91.00	104.00
11	H	88	A	O3'-P-O5'	-6.84	91.00	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	H	93	A	O3'-P-O5'	-6.83	91.03	104.00
11	H	78	C	O3'-P-O5'	-6.82	91.04	104.00
11	H	73	C	O3'-P-O5'	-6.82	91.05	104.00
5	A	1109	LEU	CA-CB-CG	6.81	130.97	115.30
11	H	55	U	O3'-P-O5'	-6.81	91.06	104.00
11	H	83	A	O3'-P-O5'	-6.81	91.06	104.00
11	H	67	C	O3'-P-O5'	-6.81	91.07	104.00
11	H	181	G	O3'-P-O5'	-6.80	91.07	104.00
11	H	92	U	O3'-P-O5'	-6.80	91.08	104.00
11	H	141	C	O3'-P-O5'	-6.79	91.09	104.00
11	H	74	U	O3'-P-O5'	-6.79	91.10	104.00
6	B	40	U	N1-C2-O2	6.79	127.55	122.80
10	G	137	C	C2'-C3'-O3'	6.79	124.56	113.70
11	H	80	A	O3'-P-O5'	-6.79	91.11	104.00
11	H	180	G	O3'-P-O5'	-6.78	91.12	104.00
11	H	59	A	O3'-P-O5'	-6.78	91.12	104.00
11	H	56	A	O3'-P-O5'	-6.78	91.13	104.00
11	H	79	G	O3'-P-O5'	-6.77	91.13	104.00
11	H	57	A	O3'-P-O5'	-6.77	91.14	104.00
10	G	-6	C	N3-C2-O2	-6.75	117.17	121.90
11	H	69	U	O3'-P-O5'	-6.75	91.17	104.00
11	H	148	C	O3'-P-O5'	-6.75	91.17	104.00
11	H	182	U	O3'-P-O5'	-6.75	91.18	104.00
11	H	149	A	O3'-P-O5'	-6.74	91.19	104.00
11	H	89	U	O3'-P-O5'	-6.74	91.20	104.00
11	H	72	U	O3'-P-O5'	-6.74	91.20	104.00
11	H	91	U	O3'-P-O5'	-6.73	91.21	104.00
11	H	183	G	O3'-P-O5'	-6.73	91.21	104.00
11	H	58	U	O3'-P-O5'	-6.73	91.22	104.00
11	H	70	C	O3'-P-O5'	-6.72	91.22	104.00
11	H	71	C	O3'-P-O5'	-6.72	91.23	104.00
11	H	68	G	O3'-P-O5'	-6.72	91.24	104.00
11	H	81	G	O3'-P-O5'	-6.71	91.24	104.00
11	H	90	A	O3'-P-O5'	-6.71	91.24	104.00
11	H	155	C	P-O3'-C3'	6.71	127.75	119.70
6	B	20	G	O4'-C1'-N9	6.70	113.56	108.20
9	F	60	C	C5-C6-N1	6.69	124.35	121.00
11	H	77	C	O3'-P-O5'	-6.69	91.28	104.00
16	O	193	LEU	CA-CB-CG	6.69	130.68	115.30
40	q	46	PRO	N-CA-CB	6.64	111.27	103.30
9	F	61	C	C6-N1-C2	-6.58	117.67	120.30
39	K	90	PRO	N-CA-CB	6.58	111.19	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	H	29	A	P-O3'-C3'	6.53	127.53	119.70
6	B	43	U	N1-C2-O2	6.50	127.35	122.80
40	r	46	PRO	N-CA-CB	6.49	111.08	103.30
2	w	114	LYS	N-CA-C	-6.42	93.67	111.00
40	q	60	PRO	N-CA-CB	6.40	110.98	103.30
10	G	-6	C	C6-N1-C1'	-6.38	113.14	120.80
5	A	422	LEU	CB-CG-CD2	-6.37	100.17	111.00
39	K	78	PRO	N-CA-CB	6.37	110.94	103.30
10	G	131	U	C2'-C3'-O3'	-6.36	95.51	109.50
36	o	5	THR	N-CA-CB	-6.30	98.34	110.30
26	I	589	PRO	N-CA-CB	6.29	110.85	103.30
6	B	36	C	C6-N1-C2	-6.26	117.80	120.30
26	I	475	PRO	N-CA-CB	6.25	110.80	103.30
7	C	172	PHE	CD1-CE1-CZ	-6.21	112.65	120.10
6	B	36	C	C5-C6-N1	6.21	124.10	121.00
7	C	105	MET	CA-CB-CG	6.20	123.83	113.30
6	B	43	U	N3-C2-O2	-6.18	117.88	122.20
13	L	558	PRO	N-CA-CB	6.16	110.70	103.30
9	F	38	G	C6-C5-N7	-6.16	126.71	130.40
6	B	23	C	C6-N1-C1'	-6.15	113.42	120.80
12	J	637	PRO	N-CA-CB	6.15	110.68	103.30
11	H	165	A	O4'-C1'-N9	-6.14	103.29	108.20
26	I	162	PRO	N-CA-CB	6.10	110.62	103.30
26	I	232	PRO	N-CA-CB	6.10	110.61	103.30
26	I	371	PRO	N-CA-CB	6.09	110.61	103.30
10	G	13	C	C5-C6-N1	6.09	124.04	121.00
26	I	394	PRO	N-CA-CB	6.08	110.59	103.30
10	G	16	G	P-O3'-C3'	6.07	126.98	119.70
26	I	788	PRO	N-CA-CB	6.06	110.57	103.30
26	I	177	PRO	N-CA-CB	6.06	110.57	103.30
15	N	119	CYS	CA-CB-SG	6.05	124.89	114.00
26	I	816	PRO	N-CA-CB	6.04	110.55	103.30
13	L	546	PRO	N-CA-CB	6.03	110.54	103.30
12	J	670	PRO	N-CA-CB	6.02	110.53	103.30
12	J	220	LEU	CA-CB-CG	6.01	129.13	115.30
5	A	1405	LEU	CA-CB-CG	6.00	129.09	115.30
12	J	523	PRO	N-CA-CB	6.00	110.49	103.30
11	H	162	U	N1-C2-O2	5.99	126.99	122.80
11	H	104	U	C2'-C3'-O3'	5.97	123.25	113.70
13	L	594	PRO	N-CA-CB	5.96	110.46	103.30
13	L	563	PRO	N-CA-CB	5.96	110.45	103.30
26	I	160	PRO	N-CA-CB	5.96	110.45	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	H	172	C	P-O3'-C3'	5.95	126.84	119.70
6	B	36	C	N3-C2-O2	-5.93	117.75	121.90
40	r	19	PRO	N-CA-CB	5.92	110.41	103.30
12	J	604	PRO	N-CA-CB	5.91	110.39	103.30
26	I	518	PRO	N-CA-CB	5.89	110.37	103.30
26	I	387	PRO	N-CA-CB	5.88	110.35	103.30
11	H	14	C	N1-C2-O2	5.87	122.42	118.90
6	B	55	C	N3-C2-O2	-5.86	117.80	121.90
22	V	539	LEU	CA-CB-CG	5.85	128.75	115.30
40	q	19	PRO	N-CA-CB	5.84	110.31	103.30
12	J	675	PRO	N-CA-CB	5.83	110.30	103.30
13	L	548	PRO	N-CA-CB	5.82	110.29	103.30
36	o	27	ARG	CB-CA-C	-5.82	98.76	110.40
6	B	40	U	N3-C2-O2	-5.80	118.14	122.20
9	F	25	C	P-O3'-C3'	5.79	126.65	119.70
12	J	551	PRO	N-CA-CB	5.77	110.23	103.30
9	F	38	G	N3-C4-N9	5.77	129.46	126.00
22	V	489	LEU	CA-CB-CG	5.76	128.54	115.30
12	J	488	PRO	N-CA-CB	5.75	110.20	103.30
12	J	566	PRO	N-CA-CB	5.74	110.19	103.30
13	L	564	PRO	N-CA-CB	5.74	110.19	103.30
9	F	60	C	N3-C2-O2	-5.71	117.90	121.90
13	L	620	PRO	N-CA-CB	5.70	110.14	103.30
6	B	40	U	C2-N1-C1'	5.70	124.54	117.70
26	I	588	PRO	N-CA-CB	5.69	110.12	103.30
9	F	26	U	C6-N1-C2	-5.68	117.59	121.00
11	H	156	U	P-O3'-C3'	-5.68	112.88	119.70
6	B	52	U	N3-C2-O2	-5.65	118.25	122.20
7	C	93	ILE	CG1-CB-CG2	-5.64	98.99	111.40
25	Z	82	LEU	CA-CB-CG	5.64	128.28	115.30
12	J	205	LEU	C-N-CA	5.63	135.76	121.70
9	F	60	C	N1-C2-O2	5.59	122.26	118.90
12	J	522	PRO	N-CA-CB	5.59	110.01	103.30
23	W	251	GLY	N-CA-C	-5.59	99.12	113.10
36	o	58	ASP	N-CA-CB	-5.56	100.58	110.60
26	I	463	PRO	N-CA-CB	5.55	109.96	103.30
23	W	165	LEU	CA-CB-CG	5.53	128.03	115.30
5	A	1889	LEU	CA-CB-CG	5.53	128.02	115.30
9	F	37	C	O4'-C1'-N1	5.53	112.62	108.20
6	B	23	C	C6-N1-C2	-5.51	118.10	120.30
10	G	6	A	N7-C8-N9	5.51	116.55	113.80
39	K	93	SER	N-CA-CB	-5.50	102.25	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	20	G	C4-N9-C1'	5.47	133.61	126.50
26	I	761	PRO	N-CA-CB	5.46	109.86	103.30
14	M	186	LEU	CB-CG-CD1	-5.45	101.74	111.00
7	C	943	LEU	CA-CB-CG	5.41	127.73	115.30
10	G	17	U	C5-C6-N1	5.37	125.39	122.70
10	G	18	A	C6-N1-C2	5.37	121.82	118.60
36	o	47	ILE	N-CA-CB	5.36	123.13	110.80
26	I	625	PRO	N-CA-CB	5.36	109.73	103.30
12	J	187	VAL	C-N-CA	5.36	135.09	121.70
9	F	31	U	N3-C2-O2	-5.35	118.46	122.20
9	F	31	U	N1-C2-O2	5.34	126.54	122.80
5	A	623	LYS	N-CA-C	-5.34	96.58	111.00
11	H	156	U	OP2-P-O3'	5.31	116.87	105.20
6	B	58	U	N3-C2-O2	-5.30	118.49	122.20
20	T	401	PRO	C-N-CA	5.30	134.96	121.70
6	B	56	C	N1-C2-O2	5.30	122.08	118.90
9	F	89	U	N3-C2-O2	-5.30	118.49	122.20
9	F	26	U	N3-C2-O2	-5.29	118.50	122.20
10	G	5	G	C4-N9-C1'	5.28	133.36	126.50
7	C	298	LEU	CA-CB-CG	5.25	127.38	115.30
10	G	1	G	C2'-C3'-O3'	5.24	122.09	113.70
5	A	1763	LEU	CA-CB-CG	5.22	127.31	115.30
11	H	157	G	O4'-C1'-N9	-5.22	104.03	108.20
2	w	115	GLY	N-CA-C	5.20	126.11	113.10
11	H	162	U	C2-N3-C4	-5.18	123.89	127.00
24	X	85	LEU	CB-CG-CD1	-5.18	102.19	111.00
9	F	60	C	C2-N1-C1'	5.17	124.49	118.80
15	N	101	CYS	CA-CB-SG	-5.17	104.69	114.00
11	H	157	G	P-O5'-C5'	-5.16	112.64	120.90
6	B	21	A	OP2-P-O3'	5.16	116.54	105.20
12	J	195	LEU	CA-CB-CG	5.16	127.16	115.30
11	H	160	A	C4'-C3'-C2'	-5.14	97.46	102.60
5	A	1090	ARG	NE-CZ-NH2	-5.14	117.73	120.30
11	H	13	C	N3-C2-O2	-5.13	118.31	121.90
10	G	-12	G	P-O3'-C3'	5.12	125.85	119.70
6	B	55	C	N1-C2-O2	5.12	121.97	118.90
9	F	26	U	P-O3'-C3'	5.12	125.84	119.70
9	F	38	G	C4-N9-C1'	5.11	133.15	126.50
18	R	275	LEU	CA-CB-CG	5.11	127.04	115.30
11	H	160	A	P-O5'-C5'	-5.10	112.74	120.90
11	H	156	U	C4'-C3'-C2'	5.10	107.70	102.60
11	H	29	A	OP1-P-O3'	5.09	116.39	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	V	467	LEU	CA-CB-CG	5.08	126.98	115.30
11	H	176	G	OP1-P-OP2	-5.06	112.01	119.60
9	F	52	U	N3-C2-O2	-5.04	118.67	122.20
19	S	106	ASP	CB-CG-OD1	5.04	122.84	118.30
23	W	442	LEU	CA-CB-CG	5.02	126.84	115.30
9	F	89	U	N1-C2-O2	5.00	126.30	122.80

There are no chirality outliers.

All (49) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	A	1070	ASP	Peptide
5	A	1091	TYR	Peptide
5	A	1209	HIS	Peptide
5	A	1502	PHE	Peptide
5	A	851	SER	Peptide
5	A	941	LYS	Peptide
7	C	103	THR	Peptide
7	C	167	TYR	Peptide
7	C	439	PRO	Peptide
7	C	456	GLY	Peptide
7	C	534	VAL	Peptide
7	C	560	VAL	Peptide
7	C	93	ILE	Peptide
41	D	430	LEU	Peptide
8	E	192	ASN	Peptide
11	H	40	C	Sidechain
12	J	205	LEU	Peptide
12	J	240	THR	Peptide
12	J	241	VAL	Peptide
14	M	124	PHE	Peptide
16	O	133	PRO	Peptide
17	P	204	GLN	Peptide
18	R	183	GLN	Peptide
18	R	185	GLY	Peptide
20	T	185	MET	Peptide
20	T	400	PHE	Peptide
20	T	457	GLY	Peptide
23	W	198	LYS	Peptide
23	W	242	HIS	Peptide
23	W	245	GLU	Peptide
38	Y	1098	LYS	Peptide

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Mol	Chain	Res	Type	Group
38	Y	1127	LEU	Peptide
38	Y	1163	ARG	Peptide
38	Y	1187	THR	Peptide
38	Y	515	ASP	Peptide
38	Y	550	TYR	Peptide
38	Y	563	GLU	Peptide
38	Y	636	CYS	Peptide
38	Y	662	THR	Peptide
38	Y	811	PRO	Peptide
38	Y	855	VAL	Peptide
38	Y	868	LYS	Peptide
38	Y	938	ASN	Peptide
38	Y	963	THR	Peptide
38	Y	993	LEU	Peptide
25	Z	135	GLU	Peptide
25	Z	92	GLN	Peptide
32	d	112	ASN	Peptide
32	k	112	ASN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	v	711	0	299	0	0
2	w	445	0	203	0	0
3	u	1907	0	845	0	0
4	x	124	0	51	0	0
5	A	17837	0	17053	235	0
6	B	2040	0	1034	51	0
7	C	7066	0	7084	130	0
8	E	2366	0	2303	65	0
9	F	2075	0	1048	27	0
10	G	1549	0	784	51	0
11	H	2966	0	1505	227	0
12	J	3829	0	2907	38	0
13	L	3064	0	2521	40	0
14	M	1098	0	1082	25	0
15	N	1184	0	1189	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	O	2296	0	2284	36	0
17	P	929	0	910	6	0
18	R	2073	0	2119	36	0
19	S	1236	0	1210	23	0
20	T	2461	0	2420	69	0
21	U	193	0	196	4	0
22	V	2765	0	1955	17	0
23	W	4122	0	4031	109	0
24	X	701	0	631	30	0
25	Z	1999	0	1951	35	0
26	I	2782	0	1245	52	0
27	y	390	0	190	0	0
28	Q	6562	0	2836	5	0
29	a	399	0	173	0	0
29	h	398	0	172	0	0
30	b	424	0	179	0	0
30	i	424	0	179	0	0
31	c	406	0	170	0	0
31	j	406	0	170	0	0
32	d	480	0	200	0	0
32	k	422	0	175	0	0
33	f	361	0	158	0	0
33	m	356	0	156	0	0
34	e	391	0	163	0	0
34	l	391	0	163	0	0
35	g	363	0	160	0	0
35	n	339	0	145	0	0
36	o	804	0	350	0	0
37	p	464	0	205	0	0
38	Y	2917	0	857	9	0
39	K	757	0	338	19	0
40	q	659	0	296	0	0
40	r	654	0	294	0	0
40	s	335	0	168	0	0
40	t	335	0	168	0	0
41	D	8530	0	3747	8	0
42	A	36	0	6	3	0
43	C	32	0	12	2	0
44	C	1	0	0	0	0
44	F	6	0	0	0	0
44	Q	2	0	0	0	0
45	N	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	O	3	0	0	0	0
45	Z	1	0	0	0	0
46	Q	31	0	12	0	0
All	All	97900	0	70702	1177	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 8.

All (1177) 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)
7:C:104:LEU:CG	7:C:104:LEU:CD1	1.74	1.61
12:J:466:ARG:CB	26:I:607:GLY:HA2	1.44	1.47
8:E:56:GLN:NE2	8:E:97:GLY:HA2	1.35	1.40
7:C:172:PHE:CD1	7:C:172:PHE:CG	2.10	1.39
7:C:172:PHE:CG	7:C:172:PHE:CD2	2.10	1.39
23:W:257:ILE:HD12	23:W:258:PRO:CD	1.51	1.36
23:W:257:ILE:CD1	23:W:258:PRO:HD2	1.54	1.34
11:H:150:U:O3'	24:X:124:THR:HG22	1.31	1.27
26:I:331:LEU:CB	26:I:340:ARG:CB	2.12	1.26
39:K:113:GLN:O	39:K:117:GLN:CB	1.87	1.22
23:W:258:PRO:CG	23:W:265:LEU:HD22	1.74	1.16
20:T:342:GLU:CB	20:T:343:PRO:HD2	1.63	1.15
23:W:258:PRO:HG3	23:W:265:LEU:CD2	1.74	1.15
20:T:399:LYS:HB2	20:T:406:ILE:HD11	1.14	1.13
12:J:427:LYS:NZ	26:I:579:LEU:CB	2.12	1.13
26:I:612:ALA:CB	26:I:623:VAL:CB	2.26	1.12
12:J:484:VAL:CB	26:I:642:ILE:CB	2.28	1.12
39:K:112:ALA:O	39:K:116:HIS:CB	1.98	1.11
7:C:104:LEU:CD1	7:C:104:LEU:CD2	2.30	1.10
26:I:296:PHE:HA	26:I:305:SER:CB	1.80	1.10
26:I:346:ASN:CB	28:Q:524:LYS:CB	2.30	1.10
11:H:150:U:H5"	24:X:124:THR:CB	1.81	1.10
12:J:466:ARG:CB	26:I:607:GLY:CA	2.30	1.09
12:J:427:LYS:CE	26:I:579:LEU:CB	2.30	1.09
10:G:138:A:C2	11:H:39:U:O2	2.07	1.08
26:I:612:ALA:HB2	26:I:623:VAL:CB	1.84	1.07
11:H:150:U:H5"	24:X:124:THR:HB	1.31	1.07
23:W:257:ILE:HD12	23:W:258:PRO:N	1.67	1.07
11:H:156:U:H6	11:H:156:U:H5"	1.09	1.07
11:H:150:U:H5"	24:X:124:THR:CG2	1.84	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:104:LEU:CB	7:C:104:LEU:HG	1.86	1.06
8:E:56:GLN:HE22	8:E:97:GLY:CA	1.67	1.05
11:H:151:C:OP1	24:X:123:GLN:HB2	1.55	1.03
20:T:342:GLU:HB3	20:T:343:PRO:CD	1.88	1.03
8:E:60:MET:HG3	8:E:353:MET:SD	1.99	1.03
7:C:104:LEU:HD11	7:C:104:LEU:HD21	1.40	1.01
8:E:56:GLN:NE2	8:E:97:GLY:CA	2.23	0.99
5:A:1976:TRP:O	5:A:1980:GLU:HG3	1.62	0.99
11:H:106:G:H4'	11:H:107:A:OP1	1.62	0.99
23:W:257:ILE:HD12	23:W:258:PRO:HD2	1.05	0.98
24:X:120:ALA:O	24:X:124:THR:HG23	1.64	0.97
38:Y:405:MET:HE3	38:Y:411:LEU:HD23	1.46	0.97
11:H:151:C:P	24:X:124:THR:HG22	2.05	0.96
8:E:60:MET:HB3	8:E:353:MET:HB2	1.45	0.96
11:H:156:U:H5"	11:H:156:U:C6	2.02	0.94
5:A:1673:SER:CB	25:Z:164:ASP:OD1	2.15	0.94
5:A:1945:VAL:HG11	5:A:1990:ASP:CG	1.86	0.94
11:H:150:U:C5'	24:X:124:THR:HB	1.97	0.93
11:H:150:U:OP1	24:X:124:THR:HB	1.69	0.93
23:W:257:ILE:HD13	23:W:258:PRO:HD2	1.51	0.92
8:E:54:SER:N	8:E:96:TYR:HE1	1.66	0.92
11:H:108:G:H2'	11:H:109:C:H6	1.31	0.92
16:O:72:GLN:HG3	16:O:82:GLN:HE22	1.35	0.92
11:H:106:G:H5'	11:H:106:G:H8	1.36	0.90
20:T:342:GLU:CB	20:T:343:PRO:CD	2.47	0.90
13:L:65:ARG:NH2	26:I:799:ARG:O	2.04	0.90
8:E:56:GLN:HE22	8:E:97:GLY:HA2	1.07	0.90
10:G:138:A:N1	11:H:39:U:O2	2.05	0.89
11:H:100:U:H5'	11:H:100:U:C6	2.07	0.89
10:G:129:G:O3'	23:W:541:LYS:HE3	1.72	0.88
20:T:399:LYS:CB	20:T:406:ILE:HD11	2.02	0.88
5:A:1673:SER:HB2	25:Z:164:ASP:OD1	1.74	0.88
20:T:342:GLU:HB3	20:T:343:PRO:HD2	0.91	0.88
26:I:612:ALA:HB1	26:I:623:VAL:CB	2.04	0.87
11:H:154:C:O2	11:H:176:G:N2	2.07	0.87
11:H:156:U:H6	11:H:156:U:C5'	1.89	0.86
11:H:166:G:N2	11:H:166:G:OP2	2.08	0.86
8:E:56:GLN:HE21	8:E:97:GLY:HA2	1.36	0.86
26:I:280:GLU:C	26:I:288:THR:CB	2.43	0.86
7:C:104:LEU:HB3	7:C:172:PHE:CE1	2.11	0.85
39:K:131:GLY:O	39:K:135:TRP:CB	2.24	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:Y:405:MET:CE	38:Y:411:LEU:HD23	2.06	0.85
38:Y:405:MET:CE	38:Y:411:LEU:CD2	2.54	0.85
8:E:54:SER:N	8:E:96:TYR:CE1	2.44	0.85
7:C:104:LEU:CD1	7:C:104:LEU:HD21	2.03	0.84
26:I:280:GLU:O	26:I:288:THR:CB	2.25	0.84
11:H:41:U:H5"	11:H:41:U:H6	1.43	0.83
11:H:98:G:H4'	11:H:98:G:OP2	1.78	0.83
11:H:152:G:N2	11:H:153:A:N7	2.26	0.83
12:J:427:LYS:HE2	26:I:579:LEU:CB	2.09	0.83
6:B:80:U:H2'	6:B:80:U:OP1	1.79	0.83
11:H:150:U:C3'	24:X:124:THR:HG22	2.10	0.81
11:H:152:G:H5"	11:H:153:A:OP2	1.80	0.81
39:K:114:LEU:O	39:K:118:ALA:N	2.13	0.81
11:H:106:G:H5'	11:H:106:G:C8	2.16	0.81
5:A:1831:LYS:HG2	10:G:2:U:OP2	1.80	0.80
11:H:151:C:OP2	24:X:124:THR:HA	1.80	0.80
23:W:265:LEU:HD23	23:W:300:SER:CB	2.12	0.80
10:G:126:C:H4'	10:G:127:U:OP1	1.82	0.79
11:H:108:G:H2'	11:H:109:C:C6	2.17	0.79
10:G:130:A:O2'	10:G:131:U:OP2	1.99	0.79
23:W:252:ARG:HH11	23:W:252:ARG:HG2	1.46	0.79
11:H:153:A:H2'	11:H:154:C:H5'	1.65	0.78
10:G:138:A:H2	11:H:39:U:O2	1.65	0.78
5:A:1980:GLU:OE1	25:Z:347:PRO:HD2	1.84	0.78
8:E:61:LEU:HG	8:E:62:LEU:N	1.97	0.78
11:H:150:U:OP1	24:X:124:THR:CB	2.32	0.78
38:Y:405:MET:HE3	38:Y:411:LEU:CD2	2.14	0.78
10:G:142:U:O2'	10:G:143:U:OP1	2.01	0.77
28:Q:523:ALA:HB3	28:Q:534:ARG:H	1.48	0.77
5:A:1979:VAL:HA	5:A:1982:GLN:OE1	1.83	0.77
20:T:342:GLU:OE2	20:T:342:GLU:HA	1.82	0.77
11:H:107:A:N3	11:H:107:A:H3'	2.00	0.77
11:H:177:A:H5"	11:H:178:A:OP1	1.84	0.77
12:J:427:LYS:HZ1	26:I:579:LEU:CB	1.95	0.77
20:T:399:LYS:HB2	20:T:406:ILE:CD1	2.07	0.76
11:H:150:U:H5"	24:X:124:THR:HG21	1.66	0.76
6:B:75:G:N7	6:B:76:A:C8	2.54	0.76
11:H:143:A:H3'	11:H:143:A:N3	2.00	0.76
12:J:427:LYS:HZ3	26:I:579:LEU:CB	1.95	0.76
16:O:72:GLN:HG3	16:O:82:GLN:NE2	2.01	0.76
5:A:1945:VAL:CG1	5:A:1990:ASP:CG	2.55	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:474:LEU:HA	7:C:498:SER:O	1.86	0.75
6:B:72:U:H1'	6:B:74:U:H1'	1.68	0.75
6:B:81:U:O2'	6:B:82:A:OP2	2.02	0.75
10:G:129:G:H4'	23:W:541:LYS:CD	2.16	0.75
20:T:346:ILE:HD12	20:T:356:LEU:HD12	1.66	0.75
7:C:104:LEU:CG	7:C:104:LEU:CB	2.64	0.75
26:I:720:ILE:O	26:I:721:LYS:CB	2.34	0.74
12:J:493:ALA:HB1	12:J:499:ARG:CB	2.18	0.74
11:H:153:A:C2'	11:H:154:C:H5'	2.17	0.74
23:W:258:PRO:HB2	23:W:265:LEU:HD13	1.69	0.74
11:H:150:U:P	24:X:124:THR:HB	2.28	0.74
15:N:38:GLU:OE2	15:N:38:GLU:HA	1.87	0.74
11:H:151:C:OP1	24:X:123:GLN:CB	2.36	0.73
11:H:41:U:H2'	11:H:42:G:C8	2.23	0.73
12:J:463:GLY:O	26:I:610:ARG:CB	2.37	0.73
5:A:1945:VAL:CG1	5:A:1990:ASP:OD2	2.37	0.73
23:W:541:LYS:HB2	23:W:541:LYS:HZ2	1.54	0.73
11:H:179:C:H2'	11:H:180:G:H8	1.53	0.72
7:C:104:LEU:HB2	7:C:172:PHE:CD1	2.25	0.72
11:H:153:A:H2'	11:H:154:C:C5'	2.19	0.72
5:A:1673:SER:HB3	25:Z:164:ASP:OD1	1.88	0.72
11:H:150:U:O3'	24:X:124:THR:CG2	2.24	0.72
6:B:74:U:O4	6:B:75:G:O6	2.07	0.71
7:C:104:LEU:HB2	7:C:172:PHE:CG	2.25	0.71
11:H:39:U:C5'	11:H:39:U:H6	2.03	0.71
39:K:130:HIS:O	39:K:134:ALA:HB3	1.90	0.71
8:E:56:GLN:HE22	8:E:97:GLY:C	1.93	0.71
11:H:151:C:P	24:X:124:THR:CG2	2.78	0.71
5:A:1946:ASN:HD22	5:A:1986:LEU:HD11	1.54	0.71
11:H:105:G:N3	11:H:105:G:H2'	2.05	0.71
10:G:138:A:N1	11:H:39:U:C2	2.58	0.71
11:H:151:C:OP1	24:X:120:ALA:O	2.09	0.71
6:B:96:A:C6	6:B:97:G:C5	2.78	0.71
39:K:135:TRP:O	39:K:136:LYS:CB	2.38	0.71
7:C:104:LEU:HG	7:C:172:PHE:CE2	2.26	0.70
11:H:152:G:OP2	24:X:123:GLN:NE2	2.19	0.70
6:B:78:U:H6	6:B:78:U:H3'	1.57	0.70
23:W:252:ARG:HG3	23:W:253:SER:N	2.05	0.70
28:Q:523:ALA:HB3	28:Q:534:ARG:N	2.07	0.70
11:H:154:C:H2'	11:H:155:C:C6	2.26	0.70
23:W:258:PRO:HD2	23:W:266:ARG:HH12	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1935:ARG:HH21	25:Z:348:THR:HG21	1.56	0.69
13:L:65:ARG:CZ	26:I:799:ARG:O	2.40	0.69
11:H:153:A:N6	11:H:177:A:C2	2.60	0.69
5:A:671:THR:O	5:A:676:ARG:NH1	2.26	0.69
11:H:97:G:H4'	11:H:99:A:OP1	1.91	0.69
11:H:150:U:H3	11:H:181:G:H1	1.41	0.68
23:W:257:ILE:CD1	23:W:258:PRO:CD	2.33	0.68
20:T:356:LEU:HD22	20:T:366:VAL:HB	1.74	0.68
11:H:150:U:C5'	24:X:124:THR:CG2	2.69	0.68
10:G:137:C:C5'	10:G:137:C:H6	2.06	0.68
12:J:512:GLU:CB	26:I:640:ALA:N	2.57	0.68
13:L:65:ARG:NH2	26:I:799:ARG:HA	2.09	0.68
11:H:152:G:O3'	11:H:153:A:O4'	2.11	0.67
11:H:143:A:H2'	11:H:144:C:H6	1.59	0.67
13:L:28:LYS:HE2	13:L:50:TRP:HE1	1.60	0.67
23:W:265:LEU:HD23	23:W:300:SER:HB2	1.76	0.67
20:T:329:HIS:ND1	20:T:349:SER:OG	2.27	0.67
26:I:337:LEU:CB	26:I:363:ARG:O	2.43	0.67
23:W:266:ARG:HD3	23:W:266:ARG:N	2.10	0.67
11:H:108:G:O2'	11:H:109:C:H5'	1.95	0.67
11:H:151:C:O2	11:H:152:G:C8	2.48	0.67
39:K:113:GLN:O	39:K:117:GLN:N	2.27	0.67
5:A:663:ARG:NH1	9:F:64:U:OP2	2.28	0.66
7:C:623:GLU:H	7:C:941:LYS:HZ2	1.41	0.66
6:B:96:A:O2'	6:B:97:G:H5'	1.95	0.66
20:T:270:VAL:HB	20:T:284:TYR:HB2	1.77	0.66
11:H:67:C:H42	11:H:85:A:H61	1.44	0.66
13:L:65:ARG:NE	26:I:799:ARG:O	2.29	0.66
11:H:151:C:H2'	11:H:152:G:H8	1.59	0.66
23:W:541:LYS:HB2	23:W:541:LYS:NZ	2.10	0.66
11:H:151:C:C2	11:H:152:G:C8	2.84	0.66
6:B:96:A:C6	6:B:97:G:C6	2.84	0.66
5:A:761:ILE:HD12	5:A:775:ASN:HD22	1.61	0.66
20:T:314:ILE:HD11	20:T:326:LEU:HD21	1.78	0.65
11:H:153:A:C3'	11:H:154:C:H5'	2.25	0.65
26:I:296:PHE:CA	26:I:305:SER:CB	2.66	0.65
11:H:75:A:H61	11:H:77:C:H42	1.43	0.65
23:W:445:TRP:HE1	23:W:452:ASP:HB3	1.62	0.65
5:A:1594:CYS:SG	25:Z:268:ARG:NH2	2.68	0.65
23:W:252:ARG:HH11	23:W:252:ARG:CG	2.10	0.65
5:A:188:LEU:HD22	5:A:567:GLY:HA2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:56:GLN:HG2	8:E:57:ALA:N	2.11	0.65
5:A:1699:THR:HA	5:A:1717:ASN:HD22	1.62	0.65
5:A:44:ARG:HH22	8:E:286:LYS:HB2	1.60	0.65
16:O:78:LYS:O	16:O:97:ARG:NH2	2.29	0.65
5:A:1945:VAL:HG13	5:A:1990:ASP:OD2	1.97	0.65
5:A:1437:ARG:NH1	5:A:1455:TRP:O	2.30	0.64
7:C:817:TYR:O	7:C:821:LEU:HB2	1.97	0.64
11:H:98:G:N3	11:H:98:G:H3'	2.13	0.64
23:W:258:PRO:HB2	23:W:265:LEU:CD1	2.26	0.64
11:H:153:A:H3'	11:H:154:C:H5'	1.79	0.64
20:T:282:ARG:HB2	20:T:320:LYS:HD3	1.79	0.64
10:G:129:G:C4'	23:W:541:LYS:HE3	2.28	0.64
20:T:314:ILE:HD12	20:T:324:HIS:HB2	1.78	0.64
7:C:829:GLU:HB2	7:C:907:VAL:HG22	1.80	0.64
14:M:239:ARG:HD3	26:I:817:GLU:CB	2.28	0.64
23:W:313:ILE:HB	23:W:328:PHE:HB2	1.80	0.63
11:H:147:G:H2'	11:H:148:C:H6	1.62	0.63
20:T:458:SER:OG	20:T:459:LEU:N	2.32	0.63
23:W:258:PRO:HG3	23:W:265:LEU:HD22	0.82	0.63
5:A:270:ASN:HD21	21:U:8:PRO:HB3	1.63	0.63
7:C:224:GLY:HA3	7:C:438:ILE:HD12	1.81	0.63
10:G:137:C:H2'	10:G:138:A:C8	2.34	0.63
16:O:50:ARG:NH1	16:O:122:GLU:OE1	2.32	0.63
41:D:1992:GLU:HA	41:D:1995:ALA:HB3	1.80	0.63
5:A:200:ASP:OD1	5:A:240:ARG:NH2	2.32	0.63
11:H:154:C:H2'	11:H:155:C:H6	1.62	0.63
5:A:1986:LEU:HD23	5:A:1986:LEU:C	2.19	0.62
5:A:1615:HIS:HB3	5:A:1618:LYS:HB3	1.82	0.62
5:A:1667:ARG:HH12	5:A:1674:HIS:HA	1.64	0.62
12:J:512:GLU:CB	26:I:640:ALA:HA	2.30	0.62
23:W:485:ILE:HB	23:W:502:PHE:HB2	1.80	0.62
14:M:178:GLU:OE2	14:M:181:ARG:NH2	2.32	0.62
5:A:1476:GLN:OE1	22:V:457:ARG:NH1	2.32	0.62
11:H:112:G:H2'	11:H:113:G:H8	1.64	0.62
11:H:157:G:H8	11:H:157:G:H5"	1.65	0.62
5:A:907:PRO:HG2	5:A:1032:ARG:HH21	1.65	0.62
39:K:134:ALA:O	39:K:136:LYS:N	2.33	0.62
8:E:61:LEU:HG	8:E:62:LEU:H	1.64	0.62
11:H:18:U:OP2	14:M:221:LYS:NZ	2.32	0.62
11:H:151:C:OP2	24:X:124:THR:CA	2.48	0.62
11:H:152:G:C2	11:H:153:A:C5	2.87	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:443:VAL:HG12	5:A:610:HIS:HB3	1.81	0.62
6:B:74:U:N3	6:B:75:G:C6	2.68	0.62
11:H:143:A:H2'	11:H:144:C:C6	2.35	0.62
8:E:217:ILE:HB	8:E:231:MET:HB2	1.81	0.62
11:H:156:U:C6	11:H:156:U:C5'	2.72	0.62
5:A:974:ASN:HB2	5:A:1178:TYR:HB3	1.81	0.62
42:A:3000:IHP:O24	25:Z:167:ARG:NH2	2.29	0.62
19:S:72:ARG:HD3	23:W:90:ALA:HB3	1.81	0.62
5:A:1809:ILE:HB	5:A:1818:PHE:HB2	1.81	0.61
23:W:265:LEU:CD2	23:W:300:SER:HB2	2.29	0.61
9:F:46:G:OP1	13:L:169:ARG:NH1	2.32	0.61
13:L:65:ARG:HG2	26:I:803:SER:CB	2.30	0.61
13:L:764:PRO:O	13:L:765:ARG:CB	2.48	0.61
11:H:142:C:C2'	11:H:143:A:H5'	2.30	0.61
11:H:166:G:H2'	11:H:166:G:N3	2.15	0.61
23:W:341:ASN:OD1	23:W:388:GLN:NE2	2.32	0.61
5:A:274:PRO:HG3	21:U:1:MET:HB3	1.83	0.61
7:C:737:PRO:HB3	7:C:775:ARG:HB3	1.82	0.61
19:S:131:ARG:NH1	19:S:132:VAL:O	2.34	0.61
12:J:466:ARG:CB	26:I:606:TRP:O	2.47	0.61
16:O:234:LEU:HB2	16:O:272:ILE:HB	1.81	0.61
5:A:419:ARG:NH2	5:A:423:ASP:O	2.33	0.61
15:N:101:CYS:SG	15:N:102:CYS:N	2.73	0.61
15:N:120:ARG:HH11	15:N:142:CYS:CB	2.13	0.61
23:W:258:PRO:CD	23:W:266:ARG:HH12	2.12	0.61
11:H:153:A:N6	11:H:177:A:H2	1.98	0.61
39:K:124:LEU:O	39:K:128:SER:N	2.27	0.61
7:C:172:PHE:CE2	7:C:172:PHE:CZ	2.89	0.61
8:E:90:ILE:HB	8:E:105:LEU:HB2	1.81	0.61
9:F:29:A:N6	10:G:17:U:OP2	2.34	0.60
11:H:151:C:P	24:X:124:THR:N	2.74	0.60
20:T:210:ILE:HG12	20:T:221:THR:HG22	1.83	0.60
20:T:349:SER:OG	20:T:351:ASP:OD1	2.17	0.60
5:A:1248:LEU:O	5:A:1298:ARG:NH1	2.34	0.60
11:H:108:G:O5'	11:H:108:G:H8	1.84	0.60
23:W:391:PHE:O	23:W:402:GLN:HA	2.01	0.60
10:G:130:A:O2'	10:G:131:U:P	2.60	0.60
23:W:565:LYS:HD2	23:W:577:LEU:HD21	1.83	0.60
25:Z:124:GLY:HA3	25:Z:149:ILE:HG23	1.83	0.60
22:V:628:ILE:HG12	22:V:640:THR:HB	1.84	0.60
5:A:43:LYS:O	5:A:49:ARG:NH1	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:155:ALA:O	13:L:159:LEU:HB2	2.00	0.60
7:C:684:LYS:HB3	7:C:795:VAL:HB	1.82	0.60
5:A:506:LEU:O	5:A:510:ARG:HB2	2.02	0.60
7:C:449:ILE:HG13	7:C:465:MET:HB3	1.84	0.60
8:E:144:VAL:HG12	8:E:145:LYS:HG3	1.84	0.60
10:G:138:A:O5'	10:G:138:A:H8	1.83	0.59
14:M:239:ARG:HG2	26:I:817:GLU:CB	2.32	0.59
20:T:347:THR:HG22	20:T:357:TRP:HE1	1.66	0.59
39:K:112:ALA:O	39:K:116:HIS:N	2.35	0.59
23:W:436:THR:HG21	23:W:464:MET:HB2	1.85	0.59
5:A:975:VAL:HB	5:A:1099:PHE:HB2	1.83	0.59
5:A:1946:ASN:ND2	5:A:1986:LEU:HD21	2.17	0.59
8:E:274:VAL:HG12	8:E:275:LYS:HG3	1.83	0.59
15:N:40:LYS:CG	15:N:41:ARG:H	2.15	0.59
7:C:277:LYS:NZ	7:C:864:PRO:O	2.36	0.59
10:G:134:U:C5'	10:G:135:G:OP2	2.51	0.59
11:H:104:U:H6	11:H:104:U:H3'	1.66	0.59
5:A:1860:GLN:HG2	5:A:1883:VAL:HB	1.85	0.59
10:G:134:U:C5	10:G:135:G:N2	2.71	0.59
5:A:1136:ARG:HA	5:A:1139:ARG:HE	1.67	0.58
6:B:96:A:N6	6:B:97:G:C6	2.71	0.58
10:G:137:C:C5'	10:G:137:C:C6	2.85	0.58
23:W:265:LEU:HD21	23:W:302:HIS:HB2	1.84	0.58
16:O:197:ASN:HB3	16:O:200:ASP:HB2	1.84	0.58
19:S:72:ARG:NH2	23:W:73:ASP:O	2.35	0.58
20:T:345:ILE:HD11	20:T:359:LEU:HD13	1.85	0.58
23:W:304:LEU:HB3	23:W:316:TRP:HB2	1.85	0.58
15:N:118:ILE:HD13	15:N:132:ILE:CG2	2.32	0.58
7:C:245:HIS:O	7:C:249:GLU:HB2	2.03	0.58
9:F:49:G:OP1	13:L:33:ARG:NH1	2.37	0.58
5:A:650:ARG:HH21	5:A:651:TRP:HE1	1.51	0.58
5:A:1784:ASN:HD22	5:A:1897:LEU:HD12	1.69	0.58
7:C:343:LEU:HD13	7:C:373:ILE:HD11	1.85	0.58
15:N:118:ILE:HD13	15:N:132:ILE:HG23	1.86	0.58
20:T:261:LEU:HB2	20:T:273:TRP:HB2	1.85	0.58
6:B:13:C:C2	6:B:65:G:C2	2.92	0.57
7:C:221:ILE:HG23	7:C:495:ARG:HB2	1.84	0.57
10:G:129:G:H4'	23:W:541:LYS:HD2	1.86	0.57
11:H:105:G:N1	11:H:107:A:H5'	2.19	0.57
6:B:96:A:C5	6:B:97:G:N7	2.73	0.57
7:C:104:LEU:CB	7:C:172:PHE:CE1	2.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:13:ASN:HA	19:S:25:LEU:O	2.03	0.57
20:T:250:ARG:NH1	20:T:266:GLU:OE2	2.36	0.57
13:L:65:ARG:NH2	26:I:799:ARG:CA	2.67	0.57
19:S:26:GLU:OE1	19:S:131:ARG:NH2	2.37	0.57
20:T:356:LEU:CD2	20:T:366:VAL:HB	2.34	0.57
5:A:1781:ASP:HB3	5:A:1808:PHE:HB3	1.86	0.57
6:B:40:U:H3	10:G:-1:G:H22	1.52	0.57
6:B:87:A:H2'	6:B:87:A:N3	2.19	0.57
13:L:263:ASP:OD2	14:M:199:ARG:NH2	2.33	0.57
5:A:617:ASN:HB2	5:A:622:GLY:O	2.04	0.57
10:G:127:U:P	23:W:547:LYS:NZ	2.78	0.57
5:A:474:ARG:HD2	6:B:14:U:H5'	1.86	0.57
5:A:1072:LEU:HD22	5:A:1087:LEU:HD22	1.86	0.57
7:C:846:VAL:HG22	7:C:887:LEU:HD11	1.86	0.57
11:H:152:G:N2	11:H:153:A:C5	2.73	0.57
11:H:154:C:O2'	11:H:155:C:H5'	2.04	0.57
16:O:72:GLN:CG	16:O:82:GLN:NE2	2.67	0.57
23:W:347:PHE:HD2	23:W:359:TRP:HB2	1.68	0.57
39:K:113:GLN:O	39:K:117:GLN:CA	2.53	0.57
6:B:96:A:C2'	6:B:97:G:H5'	2.34	0.57
11:H:169:C:O5'	11:H:169:C:H6	1.88	0.57
19:S:102:ASN:ND2	19:S:108:ASN:OD1	2.29	0.57
20:T:318:ARG:HD3	20:T:319:THR:HG23	1.87	0.57
25:Z:121:GLU:HB2	25:Z:130:LYS:HD3	1.87	0.57
5:A:798:GLY:HA3	18:R:281:ASN:HD22	1.70	0.57
20:T:272:CYS:HB3	20:T:282:ARG:HG2	1.86	0.57
6:B:78:U:H3'	6:B:78:U:C6	2.40	0.56
11:H:77:C:H2'	11:H:78:C:H6	1.70	0.56
11:H:179:C:H2'	11:H:180:G:C8	2.38	0.56
23:W:258:PRO:CB	23:W:265:LEU:HD13	2.35	0.56
5:A:1193:GLU:HB3	5:A:1231:ARG:HB3	1.86	0.56
5:A:1386:TRP:HB3	38:Y:410:VAL:HG21	1.88	0.56
7:C:172:PHE:CD2	7:C:172:PHE:CE2	2.93	0.56
8:E:239:THR:O	8:E:290:ARG:NH1	2.37	0.56
10:G:136:U:OP2	10:G:136:U:H6	1.88	0.56
11:H:71:C:C2	11:H:72:U:C5	2.94	0.56
11:H:77:C:C2	11:H:78:C:C5	2.93	0.56
11:H:141:C:C2	11:H:142:C:C5	2.94	0.56
11:H:149:A:H2'	11:H:150:U:H6	1.71	0.56
20:T:311:THR:HG22	20:T:327:SER:HB3	1.88	0.56
11:H:181:G:H2'	11:H:182:U:H6	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:27:CYS:SG	16:O:83:THR:OG1	2.63	0.56
6:B:96:A:C4	6:B:97:G:C8	2.93	0.56
11:H:73:C:C2	11:H:74:U:C5	2.94	0.56
11:H:183:G:H2'	11:H:184:C:H6	1.71	0.56
20:T:312:ALA:HB3	20:T:326:LEU:HD12	1.87	0.56
8:E:94:ASN:HB2	8:E:99:CYS:HA	1.88	0.56
11:H:72:U:C2	11:H:73:C:C5	2.94	0.56
11:H:83:A:H2'	11:H:84:C:H6	1.71	0.56
12:J:466:ARG:CA	26:I:607:GLY:HA2	2.29	0.56
5:A:409:ARG:HH11	6:B:25:C:H2'	1.71	0.56
7:C:104:LEU:CB	7:C:172:PHE:CZ	2.89	0.56
11:H:70:C:C2	11:H:71:C:C5	2.93	0.56
11:H:70:C:H2'	11:H:71:C:H6	1.70	0.56
12:J:344:GLN:HG2	14:M:132:LEU:HD21	1.87	0.56
5:A:788:GLN:HG2	5:A:1024:HIS:HB3	1.88	0.56
11:H:57:A:H2'	11:H:58:U:H6	1.70	0.56
11:H:69:U:C2	11:H:70:C:C5	2.94	0.56
11:H:73:C:H2'	11:H:74:U:H6	1.70	0.56
15:N:120:ARG:NH1	15:N:142:CYS:HB3	2.20	0.56
23:W:330:GLY:O	23:W:357:LYS:NZ	2.37	0.56
11:H:152:G:N2	11:H:153:A:C8	2.73	0.56
5:A:112:GLN:HE21	5:A:189:GLU:HA	1.71	0.56
8:E:60:MET:HB3	8:E:353:MET:CB	2.27	0.56
11:H:91:U:C2	11:H:92:U:C5	2.94	0.56
23:W:531:LYS:HG2	23:W:547:LYS:HA	1.88	0.56
25:Z:285:TYR:HD1	25:Z:292:MET:HG2	1.71	0.56
11:H:54:U:C2	11:H:55:U:C5	2.94	0.55
11:H:68:G:H2'	11:H:69:U:H6	1.71	0.55
11:H:150:U:H2'	11:H:151:C:H6	1.71	0.55
16:O:223:LEU:HD22	16:O:285:GLU:HG2	1.86	0.55
18:R:94:GLY:O	19:S:141:ARG:NH1	2.38	0.55
18:R:106:GLN:HG2	18:R:110:LYS:HD3	1.88	0.55
5:A:1986:LEU:HD23	5:A:1986:LEU:O	2.07	0.55
11:H:141:C:H2'	11:H:142:C:H6	1.71	0.55
13:L:59:LYS:HA	14:M:243:VAL:H	1.71	0.55
7:C:813:ARG:NH2	7:C:817:TYR:OH	2.40	0.55
11:H:91:U:H2'	11:H:92:U:H6	1.71	0.55
11:H:150:U:C2	11:H:151:C:C5	2.94	0.55
11:H:183:G:C4	11:H:184:C:C5	2.94	0.55
15:N:40:LYS:CG	15:N:41:ARG:N	2.70	0.55
18:R:91:ASP:OD1	18:R:91:ASP:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1980:GLU:OE1	25:Z:347:PRO:HG2	2.06	0.55
6:B:20:G:H1'	6:B:21:A:H5"	1.89	0.55
6:B:74:U:H5'	6:B:75:G:O5'	2.07	0.55
7:C:488:VAL:HG13	7:C:609:LYS:HE2	1.87	0.55
5:A:1431:ALA:O	5:A:1434:LYS:NZ	2.40	0.55
11:H:40:C:H2'	11:H:41:U:C6	2.40	0.55
11:H:90:A:H2'	11:H:91:U:H6	1.71	0.55
11:H:147:G:C4	11:H:148:C:C5	2.94	0.55
11:H:69:U:H2'	11:H:70:C:H6	1.71	0.55
11:H:88:A:H2'	11:H:89:U:H6	1.70	0.55
5:A:608:LEU:HD13	5:A:632:ALA:HB1	1.87	0.55
5:A:1773:SER:O	5:A:1813:ARG:NH1	2.37	0.55
11:H:54:U:H2'	11:H:55:U:H6	1.71	0.55
11:H:71:C:H2'	11:H:72:U:H6	1.70	0.55
11:H:90:A:C4	11:H:91:U:C5	2.95	0.55
18:R:145:GLU:OE1	18:R:148:ARG:NH2	2.40	0.55
5:A:1593:LEU:HD12	5:A:1664:ILE:HD11	1.89	0.55
7:C:172:PHE:CD1	7:C:172:PHE:CE1	2.95	0.55
8:E:196:VAL:HA	8:E:212:GLY:HA2	1.88	0.55
11:H:149:A:C4	11:H:150:U:C5	2.95	0.55
5:A:293:TRP:HB2	5:A:1136:ARG:HH22	1.71	0.55
5:A:1491:LYS:O	5:A:1710:ASN:ND2	2.40	0.55
5:A:1816:GLN:HE21	5:A:1916:LEU:HD21	1.71	0.55
7:C:312:SER:OG	43:C:1500:GTP:N7	2.40	0.55
11:H:59:A:H2'	11:H:60:U:H6	1.70	0.55
11:H:171:U:H6	11:H:171:U:H5'	1.72	0.55
5:A:909:TYR:HB2	5:A:1033:GLY:HA3	1.89	0.54
5:A:1476:GLN:NE2	25:Z:85:GLN:OE1	2.37	0.54
6:B:85:C:H3'	6:B:85:C:OP1	2.07	0.54
7:C:169:ASP:HB2	7:C:174:GLU:HB3	1.89	0.54
10:G:137:C:H6	10:G:137:C:O5'	1.90	0.54
11:H:68:G:C4	11:H:69:U:C5	2.95	0.54
11:H:181:G:C4	11:H:182:U:C5	2.95	0.54
14:M:226:TYR:O	14:M:230:THR:N	2.39	0.54
26:I:280:GLU:CB	26:I:288:THR:CB	2.85	0.54
7:C:561:LYS:NZ	7:C:614:TYR:O	2.36	0.54
11:H:72:U:H2'	11:H:73:C:H6	1.71	0.54
16:O:239:LEU:O	16:O:296:ARG:NH1	2.34	0.54
23:W:268:THR:HG22	23:W:270:PRO:HD2	1.88	0.54
5:A:680:HIS:NE2	5:A:684:GLU:OE2	2.40	0.54
6:B:100:C:H2'	6:B:101:U:C6	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:172:PHE:CD1	7:C:172:PHE:HA	2.43	0.54
15:N:97:TYR:HA	15:N:120:ARG:HH22	1.72	0.54
23:W:505:HIS:HB2	23:W:527:ASP:HB3	1.88	0.54
10:G:129:G:C3'	23:W:541:LYS:HE3	2.37	0.54
11:H:57:A:C4	11:H:58:U:C5	2.95	0.54
11:H:153:A:C3'	11:H:154:C:C5'	2.86	0.54
16:O:173:CYS:HB3	23:W:206:ALA:HB3	1.89	0.54
5:A:942:PRO:HD3	5:A:1091:TYR:HA	1.88	0.54
11:H:83:A:C4	11:H:84:C:C5	2.95	0.54
11:H:88:A:C4	11:H:89:U:C5	2.95	0.54
41:D:1048:VAL:O	41:D:1050:GLU:N	2.40	0.54
5:A:1980:GLU:OE1	25:Z:347:PRO:CD	2.54	0.54
7:C:143:THR:HG23	7:C:168:THR:HB	1.89	0.54
12:J:214:ILE:HG23	12:J:219:GLU:HB2	1.89	0.54
5:A:361:HIS:NE2	7:C:283:ASP:OD2	2.40	0.54
7:C:104:LEU:CB	7:C:172:PHE:CD1	2.91	0.54
8:E:208:ILE:HG23	8:E:220:TRP:HB2	1.89	0.54
11:H:59:A:C4	11:H:60:U:C5	2.95	0.54
20:T:185:MET:SD	20:T:442:ARG:NH1	2.80	0.54
5:A:1433:ASP:OD1	5:A:1439:ARG:NH2	2.40	0.54
8:E:304:SER:H	8:E:330:ILE:HB	1.72	0.54
22:V:483:GLU:O	22:V:486:THR:OG1	2.24	0.54
5:A:58:LYS:NZ	5:A:479:THR:O	2.34	0.54
5:A:1210:LYS:HG3	22:V:509:LEU:HD13	1.90	0.54
5:A:1945:VAL:HG11	5:A:1990:ASP:OD2	2.02	0.54
20:T:346:ILE:CD1	20:T:356:LEU:HD12	2.36	0.54
5:A:1904:ASP:OD1	24:X:86:ARG:NH2	2.40	0.53
6:B:79:C:H2'	6:B:79:C:O2	2.07	0.53
23:W:442:LEU:HB2	23:W:456:ILE:HB	1.89	0.53
5:A:266:SER:OG	5:A:271:MET:O	2.23	0.53
5:A:579:GLN:HG3	5:A:629:PHE:H	1.74	0.53
5:A:781:ARG:HH21	11:H:24:A:H5"	1.73	0.53
7:C:718:PHE:HB3	7:C:724:TRP:HB3	1.91	0.53
8:E:171:SER:OG	8:E:173:ASP:OD1	2.27	0.53
25:Z:179:MET:O	25:Z:182:VAL:HB	2.08	0.53
25:Z:342:HIS:HB3	25:Z:345:ALA:HB3	1.91	0.53
5:A:1132:LYS:HA	5:A:1139:ARG:HH12	1.73	0.53
5:A:1889:LEU:HB2	5:A:2013:GLY:HA3	1.90	0.53
23:W:257:ILE:HD12	23:W:257:ILE:C	2.25	0.53
5:A:48:LYS:HG3	5:A:49:ARG:HD2	1.90	0.53
5:A:1807:ILE:HB	5:A:1820:LYS:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1942:ALA:CB	5:A:1983:LEU:HD22	2.37	0.53
6:B:78:U:O2'	6:B:79:C:OP1	2.21	0.53
7:C:704:VAL:HG23	7:C:705:VAL:HG22	1.91	0.53
16:O:88:LEU:O	18:R:183:GLN:NE2	2.42	0.53
25:Z:273:LYS:HB3	25:Z:292:MET:HG3	1.90	0.53
5:A:725:PRO:HB2	18:R:272:GLY:HA3	1.90	0.53
12:J:343:GLU:HG3	12:J:369:PHE:HZ	1.73	0.53
7:C:501:ILE:O	7:C:543:ARG:HA	2.09	0.53
20:T:346:ILE:HD12	20:T:356:LEU:CD1	2.38	0.53
22:V:603:LEU:HD12	22:V:639:LEU:HD13	1.91	0.53
6:B:13:C:C2	6:B:65:G:N2	2.77	0.53
19:S:11:PRO:O	19:S:29:TRP:NE1	2.31	0.53
5:A:79:ARG:O	5:A:82:ARG:HB2	2.09	0.53
5:A:829:PRO:O	5:A:882:LYS:NZ	2.38	0.53
7:C:104:LEU:CB	7:C:172:PHE:CE2	2.92	0.53
9:F:28:A:H1'	15:N:40:LYS:O	2.09	0.53
5:A:65:HIS:HD2	15:N:46:LEU:HD22	1.73	0.53
20:T:210:ILE:HG13	20:T:480:ALA:HB2	1.91	0.53
7:C:259:LYS:HG2	43:C:1500:GTP:C6	2.43	0.52
11:H:147:G:H2'	11:H:148:C:C6	2.43	0.52
8:E:160:ALA:HB2	8:E:166:LEU:H	1.72	0.52
11:H:153:A:H3'	11:H:154:C:C5'	2.38	0.52
6:B:96:A:N6	6:B:97:G:O6	2.42	0.52
23:W:265:LEU:HD23	23:W:300:SER:OG	2.08	0.52
25:Z:127:THR:OG1	25:Z:153:GLU:OE1	2.26	0.52
6:B:71:C:H5"	6:B:72:U:C6	2.45	0.52
23:W:392:VAL:HG22	23:W:402:GLN:HG2	1.92	0.52
19:S:41:GLU:OE2	19:S:44:ARG:NH2	2.41	0.52
23:W:427:VAL:HG23	23:W:490:ALA:HB1	1.91	0.52
11:H:39:U:H6	11:H:39:U:H5"	1.72	0.52
20:T:353:THR:HG22	20:T:369:THR:HG22	1.91	0.52
18:R:61:GLY:HA2	19:S:136:ILE:HB	1.90	0.52
25:Z:87:PRO:HB2	25:Z:91:LYS:HD3	1.91	0.52
5:A:57:GLN:NE2	5:A:59:GLU:OE2	2.37	0.52
9:F:14:C:H2'	9:F:15:A:H8	1.73	0.52
10:G:136:U:OP2	10:G:136:U:C6	2.62	0.52
10:G:137:C:C6	10:G:137:C:H5"	2.45	0.52
11:H:108:G:C4	11:H:109:C:C5	2.98	0.52
12:J:355:ARG:HH21	14:M:139:THR:HG23	1.75	0.52
5:A:855:ARG:HD2	5:A:1523:ARG:HH12	1.75	0.52
5:A:2090:ILE:HA	5:A:2223:CYS:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:75:G:C8	6:B:76:A:C8	2.97	0.52
7:C:172:PHE:CE1	7:C:172:PHE:CZ	2.98	0.52
7:C:508:LYS:HE3	7:C:510:LEU:HD21	1.91	0.52
22:V:456:ARG:HG3	22:V:492:MET:HG3	1.92	0.52
23:W:265:LEU:HG	23:W:300:SER:HB2	1.90	0.52
8:E:326:HIS:HD1	8:E:346:SER:HG	1.56	0.51
9:F:22:A:H5"	15:N:115:THR:OG1	2.10	0.51
13:L:526:ARG:CB	13:L:594:PRO:CB	2.88	0.51
23:W:354:ARG:NH1	23:W:373:ARG:O	2.44	0.51
39:K:114:LEU:O	39:K:118:ALA:HB2	2.10	0.51
6:B:99:C:H2'	6:B:100:C:C6	2.45	0.51
11:H:143:A:N3	11:H:143:A:C3'	2.73	0.51
11:H:150:U:O5'	24:X:124:THR:HB	2.10	0.51
5:A:1921:ASP:HB3	5:A:1966:HIS:CD2	2.44	0.51
6:B:46:U:O2	21:U:11:ARG:NH2	2.43	0.51
8:E:80:THR:HA	8:E:93:TRP:O	2.11	0.51
20:T:307:SER:OG	20:T:308:ARG:N	2.44	0.51
23:W:265:LEU:CG	23:W:300:SER:HB2	2.40	0.51
8:E:259:VAL:HB	8:E:277:PHE:HB2	1.92	0.51
13:L:696:LEU:HA	39:K:110:SER:CB	2.40	0.51
23:W:500:LYS:HA	23:W:540:THR:HG21	1.93	0.51
5:A:71:ARG:NH1	15:N:34:THR:HG22	2.26	0.51
5:A:658:ARG:NH1	9:F:67:G:OP1	2.35	0.51
8:E:91:LEU:HD22	8:E:101:ASN:HD21	1.74	0.51
11:H:105:G:N3	11:H:105:G:C2'	2.72	0.51
12:J:466:ARG:CB	26:I:610:ARG:CB	2.89	0.51
5:A:1776:ILE:HB	5:A:1858:PRO:HA	1.92	0.51
10:G:127:U:P	23:W:547:LYS:HZ3	2.33	0.51
11:H:108:G:C4	11:H:109:C:C6	2.98	0.51
23:W:266:ARG:N	23:W:266:ARG:CD	2.73	0.51
26:I:729:SER:O	26:I:732:ALA:HB3	2.09	0.51
10:G:130:A:HO2'	10:G:131:U:P	2.34	0.51
5:A:584:HIS:HE1	42:A:3000:IHP:O22	1.93	0.51
7:C:734:ALA:HB2	7:C:767:VAL:HG22	1.93	0.51
7:C:926:ALA:HA	7:C:929:LEU:HG	1.92	0.51
20:T:477:LEU:HB3	20:T:489:TYR:HB2	1.92	0.51
5:A:552:ARG:NH1	5:A:589:THR:O	2.44	0.51
5:A:711:GLN:HE22	11:H:18:U:H3'	1.76	0.51
12:J:512:GLU:CB	26:I:640:ALA:CA	2.88	0.51
18:R:52:PRO:HB3	18:R:57:ASP:HB3	1.93	0.51
5:A:109:PRO:HG3	5:A:630:TRP:HE1	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:78:U:C6	6:B:78:U:C3'	2.94	0.50
7:C:445:ALA:HA	7:C:448:LYS:HB3	1.93	0.50
23:W:267:SER:O	23:W:268:THR:O	2.28	0.50
7:C:448:LYS:O	7:C:452:THR:HB	2.11	0.50
7:C:622:GLU:OE1	7:C:941:LYS:NZ	2.38	0.50
15:N:18:ILE:HG21	15:N:70:ILE:HD11	1.93	0.50
15:N:120:ARG:NH1	15:N:142:CYS:CB	2.75	0.50
23:W:552:VAL:HG13	23:W:571:TRP:CD1	2.46	0.50
25:Z:122:ASN:O	25:Z:138:ARG:NH2	2.44	0.50
5:A:329:LEU:HD12	7:C:177:ARG:HD2	1.92	0.50
5:A:425:PRO:HG3	6:B:26:A:H5'	1.93	0.50
7:C:104:LEU:CB	7:C:172:PHE:CD2	2.94	0.50
20:T:427:LEU:HB3	20:T:439:TRP:HB2	1.93	0.50
23:W:252:ARG:HD2	23:W:257:ILE:HG22	1.94	0.50
5:A:108:MET:O	5:A:110:TRP:N	2.44	0.50
5:A:663:ARG:NH2	9:F:65:G:N7	2.58	0.50
6:B:74:U:N3	6:B:75:G:C5	2.80	0.50
12:J:294:HIS:CD2	13:L:227:THR:HG1	2.29	0.50
13:L:48:ALA:O	13:L:52:GLU:CB	2.60	0.50
20:T:289:SER:OG	20:T:308:ARG:NE	2.36	0.50
23:W:387:LYS:HD3	23:W:390:LEU:HD12	1.93	0.50
23:W:534:ILE:HB	23:W:544:SER:HB3	1.94	0.50
23:W:541:LYS:NZ	23:W:541:LYS:CB	2.73	0.50
11:H:100:U:H4'	11:H:101:U:H5'	1.93	0.50
16:O:176:GLY:HA2	23:W:206:ALA:HB2	1.94	0.50
16:O:283:ALA:O	16:O:287:SER:HB3	2.11	0.50
5:A:658:ARG:NH2	9:F:65:G:OP2	2.43	0.50
7:C:725:ASP:O	7:C:729:ALA:N	2.43	0.50
10:G:129:G:H4'	23:W:541:LYS:CE	2.41	0.50
20:T:213:GLU:HG3	20:T:218:TRP:CE2	2.47	0.50
8:E:69:VAL:HG11	8:E:351:LEU:HD21	1.94	0.50
10:G:129:G:C4'	23:W:541:LYS:CE	2.90	0.50
11:H:168:A:H3'	11:H:169:C:C5	2.47	0.50
5:A:1318:THR:HB	5:A:1324:GLY:HA3	1.94	0.50
5:A:1676:ILE:HD13	5:A:1706:ASP:HB2	1.93	0.50
7:C:129:ILE:HG22	7:C:199:LEU:HB3	1.93	0.50
8:E:258:THR:HG22	8:E:260:ARG:HG3	1.94	0.50
5:A:160:HIS:HE1	25:Z:170:TRP:HA	1.77	0.50
5:A:161:PHE:CE2	5:A:626:GLY:HA2	2.47	0.50
5:A:1137:ASP:O	5:A:1141:ARG:NH1	2.43	0.50
13:L:65:ARG:NH2	26:I:799:ARG:C	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:530:LYS:NZ	22:V:564:VAL:O	2.45	0.50
5:A:380:LEU:HD12	5:A:384:VAL:HG21	1.92	0.49
5:A:1949:ARG:NH2	24:X:62:GLU:OE1	2.45	0.49
7:C:168:THR:HG23	7:C:184:THR:HB	1.93	0.49
12:J:427:LYS:HE3	26:I:579:LEU:CB	2.36	0.49
12:J:466:ARG:CB	26:I:606:TRP:C	2.80	0.49
5:A:224:THR:N	6:B:12:U:OP1	2.39	0.49
5:A:409:ARG:HE	5:A:413:LEU:HD21	1.77	0.49
7:C:485:ASP:OD1	7:C:485:ASP:N	2.44	0.49
9:F:78:A:OP2	13:L:170:LYS:NZ	2.38	0.49
9:F:85:U:H5'	14:M:193:ARG:HD2	1.94	0.49
11:H:110:A:H2'	11:H:111:G:C2	2.46	0.49
23:W:252:ARG:CG	23:W:252:ARG:NH1	2.73	0.49
39:K:114:LEU:O	39:K:118:ALA:CB	2.60	0.49
7:C:137:HIS:HB3	7:C:140:HIS:CD2	2.47	0.49
7:C:834:VAL:HG21	7:C:883:PHE:HE2	1.78	0.49
18:R:151:LEU:HD22	20:T:323:VAL:HG11	1.92	0.49
5:A:1275:ARG:HD2	5:A:1375:TRP:CE2	2.47	0.49
7:C:171:LEU:HD11	7:C:182:LYS:HD2	1.94	0.49
7:C:774:THR:HA	7:C:784:ILE:HD12	1.94	0.49
5:A:1275:ARG:NH1	5:A:1373:GLN:O	2.39	0.49
5:A:1984:LYS:HG2	5:A:1988:LEU:HD12	1.94	0.49
6:B:79:C:C6	6:B:79:C:C5'	2.95	0.49
9:F:21:U:H1'	15:N:121:VAL:CG2	2.42	0.49
9:F:21:U:O4'	15:N:121:VAL:HG23	2.12	0.49
16:O:26:THR:HG22	16:O:155:PRO:HB3	1.93	0.49
5:A:1972:THR:OG1	5:A:1975:GLU:OE1	2.24	0.49
7:C:476:CYS:HB2	7:C:565:ILE:HB	1.95	0.49
7:C:747:ASP:HB3	7:C:791:ILE:HB	1.94	0.49
10:G:126:C:O3'	23:W:547:LYS:NZ	2.46	0.49
15:N:119:CYS:SG	15:N:139:CYS:HB3	2.53	0.49
23:W:531:LYS:HD3	23:W:547:LYS:HG2	1.93	0.49
16:O:56:ARG:HG2	16:O:67:LYS:HB3	1.95	0.49
28:Q:523:ALA:O	28:Q:532:PRO:HA	2.13	0.49
5:A:118:VAL:HG21	5:A:487:LEU:HD12	1.94	0.49
5:A:1576:ILE:O	5:A:1746:ARG:NH1	2.38	0.49
5:A:1894:GLN:NE2	24:X:69:GLY:O	2.46	0.49
14:M:239:ARG:CG	26:I:817:GLU:CB	2.91	0.49
16:O:34:ILE:HB	18:R:197:ILE:HG12	1.94	0.49
5:A:379:GLU:HG2	7:C:355:LYS:HB3	1.92	0.49
5:A:1215:ASN:HB3	5:A:1224:ARG:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:44:A:O2'	10:G:-5:G:N2	2.43	0.49
14:M:210:TYR:HB3	14:M:219:ASN:HD22	1.78	0.49
17:P:13:ARG:NH1	20:T:329:HIS:O	2.45	0.49
18:R:132:LEU:HA	20:T:399:LYS:HE3	1.95	0.49
20:T:342:GLU:CG	20:T:343:PRO:CD	2.91	0.49
12:J:221:ASN:ND2	13:L:211:ASN:OD1	2.46	0.48
13:L:65:ARG:HE	26:I:803:SER:CB	2.26	0.48
18:R:107:SER:OG	18:R:109:ASP:OD1	2.28	0.48
20:T:339:GLN:NE2	20:T:342:GLU:O	2.45	0.48
5:A:1066:GLN:CG	38:Y:423:THR:O	2.61	0.48
5:A:1615:HIS:HD2	5:A:1616:PRO:HD2	1.78	0.48
7:C:135:CYS:HB2	7:C:242:LEU:HD13	1.95	0.48
7:C:137:HIS:HB2	7:C:239:THR:HG23	1.94	0.48
11:H:107:A:N3	11:H:107:A:C3'	2.74	0.48
20:T:422:ASN:HB3	20:T:424:ASP:H	1.78	0.48
5:A:699:GLU:OE1	18:R:235:ARG:NH2	2.46	0.48
13:L:784:LEU:CB	39:K:195:ILE:CB	2.90	0.48
18:R:74:LEU:HD23	18:R:75:ASP:H	1.76	0.48
5:A:1610:GLN:NE2	5:A:1612:GLU:OE2	2.46	0.48
23:W:258:PRO:CB	23:W:265:LEU:CD1	2.91	0.48
6:B:96:A:C2	6:B:97:G:C4	3.02	0.48
5:A:768:ASP:OD1	6:B:40:U:O2'	2.27	0.48
5:A:854:SER:OG	5:A:855:ARG:N	2.47	0.48
8:E:233:GLY:O	8:E:260:ARG:NH1	2.46	0.48
8:E:92:LEU:HD12	8:E:103:ALA:HB3	1.93	0.48
10:G:136:U:H2'	10:G:137:C:C5	2.49	0.48
20:T:394:ASN:OD1	20:T:396:LYS:NZ	2.47	0.48
5:A:1865:ARG:NH1	10:G:147:C:OP1	2.47	0.48
11:H:101:U:H4'	11:H:102:U:OP1	2.14	0.48
13:L:59:LYS:HG2	14:M:243:VAL:HA	1.96	0.48
16:O:276:THR:HG23	16:O:279:ALA:H	1.78	0.48
8:E:260:ARG:HG2	8:E:276:ILE:HG12	1.96	0.48
11:H:151:C:OP2	24:X:124:THR:N	2.46	0.48
13:L:74:LEU:HD23	13:L:77:LEU:HD12	1.94	0.48
5:A:325:HIS:HD2	5:A:326:HIS:HD2	1.60	0.47
5:A:522:PHE:O	5:A:548:ARG:NH2	2.38	0.47
5:A:1768:TYR:CZ	5:A:2012:LEU:HD11	2.49	0.47
7:C:226:VAL:HA	7:C:254:THR:O	2.14	0.47
5:A:211:GLN:OE1	5:A:214:ARG:NH1	2.47	0.47
5:A:1214:TRP:CE2	5:A:1230:LEU:HD11	2.49	0.47
5:A:1219:GLU:O	5:A:1222:LYS:NZ	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1560:ILE:HG21	5:A:1573:LEU:HD13	1.95	0.47
20:T:248:THR:HB	20:T:266:GLU:HG3	1.95	0.47
28:Q:523:ALA:CB	28:Q:534:ARG:O	2.63	0.47
5:A:356:ILE:HD13	7:C:867:PRO:HD3	1.96	0.47
5:A:1831:LYS:HG2	10:G:2:U:P	2.53	0.47
5:A:1962:THR:HG22	5:A:1969:PRO:HA	1.96	0.47
7:C:440:SER:O	7:C:443:VAL:N	2.47	0.47
11:H:44:U:H2'	11:H:45:C:C6	2.48	0.47
12:J:323:LEU:HD22	14:M:179:ILE:HG22	1.96	0.47
14:M:237:LEU:HD11	18:R:264:LEU:HD22	1.95	0.47
19:S:18:THR:HG22	19:S:159:ILE:HG12	1.96	0.47
7:C:506:PRO:HA	7:C:526:THR:HA	1.96	0.47
7:C:938:ARG:HE	7:C:945:GLU:HA	1.80	0.47
8:E:167:VAL:HB	8:E:179:TRP:HB2	1.96	0.47
11:H:42:G:H8	11:H:42:G:O5'	1.98	0.47
11:H:151:C:C2	11:H:152:G:N7	2.82	0.47
18:R:185:GLY:O	18:R:187:ALA:N	2.47	0.47
23:W:258:PRO:HD2	23:W:266:ARG:NH1	2.28	0.47
5:A:1775:GLN:HG2	5:A:1859:LYS:HD2	1.97	0.47
6:B:93:U:H4'	6:B:94:U:H5"	1.97	0.47
10:G:138:A:H2'	10:G:139:U:C6	2.49	0.47
14:M:221:LYS:HE3	18:R:249:PRO:HB3	1.96	0.47
5:A:1251:SER:O	5:A:1298:ARG:NH2	2.33	0.47
16:O:123:ARG:NH1	18:R:222:PRO:O	2.46	0.47
5:A:62:PRO:HG3	15:N:53:HIS:CD2	2.50	0.47
5:A:425:PRO:HB2	5:A:428:LYS:HB2	1.97	0.47
10:G:129:G:H4'	23:W:541:LYS:HE3	1.95	0.47
11:H:153:A:C8	11:H:154:C:H5'	2.50	0.47
16:O:27:CYS:SG	16:O:66:LYS:NZ	2.81	0.47
20:T:416:ILE:HA	20:T:431:ALA:HA	1.95	0.47
22:V:565:LEU:HG	22:V:568:ILE:HD12	1.95	0.47
9:F:25:C:N4	16:O:39:GLU:OE1	2.47	0.47
10:G:145:U:HO2'	10:G:146:C:P	2.38	0.47
11:H:98:G:N3	11:H:98:G:C3'	2.78	0.47
11:H:141:C:H2'	11:H:142:C:C6	2.50	0.47
11:H:183:G:H2'	11:H:184:C:C6	2.50	0.47
20:T:342:GLU:CG	20:T:343:PRO:HD2	2.37	0.47
8:E:60:MET:CG	8:E:353:MET:SD	2.89	0.47
11:H:91:U:H2'	11:H:92:U:C6	2.50	0.47
11:H:149:A:H2'	11:H:150:U:C6	2.50	0.47
25:Z:133:CYS:SG	25:Z:134:PHE:N	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:143:GLN:NE2	5:A:207:PHE:O	2.45	0.47
5:A:668:VAL:HB	9:F:68:C:H5"	1.96	0.47
5:A:1763:LEU:HG	5:A:1862:ILE:HD13	1.96	0.47
7:C:205:THR:HB	7:C:215:VAL:HG22	1.97	0.47
11:H:41:U:H5"	11:H:41:U:C6	2.35	0.47
16:O:22:ILE:HG23	23:W:112:SER:HB3	1.97	0.47
22:V:470:GLU:OE2	22:V:513:ARG:NH1	2.47	0.47
5:A:1350:ILE:HD12	22:V:470:GLU:HG3	1.97	0.46
5:A:1806:ALA:HA	5:A:1820:LYS:O	2.14	0.46
9:F:82:A:N6	11:H:19:G:OP1	2.48	0.46
10:G:134:U:H5"	10:G:135:G:OP2	2.15	0.46
11:H:38:A:H2'	11:H:39:U:H5"	1.97	0.46
11:H:72:U:H2'	11:H:73:C:C6	2.50	0.46
19:S:52:LYS:HE3	19:S:156:ASP:HA	1.97	0.46
22:V:536:ILE:H	22:V:536:ILE:HG13	1.49	0.46
7:C:448:LYS:O	7:C:452:THR:CB	2.63	0.46
7:C:692:LEU:HD12	7:C:786:ASN:HA	1.96	0.46
13:L:48:ALA:O	13:L:52:GLU:HB3	2.15	0.46
25:Z:334:ALA:O	25:Z:338:GLY:N	2.44	0.46
12:J:466:ARG:CB	26:I:607:GLY:N	2.75	0.46
14:M:239:ARG:CD	26:I:817:GLU:CB	2.92	0.46
23:W:524:ILE:HD11	23:W:558:TRP:HE3	1.79	0.46
5:A:856:LEU:HD23	5:A:860:GLN:HB3	1.97	0.46
7:C:156:GLU:OE2	7:C:167:TYR:OH	2.33	0.46
8:E:326:HIS:CE1	8:E:346:SER:HG	2.32	0.46
11:H:57:A:H2'	11:H:58:U:C6	2.50	0.46
11:H:150:U:H2'	11:H:151:C:C6	2.49	0.46
18:R:127:ALA:HB2	20:T:442:ARG:HD3	1.97	0.46
5:A:103:LEU:HD11	5:A:554:THR:HG22	1.97	0.46
11:H:41:U:H6	11:H:41:U:C5'	2.20	0.46
11:H:90:A:H2'	11:H:91:U:C6	2.50	0.46
11:H:182:U:H2'	11:H:183:G:H8	1.81	0.46
12:J:193:GLN:O	12:J:196:ARG:HB3	2.16	0.46
12:J:221:ASN:HD22	12:J:221:ASN:HA	1.54	0.46
23:W:400:ILE:HD12	23:W:445:TRP:CZ3	2.51	0.46
23:W:506:MET:H	23:W:527:ASP:HB2	1.81	0.46
5:A:976:MET:HG2	5:A:1187:PHE:HB3	1.97	0.46
5:A:1045:GLY:HA3	5:A:1090:ARG:NH2	2.29	0.46
5:A:542:ASN:O	5:A:546:LEU:HB2	2.15	0.46
5:A:944:ASP:HA	5:A:1437:ARG:HE	1.81	0.46
5:A:1312:PRO:HG2	5:A:1314:VAL:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:698:GLU:O	7:C:702:ASN:N	2.49	0.46
8:E:338:ASP:OD1	8:E:338:ASP:N	2.49	0.46
9:F:21:U:OP1	15:N:116:ASN:ND2	2.49	0.46
11:H:70:C:H2'	11:H:71:C:C6	2.49	0.46
11:H:104:U:H4'	11:H:105:G:C4'	2.45	0.46
11:H:108:G:H8	11:H:108:G:P	2.39	0.46
11:H:181:G:H2'	11:H:182:U:C6	2.50	0.46
22:V:539:LEU:HD12	22:V:544:LEU:HD23	1.98	0.46
23:W:400:ILE:HD11	23:W:421:VAL:HG11	1.98	0.46
5:A:320:TYR:OH	7:C:634:GLU:OE2	2.30	0.46
5:A:852:VAL:O	5:A:854:SER:N	2.49	0.46
5:A:1418:ARG:HE	5:A:1464:LEU:HD23	1.80	0.46
8:E:98:ASP:HB3	8:E:100:ASP:OD1	2.16	0.46
11:H:81:G:H2'	11:H:82:G:H8	1.80	0.46
11:H:142:C:H2'	11:H:143:A:H5'	1.98	0.46
14:M:209:ASP:HB2	18:R:263:PRO:HG3	1.98	0.46
41:D:1349:GLY:HA2	41:D:1491:SER:O	2.16	0.46
7:C:935:ILE:O	7:C:939:ARG:N	2.46	0.46
11:H:68:G:H2'	11:H:69:U:C6	2.50	0.46
11:H:69:U:H2'	11:H:70:C:C6	2.49	0.46
11:H:78:C:H2'	11:H:79:G:H8	1.81	0.46
13:L:140:ASP:OD1	13:L:140:ASP:N	2.49	0.46
23:W:434:VAL:HG21	23:W:476:LEU:HD11	1.98	0.46
11:H:152:G:O2'	11:H:153:A:H1'	2.16	0.46
16:O:236:VAL:O	16:O:269:CYS:HA	2.16	0.46
11:H:56:A:H2'	11:H:57:A:H8	1.81	0.45
11:H:104:U:H3'	11:H:104:U:C6	2.49	0.45
26:I:712:VAL:O	26:I:715:GLY:N	2.49	0.45
5:A:359:ILE:HA	7:C:864:PRO:HB3	1.97	0.45
5:A:603:ARG:O	5:A:606:LYS:HB2	2.16	0.45
5:A:1242:ASN:OD1	5:A:1245:ARG:NH2	2.42	0.45
11:H:54:U:H2'	11:H:55:U:C6	2.50	0.45
11:H:71:C:H2'	11:H:72:U:C6	2.50	0.45
5:A:696:MET:HB2	5:A:696:MET:HE3	1.81	0.45
5:A:1382:SER:HA	5:A:1415:GLY:HA2	1.98	0.45
5:A:1945:VAL:HG11	5:A:1990:ASP:CB	2.46	0.45
7:C:104:LEU:CB	7:C:172:PHE:CG	2.97	0.45
7:C:227:LEU:HB3	7:C:255:VAL:HG22	1.98	0.45
9:F:1:G:O2'	15:N:99:ASN:ND2	2.50	0.45
10:G:137:C:C5	10:G:137:C:OP2	2.69	0.45
11:H:102:U:OP2	11:H:102:U:H3'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:171:U:H2'	11:H:172:C:O4'	2.16	0.45
41:D:441:GLY:O	41:D:693:THR:N	2.36	0.45
5:A:2121:ARG:O	5:A:2154:HIS:HA	2.15	0.45
7:C:87:GLN:HE21	20:T:239:LYS:HB3	1.81	0.45
11:H:88:A:H2'	11:H:89:U:C6	2.50	0.45
11:H:92:U:H2'	11:H:93:A:H8	1.82	0.45
18:R:303:GLU:OE2	18:R:307:GLN:NE2	2.49	0.45
8:E:75:HIS:NE2	8:E:121:GLY:O	2.46	0.45
11:H:58:U:H2'	11:H:59:A:H8	1.82	0.45
11:H:74:U:H2'	11:H:75:A:H8	1.81	0.45
11:H:79:G:H2'	11:H:80:A:H8	1.81	0.45
11:H:82:G:H2'	11:H:83:A:H8	1.81	0.45
16:O:280:ALA:HB1	16:O:302:TRP:HH2	1.81	0.45
5:A:338:VAL:HG12	7:C:262:ARG:HH21	1.82	0.45
6:B:96:A:N1	6:B:97:G:C5	2.84	0.45
9:F:22:A:OP2	23:W:130:ARG:NH2	2.50	0.45
10:G:139:U:O4	10:G:140:A:N6	2.50	0.45
11:H:73:C:H2'	11:H:74:U:C6	2.50	0.45
11:H:148:C:H2'	11:H:149:A:H8	1.82	0.45
13:L:28:LYS:NZ	18:R:273:ARG:HH22	2.15	0.45
15:N:118:ILE:CD1	15:N:132:ILE:HG23	2.46	0.45
16:O:68:THR:HA	16:O:83:THR:HG22	1.99	0.45
18:R:94:GLY:HA3	19:S:141:ARG:HD3	1.97	0.45
5:A:1908:LYS:HE3	23:W:448:ASP:HB3	1.98	0.45
7:C:566:THR:OG1	7:C:567:GLU:N	2.50	0.45
7:C:604:LEU:HD23	7:C:607:LEU:HD12	1.98	0.45
8:E:95:VAL:HB	8:E:96:TYR:HD2	1.81	0.45
11:H:89:U:H2'	11:H:90:A:H8	1.82	0.45
11:H:100:U:C6	11:H:100:U:C5'	2.93	0.45
5:A:1980:GLU:OE1	25:Z:347:PRO:CG	2.64	0.45
7:C:158:ARG:HB2	7:C:165:LEU:HB3	1.99	0.45
10:G:120:G:O4'	26:I:316:GLU:O	2.34	0.45
11:H:80:A:H2'	11:H:81:G:H8	1.81	0.45
15:N:118:ILE:H	15:N:118:ILE:HG13	1.62	0.45
16:O:233:THR:HA	16:O:272:ILE:O	2.17	0.45
6:B:69:A:N6	6:B:70:A:N3	2.64	0.45
7:C:94:ILE:H	7:C:94:ILE:HG13	1.45	0.45
7:C:887:LEU:HD23	7:C:897:SER:HB2	1.98	0.45
11:H:67:C:H2'	11:H:68:G:H8	1.81	0.45
19:S:72:ARG:HH22	23:W:74:PRO:HA	1.82	0.45
20:T:373:LYS:HD2	20:T:392:PRO:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:221:ILE:O	7:C:495:ARG:NH1	2.50	0.45
12:J:466:ARG:HA	26:I:606:TRP:C	2.37	0.45
13:L:52:GLU:OE2	13:L:134:THR:OG1	2.34	0.45
13:L:717:MET:O	13:L:721:LEU:N	2.48	0.45
20:T:418:THR:HG21	20:T:468:CYS:H	1.81	0.45
23:W:257:ILE:HG23	23:W:257:ILE:O	2.17	0.45
23:W:267:SER:O	23:W:268:THR:C	2.56	0.45
23:W:514:VAL:HA	23:W:524:ILE:O	2.16	0.45
39:K:112:ALA:O	39:K:116:HIS:CA	2.62	0.45
5:A:1986:LEU:C	5:A:1986:LEU:CD2	2.85	0.44
11:H:106:G:C4'	11:H:107:A:OP1	2.45	0.44
22:V:499:GLN:HG2	25:Z:72:TRP:CG	2.52	0.44
41:D:721:VAL:HA	41:D:825:THR:O	2.17	0.44
8:E:355:GLU:H	23:W:82:ASN:ND2	2.16	0.44
11:H:84:C:H2'	11:H:85:A:H8	1.82	0.44
11:H:93:A:H2'	11:H:94:A:H8	1.82	0.44
17:P:204:GLN:O	17:P:206:LYS:N	2.50	0.44
23:W:420:ALA:O	23:W:438:ASP:N	2.46	0.44
5:A:417:ARG:NH1	6:B:58:U:O3'	2.44	0.44
6:B:20:G:H8	6:B:21:A:H2'	1.81	0.44
7:C:63:LYS:HE3	7:C:65:TYR:HE1	1.82	0.44
9:F:23:U:OP1	15:N:115:THR:HG21	2.17	0.44
11:H:180:G:H2'	11:H:181:G:H8	1.81	0.44
13:L:699:ASN:CB	39:K:114:LEU:CB	2.95	0.44
7:C:112:THR:HG23	7:C:154:HIS:CD2	2.53	0.44
11:H:55:U:H2'	11:H:56:A:H8	1.82	0.44
11:H:59:A:H2'	11:H:60:U:C6	2.50	0.44
11:H:170:C:C6	11:H:170:C:OP2	2.70	0.44
12:J:251:TRP:CE3	12:J:252:GLU:HG3	2.53	0.44
18:R:64:PHE:H	18:R:71:GLN:HE22	1.65	0.44
20:T:405:PHE:O	20:T:405:PHE:CD1	2.70	0.44
23:W:181:PHE:HD1	23:W:200:VAL:HG12	1.83	0.44
23:W:264:ASN:ND2	23:W:267:SER:HB2	2.32	0.44
38:Y:405:MET:CE	38:Y:411:LEU:HD21	2.43	0.44
5:A:348:PRO:HB3	5:A:394:TYR:CZ	2.52	0.44
5:A:1497:THR:OG1	5:A:1499:GLU:OE1	2.26	0.44
42:A:3000:IHP:H3	42:A:3000:IHP:O32	2.17	0.44
11:H:153:A:C2'	11:H:154:C:C5'	2.86	0.44
13:L:55:ASP:HB3	13:L:58:ILE:HG13	2.00	0.44
14:M:162:PRO:HA	14:M:167:LEU:HD12	1.98	0.44
18:R:105:GLY:HA3	18:R:225:PRO:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:294:LEU:HD12	20:T:303:LEU:HD11	2.00	0.44
23:W:462:HIS:CE1	23:W:482:ASP:HB3	2.52	0.44
5:A:89:LEU:O	5:A:92:LEU:HB3	2.18	0.44
5:A:121:HIS:HD2	18:R:207:MET:HG3	1.82	0.44
5:A:721:LYS:O	5:A:781:ARG:NH1	2.51	0.44
5:A:1214:TRP:NE1	5:A:1276:GLU:OE1	2.50	0.44
11:H:83:A:H2'	11:H:84:C:C6	2.49	0.44
19:S:58:LYS:HE2	19:S:144:MET:HG2	2.00	0.44
5:A:620:PRO:HG2	25:Z:134:PHE:HE2	1.83	0.44
5:A:1494:TYR:HB3	5:A:1744:ARG:HD3	2.00	0.44
5:A:2008:ARG:O	5:A:2012:LEU:HB2	2.18	0.44
7:C:82:GLN:HE21	20:T:238:LEU:H	1.66	0.44
7:C:311:SER:HB3	7:C:316:ILE:HB	2.00	0.44
11:H:77:C:H2'	11:H:78:C:C6	2.50	0.44
11:H:143:A:OP2	11:H:143:A:C2	2.71	0.44
18:R:136:ASP:HB3	18:R:138:GLU:H	1.82	0.44
8:E:299:LYS:HE3	8:E:320:LEU:HD13	1.99	0.44
8:E:346:SER:OG	8:E:348:ASP:OD1	2.36	0.44
11:H:169:C:O5'	11:H:169:C:C6	2.70	0.44
15:N:118:ILE:CD1	15:N:132:ILE:CG2	2.95	0.44
9:F:21:U:C1'	15:N:121:VAL:CG2	2.96	0.44
9:F:28:A:C1'	15:N:40:LYS:O	2.66	0.44
11:H:108:G:C5	11:H:109:C:C5	3.06	0.44
11:H:114:A:C8	11:H:114:A:OP2	2.70	0.44
11:H:153:A:H2'	11:H:154:C:H5"	2.00	0.44
12:J:232:GLU:OE2	12:J:267:ARG:NH2	2.44	0.44
12:J:338:GLU:OE2	14:M:164:SER:OG	2.28	0.44
5:A:787:GLU:OE2	5:A:790:ARG:NH2	2.43	0.43
5:A:1286:ASP:OD1	5:A:1354:ARG:NH2	2.51	0.43
11:H:150:U:C4'	24:X:124:THR:HG22	2.48	0.43
11:H:154:C:O2'	11:H:155:C:C5'	2.66	0.43
20:T:354:ILE:HD11	20:T:389:SER:CB	2.48	0.43
5:A:106:MET:HA	5:A:107:PRO:HD3	1.84	0.43
5:A:1199:LYS:HD3	5:A:1206:GLU:HG3	2.00	0.43
8:E:336:HIS:CD2	8:E:337:PRO:HD2	2.52	0.43
9:F:21:U:C1'	15:N:121:VAL:HG23	2.48	0.43
13:L:703:MET:O	13:L:707:ALA:HB3	2.18	0.43
20:T:289:SER:OG	20:T:290:ALA:N	2.51	0.43
26:I:433:ALA:O	26:I:437:CYS:N	2.50	0.43
7:C:101:LYS:HG2	7:C:172:PHE:HE2	1.83	0.43
7:C:107:GLN:HG3	7:C:108:THR:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:143:U:H2'	10:G:145:U:C5	2.53	0.43
20:T:297:HIS:HB2	20:T:302:VAL:HG12	2.00	0.43
5:A:1070:ASP:OD1	5:A:1073:SER:OG	2.28	0.43
7:C:747:ASP:OD1	7:C:747:ASP:N	2.50	0.43
11:H:178:A:N3	11:H:178:A:H2'	2.33	0.43
16:O:133:PRO:HB2	16:O:136:MET:HB3	2.00	0.43
20:T:345:ILE:O	20:T:357:TRP:HD1	2.01	0.43
7:C:134:LEU:HD23	7:C:226:VAL:HB	2.00	0.43
7:C:296:GLU:HB2	7:C:299:ILE:HD11	2.01	0.43
10:G:134:U:H3'	10:G:135:G:H21	1.84	0.43
11:H:104:U:C6	11:H:104:U:C3'	3.01	0.43
11:H:157:G:H2'	11:H:158:G:O4'	2.18	0.43
11:H:166:G:OP2	11:H:166:G:C2	2.72	0.43
7:C:264:ILE:HG12	7:C:378:TYR:CE1	2.53	0.43
9:F:17:C:H2'	9:F:18:A:H8	1.84	0.43
11:H:142:C:O2'	11:H:143:A:H5'	2.18	0.43
12:J:228:ARG:NE	12:J:252:GLU:OE2	2.51	0.43
6:B:74:U:O2	6:B:74:U:H2'	2.18	0.43
12:J:213:LYS:HA	13:L:243:ARG:HA	2.01	0.43
15:N:133:GLU:OE2	15:N:140:ARG:NH2	2.36	0.43
16:O:76:LYS:HG2	23:W:111:LEU:HD22	2.00	0.43
18:R:119:LEU:HD21	18:R:230:MET:HB3	2.01	0.43
19:S:72:ARG:HG3	23:W:72:LEU:HD13	2.00	0.43
5:A:624:GLY:HA2	5:A:625:PRO:HD3	1.69	0.43
5:A:1130:ASN:HB3	5:A:1132:LYS:HE3	2.00	0.43
5:A:1803:ILE:HG13	5:A:1804:ASN:H	1.84	0.43
7:C:242:LEU:HD23	7:C:242:LEU:HA	1.87	0.43
7:C:255:VAL:HG21	7:C:285:VAL:HG11	2.00	0.43
13:L:53:TRP:HD1	13:L:54:LEU:HD12	1.84	0.43
15:N:37:HIS:CG	15:N:37:HIS:O	2.70	0.43
16:O:196:GLN:HE22	16:O:209:VAL:HG23	1.83	0.43
23:W:360:ASP:HB2	23:W:367:ILE:HD11	2.01	0.43
23:W:452:ASP:OD1	23:W:452:ASP:N	2.52	0.43
13:L:227:THR:O	13:L:227:THR:OG1	2.37	0.43
19:S:55:ARG:HH21	19:S:57:ILE:HD11	1.82	0.43
5:A:893:GLU:OE2	5:A:1018:ASN:ND2	2.52	0.43
7:C:669:THR:HG22	7:C:690:GLU:HG3	2.01	0.43
8:E:59:ILE:HD12	8:E:59:ILE:HA	1.87	0.43
8:E:178:LEU:HB2	8:E:188:GLN:HB3	2.01	0.43
8:E:310:TYR:HE1	8:E:322:LYS:HG3	1.84	0.43
13:L:65:ARG:CG	26:I:803:SER:CB	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:125:SER:HB3	18:R:239:VAL:HG22	2.00	0.43
16:O:235:TYR:HD2	16:O:301:LYS:HB2	1.84	0.43
23:W:348:LEU:HD11	23:W:356:LEU:HD21	2.00	0.43
5:A:549:GLU:HB3	5:A:591:MET:HG2	2.00	0.42
8:E:277:PHE:HE1	8:E:317:ARG:HG2	1.83	0.42
11:H:43:U:H2'	11:H:44:U:C6	2.53	0.42
15:N:118:ILE:HD13	15:N:132:ILE:HG21	2.01	0.42
15:N:120:ARG:HA	15:N:120:ARG:HD2	1.43	0.42
7:C:80:ILE:HG22	7:C:82:GLN:HG2	2.01	0.42
7:C:924:GLN:HG3	7:C:932:GLU:HG3	2.01	0.42
8:E:307:ARG:NE	8:E:326:HIS:O	2.42	0.42
10:G:119:G:H4'	10:G:120:G:OP1	2.19	0.42
15:N:40:LYS:HE2	15:N:40:LYS:HB2	1.26	0.42
23:W:258:PRO:CG	23:W:266:ARG:NH1	2.82	0.42
5:A:25:MET:SD	8:E:215:ASN:ND2	2.91	0.42
11:H:106:G:C8	11:H:106:G:C5'	2.96	0.42
22:V:455:PHE:O	22:V:459:ILE:HG12	2.19	0.42
5:A:167:PRO:HA	5:A:168:PRO:HD3	1.90	0.42
5:A:1891:LEU:HD22	5:A:1937:ILE:HD12	2.01	0.42
7:C:160:ARG:NH1	7:C:410:LEU:HD22	2.34	0.42
7:C:711:ARG:NH2	7:C:730:ARG:O	2.37	0.42
11:H:39:U:H2'	11:H:40:C:C6	2.55	0.42
18:R:177:ILE:HG13	18:R:197:ILE:HB	2.01	0.42
23:W:399:LYS:HA	23:W:414:TYR:O	2.19	0.42
23:W:530:GLY:HA2	23:W:552:VAL:HA	2.01	0.42
38:Y:399:LYS:HB2	38:Y:399:LYS:HE3	1.59	0.42
5:A:523:ASN:OD1	5:A:552:ARG:NH2	2.53	0.42
6:B:74:U:C4	6:B:75:G:C6	3.07	0.42
8:E:181:ILE:HG13	8:E:182:ARG:HG3	2.00	0.42
11:H:112:G:H2'	11:H:113:G:C8	2.50	0.42
16:O:31:ASN:O	18:R:195:ARG:NH1	2.52	0.42
17:P:54:VAL:HG13	17:P:59:PHE:HZ	1.83	0.42
22:V:540:GLU:O	22:V:544:LEU:N	2.45	0.42
25:Z:265:LEU:HB3	25:Z:266:ARG:H	1.71	0.42
5:A:569:VAL:HG12	5:A:573:GLN:HB2	2.02	0.42
5:A:793:ASN:HD22	7:C:60:HIS:CD2	2.38	0.42
5:A:1017:ILE:HD11	5:A:1031:ILE:HD11	2.02	0.42
7:C:277:LYS:HD2	7:C:865:GLY:HA3	2.00	0.42
7:C:442:LYS:HG2	7:C:468:CYS:HB2	2.02	0.42
11:H:155:C:H2'	11:H:156:U:H5"	2.02	0.42
15:N:22:LEU:HD23	15:N:22:LEU:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:121:VAL:HA	15:N:122:PRO:HD3	1.88	0.42
23:W:258:PRO:CG	23:W:265:LEU:HD13	2.49	0.42
25:Z:84:HIS:ND1	25:Z:85:GLN:OE1	2.53	0.42
5:A:1260:VAL:HG21	5:A:1325:LEU:HB3	2.01	0.42
7:C:264:ILE:HG21	7:C:381:LEU:HD12	2.01	0.42
8:E:96:TYR:N	8:E:96:TYR:CD2	2.88	0.42
13:L:83:ARG:HA	13:L:83:ARG:HD3	1.87	0.42
5:A:67:ARG:HD2	15:N:33:GLU:OE2	2.20	0.42
5:A:451:LEU:HD23	5:A:451:LEU:HA	1.89	0.42
5:A:1275:ARG:NH2	5:A:1464:LEU:O	2.43	0.42
8:E:60:MET:C	8:E:60:MET:SD	2.96	0.42
8:E:95:VAL:C	8:E:96:TYR:CD2	2.93	0.42
12:J:287:MET:HB3	14:M:186:LEU:HD11	2.00	0.42
12:J:311:GLN:HG3	14:M:131:GLN:HG2	2.02	0.42
15:N:22:LEU:HD11	15:N:60:ILE:HD11	2.02	0.42
18:R:113:TYR:OH	20:T:402:ASP:O	2.33	0.42
26:I:712:VAL:O	26:I:713:ARG:C	2.57	0.42
5:A:156:ARG:HD3	25:Z:153:GLU:HG2	2.02	0.42
5:A:723:ASN:ND2	5:A:788:GLN:OE1	2.52	0.42
10:G:137:C:OP2	10:G:137:C:H5	2.02	0.42
14:M:176:THR:HA	14:M:179:ILE:HG12	2.02	0.42
38:Y:411:LEU:HD23	38:Y:411:LEU:HA	1.84	0.42
5:A:546:LEU:HD22	5:A:648:LEU:HD11	2.02	0.42
5:A:1507:SER:HB2	5:A:1511:GLU:HG3	2.01	0.42
6:B:63:A:H2'	6:B:64:G:C8	2.55	0.42
9:F:22:A:C8	15:N:121:VAL:HG21	2.54	0.42
10:G:142:U:HO2'	10:G:143:U:P	2.38	0.42
15:N:102:CYS:HB3	15:N:104:ARG:H	1.84	0.42
18:R:175:GLN:NE2	18:R:176:TYR:O	2.52	0.42
19:S:102:ASN:H	19:S:126:HIS:CE1	2.38	0.42
20:T:371:HIS:NE2	20:T:389:SER:OG	2.35	0.42
22:V:459:ILE:HD12	22:V:489:LEU:HD23	2.00	0.42
25:Z:79:ARG:O	25:Z:81:THR:N	2.53	0.42
5:A:533:LYS:NZ	10:G:5:G:OP2	2.34	0.41
5:A:1772:PHE:HB3	25:Z:320:ASP:HB2	2.01	0.41
6:B:78:U:HO2'	6:B:79:C:P	2.37	0.41
7:C:62:ASP:OD1	7:C:62:ASP:N	2.33	0.41
7:C:131:ASN:HB3	7:C:222:SER:HA	2.01	0.41
8:E:81:LEU:HB2	8:E:93:TRP:HB2	2.02	0.41
8:E:161:ARG:HH22	8:E:243:LEU:HD12	1.85	0.41
12:J:242:ILE:HD13	12:J:275:ASN:ND2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:314:ILE:CD1	20:T:326:LEU:HD21	2.47	0.41
20:T:329:HIS:ND1	20:T:349:SER:CB	2.82	0.41
23:W:475:TRP:CD1	23:W:489:GLY:HA2	2.55	0.41
5:A:1807:ILE:HG12	5:A:1841:THR:HG23	2.02	0.41
7:C:623:GLU:H	7:C:941:LYS:NZ	2.14	0.41
8:E:340:PRO:HB2	8:E:356:ILE:HB	2.01	0.41
10:G:21:A:N6	16:O:91:GLY:O	2.43	0.41
13:L:262:LYS:HE3	13:L:266:HIS:CE1	2.55	0.41
19:S:20:MET:HG3	19:S:142:VAL:HG22	2.02	0.41
21:U:23:LEU:HD12	22:V:477:LEU:HD13	2.02	0.41
23:W:305:LEU:HD21	23:W:313:ILE:HG23	2.02	0.41
26:I:296:PHE:CB	26:I:305:SER:O	2.68	0.41
5:A:99:VAL:HG13	5:A:554:THR:HG21	2.02	0.41
5:A:531:THR:HG23	5:A:534:GLU:H	1.84	0.41
5:A:620:PRO:HG2	25:Z:134:PHE:CE2	2.55	0.41
5:A:762:ARG:NH2	17:P:227:TYR:OH	2.53	0.41
5:A:1490:PHE:O	5:A:1493:THR:OG1	2.35	0.41
5:A:1976:TRP:HA	5:A:1979:VAL:HG22	2.03	0.41
13:L:699:ASN:HA	39:K:114:LEU:CB	2.50	0.41
14:M:212:ASN:HB3	14:M:215:ASN:H	1.85	0.41
23:W:126:GLU:HB3	23:W:130:ARG:NH1	2.35	0.41
5:A:866:LEU:HD12	5:A:913:PRO:HB2	2.02	0.41
5:A:1174:PHE:HE2	5:A:1176:SER:HB2	1.85	0.41
11:H:113:G:C2'	11:H:114:A:H5'	2.50	0.41
19:S:24:VAL:HB	19:S:134:GLN:HB3	2.02	0.41
5:A:506:LEU:O	5:A:510:ARG:CB	2.68	0.41
5:A:955:TRP:HE1	5:A:976:MET:HE3	1.85	0.41
8:E:294:SER:HB3	8:E:299:LYS:HB2	2.02	0.41
11:H:43:U:OP2	11:H:43:U:C6	2.74	0.41
11:H:151:C:OP1	24:X:124:THR:N	2.54	0.41
5:A:764:GLY:HA2	5:A:1245:ARG:NH1	2.36	0.41
7:C:441:PRO:O	7:C:445:ALA:HB2	2.20	0.41
11:H:157:G:H5"	11:H:157:G:C8	2.50	0.41
39:K:18:TYR:CB	39:K:168:LYS:HA	2.50	0.41
5:A:555:LYS:NZ	5:A:559:ASP:OD2	2.43	0.41
6:B:70:A:H5"	6:B:70:A:H8	1.85	0.41
23:W:84:THR:O	23:W:87:THR:OG1	2.35	0.41
10:G:163:C:H2'	10:G:164:A:O4'	2.20	0.41
11:H:37:U:H2'	11:H:38:A:H8	1.85	0.41
15:N:120:ARG:HH11	15:N:142:CYS:HB2	1.86	0.41
16:O:240:GLY:H	16:O:268:GLN:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:707:ARG:HG2	17:P:9:PHE:CZ	2.56	0.41
5:A:835:ASP:OD1	5:A:921:TYR:OH	2.33	0.41
5:A:1088:PHE:HD1	5:A:1097:ILE:HG12	1.85	0.41
5:A:1590:VAL:HG22	5:A:1664:ILE:HD12	2.03	0.41
5:A:2332:ASP:O	5:A:2334:TYR:N	2.54	0.41
7:C:87:GLN:HA	7:C:88:PRO:HD2	1.97	0.41
7:C:743:ASN:HB3	7:C:770:PHE:CZ	2.56	0.41
11:H:152:G:H2'	11:H:153:A:C1'	2.51	0.41
16:O:110:SER:OG	16:O:113:ASN:ND2	2.53	0.41
23:W:97:ASN:OD1	23:W:97:ASN:N	2.54	0.41
23:W:304:LEU:HD11	23:W:567:ILE:HG21	2.02	0.41
23:W:387:LYS:NZ	23:W:430:ASN:OD1	2.49	0.41
23:W:393:ALA:HB3	23:W:403:TRP:HZ3	1.86	0.41
25:Z:178:HIS:O	25:Z:181:ILE:HB	2.21	0.41
41:D:538:ILE:O	41:D:585:ILE:HA	2.21	0.41
41:D:577:LYS:O	41:D:581:SER:N	2.54	0.41
5:A:192:GLN:H	5:A:192:GLN:HG2	1.69	0.41
5:A:1790:ILE:HD13	24:X:76:SER:HB2	2.03	0.41
7:C:618:THR:HB	7:C:630:LEU:HB2	2.03	0.41
7:C:637:LEU:HD23	7:C:637:LEU:HA	1.94	0.41
7:C:833:PHE:HB2	7:C:902:HIS:ND1	2.36	0.41
9:F:17:C:H2'	9:F:18:A:C8	2.56	0.41
11:H:102:U:OP2	11:H:102:U:H2'	2.21	0.41
20:T:366:VAL:HG21	20:T:402:ASP:HA	2.03	0.41
23:W:341:ASN:HB3	23:W:344:GLY:H	1.86	0.41
5:A:913:PRO:HA	5:A:916:LYS:HD3	2.04	0.40
5:A:1244:VAL:HG11	5:A:1291:CYS:HB3	2.03	0.40
5:A:1820:LYS:HD3	5:A:1914:MET:HE1	2.02	0.40
5:A:1946:ASN:HD22	5:A:1986:LEU:HD21	1.83	0.40
7:C:101:LYS:HG2	7:C:172:PHE:CE2	2.56	0.40
7:C:112:THR:H	7:C:155:PRO:HD2	1.87	0.40
7:C:169:ASP:OD1	7:C:169:ASP:N	2.54	0.40
7:C:843:VAL:HG13	7:C:871:ILE:HD11	2.03	0.40
11:H:152:G:H2'	11:H:152:G:N3	2.36	0.40
11:H:153:A:C8	11:H:154:C:O4'	2.74	0.40
12:J:493:ALA:CB	12:J:499:ARG:CB	2.96	0.40
16:O:230:THR:H	16:O:277:ARG:NH1	2.18	0.40
19:S:136:ILE:HA	19:S:139:VAL:HG12	2.03	0.40
20:T:193:PRO:HD2	20:T:495:ALA:HB1	2.03	0.40
20:T:483:ASP:OD1	20:T:485:THR:OG1	2.34	0.40
25:Z:106:VAL:HG12	25:Z:153:GLU:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:162:ASP:HB2	25:Z:165:GLY:H	1.85	0.40
5:A:1591:MET:HE3	5:A:1595:GLN:HG3	2.03	0.40
6:B:85:C:H3'	6:B:85:C:P	2.61	0.40
7:C:706:GLN:HG3	7:C:707:ILE:H	1.86	0.40
8:E:253:ASN:HB3	8:E:259:VAL:HG13	2.02	0.40
8:E:295:PRO:HG3	8:E:337:PRO:HA	2.03	0.40
16:O:64:ARG:HD2	16:O:163:HIS:CE1	2.56	0.40
17:P:66:ARG:HH22	20:T:217:GLN:HE22	1.68	0.40
19:S:25:LEU:HA	19:S:132:VAL:HA	2.03	0.40
23:W:162:ASN:HB3	23:W:165:LEU:HG	2.03	0.40
5:A:155:LYS:HZ3	5:A:624:GLY:H	1.69	0.40
5:A:1241:HIS:HB2	5:A:1287:LEU:HD21	2.02	0.40
5:A:1590:VAL:HG11	5:A:1614:ILE:HD11	2.04	0.40
7:C:104:LEU:HG	7:C:172:PHE:CD2	2.56	0.40
7:C:231:ALA:O	7:C:277:LYS:HE3	2.21	0.40
7:C:263:LEU:HD23	7:C:267:LEU:HD12	2.02	0.40
11:H:149:A:C6	11:H:150:U:C4	3.09	0.40
11:H:183:G:C6	11:H:184:C:N4	2.89	0.40
15:N:70:ILE:HG12	15:N:74:LEU:HD23	2.03	0.40
20:T:314:ILE:O	20:T:323:VAL:N	2.54	0.40
5:A:1803:ILE:O	5:A:1824:THR:HG22	2.22	0.40
7:C:104:LEU:CG	7:C:172:PHE:CE2	3.01	0.40
7:C:506:PRO:HG2	7:C:568:PRO:HG3	2.03	0.40
11:H:57:A:C6	11:H:58:U:C4	3.10	0.40
13:L:176:LEU:HD22	23:W:440:LYS:HE3	2.04	0.40
18:R:91:ASP:HB3	18:R:97:LYS:HE3	2.02	0.40
19:S:142:VAL:HG13	19:S:157:VAL:HG11	2.04	0.40
20:T:438:LEU:HB2	20:T:448:GLN:HB3	2.03	0.40
26:I:729:SER:HA	26:I:732:ALA:HB3	2.04	0.40
41:D:420:SER:CB	41:D:622:ASP:HA	2.52	0.40
5:A:156:ARG:NH1	25:Z:153:GLU:OE2	2.55	0.40
5:A:796:LYS:HD3	18:R:279:HIS:HE1	1.87	0.40
5:A:1330:MET:HG3	5:A:1367:ASN:OD1	2.21	0.40
5:A:1403:LEU:HD23	5:A:1403:LEU:HA	1.92	0.40
7:C:104:LEU:HB3	7:C:172:PHE:CZ	2.56	0.40
8:E:95:VAL:C	8:E:96:TYR:HD2	2.25	0.40
8:E:95:VAL:HG23	8:E:96:TYR:H	1.85	0.40
8:E:282:HIS:NE2	8:E:289:LEU:HD12	2.36	0.40
20:T:320:LYS:HB2	20:T:320:LYS:HE3	1.85	0.40
26:I:520:ILE:O	26:I:524:TYR:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	v	142/148 (96%)	138 (97%)	4 (3%)	0	100 100
2	w	89/174 (51%)	87 (98%)	1 (1%)	1 (1%)	12 44
3	u	384/411 (93%)	372 (97%)	9 (2%)	3 (1%)	16 51
4	x	23/703 (3%)	22 (96%)	1 (4%)	0	100 100
5	A	2247/2335 (96%)	2091 (93%)	147 (6%)	9 (0%)	30 66
7	C	892/972 (92%)	798 (90%)	90 (10%)	4 (0%)	30 66
8	E	301/357 (84%)	273 (91%)	28 (9%)	0	100 100
12	J	530/848 (62%)	491 (93%)	32 (6%)	7 (1%)	10 39
13	L	436/802 (54%)	405 (93%)	27 (6%)	4 (1%)	14 49
14	M	128/243 (53%)	124 (97%)	3 (2%)	1 (1%)	16 51
15	N	141/144 (98%)	126 (89%)	13 (9%)	2 (1%)	9 37
16	O	283/420 (67%)	260 (92%)	22 (8%)	1 (0%)	30 66
17	P	104/229 (45%)	86 (83%)	15 (14%)	3 (3%)	3 20
18	R	255/536 (48%)	229 (90%)	24 (9%)	2 (1%)	16 51
19	S	157/166 (95%)	148 (94%)	9 (6%)	0	100 100
20	T	311/514 (60%)	281 (90%)	23 (7%)	7 (2%)	5 26
21	U	24/2752 (1%)	23 (96%)	1 (4%)	0	100 100
22	V	444/908 (49%)	429 (97%)	14 (3%)	1 (0%)	44 77
23	W	506/579 (87%)	441 (87%)	60 (12%)	5 (1%)	13 46
24	X	90/184 (49%)	84 (93%)	6 (7%)	0	100 100
25	Z	238/586 (41%)	214 (90%)	24 (10%)	0	100 100
26	I	498/855 (58%)	481 (97%)	10 (2%)	7 (1%)	9 37
27	y	77/301 (26%)	75 (97%)	2 (3%)	0	100 100
28	Q	1308/1485 (88%)	1282 (98%)	26 (2%)	0	100 100
29	a	77/126 (61%)	76 (99%)	1 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
29	h	77/126 (61%)	76 (99%)	1 (1%)	0	100 100
30	b	84/231 (36%)	82 (98%)	2 (2%)	0	100 100
30	i	84/231 (36%)	82 (98%)	2 (2%)	0	100 100
31	c	80/119 (67%)	77 (96%)	3 (4%)	0	100 100
31	j	80/119 (67%)	77 (96%)	3 (4%)	0	100 100
32	d	95/118 (80%)	91 (96%)	4 (4%)	0	100 100
32	k	81/118 (69%)	78 (96%)	3 (4%)	0	100 100
33	f	72/86 (84%)	69 (96%)	3 (4%)	0	100 100
33	m	71/86 (83%)	68 (96%)	3 (4%)	0	100 100
34	e	77/92 (84%)	76 (99%)	1 (1%)	0	100 100
34	l	77/92 (84%)	76 (99%)	1 (1%)	0	100 100
35	g	72/76 (95%)	70 (97%)	2 (3%)	0	100 100
35	n	65/76 (86%)	59 (91%)	4 (6%)	2 (3%)	3 19
36	o	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	10 39
37	p	92/225 (41%)	90 (98%)	2 (2%)	0	100 100
38	Y	709/1220 (58%)	616 (87%)	61 (9%)	32 (4%)	2 12
39	K	144/225 (64%)	129 (90%)	8 (6%)	7 (5%)	2 10
40	q	130/504 (26%)	119 (92%)	7 (5%)	4 (3%)	3 19
40	r	129/504 (26%)	119 (92%)	8 (6%)	2 (2%)	8 34
40	s	65/504 (13%)	62 (95%)	2 (3%)	1 (2%)	8 36
40	t	65/504 (13%)	64 (98%)	0	1 (2%)	8 36
41	D	1720/2136 (80%)	1633 (95%)	84 (5%)	3 (0%)	44 77
All	All	13914/24425 (57%)	12995 (93%)	808 (6%)	111 (1%)	19 51

All (111) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	u	383	ASN
15	N	36	PRO
18	R	233	PRO
20	T	343	PRO
20	T	458	SER
23	W	268	THR
26	I	463	PRO

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Mol	Chain	Res	Type
26	I	721	LYS
26	I	797	PHE
38	Y	531	MET
38	Y	610	ARG
38	Y	855	VAL
38	Y	944	ASP
38	Y	995	MET
38	Y	1090	LYS
38	Y	1098	LYS
38	Y	1099	SER
38	Y	1129	ASP
38	Y	1145	GLN
38	Y	1164	GLU
39	K	78	PRO
39	K	90	PRO
39	K	135	TRP
40	q	59	HIS
40	q	60	PRO
40	s	71	ILE
40	t	69	THR
41	D	957	VAL
41	D	1584	ILE
2	w	115	GLY
3	u	340	GLY
3	u	385	ASP
7	C	94	ILE
12	J	188	GLN
12	J	241	VAL
12	J	709	VAL
13	L	765	ARG
15	N	37	HIS
17	P	205	LYS
18	R	186	VAL
23	W	243	VAL
23	W	258	PRO
26	I	618	ARG
26	I	634	ILE
36	o	160	LYS
38	Y	517	GLU
38	Y	845	SER
38	Y	870	GLY
38	Y	1182	LYS

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Mol	Chain	Res	Type
39	K	136	LYS
39	K	172	LEU
40	q	9	ASN
12	J	205	LEU
17	P	48	GLN
20	T	186	PRO
20	T	328	GLY
26	I	752	ALA
35	n	6	PRO
38	Y	524	ASN
38	Y	550	TYR
38	Y	806	GLU
38	Y	994	ILE
38	Y	1055	ASN
38	Y	1056	LYS
40	q	19	PRO
40	r	9	ASN
5	A	1092	ILE
5	A	1190	CYS
12	J	604	PRO
13	L	585	TYR
20	T	406	ILE
23	W	74	PRO
26	I	617	GLU
35	n	8	GLU
36	o	32	PRO
38	Y	590	THR
38	Y	663	ASP
38	Y	722	ALA
38	Y	835	VAL
39	K	65	ILE
5	A	56	ALA
5	A	108	MET
5	A	570	ASP
12	J	341	PRO
14	M	125	SER
22	V	597	PRO
38	Y	811	PRO
5	A	109	PRO
5	A	853	LYS
5	A	1503	TRP
13	L	763	ILE

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Mol	Chain	Res	Type
16	O	20	PHE
17	P	11	PRO
38	Y	523	ALA
38	Y	856	ASP
38	Y	1157	THR
7	C	87	GLN
7	C	441	PRO
13	L	764	PRO
38	Y	738	PRO
38	Y	1137	PRO
39	K	17	PRO
40	r	65	PRO
5	A	852	VAL
12	J	206	LEU
20	T	185	MET
20	T	401	PRO
38	Y	521	ILE
23	W	271	PRO
41	D	585	ILE
7	C	440	SER

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	1795/2108 (85%)	1780 (99%)	15 (1%)	79 90
7	C	793/866 (92%)	786 (99%)	7 (1%)	75 89
8	E	259/300 (86%)	254 (98%)	5 (2%)	52 79
12	J	241/751 (32%)	239 (99%)	2 (1%)	79 90
13	L	208/709 (29%)	204 (98%)	4 (2%)	52 79
14	M	117/209 (56%)	113 (97%)	4 (3%)	32 66
15	N	130/130 (100%)	124 (95%)	6 (5%)	23 56
16	O	255/361 (71%)	250 (98%)	5 (2%)	50 78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	P	99/203 (49%)	98 (99%)	1 (1%)	73 88
18	R	219/457 (48%)	212 (97%)	7 (3%)	34 67
19	S	129/134 (96%)	129 (100%)	0	100 100
20	T	269/441 (61%)	261 (97%)	8 (3%)	36 69
21	U	21/2432 (1%)	20 (95%)	1 (5%)	21 55
22	V	140/838 (17%)	136 (97%)	4 (3%)	37 70
23	W	447/502 (89%)	434 (97%)	13 (3%)	37 70
24	X	62/157 (40%)	57 (92%)	5 (8%)	9 34
25	Z	214/520 (41%)	210 (98%)	4 (2%)	52 79
38	Y	8/1085 (1%)	5 (62%)	3 (38%)	0 0
All	All	5406/12203 (44%)	5312 (98%)	94 (2%)	56 81

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	258	PHE
5	A	409	ARG
5	A	623	LYS
5	A	642	ARG
5	A	762	ARG
5	A	994	ASN
5	A	1090	ARG
5	A	1341	ARG
5	A	1393	ARG
5	A	1402	ARG
5	A	1543	ASN
5	A	1763	LEU
5	A	1774	ASN
5	A	1984	LYS
5	A	1985	ASP
7	C	105	MET
7	C	158	ARG
7	C	256	CYS
7	C	297	ASN
7	C	308	CYS
7	C	495	ARG
7	C	678	THR
8	E	54	SER

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Mol	Chain	Res	Type
8	E	56	GLN
8	E	59	ILE
8	E	60	MET
8	E	99	CYS
12	J	201	ARG
12	J	221	ASN
13	L	41	LYS
13	L	181	ARG
13	L	227	THR
13	L	240	ARG
14	M	181	ARG
14	M	184	ILE
14	M	212	ASN
14	M	215	ASN
15	N	38	GLU
15	N	40	LYS
15	N	119	CYS
15	N	120	ARG
15	N	121	VAL
15	N	130	ARG
16	O	45	CYS
16	O	73	THR
16	O	75	SER
16	O	147	LEU
16	O	222	ARG
17	P	212	ASN
18	R	74	LEU
18	R	78	ARG
18	R	95	LYS
18	R	212	PHE
18	R	258	LYS
18	R	276	GLN
18	R	312	MET
20	T	327	SER
20	T	339	GLN
20	T	342	GLU
20	T	344	GLN
20	T	356	LEU
20	T	404	SER
20	T	406	ILE
20	T	412	HIS
21	U	23	LEU

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Mol	Chain	Res	Type
22	V	458	THR
22	V	539	LEU
22	V	583	VAL
22	V	597	PRO
23	W	129	ARG
23	W	182	LYS
23	W	252	ARG
23	W	257	ILE
23	W	260	ASP
23	W	266	ARG
23	W	322	ARG
23	W	492	ASN
23	W	495	ARG
23	W	500	LYS
23	W	529	ASN
23	W	541	LYS
23	W	552	VAL
24	X	103	GLN
24	X	104	LYS
24	X	105	LEU
24	X	109	PHE
24	X	113	LEU
25	Z	116	ARG
25	Z	122	ASN
25	Z	164	ASP
25	Z	166	LYS
38	Y	404	GLN
38	Y	405	MET
38	Y	411	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	97	HIS
5	A	160	HIS
5	A	181	ASN
5	A	270	ASN
5	A	294	ASN
5	A	326	HIS
5	A	328	HIS
5	A	579	GLN
5	A	617	ASN

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Mol	Chain	Res	Type
5	A	723	ASN
5	A	775	ASN
5	A	994	ASN
5	A	1069	ASN
5	A	1075	GLN
5	A	1460	HIS
5	A	1615	HIS
5	A	1717	ASN
5	A	1774	ASN
5	A	1816	GLN
5	A	1946	ASN
7	C	60	HIS
7	C	82	GLN
7	C	154	HIS
7	C	297	ASN
7	C	548	ASN
7	C	627	HIS
7	C	642	HIS
7	C	924	GLN
8	E	56	GLN
8	E	94	ASN
8	E	101	ASN
8	E	202	ASN
8	E	287	ASN
12	J	221	ASN
12	J	238	ASN
12	J	331	GLN
12	J	347	HIS
13	L	211	ASN
13	L	266	HIS
14	M	212	ASN
15	N	99	ASN
16	O	72	GLN
16	O	82	GLN
16	O	163	HIS
16	O	251	HIS
17	P	29	GLN
17	P	212	ASN
18	R	71	GLN
18	R	175	GLN
18	R	276	GLN
18	R	279	HIS

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Mol	Chain	Res	Type
19	S	134	GLN
20	T	278	ASN
20	T	339	GLN
20	T	384	HIS
20	T	446	ASN
23	W	82	ASN
23	W	103	GLN
23	W	119	HIS
23	W	462	HIS
23	W	492	ASN
23	W	529	ASN
24	X	103	GLN
24	X	116	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	G	82/273 (30%)	44 (53%)	7 (8%)
11	H	133/188 (70%)	45 (33%)	9 (6%)
6	B	96/117 (82%)	46 (47%)	8 (8%)
9	F	96/107 (89%)	33 (34%)	6 (6%)
All	All	407/685 (59%)	168 (41%)	30 (7%)

All (168) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	B	9	G
6	B	10	U
6	B	13	C
6	B	19	A
6	B	20	G
6	B	21	A
6	B	22	U
6	B	24	G
6	B	25	C
6	B	26	A
6	B	28	A
6	B	33	U
6	B	36	C
6	B	38	C
6	B	40	U

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Mol	Chain	Res	Type
6	B	45	C
6	B	47	A
6	B	52	U
6	B	57	G
6	B	66	A
6	B	67	A
6	B	71	C
6	B	72	U
6	B	73	C
6	B	74	U
6	B	75	G
6	B	76	A
6	B	77	G
6	B	78	U
6	B	79	C
6	B	80	U
6	B	81	U
6	B	82	A
6	B	83	A
6	B	84	C
6	B	85	C
6	B	86	C
6	B	87	A
6	B	88	A
6	B	89	U
6	B	90	U
6	B	91	U
6	B	92	U
6	B	94	U
6	B	95	G
6	B	96	A
9	F	6	C
9	F	7	G
9	F	9	U
9	F	10	U
9	F	12	G
9	F	26	U
9	F	27	A
9	F	28	A
9	F	29	A
9	F	33	G
9	F	34	G

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Mol	Chain	Res	Type
9	F	37	C
9	F	38	G
9	F	46	G
9	F	49	G
9	F	51	U
9	F	54	G
9	F	58	G
9	F	59	G
9	F	60	C
9	F	61	C
9	F	68	C
9	F	69	A
9	F	74	U
9	F	79	C
9	F	81	C
9	F	82	A
9	F	83	A
9	F	84	A
9	F	85	U
9	F	86	U
9	F	87	C
9	F	89	U
10	G	-11	G
10	G	-7	C
10	G	-6	C
10	G	-1	G
10	G	2	U
10	G	5	G
10	G	8	C
10	G	11	A
10	G	13	C
10	G	17	U
10	G	18	A
10	G	21	A
10	G	22	C
10	G	23	U
10	G	25	G
10	G	27	U
10	G	120	G
10	G	123	U
10	G	124	U
10	G	125	C

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Mol	Chain	Res	Type
10	G	126	C
10	G	127	U
10	G	128	U
10	G	129	G
10	G	130	A
10	G	131	U
10	G	134	U
10	G	135	G
10	G	136	U
10	G	137	C
10	G	138	A
10	G	139	U
10	G	140	A
10	G	141	C
10	G	142	U
10	G	143	U
10	G	144	A
10	G	145	U
10	G	146	C
10	G	149	G
10	G	163	C
10	G	164	A
10	G	166	A
10	G	167	G
11	H	14	C
11	H	15	U
11	H	16	U
11	H	17	U
11	H	19	G
11	H	20	G
11	H	24	A
11	H	25	G
11	H	29	A
11	H	30	A
11	H	31	G
11	H	33	G
11	H	38	A
11	H	39	U
11	H	40	C
11	H	41	U
11	H	42	G
11	H	43	U

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Mol	Chain	Res	Type
11	H	98	G
11	H	99	A
11	H	100	U
11	H	101	U
11	H	102	U
11	H	103	U
11	H	104	U
11	H	105	G
11	H	106	G
11	H	107	A
11	H	111	G
11	H	112	G
11	H	114	A
11	H	115	G
11	H	143	A
11	H	147	G
11	H	152	G
11	H	153	A
11	H	154	C
11	H	156	U
11	H	157	G
11	H	168	A
11	H	170	C
11	H	171	U
11	H	177	A
11	H	178	A
11	H	179	C

All (30) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	B	20	G
6	B	21	A
6	B	78	U
6	B	79	C
6	B	80	U
6	B	88	A
6	B	92	U
6	B	95	G
9	F	5	U
9	F	25	C
9	F	26	U

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Mol	Chain	Res	Type
9	F	33	G
9	F	50	A
9	F	58	G
10	G	-12	G
10	G	1	G
10	G	16	G
10	G	21	A
10	G	137	C
10	G	138	A
10	G	142	U
11	H	29	A
11	H	39	U
11	H	40	C
11	H	100	U
11	H	104	U
11	H	105	G
11	H	106	G
11	H	156	U
11	H	168	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	SEP	R	232	18	8,9,10	1.47	1 (12%)	8,12,14	2.47	2 (25%)
18	SEP	R	224	18	8,9,10	0.81	0	8,12,14	1.48	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	SEP	R	232	18	-	1/5/8/10	-
18	SEP	R	224	18	-	1/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	232	SEP	P-O1P	3.18	1.60	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	R	232	SEP	P-OG-CB	-5.11	104.21	118.30
18	R	232	SEP	OG-CB-CA	4.37	112.39	108.14
18	R	224	SEP	OG-CB-CA	-2.59	105.63	108.14

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 16 are monoatomic - leaving 3 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	$\#\|Z\|>2$
46	ATP	Q	1501	44	26,33,33	1.73	8 (30%)	31,52,52	1.87	10 (32%)
42	IHP	A	3000	-	36,36,36	0.83	0	54,60,60	1.05	2 (3%)
43	GTP	C	1500	44	26,34,34	1.34	3 (11%)	32,54,54	1.51	7 (21%)

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
46	ATP	Q	1501	44	-	4/18/38/38	0/3/3/3
42	IHP	A	3000	-	-	7/30/54/54	0/1/1/1
43	GTP	C	1500	44	-	4/18/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	C	1500	GTP	C5-C6	-4.30	1.38	1.47
46	Q	1501	ATP	C2'-C1'	-3.61	1.48	1.53
46	Q	1501	ATP	C4-N3	3.59	1.40	1.35
46	Q	1501	ATP	C6-N6	3.25	1.45	1.34
46	Q	1501	ATP	C2'-C3'	-2.78	1.45	1.53
46	Q	1501	ATP	O2'-C2'	-2.27	1.37	1.43
43	C	1500	GTP	C5-C4	-2.23	1.37	1.43
46	Q	1501	ATP	C3'-C4'	-2.22	1.47	1.53
46	Q	1501	ATP	O3'-C3'	-2.11	1.38	1.43
43	C	1500	GTP	O4'-C4'	-2.08	1.40	1.45
46	Q	1501	ATP	C2-N3	2.08	1.35	1.32

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	Q	1501	ATP	PB-O3B-PG	-5.52	113.89	132.83
46	Q	1501	ATP	N3-C2-N1	-4.26	122.02	128.68
43	C	1500	GTP	C5-C6-N1	3.52	120.18	113.95
43	C	1500	GTP	C8-N7-C5	3.16	109.00	102.99
43	C	1500	GTP	C2-N1-C6	-3.07	119.44	125.10
43	C	1500	GTP	PA-O3A-PB	-3.07	122.28	132.83
46	Q	1501	ATP	PA-O3A-PB	-2.58	123.97	132.83
46	Q	1501	ATP	C1'-N9-C4	-2.51	122.22	126.64
46	Q	1501	ATP	O2G-PG-O1G	-2.39	101.31	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	C	1500	GTP	O6-C6-C5	-2.38	119.73	124.37
46	Q	1501	ATP	O2A-PA-O1A	-2.36	100.58	112.24
42	A	3000	IHP	O13-C3-C2	2.36	114.24	108.69
46	Q	1501	ATP	O2G-PG-O3B	2.31	112.39	104.64
43	C	1500	GTP	PB-O3B-PG	-2.20	125.28	132.83
46	Q	1501	ATP	O5'-C5'-C4'	2.11	116.25	108.99
42	A	3000	IHP	O44-P4-O34	2.10	115.67	107.64
46	Q	1501	ATP	O2B-PB-O1B	-2.09	101.93	112.24
43	C	1500	GTP	C2'-C3'-C4'	2.07	106.66	102.64
46	Q	1501	ATP	O3G-PG-O3B	2.06	111.56	104.64

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
42	A	3000	IHP	C2-O12-P2-O22
42	A	3000	IHP	C6-O16-P6-O26
43	C	1500	GTP	PB-O3B-PG-O3G
46	Q	1501	ATP	C5'-O5'-PA-O1A
46	Q	1501	ATP	C5'-O5'-PA-O2A
43	C	1500	GTP	C3'-C4'-C5'-O5'
43	C	1500	GTP	O4'-C4'-C5'-O5'
42	A	3000	IHP	C4-O14-P4-O44
42	A	3000	IHP	C6-O16-P6-O36
42	A	3000	IHP	C3-C2-O12-P2
46	Q	1501	ATP	PB-O3A-PA-O2A
42	A	3000	IHP	C2-C1-O11-P1
42	A	3000	IHP	C4-O14-P4-O34
46	Q	1501	ATP	C5'-O5'-PA-O3A
43	C	1500	GTP	PB-O3A-PA-O2A

There are no ring outliers.

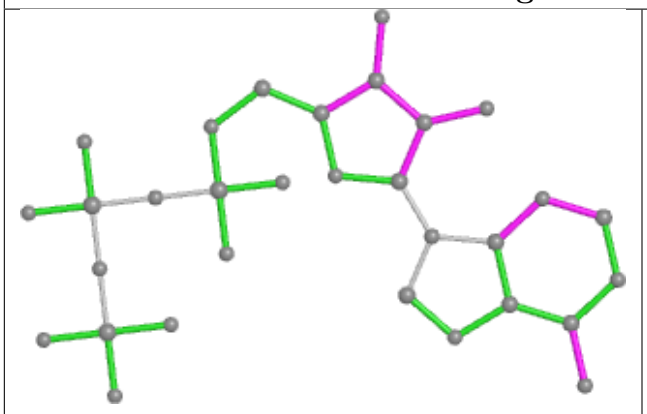
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	A	3000	IHP	3	0
43	C	1500	GTP	2	0

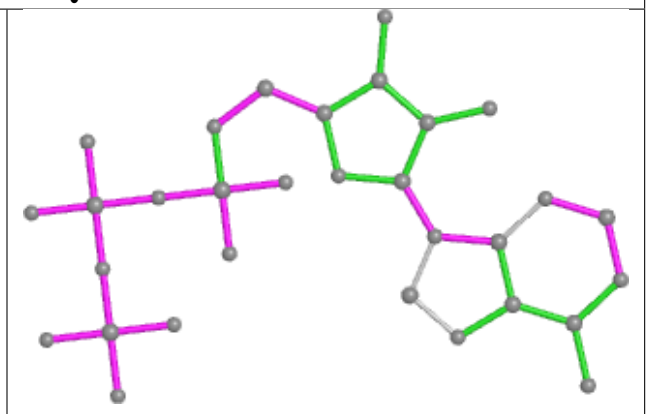
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

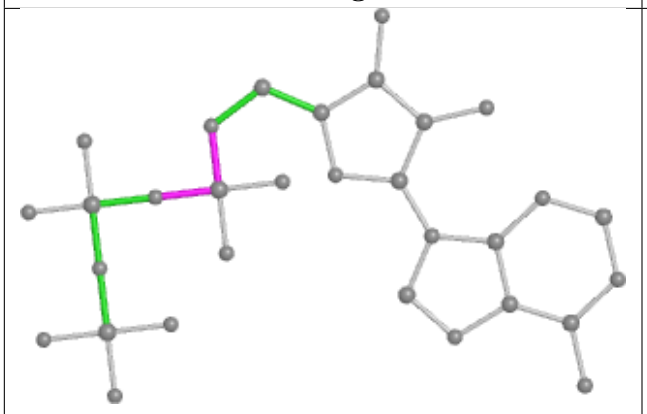
Ligand ATP Q 1501



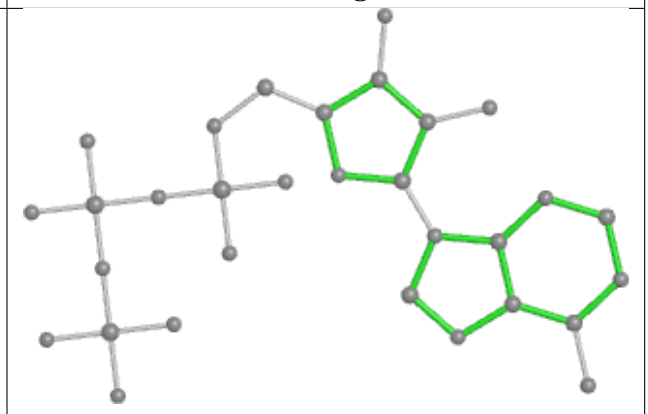
Bond lengths



Bond angles

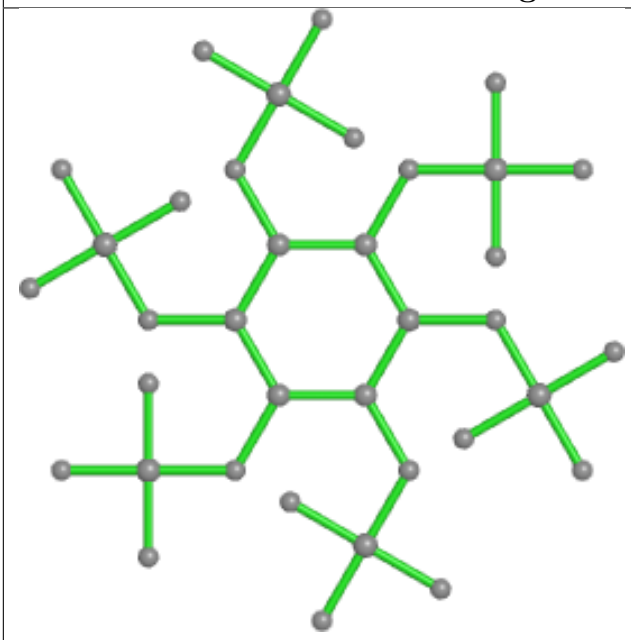


Torsions

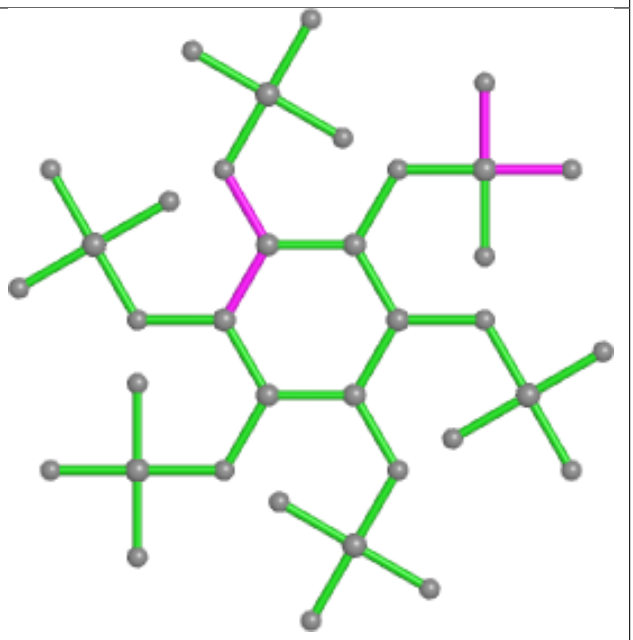


Rings

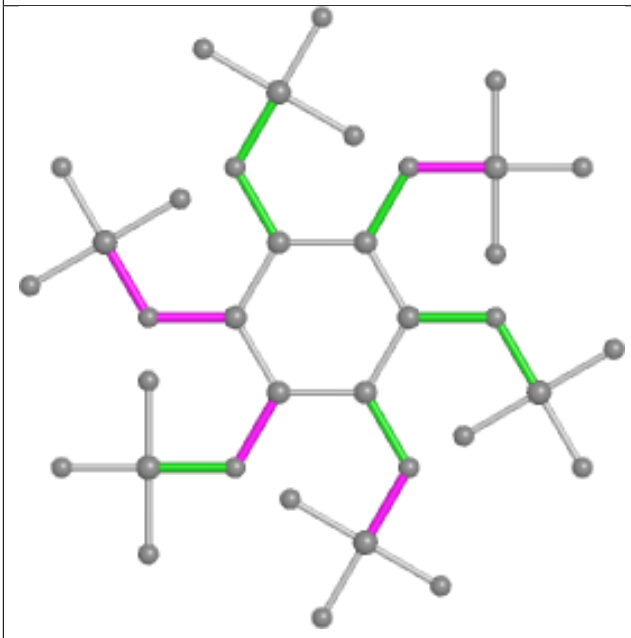
Ligand IHP A 3000



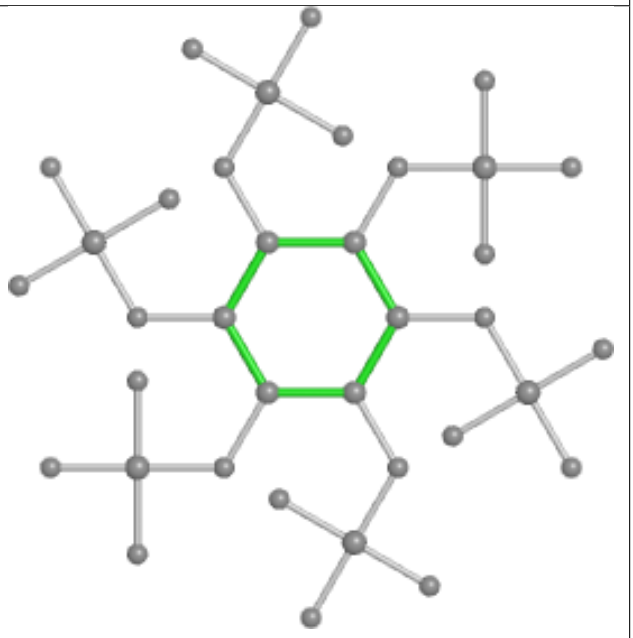
Bond lengths



Bond angles

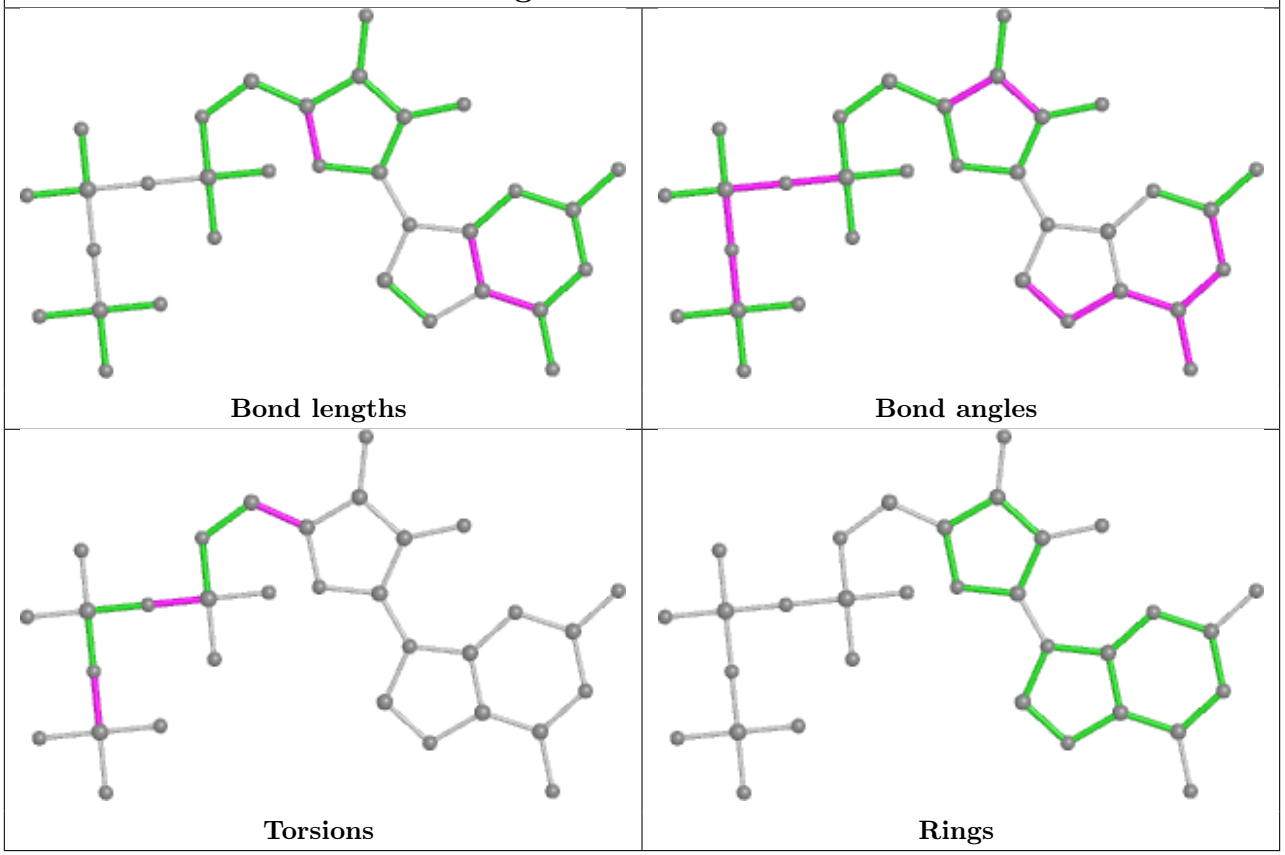


Torsions



Rings

Ligand GTP C 1500



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

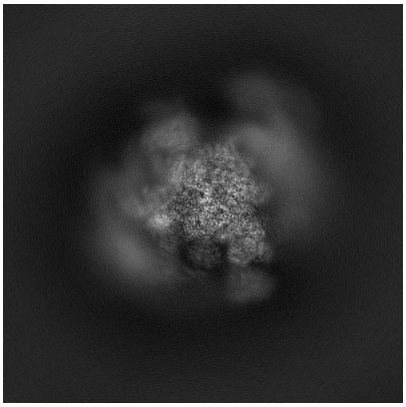
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9645. These allow visual inspection of the internal detail of the map and identification of artifacts.

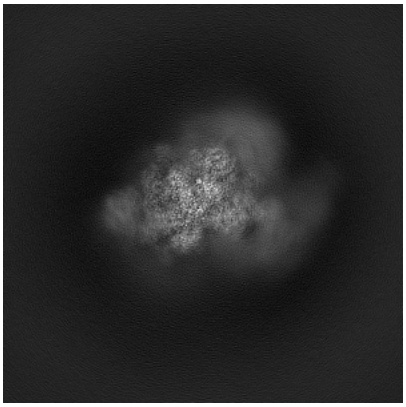
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

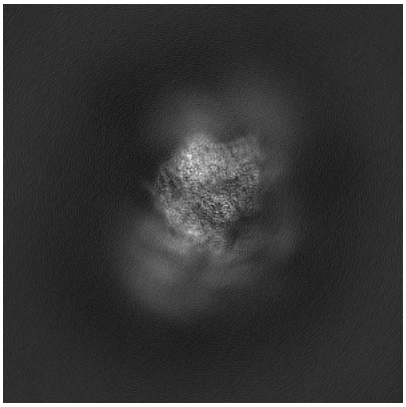
6.1.1 Primary map



X



Y

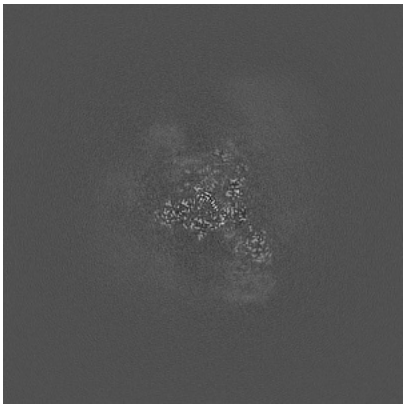


Z

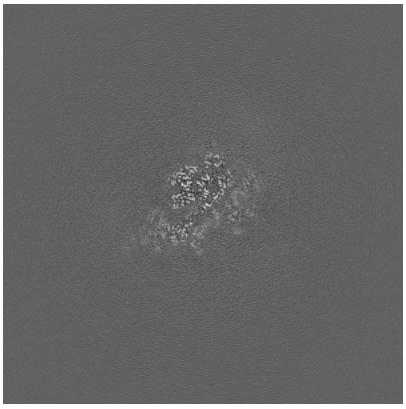
The images above show the map projected in three orthogonal directions.

6.2 Central slices

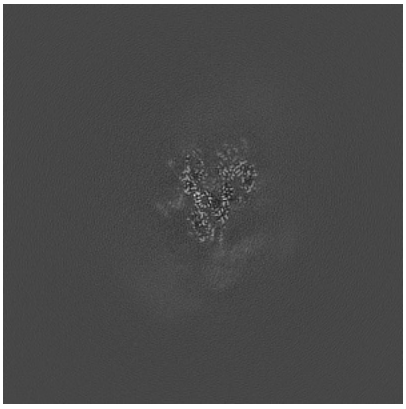
6.2.1 Primary map



X Index: 200



Y Index: 200

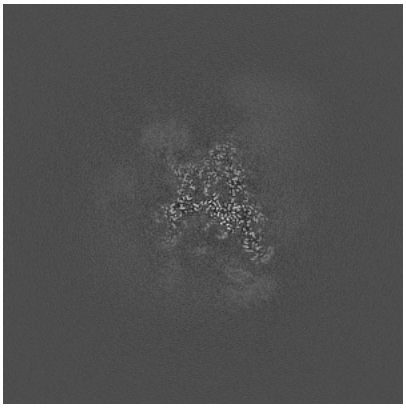


Z Index: 200

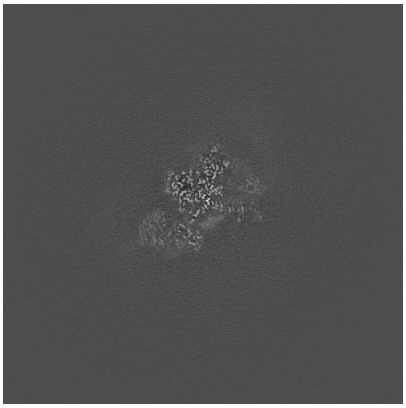
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

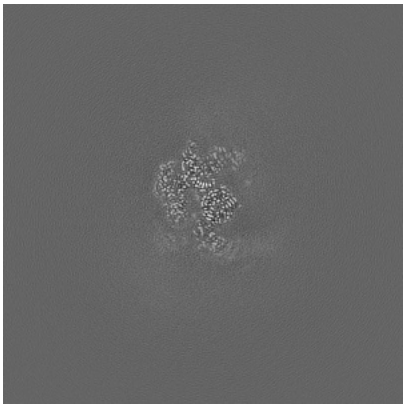
6.3.1 Primary map



X Index: 193



Y Index: 205

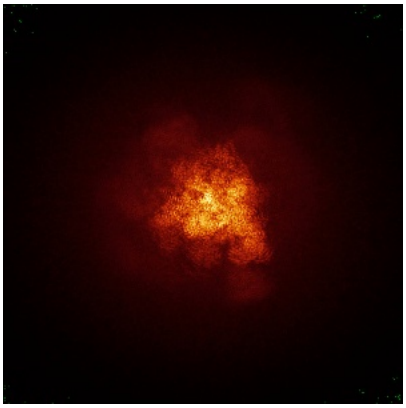


Z Index: 180

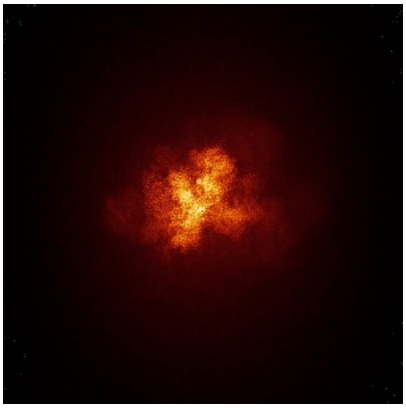
The images above show the largest variance slices of the map in three orthogonal directions.

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

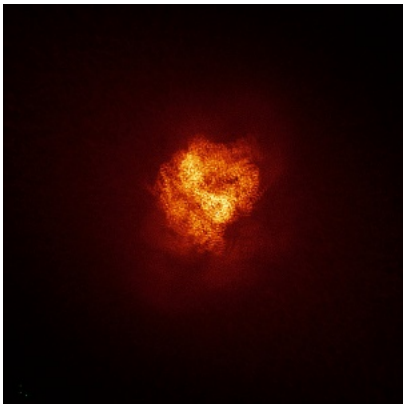
6.4.1 Primary map



X



Y

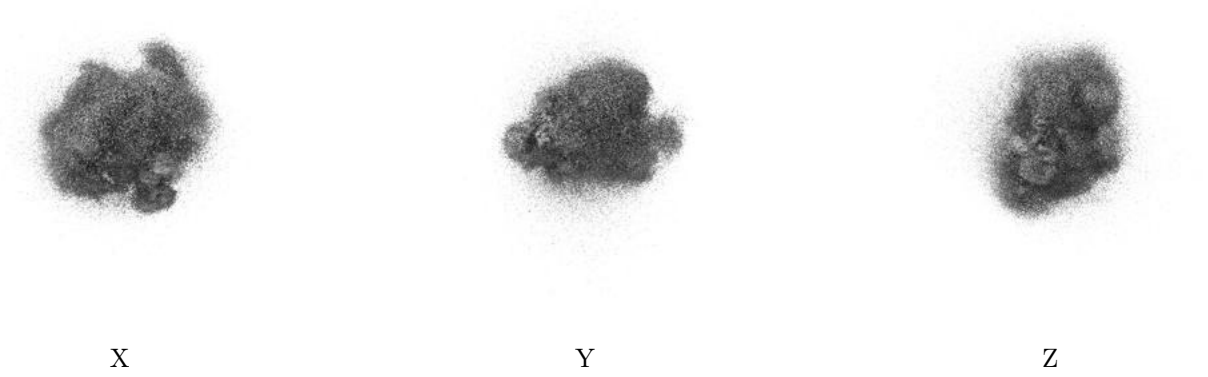


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

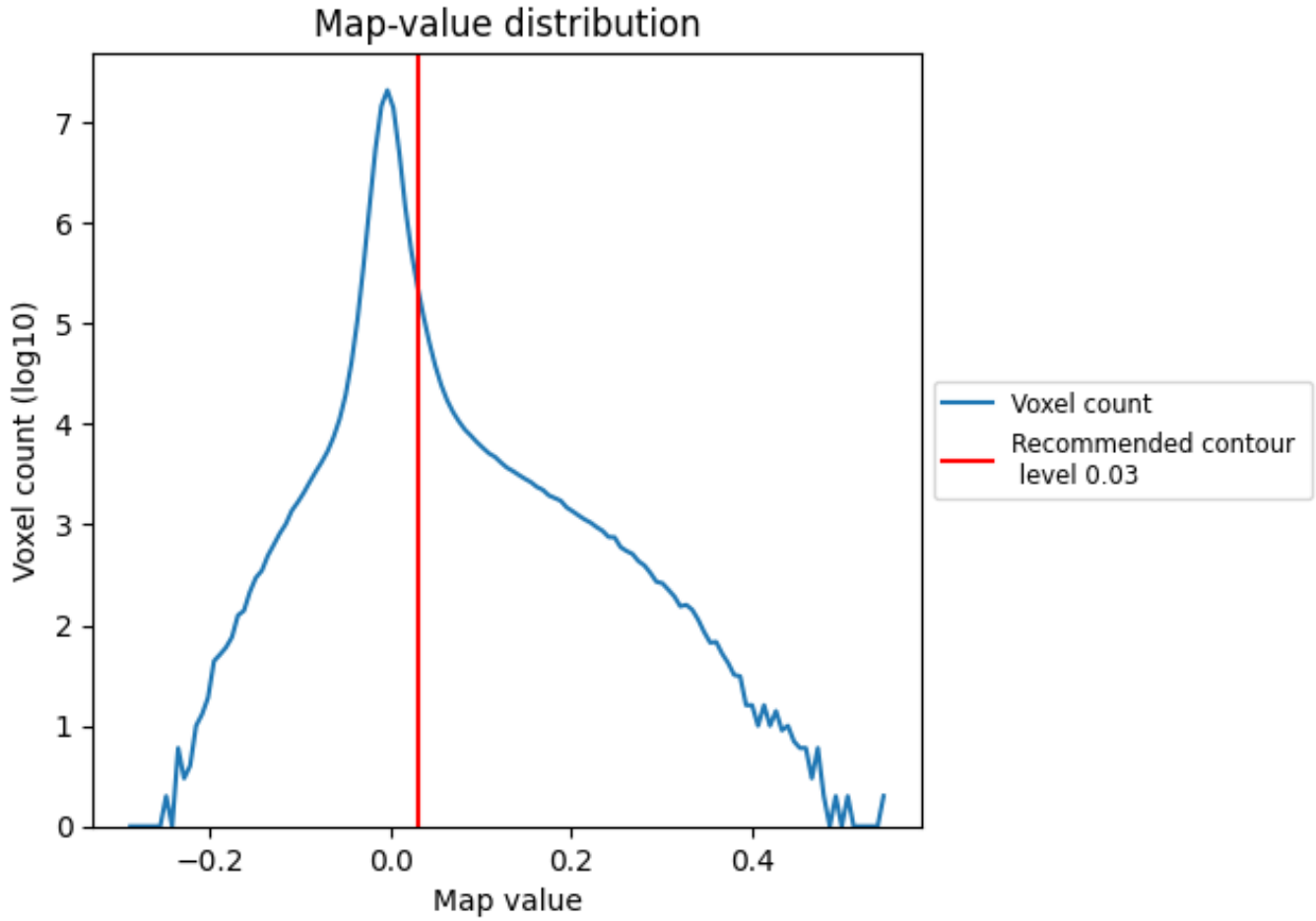
6.6 Mask visualisation (i)

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

7 Map analysis

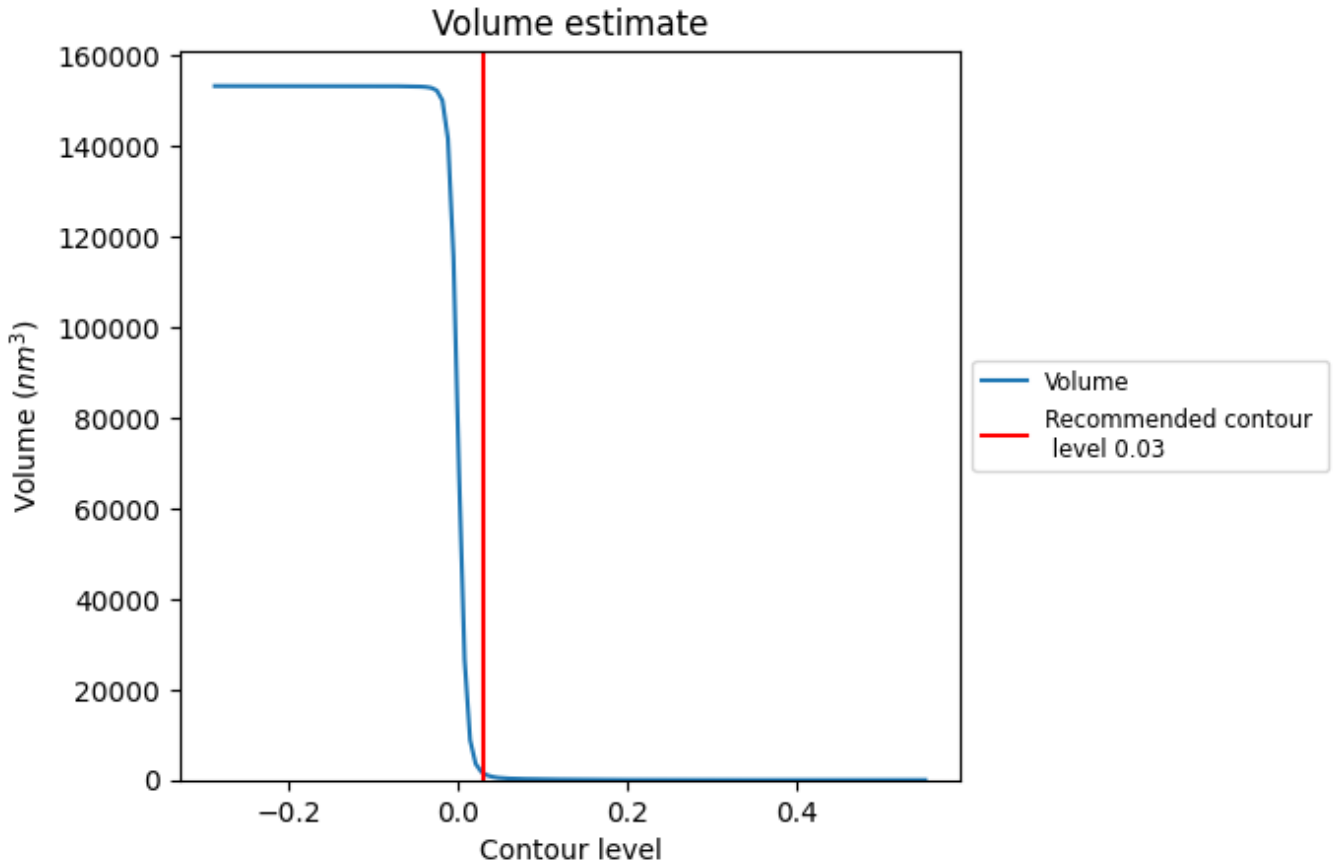
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

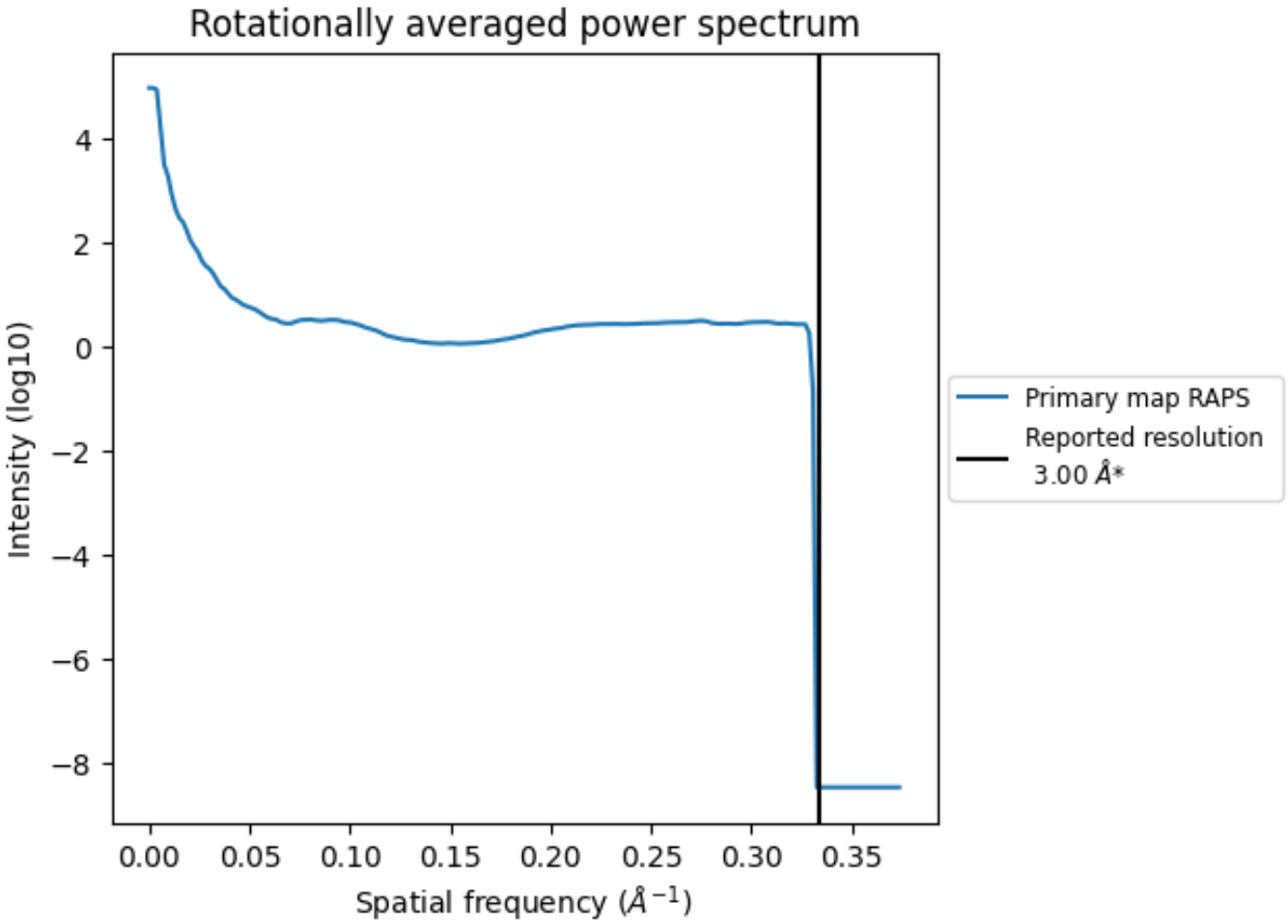
7.2 Volume estimate



The volume at the recommended contour level is 1504 nm^3; this corresponds to an approximate mass of 1358 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 0.333 Å^{-1}

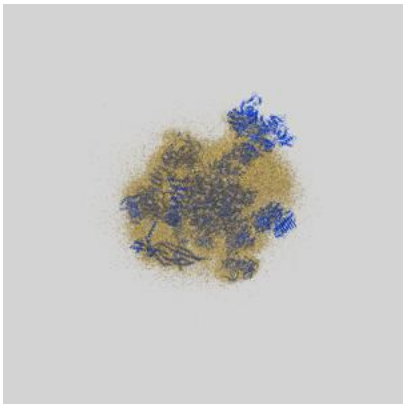
8 Fourier-Shell correlation (i)

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

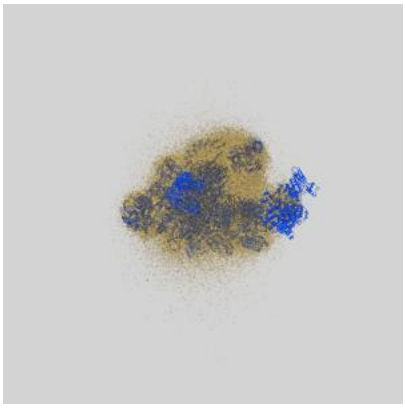
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9645 and PDB model 6ICZ. Per-residue inclusion information can be found in section 3 on page 14.

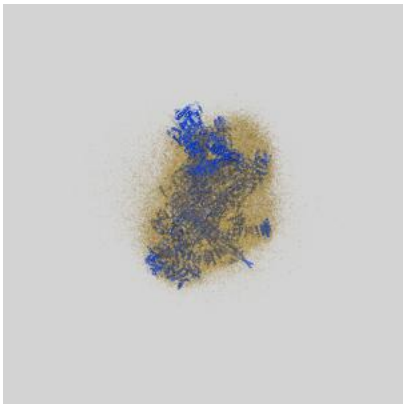
9.1 Map-model overlay



X



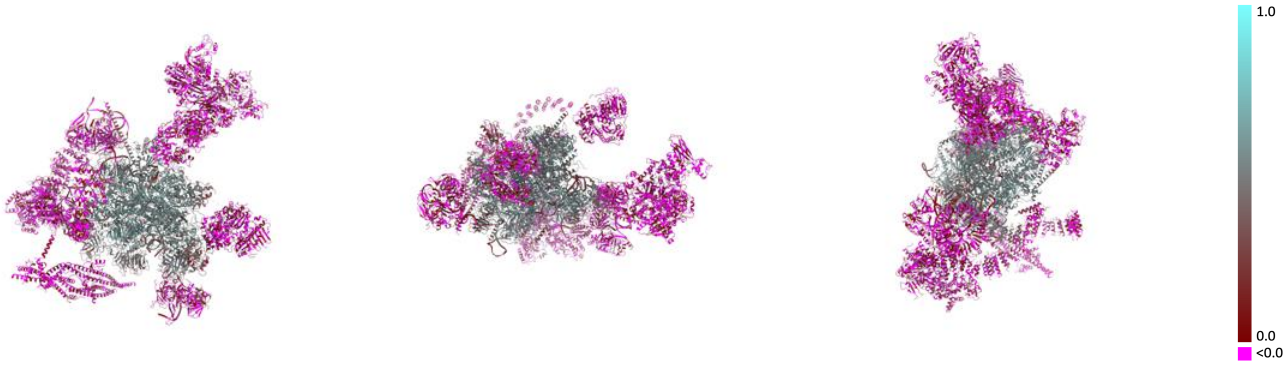
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

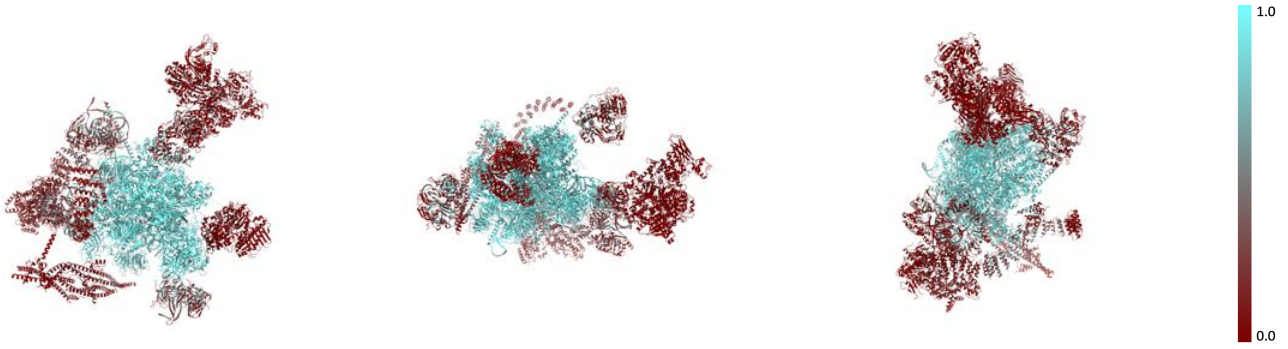
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

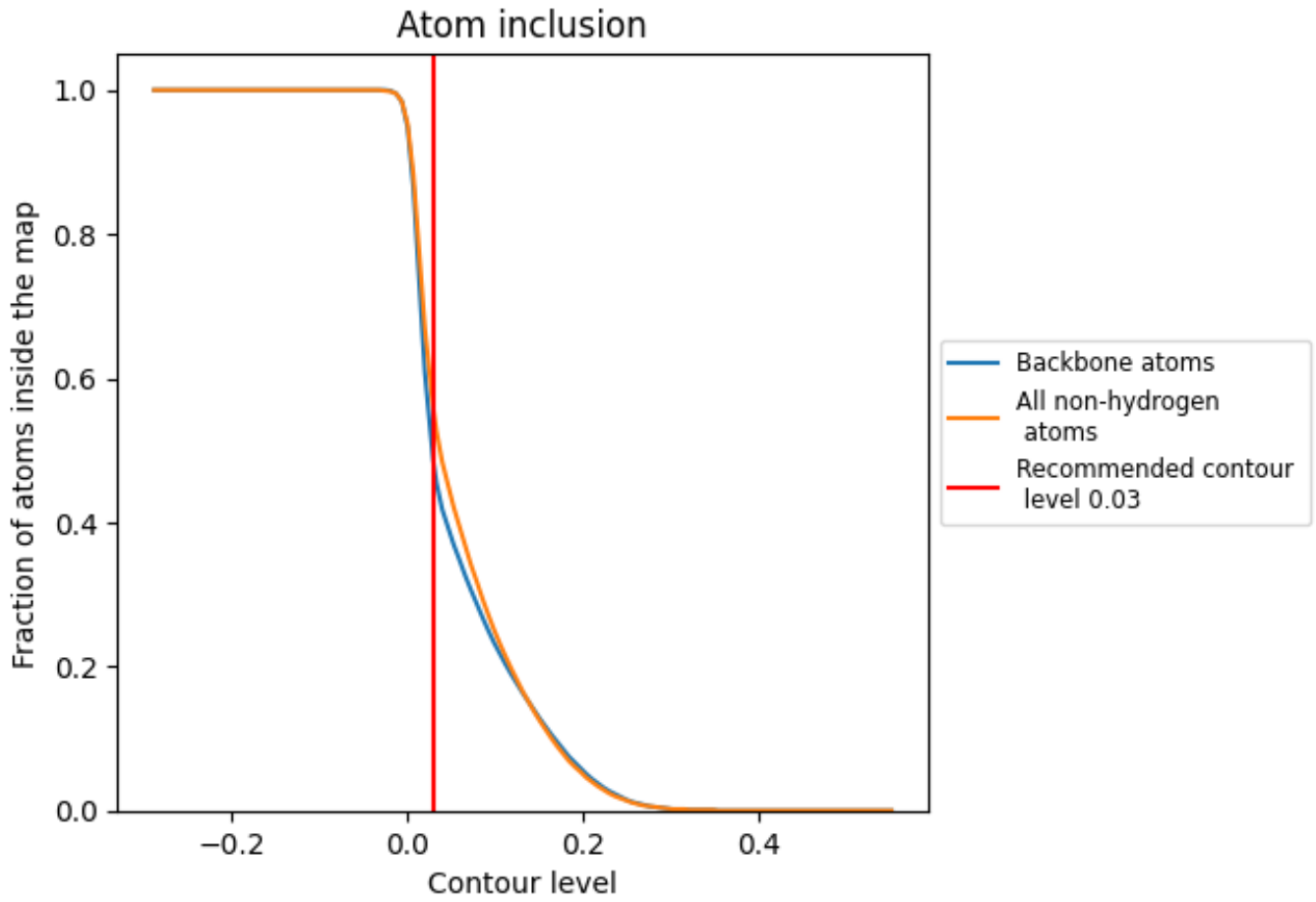
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 49% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5600	0.2840
A	0.8720	0.5070
B	0.7660	0.3530
C	0.8960	0.4650
D	0.0170	0.0020
E	0.8600	0.4140
F	0.9330	0.4850
G	0.7650	0.3440
H	0.4880	0.1340
I	0.2180	0.0190
J	0.5970	0.3190
K	0.1120	-0.0060
L	0.6000	0.3280
M	0.8730	0.4830
N	0.9350	0.5390
O	0.8170	0.4200
P	0.8340	0.4750
Q	0.0290	0.0020
R	0.8770	0.4780
S	0.8670	0.4200
T	0.9650	0.5840
U	0.8240	0.5200
V	0.4890	0.2780
W	0.8310	0.4190
X	0.5930	0.3250
Y	0.2630	0.0450
Z	0.7970	0.4390
a	0.3460	0.0120
b	0.3260	0.0300
c	0.2930	0.0150
d	0.3210	0.0150
e	0.3220	0.0560
f	0.3020	0.0360
g	0.3000	0.0160
h	0.1990	-0.0100

Continued on next page...

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Chain	Atom inclusion	Q-score
i	0.2030	0.0080
j	0.3640	0.0370
k	0.2940	-0.0060
l	0.3040	0.0530
m	0.3820	0.0410
n	0.2270	-0.0020
o	0.1490	0.0120
p	0.2390	-0.0180
q	0.0430	-0.0060
r	0.0690	0.0010
s	0.1190	0.0440
t	0.0570	-0.0170
u	0.0290	-0.0080
v	0.0010	0.0100
w	0.0000	0.0450
x	0.0000	0.0520
y	0.1870	-0.0070