Full wwPDB EM Validation Report ⓘ

Jul 31, 2024 – 11:10 AM JST

PDB ID	:	8I0P
EMDB ID	:	EMD-35105
Title	:	The cryo-EM structure of human pre-Bact complex
Authors	:	Zhan, X.; Lu, Y.; Shi, Y.
Deposited on	:	2023-01-11
Resolution	:	3.40 Å(reported)

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

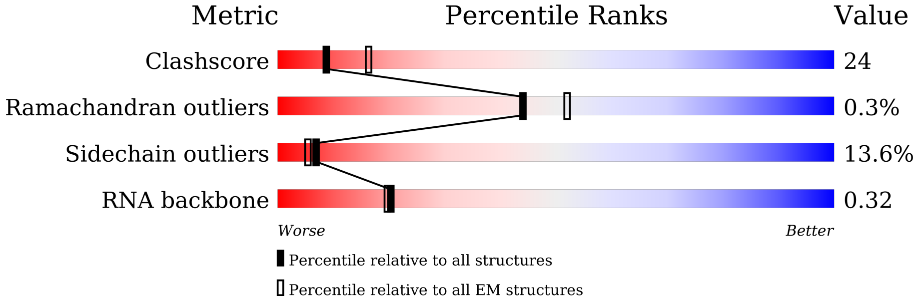
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance ⓘ

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

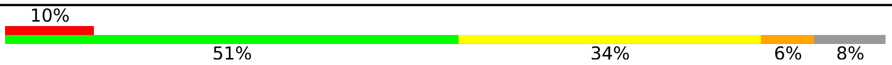
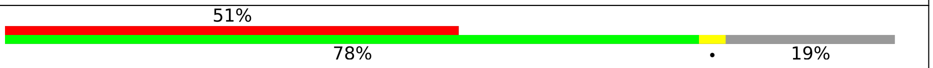
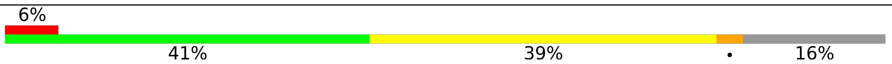
The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	2335	
2	B	117	
3	C	972	
4	D	2136	
5	E	357	
6	F	107	
7	G	220	

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Mol	Chain	Length	Quality of chain
8	H	188	16% 20% 48% 18% • 12%
9	I	855	17% 65% • 31%
10	J	848	15% 13% • 71%
11	K	393	11% 48% 26% 5% 21%
12	L	802	7% • • 88%
13	N	144	11% 89% • 7%
14	O	420	• 60% 5% 35%
15	P	229	10% 7% • 82%
16	Q	1485	36% 86% • 11%
17	R	536	20% 11% • 64%
18	T	514	24% 31% 7% 38%
19	X	396	• 17% 20% • 61%
20	Y	322	15% 18% • 63%
21	Z	619	6% • 91%
22	1	1304	35% 34% 6% 24%
23	3	1217	43% 44% 10% •
24	o	255	6% 64% 36%
25	p	225	• 75% 25%
26	c	118	18% 82% 18%
26	h	118	8% 80% • 19%
27	d	86	23% 86% 14%
27	i	86	5% 84% 16%
28	a	240	7% 35% 65%
28	m	240	• 34% 66%
29	g	126	15% 64% 36%

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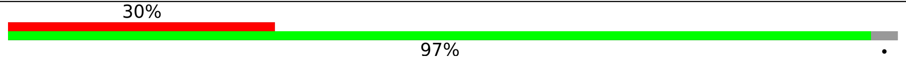
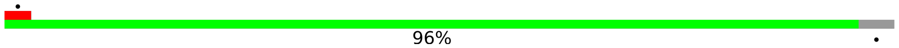
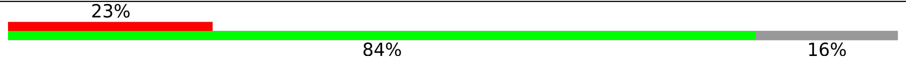
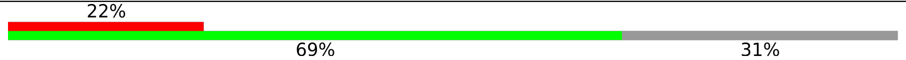
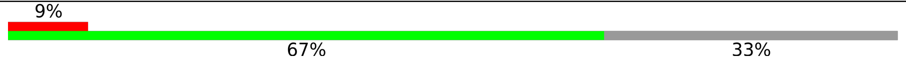
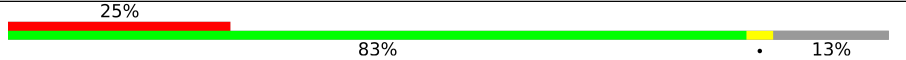
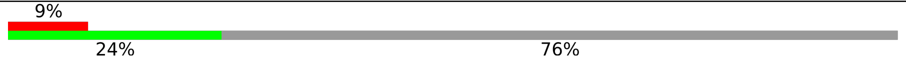
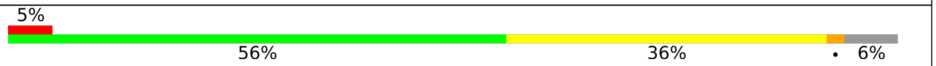
Mol	Chain	Length	Quality of chain
29	l	126	
30	f	76	
30	k	76	
31	e	92	
31	j	92	
32	b	119	
32	n	119	
33	w	501	
34	u	793	
35	2	895	
36	4	424	
37	6	125	
38	7	110	
39	5	86	
40	9	520	
41	8	904	
42	y	301	
43	v	464	
44	z	25	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	SEP	1	129	-	-	X	-

2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 103887 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2149	16165	10296	2906	2900	63	0	0

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	98	2066	925	347	696	98	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	896	7077	4528	1176	1338	35	0	0

- Molecule 4 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	1722	8528	5084	1722	1722	0	0

- Molecule 5 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	299	2338	1470	410	445	13	0	0

- Molecule 6 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	F	95	2035	910	377	653	95	0	0

- Molecule 7 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	G	63	1321	592	217	449	63	0	0

- Molecule 8 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	H	165	3497	1562	600	1170	165	0	0

- Molecule 9 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	I	593	2991	1805	593	593	0	0

- Molecule 10 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	249	2116	1355	380	375	6	0	0

- Molecule 11 is a protein called DNA/RNA-binding protein KIN17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	312	2173	1338	413	412	10	0	0

- Molecule 12 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	99	829	532	149	144	4	0	0

- Molecule 13 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	N	134	662	394	134	134	0	0

- Molecule 14 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	O	271	1340	798	271	271	0	0

- Molecule 15 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	P	42	362	231	63	66	2	0	0

- Molecule 16 is a protein called RNA helicase aquarius.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	Q	1329	6730	4072	1329	1329	0	0

- Molecule 17 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	R	192	1520	937	278	297	8	0	0

- Molecule 18 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	T	320	2507	1582	456	462	7	0	0

- Molecule 19 is a protein called Smad nuclear-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	X	154	1279	819	231	227	2	0	0

- Molecule 20 is a protein called RNA-binding motif protein, X-linked 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	Y	118	948	605	163	176	4	0	0

- Molecule 21 is a protein called BUD13 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	Z	55	Total 439	C 282	N 85	O 72	0	0

- Molecule 22 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	1	993	Total 7845	C 5003	N 1360	O 1435	P 1	S 46	0	0

- Molecule 23 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	3	1180	Total 9240	C 5868	N 1569	O 1758	S 45	0	0

- Molecule 24 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	o	162	Total 816	C 492	N 162	O 162	0	0

- Molecule 25 is a protein called U2 small nuclear ribonucleoprotein B".

Mol	Chain	Residues	Atoms				AltConf	Trace
25	p	169	Total 851	C 513	N 169	O 169	0	0

- Molecule 26 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	h	95	Total 482	C 292	N 95	O 95	0	0
26	c	97	Total 388	C 194	N 97	O 97	0	0

- Molecule 27 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	i	72	Total 359	C 215	N 72	O 72	0	0
27	d	74	Total 296	C 148	N 74	O 74	0	0

- Molecule 28 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	m	82	Total	C	N	O	0	0
			413	249	82	82		
28	a	84	Total	C	N	O	0	0
			336	168	84	84		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
29	l	83	Total	C	N	O	0	0
			415	249	83	83		
29	g	81	Total	C	N	O	0	0
			324	162	81	81		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
30	k	73	Total	C	N	O	0	0
			364	218	73	73		
30	f	74	Total	C	N	O	0	0
			296	148	74	74		

- Molecule 31 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	j	81	Total	C	N	O	0	0
			403	241	81	81		
31	e	77	Total	C	N	O	0	0
			308	154	77	77		

- Molecule 32 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	n	80	Total	C	N	O	0	0
			402	242	80	80		
32	b	82	Total	C	N	O	0	0
			328	164	82	82		

- Molecule 33 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	w	434	Total 2275	C 1287	N 491	O 493	S 4	0	0

- Molecule 34 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	u	187	Total 834	C 460	N 187	O 187	0	0

- Molecule 35 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	2	231	Total 1651	C 1037	N 309	O 301	S 4	0	0

- Molecule 36 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	4	161	Total 792	C 470	N 161	O 161	0	0

- Molecule 37 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	6	109	Total 906	C 582	N 157	O 163	S 4	0	0

- Molecule 38 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	7	105	Total 811	C 502	N 145	O 151	S 13	0	0

- Molecule 39 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	5	81	Total 669	C 422	N 117	O 124	S 6	0	0

- Molecule 40 is a protein called RING-type E3 ubiquitin-protein ligase PPIL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	9	384	Total	C	N	O	S	0	0
			2681	1665	484	524	8		

- Molecule 41 is a protein called Serine/arginine repetitive matrix protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	8	115	Total	C	N	O	S	0	0
			931	602	154	170	5		

- Molecule 42 is a protein called Peptidyl-prolyl cis-trans isomerase E.

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

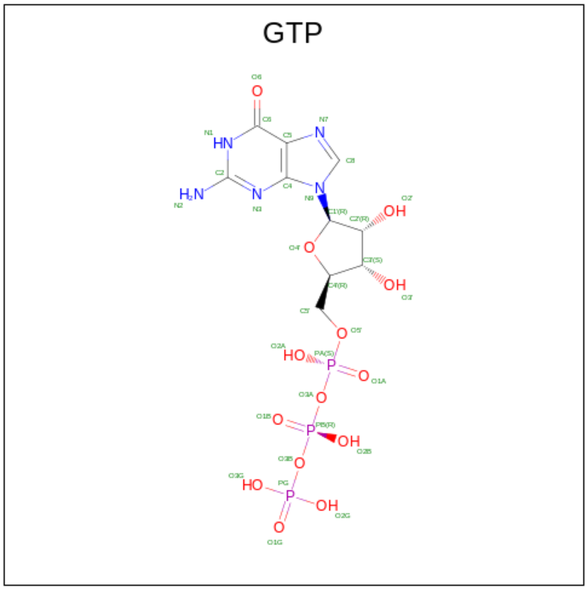
- Molecule 43 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	166	Total	C	N	O	S	0	0
			997	576	211	207	3		

- Molecule 44 is a protein called Unknown polymer.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	z	25	Total	C	N	O	0	0
			124	74	25	25		

- Molecule 45 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 46 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
46	C	1	1	1	0

- Molecule 47 is ZINC ION (three-letter code: ZN) (formula: Zn).

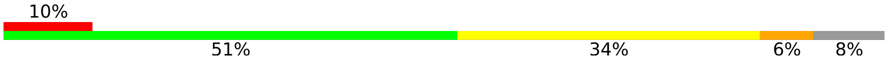
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
47	K	1	1	1	0
47	7	3	3	3	0

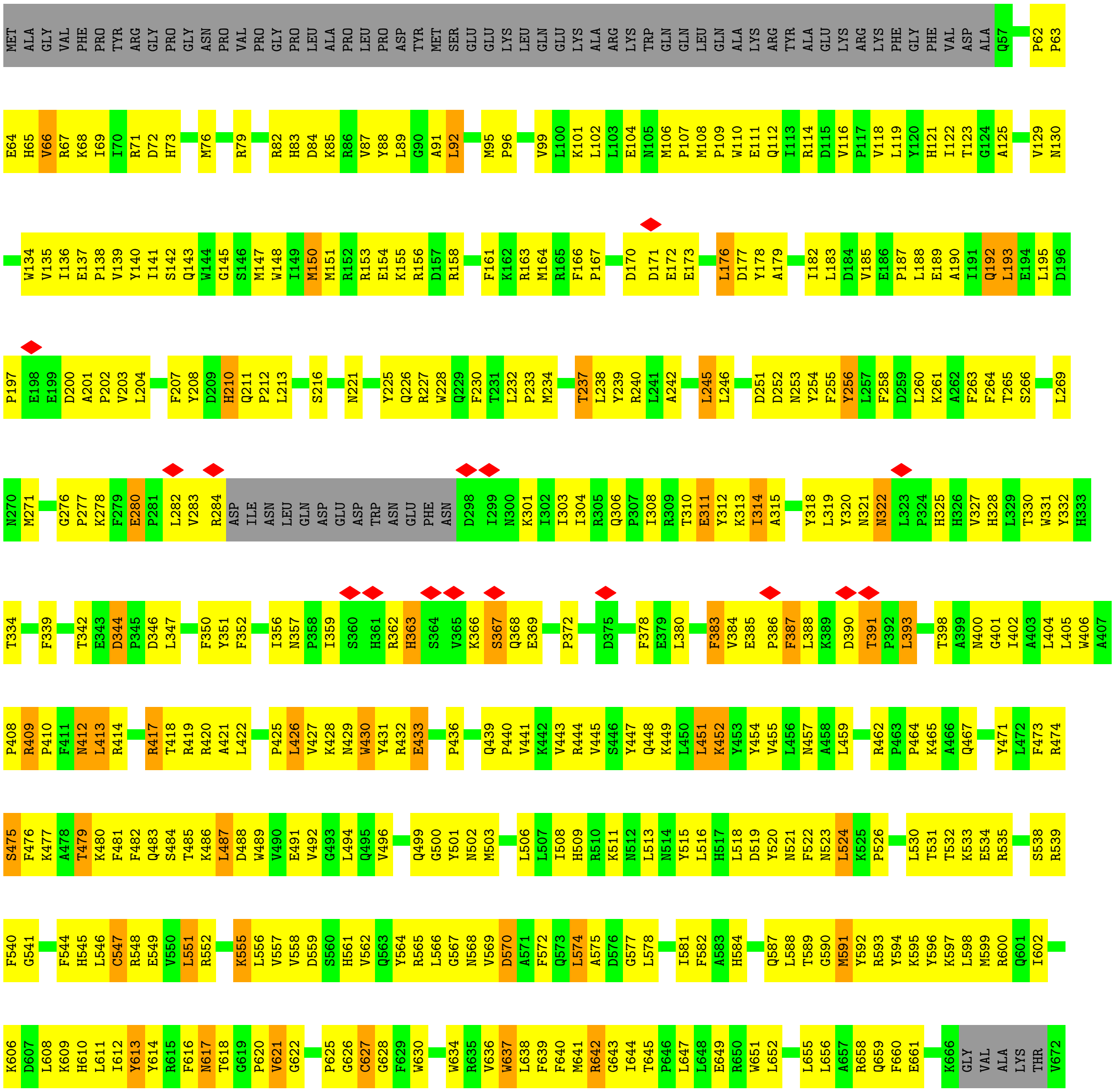
3 Residue-property plots ⓘ

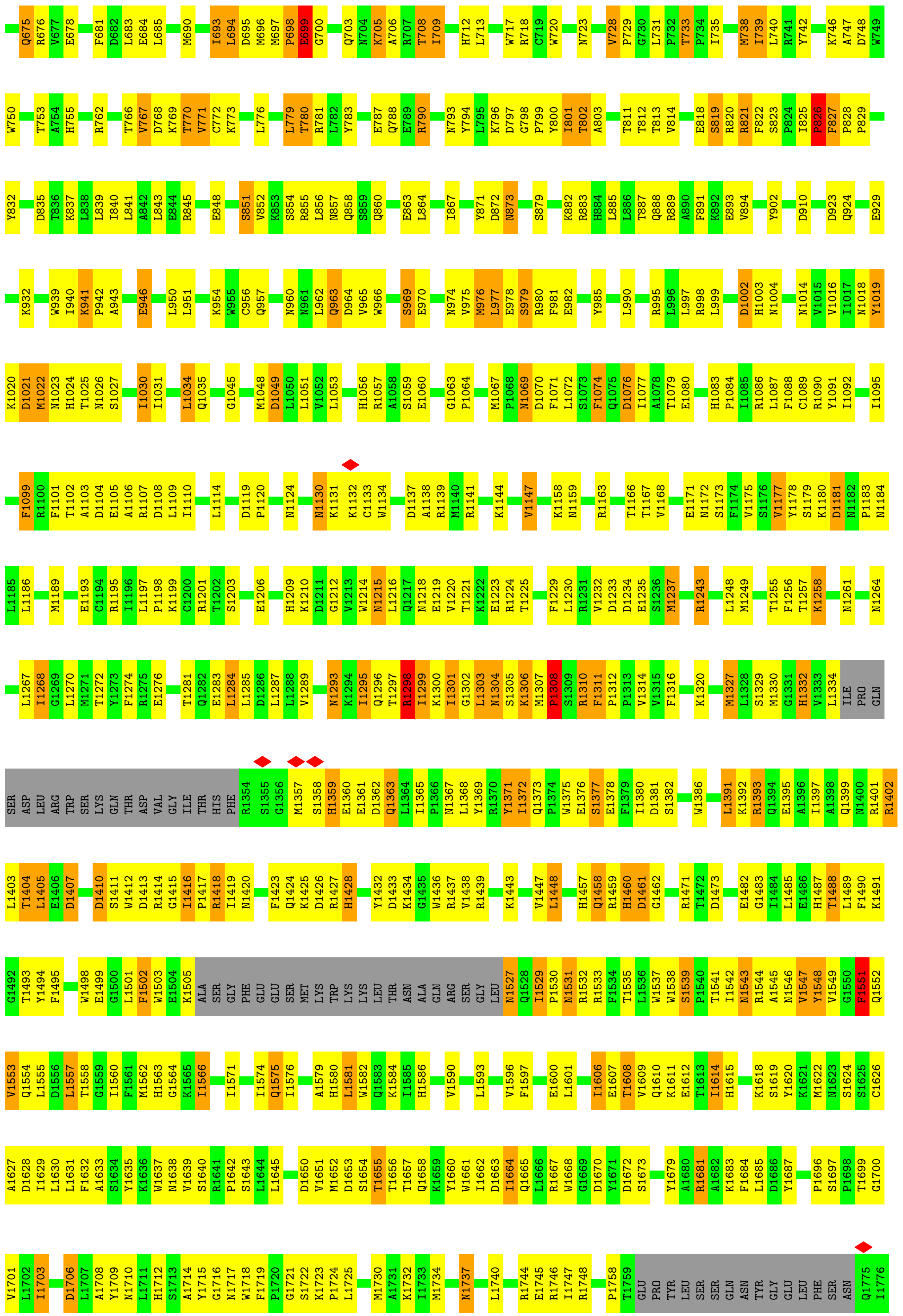
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Pre-mRNA-processing-splicing factor 8

Chain A:






Q675 R676 V677 E678 F681 D682 L683 E684 L685 M690 I693 L694 D695 M696 M697 P698 E699 G700 Q703 N704 K705 A706 R707 T708 I709 H712 L713 W717 R718 C719 W720 N723 V728 P729 G730 L731 P732 T733 P734 I735 M738 I739 L740 R741 Y742 K746 A747 D748 W749
W750 T753 A754 H755 R762 T766 V767 D768 K769 T770 V771 C772 K773 L776 L779 T780 R781 L782 Y783 E787 Q788 E789 R790 N793 Y794 L795 K796 D797 G798 P799 Y800 I801 T802 A803 T811 T812 T813 V814 E818 S819 R820 R821 F822 S823 P824 I825 P826 F827 P828 P829
Y832 D835 T836 K837 L838 L839 I840 L841 A842 L843 E844 R845 E848 S851 V852 K853 S854 R855 L856 N857 Q858 S859 Q860 E863 L864 I867 Y871 D872 N873 S879 K882 R883 H884 L885 L886 T887 Q888 R889 A890 F891 K892 E893 V894 Y902 D910 D923 Q924 E929
K932 W939 I940 K941 P942 A943 E946 L950 L951 K954 W955 C956 Q957 N960 N961 L962 Q963 D964 V965 W966 S969 E970 N974 V975 M976 L977 E978 S979 R980 F981 E982 Y985 L990 R995 L996 L997 R998 L999 D1002 H1003 N1004 N1014 V1015 V1016 I1017 N1018 Y1019
K1020 D1021 M1022 N1023 H1024 T1025 N1026 S1027 I1030 I1031 L1034 Q1035 G1045 M1048 D1049 L1050 L1051 V1052 L1053 H1056 R1057 A1058 S1059 E1060 G1063 P1064 M1067 P1068 N1069 D1070 F1071 L1072 S1073 F1074 Q1075 D1076 I1077 A1078 T1079 E1080 H1083 P1084 I1085 R1086 L1087 F1088 C1089 R1090 Y1091 I1092 I1095
F1099 R1100 F1101 T1102 A1103 D1104 E1105 A1106 R1107 D1108 L1109 I1110 L1114 D1119 P1120 N1124 N1130 K1131 K1132 C1133 W1134 D1137 A1138 R1139 M1140 R1141 K1144 V1147 K1158 N1159 R1163 T1166 T1167 V1168 E1171 N1172 S1173 F1174 V1175 S1176 V1177 Y1178 S1179 K1180 D1181 N1182 P1183 N1184
L1185 L1186 M1189 E1193 C1194 R1195 I1196 L1197 P1198 K1199 C1200 R1201 T1202 S1203 E1206 H1209 K1210 D1211 G1212 V1213 W1214 N1215 L1216 Q1217 N1218 E1219 V1220 T1221 K1222 E1223 R1224 T1225 F1229 L1230 R1231 V1232 D1233 D1234 E1235 S1236 M1237 R1243 L1248 M1249 T1255 F1256 T1257 K1258 N1261 N1264
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SER ASP LEU ARG TRP SER LYS GLN THR ASP VAL GLY ILE THR HIS PHE R1354 S1355 G1356 M1357 S1358 H1359 E1360 E1361 D1362 Q1363 L1364 I1365 P1366 N1367 L1368 Y1369 R1370 Y1371 I1372 Q1373 P1374 W1375 E1376 S1377 E1378 F1379 I1380 D1381 S1382 W1386 L1391 K1392 R1393 Q1394 E1395 A1396 I1397 A1398 Q1399 N1400 R1401 R1402
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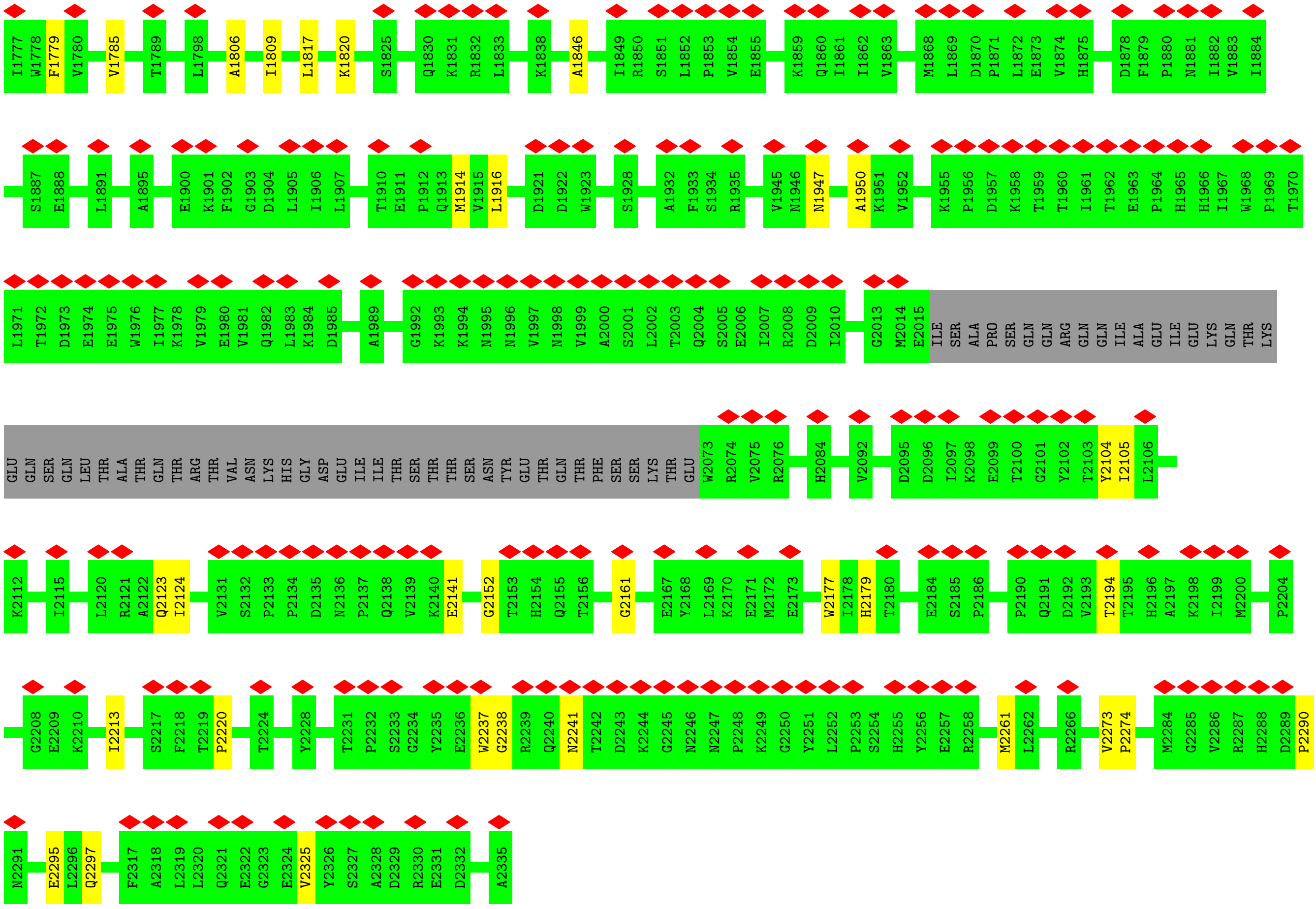
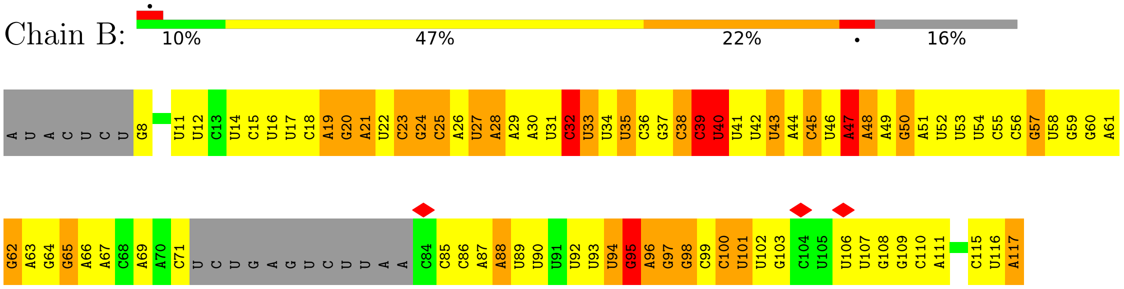
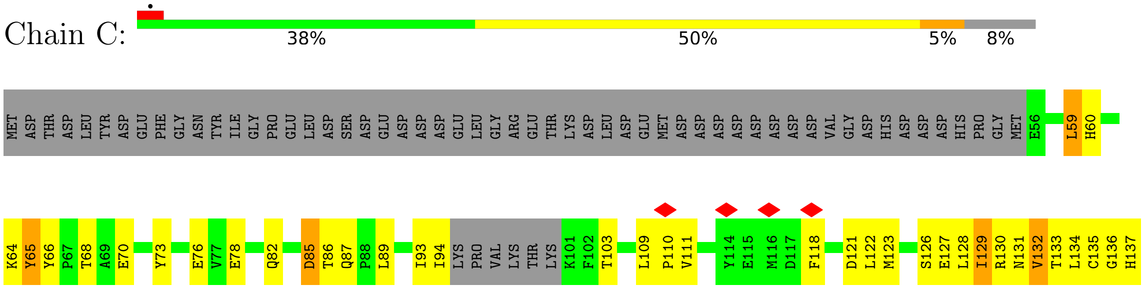
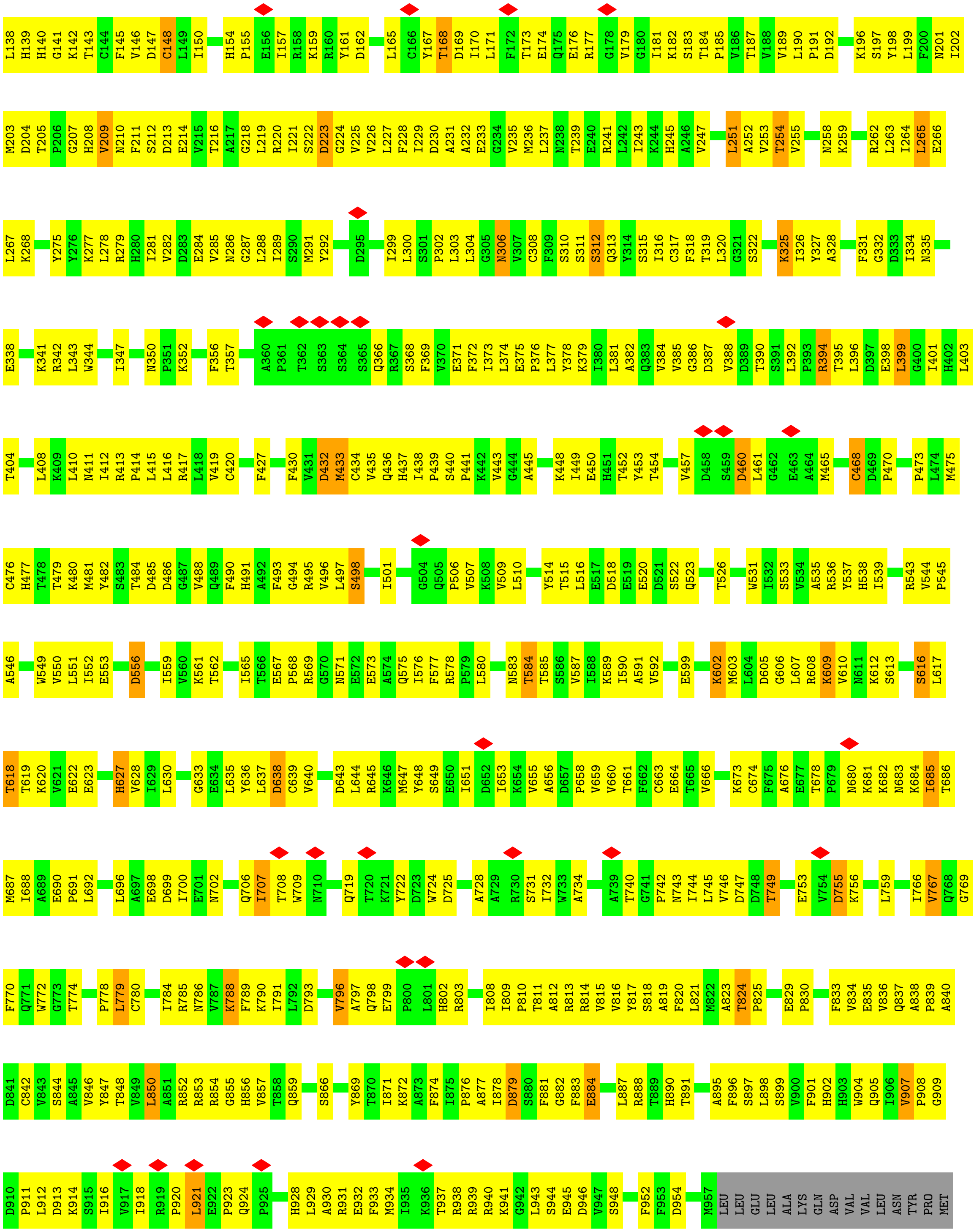


- Molecule 2: U5 snRNA

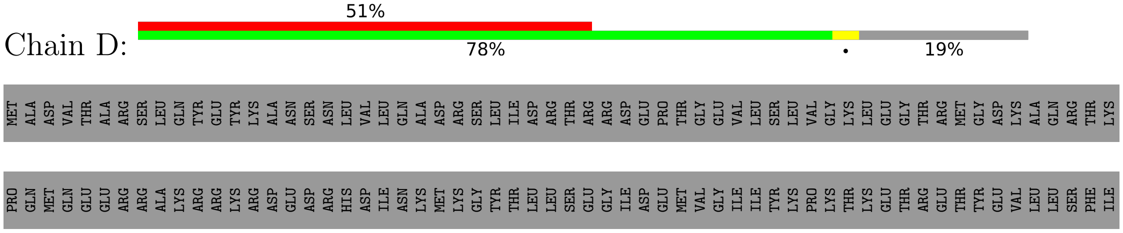


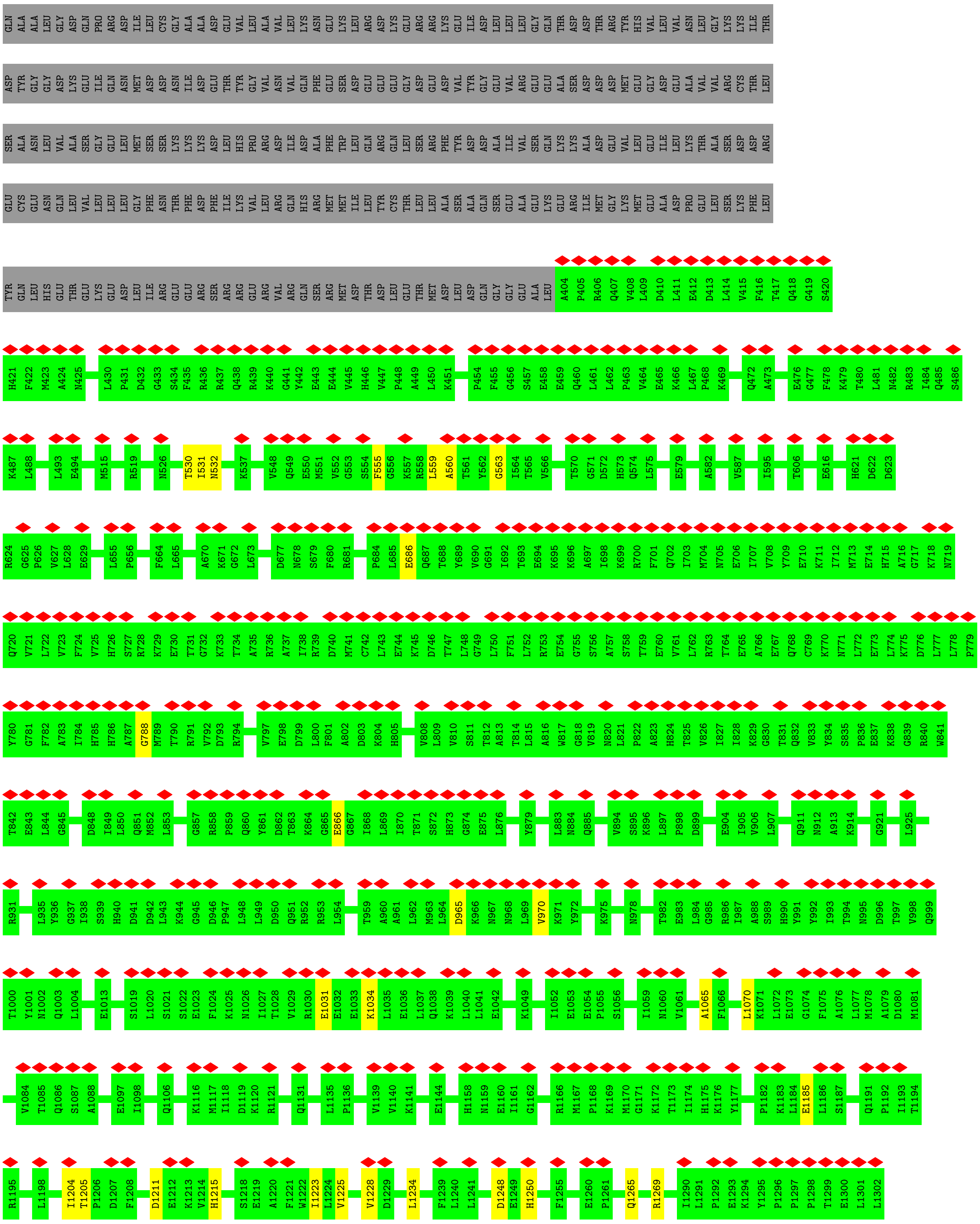
- Molecule 3: 116 kDa U5 small nuclear ribonucleoprotein component





- Molecule 4: U5 small nuclear ribonucleoprotein 200 kDa helicase

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ASP TYR GLY GLY ASP LYS GLU ILE GLN ASN MET ASP ASP ASN ILE ASP GLU THR TYR GLY VAL ASN VAL GLN PHE GLU SER ASP GLU GLU GLU GLY ASP GLU ASP VAL TYR GLY GLU VAL ARG GLU GLU ALA SER ASP ASP ASP MET GLU GLY ASP GLU ALA VAL VAL ARG CYS THR LEU
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TYR GLN LEU HIS GLU THR GLU LYS GLU ASP LEU ILE ARG GLU GLU ARG SER ARG ARG GLU ARG VAL ARG GLN SER ARG MET ASP THR ASP LEU GLU THR MET ASP LEU ASP GLN GLY GLY GLU ALA LEU A404 P405 R406 Q407 V408 L409 D410 L411 E412 D413 L414 V415 F416 T417 Q418 G419 S420
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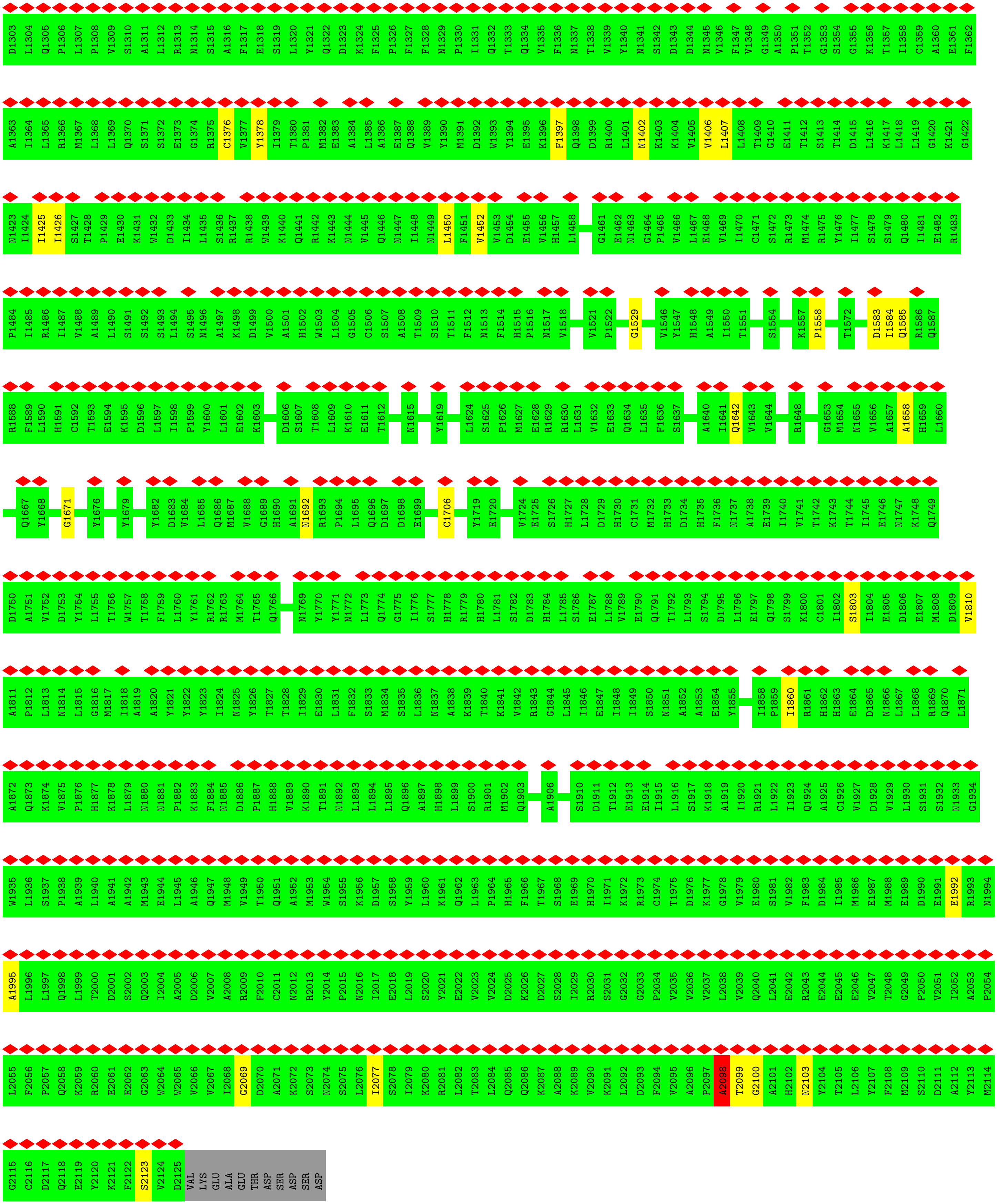
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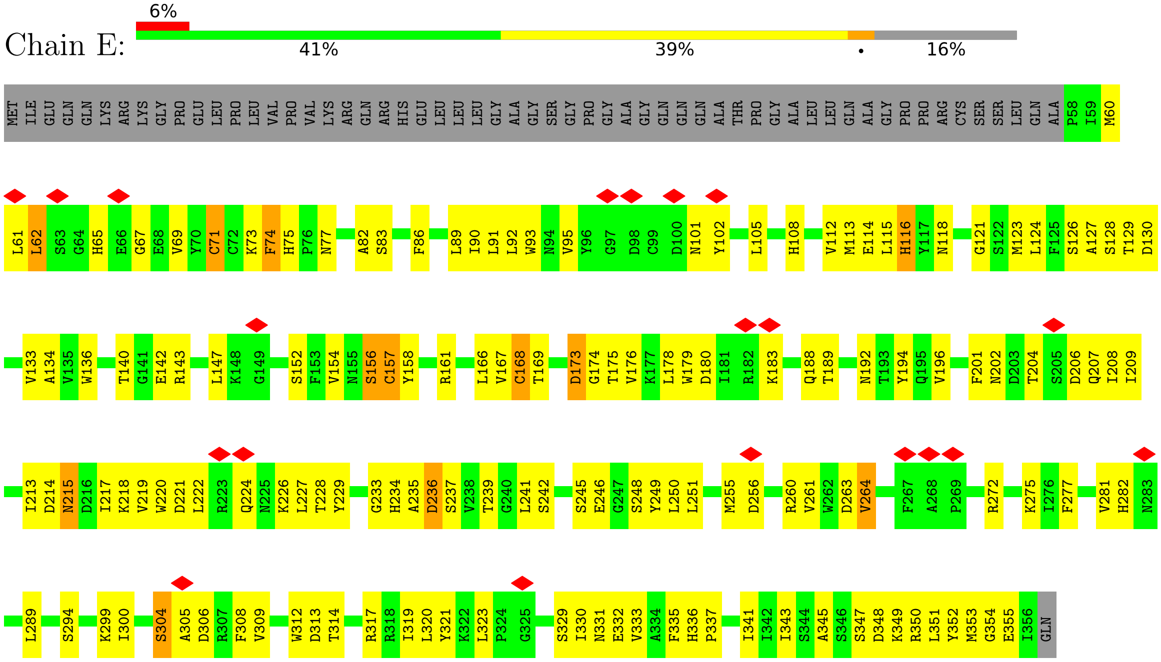
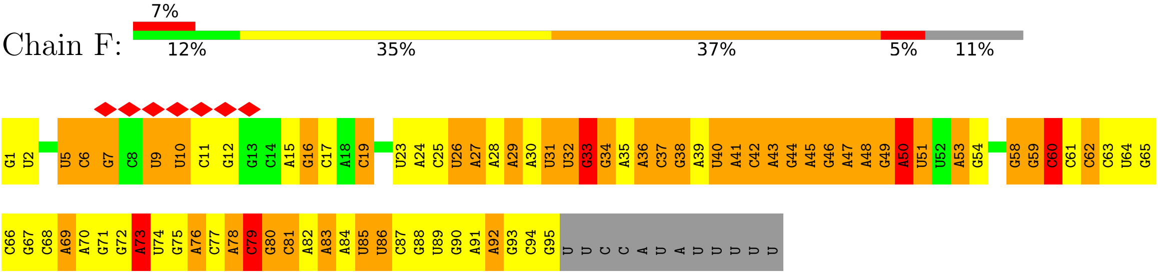
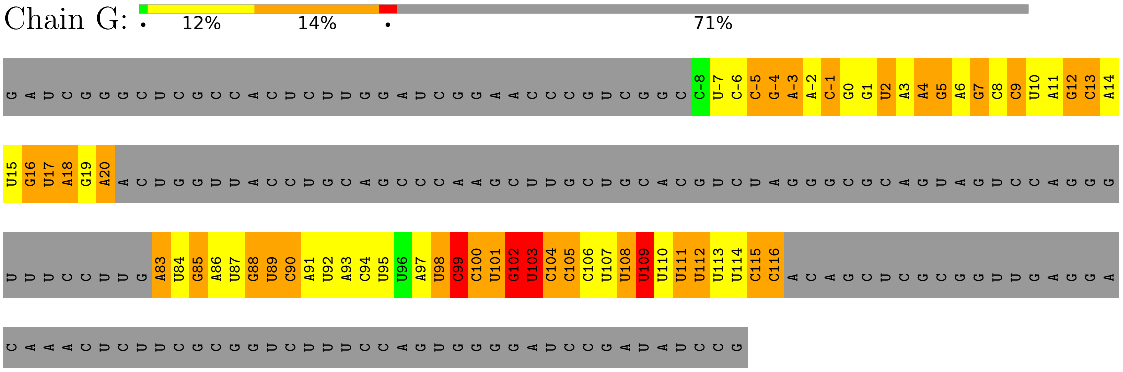
- Molecule 5: U5 small nuclear ribonucleoprotein 40 kDa protein



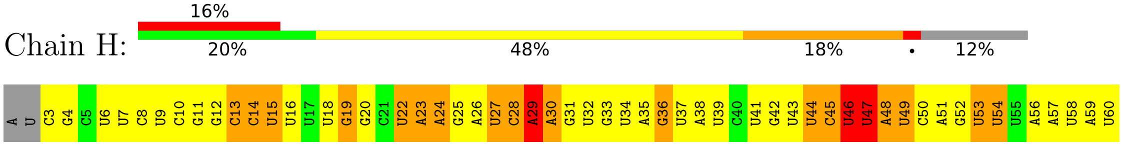
- Molecule 6: U6 snRNA

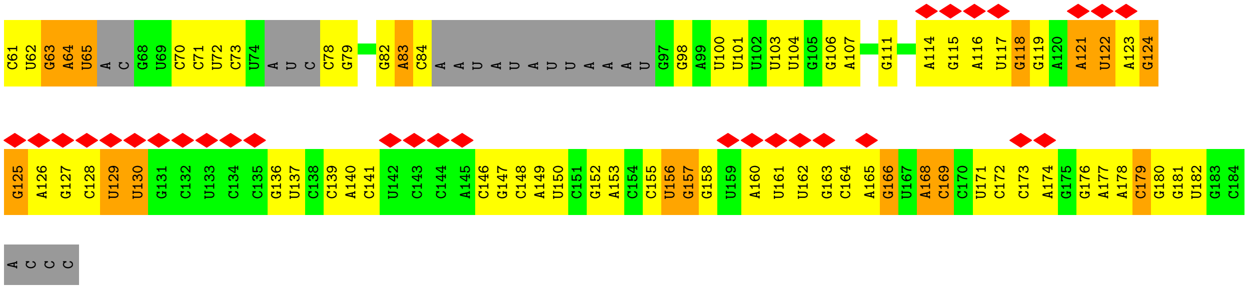


- Molecule 7: pre-mRNA

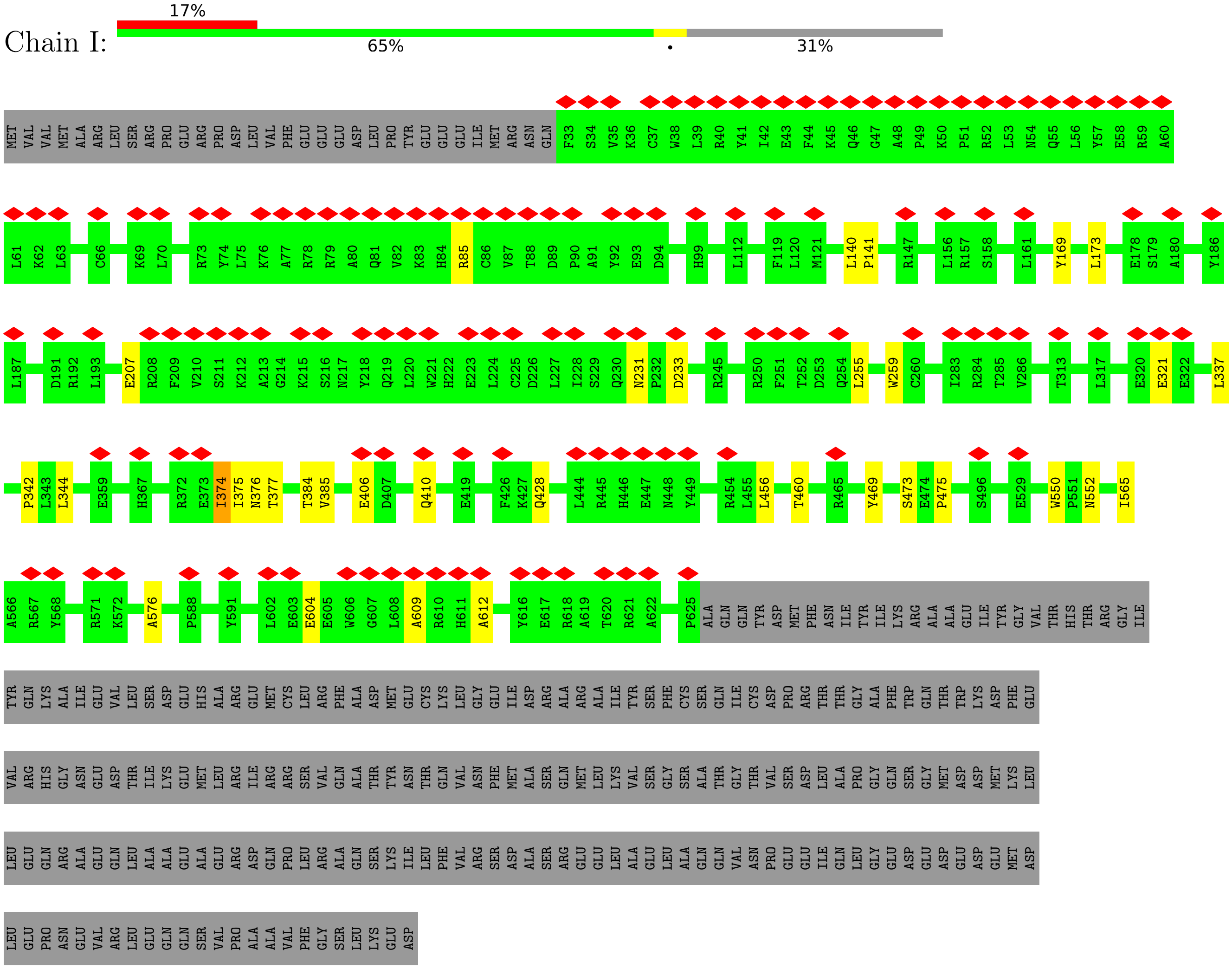


- Molecule 8: U2 snRNA

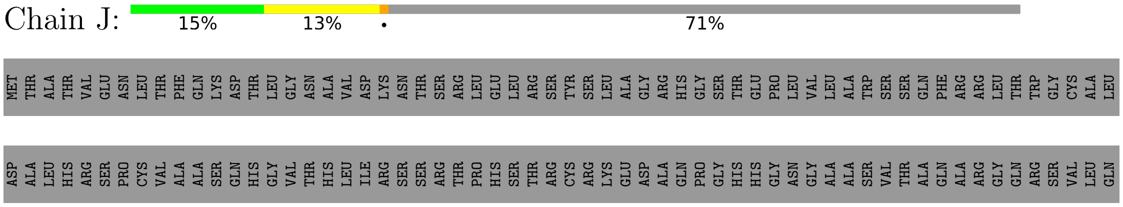


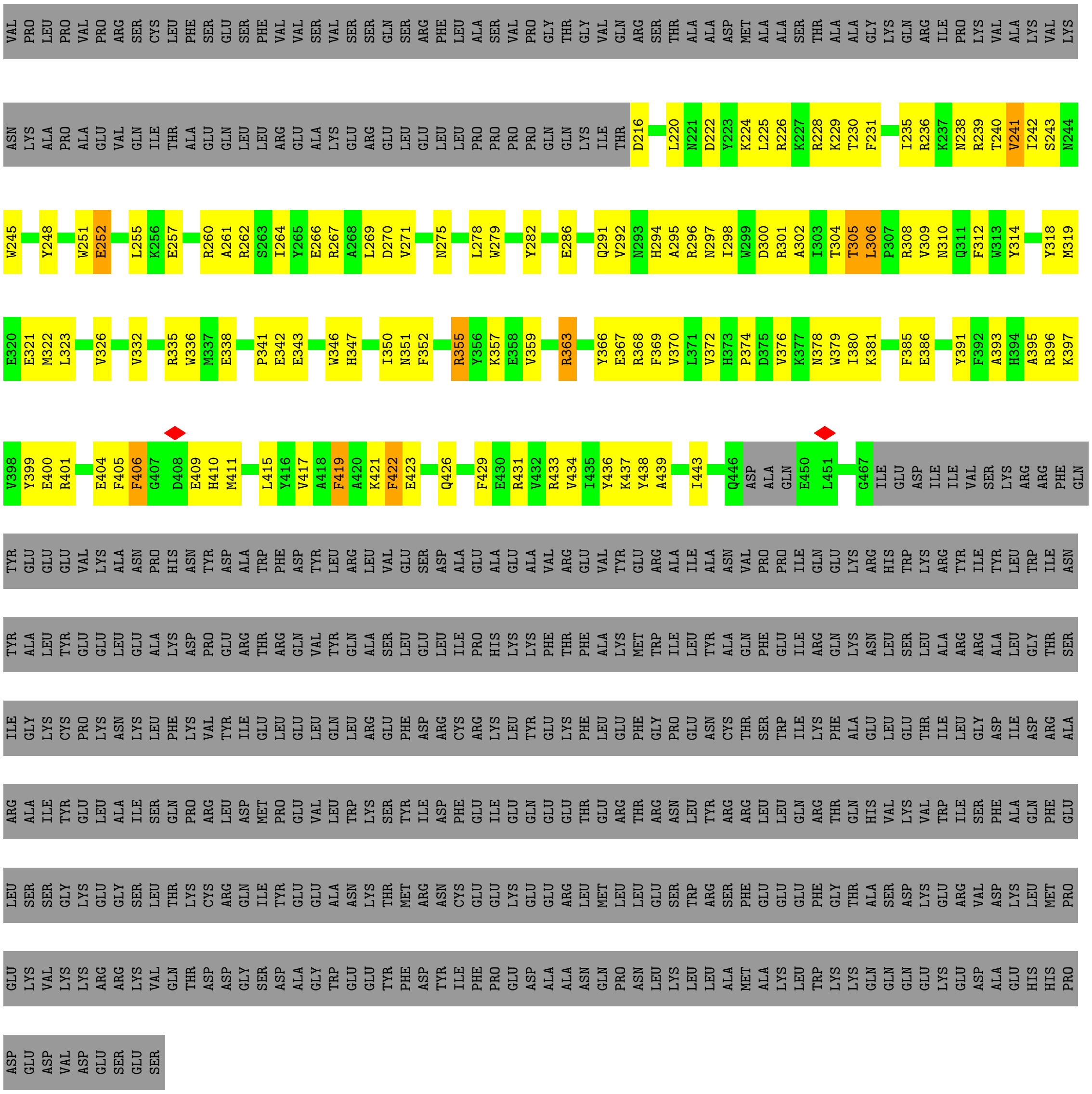


- Molecule 9: Pre-mRNA-splicing factor SYF1

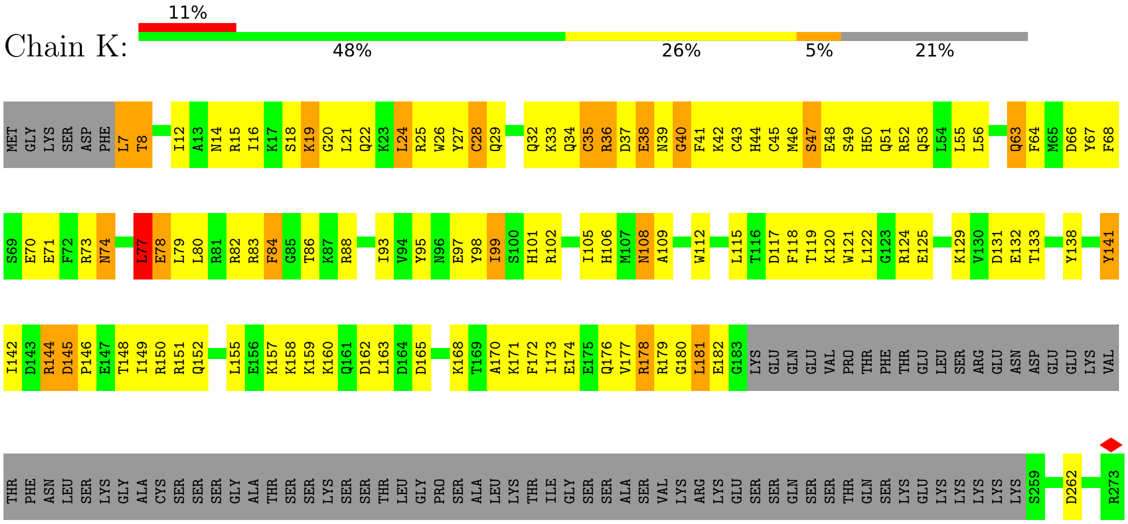


- Molecule 10: Crooked neck-like protein 1

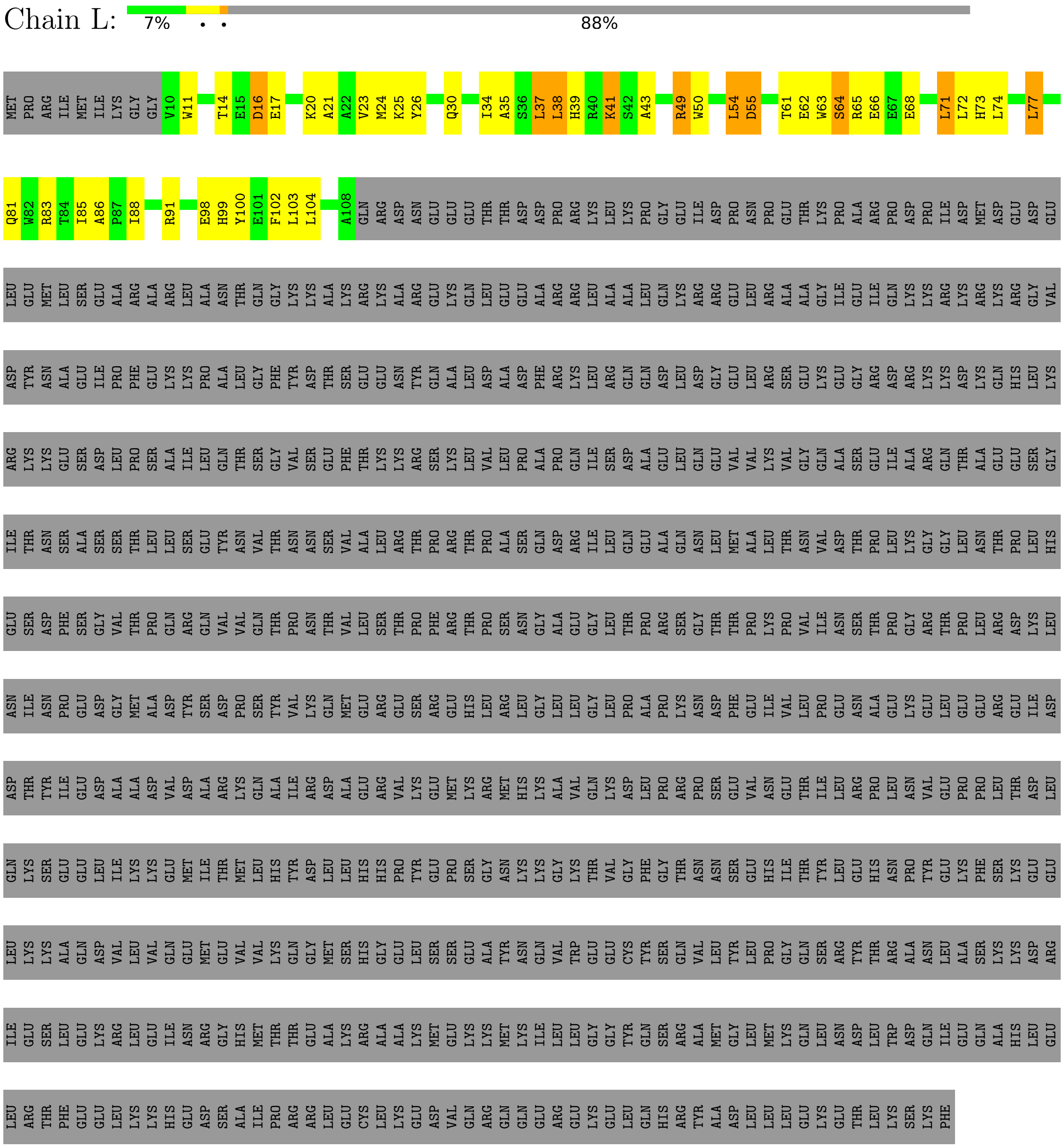




- Molecule 11: DNA/RNA-binding protein KIN17

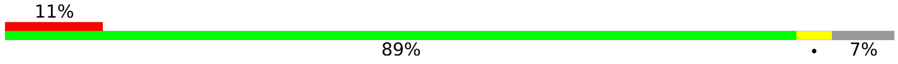


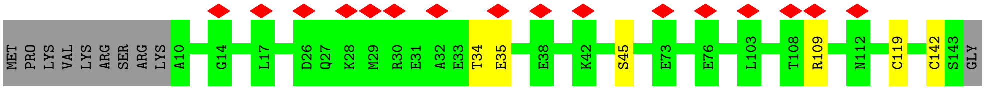
- Molecule 12: Cell division cycle 5-like protein



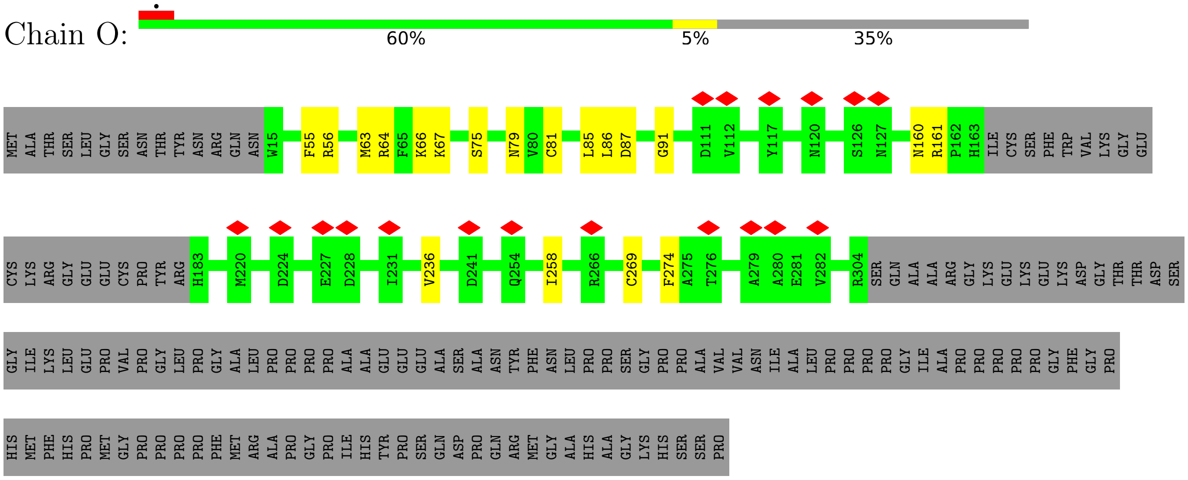
- Molecule 13: Protein BUD31 homolog

Chain N:

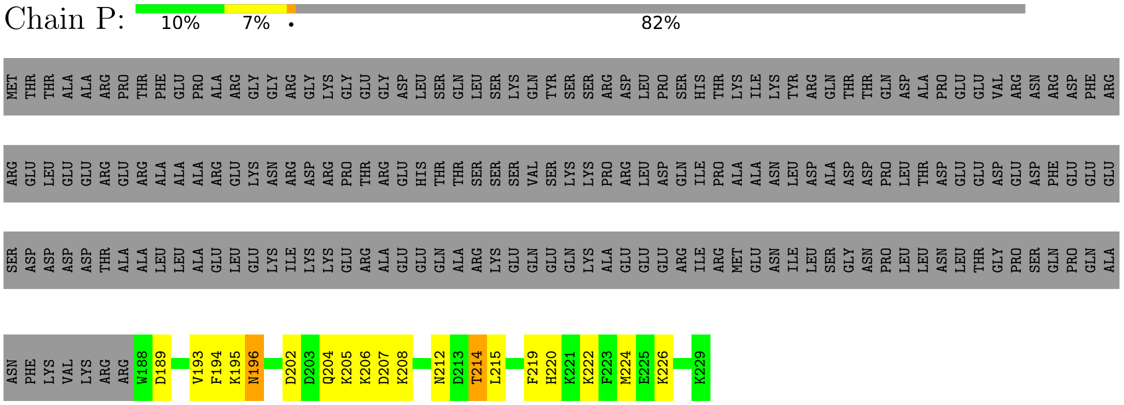




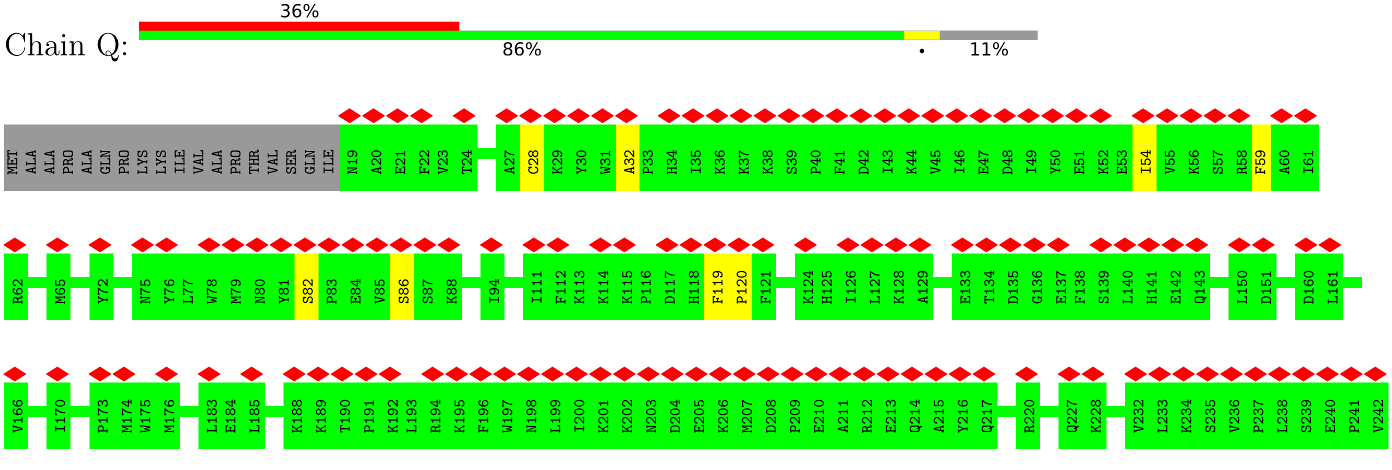
- Molecule 14: Pre-mRNA-splicing factor RBM22

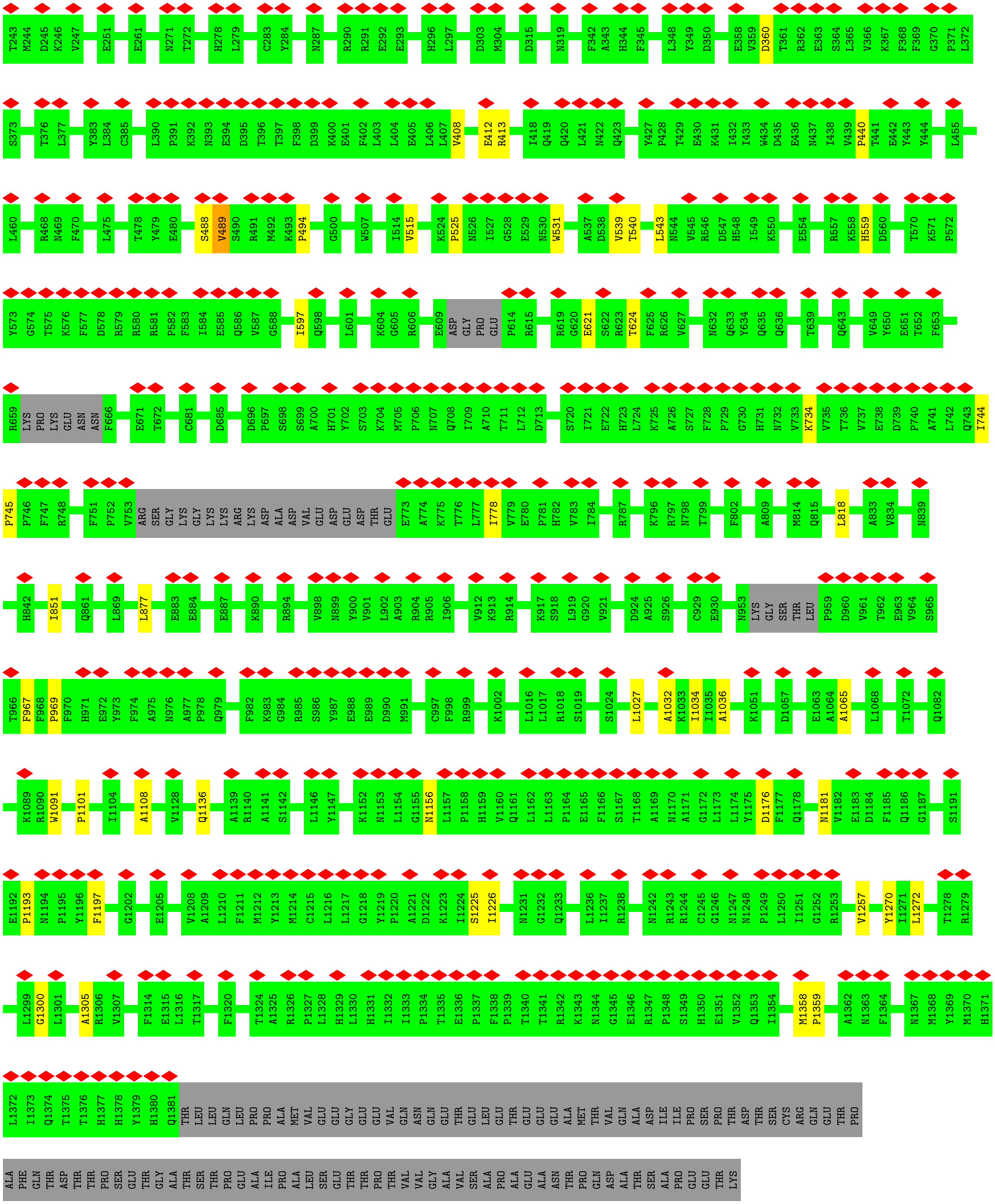


- Molecule 15: Spliceosome-associated protein CWC15 homolog



- Molecule 16: RNA helicase aquarius





- Molecule 17: SNW domain-containing protein 1

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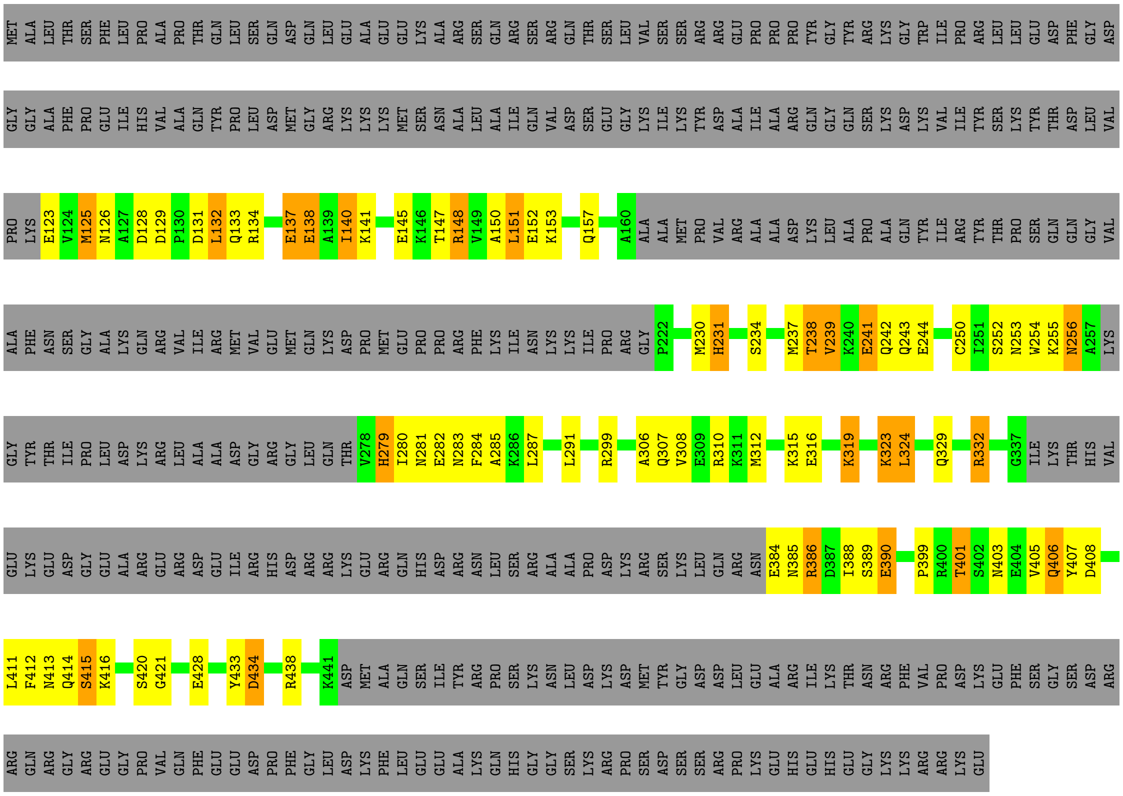
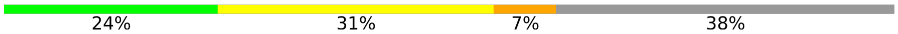
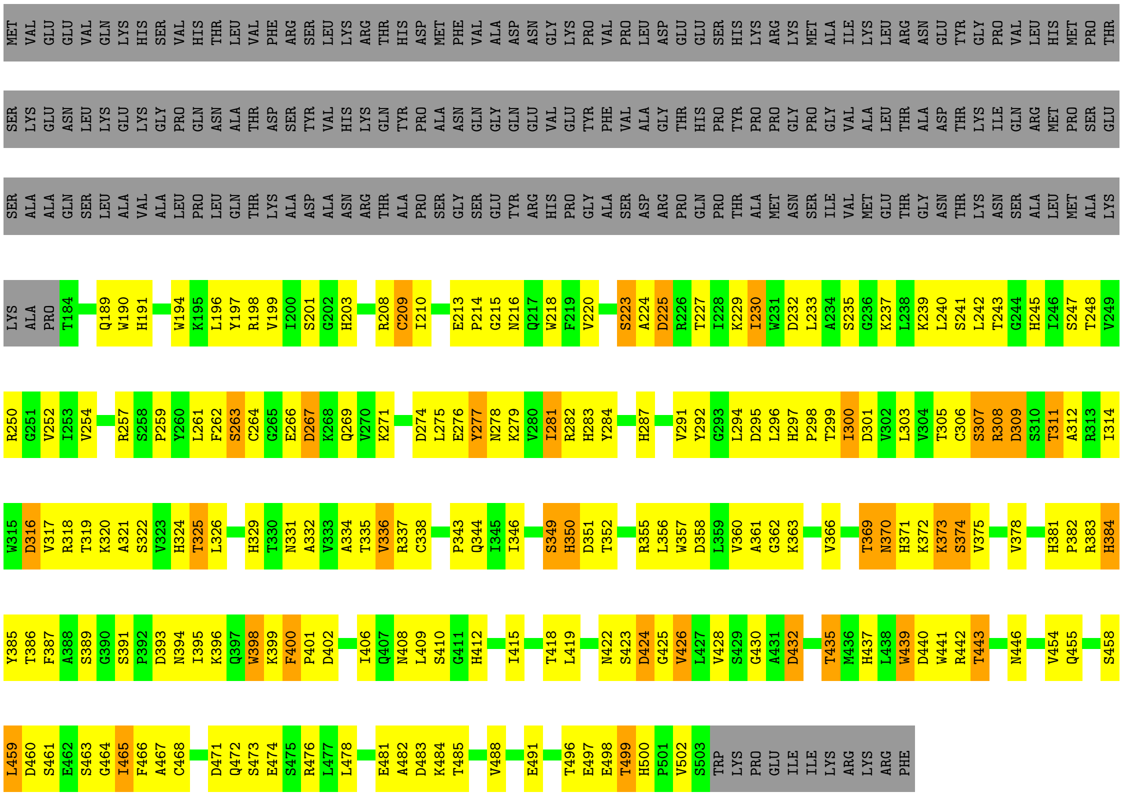


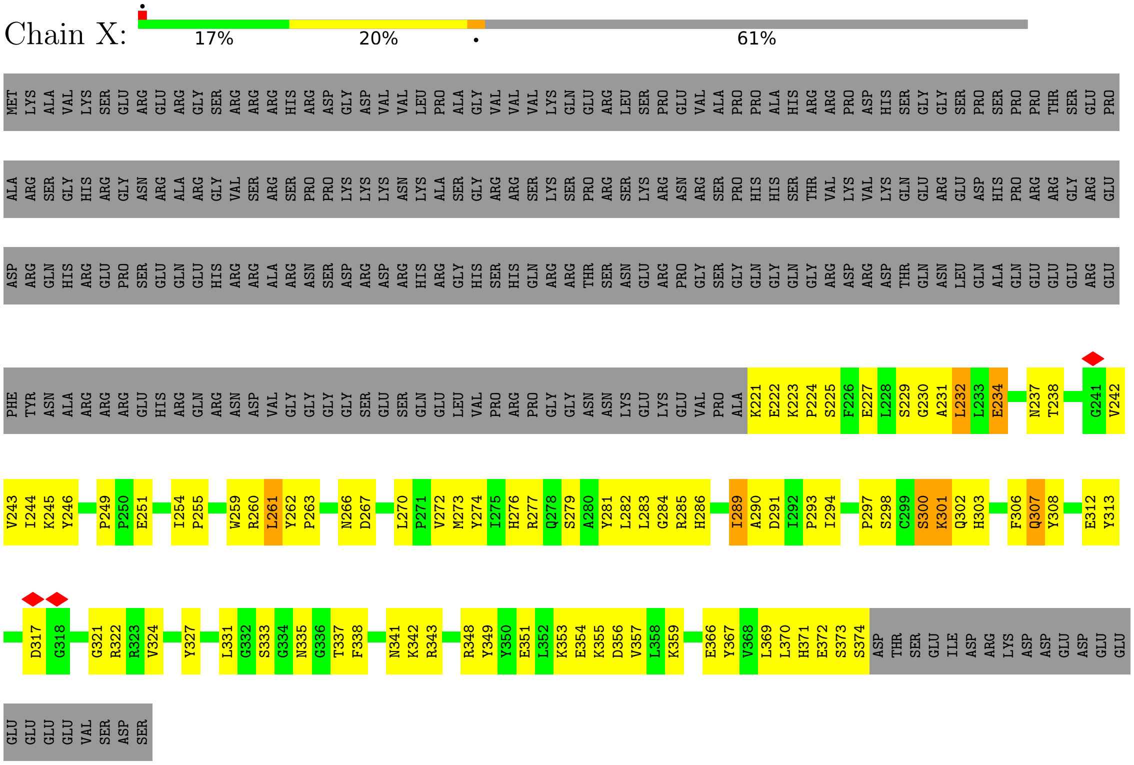
- Molecule 18: Pleiotropic regulator 1

Chain T:

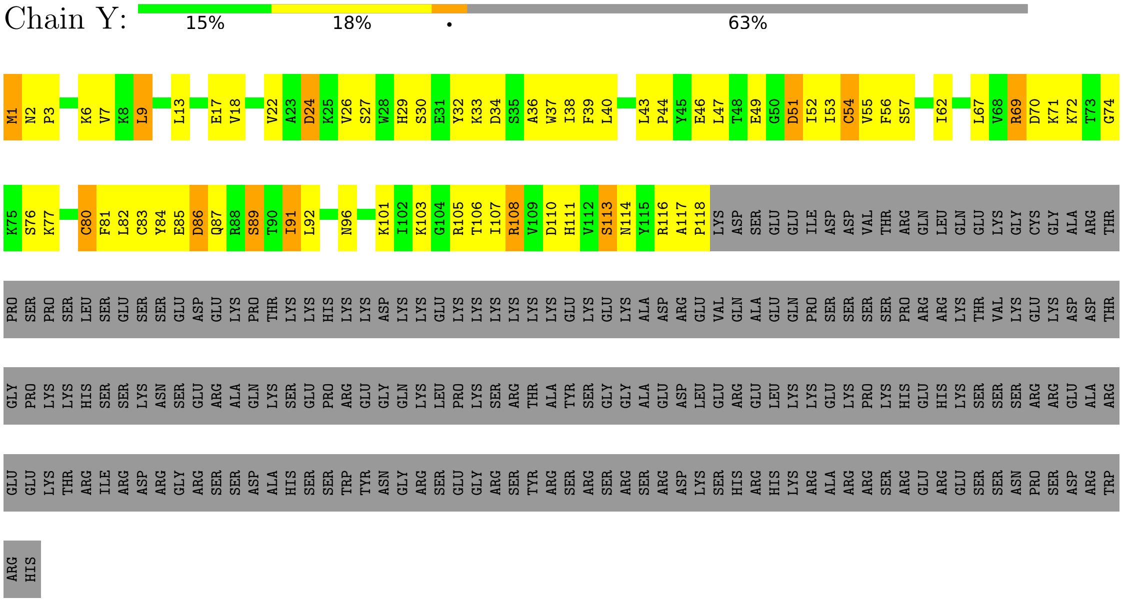




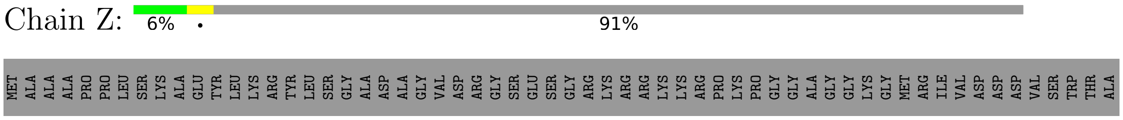
- Molecule 19: Smad nuclear-interacting protein 1

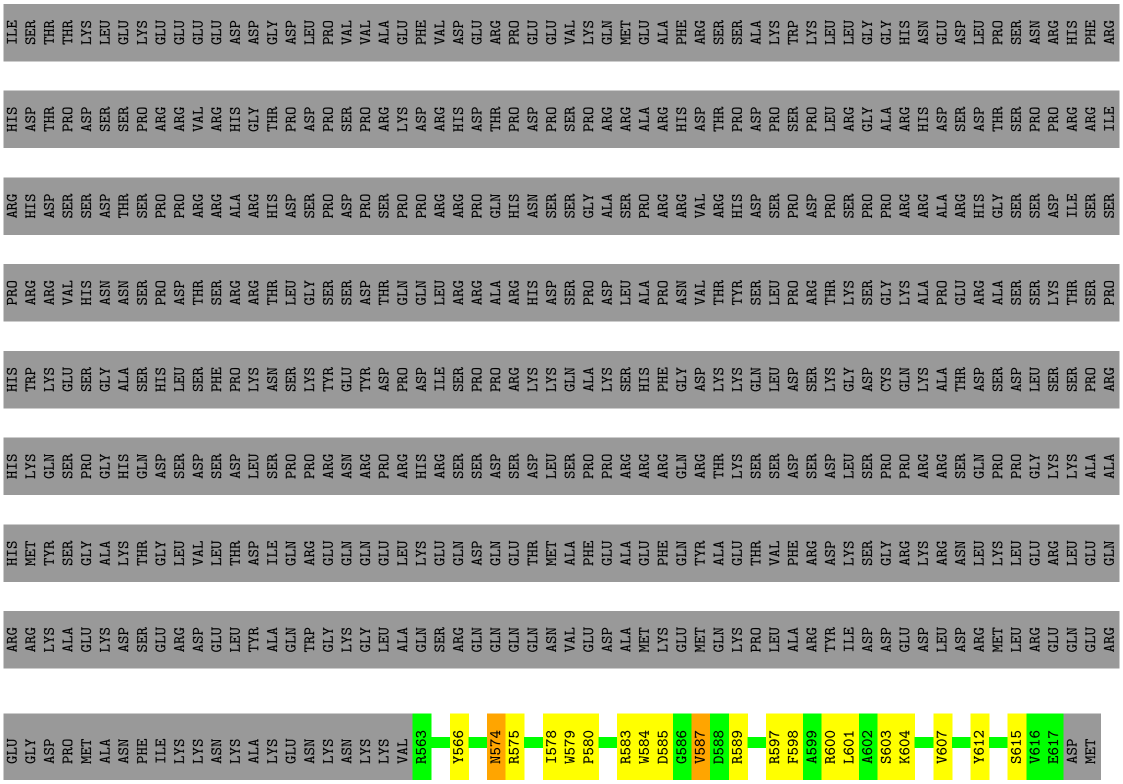


- Molecule 20: RNA-binding motif protein, X-linked 2



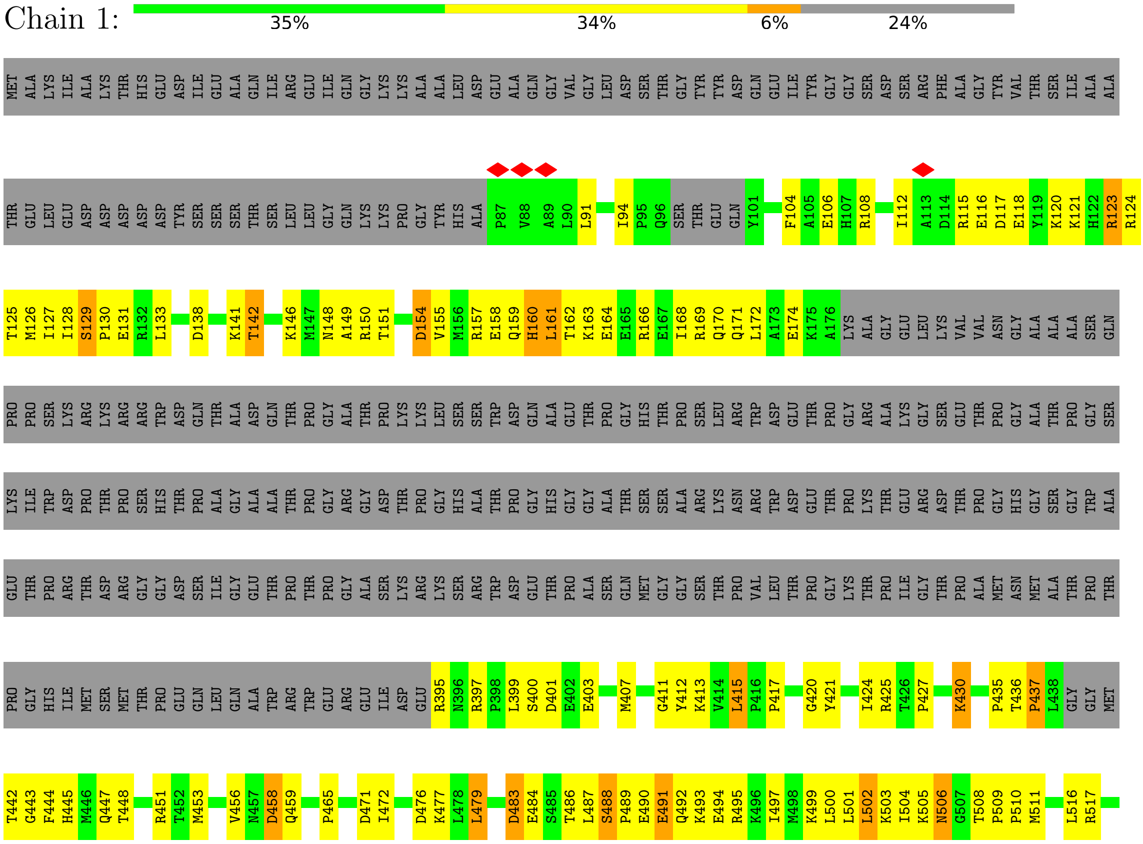
- Molecule 21: BUD13 homolog

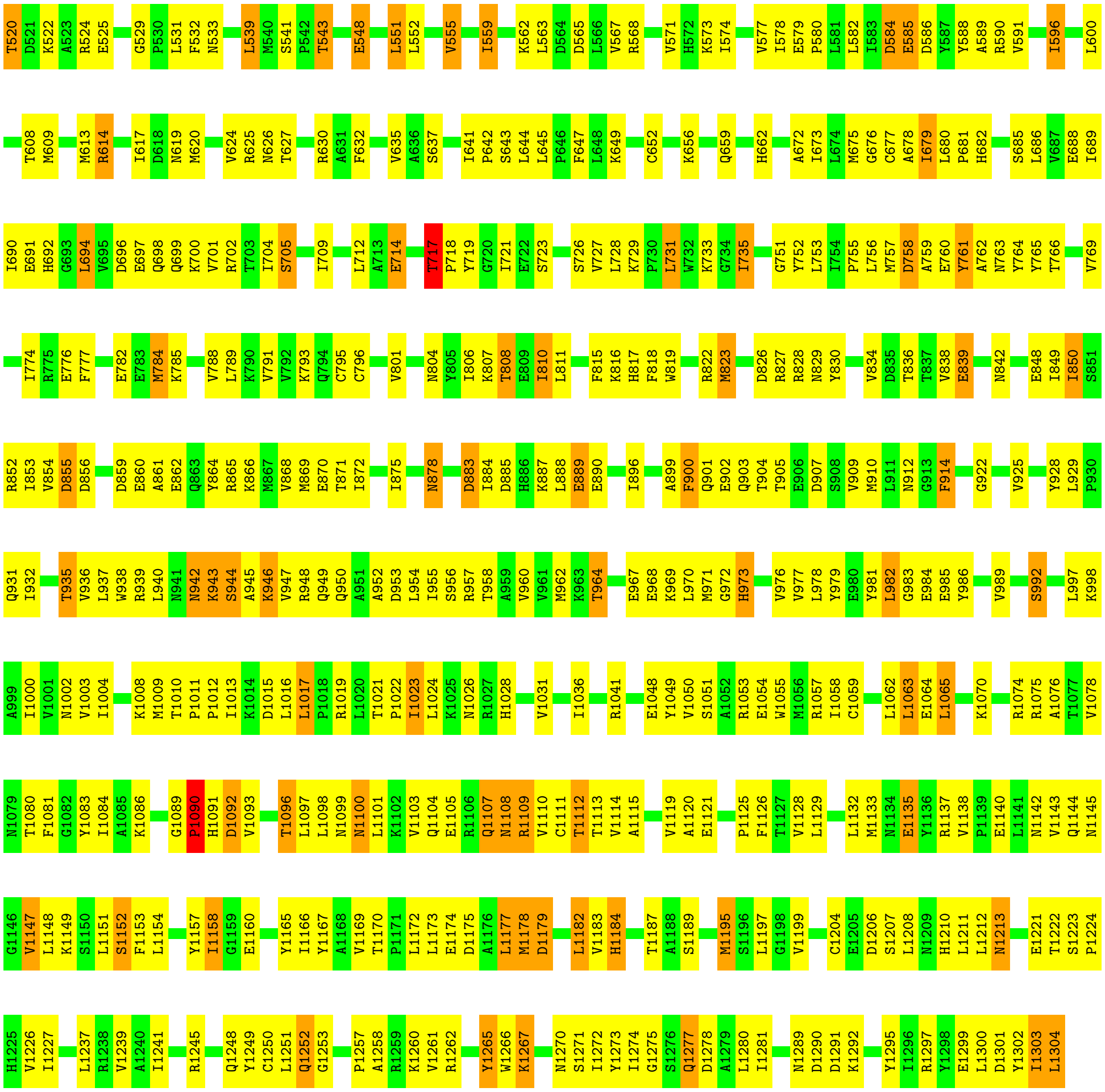




- Molecule 22: Splicing factor 3B subunit 1

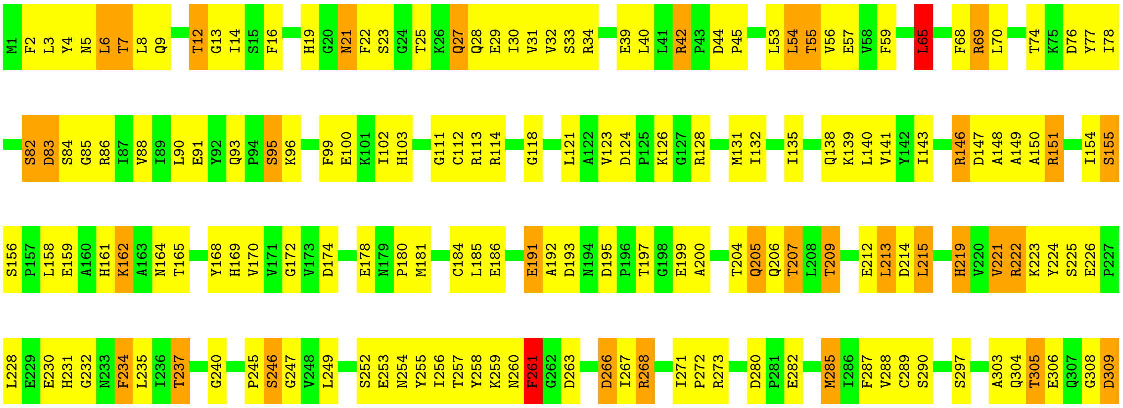
Chain 1:

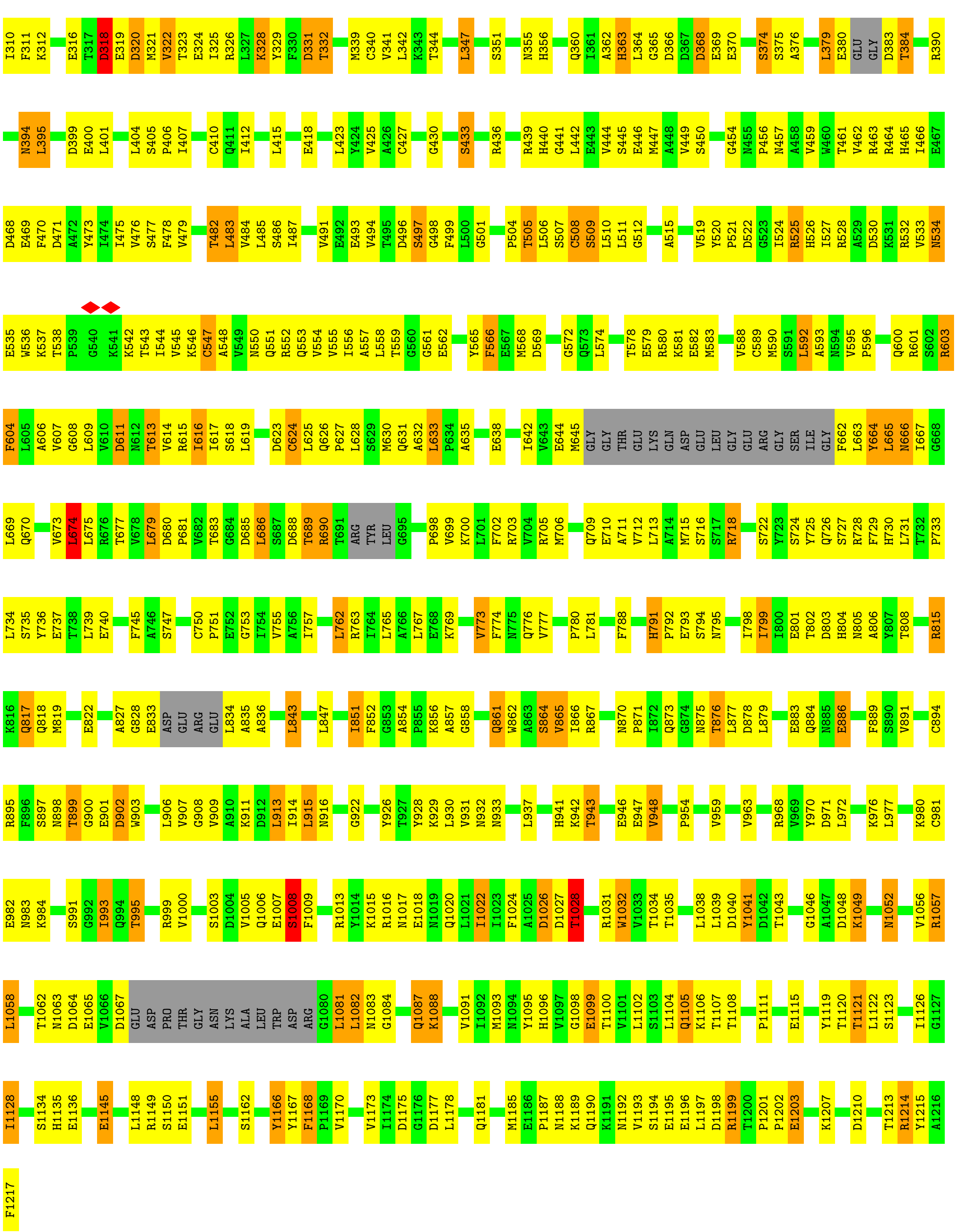




- Molecule 23: Splicing factor 3B subunit 3

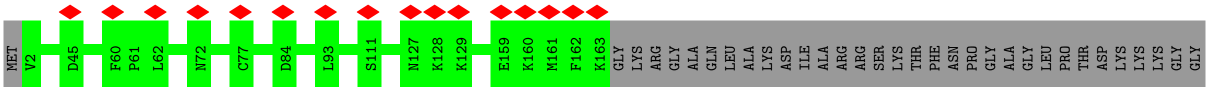
Chain 3:





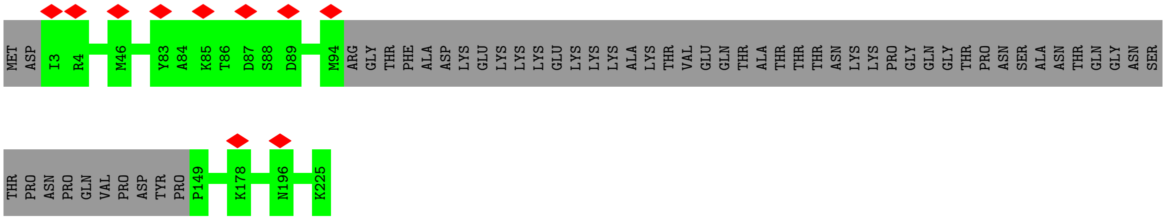
- Molecule 24: U2 small nuclear ribonucleoprotein A’

Chain o:



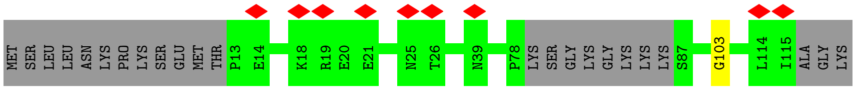
- Molecule 25: U2 small nuclear ribonucleoprotein B"

Chain p:



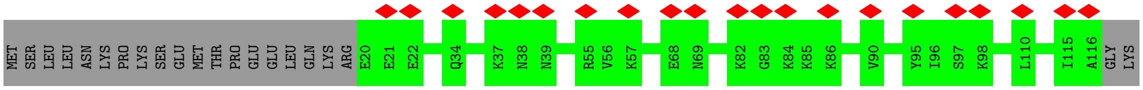
- Molecule 26: Small nuclear ribonucleoprotein Sm D2

Chain h:



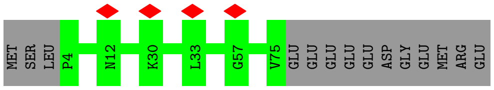
- Molecule 26: Small nuclear ribonucleoprotein Sm D2

Chain c:



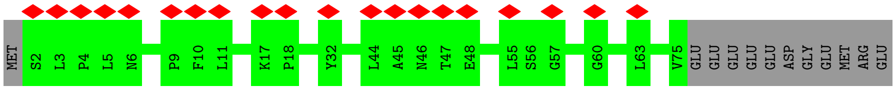
- Molecule 27: Small nuclear ribonucleoprotein F

Chain i:



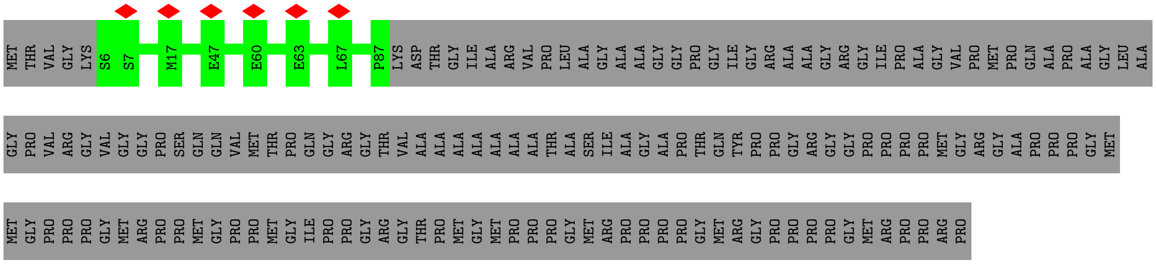
- Molecule 27: Small nuclear ribonucleoprotein F

Chain d:



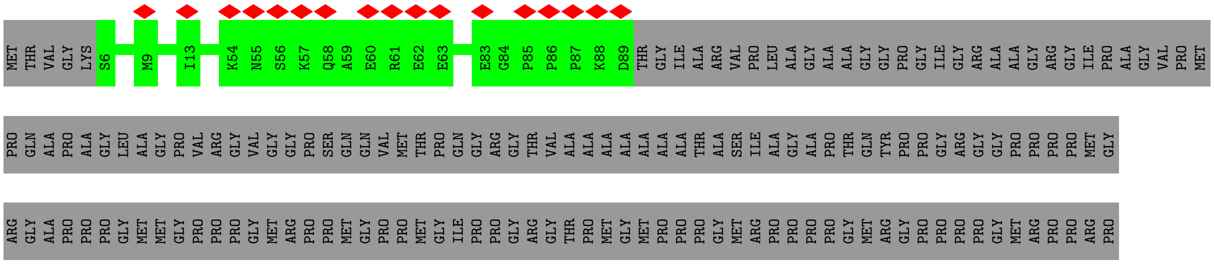
- Molecule 28: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain m:



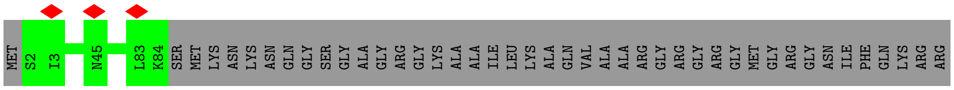
- Molecule 28: Small nuclear ribonucleoprotein-associated proteins B and B’

Chain a:



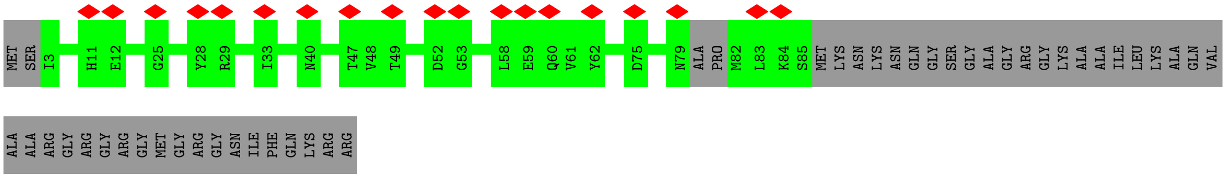
- Molecule 29: Small nuclear ribonucleoprotein Sm D3

Chain l:



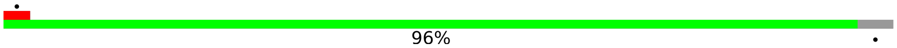
- Molecule 29: Small nuclear ribonucleoprotein Sm D3

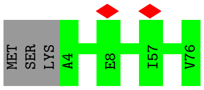
Chain g:



- Molecule 30: Small nuclear ribonucleoprotein G

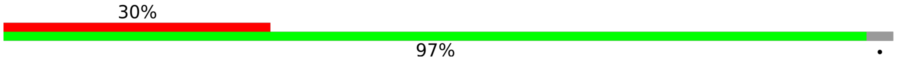
Chain k:

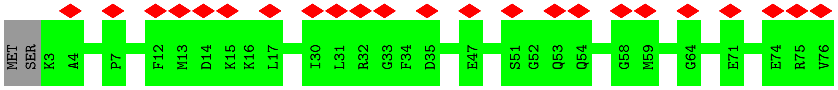




- Molecule 30: Small nuclear ribonucleoprotein G

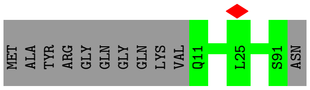
Chain f:





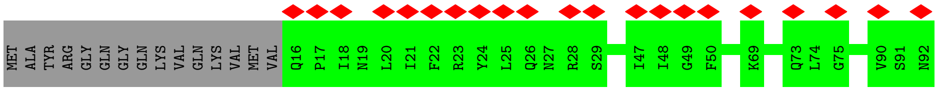
- Molecule 31: Small nuclear ribonucleoprotein E

Chain j:



- Molecule 31: Small nuclear ribonucleoprotein E

Chain e:

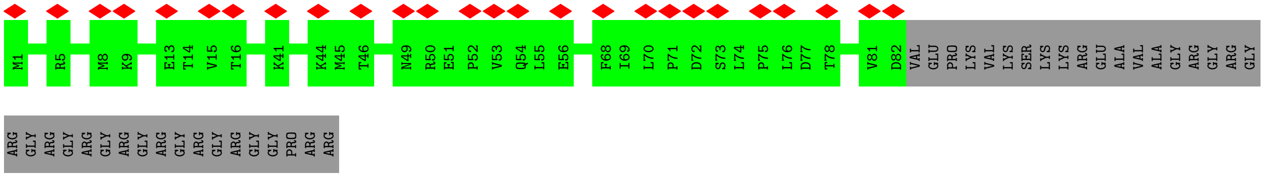


- Molecule 32: Small nuclear ribonucleoprotein Sm D1

Chain n:

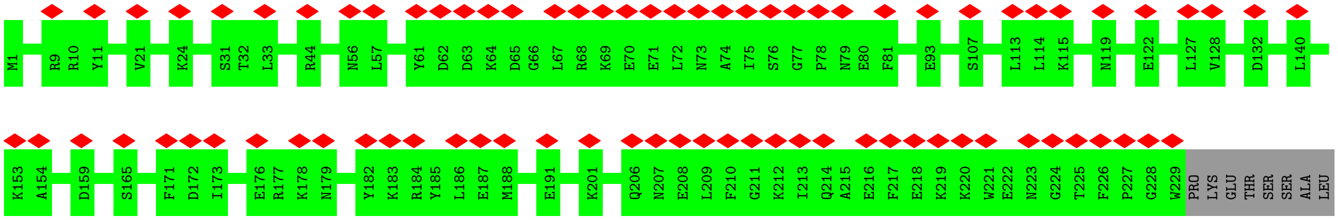
- Molecule 32: Small nuclear ribonucleoprotein Sm D1

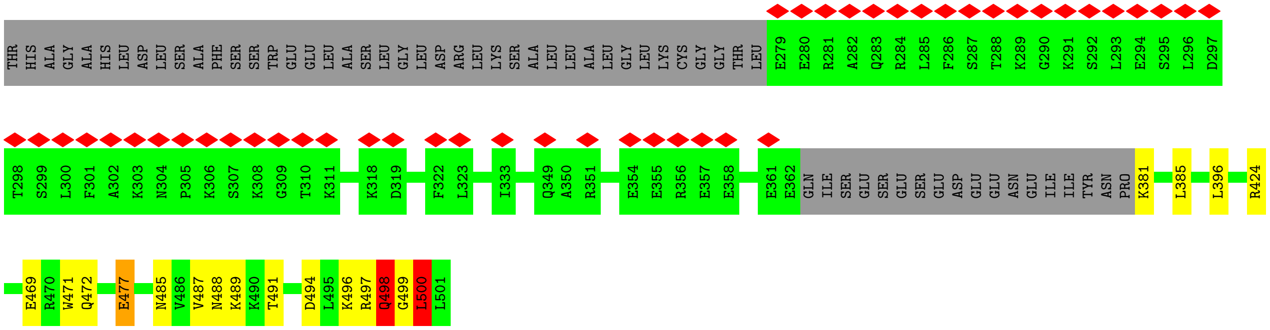
Chain b:



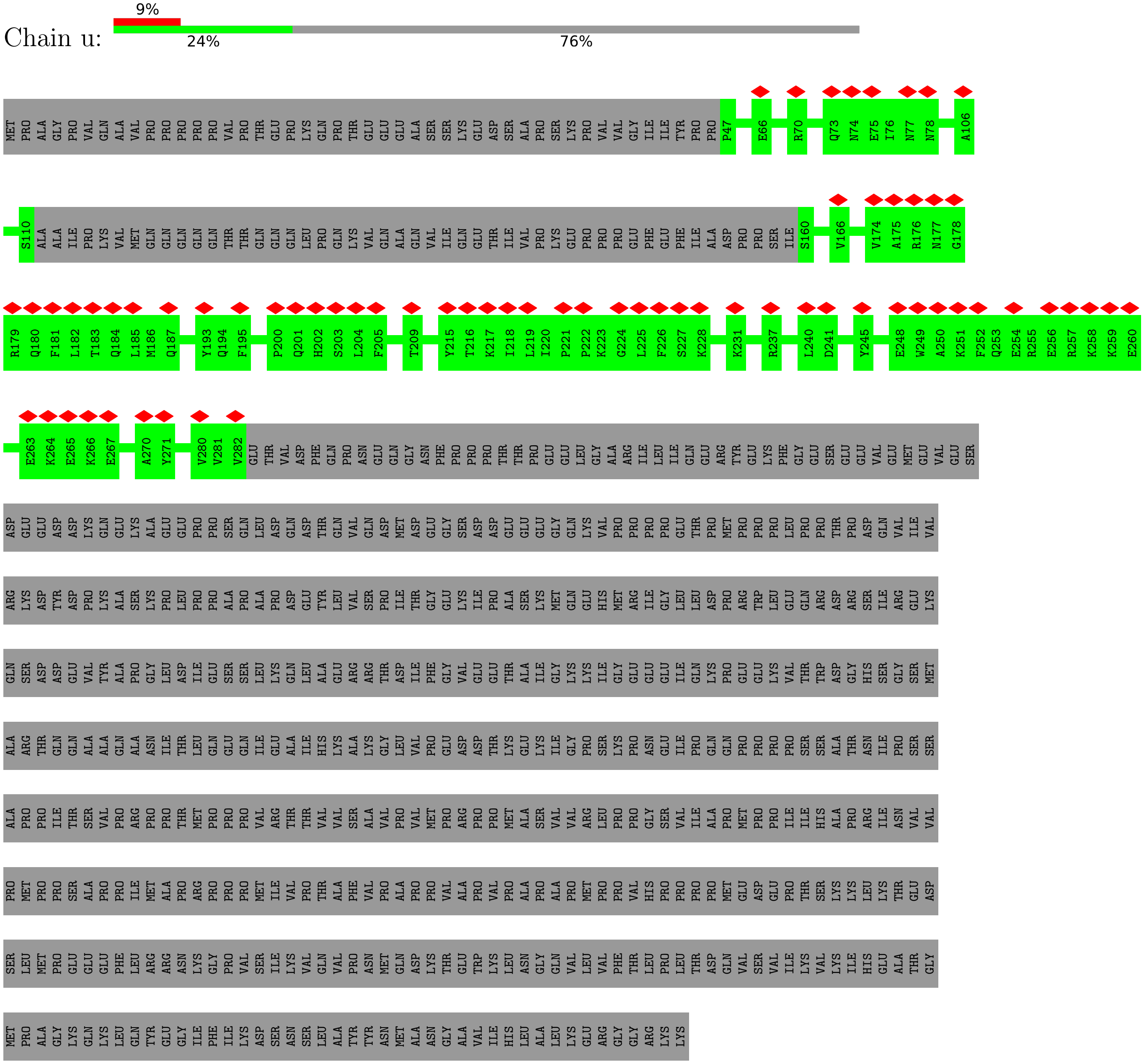
- Molecule 33: Splicing factor 3A subunit 3

Chain w:

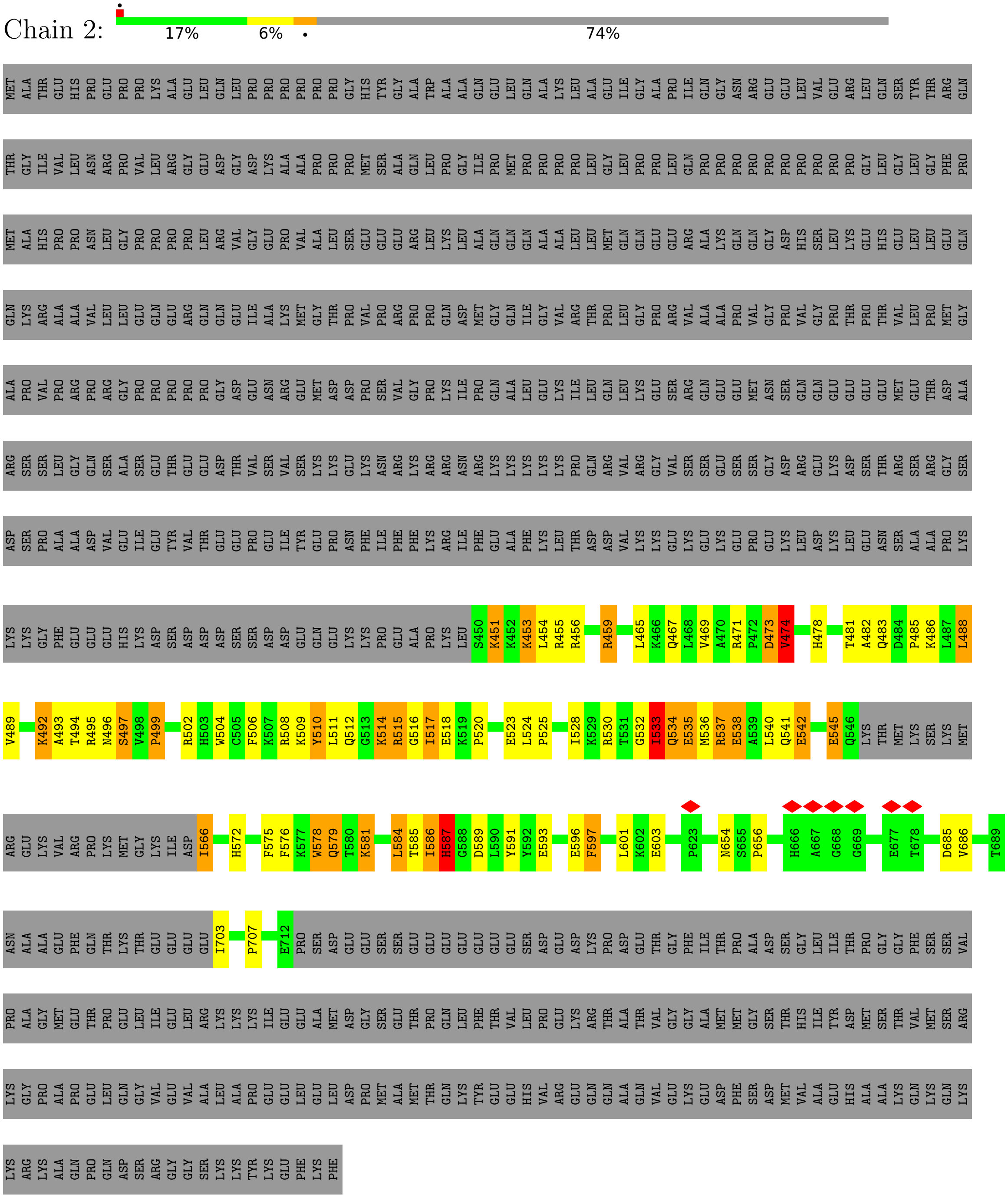




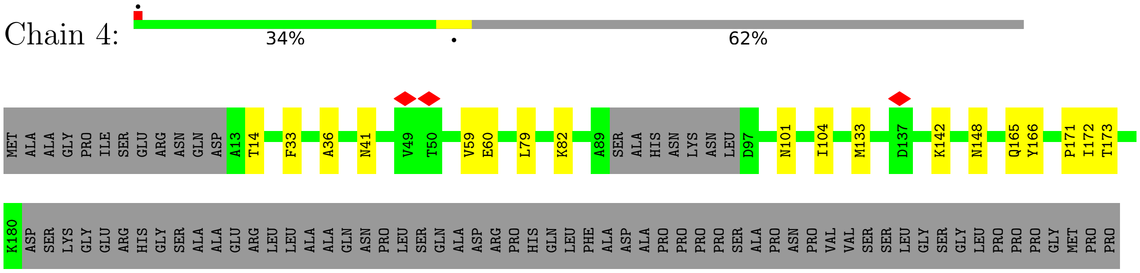
- Molecule 34: Splicing factor 3A subunit 1

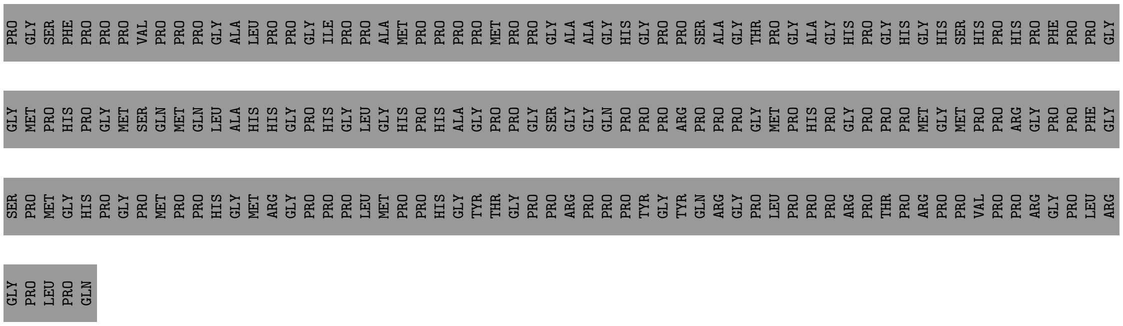


- Molecule 35: Splicing factor 3B subunit 2

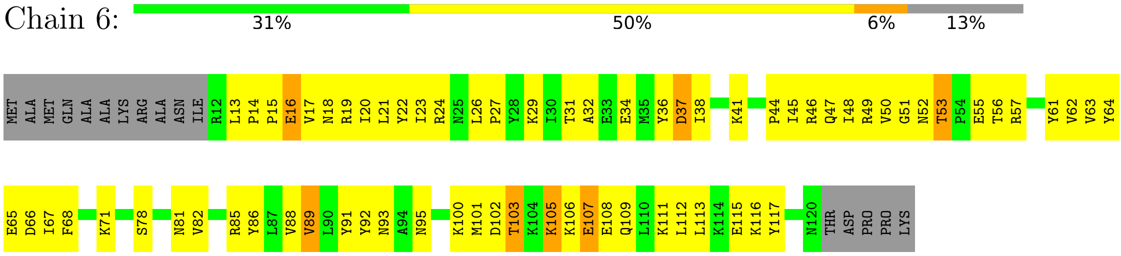


- Molecule 36: Splicing factor 3B subunit 4

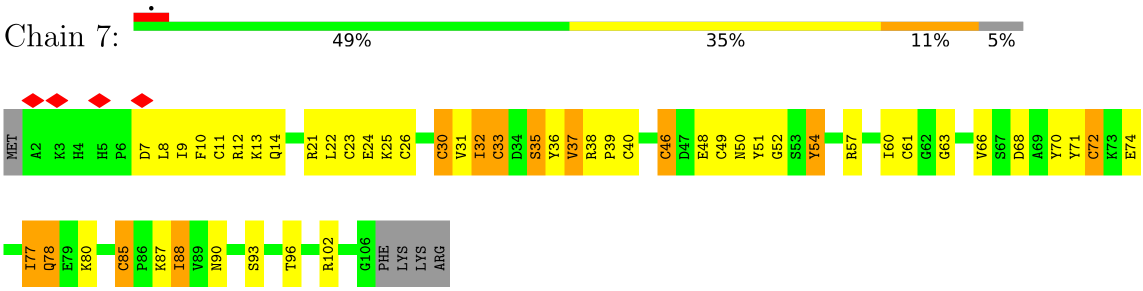




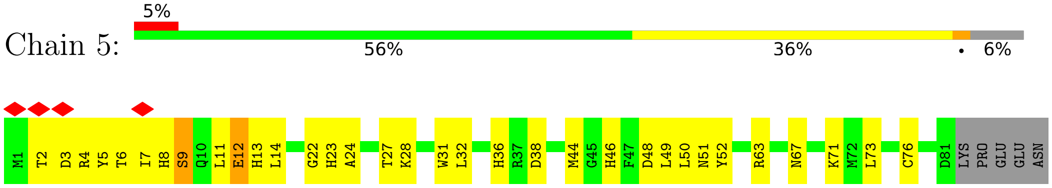
- Molecule 37: Splicing factor 3B subunit 6



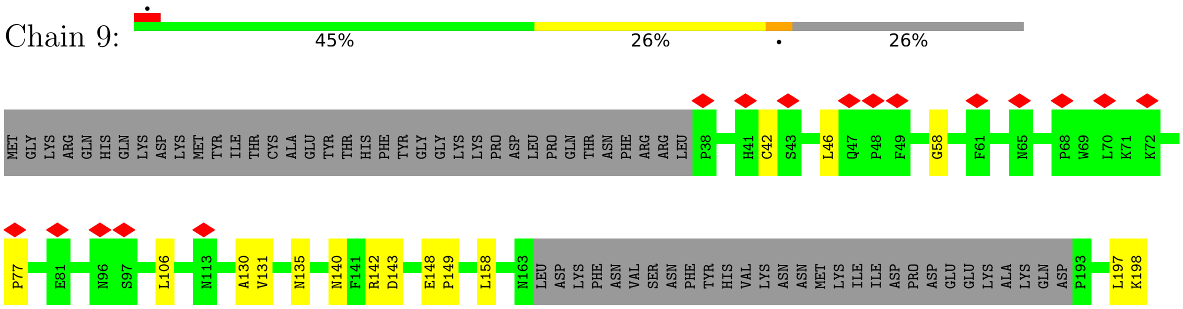
- Molecule 38: PHD finger-like domain-containing protein 5A

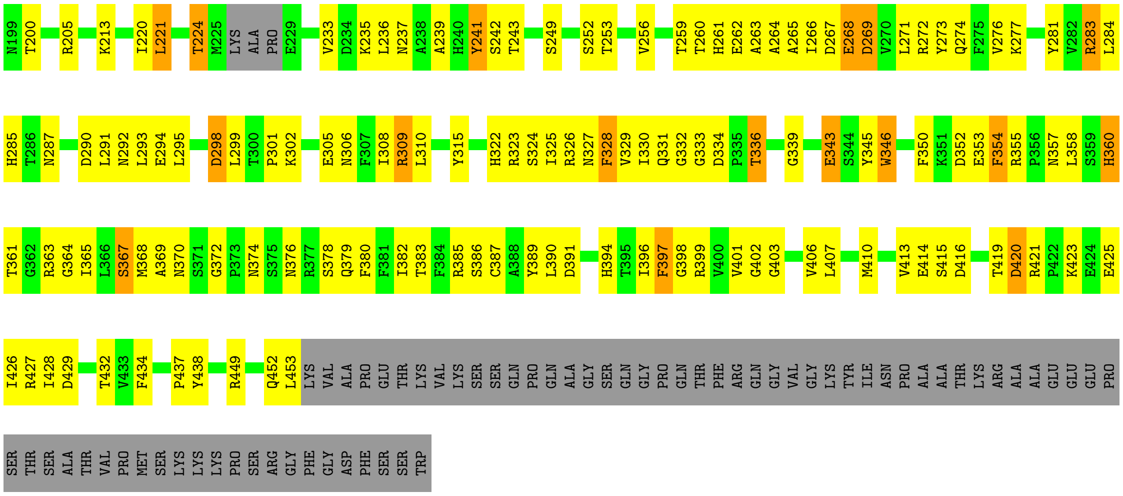


- Molecule 39: Splicing factor 3B subunit 5



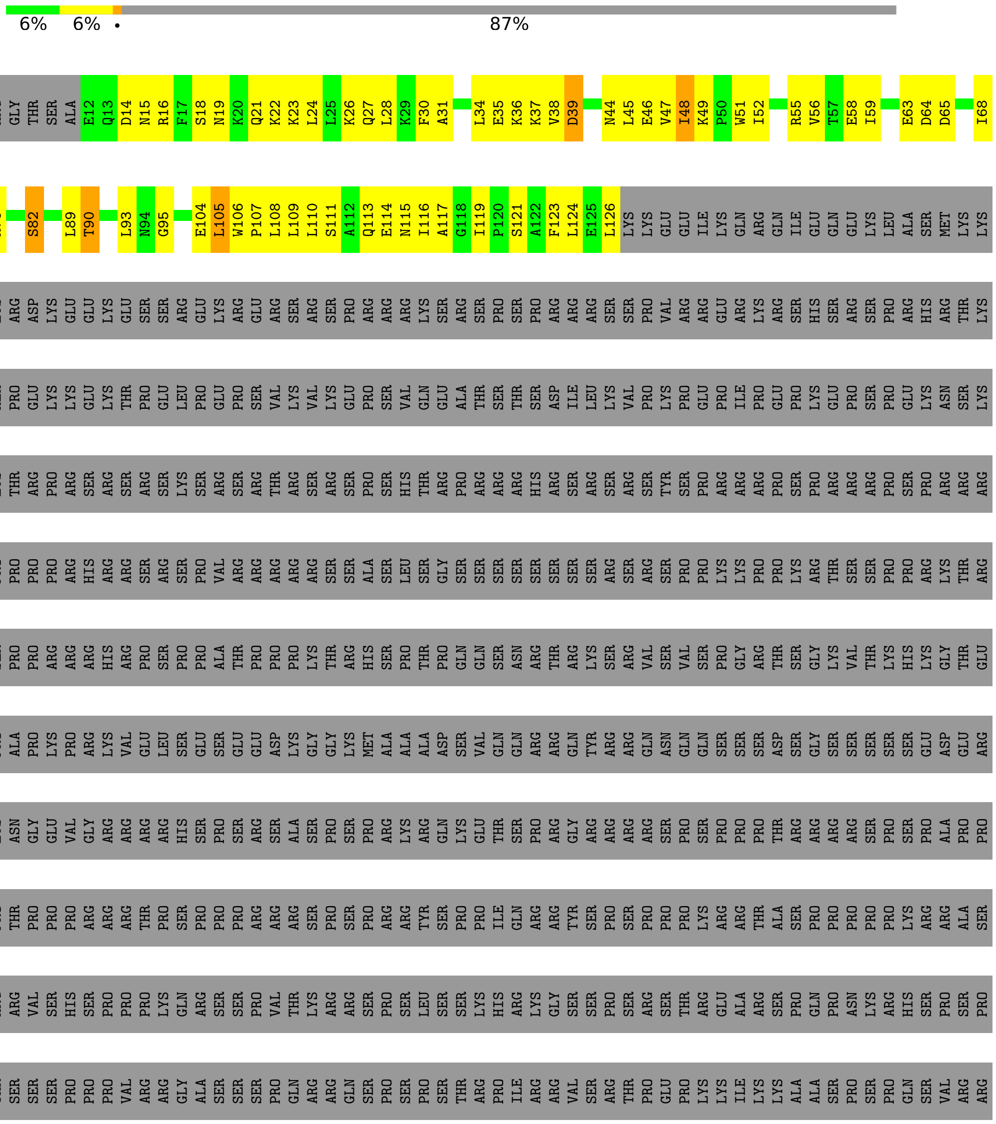
- Molecule 40: RING-type E3 ubiquitin-protein ligase PPIL2

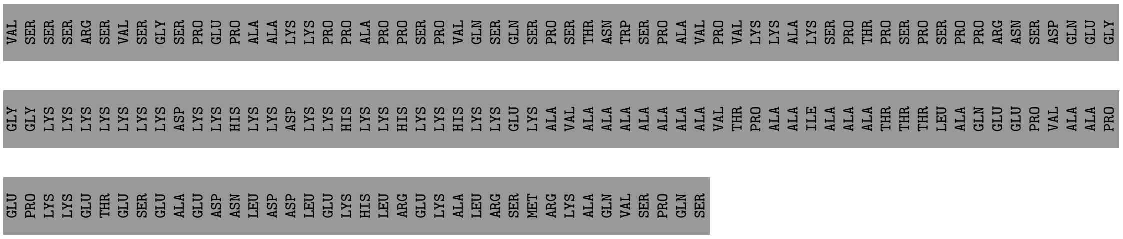




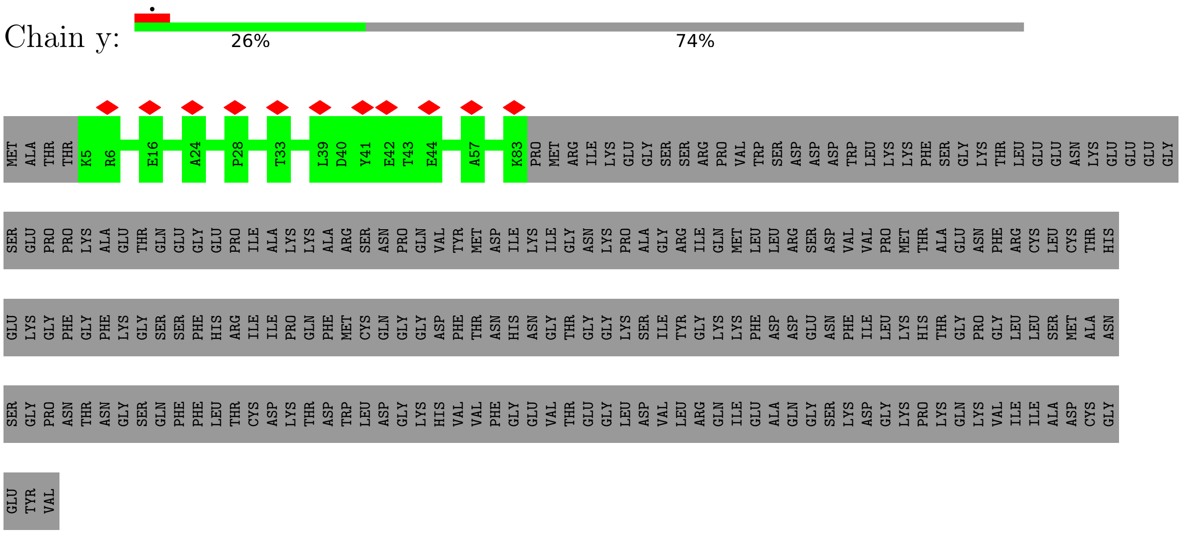
- Molecule 41: Serine/arginine repetitive matrix protein 1

Chain 8:

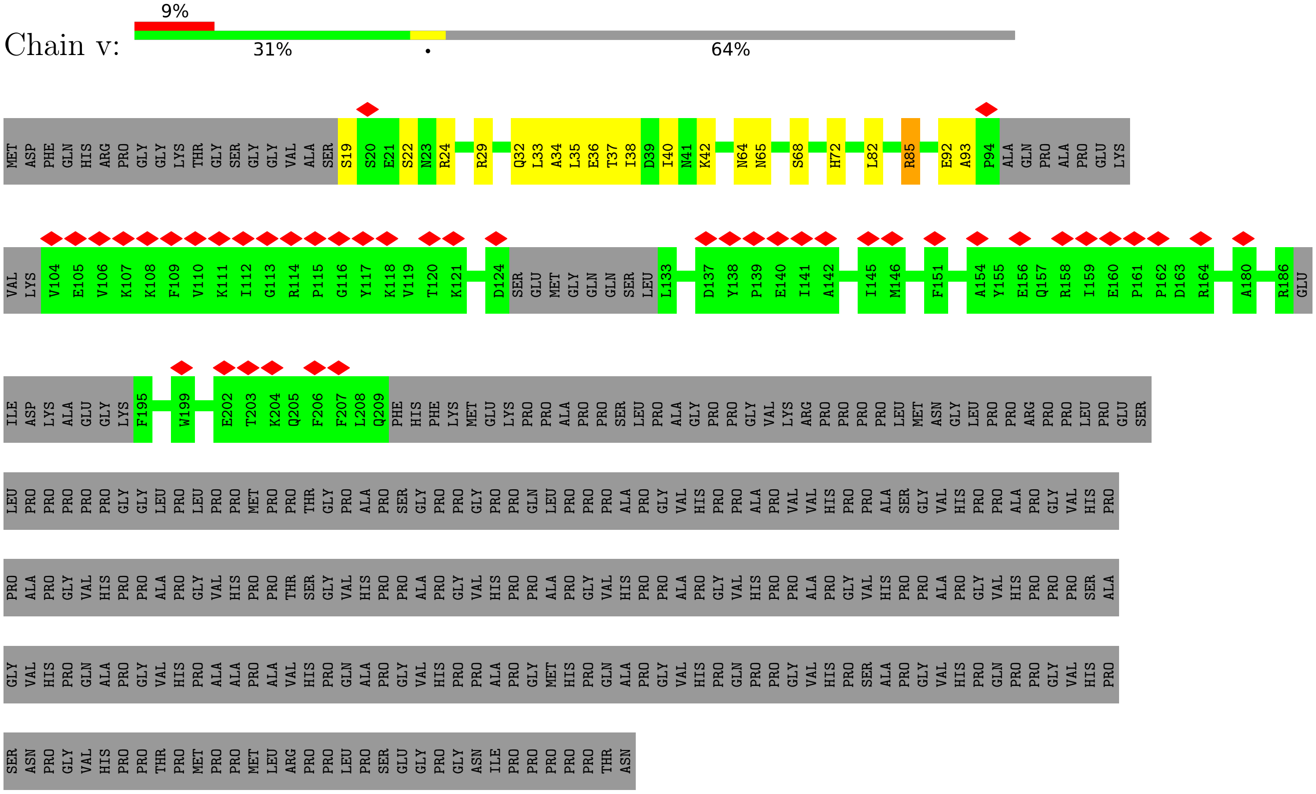




- Molecule 42: Peptidyl-prolyl cis-trans isomerase E

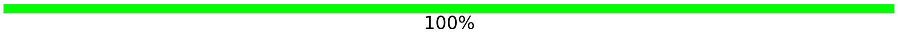


- Molecule 43: Splicing factor 3A subunit 2



- Molecule 44: Unknown polymer

Chain z:



There are no outlier residues recorded for this chain.

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46696	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 $(e^-/\text{Å}^2)$	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.456	Depositor
Minimum map value	-1.255	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.19	Depositor
Map size (Å)	516.96, 516.96, 516.96	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.077, 1.077, 1.077	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.71	2/16545 (0.0%)	0.65	9/22533 (0.0%)
2	B	0.51	0/2303	1.11	9/3579 (0.3%)
3	C	0.33	0/7237	0.54	1/9834 (0.0%)
4	D	0.24	0/8527	0.44	0/11887
5	E	0.31	0/2392	0.53	0/3242
6	F	0.61	1/2279 (0.0%)	1.20	16/3551 (0.5%)
7	G	0.83	0/1470	1.27	11/2281 (0.5%)
8	H	0.67	0/3900	1.03	9/6065 (0.1%)
9	I	0.25	0/3013	0.47	0/4223
10	J	0.36	0/2171	0.48	0/2929
11	K	0.37	0/2203	0.62	2/2983 (0.1%)
12	L	0.70	0/850	0.63	0/1146
13	N	0.24	0/661	0.41	0/919
14	O	0.25	0/1338	0.45	0/1861
15	P	0.73	0/369	0.63	0/489
16	Q	0.24	0/6796	0.43	0/9527
17	R	0.55	0/1544	0.64	0/2074
18	T	0.65	0/2574	0.66	0/3511
19	X	0.37	0/1312	0.51	0/1769
20	Y	0.60	0/966	0.54	0/1303
21	Z	0.48	0/455	0.54	0/617
22	1	0.83	6/7983 (0.1%)	0.71	4/10805 (0.0%)
23	3	0.99	6/9428 (0.1%)	0.75	5/12794 (0.0%)
24	o	0.23	0/821	0.46	0/1149
25	p	0.27	0/857	0.46	0/1196
26	c	0.24	0/387	0.52	0/482
26	h	0.25	0/485	0.46	0/677
27	d	0.25	0/295	0.54	0/367
27	i	0.26	0/362	0.48	0/502
28	a	0.25	0/335	0.54	0/417
28	m	0.26	0/416	0.52	0/581
29	g	0.24	0/322	0.53	0/399

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
29	l	0.26	0/417	0.45	0/581
30	f	0.24	0/295	0.54	0/367
30	k	0.26	0/366	0.52	0/509
31	e	0.23	0/307	0.50	0/382
31	j	0.24	0/403	0.45	0/561
32	b	0.24	0/327	0.53	0/407
32	n	0.23	0/404	0.50	0/564
33	w	0.55	1/2311 (0.0%)	0.82	8/3008 (0.3%)
34	u	0.24	0/842	0.42	0/1110
35	2	0.90	4/1679 (0.2%)	1.10	15/2267 (0.7%)
36	4	0.27	0/790	0.48	0/1095
37	6	0.49	0/925	0.55	0/1247
38	7	0.78	1/825 (0.1%)	0.62	1/1106 (0.1%)
39	5	1.20	1/688 (0.1%)	0.74	1/930 (0.1%)
40	9	0.34	0/2723	0.53	0/3697
41	8	0.52	0/946	0.56	0/1270
42	y	0.26	0/389	0.46	0/540
43	v	0.78	2/1010 (0.2%)	1.10	5/1326 (0.4%)
All	All	0.60	24/106243 (0.0%)	0.68	96/146659 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11
4	D	0	1
5	E	0	1
9	I	0	4
11	K	0	2
16	Q	0	1
22	1	0	8
23	3	0	3
33	w	0	1
35	2	0	1
40	9	0	1
43	v	0	1
All	All	0	35

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	1090	PRO	N-CA	11.88	1.67	1.47
35	2	485	PRO	N-CA	10.71	1.65	1.47
43	v	93	ALA	C-N	9.29	1.51	1.34
35	2	510	TYR	C-O	8.64	1.39	1.23
1	A	827	PHE	C-N	8.37	1.50	1.34
33	w	496	LYS	C-O	7.99	1.38	1.23
1	A	750	TRP	CB-CG	-7.00	1.37	1.50
35	2	497	SER	CA-CB	-6.47	1.43	1.52
22	1	1302	TYR	CD2-CE2	-6.30	1.29	1.39
35	2	499	PRO	C-O	-6.00	1.11	1.23
6	F	73	A	N9-C4	-5.98	1.34	1.37
38	7	72	CYS	CB-SG	-5.96	1.72	1.81
22	1	1189	SER	CA-CB	-5.82	1.44	1.52
23	3	1032	TRP	CB-CG	-5.70	1.40	1.50
23	3	31	VAL	CB-CG2	-5.42	1.41	1.52
43	v	68	SER	CA-CB	-5.39	1.44	1.52
39	5	31	TRP	CB-CG	-5.38	1.40	1.50
23	3	1170	VAL	CB-CG2	-5.31	1.41	1.52
23	3	1173	VAL	CB-CG1	-5.26	1.41	1.52
22	1	1089	GLY	C-N	5.26	1.44	1.34
22	1	1250	CYS	CB-SG	-5.23	1.73	1.81
22	1	1265	TYR	CD1-CE1	-5.20	1.31	1.39
23	3	31	VAL	CB-CG1	-5.08	1.42	1.52
23	3	1167	TYR	CE1-CZ	-5.04	1.31	1.38

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	w	500	LEU	C-N-CA	-9.80	97.21	121.70
35	2	502	ARG	CG-CD-NE	-8.83	93.25	111.80
6	F	33	G	N3-C4-N9	-8.47	120.92	126.00
35	2	502	ARG	CB-CA-C	-8.28	93.85	110.40
6	F	60	C	N1-C2-O2	8.26	123.86	118.90
7	G	109	U	C2-N1-C1’	8.24	127.58	117.70
43	v	65	ASN	CB-CA-C	-7.53	95.34	110.40
33	w	494	ASP	CB-CA-C	-7.45	95.50	110.40
23	3	65	LEU	CA-CB-CG	7.44	132.41	115.30
6	F	60	C	C2-N1-C1’	7.37	126.90	118.80
23	3	674	LEU	CA-CB-CG	7.28	132.04	115.30
35	2	587	HIS	C-N-CA	7.22	137.47	122.30
35	2	485	PRO	CA-N-CD	-6.99	101.72	111.50
6	F	33	G	C4-N9-C1’	-6.96	117.45	126.50
2	B	32	C	C5-C6-N1	6.92	124.46	121.00

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1551	PHE	CB-CA-C	-6.86	96.68	110.40
8	H	14	C	N1-C2-O2	6.82	122.99	118.90
6	F	33	G	N3-C4-C5	6.79	132.00	128.60
35	2	492	LYS	CB-CA-C	-6.75	96.91	110.40
6	F	60	C	N3-C2-O2	-6.74	117.18	121.90
22	1	1090	PRO	CA-N-CD	-6.71	102.10	111.50
8	H	47	U	O4'-C1'-N1	6.69	113.55	108.20
33	w	498	GLN	C-N-CA	6.68	136.33	122.30
2	B	32	C	C6-N1-C2	-6.67	117.63	120.30
7	G	103	U	C2-N1-C1'	6.59	125.61	117.70
43	v	85	ARG	CB-CA-C	-6.58	97.25	110.40
6	F	33	G	C8-N9-C1'	6.56	135.53	127.00
8	H	29	A	OP1-P-O3'	6.48	119.45	105.20
2	B	39	C	OP1-P-O3'	6.45	119.40	105.20
33	w	499	GLY	C-N-CA	-6.44	105.60	121.70
1	A	694	LEU	CA-CB-CG	-6.41	100.56	115.30
6	F	33	G	N3-C2-N2	-6.40	115.42	119.90
43	v	72	HIS	CB-CA-C	-6.31	97.79	110.40
8	H	47	U	N1-C1'-C2'	6.28	122.16	114.00
7	G	9	C	C2-N3-C4	6.25	123.03	119.90
35	2	494	THR	CB-CA-C	-6.20	94.85	111.60
43	v	34	ALA	N-CA-CB	6.19	118.77	110.10
6	F	79	C	OP1-P-O3'	6.17	118.77	105.20
35	2	510	TYR	CB-CA-C	6.13	122.67	110.40
23	3	1028	THR	CB-CA-C	-6.13	95.06	111.60
7	G	99	C	C2-N1-C1'	6.12	125.53	118.80
2	B	47	A	O4'-C1'-N9	6.11	113.09	108.20
8	H	47	U	C4'-C3'-O3'	6.07	125.14	113.00
33	w	477	GLU	CB-CA-C	-6.04	98.32	110.40
8	H	46	U	C2'-C3'-O3'	6.02	123.34	113.70
33	w	500	LEU	O-C-N	6.02	132.33	122.70
2	B	40	U	O5'-P-OP1	-5.93	100.36	105.70
3	C	921	LEU	C-N-CA	-5.90	106.95	121.70
1	A	826	PRO	N-CA-CB	-5.86	96.15	102.60
35	2	597	PHE	CB-CA-C	-5.85	98.70	110.40
7	G	109	U	C6-N1-C1'	-5.84	113.03	121.20
22	1	1065	LEU	CA-CB-CG	-5.76	102.05	115.30
1	A	1448	LEU	CA-CB-CG	-5.68	102.24	115.30
6	F	33	G	C6-C5-N7	5.67	133.80	130.40
43	v	36	GLU	CB-CA-C	-5.67	99.07	110.40
1	A	524	LEU	CA-CB-CG	5.64	128.28	115.30
2	B	101	U	C5-C6-N1	5.64	125.52	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	779	LEU	CA-CB-CG	-5.62	102.38	115.30
35	2	485	PRO	N-CA-C	-5.59	97.55	112.10
7	G	109	U	C5-C6-N1	5.57	125.48	122.70
22	1	1187	THR	CA-CB-OG1	-5.56	97.33	109.00
1	A	821	ARG	CG-CD-NE	-5.53	100.18	111.80
8	H	46	U	C4'-C3'-O3'	-5.53	97.79	109.40
7	G	9	C	C5-C6-N1	5.51	123.75	121.00
6	F	33	G	N1-C2-N2	5.50	121.15	116.20
1	A	1298	ARG	CG-CD-NE	-5.49	100.27	111.80
11	K	181	LEU	CA-CB-CG	5.47	127.89	115.30
6	F	19	C	C2-N1-C1'	5.43	124.78	118.80
6	F	60	C	C6-N1-C2	-5.41	118.14	120.30
23	3	1026	ASP	CA-CB-CG	-5.39	101.53	113.40
7	G	99	C	C6-N1-C1'	-5.39	114.33	120.80
6	F	79	C	P-O3'-C3'	5.38	126.15	119.70
22	1	1213	ASN	CB-CA-C	-5.37	99.67	110.40
7	G	103	U	C5-C6-N1	5.34	125.37	122.70
6	F	50	A	OP1-P-O3'	5.33	116.92	105.20
38	7	72	CYS	CA-CB-SG	-5.33	104.42	114.00
11	K	77	LEU	CA-CB-CG	5.25	127.36	115.30
7	G	109	U	N1-C2-O2	5.23	126.46	122.80
39	5	49	LEU	CB-CG-CD2	-5.23	102.10	111.00
8	H	29	A	P-O3'-C3'	5.23	125.97	119.70
6	F	73	A	C2-N3-C4	-5.22	107.99	110.60
2	B	100	C	C5-C6-N1	5.21	123.61	121.00
35	2	516	GLY	N-CA-C	5.21	126.13	113.10
35	2	506	PHE	CB-CA-C	-5.19	100.02	110.40
35	2	515	ARG	C-N-CA	5.19	133.19	122.30
8	H	46	U	C3'-C2'-O2'	5.16	128.26	113.30
33	w	424	ARG	NE-CZ-NH1	5.15	122.87	120.30
35	2	510	TYR	N-CA-CB	-5.13	101.37	110.60
7	G	102	G	C4-N9-C1'	5.10	133.13	126.50
33	w	500	LEU	CB-CA-C	-5.08	100.55	110.20
23	3	158	LEU	CA-CB-CG	-5.05	103.68	115.30
2	B	95	G	C4-N9-C1'	5.05	133.07	126.50
2	B	32	C	C2-N1-C1'	5.04	124.35	118.80
35	2	511	LEU	CB-CA-C	5.03	119.76	110.20
1	A	1270	LEU	CA-CB-CG	-5.03	103.74	115.30
35	2	510	TYR	CA-C-O	5.00	130.60	120.10

There are no chirality outliers.

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	1	1101	LEU	Peptide
22	1	1107	GLN	Peptide
22	1	1108	ASN	Peptide
22	1	1177	LEU	Mainchain
22	1	415	LEU	Peptide
22	1	717	THR	Peptide
22	1	943	LYS	Peptide
22	1	944	SER	Peptide
35	2	493	ALA	Mainchain
23	3	261	PHE	Peptide
23	3	318	ASP	Peptide
23	3	916	ASN	Peptide
40	9	343	GLU	Peptide
1	A	1019	TYR	Peptide
1	A	109	PRO	Peptide
1	A	1543	ASN	Mainchain
1	A	166	PHE	Peptide
1	A	346	ASP	Peptide
1	A	698	PRO	Peptide
1	A	699	GLU	Peptide
1	A	700	GLY	Peptide
1	A	801	ILE	Peptide
1	A	940	ILE	Peptide
1	A	941	LYS	Peptide
4	D	2098	ALA	Peptide
5	E	192	ASN	Peptide
9	I	321	GLU	Peptide
9	I	337	LEU	Peptide
9	I	374	ILE	Peptide
9	I	384	THR	Peptide
11	K	275	ALA	Peptide
11	K	36	ARG	Peptide
16	Q	488	SER	Peptide
43	v	64	ASN	Mainchain
33	w	498	GLN	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	16165	0	14621	961	0
2	B	2066	0	1047	127	0
3	C	7077	0	7067	504	0
4	D	8528	0	3745	30	0
5	E	2338	0	2275	120	0
6	F	2035	0	1028	165	0
7	G	1321	0	673	134	0
8	H	3497	0	1770	121	0
9	I	2991	0	1473	16	0
10	J	2116	0	1977	94	0
11	K	2173	0	1770	124	0
12	L	829	0	837	47	0
13	N	662	0	284	5	0
14	O	1340	0	581	11	0
15	P	362	0	356	19	0
16	Q	6730	0	3268	29	0
17	R	1520	0	1482	98	0
18	T	2507	0	2451	192	0
19	X	1279	0	1284	79	0
20	Y	948	0	954	61	0
21	Z	439	0	410	16	0
22	1	7845	0	7915	480	0
23	3	9240	0	9164	524	0
24	o	816	0	386	0	0
25	p	851	0	423	0	0
26	c	388	0	102	0	0
26	h	482	0	220	0	0
27	d	296	0	87	0	0
27	i	359	0	179	0	0
28	a	336	0	89	0	0
28	m	413	0	194	0	0
29	g	324	0	89	0	0
29	l	415	0	198	0	0
30	f	296	0	84	0	0
30	k	364	0	176	0	0
31	e	308	0	83	0	0
31	j	403	0	173	0	0
32	b	328	0	89	0	0
32	n	402	0	184	0	0
33	w	2275	0	1347	0	0
34	u	834	0	325	0	0
35	2	1651	0	1438	155	0
36	4	792	0	367	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	6	906	0	913	66	0
38	7	811	0	789	42	0
39	5	669	0	631	26	0
40	9	2681	0	2270	133	0
41	8	931	0	960	60	0
42	y	390	0	190	0	0
43	v	997	0	745	0	0
44	z	124	0	26	0	0
45	C	32	0	12	7	0
46	C	1	0	0	0	0
47	7	3	0	0	0	0
47	K	1	0	0	0	0
All	All	103887	0	79201	4037	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 24.

All (4037) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1308:PRO:HB3	1:A:1548:TYR:CE2	1.15	1.65
35:2:530:ARG:HG2	35:2:578:TRP:CH2	1.15	1.64
35:2:530:ARG:CG	35:2:578:TRP:HH2	1.19	1.53
35:2:530:ARG:CG	35:2:578:TRP:CH2	1.89	1.53
35:2:530:ARG:HG2	35:2:578:TRP:CZ3	1.46	1.50
1:A:1307:MET:SD	1:A:1308:PRO:HD2	1.48	1.49
1:A:1308:PRO:CB	1:A:1548:TYR:CE2	1.93	1.48
23:3:146:ARG:HD3	23:3:150:ALA:CB	1.47	1.43
22:1:1090:PRO:N	22:1:1090:PRO:CA	1.67	1.42
35:2:533:ILE:HD11	35:2:566:ILE:CD1	1.50	1.41
1:A:1307:MET:SD	1:A:1308:PRO:CD	2.13	1.34
1:A:1308:PRO:HB3	1:A:1548:TYR:CD2	1.61	1.32
22:1:1210:HIS:CE1	35:2:585:THR:HG23	1.65	1.31
1:A:1545:ALA:HB2	1:A:1563:HIS:CG	1.66	1.29
7:G:99:C:N4	8:H:32:U:H3	1.29	1.28
1:A:1308:PRO:CB	1:A:1548:TYR:CD2	2.16	1.23
12:L:38:LEU:CD1	12:L:41:LYS:HG2	1.69	1.23
2:B:8:G:H1	2:B:69:A:N6	1.38	1.22
23:3:146:ARG:CD	23:3:150:ALA:HB1	1.71	1.21
1:A:1545:ALA:HB2	1:A:1563:HIS:CD2	1.75	1.20
6:F:85:U:H3	8:H:14:C:N4	1.42	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1545:ALA:HB2	1:A:1563:HIS:CE1	1.79	1.16
12:L:38:LEU:HD12	12:L:41:LYS:HG2	1.17	1.15
1:A:1308:PRO:CB	1:A:1548:TYR:HE2	1.41	1.14
23:3:146:ARG:CD	23:3:150:ALA:CB	2.25	1.13
23:3:146:ARG:HG2	23:3:150:ALA:HA	1.30	1.13
23:3:146:ARG:NE	23:3:150:ALA:HB1	1.67	1.09
22:1:129:SEP:O2P	22:1:573:LYS:NZ	1.85	1.09
1:A:1545:ALA:HB2	1:A:1563:HIS:ND1	1.68	1.07
35:2:533:ILE:HD11	35:2:566:ILE:HD11	1.36	1.07
23:3:146:ARG:HD3	23:3:150:ALA:HB2	1.34	1.07
22:1:1210:HIS:CE1	35:2:585:THR:H	1.71	1.07
23:3:146:ARG:CG	23:3:150:ALA:HA	1.84	1.06
22:1:1182:LEU:H	22:1:1182:LEU:HD12	1.20	1.06
35:2:533:ILE:CD1	35:2:566:ILE:CD1	2.34	1.05
35:2:533:ILE:HD11	35:2:566:ILE:HD12	1.15	1.05
11:K:360:ILE:O	20:Y:72:LYS:HE2	1.55	1.04
35:2:530:ARG:HG3	35:2:578:TRP:HH2	1.19	1.04
1:A:1545:ALA:CB	1:A:1563:HIS:CG	2.40	1.03
35:2:465:LEU:O	35:2:469:VAL:CG2	2.07	1.02
1:A:1304:ASN:OD1	1:A:1548:TYR:CE1	2.12	1.02
12:L:38:LEU:HD12	12:L:41:LYS:CG	1.89	1.02
22:1:1210:HIS:HE1	35:2:585:THR:CG2	1.72	1.02
1:A:1304:ASN:OD1	1:A:1548:TYR:CZ	2.12	1.01
35:2:469:VAL:HG11	35:2:489:VAL:HG11	1.38	1.00
35:2:465:LEU:O	35:2:469:VAL:HG23	1.62	1.00
14:O:55:PHE:O	14:O:67:LYS:HA	1.63	0.99
23:3:146:ARG:HH21	23:3:146:ARG:HB2	1.26	0.99
35:2:533:ILE:CD1	35:2:566:ILE:HD12	1.90	0.99
22:1:1137:ARG:HH22	35:2:534:GLN:HG2	1.27	0.98
1:A:827:PHE:HB2	1:A:1002:ASP:OD2	1.65	0.97
18:T:245:HIS:HE2	18:T:263:SER:HG	1.12	0.96
11:K:362:GLU:CB	20:Y:71:LYS:HG2	1.95	0.96
23:3:146:ARG:HD3	23:3:150:ALA:HB1	1.30	0.96
22:1:1210:HIS:HE1	35:2:585:THR:HG23	0.80	0.96
1:A:1308:PRO:HB2	1:A:1548:TYR:CD2	1.99	0.96
1:A:508:ILE:HG23	1:A:513:LEU:HB2	1.47	0.96
6:F:33:G:N1	7:G:14:A:C6	2.34	0.95
1:A:1545:ALA:HB2	1:A:1563:HIS:NE2	1.80	0.95
2:B:17:U:H3	2:B:60:G:H1	1.16	0.94
6:F:33:G:C6	7:G:14:A:N6	2.36	0.93
3:C:686:THR:HB	3:C:793:ASP:HB3	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:9:449:ARG:HA	40:9:452:GLN:HE21	1.35	0.92
35:2:533:ILE:CD1	35:2:566:ILE:HD11	2.00	0.91
35:2:530:ARG:HG3	35:2:578:TRP:CH2	1.93	0.91
6:F:85:U:H3	8:H:14:C:H42	0.91	0.90
11:K:362:GLU:CB	20:Y:71:LYS:CG	2.48	0.90
22:1:1036:ILE:HD11	22:1:1065:LEU:HD13	1.53	0.90
6:F:85:U:O2	8:H:14:C:N3	2.05	0.90
8:H:56:A:O2'	35:2:481:THR:HG21	1.70	0.89
18:T:292:TYR:OH	18:T:308:ARG:HD3	1.71	0.89
19:X:312:GLU:HG2	19:X:322:ARG:HG2	1.54	0.89
17:R:241:GLU:HA	17:R:244:GLU:HB2	1.53	0.89
1:A:1410:ASP:OD1	1:A:1410:ASP:N	2.06	0.88
23:3:555:VAL:HG23	23:3:592:LEU:HD22	1.55	0.88
3:C:182:LYS:HG3	3:C:214:GLU:HG2	1.55	0.88
23:3:456:PRO:HA	23:3:478:PHE:HA	1.55	0.88
22:1:1108:ASN:ND2	22:1:1111:CYS:SG	2.46	0.88
1:A:1407:ASP:OD1	1:A:1407:ASP:N	2.07	0.87
1:A:188:LEU:HD22	1:A:567:GLY:HA2	1.57	0.87
23:3:902:ASP:OD2	23:3:929:LYS:NZ	2.08	0.87
35:2:451:LYS:H	35:2:451:LYS:HD2	1.40	0.87
1:A:1304:ASN:OD1	1:A:1548:TYR:OH	1.93	0.86
23:3:552:ARG:NE	23:3:568:MET:O	2.07	0.86
1:A:158:ARG:HH21	1:A:572:PHE:HB2	1.40	0.86
3:C:452:THR:HG22	3:C:577:PHE:HB3	1.54	0.86
22:1:967:GLU:HB3	22:1:970:LEU:HB3	1.56	0.86
35:2:530:ARG:CG	35:2:578:TRP:CZ3	2.33	0.86
35:2:585:THR:HB	35:2:589:ASP:OD2	1.74	0.86
17:R:148:ARG:CZ	17:R:148:ARG:HB3	2.05	0.86
3:C:258:ASN:HD21	3:C:312:SER:HB3	1.38	0.86
18:T:292:TYR:CE1	18:T:308:ARG:HB2	2.11	0.86
1:A:1307:MET:SD	1:A:1308:PRO:HD3	2.14	0.86
3:C:590:ILE:HB	3:C:637:LEU:HD21	1.57	0.86
6:F:30:A:OP2	7:G:16:G:N2	2.07	0.86
1:A:1308:PRO:CG	1:A:1548:TYR:HE2	1.88	0.85
22:1:1210:HIS:HE1	35:2:585:THR:H	1.19	0.85
11:K:21:LEU:HD11	11:K:102:ARG:HG2	1.56	0.85
23:3:114:ARG:NH1	39:5:38:ASP:OD1	2.09	0.85
23:3:146:ARG:HH21	23:3:146:ARG:CB	1.88	0.85
35:2:469:VAL:HG11	35:2:489:VAL:CG1	2.06	0.85
17:R:329:GLN:HE22	17:R:332:ARG:HD2	1.42	0.85
23:3:461:THR:HA	23:3:473:TYR:O	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1220:VAL:HG23	1:A:1221:THR:HG23	1.58	0.85
35:2:581:LYS:HB3	35:2:581:LYS:HZ2	1.42	0.84
1:A:110:TRP:O	1:A:192:GLN:NE2	2.10	0.84
22:1:154:ASP:O	22:1:158:GLU:HG3	1.77	0.84
23:3:805:ASN:ND2	23:3:858:GLY:O	2.10	0.84
1:A:1256:PHE:CD1	1:A:1299:ILE:CG2	2.60	0.84
11:K:146:PRO:HB2	11:K:150:ARG:HH21	1.42	0.84
11:K:360:ILE:O	20:Y:72:LYS:CE	2.25	0.84
23:3:700:LYS:NZ	23:3:740:GLU:O	2.11	0.84
7:G:-3:A:H2’	7:G:-2:A:H8	1.41	0.84
23:3:93:GLN:NE2	23:3:100:GLU:OE1	2.10	0.84
23:3:617:ILE:HG12	23:3:627:PRO:HA	1.59	0.84
18:T:422:ASN:HB3	18:T:426:VAL:HG23	1.60	0.84
35:2:530:ARG:O	35:2:530:ARG:HD3	1.78	0.84
19:X:232:LEU:HD21	20:Y:51:ASP:HB3	1.60	0.84
23:3:675:LEU:HG	23:3:688:ASP:HB3	1.59	0.84
1:A:982:GLU:OE2	1:A:1172:ASN:ND2	2.10	0.84
1:A:1299:ILE:HD13	1:A:1316:PHE:CE1	2.13	0.84
22:1:1252:GLN:NE2	35:2:492:LYS:HA	1.91	0.83
1:A:1545:ALA:CB	1:A:1563:HIS:CD2	2.59	0.83
3:C:396:LEU:HD13	3:C:403:LEU:HD13	1.60	0.83
17:R:389:SER:O	19:X:348:ARG:NE	2.10	0.83
8:H:78:C:H2’	8:H:79:G:H8	1.42	0.83
18:T:394:ASN:ND2	18:T:410:SER:OG	2.11	0.83
7:G:90:C:H2’	7:G:91:A:C8	2.14	0.83
35:2:473:ASP:OD1	35:2:473:ASP:N	2.07	0.83
1:A:617:ASN:ND2	1:A:622:GLY:O	2.12	0.83
1:A:1545:ALA:CB	1:A:1563:HIS:CE1	2.61	0.83
6:F:38:G:N2	7:G:9:C:O2	2.12	0.83
35:2:581:LYS:HD2	35:2:581:LYS:O	1.78	0.82
22:1:806:ILE:HA	22:1:810:ILE:HG13	1.61	0.82
22:1:1126:PHE:CE2	35:2:572:HIS:HD2	1.96	0.82
1:A:393:LEU:HA	3:C:379:LYS:HG2	1.62	0.82
35:2:537:ARG:HH11	35:2:537:ARG:HG3	1.44	0.82
1:A:1298:ARG:HB3	1:A:1298:ARG:NH2	1.94	0.82
18:T:287:HIS:HE2	18:T:305:THR:HG1	1.28	0.82
20:Y:24:ASP:OD1	20:Y:24:ASP:N	2.10	0.82
23:3:828:GLY:O	23:3:834:LEU:N	2.12	0.82
18:T:316:ASP:OD1	18:T:319:THR:N	2.13	0.81
22:1:699:GLN:OE1	22:1:702:ARG:NH2	2.11	0.81
23:3:726:GLN:O	23:3:728:ARG:NH2	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:2:575:PHE:O	35:2:579:GLN:NE2	2.12	0.81
3:C:399:LEU:HB3	3:C:401:ILE:HG12	1.62	0.81
1:A:539:ARG:HH12	7:G:-1:C:H5”	1.44	0.81
18:T:245:HIS:NE2	18:T:263:SER:OG	2.12	0.81
11:K:73:ARG:HH12	11:K:77:LEU:HD11	1.44	0.81
3:C:237:LEU:HD22	3:C:898:LEU:HD22	1.62	0.81
21:Z:585:ASP:OD2	21:Z:589:ARG:NH2	2.12	0.81
23:3:499:PHE:O	23:3:525:ARG:NH1	2.13	0.81
1:A:232:LEU:HD22	1:A:404:LEU:HD13	1.62	0.81
17:R:386:ARG:NH2	19:X:356:ASP:OD2	2.13	0.81
41:8:121:SER:HA	41:8:124:LEU:HD12	1.62	0.81
22:1:129:SEP:HB3	22:1:130:PRO:HD2	1.64	0.81
22:1:571:VAL:HG22	22:1:600:LEU:HD11	1.63	0.81
23:3:70:LEU:HD12	23:3:146:ARG:HH22	1.46	0.81
8:H:155:C:N3	8:H:176:G:N2	2.29	0.80
12:L:38:LEU:HD11	12:L:41:LYS:HG2	1.63	0.80
3:C:85:ASP:OD1	3:C:85:ASP:N	2.13	0.80
22:1:157:ARG:NH1	37:6:103:THR:OG1	2.14	0.80
35:2:581:LYS:H	35:2:581:LYS:HZ3	1.25	0.80
37:6:113:LEU:HA	37:6:116:LYS:HE3	1.63	0.80
22:1:141:LYS:NZ	22:1:142:THR:O	2.15	0.80
22:1:1137:ARG:NH2	35:2:534:GLN:HG2	1.96	0.80
5:E:341:ILE:HG12	5:E:355:GLU:HG3	1.64	0.80
18:T:386:THR:HG22	18:T:399:LYS:HA	1.63	0.80
6:F:38:G:C2	7:G:9:C:C2	2.70	0.80
22:1:1248:GLN:OE1	35:2:587:HIS:HE1	1.65	0.80
10:J:238:ASN:HB3	10:J:240:THR:HG22	1.64	0.80
23:3:146:ARG:CG	23:3:150:ALA:CA	2.59	0.79
1:A:319:LEU:HD22	3:C:637:LEU:HG	1.64	0.79
1:A:1308:PRO:CB	1:A:1548:TYR:HD2	1.86	0.79
1:A:1545:ALA:CB	1:A:1563:HIS:ND1	2.43	0.79
3:C:509:VAL:HG12	3:C:565:ILE:HG12	1.64	0.79
40:9:236:LEU:HD22	40:9:452:GLN:HE22	1.46	0.79
4:D:1376:CYS:HA	4:D:1450:LEU:O	1.82	0.79
6:F:38:G:N1	7:G:9:C:N3	2.31	0.79
22:1:1178:MET:CE	35:2:591:TYR:CE2	2.66	0.79
11:K:39:ASN:OD1	11:K:43:CYS:N	2.16	0.79
3:C:589:LYS:HE2	3:C:628:VAL:HG11	1.62	0.79
3:C:347:ILE:HD11	3:C:356:PHE:HB3	1.65	0.79
8:H:54:U:O2	8:H:59:A:N6	2.16	0.79
35:2:514:LYS:N	35:2:593:GLU:OE1	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1:138:ASP:HB3	22:1:141:LYS:HB3	1.63	0.79
23:3:609:LEU:HB2	23:3:611:ASP:HB3	1.64	0.79
22:1:1137:ARG:HH22	35:2:534:GLN:CG	1.96	0.78
23:3:553:GLN:NE2	23:3:600:GLN:O	2.16	0.78
22:1:626:ASN:OD1	22:1:630:ARG:NH1	2.17	0.78
23:3:1048:ASP:OD1	23:3:1049:LYS:N	2.16	0.78
5:E:90:ILE:HB	5:E:105:LEU:HB2	1.65	0.78
1:A:401:GLY:HA3	3:C:386:GLY:HA2	1.65	0.78
23:3:581:LYS:NZ	23:3:583:MET:SD	2.56	0.78
1:A:979:SER:OG	1:A:980:ARG:N	2.13	0.78
23:3:483:LEU:HD23	23:3:485:LEU:HD11	1.65	0.78
23:3:932:ASN:O	23:3:933:ASN:ND2	2.17	0.78
23:3:206:GLN:NE2	23:3:232:GLY:H	1.80	0.78
22:1:1210:HIS:CE1	35:2:585:THR:CG2	2.54	0.78
1:A:535:ARG:NH2	1:A:1551:PHE:HE1	1.82	0.78
3:C:441:PRO:HB3	3:C:495:ARG:HH22	1.48	0.78
18:T:350:HIS:HA	18:T:374:SER:HB2	1.65	0.77
23:3:554:VAL:HB	23:3:566:PHE:HB2	1.66	0.77
23:3:943:THR:HG21	23:3:977:LEU:HB2	1.66	0.77
41:8:115:ASN:OD1	41:8:116:ILE:N	2.17	0.77
1:A:1021:ASP:N	1:A:1021:ASP:OD1	2.14	0.77
22:1:859:ASP:OD1	22:1:860:GLU:N	2.17	0.77
23:3:946:GLU:OE1	23:3:946:GLU:N	2.16	0.77
1:A:1303:LEU:HD13	1:A:1303:LEU:N	2.00	0.77
12:L:41:LYS:HA	12:L:41:LYS:CE	2.15	0.77
23:3:941:HIS:CD2	23:3:976:LYS:HA	2.19	0.77
20:Y:53:ILE:HG23	20:Y:62:ILE:HD12	1.65	0.77
7:G:111:U:O2	20:Y:105:ARG:NH2	2.16	0.77
23:3:146:ARG:HD3	23:3:150:ALA:CA	2.15	0.77
23:3:473:TYR:HB3	23:3:475:ILE:HD11	1.66	0.77
23:3:155:SER:OG	23:3:156:SER:N	2.13	0.77
22:1:758:ASP:N	22:1:758:ASP:OD1	2.16	0.77
23:3:745:PHE:HB2	23:3:755:VAL:HG23	1.65	0.77
3:C:304:LEU:O	3:C:436:GLN:NE2	2.18	0.77
16:Q:1270:TYR:HA	16:Q:1300:GLY:O	1.84	0.77
1:A:82:ARG:NH1	7:G:16:G:O6	2.18	0.77
6:F:32:U:H3	7:G:15:U:H3	1.29	0.77
23:3:34:ARG:NH1	23:3:39:GLU:OE1	2.18	0.77
23:3:528:ARG:NH1	23:3:572:GLY:O	2.17	0.77
22:1:1074:ARG:NH1	22:1:1107:GLN:OE1	2.17	0.76
22:1:1126:PHE:HA	35:2:575:PHE:CD2	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:550:ASN:HD21	23:3:595:VAL:H	1.30	0.76
6:F:69:A:H3’	6:F:70:A:H8	1.50	0.76
1:A:420:ARG:NH1	2:B:56:C:O2’	2.18	0.76
6:F:30:A:N6	7:G:17:U:O5’	2.18	0.76
23:3:473:TYR:OH	23:3:497:SER:O	2.02	0.76
6:F:26:U:H3’	6:F:27:A:H5”	1.66	0.76
22:1:1277:GLN:NE2	22:1:1277:GLN:O	2.18	0.76
23:3:27:GLN:OE1	23:3:42:ARG:NH1	2.18	0.76
23:3:926:TYR:HB3	23:3:928:TYR:HE2	1.51	0.76
8:H:29:A:H1’	8:H:30:A:H5’	1.68	0.76
1:A:457:ASN:ND2	2:B:28:A:OP2	2.18	0.76
3:C:813:ARG:NH2	40:9:106:LEU:O	2.18	0.76
1:A:79:ARG:HH22	6:F:29:A:H5’	1.51	0.75
1:A:1312:PRO:HG3	1:A:1541:THR:HG22	1.68	0.75
3:C:448:LYS:O	3:C:452:THR:HB	1.86	0.75
6:F:38:G:C2	7:G:9:C:O2	2.39	0.75
23:3:444:VAL:HG11	23:3:736:TYR:HB2	1.68	0.75
2:B:42:U:O4	7:G:-2:A:N6	2.17	0.75
3:C:313:GLN:HB2	45:C:1500:GTP:C5	2.21	0.75
19:X:234:GLU:O	19:X:238:THR:OG1	2.05	0.75
22:1:1248:GLN:OE1	35:2:587:HIS:CE1	2.39	0.75
23:3:547:CYS:HA	23:3:555:VAL:O	1.85	0.75
23:3:590:MET:HG2	23:3:607:VAL:HA	1.68	0.75
35:2:586:ILE:O	35:2:586:ILE:HD13	1.85	0.75
23:3:631:GLN:NE2	23:3:632:ALA:O	2.19	0.75
1:A:684:GLU:OE2	18:T:308:ARG:NH2	2.19	0.75
35:2:465:LEU:O	35:2:469:VAL:HG21	1.86	0.75
1:A:837:LYS:HD3	1:A:1432:TYR:HE2	1.51	0.75
1:A:1261:ASN:ND2	17:R:428:GLU:O	2.17	0.75
35:2:581:LYS:H	35:2:581:LYS:NZ	1.85	0.75
1:A:315:ALA:O	1:A:330:THR:OG1	2.05	0.75
22:1:1210:HIS:CE1	35:2:585:THR:N	2.53	0.75
1:A:873:ASN:N	1:A:873:ASN:OD1	2.20	0.74
3:C:225:VAL:HB	3:C:251:LEU:HD12	1.67	0.74
3:C:255:VAL:HG23	3:C:300:LEU:HD22	1.68	0.74
1:A:425:PRO:HB2	1:A:428:LYS:HB2	1.69	0.74
7:G:98:U:O4	8:H:33:G:N1	2.19	0.74
1:A:1601:LEU:HD12	1:A:1606:ILE:HB	1.69	0.74
6:F:65:G:H21	6:F:69:A:H2	1.35	0.74
1:A:1171:GLU:OE1	1:A:1171:GLU:N	2.20	0.74
3:C:664:GLU:O	3:C:785:ARG:N	2.19	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:197:TYR:OH	18:T:476:ARG:NH1	2.20	0.74
1:A:62:PRO:HB2	1:A:64:GLU:HG2	1.67	0.74
1:A:1301:ILE:O	1:A:1301:ILE:HD13	1.88	0.74
3:C:496:VAL:HB	3:C:546:ALA:HA	1.68	0.74
35:2:509:LYS:HB2	35:2:512:GLN:HB3	1.68	0.74
3:C:170:ILE:HD11	3:C:535:ALA:HB1	1.68	0.74
9:I:169:TYR:O	9:I:173:LEU:CB	2.35	0.74
6:F:33:G:C2	7:G:14:A:C6	2.75	0.74
23:3:1100:THR:OG1	39:5:48:ASP:OD2	2.05	0.74
7:G:99:C:N4	8:H:32:U:N3	2.05	0.74
17:R:407:TYR:HB3	17:R:411:LEU:HD12	1.69	0.74
22:1:984:GLU:OE2	22:1:986:TYR:N	2.20	0.74
23:3:5:ASN:ND2	23:3:1095:TYR:OH	2.21	0.74
35:2:517:ILE:N	35:2:517:ILE:HD12	2.03	0.74
1:A:821:ARG:HG2	1:A:821:ARG:NH1	2.00	0.74
22:1:458:ASP:O	22:1:459:GLN:NE2	2.21	0.74
3:C:76:GLU:OE1	3:C:76:GLU:N	2.18	0.73
5:E:251:LEU:HD13	5:E:300:ILE:HD13	1.70	0.73
12:L:74:LEU:O	12:L:77:LEU:N	2.20	0.73
1:A:1201:ARG:O	1:A:1203:SER:N	2.20	0.73
12:L:38:LEU:HD23	12:L:38:LEU:H	1.53	0.73
23:3:399:ASP:OD1	23:3:400:GLU:N	2.21	0.73
39:5:11:LEU:HD22	39:5:23:HIS:HB2	1.70	0.73
1:A:939:TRP:NE1	1:A:1049:ASP:OD2	2.21	0.73
17:R:148:ARG:HA	17:R:151:LEU:HD23	1.70	0.73
5:E:208:ILE:O	5:E:219:VAL:HA	1.89	0.73
10:J:224:LYS:NZ	10:J:257:GLU:OE2	2.21	0.73
22:1:129:SEP:HB3	22:1:130:PRO:CD	2.19	0.73
35:2:537:ARG:HG3	35:2:537:ARG:NH1	2.01	0.73
22:1:838:VAL:O	22:1:842:ASN:ND2	2.21	0.73
17:R:137:GLU:CD	17:R:137:GLU:H	1.92	0.73
17:R:434:ASP:N	17:R:434:ASP:OD1	2.20	0.73
22:1:931:GLN:O	22:1:935:THR:OG1	2.07	0.73
22:1:1212:LEU:HD12	22:1:1212:LEU:O	1.88	0.73
23:3:525:ARG:HG3	23:3:533:VAL:HG13	1.70	0.73
1:A:1308:PRO:HB2	1:A:1548:TYR:CE2	2.11	0.73
2:B:20:G:N1	2:B:58:U:O2	2.20	0.73
20:Y:92:LEU:O	20:Y:96:ASN:ND2	2.20	0.73
1:A:578:LEU:HA	1:A:581:ILE:HD12	1.70	0.73
23:3:430:GLY:O	23:3:433:SER:OG	2.06	0.73
6:F:38:G:N2	7:G:9:C:C2	2.57	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:38:G:N1	7:G:9:C:C2	2.57	0.72
20:Y:113:SER:OG	20:Y:114:ASN:ND2	2.22	0.72
22:1:491:GLU:OE2	22:1:492:GLN:N	2.22	0.72
22:1:694:LEU:HD11	22:1:731:LEU:HD23	1.71	0.72
23:3:266:ASP:OD1	23:3:266:ASP:N	2.20	0.72
23:3:1013:ARG:NH1	23:3:1065:GLU:OE2	2.22	0.72
1:A:798:GLY:HA3	17:R:281:ASN:HD22	1.54	0.72
3:C:318:PHE:HE1	3:C:373:ILE:HD13	1.52	0.72
23:3:685:ASP:OD1	23:3:686:LEU:N	2.22	0.72
1:A:471:TYR:HB3	1:A:474:ARG:HG3	1.71	0.72
3:C:685:ILE:HD11	3:C:811:THR:HG23	1.69	0.72
22:1:476:ASP:OD1	22:1:477:LYS:N	2.22	0.72
22:1:848:GLU:OE2	22:1:852:ARG:NE	2.23	0.72
22:1:1289:ASN:HB3	22:1:1295:TYR:H	1.53	0.72
1:A:639:PHE:O	2:B:28:A:O2’	2.05	0.72
1:A:941:LYS:NZ	1:A:946:GLU:OE2	2.23	0.72
3:C:913:ASP:HB3	3:C:916:ILE:HG13	1.70	0.72
1:A:798:GLY:HA2	17:R:284:PHE:HE2	1.55	0.72
2:B:58:U:H2’	2:B:59:G:H8	1.53	0.72
3:C:94:ILE:HG21	18:T:259:PRO:HB3	1.71	0.72
3:C:454:THR:OG1	3:C:576:ILE:O	2.06	0.72
3:C:495:ARG:HB3	3:C:549:TRP:HD1	1.53	0.72
18:T:287:HIS:NE2	18:T:305:THR:OG1	2.19	0.72
20:Y:86:ASP:OD1	20:Y:89:SER:OG	2.08	0.72
22:1:1262:ARG:NH1	39:5:24:ALA:O	2.23	0.72
23:3:946:GLU:OE2	23:3:968:ARG:NH2	2.20	0.72
18:T:329:HIS:ND1	18:T:351:ASP:OD2	2.20	0.72
1:A:2104:TYR:O	1:A:2261:MET:HA	1.90	0.72
19:X:298:SER:O	19:X:335:ASN:ND2	2.22	0.72
23:3:21:ASN:N	23:3:76:ASP:OD2	2.21	0.72
41:8:14:ASP:OD1	41:8:16:ARG:N	2.23	0.72
1:A:66:VAL:HG11	1:A:485:THR:HG21	1.72	0.72
22:1:1260:LYS:NZ	35:2:504:TRP:O	2.16	0.72
23:3:263:ASP:OD1	23:3:263:ASP:N	2.21	0.72
23:3:1008:SER:OG	23:3:1027:ASP:OD2	2.08	0.72
1:A:1551:PHE:HB3	1:A:1553:VAL:HG23	1.72	0.71
23:3:280:ASP:H	23:3:857:ALA:HB3	1.54	0.71
6:F:75:G:OP2	6:F:75:G:N2	2.22	0.71
8:H:139:C:H2’	8:H:140:A:H8	1.55	0.71
18:T:349:SER:OG	18:T:350:HIS:N	2.21	0.71
22:1:1178:MET:HE3	35:2:591:TYR:CE2	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:698:GLU:O	3:C:702:ASN:ND2	2.22	0.71
22:1:1064:GLU:OE1	22:1:1064:GLU:N	2.22	0.71
1:A:63:PRO:HB2	1:A:67:ARG:HH22	1.55	0.71
6:F:79:C:H4'	6:F:80:G:OP1	1.90	0.71
40:9:352:ASP:OD1	40:9:376:ASN:ND2	2.23	0.71
1:A:1373:GLN:NE2	1:A:1377:SER:OG	2.22	0.71
3:C:313:GLN:O	3:C:417:ARG:NH1	2.24	0.71
22:1:804:ASN:O	22:1:808:THR:OG1	2.08	0.71
23:3:1017:ASN:OD1	23:3:1018:GLU:N	2.23	0.71
22:1:1092:ASP:N	22:1:1092:ASP:OD1	2.22	0.71
14:O:81:CYS:O	14:O:85:LEU:N	2.23	0.71
20:Y:32:TYR:O	20:Y:87:GLN:NE2	2.23	0.71
22:1:1054:GLU:OE1	22:1:1057:ARG:NH1	2.24	0.71
35:2:530:ARG:HG2	35:2:578:TRP:HZ3	1.47	0.71
37:6:47:GLN:OE1	37:6:49:ARG:NE	2.24	0.71
19:X:263:PRO:HB2	19:X:270:LEU:HB2	1.73	0.71
22:1:884:ILE:HG23	22:1:888:LEU:HB3	1.73	0.71
22:1:1252:GLN:OE1	35:2:499:PRO:HA	1.91	0.71
1:A:276:GLY:O	1:A:448:GLN:NE2	2.23	0.71
1:A:578:LEU:HB2	1:A:630:TRP:CD1	2.26	0.71
23:3:206:GLN:HE21	23:3:232:GLY:H	1.36	0.71
1:A:96:PRO:HB2	1:A:645:THR:HG23	1.73	0.71
1:A:200:ASP:OD1	1:A:240:ARG:NH1	2.24	0.70
3:C:599:GLU:HG2	3:C:651:ILE:HD12	1.72	0.70
35:2:532:GLY:O	35:2:535:GLU:N	2.24	0.70
1:A:363:HIS:HD2	3:C:284:GLU:HA	1.56	0.70
1:A:902:TYR:OH	1:A:1249:MET:SD	2.46	0.70
10:J:275:ASN:OD1	10:J:278:LEU:N	2.23	0.70
22:1:946:LYS:HD2	22:1:946:LYS:H	1.57	0.70
23:3:705:ARG:HA	23:3:710:GLU:HA	1.73	0.70
6:F:46:G:H5”	11:K:19:LYS:HD3	1.71	0.70
40:9:287:ASN:ND2	40:9:425:GLU:O	2.24	0.70
1:A:1622:MET:O	1:A:1687:TYR:OH	2.10	0.70
2:B:50:G:H2'	2:B:51:A:O4'	1.91	0.70
19:X:224:PRO:HG3	20:Y:69:ARG:HD2	1.72	0.70
23:3:487:ILE:HA	23:3:491:VAL:HG13	1.74	0.70
37:6:17:VAL:HG13	37:6:67:ILE:HD11	1.73	0.70
36:4:79:LEU:N	36:4:82:LYS:O	2.24	0.70
3:C:210:ASN:HB3	3:C:636:TYR:HB2	1.74	0.70
3:C:366:GLN:HG3	3:C:371:GLU:HB2	1.71	0.70
19:X:286:HIS:HB2	19:X:301:LYS:HG2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1404:THR:OG1	1:A:1405:LEU:N	2.25	0.70
1:A:1655:THR:OG1	1:A:1656:THR:N	2.23	0.70
11:K:98:TYR:OH	11:K:105:ILE:N	2.20	0.70
17:R:299:ARG:NH1	22:1:447:GLN:O	2.24	0.70
1:A:1166:THR:OG1	1:A:1167:THR:N	2.18	0.70
1:A:1415:GLY:O	1:A:1418:ARG:NH1	2.25	0.70
2:B:97:G:H1	2:B:116:U:H3	1.37	0.70
11:K:40:GLY:O	11:K:44:HIS:CD2	2.45	0.70
17:R:407:TYR:HB2	17:R:412:PHE:HE1	1.57	0.70
1:A:1554:GLN:OE1	1:A:1622:MET:CE	2.40	0.70
4:D:1204:ILE:O	4:D:1250:HIS:N	2.22	0.70
5:E:202:ASN:ND2	5:E:204:THR:OG1	2.24	0.70
18:T:424:ASP:OD1	18:T:424:ASP:N	2.24	0.70
19:X:354:GLU:HG2	19:X:355:LYS:HG3	1.73	0.70
22:1:471:ASP:OD2	22:1:505:LYS:NZ	2.24	0.70
35:2:451:LYS:H	35:2:451:LYS:CD	2.02	0.70
35:2:581:LYS:HZ3	35:2:581:LYS:N	1.90	0.70
1:A:835:ASP:N	1:A:835:ASP:OD1	2.23	0.69
1:A:837:LYS:HD3	1:A:1432:TYR:CE2	2.27	0.69
1:A:1110:ILE:HG22	1:A:1114:LEU:HD12	1.74	0.69
2:B:29:A:H2’	2:B:30:A:H8	1.57	0.69
22:1:1133:MET:SD	35:2:528:ILE:HD11	2.32	0.69
23:3:368:ASP:OD1	23:3:368:ASP:N	2.17	0.69
40:9:360:HIS:NE2	40:9:394:HIS:O	2.25	0.69
10:J:236:ARG:HA	10:J:239:ARG:CZ	2.22	0.69
17:R:134:ARG:HH22	18:T:383:ARG:HA	1.56	0.69
23:3:561:GLY:O	23:3:582:GLU:HA	1.93	0.69
1:A:499:GLN:O	1:A:503:MET:HG2	1.93	0.69
6:F:36:A:N6	7:G:10:U:C2	2.60	0.69
11:K:121:TRP:HA	11:K:124:ARG:HH21	1.56	0.69
19:X:255:PRO:HA	19:X:324:VAL:HG11	1.73	0.69
23:3:285:MET:SD	23:3:305:THR:OG1	2.49	0.69
23:3:1150:SER:OG	23:3:1151:GLU:OE1	2.09	0.69
1:A:1298:ARG:C	1:A:1298:ARG:HH21	1.95	0.69
2:B:98:G:H2’	2:B:99:C:C6	2.28	0.69
11:K:360:ILE:C	20:Y:72:LYS:HE2	2.13	0.69
17:R:281:ASN:OD1	17:R:282:GLU:N	2.25	0.69
23:3:146:ARG:CD	23:3:150:ALA:CA	2.70	0.69
23:3:351:SER:OG	23:3:355:ASN:O	2.10	0.69
23:3:736:TYR:HE2	23:3:739:LEU:HD21	1.56	0.69
23:3:854:ALA:HB1	23:3:856:LYS:HD2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1:1108:ASN:HB2	22:1:1111:CYS:H	1.57	0.69
23:3:550:ASN:OD1	23:3:551:GLN:N	2.24	0.69
23:3:895:ARG:NH1	23:3:901:GLU:OE2	2.25	0.69
1:A:1670:ASP:OD1	1:A:1673:SER:N	2.25	0.69
8:H:50:C:H2'	8:H:51:A:C8	2.28	0.69
23:3:527:ILE:HA	23:3:532:ARG:O	1.93	0.69
1:A:1375:TRP:O	1:A:1378:GLU:N	2.25	0.69
5:E:304:SER:H	5:E:330:ILE:HB	1.56	0.69
7:G:91:A:H2'	7:G:92:U:C6	2.27	0.69
11:K:67:TYR:O	11:K:71:GLU:HG2	1.91	0.69
19:X:281:TYR:HB2	19:X:306:PHE:HB3	1.74	0.69
23:3:380:GLU:O	23:3:383:ASP:N	2.26	0.69
1:A:1684:PHE:HB3	1:A:1715:TYR:HD2	1.57	0.69
22:1:1017:LEU:HD21	22:1:1058:ILE:HD11	1.75	0.69
38:7:11:CYS:HB3	38:7:85:CYS:HB3	1.74	0.69
1:A:145:GLY:HA2	1:A:245:LEU:HD21	1.75	0.69
2:B:30:A:H2'	2:B:31:U:H6	1.56	0.69
3:C:300:LEU:HD23	3:C:306:ASN:HB2	1.73	0.69
7:G:-3:A:H2'	7:G:-2:A:C8	2.26	0.69
12:L:38:LEU:CD1	12:L:41:LYS:CG	2.57	0.69
1:A:1256:PHE:CG	1:A:1299:ILE:CG2	2.76	0.69
1:A:1437:ARG:NH2	1:A:1461:ASP:OD2	2.26	0.69
3:C:556:ASP:HA	3:C:559:ILE:HD12	1.75	0.69
5:E:224:GLN:HG3	5:E:226:LYS:H	1.59	0.69
19:X:237:ASN:ND2	19:X:244:ILE:O	2.25	0.69
20:Y:49:GLU:N	20:Y:49:GLU:OE2	2.25	0.69
37:6:18:ASN:OD1	37:6:19:ARG:N	2.25	0.69
2:B:18:C:O2	2:B:59:G:N2	2.20	0.68
3:C:879:ASP:OD1	3:C:879:ASP:N	2.25	0.68
22:1:400:SER:N	22:1:403:GLU:OE1	2.26	0.68
23:3:146:ARG:HB2	23:3:146:ARG:NH2	2.04	0.68
23:3:282:GLU:OE1	23:3:282:GLU:N	2.26	0.68
1:A:266:SER:OG	1:A:271:MET:O	2.08	0.68
1:A:318:TYR:HD1	3:C:645:ARG:HH11	1.40	0.68
2:B:100:C:H2'	2:B:101:U:C6	2.27	0.68
17:R:238:THR:O	17:R:242:GLN:HB2	1.94	0.68
22:1:158:GLU:O	22:1:162:THR:HG23	1.93	0.68
1:A:398:THR:HA	3:C:386:GLY:HA3	1.74	0.68
22:1:901:GLN:HA	22:1:939:ARG:HH22	1.58	0.68
1:A:1022:MET:C	1:A:1023:ASN:HD22	1.97	0.68
3:C:64:LYS:HE3	15:P:206:LYS:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Y:80:CYS:SG	20:Y:81:PHE:N	2.65	0.68
3:C:128:LEU:HD21	3:C:196:LYS:HE3	1.76	0.68
23:3:644:GLU:HG3	23:3:662:PHE:HB3	1.75	0.68
1:A:443:VAL:HG12	1:A:610:HIS:HB3	1.76	0.68
1:A:1310:ARG:HB3	1:A:1310:ARG:CZ	2.23	0.68
3:C:392:LEU:O	3:C:396:LEU:HG	1.93	0.68
3:C:531:TRP:HB3	3:C:538:HIS:HB3	1.76	0.68
6:F:42:C:H42	7:G:6:A:N6	1.91	0.68
23:3:146:ARG:CG	23:3:146:ARG:HH21	2.06	0.68
1:A:462:ARG:HH21	1:A:465:LYS:HG2	1.58	0.68
1:A:643:GLY:N	2:B:28:A:O2’	2.27	0.68
2:B:8:G:N1	2:B:69:A:N6	2.13	0.68
3:C:286:ASN:HB3	3:C:299:ILE:HG23	1.75	0.68
4:D:2098:ALA:O	4:D:2100:GLY:N	2.27	0.68
6:F:85:U:C2	8:H:14:C:N3	2.60	0.68
6:F:86:U:C2	8:H:12:G:O6	2.47	0.68
7:G:98:U:H3	8:H:33:G:H22	1.40	0.68
23:3:971:ASP:OD1	23:3:972:LEU:N	2.25	0.68
23:3:1136:GLU:OE1	23:3:1136:GLU:N	2.21	0.68
8:H:165:A:O2’	8:H:166:G:O4’	2.12	0.68
17:R:148:ARG:HG2	17:R:148:ARG:HH21	1.59	0.68
18:T:325:THR:O	18:T:325:THR:OG1	2.11	0.68
23:3:878:ASP:OD1	23:3:879:LEU:N	2.25	0.68
38:7:11:CYS:SG	38:7:13:LYS:HG3	2.34	0.68
38:7:35:SER:OG	38:7:36:TYR:N	2.24	0.68
1:A:150:MET:HG3	1:A:572:PHE:HE1	1.59	0.68
1:A:1580:HIS:HB2	1:A:1584:LYS:HE3	1.76	0.68
5:E:239:THR:HB	5:E:289:LEU:H	1.57	0.68
22:1:1078:VAL:HG11	22:1:1114:VAL:HG12	1.75	0.68
40:9:276:VAL:HG21	40:9:438:TYR:CD1	2.29	0.68
1:A:1488:THR:OG1	1:A:1489:LEU:N	2.25	0.68
23:3:498:GLY:O	23:3:525:ARG:NH2	2.27	0.68
1:A:467:GLN:NE2	2:B:57:G:O6	2.27	0.67
5:E:304:SER:OG	5:E:305:ALA:N	2.26	0.67
18:T:213:GLU:HG2	18:T:214:PRO:HD2	1.76	0.67
19:X:279:SER:O	19:X:307:GLN:NE2	2.27	0.67
22:1:944:SER:HB2	22:1:948:ARG:CZ	2.24	0.67
40:9:425:GLU:OE1	40:9:427:ARG:NH1	2.27	0.67
3:C:589:LYS:HG3	3:C:630:LEU:HD23	1.75	0.67
6:F:33:G:N1	7:G:14:A:C5	2.62	0.67
18:T:213:GLU:CD	18:T:215:GLY:H	1.96	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:1013:ARG:NH2	23:3:1064:ASP:OD1	2.26	0.67
14:O:63:MET:HA	14:O:161:ARG:HA	1.75	0.67
23:3:947:GLU:HG3	23:3:948:VAL:H	1.60	0.67
38:7:8:LEU:HA	38:7:90:ASN:HD21	1.58	0.67
1:A:104:GLU:HG3	1:A:638:LEU:HD13	1.74	0.67
1:A:253:ASN:OD1	3:C:888:ARG:NH2	2.28	0.67
3:C:230:ASP:OD2	3:C:262:ARG:NH2	2.27	0.67
6:F:62:C:O2'	11:K:38:GLU:OE2	2.11	0.67
10:J:319:MET:O	10:J:323:LEU:HG	1.95	0.67
11:K:79:LEU:HD11	11:K:97:GLU:HG3	1.74	0.67
22:1:1108:ASN:HB3	22:1:1110:VAL:HB	1.74	0.67
22:1:1278:ASP:OD2	23:3:112:CYS:N	2.28	0.67
37:6:46:ARG:HB3	37:6:63:VAL:HG12	1.76	0.67
3:C:320:LEU:HD21	3:C:344:TRP:HB2	1.76	0.67
22:1:614:ARG:HG3	22:1:647:PHE:HZ	1.58	0.67
1:A:429:ASN:ND2	1:A:432:ARG:HH11	1.91	0.67
1:A:1531:ASN:OD1	1:A:1531:ASN:N	2.24	0.67
3:C:241:ARG:NH2	3:C:583:ASN:O	2.27	0.67
3:C:475:MET:HB2	3:C:498:SER:HB2	1.75	0.67
6:F:85:U:N3	8:H:14:C:N4	2.25	0.67
11:K:360:ILE:O	20:Y:72:LYS:HG3	1.95	0.67
19:X:277:ARG:NH2	22:1:437:PRO:HA	2.09	0.67
2:B:33:U:H1'	18:T:279:LYS:HD3	1.77	0.67
3:C:259:LYS:HB3	3:C:262:ARG:HG3	1.76	0.67
3:C:645:ARG:NH2	3:C:653:ILE:O	2.27	0.67
10:J:241:VAL:HG22	10:J:243:SER:H	1.58	0.67
38:7:46:CYS:HB3	38:7:85:CYS:HB2	1.77	0.67
1:A:101:LYS:HG3	1:A:473:PHE:HE2	1.59	0.67
2:B:29:A:H2'	2:B:30:A:C8	2.30	0.67
5:E:114:GLU:OE2	5:E:157:CYS:N	2.25	0.67
1:A:617:ASN:HA	1:A:621:VAL:HG22	1.76	0.67
12:L:38:LEU:HD12	12:L:41:LYS:CB	2.25	0.67
12:L:41:LYS:HA	12:L:41:LYS:HE3	1.75	0.67
17:R:385:ASN:O	17:R:386:ARG:NH1	2.28	0.67
18:T:245:HIS:ND1	18:T:267:ASP:OD2	2.28	0.67
22:1:659:GLN:OE1	22:1:659:GLN:N	2.28	0.67
23:3:578:THR:O	23:3:580:ARG:NH1	2.28	0.67
1:A:582:PHE:CE2	1:A:634:TRP:HB2	2.30	0.67
22:1:1004:ILE:HD11	22:1:1008:LYS:HB2	1.76	0.67
12:L:66:GLU:OE1	12:L:66:GLU:N	2.24	0.66
20:Y:54:CYS:HB3	21:Z:585:ASP:HB2	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1:793:LYS:HB2	22:1:836:THR:HG22	1.77	0.66
23:3:507:SER:OG	23:3:509:SER:OG	2.12	0.66
1:A:508:ILE:HG22	1:A:509:HIS:HD2	1.60	0.66
1:A:535:ARG:NH2	1:A:1551:PHE:CE1	2.62	0.66
1:A:802:THR:OG1	1:A:803:ALA:N	2.23	0.66
1:A:1119:ASP:OD2	1:A:1124:ASN:ND2	2.28	0.66
6:F:78:A:H5”	6:F:79:C:H5	1.60	0.66
17:R:332:ARG:NH2	19:X:267:ASP:H	1.93	0.66
22:1:942:ASN:ND2	22:1:943:LYS:O	2.27	0.66
23:3:858:GLY:HA3	23:3:861:GLN:HG3	1.77	0.66
37:6:34:GLU:O	37:6:38:ILE:HG13	1.95	0.66
1:A:1580:HIS:O	1:A:1584:LYS:HG2	1.96	0.66
2:B:99:C:H2’	2:B:100:C:C6	2.31	0.66
22:1:1076:ALA:O	22:1:1080:THR:HG23	1.96	0.66
23:3:21:ASN:HD22	23:3:28:GLN:HG3	1.60	0.66
35:2:536:MET:SD	35:2:536:MET:N	2.67	0.66
1:A:344:ASP:N	1:A:344:ASP:OD1	2.26	0.66
1:A:401:GLY:HA2	1:A:404:LEU:HD12	1.76	0.66
1:A:1102:THR:OG1	1:A:1104:ASP:OD1	2.10	0.66
3:C:387:ASP:OD1	3:C:390:THR:OG1	2.11	0.66
3:C:470:PRO:HB3	3:C:545:PRO:HB3	1.77	0.66
3:C:731:SER:HB2	3:C:747:ASP:HB3	1.76	0.66
20:Y:110:ASP:OD1	20:Y:111:HIS:N	2.29	0.66
1:A:1256:PHE:CD1	1:A:1299:ILE:HG22	2.31	0.66
3:C:602:LYS:HD2	3:C:651:ILE:HD11	1.76	0.66
8:H:50:C:H2’	8:H:51:A:H8	1.59	0.66
22:1:698:GLN:O	22:1:702:ARG:NH1	2.29	0.66
23:3:854:ALA:O	23:3:856:LYS:N	2.29	0.66
1:A:843:LEU:HD22	1:A:867:ILE:HG23	1.78	0.66
2:B:23:C:H1’	2:B:24:G:H2’	1.78	0.66
18:T:399:LYS:HB2	18:T:406:ILE:HD11	1.76	0.66
22:1:855:ASP:OD1	22:1:855:ASP:N	2.15	0.66
23:3:1194:SER:OG	23:3:1199:ARG:O	2.13	0.66
1:A:253:ASN:ND2	1:A:334:THR:O	2.25	0.66
2:B:18:C:N3	2:B:59:G:N1	2.41	0.66
11:K:14:ASN:O	11:K:18:SER:OG	2.13	0.66
12:L:77:LEU:HD21	17:R:285:ALA:HA	1.77	0.66
17:R:332:ARG:HH22	19:X:267:ASP:H	1.42	0.66
18:T:247:SER:OG	18:T:248:THR:N	2.22	0.66
40:9:360:HIS:HA	40:9:365:ILE:HG13	1.78	0.66
3:C:279:ARG:HA	3:C:282:VAL:HG12	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1:899:ALA:O	22:1:903:GLN:NE2	2.28	0.66
1:A:733:THR:HG22	40:9:241:TYR:HA	1.76	0.66
1:A:1018:ASN:OD1	1:A:1019:TYR:N	2.28	0.66
1:A:2105:ILE:O	1:A:2141:GLU:HA	1.96	0.66
3:C:322:SER:O	3:C:326:ILE:HG13	1.96	0.66
35:2:534:GLN:CA	35:2:534:GLN:HE21	2.07	0.66
18:T:356:LEU:HD13	18:T:366:VAL:HB	1.77	0.65
1:A:1256:PHE:CD1	1:A:1299:ILE:HG23	2.29	0.65
18:T:264:CYS:HB2	18:T:291:VAL:HG11	1.78	0.65
20:Y:7:VAL:HG23	20:Y:108:ARG:HB3	1.78	0.65
23:3:304:GLN:HE21	23:3:308:GLY:HA2	1.61	0.65
37:6:37:ASP:O	37:6:41:LYS:NZ	2.29	0.65
1:A:522:PHE:O	1:A:552:ARG:NH2	2.21	0.65
1:A:755:HIS:CE1	15:P:220:HIS:HD1	2.14	0.65
3:C:749:THR:O	3:C:749:THR:OG1	2.14	0.65
7:G:99:C:H42	8:H:32:U:H3	0.66	0.65
23:3:457:ASN:OD1	23:3:477:SER:OG	2.13	0.65
19:X:353:LYS:HG3	19:X:354:GLU:H	1.61	0.65
22:1:649:LYS:HG2	22:1:689:ILE:HG12	1.79	0.65
22:1:1107:GLN:N	22:1:1108:ASN:OD1	2.29	0.65
23:3:1043:THR:HG22	23:3:1057:ARG:HB2	1.79	0.65
23:3:1056:VAL:HG22	23:3:1091:VAL:HG22	1.78	0.65
1:A:1209:HIS:CD2	1:A:1210:LYS:HE2	2.31	0.65
10:J:396:ARG:NH2	10:J:423:GLU:OE2	2.30	0.65
11:K:27:TYR:HA	11:K:34:GLN:HA	1.78	0.65
23:3:394:ASN:OD1	23:3:394:ASN:N	2.29	0.65
1:A:136:ILE:HG12	1:A:228:TRP:HB3	1.79	0.65
1:A:163:ARG:HD3	1:A:625:PRO:HB3	1.77	0.65
1:A:369:GLU:HG3	3:C:303:LEU:HD22	1.79	0.65
1:A:857:ASN:HB3	1:A:860:GLN:HG3	1.77	0.65
1:A:1167:THR:OG1	1:A:1168:VAL:N	2.26	0.65
22:1:492:GLN:HA	22:1:495:ARG:HD3	1.78	0.65
22:1:902:GLU:O	22:1:903:GLN:NE2	2.29	0.65
23:3:82:SER:HG	23:3:84:SER:H	1.44	0.65
23:3:138:GLN:HG2	23:3:161:HIS:CE1	2.31	0.65
23:3:706:MET:HE1	23:3:767:LEU:HB2	1.78	0.65
22:1:565:ASP:O	22:1:568:ARG:HG3	1.96	0.65
1:A:357:ASN:ND2	3:C:866:SER:O	2.30	0.65
1:A:1638:ASN:HA	1:A:1656:THR:HA	1.79	0.65
3:C:110:PRO:HD2	3:C:537:TYR:CZ	2.32	0.65
3:C:253:VAL:HG11	3:C:289:ILE:HD11	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:490:PHE:HE2	3:C:612:LYS:HB3	1.62	0.65
5:E:127:ALA:HB1	5:E:154:VAL:HG12	1.79	0.65
7:G:-2:A:H2'	7:G:-1:C:H6	1.61	0.65
7:G:8:C:H2'	7:G:9:C:H6	1.61	0.65
15:P:195:LYS:HB3	40:9:198:LYS:HB2	1.78	0.65
22:1:977:VAL:HG12	22:1:981:TYR:HE2	1.62	0.65
18:T:370:ASN:OD1	18:T:370:ASN:N	2.30	0.65
18:T:455:GLN:HG3	18:T:485:THR:HG21	1.79	0.65
8:H:126:A:H2'	8:H:127:G:C8	2.31	0.65
23:3:614:VAL:HG12	23:3:633:LEU:HD21	1.79	0.65
23:3:1107:THR:OG1	23:3:1108:THR:N	2.30	0.65
37:6:47:GLN:HE22	37:6:49:ARG:HH21	1.44	0.65
1:A:693:ILE:O	1:A:696:MET:N	2.29	0.64
1:A:1181:ASP:OD1	1:A:1181:ASP:N	2.28	0.64
3:C:663:CYS:HB3	3:C:785:ARG:HB2	1.79	0.64
40:9:333:GLY:O	40:9:378:SER:OG	2.13	0.64
1:A:447:TYR:CE2	1:A:611:LEU:HD13	2.32	0.64
1:A:582:PHE:CD2	1:A:630:TRP:HB2	2.33	0.64
1:A:1434:LYS:O	1:A:1439:ARG:NH1	2.25	0.64
2:B:30:A:H2'	2:B:31:U:C6	2.32	0.64
7:G:91:A:H2'	7:G:92:U:H6	1.63	0.64
19:X:222:GLU:HG2	20:Y:69:ARG:HH12	1.61	0.64
22:1:619:ASN:OD1	22:1:620:MET:N	2.31	0.64
22:1:839:GLU:HA	22:1:842:ASN:HD22	1.62	0.64
23:3:550:ASN:ND2	23:3:593:ALA:O	2.31	0.64
1:A:254:TYR:HE2	1:A:433:GLU:HA	1.62	0.64
3:C:111:VAL:HG13	3:C:155:PRO:HD2	1.79	0.64
6:F:44:G:H21	7:G:5:G:H22	1.43	0.64
10:J:252:GLU:OE2	10:J:260:ARG:HD3	1.97	0.64
11:K:35:CYS:HB3	11:K:40:GLY:HA2	1.77	0.64
35:2:514:LYS:CA	35:2:593:GLU:OE1	2.46	0.64
1:A:387:PHE:HE1	3:C:326:ILE:HG22	1.62	0.64
1:A:1310:ARG:HG2	1:A:1310:ARG:HH21	1.61	0.64
1:A:1330:MET:HE1	1:A:1369:TYR:HB2	1.80	0.64
3:C:223:ASP:OD1	3:C:223:ASP:N	2.28	0.64
3:C:224:GLY:HA3	3:C:438:ILE:HD12	1.78	0.64
3:C:853:ARG:O	3:C:876:PRO:HD2	1.97	0.64
23:3:447:MET:HE3	23:3:750:CYS:HA	1.80	0.64
41:8:105:LEU:O	41:8:108:LEU:N	2.31	0.64
23:3:84:SER:OG	23:3:85:GLY:N	2.31	0.64
23:3:1145:GLU:OE2	23:3:1149:ARG:NH2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:846:VAL:HG22	3:C:887:LEU:HD11	1.80	0.64
9:I:609:ALA:HA	9:I:612:ALA:HB3	1.79	0.64
10:J:297:ASN:O	10:J:301:ARG:HG3	1.98	0.64
19:X:282:LEU:N	19:X:291:ASP:OD2	2.23	0.64
17:R:150:ALA:CB	18:T:360:VAL:HG21	2.28	0.64
18:T:257:ARG:NH2	18:T:297:HIS:O	2.31	0.64
20:Y:56:PHE:O	20:Y:84:TYR:OH	2.11	0.64
22:1:1126:PHE:HA	35:2:575:PHE:HD2	1.59	0.64
35:2:581:LYS:HB3	35:2:581:LYS:NZ	2.13	0.64
40:9:365:ILE:HB	40:9:383:THR:OG1	1.98	0.64
5:E:219:VAL:HB	5:E:229:TYR:HB2	1.79	0.64
7:G:-2:A:H2'	7:G:-1:C:C6	2.33	0.64
22:1:489:PRO:O	22:1:492:GLN:N	2.30	0.64
23:3:581:LYS:HD2	23:3:625:LEU:HD22	1.79	0.64
1:A:634:TRP:NE1	1:A:638:LEU:HD11	2.12	0.64
6:F:40:U:C2	6:F:41:A:C8	2.86	0.64
7:G:6:A:H8	7:G:7:G:N7	1.96	0.64
9:I:374:ILE:O	9:I:376:ASN:N	2.31	0.64
17:R:306:ALA:HB1	17:R:310:ARG:HH12	1.63	0.64
22:1:1257:PRO:HB3	35:2:481:THR:OG1	1.98	0.64
23:3:320:ASP:OD1	23:3:320:ASP:N	2.29	0.64
23:3:999:ARG:HH11	23:3:1024:PHE:HZ	1.46	0.64
23:3:1188:ASN:OD1	23:3:1188:ASN:N	2.28	0.64
1:A:135:VAL:HA	1:A:225:TYR:CE2	2.32	0.63
8:H:43:U:H2'	8:H:44:U:C5	2.33	0.63
18:T:203:HIS:CE1	18:T:229:LYS:HD2	2.33	0.63
18:T:213:GLU:HG3	18:T:218:TRP:CE2	2.33	0.63
1:A:108:MET:HG2	1:A:114:ARG:HH22	1.62	0.63
1:A:559:ASP:HA	1:A:562:VAL:HB	1.80	0.63
1:A:589:THR:OG1	1:A:591:MET:SD	2.49	0.63
3:C:460:ASP:OD1	3:C:460:ASP:N	2.29	0.63
10:J:434:VAL:O	10:J:438:TYR:HB3	1.99	0.63
18:T:394:ASN:ND2	18:T:408:ASN:OD1	2.31	0.63
40:9:242:SER:HA	40:9:263:ALA:HA	1.81	0.63
3:C:212:SER:O	3:C:216:THR:HG23	1.98	0.63
17:R:148:ARG:HH21	17:R:148:ARG:CG	2.12	0.63
23:3:316:GLU:OE2	23:3:326:ARG:NH2	2.32	0.63
1:A:200:ASP:HA	1:A:237:THR:HG21	1.79	0.63
1:A:508:ILE:HG22	1:A:509:HIS:CD2	2.33	0.63
2:B:62:G:H2'	2:B:63:A:C8	2.32	0.63
3:C:210:ASN:OD1	3:C:633:GLY:HA3	1.99	0.63

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
5:E:221:ASP:HB3	5:E:224:GLN:HG2	1.81	0.63
22:1:1145:ASN:ND2	22:1:1183:VAL:HG11	2.14	0.63
1:A:67:ARG:NH2	1:A:487:LEU:HD23	2.13	0.63
1:A:145:GLY:HA3	1:A:242:ALA:HA	1.80	0.63
1:A:1947:ASN:HA	1:A:1950:ALA:HB3	1.81	0.63
6:F:15:A:H2'	6:F:16:G:C8	2.34	0.63
8:H:50:C:N3	8:H:64:A:N6	2.46	0.63
1:A:1660:TYR:OH	1:A:1717:ASN:O	2.17	0.63
5:E:336:HIS:HB2	5:E:341:ILE:HB	1.81	0.63
8:H:70:C:H2'	8:H:71:C:C6	2.34	0.63
8:H:78:C:H2'	8:H:79:G:C8	2.29	0.63
11:K:179:ARG:HA	11:K:182:GLU:OE2	1.99	0.63
22:1:1133:MET:SD	35:2:528:ILE:CD1	2.87	0.63
1:A:1491:LYS:O	1:A:1710:ASN:ND2	2.32	0.63
1:A:1579:ALA:O	1:A:1584:LYS:NZ	2.24	0.63
3:C:911:PRO:HG2	3:C:912:LEU:HD12	1.80	0.63
23:3:260:ASN:OD1	23:3:261:PHE:N	2.32	0.63
23:3:552:ARG:HH21	23:3:569:ASP:HA	1.64	0.63
1:A:277:PRO:HD3	1:A:451:LEU:HB3	1.80	0.63
1:A:301:LYS:HG2	3:C:939:ARG:HB3	1.81	0.63
2:B:31:U:H2'	2:B:32:C:C6	2.34	0.63
1:A:799:PRO:HD3	17:R:284:PHE:CD2	2.34	0.63
1:A:1076:ASP:OD1	1:A:1077:ILE:N	2.31	0.63
8:H:139:C:H2'	8:H:140:A:C8	2.34	0.63
10:J:343:GLU:OE1	10:J:378:ASN:ND2	2.19	0.63
22:1:543:THR:O	22:1:543:THR:OG1	2.14	0.63
35:2:537:ARG:HH11	35:2:537:ARG:CG	2.10	0.63
40:9:367:SER:HB2	40:9:394:HIS:HB3	1.81	0.63
1:A:76:MET:HE3	1:A:502:ASN:HB3	1.80	0.62
1:A:1209:HIS:HD2	1:A:1210:LYS:H	1.47	0.62
1:A:1307:MET:HA	1:A:1307:MET:CE	2.29	0.62
3:C:122:LEU:HB3	3:C:199:LEU:HD22	1.79	0.62
3:C:381:LEU:HD22	3:C:416:LEU:HD11	1.80	0.62
3:C:780:CYS:HB3	3:C:934:MET:HG2	1.81	0.62
18:T:295:ASP:OD1	18:T:296:LEU:N	2.31	0.62
20:Y:101:LYS:HG2	20:Y:106:THR:HG22	1.81	0.62
23:3:550:ASN:HD21	23:3:595:VAL:N	1.97	0.62
40:9:370:ASN:ND2	40:9:372:GLY:O	2.32	0.62
5:E:65:HIS:HD2	5:E:351:LEU:HD11	1.64	0.62
22:1:826:ASP:OD1	22:1:827:ARG:N	2.32	0.62
1:A:501:TYR:HE1	1:A:518:LEU:HB3	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1596:VAL:O	1:A:1600:GLU:HG2	2.00	0.62
18:T:415:ILE:O	18:T:432:ASP:N	2.31	0.62
19:X:327:TYR:HD1	19:X:349:TYR:HB3	1.65	0.62
23:3:405:SER:HB2	23:3:1123:SER:O	1.99	0.62
23:3:477:SER:HB2	23:3:504:PRO:HA	1.81	0.62
23:3:700:LYS:HE2	23:3:702:PHE:HZ	1.63	0.62
3:C:139:HIS:O	3:C:259:LYS:NZ	2.32	0.62
3:C:448:LYS:O	3:C:452:THR:CB	2.47	0.62
11:K:47:SER:HG	11:K:49:SER:HG	1.34	0.62
1:A:112:GLN:HG3	1:A:190:ALA:HB2	1.80	0.62
1:A:118:VAL:HG22	1:A:129:VAL:HA	1.82	0.62
1:A:1134:TRP:NE1	1:A:1193:GLU:OE2	2.31	0.62
3:C:139:HIS:HB3	45:C:1500:GTP:H5”	1.81	0.62
17:R:123:GLU:OE1	17:R:125:MET:N	2.32	0.62
38:7:23:CYS:SG	38:7:26:CYS:N	2.64	0.62
1:A:690:MET:HA	1:A:694:LEU:HD12	1.82	0.62
3:C:129:ILE:HD12	3:C:441:PRO:HG2	1.80	0.62
3:C:607:LEU:HD21	3:C:644:LEU:HD22	1.82	0.62
17:R:332:ARG:NH2	19:X:366:GLU:OE1	2.32	0.62
18:T:213:GLU:HG3	18:T:218:TRP:CZ2	2.35	0.62
1:A:170:ASP:HB3	1:A:173:GLU:HB2	1.80	0.62
1:A:518:LEU:HD11	1:A:522:PHE:HA	1.82	0.62
1:A:569:VAL:HG23	1:A:570:ASP:H	1.64	0.62
1:A:1272:THR:HG22	1:A:1372:ILE:HD11	1.81	0.62
1:A:1551:PHE:CB	1:A:1553:VAL:HG23	2.29	0.62
1:A:1629:ILE:O	1:A:1661:TRP:HA	1.98	0.62
3:C:854:ARG:HB3	3:C:876:PRO:HG2	1.80	0.62
8:H:70:C:H2’	8:H:71:C:H6	1.65	0.62
18:T:190:TRP:NE1	18:T:500:HIS:O	2.33	0.62
21:Z:600:ARG:HH22	21:Z:601:LEU:HD13	1.64	0.62
23:3:209:THR:O	23:3:209:THR:OG1	2.15	0.62
35:2:581:LYS:HD2	35:2:581:LYS:C	2.19	0.62
1:A:1734:MET:SD	1:A:1734:MET:N	2.73	0.62
3:C:664:GLU:HB3	3:C:820:PHE:CZ	2.35	0.62
22:1:1054:GLU:O	22:1:1058:ILE:HG13	2.00	0.62
22:1:1126:PHE:O	35:2:575:PHE:HE2	1.82	0.62
1:A:197:PRO:HA	1:A:204:LEU:HD13	1.81	0.62
1:A:261:LYS:HA	1:A:328:HIS:CD2	2.35	0.62
1:A:1295:ILE:HD13	1:A:1295:ILE:C	2.20	0.62
1:A:1607:GLU:N	1:A:1632:PHE:O	2.25	0.62
6:F:41:A:H2’	6:F:42:C:C6	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:82:G:H2'	8:H:83:A:H8	1.65	0.62
22:1:1133:MET:CE	35:2:528:ILE:HD12	2.29	0.62
23:3:146:ARG:HE	23:3:150:ALA:HB1	1.61	0.62
23:3:186:GLU:O	23:3:206:GLN:HB2	1.99	0.62
2:B:52:U:H2'	2:B:53:U:H6	1.65	0.62
2:B:62:G:H2'	2:B:63:A:H8	1.65	0.62
11:K:73:ARG:NH1	11:K:77:LEU:HD11	2.14	0.62
41:8:64:ASP:O	41:8:68:ILE:HG12	2.00	0.62
1:A:350:PHE:HA	3:C:268:LYS:HB3	1.81	0.61
3:C:749:THR:O	3:C:753:GLU:N	2.33	0.61
6:F:47:A:H3'	6:F:48:A:H4'	1.81	0.61
12:L:62:GLU:OE1	12:L:62:GLU:N	2.33	0.61
20:Y:1:MET:HE3	20:Y:6:LYS:HE2	1.81	0.61
22:1:584:ASP:O	22:1:590:ARG:NH2	2.31	0.61
41:8:47:VAL:HG13	41:8:48:ILE:HG12	1.82	0.61
11:K:159:LYS:HA	11:K:162:ASP:OD2	2.00	0.61
22:1:1262:ARG:HH12	35:2:483:GLN:NE2	1.98	0.61
23:3:370:GLU:OE2	23:3:390:ARG:NH1	2.32	0.61
23:3:462:VAL:HG21	23:3:508:CYS:HB2	1.81	0.61
23:3:553:GLN:OE1	23:3:553:GLN:N	2.33	0.61
23:3:727:SER:O	23:3:728:ARG:NH1	2.34	0.61
23:3:730:HIS:HE1	23:3:773:VAL:HG13	1.63	0.61
1:A:467:GLN:HB3	2:B:19:A:N6	2.15	0.61
8:H:124:G:H2'	8:H:125:G:C8	2.36	0.61
17:R:152:GLU:HA	17:R:152:GLU:OE2	1.98	0.61
23:3:545:VAL:HG12	23:3:546:LYS:HG2	1.82	0.61
3:C:203:MET:HG2	3:C:218:GLY:HA3	1.83	0.61
18:T:292:TYR:HE1	18:T:308:ARG:HB2	1.65	0.61
18:T:412:HIS:ND1	18:T:437:HIS:HB2	2.15	0.61
22:1:1074:ARG:O	22:1:1078:VAL:HG23	1.99	0.61
23:3:1175:ASP:OD1	23:3:1177:ASP:N	2.34	0.61
1:A:134:TRP:CZ3	1:A:420:ARG:HG3	2.35	0.61
1:A:582:PHE:HD2	1:A:630:TRP:HB2	1.65	0.61
1:A:1057:ARG:NH1	1:A:1060:GLU:OE1	2.31	0.61
3:C:774:THR:HA	3:C:784:ILE:HD12	1.81	0.61
7:G:101:U:O5'	22:1:1070:LYS:NZ	2.34	0.61
17:R:238:THR:O	17:R:242:GLN:CB	2.48	0.61
19:X:371:HIS:N	19:X:374:SER:OG	2.20	0.61
23:3:95:SER:OG	23:3:96:LYS:N	2.31	0.61
37:6:82:VAL:O	37:6:85:ARG:HG2	2.01	0.61
1:A:269:LEU:HD22	1:A:321:ASN:HD21	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:75:HIS:ND1	5:E:77:ASN:OD1	2.33	0.61
5:E:209:ILE:HG21	5:E:250:LEU:HD22	1.83	0.61
18:T:308:ARG:HG2	18:T:308:ARG:NH1	2.16	0.61
23:3:55:THR:O	23:3:55:THR:OG1	2.18	0.61
40:9:397:PHE:N	40:9:397:PHE:CD1	2.68	0.61
1:A:1609:VAL:HG13	1:A:1631:LEU:HD23	1.81	0.61
6:F:86:U:O2	8:H:12:G:O6	2.18	0.61
23:3:898:ASN:OD1	23:3:899:THR:N	2.33	0.61
35:2:584:LEU:H	35:2:584:LEU:HD12	1.66	0.61
2:B:99:C:H2’	2:B:100:C:H6	1.64	0.61
7:G:-4:G:O2’	7:G:-3:A:O5’	2.18	0.61
23:3:689:THR:OG1	23:3:690:ARG:N	2.34	0.61
1:A:519:ASP:OD1	1:A:522:PHE:N	2.34	0.61
1:A:855:ARG:HG3	1:A:856:LEU:H	1.66	0.61
1:A:1308:PRO:HB2	1:A:1548:TYR:HD2	1.50	0.61
1:A:1601:LEU:HA	1:A:1606:ILE:HD12	1.80	0.61
3:C:388:VAL:HA	3:C:392:LEU:HD12	1.82	0.61
6:F:1:G:H2’	6:F:2:U:C6	2.36	0.61
11:K:33:LYS:HD2	11:K:44:HIS:CE1	2.36	0.61
22:1:953:ASP:O	22:1:956:SER:OG	2.10	0.61
23:3:566:PHE:HD2	23:3:574:LEU:HD23	1.65	0.61
40:9:416:ASP:O	40:9:420:ASP:N	2.31	0.61
2:B:37:G:N2	2:B:46:U:H1’	2.16	0.61
3:C:384:VAL:HA	3:C:392:LEU:HD11	1.82	0.61
6:F:42:C:H2’	6:F:43:A:C8	2.36	0.61
7:G:98:U:H3’	7:G:99:C:H5”	1.82	0.61
11:K:142:ILE:O	11:K:144:ARG:NH2	2.34	0.61
20:Y:86:ASP:O	20:Y:89:SER:OG	2.19	0.61
23:3:642:ILE:O	23:3:703:ARG:NH2	2.33	0.61
35:2:524:LEU:HD13	35:2:528:ILE:CG2	2.31	0.61
3:C:208:HIS:HB3	3:C:211:PHE:HD2	1.63	0.60
3:C:808:ILE:HA	3:C:811:THR:HG22	1.82	0.60
22:1:516:LEU:O	22:1:520:THR:OG1	2.17	0.60
23:3:146:ARG:CD	23:3:150:ALA:HA	2.31	0.60
1:A:828:PRO:O	1:A:882:LYS:NZ	2.33	0.60
3:C:799:GLU:HB2	3:C:802:HIS:HB3	1.82	0.60
8:H:43:U:H2’	8:H:44:U:C6	2.36	0.60
18:T:213:GLU:O	18:T:472:GLN:NE2	2.30	0.60
23:3:174:ASP:OD2	23:3:240:GLY:N	2.32	0.60
1:A:82:ARG:H	1:A:85:LYS:HZ2	1.50	0.60
1:A:372:PRO:HD3	3:C:341:LYS:HD3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:717:TRP:HZ3	1:A:747:ALA:HB2	1.65	0.60
1:A:1457:HIS:CD2	17:R:420:SER:HB3	2.36	0.60
1:A:1719:PHE:O	1:A:1722:SER:OG	2.10	0.60
6:F:36:A:C6	7:G:10:U:N3	2.69	0.60
6:F:40:U:N3	6:F:41:A:N7	2.49	0.60
18:T:375:VAL:HG22	18:T:391:SER:HB2	1.84	0.60
23:3:1007:GLU:O	23:3:1008:SER:HB2	2.00	0.60
40:9:306:ASN:OD1	40:9:345:TYR:N	2.24	0.60
1:A:82:ARG:H	1:A:85:LYS:NZ	2.00	0.60
1:A:182:ILE:HA	1:A:185:VAL:HG22	1.82	0.60
1:A:530:LEU:HB3	1:A:534:GLU:HB3	1.82	0.60
5:E:93:TRP:HA	5:E:101:ASN:HA	1.83	0.60
22:1:529:GLY:O	22:1:533:ASN:ND2	2.35	0.60
22:1:1135:GLU:O	22:1:1138:VAL:HG22	2.01	0.60
1:A:405:LEU:HD11	3:C:385:VAL:HG11	1.83	0.60
1:A:1256:PHE:H	1:A:1531:ASN:ND2	2.00	0.60
1:A:1433:ASP:OD1	1:A:1439:ARG:NH2	2.34	0.60
1:A:1639:VAL:HG13	1:A:1717:ASN:HB3	1.83	0.60
3:C:190:LEU:O	3:C:198:TYR:N	2.35	0.60
3:C:636:TYR:O	3:C:640:VAL:HG23	2.01	0.60
11:K:42:LYS:O	11:K:46:MET:HG2	2.01	0.60
12:L:16:ASP:OD2	12:L:54:LEU:HD21	2.01	0.60
18:T:311:THR:OG1	18:T:312:ALA:N	2.32	0.60
22:1:620:MET:O	22:1:625:ARG:NH1	2.34	0.60
23:3:1027:ASP:OD2	23:3:1031:ARG:NH1	2.33	0.60
1:A:1712:HIS:CE1	1:A:1734:MET:HG3	2.36	0.60
5:E:133:VAL:HG22	5:E:154:VAL:HG11	1.83	0.60
7:G:108:U:H4’	7:G:109:U:OP2	2.01	0.60
17:R:150:ALA:HB1	18:T:360:VAL:HG21	1.83	0.60
1:A:1332:HIS:NE2	1:A:1358:SER:O	2.35	0.60
3:C:302:PRO:HB2	3:C:320:LEU:HD13	1.84	0.60
7:G:115:C:N3	20:Y:116:ARG:HB2	2.16	0.60
17:R:148:ARG:HB3	17:R:148:ARG:NH2	2.17	0.60
22:1:1126:PHE:CE1	35:2:576:PHE:CZ	2.90	0.60
23:3:1040:ASP:N	23:3:1040:ASP:OD1	2.32	0.60
1:A:1416:ILE:HG22	1:A:1417:PRO:HD3	1.84	0.60
1:A:1539:SER:O	1:A:1541:THR:N	2.34	0.60
2:B:14:U:H2’	2:B:15:C:C6	2.37	0.60
8:H:161:U:O2	8:H:163:G:N2	2.35	0.60
20:Y:113:SER:HG	20:Y:114:ASN:HD22	1.50	0.60
23:3:616:ILE:O	23:3:628:LEU:N	2.23	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:699:VAL:HG22	23:3:716:SER:HB2	1.83	0.60
23:3:899:THR:OG1	23:3:900:GLY:N	2.34	0.60
35:2:534:GLN:HE21	35:2:534:GLN:C	2.05	0.60
1:A:261:LYS:HB3	1:A:328:HIS:HB3	1.83	0.60
3:C:888:ARG:HD2	3:C:896:PHE:HD1	1.67	0.60
6:F:81:C:H4’	6:F:82:A:C8	2.37	0.60
11:K:63:GLN:HG3	11:K:64:PHE:N	2.17	0.60
16:Q:515:VAL:N	16:Q:540:THR:O	2.34	0.60
40:9:236:LEU:HD22	40:9:452:GLN:NE2	2.17	0.60
1:A:564:TYR:HB2	1:A:574:LEU:HB2	1.82	0.60
1:A:768:ASP:OD1	1:A:769:LYS:N	2.35	0.60
3:C:516:LEU:HD21	3:C:573:GLU:HA	1.83	0.60
1:A:221:ASN:ND2	2:B:12:U:OP1	2.34	0.59
1:A:888:GLN:O	1:A:889:ARG:NE	2.31	0.59
2:B:18:C:H2’	2:B:19:A:H8	1.67	0.59
3:C:94:ILE:HB	18:T:276:GLU:HG3	1.84	0.59
3:C:140:HIS:NE2	3:C:233:GLU:OE1	2.31	0.59
3:C:618:THR:HB	3:C:630:LEU:HB2	1.83	0.59
6:F:36:A:O2’	6:F:37:C:H5”	2.02	0.59
22:1:1145:ASN:ND2	22:1:1183:VAL:CG1	2.65	0.59
22:1:1273:TYR:O	22:1:1277:GLN:HB3	2.00	0.59
40:9:368:MET:O	40:9:394:HIS:ND1	2.35	0.59
41:8:45:LEU:O	41:8:48:ILE:N	2.35	0.59
3:C:495:ARG:HB3	3:C:549:TRP:CD1	2.33	0.59
23:3:27:GLN:HE21	23:3:45:PRO:HG3	1.67	0.59
23:3:545:VAL:N	23:3:557:ALA:O	2.28	0.59
23:3:1043:THR:HG21	23:3:1057:ARG:HH21	1.67	0.59
1:A:941:LYS:HE2	1:A:1071:PHE:CD1	2.37	0.59
10:J:267:ARG:O	10:J:271:VAL:HG23	2.02	0.59
10:J:308:ARG:HG3	17:R:231:HIS:O	2.02	0.59
23:3:369:GLU:N	23:3:369:GLU:OE1	2.34	0.59
23:3:895:ARG:HD3	23:3:903:TRP:CE2	2.37	0.59
23:3:1203:GLU:HA	23:3:1203:GLU:OE2	2.01	0.59
40:9:268:GLU:O	40:9:271:LEU:N	2.35	0.59
1:A:768:ASP:HB3	1:A:771:VAL:HG12	1.83	0.59
1:A:1106:ALA:O	1:A:1110:ILE:HG13	2.01	0.59
4:D:1378:TYR:HA	4:D:1452:VAL:O	2.02	0.59
6:F:60:C:H2’	6:F:61:C:O4’	2.01	0.59
18:T:439:TRP:CE3	18:T:446:ASN:HB2	2.37	0.59
22:1:588:TYR:HD1	38:7:96:THR:HG22	1.66	0.59
1:A:67:ARG:NE	1:A:491:GLU:OE2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LYS:HG3	1:A:473:PHE:CE2	2.36	0.59
1:A:136:ILE:HG13	1:A:225:TYR:CE1	2.37	0.59
1:A:261:LYS:HA	1:A:328:HIS:HD2	1.68	0.59
1:A:885:LEU:O	1:A:889:ARG:NH2	2.36	0.59
3:C:209:VAL:HB	3:C:898:LEU:HD21	1.84	0.59
3:C:683:ASN:OD1	3:C:797:ALA:N	2.35	0.59
6:F:33:G:N1	7:G:14:A:N6	2.45	0.59
17:R:137:GLU:OE1	17:R:137:GLU:N	2.35	0.59
18:T:307:SER:C	18:T:309:ASP:H	2.06	0.59
22:1:1103:VAL:O	22:1:1105:GLU:N	2.36	0.59
41:8:55:ARG:O	41:8:59:ILE:HG13	2.03	0.59
1:A:251:ASP:HB2	1:A:334:THR:OG1	2.03	0.59
1:A:339:PHE:HE1	1:A:406:TRP:HB2	1.68	0.59
3:C:591:ALA:HB2	3:C:940:ARG:HH21	1.66	0.59
6:F:23:U:H2’	6:F:24:A:O4’	2.01	0.59
7:G:94:C:H2’	7:G:95:U:H6	1.68	0.59
18:T:216:ASN:ND2	18:T:473:SER:H	2.00	0.59
23:3:538:THR:HG22	23:3:558:LEU:HD11	1.84	0.59
40:9:326:ARG:HG3	40:9:327:ASN:OD1	2.03	0.59
1:A:367:SER:OG	3:C:299:ILE:HG21	2.03	0.59
3:C:603:MET:HG3	3:C:653:ILE:HG12	1.83	0.59
5:E:65:HIS:CD2	5:E:83:SER:HG	2.18	0.59
14:O:64:ARG:N	14:O:160:ASN:O	2.27	0.59
18:T:460:ASP:OD1	18:T:461:SER:N	2.35	0.59
36:4:165:GLN:O	36:4:172:ILE:N	2.35	0.59
1:A:851:SER:OG	1:A:852:VAL:N	2.36	0.59
2:B:15:C:H2’	2:B:16:U:H6	1.68	0.59
7:G:104:C:H4’	7:G:105:C:OP2	2.02	0.59
22:1:619:ASN:ND2	22:1:624:VAL:HG21	2.17	0.59
23:3:459:VAL:HG23	23:3:476:VAL:HA	1.84	0.59
23:3:669:LEU:HD22	23:3:673:VAL:HG22	1.85	0.59
1:A:995:ARG:HG3	17:R:291:LEU:HD13	1.84	0.59
2:B:58:U:H2’	2:B:59:G:C8	2.37	0.59
5:E:329:SER:O	5:E:347:SER:N	2.29	0.59
23:3:374:SER:OG	23:3:375:SER:N	2.36	0.59
23:3:406:PRO:O	23:3:427:CYS:HB2	2.02	0.59
23:3:808:THR:HG22	23:3:884:GLN:OE1	2.02	0.59
1:A:308:ILE:HG22	1:A:313:LYS:HE3	1.84	0.59
7:G:101:U:C2	7:G:102:G:H8	2.20	0.59
10:J:301:ARG:O	10:J:305:THR:OG1	2.21	0.59
22:1:117:ASP:O	22:1:121:LYS:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1:118:GLU:HG2	22:1:121:LYS:HD2	1.85	0.59
22:1:484:GLU:HA	22:1:487:LEU:HD12	1.85	0.59
23:3:463:ARG:HD3	23:3:468:ASP:HB3	1.85	0.59
40:9:360:HIS:ND1	40:9:391:ASP:OD1	2.36	0.59
2:B:97:G:H2'	2:B:98:G:C8	2.38	0.58
8:H:126:A:H2'	8:H:127:G:H8	1.67	0.58
22:1:1137:ARG:HH21	35:2:524:LEU:HD12	1.68	0.58
23:3:3:LEU:HD12	23:3:1093:MET:SD	2.42	0.58
23:3:12:THR:O	23:3:12:THR:OG1	2.17	0.58
40:9:295:LEU:HD22	40:9:397:PHE:HB2	1.84	0.58
1:A:62:PRO:HG2	1:A:65:HIS:HB2	1.84	0.58
1:A:781:ARG:HG2	1:A:1022:MET:CE	2.33	0.58
1:A:1597:PHE:CE1	1:A:1725:LEU:HD21	2.38	0.58
3:C:143:THR:OG1	3:C:204:ASP:OD2	2.21	0.58
5:E:241:LEU:HB3	5:E:250:LEU:HD11	1.84	0.58
12:L:102:PHE:HD2	12:L:103:LEU:HD23	1.68	0.58
22:1:1197:LEU:HD11	38:7:78:GLN:HE21	1.67	0.58
22:1:1301:ASP:N	22:1:1301:ASP:OD1	2.35	0.58
1:A:155:LYS:NZ	1:A:622:GLY:O	2.33	0.58
1:A:776:LEU:O	1:A:780:THR:HG22	2.03	0.58
1:A:798:GLY:HA2	17:R:284:PHE:CE2	2.37	0.58
1:A:1310:ARG:HB2	1:A:1547:VAL:HG23	1.85	0.58
1:A:1553:VAL:CG1	7:G:2:U:O2'	2.50	0.58
3:C:328:ALA:O	3:C:332:GLY:HA2	2.03	0.58
3:C:584:THR:OG1	3:C:585:THR:N	2.36	0.58
16:Q:440:PRO:HG2	16:Q:1108:ALA:HB1	1.85	0.58
22:1:559:ILE:HG13	22:1:563:LEU:HD13	1.85	0.58
22:1:785:LYS:HG2	22:1:818:PHE:HE1	1.68	0.58
35:2:530:ARG:CB	35:2:578:TRP:CZ3	2.86	0.58
3:C:122:LEU:HD13	3:C:199:LEU:HB2	1.85	0.58
23:3:118:GLY:HA2	23:3:132:ILE:HD11	1.84	0.58
40:9:360:HIS:HB2	40:9:387:CYS:O	2.03	0.58
1:A:314:ILE:O	1:A:330:THR:HG21	2.03	0.58
1:A:794:TYR:HD1	1:A:800:TYR:HE2	1.50	0.58
1:A:1026:ASN:O	1:A:1026:ASN:ND2	2.35	0.58
1:A:2177:TRP:O	1:A:2213:ILE:HA	2.03	0.58
5:E:60:MET:HB2	5:E:353:MET:HB2	1.85	0.58
22:1:952:ALA:HA	22:1:955:ILE:HD12	1.85	0.58
23:3:712:VAL:HG23	23:3:713:LEU:O	2.03	0.58
41:8:44:ASN:OD1	41:8:45:LEU:N	2.36	0.58
1:A:1402:ARG:HB3	17:R:406:GLN:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1551:PHE:H	1:A:1551:PHE:HD2	1.49	0.58
2:B:65:G:H2'	2:B:66:A:H8	1.68	0.58
22:1:784:MET:O	22:1:788:VAL:HG13	2.04	0.58
23:3:454:GLY:O	23:3:456:PRO:HD3	2.04	0.58
41:8:31:ALA:HB3	41:8:34:LEU:HD13	1.85	0.58
1:A:645:THR:O	1:A:649:GLU:HG3	2.03	0.58
3:C:133:THR:HB	3:C:225:VAL:HG23	1.85	0.58
3:C:183:SER:H	3:C:214:GLU:HB3	1.68	0.58
3:C:755:ASP:HB2	3:C:759:LEU:HD23	1.85	0.58
7:G:8:C:H2'	7:G:9:C:C6	2.38	0.58
35:2:453:LYS:HE2	35:2:456:ARG:HB2	1.86	0.58
37:6:17:VAL:HG23	37:6:91:TYR:CE1	2.39	0.58
3:C:145:PHE:HA	3:C:312:SER:HB2	1.85	0.58
3:C:916:ILE:HD13	3:C:928:HIS:HB3	1.86	0.58
11:K:112:TRP:CD1	11:K:118:PHE:HA	2.38	0.58
22:1:1212:LEU:HB2	22:1:1237:LEU:HD13	1.85	0.58
41:8:52:ILE:O	41:8:56:VAL:HG22	2.04	0.58
5:E:157:CYS:HA	5:E:168:CYS:O	2.04	0.58
6:F:78:A:H5"	6:F:79:C:C5	2.37	0.58
7:G:-4:G:C2	7:G:-3:A:C5	2.91	0.58
22:1:586:ASP:OD1	22:1:589:ALA:N	2.28	0.58
1:A:547:CYS:SG	1:A:548:ARG:N	2.77	0.58
1:A:612:ILE:O	1:A:616:PHE:HB2	2.03	0.58
1:A:2237:TRP:O	1:A:2241:ASN:CB	2.52	0.58
5:E:312:TRP:CD1	5:E:319:ILE:HG13	2.39	0.58
10:J:343:GLU:HG3	10:J:369:PHE:HE1	1.68	0.58
11:K:106:HIS:ND1	11:K:108:ASN:HB2	2.19	0.58
22:1:1212:LEU:HB2	22:1:1237:LEU:CD1	2.34	0.58
23:3:1193:VAL:O	23:3:1196:GLU:N	2.37	0.58
7:G:86:A:H2'	7:G:87:U:C6	2.39	0.57
8:H:56:A:O2'	35:2:481:THR:CG2	2.49	0.57
11:K:33:LYS:CG	11:K:44:HIS:HE1	2.17	0.57
11:K:168:LYS:HA	11:K:171:LYS:HD2	1.86	0.57
17:R:407:TYR:HB2	17:R:412:PHE:CE1	2.39	0.57
19:X:222:GLU:HG2	20:Y:69:ARG:NH1	2.19	0.57
19:X:338:PHE:HB3	19:X:341:ASN:HA	1.85	0.57
22:1:885:ASP:OD1	22:1:887:LYS:N	2.36	0.57
22:1:1179:ASP:OD1	22:1:1184:HIS:HD2	1.86	0.57
23:3:197:THR:OG1	23:3:199:GLU:HG3	2.04	0.57
23:3:206:GLN:HE21	23:3:231:HIS:HA	1.67	0.57
23:3:747:SER:O	23:3:751:PRO:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:8:111:SER:OG	41:8:121:SER:N	2.33	0.57
1:A:1130:ASN:OD1	1:A:1130:ASN:N	2.37	0.57
1:A:1551:PHE:HD2	1:A:1551:PHE:N	2.02	0.57
3:C:237:LEU:HD13	3:C:898:LEU:HD13	1.86	0.57
6:F:36:A:C6	7:G:10:U:C2	2.91	0.57
11:K:262:ASP:CB	22:1:761:TYR:HE1	2.17	0.57
22:1:907:ASP:OD1	22:1:907:ASP:N	2.36	0.57
23:3:205:GLN:NE2	23:3:205:GLN:H	2.01	0.57
40:9:360:HIS:CE1	40:9:396:ILE:HD11	2.39	0.57
1:A:73:HIS:NE2	1:A:84:ASP:OD2	2.37	0.57
1:A:1553:VAL:HG12	1:A:1553:VAL:O	2.04	0.57
3:C:227:LEU:HD21	3:C:239:THR:HG23	1.86	0.57
3:C:556:ASP:O	3:C:612:LYS:NZ	2.29	0.57
5:E:75:HIS:HD1	5:E:77:ASN:H	1.52	0.57
10:J:439:ALA:O	10:J:443:ILE:HG12	2.03	0.57
11:K:262:ASP:CB	22:1:761:TYR:CE1	2.86	0.57
15:P:205:LYS:HD3	15:P:208:LYS:HE3	1.84	0.57
22:1:757:MET:HB3	22:1:762:ALA:HB2	1.85	0.57
23:3:267:ILE:HD12	23:3:322:VAL:HG22	1.86	0.57
40:9:233:VAL:HG22	40:9:265:ALA:HB2	1.86	0.57
1:A:684:GLU:CD	18:T:308:ARG:HH21	2.06	0.57
3:C:130:ARG:NH2	3:C:440:SER:HB3	2.19	0.57
3:C:606:GLY:HA2	3:C:609:LYS:HG3	1.86	0.57
3:C:770:PHE:HA	3:C:816:VAL:HG21	1.86	0.57
3:C:809:ILE:HB	3:C:810:PRO:HD3	1.85	0.57
3:C:836:VAL:HB	3:C:871:ILE:HB	1.86	0.57
9:I:231:ASN:O	9:I:233:ASP:N	2.35	0.57
18:T:442:ARG:HE	18:T:443:THR:HG22	1.70	0.57
22:1:718:PRO:O	22:1:719:TYR:CG	2.58	0.57
23:3:42:ARG:HH21	23:3:53:LEU:HD11	1.70	0.57
23:3:70:LEU:HD12	23:3:146:ARG:NH2	2.18	0.57
35:2:517:ILE:HD12	35:2:517:ILE:H	1.68	0.57
1:A:226:GLN:HE22	1:A:417:ARG:HH21	1.51	0.57
1:A:658:ARG:HH22	6:F:65:G:H3'	1.69	0.57
1:A:755:HIS:HE1	15:P:220:HIS:CE1	2.23	0.57
1:A:821:ARG:HG2	1:A:821:ARG:HH11	1.67	0.57
2:B:51:A:H2'	2:B:52:U:H6	1.68	0.57
3:C:150:ILE:HD13	3:C:167:TYR:CD2	2.40	0.57
3:C:192:ASP:HB2	3:C:432:ASP:OD1	2.04	0.57
3:C:208:HIS:CE1	3:C:635:LEU:HD23	2.39	0.57
3:C:237:LEU:HD21	3:C:835:GLU:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:X:313:TYR:N	19:X:321:GLY:O	2.24	0.57
22:1:1182:LEU:HD12	22:1:1182:LEU:N	2.03	0.57
1:A:405:LEU:HD21	3:C:385:VAL:HG12	1.87	0.57
1:A:762:ARG:HH12	15:P:226:LYS:HZ1	1.53	0.57
1:A:1651:VAL:HB	1:A:1653:ASP:OD1	2.03	0.57
6:F:44:G:N2	7:G:5:G:H1	2.02	0.57
6:F:66:C:H2'	6:F:67:G:C8	2.40	0.57
8:H:72:U:H2'	8:H:73:C:C6	2.40	0.57
11:K:168:LYS:HE3	23:3:1214:ARG:HH21	1.69	0.57
12:L:64:SER:OG	12:L:66:GLU:OE1	2.22	0.57
17:R:134:ARG:HG3	18:T:385:TYR:CD1	2.39	0.57
22:1:403:GLU:O	22:1:407:MET:HG2	2.04	0.57
22:1:762:ALA:O	22:1:766:THR:OG1	2.17	0.57
22:1:1291:ASP:OD1	22:1:1292:LYS:N	2.37	0.57
23:3:818:GLN:NE2	23:3:822:GLU:OE2	2.38	0.57
1:A:522:PHE:HB2	1:A:552:ARG:HG3	1.87	0.57
1:A:1330:MET:HG3	1:A:1330:MET:O	2.05	0.57
1:A:1545:ALA:CA	1:A:1563:HIS:CD2	2.87	0.57
2:B:15:C:H2'	2:B:16:U:C6	2.40	0.57
3:C:141:GLY:O	3:C:145:PHE:HB2	2.05	0.57
3:C:888:ARG:HG2	3:C:895:ALA:O	2.04	0.57
18:T:466:PHE:CE2	18:T:482:ALA:HB2	2.39	0.57
23:3:1189:LYS:HA	23:3:1192:ASN:ND2	2.18	0.57
38:7:51:TYR:CG	38:7:52:GLY:N	2.72	0.57
1:A:232:LEU:HD21	3:C:412:ILE:HD11	1.86	0.57
1:A:1199:LYS:HA	1:A:1203:SER:OG	2.05	0.57
1:A:1551:PHE:N	1:A:1551:PHE:CD2	2.72	0.57
2:B:36:C:N3	2:B:47:A:C6	2.73	0.57
8:H:46:U:O2	8:H:46:U:O2'	2.15	0.57
22:1:850:ILE:O	22:1:854:VAL:HG13	2.05	0.57
23:3:722:SER:HB2	23:3:731:LEU:HD12	1.87	0.57
40:9:365:ILE:O	40:9:382:ILE:HA	2.04	0.57
1:A:464:PRO:HD3	2:B:24:G:N7	2.20	0.57
1:A:488:ASP:OD2	1:A:565:ARG:NH1	2.35	0.57
1:A:599:MET:HA	1:A:602:ILE:HB	1.86	0.57
1:A:1554:GLN:OE1	1:A:1622:MET:HE3	2.03	0.57
6:F:40:U:H2'	6:F:41:A:C8	2.40	0.57
8:H:24:A:H5'	8:H:25:G:H5"	1.86	0.57
22:1:1258:ALA:HB3	22:1:1261:VAL:HG13	1.86	0.57
1:A:584:HIS:O	1:A:588:LEU:HG	2.05	0.57
1:A:770:THR:OG1	1:A:771:VAL:N	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:38:LEU:HD23	12:L:38:LEU:N	2.19	0.57
17:R:150:ALA:HA	17:R:153:LYS:HD2	1.86	0.57
17:R:256:ASN:OD1	17:R:256:ASN:N	2.37	0.57
22:1:160:HIS:CD2	22:1:163:LYS:HE2	2.40	0.57
22:1:1063:LEU:HD11	22:1:1096:THR:OG1	2.05	0.57
23:3:866:ILE:HD13	23:3:907:VAL:HG21	1.87	0.57
23:3:1058:LEU:HD23	23:3:1062:THR:HG21	1.87	0.57
41:8:55:ARG:NH1	41:8:58:GLU:OE2	2.37	0.57
1:A:83:HIS:O	1:A:87:VAL:HG23	2.04	0.56
1:A:405:LEU:O	3:C:413:ARG:NH1	2.35	0.56
1:A:2123:GLN:O	1:A:2152:GLY:HA3	2.05	0.56
3:C:477:HIS:CE1	3:C:577:PHE:HB2	2.40	0.56
3:C:692:LEU:HD11	3:C:744:ILE:HG13	1.86	0.56
11:K:148:THR:HG22	11:K:151:ARG:HH21	1.70	0.56
18:T:395:ILE:HD12	18:T:395:ILE:H	1.69	0.56
22:1:1120:ALA:HA	22:1:1128:VAL:HG11	1.86	0.56
22:1:1182:LEU:H	22:1:1182:LEU:CD1	1.99	0.56
23:3:870:ASN:ND2	23:3:873:GLN:H	2.02	0.56
1:A:592:TYR:HB3	1:A:598:LEU:HD22	1.88	0.56
1:A:1298:ARG:HB3	1:A:1298:ARG:HH21	1.68	0.56
3:C:347:ILE:HG13	3:C:357:THR:O	2.06	0.56
4:D:1658:ALA:O	4:D:1692:ASN:N	2.38	0.56
5:E:329:SER:OG	5:E:347:SER:OG	2.12	0.56
22:1:579:GLU:HB3	22:1:627:THR:OG1	2.05	0.56
1:A:1386:TRP:HE1	1:A:1417:PRO:HD2	1.70	0.56
1:A:1586:HIS:O	1:A:1590:VAL:HG23	2.04	0.56
3:C:159:LYS:HG2	3:C:161:TYR:H	1.70	0.56
3:C:734:ALA:HB3	3:C:767:VAL:HG21	1.87	0.56
3:C:859:GLN:HB3	3:C:872:LYS:HB2	1.86	0.56
8:H:106:G:N2	8:H:107:A:N1	2.41	0.56
10:J:235:ILE:O	10:J:239:ARG:HD3	2.05	0.56
18:T:308:ARG:HG2	18:T:308:ARG:HH11	1.69	0.56
22:1:522:LYS:HD3	22:1:525:GLU:CD	2.25	0.56
22:1:949:GLN:HB3	22:1:989:VAL:HA	1.86	0.56
23:3:174:ASP:CG	23:3:240:GLY:H	2.08	0.56
23:3:213:LEU:HD23	23:3:214:ASP:H	1.70	0.56
23:3:473:TYR:HE1	23:3:497:SER:HB2	1.70	0.56
40:9:274:GLN:O	40:9:277:LYS:HE2	2.04	0.56
1:A:106:MET:O	1:A:114:ARG:NH1	2.36	0.56
10:J:436:TYR:HD1	10:J:437:LYS:HD2	1.70	0.56
12:L:85:ILE:O	12:L:88:ILE:N	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:180:PRO:HD2	23:3:213:LEU:HB3	1.87	0.56
23:3:254:ASN:O	23:3:271:ILE:HG13	2.05	0.56
36:4:104:ILE:HA	36:4:173:THR:O	2.06	0.56
3:C:181:ILE:O	3:C:211:PHE:HB3	2.05	0.56
3:C:664:GLU:HB3	3:C:820:PHE:HZ	1.70	0.56
5:E:180:ASP:HB2	5:E:183:LYS:HD3	1.88	0.56
10:J:286:GLU:HG3	10:J:298:ILE:HD12	1.87	0.56
10:J:343:GLU:HG3	10:J:369:PHE:CE1	2.41	0.56
19:X:357:VAL:HA	19:X:367:TYR:O	2.04	0.56
22:1:698:GLN:HB3	22:1:701:VAL:HG12	1.87	0.56
23:3:446:GLU:OE1	23:3:763:ARG:HD3	2.05	0.56
40:9:363:ARG:NH2	40:9:407:LEU:HG	2.21	0.56
1:A:383:PHE:HB3	3:C:331:PHE:CD1	2.40	0.56
1:A:827:PHE:CB	1:A:1002:ASP:OD2	2.46	0.56
1:A:1056:HIS:O	1:A:1059:SER:OG	2.22	0.56
3:C:136:GLY:HA2	3:C:227:LEU:HD12	1.87	0.56
5:E:158:TYR:HD2	5:E:201:PHE:H	1.54	0.56
18:T:257:ARG:NH1	18:T:299:THR:O	2.37	0.56
22:1:936:VAL:HG12	22:1:937:LEU:HD12	1.88	0.56
22:1:944:SER:HB2	22:1:948:ARG:NE	2.21	0.56
1:A:1460:HIS:H	1:A:1460:HIS:CD2	2.22	0.56
3:C:78:GLU:OE2	18:T:198:ARG:NE	2.38	0.56
3:C:699:ASP:OD2	3:C:722:TYR:OH	2.22	0.56
21:Z:587:VAL:O	21:Z:589:ARG:NH1	2.38	0.56
22:1:1208:LEU:HB3	22:1:1241:ILE:HD11	1.86	0.56
1:A:516:LEU:HD11	1:A:538:SER:HB2	1.88	0.56
1:A:523:ASN:OD1	1:A:552:ARG:NH2	2.39	0.56
5:E:62:LEU:HD12	5:E:351:LEU:HB2	1.88	0.56
9:I:428:GLN:HA	9:I:469:TYR:H	1.70	0.56
12:L:65:ARG:NH2	12:L:68:GLU:OE1	2.39	0.56
17:R:138:GLU:HA	17:R:141:LYS:HD3	1.87	0.56
18:T:220:VAL:HG12	18:T:252:VAL:HG21	1.86	0.56
18:T:331:ASN:OD1	18:T:332:ALA:N	2.35	0.56
18:T:460:ASP:O	18:T:463:SER:OG	2.21	0.56
35:2:532:GLY:C	35:2:534:GLN:N	2.58	0.56
1:A:119:LEU:HD11	1:A:482:PHE:HB3	1.87	0.56
1:A:857:ASN:OD1	1:A:858:GLN:N	2.39	0.56
3:C:137:HIS:HB3	3:C:140:HIS:CE1	2.41	0.56
3:C:213:ASP:HB3	3:C:616:SER:HB3	1.87	0.56
6:F:63:C:H2'	6:F:64:U:H6	1.71	0.56
22:1:489:PRO:HB2	22:1:491:GLU:OE2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:542:LYS:NZ	23:3:562:GLU:OE1	2.34	0.56
1:A:150:MET:HG3	1:A:572:PHE:CE1	2.38	0.56
1:A:1199:LYS:HE2	1:A:1206:GLU:HB2	1.87	0.56
22:1:760:GLU:OE2	22:1:761:TYR:N	2.38	0.56
22:1:929:LEU:O	22:1:932:ILE:HB	2.05	0.56
22:1:1126:PHE:CE1	35:2:576:PHE:CE2	2.94	0.56
23:3:815:ARG:NH2	23:3:819:MET:SD	2.79	0.56
1:A:112:GLN:NE2	1:A:189:GLU:OE1	2.39	0.55
1:A:549:GLU:HG3	1:A:594:TYR:HE2	1.70	0.55
1:A:739:ILE:HG22	1:A:740:LEU:HD23	1.88	0.55
3:C:275:TYR:HB2	3:C:374:LEU:HD12	1.87	0.55
3:C:313:GLN:HB2	45:C:1500:GTP:C6	2.42	0.55
6:F:33:G:N2	7:G:13:C:N4	2.54	0.55
6:F:63:C:N4	6:F:72:G:O6	2.39	0.55
6:F:86:U:O2	8:H:12:G:C6	2.59	0.55
7:G:94:C:H2’	7:G:95:U:C6	2.41	0.55
10:J:242:ILE:HG22	10:J:245:TRP:CD1	2.41	0.55
11:K:119:THR:OG1	11:K:120:LYS:N	2.39	0.55
22:1:399:LEU:O	37:6:46:ARG:NH2	2.39	0.55
22:1:1257:PRO:CB	35:2:481:THR:OG1	2.54	0.55
23:3:554:VAL:CG1	23:3:556:ILE:HG23	2.36	0.55
40:9:294:GLU:O	40:9:398:GLY:HA3	2.04	0.55
1:A:362:ARG:NH1	3:C:284:GLU:OE1	2.39	0.55
1:A:557:VAL:HG22	1:A:581:ILE:HD13	1.87	0.55
1:A:854:SER:OG	1:A:855:ARG:N	2.39	0.55
2:B:65:G:H2’	2:B:66:A:C8	2.41	0.55
5:E:336:HIS:HD1	5:E:337:PRO:HD2	1.70	0.55
9:I:428:GLN:HA	9:I:469:TYR:N	2.21	0.55
10:J:332:VAL:HA	10:J:335:ARG:HD3	1.88	0.55
22:1:588:TYR:HA	22:1:591:VAL:HG12	1.87	0.55
22:1:883:ASP:OD2	22:1:883:ASP:N	2.39	0.55
23:3:383:ASP:OD1	23:3:384:THR:N	2.39	0.55
23:3:482:THR:OG1	23:3:501:GLY:O	2.24	0.55
40:9:302:LYS:HD3	40:9:350:PHE:HB2	1.88	0.55
1:A:1199:LYS:NZ	1:A:1206:GLU:OE2	2.38	0.55
2:B:98:G:H2’	2:B:99:C:H6	1.71	0.55
7:G:99:C:N4	8:H:32:U:C4	2.65	0.55
16:Q:54:ILE:O	16:Q:59:PHE:N	2.24	0.55
17:R:250:CYS:SG	17:R:252:SER:OG	2.64	0.55
18:T:358:ASP:OD2	18:T:361:ALA:N	2.39	0.55
22:1:907:ASP:HB2	22:1:909:VAL:HG12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:725:TYR:N	23:3:728:ARG:O	2.39	0.55
1:A:1074:PHE:CD2	1:A:1080:GLU:HB2	2.42	0.55
1:A:1301:ILE:O	1:A:1301:ILE:HG23	2.05	0.55
3:C:132:VAL:HA	3:C:224:GLY:O	2.06	0.55
5:E:236:ASP:HB2	5:E:256:ASP:HB2	1.89	0.55
10:J:351:ASN:CB	10:J:355:ARG:HH21	2.20	0.55
22:1:586:ASP:OD1	22:1:588:TYR:N	2.40	0.55
23:3:928:TYR:HD1	23:3:937:LEU:HB3	1.71	0.55
35:2:471:ARG:HH21	35:2:474:VAL:HG23	1.71	0.55
40:9:339:GLY:O	40:9:379:GLN:NE2	2.39	0.55
1:A:304:ILE:O	3:C:924:GLN:NE2	2.39	0.55
1:A:1473:ASP:OD1	1:A:1473:ASP:N	2.38	0.55
1:A:2161:GLY:N	1:A:2290:PRO:O	2.40	0.55
2:B:33:U:HO2'	18:T:279:LYS:HZ2	1.50	0.55
2:B:40:U:H3	7:G:0:G:H22	1.55	0.55
3:C:707:ILE:HD11	3:C:734:ALA:HA	1.88	0.55
10:J:294:HIS:HA	10:J:297:ASN:ND2	2.21	0.55
13:N:119:CYS:O	13:N:142:CYS:N	2.37	0.55
17:R:230:MET:O	18:T:370:ASN:HA	2.07	0.55
22:1:960:VAL:O	22:1:964:THR:OG1	2.23	0.55
22:1:1252:GLN:HE22	35:2:492:LYS:HA	1.70	0.55
23:3:271:ILE:HD13	23:3:287:PHE:HE2	1.71	0.55
37:6:21:LEU:HB2	37:6:62:VAL:HG23	1.89	0.55
38:7:22:LEU:O	38:7:66:VAL:HG22	2.06	0.55
1:A:378:PHE:HZ	3:C:335:ASN:HB3	1.71	0.55
1:A:429:ASN:ND2	1:A:432:ARG:HD3	2.21	0.55
1:A:1298:ARG:NH2	1:A:1298:ARG:CB	2.69	0.55
22:1:624:VAL:HA	22:1:627:THR:HG22	1.89	0.55
1:A:1307:MET:HA	1:A:1307:MET:HE2	1.88	0.55
1:A:1501:LEU:HD22	1:A:1503:TRP:HE1	1.71	0.55
2:B:61:A:H2'	2:B:62:G:O4'	2.06	0.55
3:C:174:GLU:OE1	3:C:174:GLU:N	2.40	0.55
3:C:183:SER:O	3:C:482:TYR:OH	2.19	0.55
3:C:842:CYS:HB3	3:C:891:THR:HG21	1.89	0.55
22:1:1262:ARG:HH12	35:2:483:GLN:HE21	1.55	0.55
1:A:641:MET:HA	1:A:644:ILE:HG12	1.86	0.55
1:A:1132:LYS:HA	1:A:1139:ARG:HE	1.72	0.55
1:A:1360:GLU:N	1:A:1363:GLN:OE1	2.39	0.55
7:G:6:A:C8	7:G:7:G:N7	2.74	0.55
8:H:19:G:O2'	8:H:20:G:O4'	2.23	0.55
8:H:47:U:O2	8:H:47:U:H2'	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:275:ASN:HB3	10:J:278:LEU:HB2	1.89	0.55
10:J:431:ARG:HA	10:J:434:VAL:HG12	1.89	0.55
11:K:36:ARG:HB3	11:K:37:ASP:OD1	2.06	0.55
12:L:30:GLN:HE22	17:R:256:ASN:ND2	2.05	0.55
23:3:287:PHE:HD1	23:3:303:ALA:HB1	1.69	0.55
40:9:220:ILE:O	40:9:224:THR:OG1	2.19	0.55
40:9:363:ARG:HH21	40:9:407:LEU:HG	1.71	0.55
1:A:1371:TYR:N	1:A:1371:TYR:CD1	2.75	0.55
3:C:724:TRP:CZ2	3:C:732:ILE:HD11	2.42	0.55
4:D:1671:GLY:HA3	4:D:1860:ILE:O	2.07	0.55
5:E:161:ARG:NH2	5:E:245:SER:HA	2.22	0.55
8:H:82:G:H2'	8:H:83:A:C8	2.41	0.55
11:K:115:LEU:O	11:K:119:THR:HG23	2.07	0.55
23:3:82:SER:OG	23:3:83:ASP:N	2.38	0.55
23:3:374:SER:OG	23:3:376:ALA:N	2.30	0.55
23:3:736:TYR:OH	23:3:763:ARG:HD2	2.06	0.55
23:3:1009:PHE:HZ	23:3:1046:GLY:HA3	1.71	0.55
23:3:1028:THR:HG22	23:3:1028:THR:O	2.06	0.55
40:9:269:ASP:HA	40:9:272:ARG:HE	1.71	0.55
1:A:179:ALA:HA	1:A:183:LEU:HD22	1.88	0.55
1:A:1310:ARG:CZ	1:A:1310:ARG:CB	2.85	0.55
3:C:481:MET:SD	3:C:612:LYS:HG2	2.46	0.55
9:I:255:LEU:O	9:I:259:TRP:CB	2.54	0.55
17:R:137:GLU:HA	17:R:140:ILE:HD13	1.89	0.55
17:R:239:VAL:O	17:R:243:GLN:HG3	2.07	0.55
19:X:371:HIS:H	19:X:374:SER:HG	1.53	0.55
22:1:1295:TYR:CE2	39:5:28:LYS:HE2	2.42	0.55
23:3:362:ALA:O	23:3:363:HIS:ND1	2.40	0.55
35:2:576:PHE:CD2	35:2:576:PHE:N	2.75	0.55
40:9:352:ASP:HA	40:9:376:ASN:HD21	1.72	0.55
1:A:1264:ASN:O	1:A:1268:ILE:HG12	2.07	0.54
11:K:39:ASN:O	11:K:41:PHE:N	2.40	0.54
12:L:63:TRP:HB3	12:L:68:GLU:HG3	1.89	0.54
40:9:361:THR:HG23	40:9:386:SER:HB2	1.89	0.54
1:A:118:VAL:O	1:A:484:SER:HA	2.07	0.54
1:A:143:GLN:O	1:A:147:MET:HG2	2.07	0.54
1:A:755:HIS:CE1	15:P:220:HIS:ND1	2.75	0.54
1:A:1310:ARG:HH21	1:A:1310:ARG:CG	2.18	0.54
3:C:320:LEU:HD23	3:C:343:LEU:HB3	1.89	0.54
6:F:41:A:H2'	6:F:42:C:H6	1.72	0.54
10:J:306:LEU:HD13	10:J:312:PHE:HE2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:26:TRP:HB2	11:K:35:CYS:O	2.07	0.54
17:R:132:LEU:O	18:T:385:TYR:HB3	2.07	0.54
18:T:337:ARG:HG3	18:T:378:VAL:HG23	1.88	0.54
20:Y:9:LEU:HD12	22:1:782:GLU:HG3	1.89	0.54
22:1:967:GLU:O	22:1:971:MET:N	2.34	0.54
23:3:791:HIS:C	23:3:791:HIS:CD2	2.80	0.54
23:3:894:CYS:HB3	23:3:954:PRO:HB3	1.89	0.54
1:A:91:ALA:HB2	1:A:125:ALA:HB1	1.89	0.54
1:A:119:LEU:HB2	1:A:130:ASN:HD22	1.72	0.54
1:A:814:VAL:HG23	1:A:999:LEU:HD13	1.89	0.54
1:A:1418:ARG:O	1:A:1420:ASN:N	2.40	0.54
1:A:1657:THR:HG22	1:A:1658:GLN:H	1.71	0.54
11:K:151:ARG:NH2	11:K:152:GLN:HG2	2.22	0.54
1:A:406:TRP:CH2	3:C:265:LEU:HB2	2.43	0.54
1:A:1558:THR:HB	1:A:1582:TRP:CE3	2.43	0.54
2:B:41:U:H2'	2:B:42:U:C6	2.43	0.54
3:C:142:LYS:O	3:C:146:VAL:HG23	2.07	0.54
3:C:441:PRO:CB	3:C:495:ARG:HH22	2.18	0.54
3:C:490:PHE:CD2	3:C:612:LYS:HD2	2.43	0.54
3:C:788:LYS:HD3	3:C:790:LYS:HG3	1.89	0.54
16:Q:1027:LEU:O	16:Q:1032:ALA:N	2.38	0.54
22:1:412:TYR:HB3	37:6:49:ARG:HB3	1.89	0.54
22:1:420:GLY:O	22:1:424:ILE:N	2.33	0.54
23:3:1081:LEU:HD22	23:3:1081:LEU:C	2.28	0.54
37:6:17:VAL:HG21	37:6:71:LYS:HB2	1.90	0.54
1:A:71:ARG:HD3	13:N:34:THR:HA	1.89	0.54
1:A:414:ARG:HG3	3:C:411:ASN:HA	1.90	0.54
1:A:1256:PHE:HB3	1:A:1299:ILE:HG21	1.90	0.54
3:C:700:ILE:O	3:C:740:THR:OG1	2.25	0.54
3:C:769:GLY:HA3	3:C:812:ALA:HB3	1.89	0.54
5:E:65:HIS:CD2	5:E:351:LEU:HD11	2.42	0.54
38:7:30:CYS:SG	38:7:33:CYS:N	2.81	0.54
1:A:1308:PRO:HG3	1:A:1548:TYR:HE2	1.69	0.54
1:A:1371:TYR:N	1:A:1371:TYR:HD1	2.05	0.54
1:A:1758:PRO:HA	22:1:938:TRP:CD1	2.42	0.54
3:C:317:CYS:SG	3:C:430:PHE:HB2	2.48	0.54
5:E:218:LYS:HD3	5:E:220:TRP:CZ2	2.42	0.54
18:T:209:CYS:SG	18:T:252:VAL:HG22	2.48	0.54
23:3:791:HIS:HD2	23:3:793:GLU:H	1.56	0.54
1:A:1382:SER:OG	1:A:1416:ILE:N	2.34	0.54
2:B:55:C:H2'	2:B:56:C:H6	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:38:G:C2	6:F:39:A:C5	2.96	0.54
8:H:172:C:H2'	8:H:173:C:C6	2.42	0.54
10:J:224:LYS:HE2	10:J:255:LEU:HD13	1.90	0.54
10:J:367:GLU:OE2	10:J:401:ARG:NH2	2.41	0.54
23:3:318:ASP:O	23:3:320:ASP:N	2.41	0.54
23:3:464:ARG:NH1	23:3:473:TYR:OH	2.40	0.54
23:3:670:GLN:HA	23:3:698:PRO:HA	1.89	0.54
23:3:851:ILE:HG23	23:3:852:PHE:CD2	2.43	0.54
35:2:586:ILE:CD1	35:2:586:ILE:H	2.20	0.54
40:9:325:ILE:HB	40:9:328:PHE:HB3	1.89	0.54
41:8:38:VAL:HG11	41:8:109:LEU:HD13	1.90	0.54
1:A:675:GLN:NE2	1:A:676:ARG:HG3	2.22	0.54
1:A:706:ALA:O	1:A:709:ILE:N	2.41	0.54
5:E:178:LEU:HB2	5:E:188:GLN:HG2	1.90	0.54
6:F:15:A:H2'	6:F:16:G:H8	1.72	0.54
8:H:27:U:H2'	8:H:28:C:C6	2.43	0.54
10:J:226:ARG:O	10:J:230:THR:HG23	2.07	0.54
22:1:862:GLU:OE1	22:1:904:THR:OG1	2.24	0.54
1:A:154:GLU:HG2	1:A:572:PHE:CG	2.43	0.54
1:A:508:ILE:HG13	1:A:513:LEU:HD12	1.89	0.54
1:A:698:PRO:O	1:A:699:GLU:HB2	2.08	0.54
1:A:1056:HIS:NE2	1:A:1060:GLU:OE2	2.41	0.54
22:1:816:LYS:HE3	22:1:817:HIS:CE1	2.43	0.54
40:9:380:PHE:HZ	40:9:428:ILE:HD11	1.72	0.54
1:A:171:ASP:OD1	1:A:521:ASN:ND2	2.40	0.54
1:A:769:LYS:HE2	1:A:773:LYS:HE3	1.89	0.54
1:A:1285:LEU:O	1:A:1289:VAL:HG23	2.07	0.54
3:C:109:LEU:HD21	3:C:539:ILE:HG13	1.89	0.54
5:E:112:VAL:HA	5:E:128:SER:OG	2.08	0.54
9:I:406:GLU:HA	9:I:410:GLN:HA	1.88	0.54
22:1:458:ASP:N	22:1:458:ASP:OD1	2.41	0.54
22:1:973:HIS:O	22:1:977:VAL:HG23	2.08	0.54
22:1:1167:TYR:CE1	35:2:581:LYS:HB2	2.43	0.54
40:9:361:THR:HA	40:9:386:SER:HA	1.89	0.54
1:A:89:LEU:HD13	1:A:660:PHE:HZ	1.73	0.53
1:A:494:LEU:HD21	1:A:562:VAL:HG21	1.90	0.53
1:A:1737:ASN:OD1	1:A:1740:LEU:HG	2.08	0.53
3:C:140:HIS:ND1	3:C:229:ILE:HA	2.23	0.53
3:C:673:LYS:HB3	3:C:686:THR:HG23	1.91	0.53
6:F:45:A:H4'	6:F:46:G:OP2	2.03	0.53
18:T:369:THR:O	18:T:369:THR:OG1	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:6:LEU:HD12	23:3:1128:ILE:HD11	1.90	0.53
40:9:292:ASN:HB2	40:9:402:GLY:N	2.23	0.53
1:A:203:VAL:HG22	1:A:207:PHE:HB2	1.90	0.53
1:A:561:HIS:CE1	1:A:574:LEU:HD21	2.43	0.53
1:A:738:MET:HE3	1:A:739:ILE:N	2.23	0.53
2:B:8:G:H1	2:B:69:A:H61	0.60	0.53
3:C:123:MET:SD	3:C:545:PRO:HD2	2.48	0.53
3:C:605:ASP:OD1	3:C:608:ARG:NH2	2.41	0.53
3:C:829:GLU:OE2	3:C:876:PRO:HB3	2.08	0.53
5:E:93:TRP:CD2	5:E:101:ASN:HB2	2.43	0.53
7:G:7:G:H2’	7:G:8:C:O4’	2.07	0.53
10:J:224:LYS:HD3	10:J:228:ARG:NH2	2.23	0.53
18:T:371:HIS:NE2	18:T:389:SER:OG	2.41	0.53
22:1:979:TYR:HA	22:1:982:LEU:HD22	1.88	0.53
35:2:530:ARG:HD3	35:2:530:ARG:C	2.24	0.53
1:A:391:THR:HG21	3:C:395:THR:HG23	1.90	0.53
1:A:1019:TYR:O	1:A:1021:ASP:N	2.42	0.53
1:A:1820:LYS:HA	1:A:1914:MET:HA	1.91	0.53
5:E:156:SER:O	5:E:169:THR:HA	2.07	0.53
10:J:357:LYS:HE3	10:J:359:VAL:HG22	1.90	0.53
11:K:82:ARG:HE	22:1:1051:SER:HA	1.73	0.53
40:9:352:ASP:N	40:9:374:ASN:OD1	2.36	0.53
1:A:280:GLU:HB2	2:B:48:A:O5’	2.08	0.53
1:A:1248:LEU:HD22	1:A:1298:ARG:HG3	1.90	0.53
1:A:1638:ASN:HB3	1:A:1656:THR:HG22	1.90	0.53
4:D:1225:VAL:O	4:D:1234:LEU:N	2.37	0.53
5:E:167:VAL:HB	5:E:179:TRP:HB2	1.89	0.53
18:T:394:ASN:HB2	18:T:409:LEU:O	2.08	0.53
23:3:603:ARG:HG2	23:3:604:PHE:CE2	2.43	0.53
23:3:1003:SER:O	23:3:1003:SER:OG	2.27	0.53
1:A:1382:SER:HA	1:A:1415:GLY:HA2	1.90	0.53
1:A:1428:HIS:NE2	22:1:94:ILE:HG21	2.24	0.53
2:B:38:C:H5’	2:B:39:C:H6	1.71	0.53
2:B:44:A:C2	2:B:45:C:H1’	2.43	0.53
10:J:376:VAL:O	10:J:380:ILE:HG13	2.09	0.53
11:K:83:ARG:HB2	11:K:84:PHE:CE2	2.43	0.53
22:1:563:LEU:H	22:1:563:LEU:HD12	1.74	0.53
23:3:139:LYS:O	23:3:140:LEU:HD23	2.07	0.53
23:3:613:THR:OG1	23:3:615:ARG:NH1	2.28	0.53
35:2:488:LEU:O	35:2:488:LEU:HD23	2.09	0.53
36:4:14:THR:HA	36:4:60:GLU:HA	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:THR:OG1	3:C:398:GLU:OE2	2.27	0.53
1:A:462:ARG:NH2	1:A:465:LYS:HG2	2.23	0.53
1:A:781:ARG:HG2	1:A:1022:MET:HE3	1.88	0.53
2:B:51:A:O2'	2:B:52:U:H5'	2.09	0.53
3:C:142:LYS:HA	3:C:228:PHE:CD2	2.43	0.53
3:C:335:ASN:HD22	3:C:338:GLU:HG2	1.73	0.53
3:C:506:PRO:HA	3:C:526:THR:HA	1.90	0.53
6:F:91:A:H2'	6:F:92:A:C8	2.44	0.53
18:T:261:LEU:HB3	18:T:275:LEU:HD21	1.91	0.53
22:1:1257:PRO:HG3	35:2:482:ALA:HB2	1.91	0.53
1:A:67:ARG:CZ	1:A:67:ARG:HB2	2.38	0.53
2:B:14:U:H2'	2:B:15:C:H6	1.74	0.53
3:C:306:ASN:HB3	3:C:437:HIS:CD2	2.43	0.53
3:C:856:HIS:CE1	3:C:874:PHE:HB2	2.43	0.53
8:H:121:A:C2	8:H:122:U:H5'	2.43	0.53
11:K:7:LEU:HG	11:K:8:THR:H	1.72	0.53
22:1:483:ASP:O	22:1:486:THR:OG1	2.25	0.53
35:2:535:GLU:HA	35:2:535:GLU:OE2	2.09	0.53
1:A:823:SER:O	1:A:823:SER:OG	2.25	0.53
3:C:220:ARG:HH22	3:C:580:LEU:HA	1.73	0.53
6:F:58:G:H3'	6:F:58:G:OP2	2.09	0.53
11:K:68:PHE:CD2	11:K:109:ALA:HB1	2.44	0.53
11:K:88:ARG:HD2	11:K:138:TYR:HB3	1.91	0.53
19:X:262:TYR:CZ	19:X:370:LEU:HD12	2.44	0.53
19:X:337:THR:O	19:X:343:ARG:HA	2.07	0.53
19:X:372:GLU:HG2	19:X:373:SER:N	2.24	0.53
23:3:180:PRO:HD3	23:3:215:LEU:HD11	1.91	0.53
23:3:200:ALA:O	23:3:204:THR:OG1	2.18	0.53
23:3:606:ALA:HA	23:3:616:ILE:HD12	1.91	0.53
37:6:112:LEU:O	37:6:116:LYS:HB2	2.08	0.53
1:A:1072:LEU:HD22	1:A:1087:LEU:HD22	1.90	0.53
1:A:1293:ASN:HB2	1:A:1357:MET:CE	2.39	0.53
2:B:18:C:H2'	2:B:19:A:C8	2.44	0.53
3:C:64:LYS:CE	15:P:206:LYS:HB3	2.39	0.53
3:C:183:SER:HA	3:C:205:THR:HA	1.91	0.53
3:C:680:ASN:O	3:C:682:LYS:N	2.42	0.53
17:R:148:ARG:NH2	17:R:148:ARG:CB	2.72	0.53
21:Z:574:ASN:N	21:Z:574:ASN:OD1	2.41	0.53
22:1:476:ASP:HB2	37:6:24:ARG:NH2	2.23	0.53
22:1:1252:GLN:HE21	35:2:492:LYS:HA	1.71	0.53
23:3:192:ALA:HA	23:3:200:ALA:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:207:THR:O	23:3:207:THR:OG1	2.24	0.53
40:9:420:ASP:N	40:9:420:ASP:OD1	2.41	0.53
41:8:63:GLU:OE1	41:8:63:GLU:N	2.31	0.53
1:A:339:PHE:CE1	1:A:406:TRP:HB2	2.44	0.53
1:A:385:GLU:HG2	1:A:386:PRO:HD2	1.89	0.53
1:A:1758:PRO:HA	22:1:938:TRP:NE1	2.24	0.53
23:3:246:SER:OG	23:3:247:GLY:N	2.41	0.53
37:6:22:TYR:OH	37:6:24:ARG:HD3	2.09	0.53
39:5:63:ARG:HD2	39:5:67:ASN:HD21	1.73	0.53
40:9:58:GLY:O	40:9:158:LEU:HA	2.09	0.53
1:A:1203:SER:OG	1:A:1203:SER:O	2.24	0.52
1:A:1298:ARG:HH21	1:A:1298:ARG:CB	2.21	0.52
1:A:1597:PHE:CZ	1:A:1725:LEU:HD21	2.44	0.52
1:A:1723:LYS:HB3	1:A:1724:PRO:HD3	1.91	0.52
3:C:674:CYS:HB3	3:C:818:SER:OG	2.09	0.52
3:C:813:ARG:HH21	3:C:952:PHE:HE1	1.56	0.52
6:F:58:G:H1	6:F:76:A:H61	1.57	0.52
10:J:261:ALA:HA	10:J:264:ILE:HD12	1.91	0.52
10:J:318:TYR:O	10:J:322:MET:HG3	2.09	0.52
11:K:41:PHE:HA	11:K:44:HIS:HD2	1.73	0.52
19:X:246:TYR:OH	19:X:307:GLN:OE1	2.27	0.52
22:1:1178:MET:CE	35:2:591:TYR:CZ	2.91	0.52
35:2:453:LYS:O	35:2:453:LYS:HD3	2.08	0.52
35:2:581:LYS:NZ	35:2:581:LYS:CB	2.73	0.52
1:A:119:LEU:HD21	1:A:476:PHE:HB3	1.91	0.52
1:A:266:SER:HB2	1:A:314:ILE:HD11	1.90	0.52
1:A:963:GLN:NE2	1:A:964:ASP:OD1	2.38	0.52
3:C:187:THR:OG1	3:C:533:SER:O	2.22	0.52
3:C:788:LYS:HZ3	3:C:790:LYS:HE3	1.74	0.52
6:F:38:G:C6	7:G:9:C:N3	2.76	0.52
7:G:89:U:H4'	7:G:90:C:OP2	2.08	0.52
11:K:28:CYS:HA	11:K:41:PHE:HE2	1.73	0.52
18:T:223:SER:OG	18:T:224:ALA:N	2.39	0.52
19:X:222:GLU:O	20:Y:69:ARG:NH1	2.43	0.52
35:2:578:TRP:N	35:2:578:TRP:CD1	2.76	0.52
38:7:21:ARG:NH2	38:7:68:ASP:OD1	2.42	0.52
1:A:156:ARG:HG3	1:A:620:PRO:HB2	1.91	0.52
1:A:1256:PHE:H	1:A:1531:ASN:HD21	1.56	0.52
2:B:52:U:H2'	2:B:53:U:C6	2.43	0.52
2:B:97:G:N2	2:B:117:A:H62	2.07	0.52
3:C:220:ARG:NH1	3:C:578:ARG:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:15:U:H3'	7:G:16:G:C8	2.45	0.52
18:T:250:ARG:NH2	18:T:266:GLU:OE2	2.43	0.52
22:1:170:GLN:HG2	22:1:171:GLN:NE2	2.25	0.52
23:3:530:ASP:O	23:3:532:ARG:N	2.42	0.52
40:9:284:LEU:O	40:9:290:ASP:HA	2.10	0.52
1:A:819:SER:O	1:A:819:SER:OG	2.20	0.52
1:A:1002:ASP:OD1	1:A:1004:ASN:N	2.38	0.52
3:C:898:LEU:HD23	3:C:899:SER:N	2.23	0.52
5:E:92:LEU:HB3	5:E:102:TYR:CZ	2.44	0.52
6:F:40:U:C2	6:F:41:A:N7	2.77	0.52
18:T:387:PHE:O	18:T:398:TRP:HD1	1.92	0.52
22:1:166:ARG:HH22	22:1:620:MET:HG2	1.75	0.52
22:1:823:MET:SD	22:1:829:ASN:ND2	2.82	0.52
39:5:46:HIS:O	39:5:48:ASP:N	2.41	0.52
40:9:322:HIS:CE1	40:9:334:ASP:HB2	2.44	0.52
41:8:34:LEU:HA	41:8:106:TRP:CD1	2.45	0.52
1:A:88:TYR:HB3	1:A:503:MET:SD	2.50	0.52
1:A:977:LEU:HG	1:A:978:GLU:N	2.23	0.52
1:A:1233:ASP:OD1	1:A:1234:ASP:N	2.40	0.52
1:A:1630:LEU:HD21	1:A:1696:PRO:HG3	1.91	0.52
3:C:82:GLN:HE21	3:C:82:GLN:HA	1.74	0.52
3:C:772:TRP:CZ2	40:9:130:ALA:HA	2.44	0.52
3:C:829:GLU:HG2	3:C:907:VAL:HG22	1.91	0.52
5:E:74:PHE:HE1	5:E:95:VAL:HG21	1.74	0.52
6:F:50:A:H4'	6:F:51:U:OP1	2.09	0.52
8:H:129:U:H2'	8:H:130:U:H5'	1.92	0.52
8:H:155:C:H2'	8:H:156:U:C6	2.45	0.52
10:J:228:ARG:HG2	10:J:248:TYR:OH	2.10	0.52
11:K:80:LEU:HD12	11:K:84:PHE:CD2	2.45	0.52
12:L:11:TRP:HB2	12:L:49:ARG:HH21	1.74	0.52
17:R:416:LYS:HD3	21:Z:607:VAL:HG22	1.92	0.52
39:5:48:ASP:O	39:5:51:ASN:N	2.42	0.52
40:9:329:VAL:HG12	40:9:383:THR:HA	1.91	0.52
1:A:678:GLU:OE1	1:A:678:GLU:N	2.42	0.52
1:A:969:SER:OG	1:A:970:GLU:N	2.39	0.52
3:C:914:LYS:HD3	3:C:931:ARG:HH22	1.75	0.52
5:E:220:TRP:CD2	5:E:227:LEU:HD13	2.44	0.52
10:J:245:TRP:HH2	10:J:267:ARG:HE	1.58	0.52
10:J:368:ARG:O	10:J:372:VAL:HG23	2.10	0.52
11:K:86:THR:HG22	11:K:141:TYR:O	2.10	0.52
22:1:900:PHE:HE2	22:1:954:LEU:HD22	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:21:ASN:OD1	23:3:69:ARG:NH2	2.43	0.52
23:3:465:HIS:O	23:3:468:ASP:HB2	2.10	0.52
35:2:586:ILE:HD13	35:2:586:ILE:C	2.29	0.52
40:9:360:HIS:CE1	40:9:391:ASP:HA	2.45	0.52
1:A:102:LEU:HD22	1:A:496:VAL:HG21	1.90	0.52
1:A:306:GLN:HG3	3:C:879:ASP:HB3	1.91	0.52
5:E:249:TYR:CE2	5:E:263:ASP:HB3	2.45	0.52
18:T:385:TYR:CZ	18:T:400:PHE:HB3	2.44	0.52
23:3:552:ARG:HD3	23:3:600:GLN:HB3	1.91	0.52
40:9:305:GLU:HG2	40:9:309:ARG:HD3	1.90	0.52
40:9:343:GLU:H	40:9:378:SER:HB3	1.75	0.52
1:A:634:TRP:O	1:A:638:LEU:HG	2.10	0.52
1:A:962:LEU:HB2	1:A:965:VAL:HB	1.90	0.52
2:B:51:A:H2’	2:B:52:U:C6	2.44	0.52
3:C:225:VAL:O	3:C:254:THR:OG1	2.24	0.52
5:E:73:LYS:HG3	5:E:115:LEU:O	2.09	0.52
17:R:134:ARG:NH2	18:T:382:PRO:O	2.43	0.52
22:1:123:ARG:HG3	22:1:124:ARG:HG3	1.90	0.52
22:1:609:MET:O	22:1:613:MET:HG2	2.10	0.52
22:1:1098:LEU:C	22:1:1100:ASN:H	2.14	0.52
22:1:1154:LEU:O	22:1:1158:ILE:HG23	2.10	0.52
23:3:23:SER:OG	23:3:29:GLU:OE2	2.19	0.52
35:2:586:ILE:CD1	35:2:586:ILE:N	2.72	0.52
41:8:46:GLU:CD	41:8:46:GLU:H	2.13	0.52
2:B:36:C:N4	2:B:47:A:H61	2.08	0.52
2:B:47:A:OP2	2:B:47:A:H2’	2.10	0.52
3:C:286:ASN:HB3	3:C:299:ILE:CG2	2.40	0.52
3:C:602:LYS:HB3	3:C:651:ILE:HD11	1.92	0.52
4:D:1211:ASP:O	4:D:1215:HIS:N	2.41	0.52
5:E:133:VAL:HG21	5:E:169:THR:HG21	1.92	0.52
6:F:46:G:H5’	6:F:47:A:C4’	2.40	0.52
22:1:124:ARG:C	22:1:126:MET:H	2.12	0.52
22:1:614:ARG:HG3	22:1:647:PHE:CZ	2.42	0.52
23:3:172:GLY:O	23:3:237:THR:OG1	2.28	0.52
23:3:616:ILE:HG22	23:3:628:LEU:HB2	1.91	0.52
23:3:673:VAL:HA	23:3:690:ARG:HA	1.91	0.52
1:A:1642:PRO:HA	1:A:1716:GLY:O	2.10	0.52
1:A:1708:ALA:C	1:A:1709:TYR:HD2	2.13	0.52
3:C:719:GLN:HA	3:C:724:TRP:H	1.75	0.52
3:C:724:TRP:HE1	3:C:728:ALA:HB3	1.74	0.52
4:D:1558:PRO:HA	4:D:1642:GLN:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1583:ASP:O	4:D:1585:GLN:N	2.43	0.52
5:E:294:SER:CB	5:E:299:LYS:H	2.23	0.52
10:J:300:ASP:O	10:J:304:THR:OG1	2.19	0.52
11:K:33:LYS:HB3	11:K:44:HIS:CE1	2.45	0.52
17:R:126:ASN:HB2	18:T:442:ARG:HD3	1.91	0.52
23:3:715:MET:HG2	23:3:739:LEU:HB2	1.92	0.52
35:2:533:ILE:CD1	35:2:533:ILE:N	2.73	0.52
35:2:586:ILE:HD13	35:2:586:ILE:N	2.24	0.52
1:A:1298:ARG:HB3	1:A:1298:ARG:CZ	2.41	0.51
1:A:1537:TRP:HD1	1:A:1538:TRP:CD1	2.27	0.51
3:C:70:GLU:H	3:C:70:GLU:CD	2.13	0.51
3:C:157:ILE:HD11	3:C:165:LEU:HD11	1.93	0.51
3:C:235:VAL:HG11	3:C:288:LEU:HD11	1.92	0.51
3:C:300:LEU:HA	3:C:306:ASN:ND2	2.24	0.51
3:C:789:PHE:CE2	3:C:816:VAL:HG13	2.45	0.51
3:C:937:THR:O	3:C:941:LYS:HG3	2.10	0.51
10:J:335:ARG:HA	10:J:338:GLU:OE1	2.09	0.51
16:Q:818:LEU:HA	16:Q:1091:TRP:O	2.10	0.51
22:1:1009:MET:HE3	22:1:1011:PRO:HD2	1.92	0.51
22:1:1195:MET:O	22:1:1199:VAL:HG23	2.09	0.51
23:3:147:ASP:OD1	23:3:151:ARG:N	2.41	0.51
23:3:727:SER:O	23:3:728:ARG:HG3	2.10	0.51
1:A:429:ASN:HA	1:A:432:ARG:HB2	1.91	0.51
1:A:647:LEU:HD11	1:A:651:TRP:CE2	2.45	0.51
1:A:1482:GLU:HG3	1:A:1483:GLY:H	1.74	0.51
1:A:1635:TYR:O	1:A:1658:GLN:NE2	2.34	0.51
2:B:12:U:H3	2:B:65:G:H1	1.56	0.51
5:E:343:ILE:HD11	5:E:353:MET:HE3	1.92	0.51
6:F:87:C:C2	8:H:12:G:C6	2.98	0.51
15:P:212:ASN:HD21	18:T:484:LYS:HE3	1.74	0.51
18:T:209:CYS:SG	18:T:252:VAL:N	2.83	0.51
23:3:791:HIS:NE2	23:3:793:GLU:HB2	2.25	0.51
23:3:883:GLU:HG2	23:3:884:GLN:H	1.75	0.51
1:A:102:LEU:HD22	1:A:496:VAL:HG11	1.91	0.51
1:A:545:HIS:HB3	1:A:594:TYR:CZ	2.45	0.51
1:A:1457:HIS:ND1	1:A:1460:HIS:HD2	2.09	0.51
3:C:226:VAL:HG11	3:C:430:PHE:CE1	2.45	0.51
3:C:281:ILE:O	3:C:285:VAL:HG23	2.10	0.51
4:D:1397:PHE:O	4:D:1402:ASN:N	2.44	0.51
6:F:43:A:H2'	6:F:44:G:C8	2.45	0.51
12:L:50:TRP:CE2	12:L:55:ASP:HB2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:X:245:LYS:HB2	19:X:331:LEU:HD13	1.91	0.51
19:X:260:ARG:HH22	19:X:372:GLU:HA	1.75	0.51
23:3:618:SER:H	23:3:628:LEU:HD13	1.75	0.51
35:2:533:ILE:N	35:2:533:ILE:HD13	2.25	0.51
1:A:332:TYR:HA	3:C:177:ARG:O	2.11	0.51
1:A:863:GLU:O	1:A:867:ILE:HG12	2.11	0.51
3:C:439:PRO:CB	3:C:443:VAL:HG13	2.39	0.51
5:E:140:THR:HG23	5:E:142:GLU:H	1.74	0.51
11:K:106:HIS:CE1	11:K:108:ASN:HB2	2.46	0.51
14:O:258:ILE:HA	14:O:274:PHE:HA	1.92	0.51
22:1:159:GLN:O	22:1:162:THR:OG1	2.24	0.51
22:1:1098:LEU:HD13	22:1:1135:GLU:HG2	1.92	0.51
23:3:520:TYR:HB2	23:3:521:PRO:HD2	1.92	0.51
23:3:864:SER:O	23:3:865:VAL:HG23	2.10	0.51
23:3:1052:ASN:OD1	23:3:1052:ASN:N	2.41	0.51
1:A:234:MET:O	1:A:238:LEU:HG	2.11	0.51
1:A:445:VAL:O	1:A:449:LYS:HG3	2.11	0.51
1:A:796:LYS:HD2	1:A:797:ASP:OD1	2.09	0.51
2:B:46:U:O4	2:B:47:A:N6	2.43	0.51
3:C:465:MET:HE3	3:C:475:MET:HG3	1.92	0.51
6:F:48:A:H5'	6:F:49:G:O5'	2.10	0.51
22:1:822:ARG:HB3	22:1:822:ARG:CZ	2.39	0.51
23:3:102:ILE:HG22	23:3:103:HIS:CD2	2.45	0.51
23:3:316:GLU:HG3	23:3:326:ARG:HD3	1.92	0.51
23:3:644:GLU:HB2	23:3:663:LEU:HD12	1.91	0.51
23:3:1018:GLU:O	23:3:1018:GLU:HG2	2.10	0.51
35:2:453:LYS:HE2	35:2:453:LYS:O	2.11	0.51
40:9:285:HIS:NE2	40:9:432:THR:OG1	2.29	0.51
1:A:171:ASP:HA	1:A:521:ASN:ND2	2.25	0.51
1:A:436:PRO:HB2	1:A:439:GLN:CD	2.31	0.51
1:A:1063:GLY:HA3	1:A:1069:ASN:OD1	2.11	0.51
1:A:1184:ASN:OD1	1:A:1195:ARG:HD2	2.11	0.51
12:L:98:GLU:HG3	12:L:99:HIS:N	2.25	0.51
18:T:439:TRP:N	18:T:439:TRP:CD1	2.79	0.51
22:1:400:SER:OG	22:1:401:ASP:N	2.43	0.51
23:3:328:LYS:HZ2	23:3:365:GLY:C	2.12	0.51
1:A:122:ILE:HD13	1:A:483:GLN:HG3	1.91	0.51
1:A:1295:ILE:O	1:A:1295:ILE:HG12	2.11	0.51
1:A:1298:ARG:HH21	1:A:1298:ARG:CA	2.23	0.51
1:A:1661:TRP:CE2	1:A:1700:GLY:HA3	2.46	0.51
2:B:107:U:H2'	2:B:108:G:O4'	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:69:VAL:HG23	5:E:349:LYS:HA	1.92	0.51
12:L:49:ARG:HG3	12:L:54:LEU:HD23	1.92	0.51
20:Y:3:PRO:O	20:Y:6:LYS:N	2.43	0.51
22:1:163:LYS:HG3	22:1:164:GLU:N	2.25	0.51
22:1:442:THR:OG1	22:1:443:GLY:N	2.35	0.51
22:1:1126:PHE:O	35:2:575:PHE:CE2	2.63	0.51
1:A:1103:ALA:O	1:A:1107:ARG:HG3	2.10	0.51
1:A:1412:TRP:O	1:A:1420:ASN:HB3	2.11	0.51
7:G:102:G:H4'	38:7:25:LYS:HZ3	1.76	0.51
18:T:287:HIS:CE1	18:T:307:SER:HB3	2.46	0.51
18:T:357:TRP:N	18:T:357:TRP:CD1	2.78	0.51
19:X:259:TRP:CE3	19:X:371:HIS:HB3	2.46	0.51
19:X:261:LEU:HD13	19:X:369:LEU:HD13	1.92	0.51
23:3:898:ASN:OD1	23:3:899:THR:HG22	2.10	0.51
23:3:926:TYR:HE1	23:3:942:LYS:HZ2	1.58	0.51
1:A:818:GLU:HB2	22:1:444:PHE:HD2	1.76	0.51
7:G:91:A:O5'	7:G:91:A:H8	1.94	0.51
18:T:189:GLN:HG2	18:T:190:TRP:H	1.75	0.51
18:T:343:PRO:HG3	18:T:356:LEU:HD23	1.93	0.51
18:T:385:TYR:O	18:T:400:PHE:HB2	2.10	0.51
19:X:300:SER:H	19:X:303:HIS:CE1	2.28	0.51
23:3:54:LEU:HD21	23:3:99:PHE:CE2	2.46	0.51
23:3:329:TYR:OH	23:3:332:THR:HG22	2.10	0.51
1:A:390:ASP:OD2	3:C:394:ARG:NH2	2.43	0.51
1:A:1643:SER:O	1:A:1715:TYR:HA	2.10	0.51
3:C:203:MET:HB2	3:C:549:TRP:CH2	2.46	0.51
3:C:371:GLU:HA	3:C:375:GLU:HB2	1.93	0.51
3:C:568:PRO:HB2	3:C:569:ARG:HH11	1.76	0.51
3:C:696:LEU:HD21	3:C:744:ILE:HD11	1.92	0.51
10:J:357:LYS:HG3	10:J:359:VAL:HG22	1.93	0.51
22:1:1051:SER:OG	22:1:1054:GLU:HG2	2.11	0.51
22:1:1108:ASN:CB	22:1:1111:CYS:H	2.23	0.51
23:3:328:LYS:NZ	23:3:365:GLY:O	2.37	0.51
23:3:876:THR:O	23:3:876:THR:OG1	2.29	0.51
35:2:587:HIS:C	35:2:587:HIS:CD2	2.84	0.51
35:2:656:PRO:HA	35:2:686:VAL:O	2.12	0.51
1:A:535:ARG:HH22	1:A:1551:PHE:HE1	1.54	0.50
1:A:577:GLY:O	1:A:581:ILE:HG13	2.10	0.50
3:C:610:VAL:HG13	3:C:648:TYR:HD2	1.76	0.50
3:C:830:PRO:HA	3:C:904:TRP:HA	1.93	0.50
6:F:1:G:H2'	6:F:2:U:H6	1.76	0.50

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
10:J:346:TRP:CE3	10:J:369:PHE:HB2	2.46	0.50
22:1:476:ASP:HB2	37:6:24:ARG:HH22	1.77	0.50
22:1:774:ILE:HA	22:1:777:PHE:CE2	2.46	0.50
22:1:1050:VAL:HG12	22:1:1054:GLU:HB2	1.92	0.50
22:1:1257:PRO:HG2	35:2:478:HIS:O	2.10	0.50
23:3:230:GLU:OE1	23:3:230:GLU:N	2.44	0.50
23:3:436:ARG:HH11	23:3:776:GLN:NE2	2.09	0.50
1:A:153:ARG:HG3	1:A:156:ARG:HE	1.76	0.50
1:A:414:ARG:HD3	3:C:410:LEU:O	2.11	0.50
1:A:840:ILE:HG13	22:1:104:PHE:CZ	2.46	0.50
1:A:1045:GLY:HA3	1:A:1090:ARG:NH2	2.26	0.50
1:A:1268:ILE:O	1:A:1272:THR:HG23	2.10	0.50
1:A:1310:ARG:CG	1:A:1310:ARG:NH2	2.73	0.50
3:C:89:LEU:O	18:T:278:ASN:ND2	2.36	0.50
3:C:168:THR:O	3:C:184:THR:HG21	2.11	0.50
3:C:381:LEU:O	3:C:385:VAL:HG13	2.11	0.50
5:E:336:HIS:CB	5:E:341:ILE:HB	2.41	0.50
8:H:153:A:H61	8:H:179:C:N4	2.08	0.50
11:K:145:ASP:O	11:K:149:ILE:HG13	2.11	0.50
11:K:362:GLU:CB	20:Y:71:LYS:HG3	2.35	0.50
14:O:81:CYS:N	14:O:86:LEU:O	2.26	0.50
18:T:412:HIS:NE2	18:T:435:THR:O	2.42	0.50
19:X:260:ARG:HD3	19:X:274:TYR:CE2	2.45	0.50
22:1:130:PRO:HB2	22:1:150:ARG:HD2	1.93	0.50
22:1:656:LYS:CE	41:8:65:ASP:H	2.22	0.50
22:1:984:GLU:OE2	22:1:985:GLU:N	2.44	0.50
22:1:1012:PRO:O	22:1:1015:ASP:N	2.43	0.50
23:3:505:THR:HG21	23:3:508:CYS:SG	2.51	0.50
38:7:33:CYS:SG	38:7:35:SER:HB3	2.51	0.50
38:7:37:VAL:HB	38:7:38:ARG:HG3	1.92	0.50
40:9:239:ALA:HB3	40:9:264:ALA:HB3	1.92	0.50
2:B:115:C:H2'	2:B:116:U:O4'	2.11	0.50
3:C:507:VAL:HA	3:C:568:PRO:HD3	1.93	0.50
4:D:1992:GLU:HA	4:D:1995:ALA:HB3	1.94	0.50
4:D:2069:GLY:HA2	4:D:2077:ILE:H	1.75	0.50
6:F:33:G:N2	7:G:14:A:C4	2.79	0.50
10:J:422:PHE:O	10:J:426:GLN:HG2	2.12	0.50
22:1:1224:PRO:HA	22:1:1227:ILE:HG22	1.92	0.50
1:A:210:HIS:CE1	1:A:211:GLN:HG3	2.46	0.50
1:A:1553:VAL:HG13	7:G:2:U:O2'	2.11	0.50
1:A:1639:VAL:HG21	1:A:1699:THR:HB	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:226:VAL:HG11	3:C:430:PHE:HE1	1.77	0.50
3:C:486:ASP:HB3	3:C:488:VAL:HG23	1.93	0.50
6:F:62:C:N3	6:F:73:A:C2	2.80	0.50
12:L:25:LYS:HD3	12:L:26:TYR:CE2	2.46	0.50
18:T:373:LYS:O	18:T:391:SER:OG	2.25	0.50
22:1:112:ILE:HG13	22:1:115:ARG:HH11	1.76	0.50
22:1:700:LYS:O	22:1:704:ILE:HG22	2.10	0.50
23:3:483:LEU:HG	23:3:493:GLU:HG3	1.93	0.50
39:5:36:HIS:CE1	39:5:76:CYS:SG	3.04	0.50
40:9:334:ASP:OD2	40:9:336:THR:OG1	2.29	0.50
1:A:252:ASP:H	1:A:334:THR:HG21	1.77	0.50
1:A:893:GLU:HB2	1:A:1016:VAL:O	2.12	0.50
3:C:109:LEU:HG	3:C:537:TYR:CE2	2.47	0.50
3:C:673:LYS:HB3	3:C:686:THR:CG2	2.41	0.50
6:F:37:C:H5	7:G:4:A:OP2	1.94	0.50
6:F:40:U:H2'	6:F:41:A:H8	1.76	0.50
6:F:64:U:C4	6:F:65:G:C5	2.99	0.50
16:Q:1181:ASN:HA	16:Q:1305:ALA:O	2.12	0.50
20:Y:86:ASP:OD1	20:Y:86:ASP:N	2.40	0.50
20:Y:116:ARG:HA	20:Y:116:ARG:NE	2.26	0.50
22:1:978:LEU:O	22:1:981:TYR:N	2.41	0.50
22:1:1023:ILE:O	22:1:1026:ASN:HB2	2.12	0.50
23:3:185:LEU:HG	23:3:235:LEU:HD11	1.93	0.50
23:3:288:VAL:HG23	23:3:289:CYS:H	1.76	0.50
1:A:378:PHE:CZ	3:C:335:ASN:HB3	2.46	0.50
1:A:1199:LYS:HZ3	1:A:1206:GLU:CD	2.15	0.50
1:A:1276:GLU:OE2	1:A:1375:TRP:N	2.44	0.50
1:A:1560:ILE:HG22	1:A:1668:TRP:CD1	2.46	0.50
3:C:375:GLU:O	3:C:379:LYS:HG3	2.11	0.50
3:C:796:VAL:HB	3:C:803:ARG:HH11	1.76	0.50
3:C:838:ALA:O	3:C:869:TYR:HB2	2.12	0.50
5:E:118:ASN:OD1	5:E:123:MET:HB2	2.12	0.50
6:F:9:U:O2'	6:F:10:U:O4'	2.24	0.50
6:F:34:G:C8	7:G:13:C:N4	2.79	0.50
10:J:363:ARG:NH2	10:J:386:GLU:OE1	2.44	0.50
11:K:132:GLU:HG2	11:K:133:THR:N	2.25	0.50
18:T:216:ASN:OD1	18:T:471:ASP:HB2	2.12	0.50
18:T:306:CYS:HB3	18:T:336:VAL:HG12	1.93	0.50
18:T:346:ILE:HD11	18:T:400:PHE:CZ	2.46	0.50
22:1:477:LYS:HB2	22:1:499:LYS:NZ	2.27	0.50
23:3:459:VAL:HA	23:3:475:ILE:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:548:ALA:O	23:3:555:VAL:HB	2.12	0.50
23:3:788:PHE:HB3	23:3:799:ILE:HG23	1.92	0.50
37:6:106:LYS:O	37:6:109:GLN:HG2	2.12	0.50
37:6:112:LEU:O	37:6:116:LYS:CB	2.60	0.50
1:A:82:ARG:HG2	7:G:16:G:O6	2.11	0.50
1:A:121:HIS:ND1	1:A:481:PHE:O	2.45	0.50
1:A:256:TYR:HE1	1:A:331:TRP:H	1.58	0.50
1:A:363:HIS:NE2	3:C:287:GLY:HA3	2.26	0.50
1:A:540:PHE:HB2	1:A:545:HIS:CE1	2.46	0.50
1:A:979:SER:HB2	1:A:1173:SER:HB3	1.93	0.50
3:C:742:PRO:O	3:C:786:ASN:HA	2.12	0.50
10:J:351:ASN:HB2	10:J:355:ARG:HH21	1.77	0.50
18:T:459:LEU:HA	40:9:259:THR:OG1	2.12	0.50
22:1:427:PRO:HA	22:1:430:LYS:CB	2.42	0.50
22:1:884:ILE:HG22	22:1:885:ASP:O	2.12	0.50
22:1:1010:THR:OG1	22:1:1011:PRO:HD3	2.11	0.50
22:1:1262:ARG:NH1	35:2:483:GLN:HE21	2.09	0.50
23:3:16:PHE:HB2	23:3:65:LEU:HD23	1.94	0.50
35:2:518:GLU:OE1	35:2:518:GLU:HA	2.12	0.50
37:6:22:TYR:CZ	37:6:24:ARG:HD3	2.46	0.50
40:9:235:LYS:NZ	40:9:452:GLN:HB2	2.26	0.50
40:9:236:LEU:HD23	40:9:237:ASN:H	1.77	0.50
1:A:150:MET:SD	1:A:193:LEU:HB2	2.51	0.50
1:A:825:ILE:HD13	1:A:929:GLU:HB2	1.93	0.50
1:A:1014:ASN:ND2	12:L:81:GLN:HB3	2.27	0.50
1:A:1019:TYR:O	1:A:1022:MET:N	2.45	0.50
1:A:1022:MET:O	1:A:1023:ASN:ND2	2.42	0.50
1:A:1740:LEU:O	1:A:1744:ARG:HG3	2.12	0.50
1:A:2274:PRO:HA	1:A:2295:GLU:O	2.11	0.50
2:B:32:C:C2	2:B:33:U:C5	3.00	0.50
10:J:245:TRP:CZ3	10:J:264:ILE:HG23	2.47	0.50
17:R:413:ASN:OD1	21:Z:603:SER:HB3	2.11	0.50
23:3:553:GLN:NE2	23:3:601:ARG:HA	2.27	0.50
23:3:593:ALA:HA	23:3:642:ILE:HD13	1.93	0.50
23:3:1207:LYS:HA	23:3:1210:ASP:OD2	2.11	0.50
1:A:239:TYR:CE1	1:A:408:PRO:HD2	2.46	0.50
1:A:1214:TRP:CZ2	1:A:1230:LEU:HD11	2.47	0.50
3:C:207:GLY:N	45:C:1500:GTP:O3G	2.38	0.50
6:F:36:A:N1	7:G:10:U:C4	2.80	0.50
10:J:326:VAL:HG13	10:J:352:PHE:HZ	1.77	0.50
16:Q:408:VAL:O	16:Q:412:GLU:CB	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:539:VAL:O	16:Q:624:THR:HA	2.12	0.50
18:T:223:SER:OG	18:T:225:ASP:N	2.33	0.50
19:X:284:GLY:O	19:X:294:ILE:N	2.36	0.50
22:1:856:ASP:HB3	22:1:864:TYR:HE2	1.76	0.50
22:1:1019:ARG:HA	22:1:1019:ARG:HH11	1.77	0.50
1:A:82:ARG:NE	7:G:14:A:OP2	2.45	0.49
1:A:787:GLU:O	1:A:790:ARG:N	2.44	0.49
1:A:1311:PHE:CD1	1:A:1312:PRO:HD2	2.47	0.49
1:A:1312:PRO:HG3	1:A:1541:THR:CG2	2.41	0.49
1:A:1645:LEU:HB2	1:A:1714:ALA:HB3	1.94	0.49
3:C:225:VAL:HG12	3:C:252:ALA:O	2.11	0.49
3:C:753:GLU:HG2	3:C:756:LYS:HD3	1.93	0.49
5:E:82:ALA:HB1	5:E:115:LEU:HD13	1.94	0.49
5:E:333:VAL:HA	5:E:343:ILE:O	2.12	0.49
6:F:45:A:N1	7:G:4:A:N6	2.60	0.49
8:H:125:G:H2’	8:H:126:A:C8	2.47	0.49
18:T:425:GLY:O	18:T:441:TRP:N	2.35	0.49
19:X:260:ARG:HB3	19:X:272:VAL:HG11	1.93	0.49
22:1:1090:PRO:N	22:1:1090:PRO:C	2.58	0.49
22:1:1125:PRO:HG2	22:1:1165:TYR:CE2	2.47	0.49
22:1:1178:MET:HE2	35:2:591:TYR:CZ	2.47	0.49
23:3:802:THR:HG22	23:3:803:ASP:N	2.27	0.49
37:6:81:ASN:HB2	37:6:86:TYR:HE1	1.75	0.49
1:A:770:THR:O	1:A:772:CYS:N	2.45	0.49
1:A:2273:VAL:O	1:A:2297:GLN:N	2.43	0.49
3:C:139:HIS:CE1	3:C:179:VAL:HG23	2.47	0.49
3:C:275:TYR:HA	3:C:278:LEU:HB2	1.94	0.49
3:C:836:VAL:HG22	3:C:897:SER:HB3	1.94	0.49
11:K:177:VAL:HA	23:3:690:ARG:HH22	1.77	0.49
18:T:497:GLU:OE1	18:T:497:GLU:N	2.45	0.49
19:X:260:ARG:HH12	19:X:372:GLU:N	2.10	0.49
20:Y:67:LEU:HD13	20:Y:80:CYS:HB2	1.93	0.49
23:3:249:LEU:HD22	23:3:256:ILE:HD11	1.93	0.49
40:9:243:THR:HG23	40:9:262:GLU:O	2.12	0.49
1:A:102:LEU:HA	1:A:129:VAL:HG21	1.94	0.49
1:A:409:ARG:HA	1:A:412:ASN:HD22	1.76	0.49
3:C:137:HIS:HB3	3:C:140:HIS:ND1	2.27	0.49
3:C:137:HIS:CG	3:C:138:LEU:N	2.79	0.49
3:C:497:LEU:HD12	3:C:577:PHE:CZ	2.47	0.49
3:C:590:ILE:HG21	3:C:637:LEU:HD11	1.93	0.49
5:E:69:VAL:HB	5:E:345:ALA:HB1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:275:LYS:HD3	5:E:314:THR:O	2.12	0.49
18:T:269:GLN:OE1	18:T:271:LYS:HE2	2.12	0.49
22:1:1107:GLN:OE1	22:1:1107:GLN:HA	2.13	0.49
22:1:1304:LEU:HD12	39:5:52:TYR:CE2	2.48	0.49
23:3:253:GLU:O	23:3:254:ASN:HB2	2.11	0.49
23:3:528:ARG:CB	23:3:532:ARG:HE	2.25	0.49
23:3:1201:PRO:HB2	23:3:1202:PRO:HD3	1.93	0.49
1:A:176:LEU:HD11	1:A:562:VAL:HG13	1.95	0.49
1:A:264:PHE:HB2	1:A:328:HIS:CD2	2.48	0.49
2:B:20:G:H4’	2:B:21:A:OP1	2.10	0.49
3:C:224:GLY:HA3	3:C:438:ILE:HG23	1.94	0.49
3:C:230:ASP:HB2	3:C:259:LYS:HZ1	1.77	0.49
3:C:259:LYS:HG2	45:C:1500:GTP:C6	2.46	0.49
3:C:837:GLN:HA	3:C:869:TYR:O	2.11	0.49
4:D:1529:GLY:HA2	4:D:1706:CYS:O	2.13	0.49
19:X:372:GLU:HG2	19:X:373:SER:H	1.75	0.49
22:1:1174:GLU:O	22:1:1178:MET:HG2	2.12	0.49
23:3:111:GLY:O	23:3:113:ARG:N	2.45	0.49
23:3:316:GLU:HB2	23:3:324:GLU:HG2	1.95	0.49
23:3:525:ARG:O	23:3:525:ARG:HG2	2.11	0.49
23:3:666:ASN:HD22	23:3:666:ASN:N	2.11	0.49
35:2:520:PRO:HG2	35:2:520:PRO:O	2.12	0.49
40:9:276:VAL:HG13	40:9:437:PRO:HB2	1.93	0.49
1:A:112:GLN:HB3	1:A:187:PRO:HB2	1.94	0.49
1:A:363:HIS:CD2	3:C:287:GLY:HA3	2.47	0.49
1:A:977:LEU:HB2	1:A:1175:VAL:HG22	1.95	0.49
1:A:1482:GLU:HG3	1:A:1483:GLY:N	2.27	0.49
2:B:101:U:H2’	2:B:102:U:H6	1.78	0.49
3:C:490:PHE:HD2	3:C:612:LYS:HD2	1.77	0.49
3:C:745:LEU:HD12	3:C:789:PHE:O	2.12	0.49
6:F:31:U:O4	7:G:16:G:H1’	2.13	0.49
7:G:5:G:H5’	11:K:22:GLN:HA	1.95	0.49
19:X:274:TYR:CE1	22:1:436:THR:HA	2.48	0.49
19:X:338:PHE:HB2	19:X:359:LYS:HB3	1.93	0.49
22:1:1055:TRP:HA	22:1:1055:TRP:CE3	2.47	0.49
22:1:1137:ARG:HH21	35:2:524:LEU:CD1	2.26	0.49
23:3:788:PHE:HA	23:3:798:ILE:O	2.12	0.49
23:3:833:GLU:O	23:3:835:ALA:N	2.45	0.49
23:3:1083:ASN:ND2	35:2:471:ARG:HH22	2.10	0.49
35:2:534:GLN:CA	35:2:534:GLN:NE2	2.76	0.49
38:7:10:PHE:HB2	38:7:12:ARG:NE	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:TYR:HD1	1:A:518:LEU:HD23	1.77	0.49
1:A:2194:THR:HA	1:A:2238:GLY:HA3	1.94	0.49
3:C:658:PRO:HB2	3:C:881:PHE:CZ	2.47	0.49
11:K:28:CYS:SG	11:K:50:HIS:HE1	2.35	0.49
14:O:75:SER:O	14:O:79:ASN:HA	2.13	0.49
17:R:390:GLU:H	17:R:390:GLU:CD	2.16	0.49
20:Y:54:CYS:O	20:Y:57:SER:OG	2.30	0.49
22:1:1179:ASP:OD1	22:1:1184:HIS:CD2	2.65	0.49
23:3:240:GLY:HA2	23:3:245:PRO:O	2.12	0.49
23:3:312:LYS:NZ	23:3:366:ASP:OD1	2.44	0.49
37:6:29:LYS:HG3	37:6:57:ARG:NH2	2.27	0.49
37:6:47:GLN:HG2	37:6:48:ILE:N	2.27	0.49
1:A:171:ASP:HA	1:A:521:ASN:HD22	1.77	0.49
1:A:319:LEU:HD21	3:C:638:ASP:HA	1.93	0.49
1:A:351:TYR:N	3:C:268:LYS:O	2.45	0.49
1:A:1069:ASN:OD1	1:A:1069:ASN:N	2.43	0.49
1:A:1083:HIS:ND1	1:A:1084:PRO:HD2	2.27	0.49
6:F:82:A:O2'	8:H:16:U:O4	2.22	0.49
8:H:166:G:N3	8:H:166:G:H2'	2.28	0.49
10:J:314:TYR:CE1	10:J:336:TRP:HH2	2.31	0.49
11:K:95:TYR:HB2	11:K:115:LEU:HD21	1.94	0.49
19:X:327:TYR:HB3	19:X:349:TYR:HD1	1.78	0.49
23:3:191:GLU:H	23:3:191:GLU:HG3	1.41	0.49
40:9:259:THR:OG1	40:9:259:THR:O	2.23	0.49
40:9:369:ALA:HB3	40:9:379:GLN:HB2	1.95	0.49
1:A:89:LEU:HD13	1:A:660:PHE:CZ	2.47	0.49
1:A:141:ILE:HG22	1:A:242:ALA:HB1	1.94	0.49
1:A:1303:LEU:HB3	1:A:1566:ILE:HG22	1.95	0.49
1:A:1581:LEU:HD23	1:A:1746:ARG:NH2	2.28	0.49
4:D:1185:GLU:O	4:D:1204:ILE:HA	2.12	0.49
5:E:248:SER:O	5:E:263:ASP:HA	2.13	0.49
5:E:321:TYR:HB3	5:E:323:LEU:HD21	1.95	0.49
6:F:91:A:H2'	6:F:92:A:H8	1.77	0.49
18:T:351:ASP:O	18:T:352:THR:OG1	2.25	0.49
22:1:944:SER:O	22:1:947:VAL:N	2.46	0.49
22:1:953:ASP:OD1	22:1:992:SER:HB3	2.13	0.49
23:3:288:VAL:HG23	23:3:289:CYS:N	2.28	0.49
23:3:305:THR:HG22	23:3:309:ASP:O	2.13	0.49
23:3:512:GLY:HA3	23:3:515:ALA:HB3	1.93	0.49
23:3:981:CYS:SG	23:3:982:GLU:N	2.86	0.49
35:2:524:LEU:HD13	35:2:528:ILE:HG21	1.93	0.49

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:A:827:PHE:C	1:A:827:PHE:CD2	2.86	0.49
1:A:1306:LYS:NZ	7:G:0:G:N7	2.60	0.49
1:A:1487:HIS:O	1:A:1541:THR:OG1	2.29	0.49
8:H:114:A:H2'	8:H:115:G:C8	2.48	0.49
11:K:121:TRP:CZ2	11:K:125:GLU:HG3	2.48	0.49
12:L:71:LEU:HD21	12:L:100:TYR:HB2	1.95	0.49
19:X:286:HIS:CD2	19:X:301:LYS:HD3	2.48	0.49
21:Z:574:ASN:ND2	21:Z:578:ILE:H	2.10	0.49
22:1:445:HIS:CG	22:1:445:HIS:O	2.65	0.49
22:1:889:GLU:OE2	22:1:928:TYR:OH	2.21	0.49
23:3:162:LYS:HZ2	23:3:222:ARG:NH1	2.11	0.49
39:5:11:LEU:HD12	39:5:12:GLU:N	2.28	0.49
1:A:556:LEU:HD13	1:A:588:LEU:HD13	1.95	0.49
1:A:661:GLU:N	1:A:661:GLU:OE2	2.43	0.49
1:A:1124:ASN:HD22	1:A:1144:LYS:HZ2	1.61	0.49
3:C:213:ASP:OD1	3:C:213:ASP:N	2.44	0.49
3:C:220:ARG:NH2	3:C:580:LEU:HA	2.27	0.49
3:C:265:LEU:HD21	3:C:381:LEU:HD13	1.94	0.49
3:C:834:VAL:HA	3:C:898:LEU:O	2.13	0.49
8:H:3:C:H2'	8:H:4:G:H8	1.78	0.49
19:X:282:LEU:HD23	19:X:290:ALA:HA	1.94	0.49
22:1:129:SEP:O2P	22:1:573:LYS:HG3	2.12	0.49
22:1:129:SEP:P	22:1:573:LYS:NZ	2.84	0.49
22:1:774:ILE:HA	22:1:777:PHE:HE2	1.78	0.49
22:1:1166:ILE:O	22:1:1170:THR:HG23	2.13	0.49
23:3:415:LEU:HD23	23:3:871:PRO:HG3	1.94	0.49
23:3:791:HIS:CD2	23:3:793:GLU:H	2.31	0.49
39:5:46:HIS:C	39:5:48:ASP:H	2.16	0.49
40:9:142:ARG:HA	40:9:149:PRO:HA	1.95	0.49
40:9:233:VAL:HG13	40:9:237:ASN:HB3	1.95	0.49
40:9:410:MET:O	40:9:413:VAL:HG12	2.12	0.49
1:A:1180:LYS:HA	1:A:1201:ARG:NH1	2.28	0.48
1:A:1544:ARG:HA	1:A:1670:ASP:OD2	2.13	0.48
1:A:1665:GLN:NE2	1:A:1665:GLN:HA	2.28	0.48
1:A:1699:THR:O	1:A:1699:THR:OG1	2.30	0.48
6:F:87:C:C2	6:F:88:G:C8	3.01	0.48
6:F:93:G:C2	8:H:6:U:C2	3.01	0.48
7:G:86:A:H2'	7:G:87:U:N1	2.27	0.48
8:H:26:A:H2'	8:H:27:U:C6	2.49	0.48
19:X:262:TYR:CE2	19:X:370:LEU:HD12	2.48	0.48
19:X:370:LEU:HB3	19:X:374:SER:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:271:ILE:HD13	23:3:287:PHE:CE2	2.47	0.48
23:3:603:ARG:HG2	23:3:604:PHE:CD2	2.48	0.48
23:3:711:ALA:HB1	23:3:722:SER:O	2.13	0.48
38:7:30:CYS:SG	38:7:31:VAL:N	2.85	0.48
41:8:65:ASP:O	41:8:69:GLU:HG2	2.13	0.48
1:A:200:ASP:HA	1:A:237:THR:CG2	2.43	0.48
1:A:422:LEU:HD22	1:A:638:LEU:HD12	1.93	0.48
1:A:651:TRP:NE1	6:F:66:C:C2	2.81	0.48
1:A:1159:ASN:ND2	15:P:196:ASN:HB2	2.28	0.48
1:A:1530:PRO:O	1:A:1532:ARG:N	2.43	0.48
3:C:148:CYS:HB3	3:C:427:PHE:HE2	1.78	0.48
3:C:606:GLY:HA3	3:C:649:SER:OG	2.12	0.48
10:J:370:VAL:O	10:J:374:PRO:HA	2.12	0.48
11:K:80:LEU:HA	11:K:84:PHE:CD2	2.49	0.48
16:Q:744:ILE:N	16:Q:745:PRO:HD3	2.28	0.48
17:R:282:GLU:HA	40:9:221:LEU:HD13	1.95	0.48
18:T:235:SER:O	18:T:237:LYS:HG3	2.12	0.48
18:T:314:ILE:O	18:T:322:SER:HA	2.12	0.48
23:3:666:ASN:N	23:3:666:ASN:ND2	2.61	0.48
23:3:690:ARG:HH11	23:3:690:ARG:HB2	1.77	0.48
36:4:133:MET:O	36:4:142:LYS:N	2.30	0.48
40:9:284:LEU:HD12	40:9:293:LEU:HD11	1.94	0.48
1:A:306:GLN:NE2	3:C:852:ARG:O	2.46	0.48
1:A:883:ARG:O	1:A:887:THR:HG23	2.12	0.48
1:A:1543:ASN:O	1:A:1563:HIS:CD2	2.66	0.48
1:A:1543:ASN:O	1:A:1563:HIS:HD2	1.96	0.48
3:C:183:SER:OG	3:C:214:GLU:HB3	2.12	0.48
3:C:306:ASN:HA	3:C:433:MET:HG3	1.93	0.48
3:C:767:VAL:HA	3:C:770:PHE:HB3	1.95	0.48
6:F:39:A:H2’	6:F:40:U:O4’	2.13	0.48
8:H:52:G:H2’	8:H:53:U:C6	2.48	0.48
17:R:411:LEU:O	17:R:414:GLN:HG3	2.13	0.48
23:3:128:ARG:NH2	23:3:180:PRO:HG3	2.29	0.48
23:3:138:GLN:HG2	23:3:161:HIS:ND1	2.27	0.48
23:3:1105:GLN:HG3	23:3:1106:LYS:N	2.29	0.48
41:8:28:LEU:HD23	41:8:30:PHE:CE1	2.48	0.48
1:A:428:LYS:HA	1:A:431:TYR:CZ	2.49	0.48
1:A:599:MET:SD	1:A:602:ILE:HD12	2.53	0.48
1:A:975:VAL:HG22	1:A:1177:VAL:HG13	1.95	0.48
1:A:1163:ARG:NH1	1:A:1163:ARG:HB2	2.28	0.48
1:A:1399:GLN:C	1:A:1401:ARG:H	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1403:LEU:HD11	17:R:407:TYR:CD1	2.48	0.48
1:A:1562:MET:C	1:A:1564:GLY:H	2.16	0.48
2:B:11:U:H2'	2:B:12:U:H6	1.78	0.48
2:B:47:A:O2'	2:B:48:A:H5"	2.14	0.48
3:C:131:ASN:HB2	3:C:223:ASP:OD1	2.14	0.48
3:C:139:HIS:HE1	3:C:179:VAL:HG23	1.78	0.48
5:E:233:GLY:HA3	5:E:260:ARG:NH1	2.29	0.48
6:F:40:U:N3	6:F:41:A:C5	2.81	0.48
6:F:63:C:C4	6:F:72:G:N1	2.80	0.48
6:F:85:U:C4	6:F:86:U:C4	3.01	0.48
12:L:21:ALA:O	12:L:24:MET:HG3	2.12	0.48
17:R:147:THR:OG1	18:T:360:VAL:HB	2.14	0.48
17:R:253:ASN:HB2	17:R:254:TRP:CE3	2.49	0.48
18:T:203:HIS:CE1	18:T:223:SER:HB3	2.49	0.48
18:T:371:HIS:CE1	18:T:396:LYS:HG3	2.48	0.48
19:X:254:ILE:HG22	19:X:255:PRO:HD2	1.95	0.48
19:X:353:LYS:HG3	19:X:354:GLU:N	2.27	0.48
22:1:1109:ARG:HA	22:1:1112:THR:HG23	1.94	0.48
40:9:322:HIS:O	40:9:421:ARG:HG2	2.14	0.48
1:A:66:VAL:HG13	1:A:487:LEU:HD21	1.95	0.48
1:A:508:ILE:O	1:A:513:LEU:HG	2.13	0.48
1:A:617:ASN:N	1:A:617:ASN:OD1	2.46	0.48
1:A:887:THR:OG1	1:A:888:GLN:N	2.45	0.48
3:C:93:ILE:H	3:C:93:ILE:HD12	1.78	0.48
3:C:663:CYS:SG	3:C:785:ARG:NH2	2.87	0.48
5:E:75:HIS:NE2	5:E:121:GLY:HA3	2.28	0.48
6:F:26:U:H3'	6:F:27:A:C5'	2.41	0.48
18:T:284:TYR:N	18:T:284:TYR:CD2	2.81	0.48
22:1:552:LEU:O	22:1:555:VAL:HG13	2.12	0.48
23:3:29:GLU:HG2	23:3:42:ARG:HB2	1.95	0.48
23:3:1083:ASN:HB2	35:2:495:ARG:HA	1.96	0.48
40:9:42:CYS:O	40:9:46:LEU:HA	2.13	0.48
40:9:266:ILE:HG23	40:9:267:ASP:H	1.78	0.48
1:A:140:TYR:OH	1:A:421:ALA:O	2.24	0.48
1:A:164:MET:HG3	1:A:577:GLY:HA3	1.96	0.48
1:A:347:LEU:HD22	1:A:351:TYR:CZ	2.48	0.48
1:A:409:ARG:HA	1:A:412:ASN:ND2	2.28	0.48
1:A:652:LEU:O	1:A:655:LEU:HG	2.14	0.48
1:A:1090:ARG:HG2	1:A:1091:TYR:O	2.13	0.48
1:A:1256:PHE:CG	1:A:1299:ILE:HG21	2.47	0.48
1:A:1618:LYS:HG3	1:A:1626:CYS:SG	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:130:ARG:NE	3:C:435:VAL:HG23	2.28	0.48
3:C:448:LYS:NZ	3:C:497:LEU:HD22	2.29	0.48
6:F:34:G:H2'	6:F:35:A:C4	2.49	0.48
6:F:39:A:C6	6:F:40:U:C4	3.02	0.48
10:J:370:VAL:HB	10:J:379:TRP:CD1	2.48	0.48
11:K:70:GLU:O	11:K:71:GLU:C	2.52	0.48
18:T:385:TYR:OH	18:T:401:PRO:HB3	2.14	0.48
19:X:225:SER:HB2	19:X:227:GLU:HG3	1.94	0.48
40:9:427:ARG:NE	40:9:429:ASP:OD1	2.45	0.48
1:A:280:GLU:HB2	2:B:48:A:P	2.54	0.48
2:B:42:U:H2'	2:B:43:U:O4'	2.13	0.48
3:C:142:LYS:H	45:C:1500:GTP:PB	2.37	0.48
3:C:480:LYS:O	3:C:481:MET:HG3	2.14	0.48
11:K:33:LYS:CD	11:K:44:HIS:HE1	2.25	0.48
11:K:80:LEU:HD12	11:K:84:PHE:HD2	1.79	0.48
18:T:346:ILE:HD11	18:T:400:PHE:HZ	1.78	0.48
22:1:785:LYS:O	22:1:788:VAL:HG22	2.13	0.48
22:1:1108:ASN:HB3	22:1:1110:VAL:N	2.29	0.48
23:3:146:ARG:CG	23:3:146:ARG:NH2	2.72	0.48
23:3:219:HIS:CE1	23:3:221:VAL:HG12	2.49	0.48
23:3:674:LEU:HD12	23:3:675:LEU:N	2.29	0.48
36:4:101:ASN:HA	36:4:148:ASN:HA	1.94	0.48
38:7:23:CYS:SG	38:7:25:LYS:HB3	2.53	0.48
40:9:390:LEU:HD22	40:9:394:HIS:HD2	1.78	0.48
1:A:386:PRO:HG3	3:C:372:PHE:CE1	2.49	0.48
1:A:693:ILE:O	1:A:695:ASP:N	2.47	0.48
1:A:767:VAL:HG12	1:A:1249:MET:HE2	1.94	0.48
1:A:827:PHE:CD2	1:A:828:PRO:HD2	2.48	0.48
1:A:1099:PHE:N	1:A:1099:PHE:CD2	2.80	0.48
1:A:1608:THR:HG23	1:A:1610:GLN:HE22	1.77	0.48
3:C:243:ILE:O	3:C:247:VAL:HG23	2.14	0.48
3:C:707:ILE:CD1	3:C:734:ALA:HA	2.43	0.48
3:C:778:PRO:HD3	3:C:817:TYR:CE1	2.48	0.48
5:E:67:GLY:C	5:E:349:LYS:HG2	2.34	0.48
5:E:341:ILE:HG23	5:E:354:GLY:O	2.14	0.48
6:F:89:U:H2'	6:F:90:G:C8	2.48	0.48
8:H:71:C:H2'	8:H:72:U:C6	2.49	0.48
11:K:121:TRP:CH2	11:K:125:GLU:HG3	2.49	0.48
16:Q:119:PHE:N	16:Q:120:PRO:HD2	2.29	0.48
16:Q:543:LEU:N	16:Q:621:GLU:O	2.36	0.48
22:1:532:PHE:CE1	22:1:559:ILE:HD11	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1:696:ASP:OD1	22:1:697:GLU:N	2.47	0.48
23:3:1049:LYS:HE2	39:5:52:TYR:CE1	2.49	0.48
38:7:30:CYS:SG	38:7:32:ILE:N	2.86	0.48
40:9:322:HIS:CE1	40:9:332:GLY:HA2	2.49	0.48
41:8:35:GLU:OE1	41:8:35:GLU:N	2.46	0.48
1:A:88:TYR:CE1	1:A:125:ALA:HA	2.49	0.48
1:A:485:THR:OG1	1:A:486:LYS:N	2.45	0.48
1:A:829:PRO:O	1:A:832:TYR:HB2	2.13	0.48
1:A:1109:LEU:HD23	1:A:1109:LEU:HA	1.60	0.48
1:A:1332:HIS:ND1	1:A:1357:MET:HB2	2.29	0.48
1:A:1544:ARG:H	1:A:1544:ARG:HG3	1.50	0.48
2:B:63:A:H2’	2:B:64:G:C8	2.49	0.48
3:C:136:GLY:N	3:C:142:LYS:HD3	2.29	0.48
3:C:490:PHE:CE2	3:C:612:LYS:HB3	2.47	0.48
3:C:918:ILE:HG21	3:C:932:GLU:HG3	1.96	0.48
7:G:7:G:H2’	7:G:8:C:C6	2.48	0.48
8:H:171:U:C2	8:H:172:C:C5	3.01	0.48
19:X:249:PRO:HD2	19:X:307:GLN:OE1	2.14	0.48
22:1:1133:MET:HE2	35:2:528:ILE:HD12	1.96	0.48
23:3:1032:TRP:CD1	23:3:1032:TRP:N	2.82	0.48
1:A:170:ASP:OD1	1:A:172:GLU:N	2.24	0.48
1:A:606:LYS:HZ2	1:A:610:HIS:CE1	2.31	0.48
1:A:647:LEU:HD11	1:A:651:TRP:CZ2	2.49	0.48
1:A:652:LEU:O	1:A:656:LEU:HD12	2.14	0.48
1:A:1221:THR:OG1	1:A:1223:GLU:OE1	2.23	0.48
1:A:1551:PHE:HD1	1:A:1553:VAL:CG2	2.26	0.48
1:A:1681:ARG:O	1:A:1685:LEU:HG	2.14	0.48
3:C:844:SER:O	3:C:848:THR:HG23	2.13	0.48
5:E:319:ILE:H	5:E:319:ILE:HD12	1.79	0.48
6:F:40:U:O2’	6:F:41:A:H5’	2.13	0.48
6:F:50:A:H2’	6:F:50:A:N3	2.28	0.48
8:H:44:U:H2’	8:H:45:C:C5	2.49	0.48
16:Q:28:CYS:HA	16:Q:32:ALA:HB3	1.95	0.48
16:Q:489:VAL:O	16:Q:494:PRO:HD3	2.14	0.48
18:T:395:ILE:HD12	18:T:395:ILE:N	2.29	0.48
18:T:478:LEU:HD22	18:T:488:VAL:HG22	1.95	0.48
21:Z:566:TYR:HB3	21:Z:579:TRP:CD1	2.49	0.48
22:1:130:PRO:CG	22:1:150:ARG:HD2	2.44	0.48
22:1:662:HIS:ND1	22:1:704:ILE:HG21	2.28	0.48
23:3:4:TYR:CE2	23:3:6:LEU:HD21	2.48	0.48
23:3:206:GLN:HE21	23:3:232:GLY:N	2.10	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:364:LEU:HD23	23:3:364:LEU:HA	1.67	0.48
23:3:469:GLU:HB2	23:3:470:PHE:CE2	2.49	0.48
40:9:273:TYR:CG	40:9:301:PRO:HB2	2.49	0.48
1:A:1045:GLY:HA3	1:A:1090:ARG:CZ	2.44	0.47
1:A:1104:ASP:OD1	1:A:1104:ASP:N	2.47	0.47
1:A:1683:LYS:HD3	1:A:1683:LYS:HA	1.59	0.47
2:B:54:U:H2'	2:B:55:C:C6	2.49	0.47
2:B:55:C:H2'	2:B:56:C:C6	2.48	0.47
3:C:221:ILE:HD13	3:C:494:GLY:HA2	1.96	0.47
3:C:784:ILE:HG23	3:C:820:PHE:HE1	1.78	0.47
3:C:840:ALA:HA	3:C:869:TYR:CE2	2.49	0.47
5:E:158:TYR:HD2	5:E:201:PHE:HB2	1.78	0.47
16:Q:1225:SER:O	16:Q:1272:LEU:N	2.36	0.47
22:1:944:SER:O	22:1:947:VAL:HG13	2.14	0.47
23:3:19:HIS:HD2	23:3:340:CYS:SG	2.37	0.47
23:3:146:ARG:HD3	23:3:150:ALA:HA	1.95	0.47
23:3:506:LEU:HD22	23:3:544:ILE:HG23	1.96	0.47
23:3:1034:THR:OG1	23:3:1035:THR:N	2.47	0.47
38:7:78:GLN:OE1	38:7:80:LYS:HE2	2.14	0.47
41:8:110:LEU:O	41:8:113:GLN:HG2	2.13	0.47
1:A:67:ARG:HD3	1:A:179:ALA:HB2	1.96	0.47
1:A:590:GLY:HA2	1:A:592:TYR:CE2	2.50	0.47
1:A:820:ARG:HD2	1:A:820:ARG:HA	1.61	0.47
1:A:1359:HIS:HB2	1:A:1361:GLU:O	2.13	0.47
1:A:1615:HIS:ND1	1:A:1618:LYS:HG2	2.29	0.47
1:A:1643:SER:O	1:A:1718:TRP:HZ2	1.97	0.47
2:B:101:U:H2'	2:B:102:U:C6	2.48	0.47
3:C:183:SER:HB2	3:C:203:MET:SD	2.54	0.47
3:C:706:GLN:HB3	3:C:708:THR:HG23	1.96	0.47
6:F:40:U:H3	7:G:7:G:H1	1.61	0.47
8:H:10:C:H2'	8:H:11:G:C8	2.49	0.47
9:I:604:GLU:HA	9:I:612:ALA:HB2	1.94	0.47
11:K:99:ILE:O	11:K:101:HIS:N	2.48	0.47
14:O:87:ASP:O	14:O:91:GLY:N	2.38	0.47
18:T:363:LYS:HD2	18:T:363:LYS:HA	1.57	0.47
23:3:645:MET:H	23:3:664:TYR:HE2	1.62	0.47
35:2:530:ARG:CB	35:2:578:TRP:HZ3	2.26	0.47
38:7:24:GLU:HG2	38:7:66:VAL:HG11	1.94	0.47
39:5:3:ASP:O	39:5:7:ILE:HG12	2.13	0.47
40:9:328:PHE:CG	40:9:329:VAL:HG22	2.49	0.47
41:8:115:ASN:OD1	41:8:117:ALA:N	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:TYR:CE2	3:C:882:GLY:HA3	2.50	0.47
1:A:480:LYS:HB3	13:N:109:ARG:O	2.15	0.47
3:C:335:ASN:ND2	3:C:338:GLU:HG2	2.29	0.47
3:C:388:VAL:O	3:C:392:LEU:HB2	2.14	0.47
3:C:507:VAL:HG12	3:C:567:GLU:OE2	2.14	0.47
5:E:282:HIS:NE2	5:E:289:LEU:HG	2.30	0.47
10:J:245:TRP:CE3	10:J:264:ILE:HG23	2.49	0.47
11:K:29:GLN:O	11:K:32:GLN:N	2.45	0.47
18:T:432:ASP:O	18:T:464:GLY:HA2	2.15	0.47
23:3:103:HIS:CE1	23:3:154:ILE:HG22	2.49	0.47
23:3:566:PHE:N	23:3:566:PHE:HD1	2.13	0.47
41:8:51:TRP:HB2	41:8:123:PHE:HZ	1.78	0.47
1:A:440:PRO:HG2	1:A:443:VAL:HG22	1.95	0.47
1:A:941:LYS:HG3	1:A:951:LEU:HD11	1.95	0.47
1:A:1306:LYS:HB2	1:A:1306:LYS:HE2	1.65	0.47
1:A:1576:ILE:HD11	1:A:1747:ILE:HA	1.97	0.47
1:A:1667:ARG:HD2	1:A:1679:TYR:CD2	2.49	0.47
3:C:655:VAL:HG12	3:C:656:ALA:O	2.14	0.47
3:C:796:VAL:HG23	3:C:798:GLN:HE22	1.79	0.47
6:F:5:U:H2'	6:F:7:G:O4'	2.15	0.47
6:F:36:A:H5'	7:G:11:A:N1	2.30	0.47
7:G:108:U:H5"	7:G:109:U:H5'	1.95	0.47
8:H:51:A:C6	8:H:63:G:C6	3.02	0.47
8:H:150:U:H3	8:H:181:G:H22	1.62	0.47
9:I:140:LEU:N	9:I:141:PRO:HD3	2.30	0.47
12:L:86:ALA:HB1	12:L:91:ARG:O	2.14	0.47
17:R:231:HIS:NE2	18:T:371:HIS:O	2.48	0.47
18:T:243:THR:O	18:T:243:THR:OG1	2.27	0.47
22:1:1221:GLU:OE2	22:1:1222:THR:N	2.44	0.47
23:3:519:VAL:HG13	23:3:524:ILE:HA	1.96	0.47
23:3:535:GLU:HG2	23:3:537:LYS:HZ2	1.79	0.47
23:3:804:HIS:ND1	23:3:805:ASN:HB2	2.28	0.47
40:9:323:ARG:NE	40:9:420:ASP:OD2	2.34	0.47
1:A:178:TYR:CD2	1:A:182:ILE:HB	2.49	0.47
1:A:322:ASN:ND2	3:C:655:VAL:O	2.47	0.47
1:A:426:LEU:H	1:A:426:LEU:HG	1.31	0.47
1:A:1086:ARG:C	1:A:1087:LEU:HD23	2.35	0.47
1:A:1134:TRP:HB3	1:A:1138:ALA:HB3	1.96	0.47
1:A:1179:SER:OG	1:A:1180:LYS:N	2.48	0.47
2:B:51:A:H4'	18:T:277:TYR:CE2	2.49	0.47
2:B:54:U:H2'	2:B:55:C:H6	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:87:GLN:HG3	18:T:239:LYS:O	2.14	0.47
3:C:318:PHE:CE1	3:C:373:ILE:HD13	2.41	0.47
3:C:839:PRO:HD2	3:C:842:CYS:SG	2.54	0.47
5:E:124:LEU:HB3	5:E:136:TRP:HB2	1.96	0.47
12:L:30:GLN:HE22	17:R:256:ASN:HD21	1.62	0.47
17:R:128:ASP:HB3	17:R:131:ASP:HB2	1.95	0.47
18:T:224:ALA:HA	18:T:248:THR:HG23	1.96	0.47
18:T:240:LEU:HD12	18:T:241:SER:H	1.80	0.47
20:Y:37:TRP:CZ3	20:Y:83:CYS:HB2	2.49	0.47
20:Y:44:PRO:HG2	20:Y:47:LEU:HD13	1.96	0.47
21:Z:566:TYR:CD2	21:Z:580:PRO:HG2	2.50	0.47
22:1:568:ARG:NH1	22:1:608:THR:OG1	2.47	0.47
1:A:303:ILE:HD12	3:C:659:VAL:HG21	1.97	0.47
1:A:614:TYR:O	1:A:618:THR:HG23	2.15	0.47
1:A:1086:ARG:O	1:A:1087:LEU:HD23	2.15	0.47
1:A:1545:ALA:CB	1:A:1563:HIS:NE2	2.68	0.47
1:A:1606:ILE:HA	1:A:1637:TRP:HZ2	1.79	0.47
1:A:1806:ALA:HA	1:A:1820:LYS:O	2.15	0.47
2:B:33:U:C2	2:B:34:U:C5	3.02	0.47
3:C:912:LEU:HD12	3:C:912:LEU:H	1.80	0.47
5:E:65:HIS:CE1	5:E:91:LEU:HD12	2.49	0.47
18:T:419:LEU:HA	18:T:428:VAL:O	2.15	0.47
20:Y:17:GLU:OE1	20:Y:27:SER:HA	2.14	0.47
22:1:869:MET:SD	22:1:910:MET:HA	2.55	0.47
22:1:1097:LEU:HD23	22:1:1097:LEU:HA	1.74	0.47
23:3:74:THR:OG1	23:3:74:THR:O	2.32	0.47
23:3:169:HIS:HD2	23:3:170:VAL:N	2.13	0.47
1:A:145:GLY:N	1:A:245:LEU:HD11	2.30	0.47
1:A:598:LEU:HD12	1:A:640:PHE:CZ	2.50	0.47
1:A:606:LYS:HG3	1:A:609:LYS:HZ3	1.78	0.47
2:B:8:G:C6	2:B:69:A:N6	2.77	0.47
2:B:24:G:C4	2:B:57:G:C2	3.02	0.47
2:B:47:A:N3	2:B:48:A:C8	2.83	0.47
2:B:110:C:H2’	2:B:111:A:C8	2.49	0.47
3:C:181:ILE:HA	3:C:211:PHE:CD2	2.50	0.47
3:C:209:VAL:HG21	3:C:899:SER:O	2.15	0.47
4:D:555:PHE:O	4:D:559:LEU:CB	2.63	0.47
8:H:6:U:H2’	8:H:7:U:C6	2.50	0.47
8:H:12:G:N7	8:H:13:C:C4	2.83	0.47
8:H:139:C:N4	8:H:140:A:H62	2.13	0.47
9:I:374:ILE:O	9:I:377:THR:N	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:332:VAL:HG22	10:J:335:ARG:HH11	1.78	0.47
11:K:170:ALA:HA	11:K:173:ILE:HD12	1.97	0.47
17:R:308:VAL:O	17:R:312:MET:HG3	2.14	0.47
18:T:208:ARG:HA	18:T:208:ARG:HD2	1.65	0.47
18:T:371:HIS:HE2	18:T:389:SER:HG	1.63	0.47
19:X:259:TRP:H	19:X:276:HIS:HB3	1.80	0.47
22:1:118:GLU:HA	22:1:121:LYS:CG	2.44	0.47
22:1:493:LYS:O	22:1:497:ILE:HG22	2.14	0.47
22:1:677:CYS:SG	38:7:48:GLU:HA	2.55	0.47
23:3:13:GLY:O	23:3:34:ARG:HD3	2.13	0.47
23:3:206:GLN:NE2	23:3:232:GLY:N	2.58	0.47
23:3:318:ASP:O	23:3:321:MET:N	2.48	0.47
23:3:473:TYR:CE1	23:3:497:SER:HB2	2.49	0.47
23:3:913:LEU:HA	23:3:913:LEU:HD23	1.57	0.47
37:6:47:GLN:HG2	37:6:48:ILE:H	1.79	0.47
37:6:53:THR:O	37:6:57:ARG:N	2.39	0.47
40:9:239:ALA:HA	40:9:266:ILE:HB	1.97	0.47
40:9:352:ASP:HB3	40:9:354:PHE:CZ	2.49	0.47
41:8:19:ASN:OD1	41:8:22:LYS:N	2.23	0.47
41:8:45:LEU:HA	41:8:48:ILE:HG13	1.97	0.47
1:A:242:ALA:O	1:A:246:LEU:HG	2.15	0.47
1:A:301:LYS:HD3	3:C:940:ARG:HA	1.96	0.47
1:A:891:PHE:O	12:L:83:ARG:NH2	2.38	0.47
1:A:1209:HIS:CD2	1:A:1210:LYS:H	2.29	0.47
1:A:1529:ILE:HG22	1:A:1530:PRO:HD2	1.96	0.47
1:A:1723:LYS:HE3	1:A:1723:LYS:HB2	1.72	0.47
2:B:100:C:H2’	2:B:101:U:C5	2.50	0.47
3:C:404:THR:O	3:C:408:LEU:HG	2.15	0.47
3:C:785:ARG:HA	3:C:785:ARG:HD3	1.71	0.47
7:G:7:G:H2’	7:G:8:C:H6	1.79	0.47
7:G:83:A:P	7:G:83:A:C8	3.08	0.47
7:G:88:G:C6	8:H:42:G:C6	3.03	0.47
10:J:399:TYR:HB3	10:J:419:PHE:CE2	2.49	0.47
11:K:33:LYS:CD	11:K:44:HIS:CE1	2.98	0.47
11:K:45:CYS:HA	11:K:50:HIS:HB3	1.97	0.47
11:K:74:ASN:OD1	11:K:74:ASN:N	2.48	0.47
11:K:176:GLN:O	23:3:690:ARG:NH2	2.48	0.47
23:3:212:GLU:OE1	23:3:223:LYS:HD2	2.15	0.47
37:6:19:ARG:O	37:6:63:VAL:HA	2.14	0.47
1:A:233:PRO:O	1:A:237:THR:OG1	2.32	0.47
1:A:386:PRO:HA	3:C:327:TYR:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:GLN:HA	1:A:502:ASN:ND2	2.29	0.47
1:A:685:LEU:HD11	1:A:742:TYR:HD1	1.79	0.47
1:A:800:TYR:CD1	3:C:59:LEU:HA	2.50	0.47
1:A:1457:HIS:ND1	1:A:1460:HIS:CD2	2.82	0.47
1:A:1684:PHE:CB	1:A:1715:TYR:HD2	2.27	0.47
1:A:1785:VAL:HA	1:A:1806:ALA:H	1.79	0.47
3:C:343:LEU:O	3:C:369:PHE:HB2	2.15	0.47
3:C:531:TRP:CH2	3:C:553:GLU:HB2	2.49	0.47
6:F:68:C:N4	18:T:320:LYS:HD2	2.30	0.47
7:G:93:A:C2	8:H:38:A:C2	3.02	0.47
8:H:27:U:O2’	8:H:28:C:H5’	2.15	0.47
10:J:262:ARG:NH2	10:J:291:GLN:HG2	2.29	0.47
18:T:418:THR:HG21	18:T:467:ALA:HA	1.97	0.47
22:1:477:LYS:HB2	22:1:499:LYS:HZ1	1.78	0.47
22:1:871:THR:C	22:1:875:ILE:HD12	2.36	0.47
22:1:1199:VAL:HG12	22:1:1199:VAL:O	2.15	0.47
23:3:7:THR:OG1	23:3:8:LEU:N	2.47	0.47
23:3:8:LEU:HA	23:3:8:LEU:HD12	1.69	0.47
23:3:255:TYR:CG	23:3:268:ARG:NH2	2.83	0.47
23:3:341:VAL:HG22	23:3:347:LEU:HD12	1.97	0.47
23:3:926:TYR:HB3	23:3:928:TYR:CE2	2.40	0.47
41:8:19:ASN:HD21	41:8:21:GLN:NE2	2.13	0.47
3:C:311:SER:HB2	3:C:316:ILE:HB	1.97	0.47
3:C:445:ALA:HB1	3:C:448:LYS:HZ1	1.80	0.47
8:H:52:G:H2’	8:H:53:U:H6	1.80	0.47
11:K:29:GLN:O	11:K:32:GLN:HG3	2.14	0.47
18:T:324:HIS:CE1	18:T:362:GLY:HA3	2.50	0.47
19:X:234:GLU:O	19:X:238:THR:CB	2.62	0.47
22:1:421:TYR:O	22:1:425:ARG:N	2.34	0.47
23:3:169:HIS:ND1	23:3:234:PHE:HB2	2.30	0.47
23:3:195:ASP:OD2	23:3:200:ALA:N	2.39	0.47
39:5:13:HIS:ND1	41:8:15:ASN:HB3	2.29	0.47
40:9:397:PHE:N	40:9:397:PHE:HD1	2.13	0.47
41:8:115:ASN:ND2	41:8:119:ILE:O	2.29	0.47
1:A:265:THR:HG23	1:A:327:VAL:HG13	1.96	0.46
1:A:277:PRO:HD3	1:A:451:LEU:HD13	1.96	0.46
1:A:540:PHE:O	1:A:545:HIS:NE2	2.46	0.46
1:A:1310:ARG:NH2	1:A:1310:ARG:HA	2.31	0.46
3:C:623:GLU:OE2	3:C:941:LYS:HB3	2.15	0.46
6:F:85:U:N3	8:H:14:C:C4	2.78	0.46
10:J:429:PHE:CE1	10:J:433:ARG:HG2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:280:ILE:HG22	17:R:281:ASN:O	2.15	0.46
18:T:223:SER:HG	18:T:225:ASP:H	1.54	0.46
22:1:445:HIS:O	22:1:445:HIS:ND1	2.49	0.46
22:1:878:ASN:OD1	22:1:878:ASN:N	2.47	0.46
22:1:981:TYR:O	22:1:983:GLY:N	2.48	0.46
23:3:21:ASN:ND2	23:3:28:GLN:HG3	2.29	0.46
23:3:524:ILE:HD13	23:3:566:PHE:HZ	1.80	0.46
23:3:727:SER:OG	23:3:728:ARG:NH1	2.47	0.46
37:6:81:ASN:HB2	37:6:86:TYR:CE1	2.49	0.46
1:A:1661:TRP:O	1:A:1700:GLY:CA	2.63	0.46
1:A:1662:ILE:HD12	1:A:1701:VAL:HG12	1.97	0.46
1:A:1779:PHE:O	1:A:1809:ILE:HA	2.15	0.46
2:B:88:A:H4’	2:B:94:U:O4	2.15	0.46
3:C:620:LYS:NZ	3:C:630:LEU:HD11	2.31	0.46
3:C:779:LEU:HD11	3:C:911:PRO:HG3	1.97	0.46
5:E:336:HIS:ND1	5:E:337:PRO:HD2	2.30	0.46
7:G:102:G:N2	7:G:103:U:H2’	2.31	0.46
17:R:150:ALA:HA	17:R:153:LYS:CD	2.46	0.46
22:1:539:LEU:HD12	22:1:539:LEU:HA	1.67	0.46
22:1:850:ILE:H	22:1:850:ILE:HG12	1.49	0.46
22:1:1062:LEU:HA	22:1:1062:LEU:HD23	1.67	0.46
22:1:1197:LEU:HD23	22:1:1197:LEU:HA	1.73	0.46
23:3:169:HIS:CD2	23:3:170:VAL:N	2.83	0.46
23:3:369:GLU:H	23:3:369:GLU:CD	2.18	0.46
1:A:488:ASP:O	1:A:492:VAL:HG23	2.14	0.46
1:A:595:LYS:HE2	1:A:597:LYS:HB2	1.95	0.46
1:A:1640:SER:CA	1:A:1652:MET:HA	2.44	0.46
1:A:1732:LYS:HA	1:A:1732:LYS:HD2	1.71	0.46
3:C:127:GLU:O	3:C:130:ARG:NH2	2.46	0.46
3:C:168:THR:HG22	3:C:184:THR:HG21	1.98	0.46
7:G:15:U:H3’	7:G:16:G:H8	1.80	0.46
10:J:436:TYR:CD1	10:J:437:LYS:HD2	2.51	0.46
11:K:157:LYS:HA	11:K:157:LYS:HD3	1.72	0.46
18:T:326:LEU:HB3	18:T:357:TRP:CE3	2.50	0.46
19:X:353:LYS:HE2	19:X:353:LYS:HB2	1.63	0.46
22:1:120:LYS:O	22:1:123:ARG:HB3	2.16	0.46
22:1:508:THR:OG1	22:1:510:PRO:HD2	2.15	0.46
22:1:940:LEU:HD12	22:1:940:LEU:HA	1.70	0.46
23:3:609:LEU:HD12	23:3:611:ASP:OD2	2.16	0.46
37:6:93:ASN:O	37:6:95:ASN:N	2.49	0.46
41:8:51:TRP:HB2	41:8:123:PHE:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ARG:HD3	1:A:82:ARG:HH11	1.80	0.46
1:A:263:PHE:CZ	1:A:277:PRO:HD2	2.50	0.46
1:A:1554:GLN:O	1:A:1554:GLN:HG2	2.15	0.46
1:A:1580:HIS:CB	1:A:1584:LYS:HE3	2.45	0.46
1:A:1614:ILE:HG23	1:A:1618:LYS:HB2	1.96	0.46
3:C:325:LYS:O	3:C:325:LYS:HD3	2.15	0.46
3:C:375:GLU:HG3	3:C:379:LYS:NZ	2.29	0.46
3:C:825:PRO:HG2	3:C:912:LEU:HD11	1.96	0.46
6:F:85:U:C2'	6:F:86:U:H5'	2.45	0.46
7:G:112:U:H2'	7:G:113:U:O4'	2.16	0.46
11:K:70:GLU:O	11:K:73:ARG:N	2.48	0.46
12:L:77:LEU:HD13	17:R:284:PHE:HB3	1.96	0.46
17:R:150:ALA:HB3	18:T:360:VAL:HG21	1.97	0.46
18:T:216:ASN:HD21	18:T:473:SER:H	1.63	0.46
18:T:316:ASP:OD1	18:T:318:ARG:N	2.49	0.46
19:X:303:HIS:CE1	19:X:333:SER:HB2	2.51	0.46
22:1:1051:SER:HG	22:1:1054:GLU:H	1.59	0.46
23:3:1043:THR:HG22	23:3:1057:ARG:HE	1.81	0.46
38:7:49:CYS:HB3	38:7:87:LYS:HD3	1.98	0.46
40:9:292:ASN:ND2	40:9:402:GLY:HA3	2.31	0.46
1:A:703:GLN:C	1:A:705:LYS:H	2.19	0.46
1:A:856:LEU:HD23	1:A:856:LEU:HA	1.70	0.46
1:A:1053:LEU:HD11	1:A:1088:PHE:CD2	2.50	0.46
1:A:1243:ARG:HH11	1:A:1243:ARG:HG3	1.80	0.46
1:A:1551:PHE:CD1	1:A:1553:VAL:CG2	2.98	0.46
1:A:2124:ILE:O	1:A:2179:HIS:HA	2.16	0.46
3:C:187:THR:HG23	3:C:201:ASN:OD1	2.16	0.46
3:C:232:ALA:HB3	3:C:262:ARG:NH2	2.31	0.46
3:C:448:LYS:HZ2	3:C:497:LEU:HD22	1.79	0.46
5:E:304:SER:O	5:E:330:ILE:N	2.45	0.46
8:H:48:A:H2'	8:H:49:U:C6	2.49	0.46
8:H:118:G:O6	8:H:140:A:N6	2.48	0.46
23:3:524:ILE:HG21	23:3:566:PHE:CE2	2.51	0.46
23:3:566:PHE:N	23:3:566:PHE:CD1	2.82	0.46
36:4:33:PHE:HA	36:4:36:ALA:HB3	1.97	0.46
38:7:39:PRO:HB2	38:7:70:TYR:CD1	2.50	0.46
40:9:299:LEU:HD21	40:9:357:ASN:OD1	2.16	0.46
1:A:464:PRO:CB	1:A:467:GLN:HE21	2.29	0.46
1:A:723:ASN:ND2	1:A:788:GLN:OE1	2.49	0.46
2:B:46:U:C4	2:B:47:A:N6	2.82	0.46
3:C:220:ARG:HG2	3:C:479:THR:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:133:VAL:O	5:E:147:LEU:HG	2.16	0.46
6:F:47:A:H5”	6:F:48:A:O5’	2.15	0.46
7:G:102:G:H4’	38:7:25:LYS:HE2	1.97	0.46
7:G:105:C:OP2	7:G:105:C:H3’	2.15	0.46
8:H:64:A:H2’	8:H:65:U:C6	2.51	0.46
11:K:29:GLN:C	11:K:32:GLN:H	2.18	0.46
18:T:216:ASN:OD1	18:T:472:GLN:N	2.36	0.46
19:X:255:PRO:HD2	19:X:276:HIS:O	2.16	0.46
22:1:834:VAL:HG13	22:1:871:THR:HG22	1.98	0.46
22:1:903:GLN:OE1	22:1:910:MET:HG3	2.15	0.46
22:1:984:GLU:CD	22:1:986:TYR:H	2.17	0.46
22:1:1133:MET:CE	35:2:528:ILE:CD1	2.93	0.46
22:1:1211:LEU:HD23	22:1:1211:LEU:HA	1.74	0.46
23:3:519:VAL:HG22	23:3:524:ILE:HG23	1.98	0.46
23:3:753:GLY:HA3	23:3:765:LEU:O	2.15	0.46
35:2:532:GLY:C	35:2:534:GLN:H	2.19	0.46
37:6:17:VAL:HG23	37:6:91:TYR:CZ	2.51	0.46
1:A:79:ARG:NH2	6:F:29:A:H5’	2.27	0.46
1:A:110:TRP:HB2	1:A:208:TYR:CD1	2.50	0.46
1:A:499:GLN:O	1:A:502:ASN:HB2	2.15	0.46
1:A:587:GLN:O	1:A:588:LEU:HD23	2.16	0.46
1:A:794:TYR:HD1	1:A:800:TYR:CE2	2.31	0.46
1:A:1418:ARG:HD3	1:A:1418:ARG:HA	1.32	0.46
1:A:1485:LEU:HD13	1:A:1490:PHE:CD2	2.50	0.46
2:B:40:U:H3	7:G:0:G:N2	2.14	0.46
5:E:249:TYR:CD2	5:E:263:ASP:HB3	2.51	0.46
10:J:381:LYS:HA	10:J:381:LYS:HE3	1.98	0.46
10:J:393:ALA:O	10:J:397:LYS:HG3	2.16	0.46
11:K:33:LYS:HD2	11:K:44:HIS:HE1	1.81	0.46
11:K:112:TRP:HA	11:K:117:ASP:OD2	2.16	0.46
11:K:159:LYS:O	11:K:163:LEU:HD12	2.15	0.46
17:R:416:LYS:HE2	17:R:416:LYS:HB2	1.72	0.46
23:3:780:PRO:O	23:3:781:LEU:HD23	2.15	0.46
23:3:970:TYR:HD1	23:3:977:LEU:HB3	1.80	0.46
35:2:456:ARG:HA	35:2:459:ARG:NE	2.30	0.46
40:9:330:ILE:HG21	40:9:407:LEU:HD11	1.97	0.46
40:9:367:SER:HA	40:9:396:ILE:HA	1.97	0.46
1:A:88:TYR:CZ	1:A:125:ALA:HA	2.51	0.46
1:A:283:VAL:O	1:A:284:ARG:HB2	2.15	0.46
1:A:564:TYR:HB3	1:A:574:LEU:HD13	1.97	0.46
1:A:566:LEU:HB3	1:A:568:ASN:ND2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:974:ASN:OD1	1:A:974:ASN:N	2.49	0.46
1:A:1144:LYS:HA	1:A:1147:VAL:CG1	2.46	0.46
1:A:1229:PHE:N	1:A:1229:PHE:HD1	2.14	0.46
1:A:1411:SER:O	1:A:1413:ASP:N	2.49	0.46
1:A:1712:HIS:ND1	1:A:1734:MET:HG3	2.31	0.46
3:C:142:LYS:HB2	45:C:1500:GTP:O2B	2.15	0.46
3:C:231:ALA:O	3:C:277:LYS:HE3	2.15	0.46
3:C:833:PHE:O	3:C:899:SER:HA	2.16	0.46
5:E:175:THR:HB	5:E:189:THR:HG23	1.97	0.46
5:E:277:PHE:HE1	5:E:317:ARG:HG2	1.80	0.46
5:E:348:ASP:O	5:E:350:ARG:HG3	2.16	0.46
7:G:-1:C:H2'	7:G:0:G:O4'	2.16	0.46
8:H:51:A:C4	8:H:52:G:C8	3.03	0.46
8:H:59:A:H2'	8:H:60:U:O4'	2.15	0.46
17:R:252:SER:HB3	17:R:255:LYS:H	1.81	0.46
22:1:900:PHE:CE2	22:1:954:LEU:HD22	2.50	0.46
23:3:665:LEU:HD21	23:3:667:ILE:HG13	1.97	0.46
1:A:68:LYS:NZ	13:N:45:SER:O	2.20	0.46
1:A:151:MET:HE2	1:A:628:GLY:N	2.31	0.46
1:A:462:ARG:HB3	1:A:465:LYS:HD2	1.97	0.46
1:A:1298:ARG:HD2	1:A:1298:ARG:HA	1.42	0.46
2:B:30:A:C4	2:B:31:U:C5	3.04	0.46
3:C:371:GLU:O	3:C:371:GLU:HG2	2.14	0.46
3:C:434:CYS:O	3:C:438:ILE:N	2.39	0.46
4:D:1803:SER:O	4:D:1810:VAL:HA	2.15	0.46
5:E:91:LEU:HD13	5:E:93:TRP:CZ2	2.50	0.46
7:G:15:U:H2'	7:G:16:G:O4'	2.16	0.46
7:G:19:G:H2'	7:G:19:G:N3	2.31	0.46
8:H:157:G:H2'	8:H:158:G:C8	2.51	0.46
10:J:235:ILE:HG21	10:J:245:TRP:CE2	2.51	0.46
11:K:35:CYS:HB2	11:K:44:HIS:NE2	2.31	0.46
16:Q:1136:GLN:H	16:Q:1156:ASN:HA	1.81	0.46
16:Q:1226:ILE:O	16:Q:1257:VAL:HA	2.16	0.46
22:1:400:SER:H	22:1:403:GLU:HB2	1.81	0.46
22:1:1126:PHE:HE1	35:2:576:PHE:HZ	1.64	0.46
23:3:624:CYS:SG	23:3:625:LEU:HG	2.56	0.46
23:3:999:ARG:NH1	23:3:1024:PHE:HZ	2.12	0.46
40:9:269:ASP:HA	40:9:272:ARG:HB2	1.98	0.46
41:8:111:SER:O	41:8:114:GLU:HG3	2.16	0.46
1:A:139:VAL:HG11	1:A:212:PRO:HG3	1.98	0.46
1:A:821:ARG:HH11	1:A:821:ARG:CG	2.28	0.46

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:A:1619:SER:OG	1:A:1620:TYR:N	2.49	0.46
1:A:1706:ASP:O	1:A:1710:ASN:N	2.49	0.46
7:G:98:U:H5”	7:G:99:C:OP2	2.16	0.46
8:H:47:U:H1’	8:H:48:A:C8	2.50	0.46
8:H:72:U:H2’	8:H:73:C:H6	1.80	0.46
8:H:172:C:H2’	8:H:173:C:H6	1.79	0.46
17:R:134:ARG:HH12	18:T:382:PRO:C	2.20	0.46
18:T:303:LEU:HA	18:T:303:LEU:HD23	1.67	0.46
18:T:308:ARG:HA	18:T:332:ALA:HB1	1.97	0.46
22:1:164:GLU:O	22:1:168:ILE:HG12	2.15	0.46
22:1:170:GLN:HG2	22:1:171:GLN:HE21	1.79	0.46
22:1:565:ASP:O	22:1:567:VAL:N	2.49	0.46
22:1:1126:PHE:CE2	35:2:572:HIS:CD2	2.89	0.46
22:1:1151:LEU:HD23	22:1:1151:LEU:HA	1.57	0.46
37:6:22:TYR:CE2	37:6:24:ARG:HD3	2.51	0.46
1:A:356:ILE:HD13	3:C:267:LEU:HD22	1.97	0.45
1:A:516:LEU:HD23	1:A:526:PRO:HA	1.98	0.45
1:A:843:LEU:HA	1:A:843:LEU:HD23	1.75	0.45
1:A:1571:ILE:HD11	11:K:16:ILE:HD11	1.97	0.45
2:B:108:G:H3’	2:B:109:G:H8	1.81	0.45
3:C:561:LYS:NZ	3:C:617:LEU:O	2.40	0.45
3:C:645:ARG:NH2	3:C:655:VAL:HG23	2.31	0.45
3:C:911:PRO:O	3:C:931:ARG:HD3	2.16	0.45
8:H:13:C:H6	8:H:14:C:H41	1.64	0.45
10:J:242:ILE:HA	10:J:245:TRP:HB2	1.97	0.45
10:J:292:VAL:O	10:J:296:ARG:HG3	2.16	0.45
18:T:189:GLN:HG2	18:T:190:TRP:N	2.31	0.45
18:T:308:ARG:HA	18:T:332:ALA:CB	2.45	0.45
20:Y:69:ARG:HB3	20:Y:76:SER:HA	1.98	0.45
22:1:112:ILE:HG23	22:1:115:ARG:HE	1.80	0.45
22:1:728:LEU:O	22:1:731:LEU:HB2	2.15	0.45
22:1:1080:THR:HA	22:1:1083:TYR:CD2	2.51	0.45
35:2:584:LEU:HD12	35:2:584:LEU:N	2.31	0.45
1:A:195:LEU:HB2	1:A:204:LEU:HD12	1.97	0.45
1:A:311:GLU:H	1:A:311:GLU:HG3	1.39	0.45
1:A:1303:LEU:HB3	1:A:1566:ILE:CG2	2.45	0.45
1:A:1312:PRO:O	1:A:1312:PRO:HG2	2.15	0.45
3:C:167:TYR:CE2	3:C:535:ALA:HB3	2.51	0.45
3:C:470:PRO:HB3	3:C:545:PRO:CB	2.46	0.45
4:D:560:ALA:O	4:D:563:GLY:N	2.49	0.45
4:D:1205:THR:HA	4:D:1248:ASP:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:42:C:O2'	6:F:43:A:H5'	2.17	0.45
11:K:73:ARG:NH2	11:K:74:ASN:OD1	2.48	0.45
11:K:151:ARG:HH11	11:K:155:LEU:HD12	1.80	0.45
18:T:316:ASP:N	18:T:321:ALA:O	2.35	0.45
20:Y:37:TRP:HA	20:Y:82:LEU:O	2.16	0.45
22:1:112:ILE:H	22:1:112:ILE:HD12	1.81	0.45
23:3:53:LEU:HA	23:3:53:LEU:HD23	1.56	0.45
23:3:1049:LYS:HE2	39:5:52:TYR:HE1	1.81	0.45
23:3:1096:HIS:HD2	23:3:1166:TYR:HB3	1.82	0.45
23:3:1168:PHE:N	23:3:1168:PHE:CD2	2.83	0.45
38:7:93:SER:O	38:7:96:THR:OG1	2.34	0.45
1:A:161:PHE:O	1:A:625:PRO:HG2	2.16	0.45
1:A:350:PHE:CZ	3:C:382:ALA:HB2	2.51	0.45
1:A:608:LEU:HD23	1:A:608:LEU:HA	1.78	0.45
1:A:1606:ILE:CG2	1:A:1631:LEU:HB3	2.47	0.45
1:A:1670:ASP:CG	1:A:1672:ASP:H	2.19	0.45
3:C:154:HIS:HB2	3:C:157:ILE:HG22	1.99	0.45
3:C:181:ILE:HG23	3:C:211:PHE:CE1	2.51	0.45
3:C:287:GLY:O	3:C:291:MET:HG3	2.16	0.45
3:C:610:VAL:HA	3:C:613:SER:OG	2.17	0.45
6:F:53:A:H8	6:F:53:A:OP2	2.00	0.45
7:G:95:U:C2	8:H:36:G:N2	2.85	0.45
11:K:79:LEU:HD13	11:K:98:TYR:HA	1.98	0.45
11:K:121:TRP:CA	11:K:124:ARG:HH21	2.27	0.45
19:X:261:LEU:O	19:X:263:PRO:HD3	2.16	0.45
22:1:939:ARG:HD2	22:1:939:ARG:HA	1.58	0.45
22:1:1010:THR:O	22:1:1012:PRO:HD3	2.17	0.45
22:1:1267:LYS:HE2	22:1:1267:LYS:HB2	1.24	0.45
23:3:131:MET:HB2	23:3:141:VAL:HG22	1.98	0.45
23:3:1121:THR:OG1	23:3:1122:LEU:N	2.47	0.45
40:9:266:ILE:HG23	40:9:267:ASP:N	2.31	0.45
1:A:255:PHE:CZ	1:A:432:ARG:HB3	2.51	0.45
1:A:414:ARG:HH11	3:C:415:LEU:HD11	1.82	0.45
1:A:755:HIS:CD2	15:P:219:PHE:HE2	2.34	0.45
1:A:939:TRP:CD1	1:A:939:TRP:C	2.89	0.45
1:A:1307:MET:SD	1:A:1308:PRO:N	2.84	0.45
1:A:1629:ILE:HB	1:A:1662:ILE:HB	1.98	0.45
2:B:18:C:C2	2:B:60:G:C2	3.04	0.45
2:B:18:C:N4	2:B:59:G:O6	2.49	0.45
2:B:35:U:O4	2:B:36:C:N4	2.49	0.45
3:C:189:VAL:HG13	3:C:197:SER:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:230:ASP:OD2	3:C:233:GLU:HB2	2.16	0.45
3:C:288:LEU:HA	3:C:291:MET:SD	2.56	0.45
5:E:71:CYS:HA	5:E:332:GLU:OE1	2.17	0.45
5:E:116:HIS:O	5:E:124:LEU:HD12	2.17	0.45
6:F:5:U:O3’	6:F:6:C:H4’	2.16	0.45
7:G:-3:A:C2	7:G:-2:A:C5	3.05	0.45
7:G:10:U:O4	7:G:11:A:N6	2.49	0.45
11:K:33:LYS:HB3	11:K:44:HIS:HE1	1.81	0.45
11:K:148:THR:CG2	11:K:151:ARG:HH21	2.28	0.45
12:L:38:LEU:H	12:L:38:LEU:CD2	2.20	0.45
22:1:151:THR:O	22:1:155:VAL:HG23	2.17	0.45
22:1:578:ILE:HD13	22:1:578:ILE:HA	1.73	0.45
22:1:751:GLY:HA3	22:1:791:VAL:HG22	1.97	0.45
22:1:1019:ARG:NH1	22:1:1019:ARG:O	2.49	0.45
22:1:1172:LEU:O	22:1:1175:ASP:N	2.48	0.45
22:1:1281:ILE:HA	22:1:1281:ILE:HD13	1.58	0.45
23:3:8:LEU:HB2	23:3:1126:ILE:O	2.17	0.45
23:3:457:ASN:ND2	23:3:479:VAL:HA	2.31	0.45
23:3:1098:GLY:C	23:3:1099:GLU:HG3	2.36	0.45
37:6:101:MET:HE1	37:6:106:LYS:HG2	1.99	0.45
38:7:74:GLU:O	38:7:77:ILE:N	2.44	0.45
40:9:328:PHE:CD2	40:9:329:VAL:HG13	2.52	0.45
41:8:106:TRP:N	41:8:107:PRO:HD2	2.31	0.45
1:A:409:ARG:N	1:A:410:PRO:HD2	2.31	0.45
1:A:634:TRP:HE1	1:A:638:LEU:HD11	1.80	0.45
1:A:685:LEU:HD12	1:A:685:LEU:HA	1.75	0.45
1:A:1576:ILE:O	1:A:1746:ARG:NH2	2.46	0.45
3:C:183:SER:HB3	3:C:205:THR:HG22	1.98	0.45
3:C:222:SER:OG	3:C:251:LEU:HD11	2.16	0.45
3:C:599:GLU:HG3	3:C:602:LYS:HB2	1.98	0.45
3:C:833:PHE:CZ	3:C:835:GLU:HB2	2.52	0.45
4:D:965:ASP:HA	4:D:970:VAL:O	2.17	0.45
6:F:36:A:N1	7:G:9:C:N3	2.64	0.45
6:F:41:A:O2’	6:F:42:C:H5’	2.16	0.45
6:F:43:A:H2’	6:F:44:G:N9	2.31	0.45
6:F:62:C:N3	6:F:73:A:H2	2.15	0.45
6:F:63:C:N3	6:F:72:G:N1	2.65	0.45
11:K:129:LYS:HG2	11:K:131:ASP:OD1	2.17	0.45
12:L:74:LEU:HD23	12:L:74:LEU:HA	1.60	0.45
16:Q:82:SER:O	16:Q:86:SER:N	2.50	0.45
17:R:138:GLU:CD	17:R:138:GLU:N	2.70	0.45

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
21:Z:587:VAL:HG12	21:Z:589:ARG:NH1	2.32	0.45
22:1:613:MET:HG3	22:1:632:PHE:CE2	2.52	0.45
22:1:1024:LEU:HD23	22:1:1024:LEU:HA	1.69	0.45
40:9:235:LYS:HZ1	40:9:452:GLN:HB2	1.81	0.45
40:9:287:ASN:HD21	40:9:426:ILE:HA	1.82	0.45
1:A:213:LEU:O	1:A:216:SER:OG	2.22	0.45
1:A:378:PHE:CE1	3:C:338:GLU:HB2	2.52	0.45
1:A:762:ARG:HH22	15:P:226:LYS:HZ3	1.63	0.45
1:A:1234:ASP:O	1:A:1235:GLU:C	2.55	0.45
1:A:1425:LYS:N	17:R:415:SER:O	2.42	0.45
1:A:1817:LEU:O	1:A:1916:LEU:HA	2.16	0.45
2:B:88:A:H2’	2:B:88:A:N3	2.32	0.45
3:C:86:THR:OG1	18:T:239:LYS:HA	2.16	0.45
3:C:510:LEU:HD22	3:C:514:TYR:CZ	2.51	0.45
8:H:121:A:N3	8:H:121:A:H2’	2.32	0.45
12:L:23:VAL:HG11	12:L:50:TRP:CH2	2.51	0.45
18:T:196:LEU:HD21	18:T:199:VAL:HG23	1.98	0.45
18:T:387:PHE:CE1	18:T:398:TRP:HB2	2.51	0.45
19:X:260:ARG:HH12	19:X:372:GLU:HA	1.82	0.45
22:1:415:LEU:HD22	37:6:32:ALA:HB2	1.97	0.45
22:1:807:LYS:HA	22:1:811:LEU:CD1	2.46	0.45
22:1:922:GLY:O	22:1:925:VAL:HG12	2.16	0.45
22:1:962:MET:SD	22:1:970:LEU:HD21	2.56	0.45
22:1:1110:VAL:O	22:1:1113:THR:HB	2.17	0.45
22:1:1153:PHE:O	22:1:1157:TYR:HD2	1.99	0.45
23:3:519:VAL:HG11	23:3:544:ILE:HD13	1.98	0.45
35:2:533:ILE:HD13	35:2:533:ILE:H	1.82	0.45
1:A:642:ARG:NH2	2:B:55:C:O2	2.39	0.45
1:A:1030:ILE:HG12	1:A:1031:ILE:N	2.31	0.45
1:A:1232:VAL:HG22	1:A:1274:PHE:CD1	2.52	0.45
1:A:1393:ARG:HG2	17:R:405:VAL:HG11	1.98	0.45
2:B:20:G:H2’	2:B:20:G:N3	2.31	0.45
3:C:684:LYS:HE3	3:C:793:ASP:OD2	2.17	0.45
7:G:12:G:N2	7:G:13:C:H1’	2.31	0.45
8:H:7:U:H2’	8:H:8:C:H6	1.81	0.45
10:J:396:ARG:O	10:J:400:GLU:HG2	2.17	0.45
11:K:360:ILE:O	20:Y:72:LYS:CG	2.64	0.45
17:R:299:ARG:NH1	22:1:448:THR:OG1	2.50	0.45
18:T:297:HIS:HB3	18:T:300:ILE:O	2.16	0.45
18:T:454:VAL:HB	18:T:458:SER:OG	2.16	0.45
20:Y:37:TRP:CH2	20:Y:83:CYS:HB2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1:956:SER:OG	22:1:957:ARG:N	2.49	0.45
22:1:1062:LEU:HD23	22:1:1065:LEU:HD12	1.99	0.45
23:3:128:ARG:NH2	23:3:178:GLU:O	2.49	0.45
23:3:556:ILE:O	23:3:556:ILE:HG13	2.17	0.45
23:3:644:GLU:HA	23:3:662:PHE:O	2.17	0.45
1:A:136:ILE:HG21	1:A:230:PHE:CE2	2.52	0.45
1:A:755:HIS:CD2	15:P:219:PHE:CE2	3.05	0.45
1:A:1215:ASN:HB3	1:A:1224:ARG:HE	1.81	0.45
1:A:1552:GLN:O	1:A:1554:GLN:N	2.50	0.45
3:C:143:THR:HG21	3:C:169:ASP:OD1	2.16	0.45
3:C:824:THR:O	3:C:824:THR:OG1	2.32	0.45
5:E:89:LEU:HD13	5:E:91:LEU:HG	1.98	0.45
5:E:166:LEU:HD23	5:E:201:PHE:HE1	1.81	0.45
5:E:224:GLN:NE2	5:E:228:THR:OG1	2.50	0.45
8:H:118:G:H2’	8:H:119:G:C8	2.52	0.45
10:J:225:LEU:O	10:J:229:LYS:HG3	2.16	0.45
21:Z:600:ARG:HG2	21:Z:600:ARG:HH11	1.80	0.45
22:1:169:ARG:HH11	22:1:397:ARG:HG2	1.80	0.45
22:1:643:SER:OG	22:1:644:LEU:N	2.50	0.45
22:1:685:SER:HA	22:1:688:GLU:OE1	2.16	0.45
22:1:948:ARG:NH2	22:1:984:GLU:OE1	2.49	0.45
22:1:1048:GLU:HG2	22:1:1049:TYR:N	2.31	0.45
23:3:442:LEU:HB2	23:3:734:LEU:HD22	1.98	0.45
23:3:635:ALA:HB3	23:3:669:LEU:HD23	1.99	0.45
23:3:817:GLN:HA	23:3:843:LEU:HD11	1.98	0.45
23:3:1022:ILE:HD13	23:3:1022:ILE:HA	1.59	0.45
35:2:532:GLY:O	35:2:534:GLN:N	2.49	0.45
38:7:9:ILE:O	38:7:88:ILE:HA	2.17	0.45
1:A:400:ASN:ND2	1:A:400:ASN:H	2.14	0.45
1:A:1016:VAL:HG22	1:A:1025:THR:HG22	1.98	0.45
1:A:1539:SER:O	1:A:1542:ILE:N	2.49	0.45
1:A:1661:TRP:O	1:A:1662:ILE:HD13	2.16	0.45
3:C:315:SER:O	3:C:420:CYS:HB3	2.17	0.45
3:C:416:LEU:HA	3:C:419:VAL:HG12	1.99	0.45
5:E:113:MET:N	5:E:127:ALA:O	2.49	0.45
5:E:242:SER:C	5:E:250:LEU:HD12	2.37	0.45
8:H:7:U:H2’	8:H:8:C:C6	2.52	0.45
8:H:42:G:C6	8:H:43:U:C4	3.05	0.45
10:J:326:VAL:HG13	10:J:352:PHE:CZ	2.51	0.45
16:Q:360:ASP:O	16:Q:413:ARG:N	2.48	0.45
19:X:262:TYR:CE2	19:X:370:LEU:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:X:317:ASP:OD1	19:X:317:ASP:N	2.37	0.45
21:Z:575:ARG:HG3	21:Z:597:ARG:NH1	2.32	0.45
22:1:157:ARG:O	22:1:161:LEU:HD22	2.17	0.45
22:1:579:GLU:HB2	22:1:580:PRO:HD3	1.98	0.45
22:1:838:VAL:HG12	22:1:842:ASN:HD21	1.81	0.45
22:1:860:GLU:O	22:1:865:ARG:NH2	2.46	0.45
23:3:42:ARG:NH2	23:3:53:LEU:HD11	2.32	0.45
23:3:520:TYR:CE1	23:3:522:ASP:HB2	2.52	0.45
35:2:654:ASN:O	35:2:685:ASP:N	2.36	0.45
41:8:26:LYS:HA	41:8:26:LYS:HD3	1.64	0.45
1:A:591:MET:HA	1:A:594:TYR:CD2	2.52	0.45
1:A:597:LYS:O	1:A:600:ARG:HG2	2.17	0.45
1:A:796:LYS:HG3	17:R:279:HIS:HD2	1.82	0.45
1:A:1299:ILE:HD13	1:A:1316:PHE:HE1	1.76	0.45
1:A:1538:TRP:O	1:A:1542:ILE:HG13	2.16	0.45
2:B:19:A:C2	2:B:59:G:C4	3.05	0.45
6:F:72:G:C6	6:F:73:A:C6	3.05	0.45
10:J:350:ILE:HD12	10:J:350:ILE:HA	1.84	0.45
10:J:359:VAL:HG11	10:J:391:TYR:OH	2.16	0.45
10:J:359:VAL:O	10:J:363:ARG:HG2	2.17	0.45
11:K:151:ARG:O	11:K:155:LEU:HB2	2.17	0.45
16:Q:525:PRO:HB3	16:Q:531:TRP:O	2.17	0.45
18:T:297:HIS:CE1	18:T:300:ILE:HG13	2.52	0.45
18:T:356:LEU:N	18:T:356:LEU:HD12	2.32	0.45
22:1:1140:GLU:OE1	22:1:1140:GLU:HA	2.17	0.45
23:3:305:THR:OG1	23:3:306:GLU:N	2.50	0.45
23:3:1026:ASP:OD1	23:3:1026:ASP:N	2.48	0.45
1:A:95:MET:O	1:A:99:VAL:HG23	2.17	0.44
1:A:264:PHE:HE1	1:A:455:VAL:HG13	1.82	0.44
1:A:402:ILE:HA	1:A:405:LEU:HD12	2.00	0.44
2:B:36:C:H42	2:B:47:A:H61	1.65	0.44
3:C:277:LYS:O	3:C:281:ILE:HG13	2.17	0.44
3:C:620:LYS:HE3	3:C:620:LYS:HB2	1.81	0.44
3:C:766:ILE:HG13	3:C:808:ILE:HG22	1.99	0.44
3:C:909:GLY:HA3	3:C:930:ALA:H	1.82	0.44
5:E:237:SER:O	5:E:255:MET:HG3	2.17	0.44
6:F:36:A:C2’	6:F:36:A:N3	2.80	0.44
8:H:118:G:C6	8:H:140:A:N6	2.86	0.44
16:Q:559:HIS:N	16:Q:597:ILE:O	2.50	0.44
22:1:465:PRO:HD2	22:1:502:LEU:HD21	1.99	0.44
22:1:807:LYS:HA	22:1:811:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1:1197:LEU:HD13	38:7:74:GLU:HB3	1.99	0.44
22:1:1251:LEU:HA	22:1:1251:LEU:HD23	1.62	0.44
23:3:77:TYR:HE1	23:3:91:GLU:OE1	2.00	0.44
23:3:212:GLU:HG2	23:3:213:LEU:O	2.17	0.44
41:8:38:VAL:HG22	41:8:113:GLN:OE1	2.16	0.44
1:A:92:LEU:HD12	1:A:503:MET:HB3	1.99	0.44
1:A:647:LEU:HD21	1:A:651:TRP:CH2	2.52	0.44
1:A:746:LYS:NZ	8:H:22:U:OP1	2.36	0.44
1:A:1120:PRO:HA	40:9:77:PRO:O	2.18	0.44
1:A:1206:GLU:OE2	1:A:1224:ARG:CZ	2.66	0.44
1:A:1433:ASP:HB3	1:A:1460:HIS:HE1	1.83	0.44
1:A:1661:TRP:O	1:A:1700:GLY:HA3	2.17	0.44
3:C:687:MET:HE2	3:C:745:LEU:HD11	2.00	0.44
5:E:176:VAL:HG22	5:E:196:VAL:HG11	1.98	0.44
7:G:-1:C:C4	7:G:0:G:C6	3.06	0.44
7:G:5:G:C5'	11:K:22:GLN:HA	2.47	0.44
8:H:57:A:H2'	8:H:58:U:O4'	2.16	0.44
18:T:254:VAL:HA	18:T:261:LEU:HD12	1.98	0.44
22:1:562:LYS:HA	22:1:562:LYS:HD3	1.79	0.44
22:1:1126:PHE:CZ	35:2:572:HIS:HD2	2.35	0.44
23:3:769:LYS:HA	23:3:769:LYS:HD3	1.79	0.44
23:3:1087:GLN:H	23:3:1087:GLN:HG2	1.64	0.44
23:3:1178:LEU:HA	23:3:1178:LEU:HD12	1.53	0.44
40:9:291:LEU:HD23	40:9:291:LEU:HA	1.84	0.44
1:A:158:ARG:HH22	1:A:570:ASP:HB3	1.82	0.44
1:A:822:PHE:O	1:A:822:PHE:CD2	2.70	0.44
1:A:1386:TRP:NE1	1:A:1417:PRO:HD2	2.32	0.44
1:A:1436:TRP:HH2	1:A:1437:ARG:NH2	2.16	0.44
3:C:450:GLU:HA	3:C:457:VAL:HG22	2.00	0.44
3:C:465:MET:CE	3:C:475:MET:HG3	2.47	0.44
3:C:678:THR:O	3:C:681:LYS:HD3	2.18	0.44
5:E:61:LEU:HD13	5:E:352:TYR:CZ	2.52	0.44
5:E:309:VAL:HG22	5:E:330:ILE:HG21	1.99	0.44
10:J:279:TRP:CE3	10:J:302:ALA:HB2	2.52	0.44
11:K:27:TYR:CD2	11:K:34:GLN:HB2	2.52	0.44
22:1:700:LYS:HD3	22:1:700:LYS:HA	1.66	0.44
22:1:901:GLN:HA	22:1:939:ARG:NH2	2.28	0.44
22:1:1280:LEU:HD23	22:1:1280:LEU:HA	1.59	0.44
23:3:817:GLN:HE21	23:3:818:GLN:HA	1.81	0.44
23:3:833:GLU:OE1	23:3:833:GLU:N	2.50	0.44
23:3:911:LYS:HB3	23:3:922:GLY:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:995:THR:HB	23:3:1000:VAL:HG22	1.98	0.44
23:3:1096:HIS:HD2	23:3:1166:TYR:CB	2.30	0.44
35:2:488:LEU:C	35:2:488:LEU:CD2	2.85	0.44
37:6:16:GLU:CD	37:6:16:GLU:H	2.21	0.44
41:8:34:LEU:N	41:8:35:GLU:OE1	2.50	0.44
1:A:112:GLN:HE21	1:A:190:ALA:H	1.65	0.44
1:A:380:LEU:HG	3:C:334:ILE:HD12	2.00	0.44
1:A:609:LYS:HB3	1:A:609:LYS:HE2	1.73	0.44
1:A:1267:LEU:HD12	1:A:1267:LEU:HA	1.68	0.44
1:A:1485:LEU:HA	1:A:1485:LEU:HD23	1.69	0.44
2:B:55:C:C2	2:B:56:C:C5	3.06	0.44
3:C:589:LYS:O	3:C:658:PRO:HB3	2.17	0.44
3:C:684:LYS:HB3	3:C:684:LYS:HE2	1.60	0.44
3:C:908:PRO:HD2	3:C:929:LEU:HD12	1.98	0.44
5:E:249:TYR:HB3	5:E:261:VAL:HG13	1.99	0.44
6:F:93:G:H2’	6:F:94:C:H6	1.83	0.44
7:G:109:U:H2’	7:G:109:U:O2	2.17	0.44
8:H:152:G:C6	8:H:180:G:C6	3.06	0.44
10:J:433:ARG:HD2	10:J:433:ARG:HA	1.44	0.44
11:K:82:ARG:HH21	22:1:1051:SER:N	2.15	0.44
16:Q:1065:ALA:O	16:Q:1101:PRO:HA	2.18	0.44
18:T:232:ASP:HB2	18:T:239:LYS:HD2	1.99	0.44
18:T:250:ARG:HG2	18:T:292:TYR:HA	1.98	0.44
19:X:277:ARG:HH22	22:1:437:PRO:HA	1.80	0.44
22:1:503:LYS:HG2	22:1:511:MET:HB3	1.99	0.44
22:1:1091:HIS:ND1	22:1:1091:HIS:C	2.71	0.44
23:3:644:GLU:OE2	23:3:662:PHE:HD2	2.01	0.44
23:3:942:LYS:HB2	23:3:942:LYS:HE3	1.65	0.44
23:3:1088:LYS:HB3	23:3:1088:LYS:HE2	1.71	0.44
40:9:298:ASP:OD1	40:9:299:LEU:N	2.50	0.44
40:9:360:HIS:O	40:9:387:CYS:N	2.47	0.44
41:8:37:LYS:HG2	41:8:38:VAL:N	2.33	0.44
41:8:55:ARG:HG3	41:8:59:ILE:HD11	1.98	0.44
1:A:119:LEU:HB2	1:A:130:ASN:ND2	2.33	0.44
1:A:202:PRO:O	1:A:234:MET:HE2	2.18	0.44
1:A:681:PHE:CD2	1:A:681:PHE:C	2.89	0.44
1:A:1215:ASN:ND2	1:A:1215:ASN:H	2.16	0.44
1:A:1229:PHE:N	1:A:1229:PHE:CD1	2.84	0.44
1:A:1395:GLU:O	1:A:1399:GLN:HG2	2.18	0.44
1:A:1436:TRP:CH2	1:A:1437:ARG:NH2	2.86	0.44
1:A:1443:LYS:HD3	1:A:1443:LYS:HA	1.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:688:ILE:O	3:C:789:PHE:HA	2.18	0.44
3:C:745:LEU:HD13	3:C:770:PHE:CD1	2.52	0.44
3:C:745:LEU:HD22	3:C:770:PHE:HB2	2.00	0.44
3:C:784:ILE:HG23	3:C:820:PHE:CE1	2.52	0.44
3:C:789:PHE:CD2	3:C:816:VAL:HG22	2.52	0.44
5:E:65:HIS:NE2	5:E:91:LEU:HD12	2.33	0.44
5:E:289:LEU:HD11	5:E:330:ILE:O	2.17	0.44
6:F:36:A:OP2	7:G:11:A:N6	2.39	0.44
6:F:63:C:C2	6:F:72:G:C2	3.05	0.44
7:G:102:G:H4’	38:7:25:LYS:NZ	2.32	0.44
8:H:9:U:C4	8:H:10:C:C4	3.05	0.44
8:H:52:G:C2	8:H:62:U:C2	3.06	0.44
11:K:119:THR:HA	11:K:122:LEU:HD12	1.99	0.44
17:R:237:MET:HA	17:R:241:GLU:OE2	2.16	0.44
22:1:774:ILE:HD13	22:1:777:PHE:HE2	1.83	0.44
22:1:1266:TRP:CZ3	39:5:22:GLY:HA3	2.52	0.44
23:3:608:GLY:HA2	23:3:614:VAL:HG23	2.00	0.44
23:3:908:GLY:O	23:3:909:VAL:HG23	2.17	0.44
23:3:1081:LEU:C	23:3:1081:LEU:CD2	2.85	0.44
37:6:22:TYR:OH	37:6:24:ARG:NH2	2.50	0.44
40:9:135:ASN:HA	40:9:140:ASN:O	2.17	0.44
40:9:269:ASP:HB3	40:9:272:ARG:HH21	1.82	0.44
41:8:24:LEU:O	41:8:28:LEU:HB2	2.17	0.44
1:A:256:TYR:OH	1:A:315:ALA:HB1	2.17	0.44
1:A:539:ARG:HH12	7:G:-1:C:C5’	2.23	0.44
1:A:998:ARG:NH1	1:A:1003:HIS:HB2	2.33	0.44
1:A:1300:LYS:C	1:A:1302:GLY:N	2.69	0.44
1:A:1593:LEU:O	1:A:1597:PHE:HD2	2.01	0.44
2:B:38:C:H5’	2:B:39:C:C6	2.51	0.44
3:C:231:ALA:HB1	3:C:263:LEU:HD11	1.98	0.44
3:C:368:SER:O	3:C:372:PHE:HB2	2.18	0.44
3:C:410:LEU:HB3	3:C:414:PRO:HB2	2.00	0.44
4:D:1228:VAL:HA	4:D:1265:GLN:O	2.18	0.44
4:D:2103:ASN:HA	4:D:2123:SER:HA	1.99	0.44
6:F:92:A:H2’	6:F:93:G:H8	1.81	0.44
8:H:51:A:C6	8:H:63:G:N1	2.86	0.44
8:H:125:G:H2’	8:H:126:A:H8	1.82	0.44
19:X:369:LEU:HD12	19:X:370:LEU:N	2.33	0.44
22:1:1272:ILE:O	22:1:1274:ILE:N	2.51	0.44
23:3:745:PHE:CB	23:3:755:VAL:HG23	2.44	0.44
35:2:524:LEU:HD13	35:2:528:ILE:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:2:536:MET:HG3	35:2:566:ILE:HG13	1.99	0.44
38:7:102:ARG:NE	38:7:102:ARG:HA	2.32	0.44
1:A:82:ARG:HA	1:A:85:LYS:HZ3	1.81	0.44
1:A:122:ILE:HD12	1:A:122:ILE:HA	1.84	0.44
1:A:312:TYR:CD2	3:C:882:GLY:HA3	2.53	0.44
1:A:406:TRP:HH2	3:C:265:LEU:HB2	1.80	0.44
1:A:1218:ASN:OD1	1:A:1219:GLU:N	2.51	0.44
1:A:1402:ARG:HD2	17:R:406:GLN:HB2	1.99	0.44
1:A:1439:ARG:NH1	1:A:1439:ARG:HG3	2.31	0.44
3:C:70:GLU:OE1	3:C:70:GLU:N	2.30	0.44
3:C:664:GLU:OE1	3:C:778:PRO:HD2	2.18	0.44
3:C:938:ARG:CZ	3:C:943:LEU:HB3	2.48	0.44
3:C:945:GLU:OE1	3:C:945:GLU:N	2.50	0.44
6:F:87:C:H2’	6:F:88:G:C8	2.52	0.44
16:Q:851:ILE:O	16:Q:1036:ALA:HA	2.17	0.44
17:R:403:ASN:ND2	19:X:251:GLU:HA	2.33	0.44
22:1:453:MET:O	22:1:456:VAL:HG12	2.17	0.44
22:1:681:PRO:HB3	23:3:219:HIS:CD2	2.53	0.44
22:1:717:THR:HA	22:1:756:LEU:HD11	2.00	0.44
22:1:1075:ARG:HE	22:1:1075:ARG:HB2	1.24	0.44
23:3:477:SER:HA	23:3:482:THR:HG22	1.99	0.44
23:3:631:GLN:HG2	23:3:632:ALA:N	2.33	0.44
23:3:1155:LEU:HA	23:3:1155:LEU:HD12	1.59	0.44
1:A:95:MET:N	1:A:96:PRO:HD2	2.33	0.44
1:A:142:SER:HA	1:A:242:ALA:HB2	1.99	0.44
1:A:226:GLN:HE22	1:A:417:ARG:NH2	2.14	0.44
1:A:227:ARG:HA	1:A:417:ARG:HA	2.00	0.44
1:A:441:VAL:O	1:A:445:VAL:HG23	2.17	0.44
1:A:693:ILE:HG23	1:A:697:MET:CB	2.48	0.44
2:B:106:U:H2’	2:B:107:U:C6	2.53	0.44
3:C:65:TYR:CD2	3:C:65:TYR:N	2.85	0.44
6:F:33:G:C2	7:G:14:A:C5	3.06	0.44
6:F:40:U:C4	6:F:41:A:N7	2.86	0.44
6:F:40:U:O4	6:F:41:A:N6	2.51	0.44
8:H:160:A:H2’	8:H:161:U:C6	2.53	0.44
10:J:310:ASN:ND2	10:J:342:GLU:OE2	2.49	0.44
18:T:194:TRP:CZ2	18:T:491:GLU:HG3	2.53	0.44
18:T:338:CYS:HA	18:T:344:GLN:O	2.17	0.44
19:X:230:GLY:O	19:X:234:GLU:N	2.36	0.44
19:X:285:ARG:HD2	19:X:297:PRO:HA	2.00	0.44
20:Y:70:ASP:O	20:Y:74:GLY:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1:1213:ASN:OD1	22:1:1249:TYR:OH	2.29	0.44
23:3:88:VAL:HG23	23:3:90:LEU:HD13	1.98	0.44
40:9:143:ASP:N	40:9:148:GLU:O	2.43	0.44
40:9:414:GLU:O	40:9:423:LYS:HG2	2.18	0.44
1:A:69:ILE:HA	1:A:72:ASP:OD2	2.18	0.44
1:A:79:ARG:HD3	1:A:82:ARG:NH1	2.33	0.44
1:A:140:TYR:HA	1:A:143:GLN:OE1	2.17	0.44
1:A:189:GLU:OE2	1:A:192:GLN:HG3	2.17	0.44
1:A:447:TYR:CZ	1:A:611:LEU:HD13	2.53	0.44
1:A:738:MET:HE2	1:A:738:MET:HB3	1.94	0.44
2:B:62:G:C4	2:B:63:A:C8	3.06	0.44
3:C:591:ALA:HB2	3:C:940:ARG:NH2	2.32	0.44
3:C:884:GLU:H	3:C:884:GLU:HG2	1.45	0.44
5:E:113:MET:HG2	5:E:129:THR:HG23	2.00	0.44
6:F:37:C:N4	7:G:5:G:P	2.91	0.44
6:F:41:A:H2'	6:F:42:C:O4'	2.18	0.44
6:F:49:G:H21	11:K:15:ARG:HG3	1.83	0.44
7:G:103:U:OP1	38:7:63:GLY:HA3	2.18	0.44
10:J:297:ASN:HB3	10:J:301:ARG:NH1	2.32	0.44
11:K:48:GLU:O	11:K:51:GLN:HB2	2.17	0.44
11:K:80:LEU:HA	11:K:84:PHE:HD2	1.83	0.44
22:1:676:GLY:O	22:1:678:ALA:N	2.51	0.44
22:1:1126:PHE:HE1	35:2:576:PHE:CZ	2.34	0.44
23:3:22:PHE:HE1	23:3:78:ILE:HG12	1.82	0.44
23:3:565:TYR:CD1	23:3:619:LEU:HD13	2.53	0.44
23:3:1119:TYR:CD1	23:3:1119:TYR:C	2.91	0.44
40:9:283:ARG:HB2	40:9:434:PHE:CZ	2.53	0.44
1:A:155:LYS:HB3	1:A:616:PHE:HE1	1.82	0.43
1:A:201:ALA:HA	1:A:204:LEU:HB2	1.99	0.43
1:A:511:LYS:HB3	1:A:513:LEU:HD21	2.00	0.43
1:A:731:LEU:O	40:9:241:TYR:HB3	2.18	0.43
1:A:1557:LEU:HD13	1:A:1557:LEU:HA	1.68	0.43
3:C:236:MET:HE3	3:C:835:GLU:HG2	2.00	0.43
3:C:515:THR:HA	3:C:575:GLN:HE22	1.83	0.43
3:C:533:SER:HA	3:C:538:HIS:ND1	2.33	0.43
7:G:85:G:H2'	7:G:86:A:C8	2.53	0.43
8:H:181:G:H2'	8:H:182:U:C6	2.53	0.43
17:R:137:GLU:HA	17:R:140:ILE:HG23	2.00	0.43
18:T:466:PHE:CD2	18:T:482:ALA:HB2	2.53	0.43
19:X:238:THR:HA	19:X:243:VAL:HA	2.00	0.43
22:1:169:ARG:NH1	22:1:397:ARG:HG2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:102:ILE:HD12	23:3:102:ILE:HG23	1.75	0.43
23:3:603:ARG:HH11	23:3:603:ARG:HG3	1.82	0.43
23:3:1096:HIS:CE1	23:3:1098:GLY:HA2	2.53	0.43
36:4:41:ASN:O	36:4:59:VAL:HA	2.18	0.43
37:6:44:PRO:HB2	37:6:65:GLU:HG3	2.00	0.43
40:9:294:GLU:OE2	40:9:401:VAL:HG11	2.18	0.43
1:A:202:PRO:O	1:A:234:MET:HG2	2.17	0.43
1:A:304:ILE:H	3:C:924:GLN:HE22	1.65	0.43
1:A:1034:LEU:H	1:A:1034:LEU:HG	1.65	0.43
1:A:1256:PHE:CD2	1:A:1531:ASN:ND2	2.86	0.43
1:A:1295:ILE:HD13	1:A:1296:GLN:N	2.33	0.43
1:A:1502:PHE:CZ	1:A:1505:LYS:HD3	2.53	0.43
1:A:1640:SER:HA	1:A:1652:MET:HA	2.00	0.43
3:C:173:THR:HG23	3:C:177:ARG:HE	1.84	0.43
5:E:207:GLN:HA	5:E:220:TRP:O	2.18	0.43
5:E:215:ASN:HB3	5:E:234:HIS:O	2.18	0.43
6:F:36:A:N3	6:F:36:A:H2’	2.33	0.43
6:F:38:G:P	6:F:38:G:H8	2.41	0.43
6:F:63:C:H2’	6:F:64:U:C6	2.53	0.43
6:F:69:A:H3’	6:F:70:A:C8	2.39	0.43
6:F:87:C:H2’	6:F:88:G:H8	1.84	0.43
14:O:55:PHE:O	14:O:67:LYS:CA	2.51	0.43
19:X:221:LYS:HE2	19:X:223:LYS:HE3	2.00	0.43
22:1:909:VAL:HG13	22:1:910:MET:N	2.33	0.43
22:1:1002:ASN:CG	22:1:1041:ARG:HH21	2.21	0.43
22:1:1206:ASP:OD1	22:1:1207:SER:N	2.51	0.43
23:3:135:ILE:HD13	23:3:135:ILE:HG21	1.74	0.43
40:9:243:THR:HG22	40:9:264:ALA:HA	2.00	0.43
40:9:350:PHE:CZ	40:9:376:ASN:HB3	2.52	0.43
40:9:416:ASP:HB3	40:9:419:THR:HG22	1.98	0.43
1:A:462:ARG:HE	1:A:465:LYS:HD2	1.82	0.43
1:A:694:LEU:HD13	1:A:706:ALA:HB1	2.00	0.43
1:A:705:LYS:O	1:A:708:THR:N	2.51	0.43
1:A:1661:TRP:NE1	1:A:1697:SER:O	2.52	0.43
2:B:66:A:H2’	2:B:67:A:C8	2.54	0.43
2:B:66:A:H2’	2:B:67:A:H8	1.83	0.43
3:C:103:THR:OG1	3:C:485:ASP:OD1	2.25	0.43
3:C:134:LEU:HD13	3:C:226:VAL:HB	1.99	0.43
3:C:216:THR:HB	3:C:580:LEU:HD21	2.00	0.43
5:E:61:LEU:HD12	5:E:351:LEU:O	2.17	0.43
5:E:152:SER:HB2	5:E:173:ASP:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:33:G:C2	7:G:14:A:N1	2.85	0.43
8:H:30:A:O2'	12:L:39:HIS:NE2	2.44	0.43
9:I:565:ILE:CB	9:I:576:ALA:HB1	2.48	0.43
18:T:190:TRP:HD1	18:T:502:VAL:HG23	1.82	0.43
19:X:327:TYR:CZ	19:X:351:GLU:HB2	2.54	0.43
20:Y:30:SER:O	20:Y:33:LYS:HG3	2.18	0.43
22:1:998:LYS:HD2	22:1:1002:ASN:OD1	2.19	0.43
23:3:485:LEU:HG	23:3:493:GLU:HA	2.00	0.43
40:9:131:VAL:O	40:9:135:ASN:CB	2.67	0.43
40:9:352:ASP:HB3	40:9:354:PHE:CE1	2.54	0.43
1:A:1601:LEU:O	1:A:1606:ILE:HG13	2.18	0.43
2:B:25:C:H4'	2:B:26:A:H5"	2.00	0.43
3:C:60:HIS:ND1	3:C:60:HIS:O	2.51	0.43
3:C:211:PHE:HA	3:C:213:ASP:OD1	2.18	0.43
5:E:136:TRP:CZ3	5:E:143:ARG:HB3	2.53	0.43
8:H:15:U:P	8:H:15:U:H6	2.42	0.43
10:J:231:PHE:O	10:J:235:ILE:HD12	2.18	0.43
22:1:1138:VAL:O	22:1:1140:GLU:N	2.51	0.43
23:3:287:PHE:CD1	23:3:303:ALA:HB1	2.50	0.43
23:3:440:HIS:CE1	23:3:1217:PHE:HB3	2.53	0.43
23:3:484:VAL:C	23:3:485:LEU:HD12	2.38	0.43
39:5:11:LEU:HD13	39:5:23:HIS:CG	2.53	0.43
39:5:44:MET:HE3	39:5:44:MET:HB3	1.86	0.43
1:A:63:PRO:O	1:A:66:VAL:HG13	2.18	0.43
1:A:384:VAL:HA	3:C:331:PHE:CD2	2.54	0.43
1:A:420:ARG:HH12	2:B:56:C:C2'	2.29	0.43
1:A:428:LYS:O	1:A:432:ARG:HG3	2.19	0.43
1:A:476:PHE:O	1:A:479:THR:OG1	2.29	0.43
1:A:640:PHE:CE1	1:A:644:ILE:HG21	2.54	0.43
1:A:652:LEU:HD23	1:A:655:LEU:HD21	1.99	0.43
1:A:981:PHE:HD1	1:A:981:PHE:HA	1.72	0.43
1:A:1016:VAL:HA	1:A:1024:HIS:O	2.19	0.43
1:A:1076:ASP:O	1:A:1079:THR:OG1	2.36	0.43
1:A:1258:LYS:HZ3	17:R:428:GLU:CD	2.21	0.43
1:A:1416:ILE:HG22	1:A:1417:PRO:CD	2.48	0.43
2:B:36:C:N3	2:B:47:A:N6	2.67	0.43
3:C:449:ILE:HG23	3:C:453:TYR:HB3	1.99	0.43
5:E:130:ASP:OD1	5:E:130:ASP:N	2.51	0.43
7:G:115:C:O2	20:Y:118:PRO:HG3	2.19	0.43
10:J:376:VAL:HG21	10:J:415:LEU:HB2	2.00	0.43
11:K:8:THR:O	11:K:12:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:129:ASP:O	17:R:133:GLN:HG2	2.19	0.43
18:T:307:SER:C	18:T:309:ASP:N	2.70	0.43
18:T:393:ASP:OD1	18:T:393:ASP:N	2.51	0.43
20:Y:29:HIS:ND1	20:Y:91:ILE:HG12	2.33	0.43
20:Y:39:PHE:CD1	20:Y:39:PHE:C	2.91	0.43
22:1:148:ASN:CB	37:6:100:LYS:HD2	2.49	0.43
22:1:1148:LEU:HD23	22:1:1148:LEU:HA	1.67	0.43
23:3:146:ARG:HG3	23:3:150:ALA:C	2.39	0.43
23:3:232:GLY:HA2	23:3:252:SER:HA	2.00	0.43
23:3:1039:LEU:HB2	23:3:1043:THR:OG1	2.18	0.43
37:6:36:TYR:CD2	37:6:45:ILE:HD13	2.53	0.43
40:9:302:LYS:HG3	40:9:346:TRP:CH2	2.53	0.43
41:8:51:TRP:HZ3	41:8:105:LEU:HD12	1.83	0.43
1:A:318:TYR:HD1	3:C:645:ARG:NH1	2.10	0.43
1:A:609:LYS:HE3	1:A:610:HIS:CD2	2.54	0.43
1:A:642:ARG:HD3	2:B:28:A:H1’	2.01	0.43
1:A:787:GLU:O	1:A:788:GLN:C	2.55	0.43
1:A:1576:ILE:HD13	1:A:1747:ILE:HG12	1.99	0.43
3:C:433:MET:O	3:C:436:GLN:HB3	2.19	0.43
3:C:480:LYS:HB3	3:C:493:PHE:HD2	1.84	0.43
5:E:166:LEU:HD23	5:E:201:PHE:CE1	2.54	0.43
6:F:16:G:H2’	6:F:17:C:O4’	2.18	0.43
6:F:47:A:H2’	6:F:47:A:N3	2.33	0.43
7:G:18:A:H3’	7:G:19:G:C8	2.54	0.43
7:G:19:G:N2	7:G:20:A:H1’	2.32	0.43
8:H:9:U:H2’	8:H:10:C:C6	2.53	0.43
8:H:34:U:C2	8:H:35:A:C8	3.06	0.43
8:H:173:C:H2’	8:H:174:A:O4’	2.18	0.43
12:L:104:LEU:HD23	12:L:104:LEU:HA	1.76	0.43
20:Y:40:LEU:HD23	20:Y:43:LEU:HD21	2.00	0.43
22:1:397:ARG:HD2	22:1:397:ARG:HA	1.81	0.43
22:1:552:LEU:HD23	22:1:552:LEU:HA	1.67	0.43
22:1:698:GLN:HB3	22:1:701:VAL:CG1	2.49	0.43
22:1:729:LYS:HD3	22:1:729:LYS:HA	1.61	0.43
22:1:735:ILE:HD13	22:1:735:ILE:HA	1.58	0.43
22:1:1137:ARG:NH2	35:2:524:LEU:HD12	2.33	0.43
22:1:1169:VAL:O	22:1:1170:THR:C	2.56	0.43
22:1:1300:LEU:HA	22:1:1300:LEU:HD23	1.58	0.43
37:6:24:ARG:HB2	37:6:88:VAL:HB	2.00	0.43
40:9:323:ARG:CZ	40:9:325:ILE:HD11	2.49	0.43
40:9:352:ASP:CG	40:9:374:ASN:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:PHE:CE1	1:A:459:LEU:HB2	2.54	0.43
1:A:471:TYR:O	1:A:475:SER:OG	2.36	0.43
1:A:637:TRP:CE3	1:A:637:TRP:HA	2.53	0.43
1:A:641:MET:HA	1:A:644:ILE:CG1	2.49	0.43
1:A:1215:ASN:HB3	1:A:1224:ARG:NE	2.34	0.43
1:A:1257:THR:HG23	1:A:1320:LYS:NZ	2.34	0.43
3:C:185:PRO:HB2	3:C:533:SER:OG	2.19	0.43
5:E:118:ASN:O	5:E:121:GLY:N	2.50	0.43
6:F:40:U:C2'	6:F:41:A:H5'	2.48	0.43
6:F:60:C:H6	6:F:75:G:N7	2.16	0.43
6:F:69:A:H2'	6:F:70:A:O4'	2.19	0.43
6:F:83:A:H4'	6:F:84:A:O4'	2.18	0.43
6:F:95:G:C6	8:H:4:G:C6	3.06	0.43
7:G:103:U:C2	7:G:104:C:C5	3.07	0.43
8:H:47:U:O2	8:H:47:U:C2'	2.67	0.43
11:K:121:TRP:HA	11:K:124:ARG:HE	1.82	0.43
14:O:56:ARG:HA	14:O:66:LYS:O	2.18	0.43
17:R:399:PRO:O	17:R:401:THR:N	2.52	0.43
18:T:284:TYR:OH	18:T:317:VAL:O	2.30	0.43
18:T:373:LYS:HG3	18:T:393:ASP:OD1	2.18	0.43
18:T:415:ILE:H	18:T:415:ILE:HG13	1.47	0.43
22:1:411:GLY:O	37:6:51:GLY:HA2	2.19	0.43
22:1:479:LEU:HD23	37:6:24:ARG:NH1	2.33	0.43
22:1:488:SER:N	22:1:489:PRO:HD2	2.34	0.43
22:1:1266:TRP:O	22:1:1270:ASN:ND2	2.52	0.43
35:2:523:GLU:O	35:2:523:GLU:HG3	2.13	0.43
38:7:54:TYR:HA	38:7:57:ARG:HG2	2.00	0.43
41:8:23:LYS:O	41:8:27:GLN:HG2	2.18	0.43
1:A:137:GLU:OE2	1:A:419:ARG:N	2.47	0.43
1:A:138:PRO:HB2	1:A:238:LEU:HD13	2.01	0.43
1:A:500:GLY:HA3	1:A:551:LEU:HD11	2.00	0.43
1:A:518:LEU:HG	1:A:519:ASP:O	2.18	0.43
1:A:693:ILE:HG22	1:A:694:LEU:HG	2.00	0.43
1:A:713:LEU:HD12	1:A:713:LEU:HA	1.63	0.43
1:A:1281:THR:HG22	1:A:1284:LEU:H	1.83	0.43
1:A:1439:ARG:HG3	1:A:1439:ARG:HH11	1.84	0.43
2:B:27:U:O2'	2:B:28:A:O5'	2.35	0.43
2:B:35:U:C4	2:B:36:C:N4	2.87	0.43
3:C:450:GLU:HA	3:C:457:VAL:CG2	2.49	0.43
3:C:496:VAL:O	3:C:497:LEU:HD23	2.18	0.43
3:C:666:VAL:O	3:C:691:PRO:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:778:PRO:HD3	3:C:817:TYR:CD1	2.54	0.43
4:D:1406:VAL:O	4:D:1425:ILE:HA	2.19	0.43
5:E:61:LEU:HD11	5:E:350:ARG:HB3	1.99	0.43
5:E:92:LEU:HD23	5:E:92:LEU:HA	1.89	0.43
5:E:108:HIS:NE2	5:E:134:ALA:HB3	2.34	0.43
8:H:52:G:C6	8:H:53:U:C4	3.07	0.43
10:J:406:PHE:HB3	10:J:411:MET:HE2	1.99	0.43
11:K:24:LEU:HD13	11:K:25:ARG:N	2.34	0.43
16:Q:1193:PRO:HD2	16:Q:1197:PHE:O	2.18	0.43
16:Q:1358:MET:N	16:Q:1359:PRO:HD2	2.33	0.43
17:R:287:LEU:HA	17:R:287:LEU:HD12	1.76	0.43
18:T:423:SER:HB2	18:T:474:GLU:OE1	2.18	0.43
20:Y:40:LEU:HD21	20:Y:56:PHE:CZ	2.53	0.43
20:Y:57:SER:OG	21:Z:584:TRP:HA	2.19	0.43
22:1:166:ARG:NH2	22:1:620:MET:HG2	2.34	0.43
22:1:501:LEU:HD23	22:1:501:LEU:HA	1.75	0.43
22:1:1140:GLU:O	22:1:1144:GLN:HG3	2.18	0.43
23:3:475:ILE:HG13	23:3:508:CYS:SG	2.58	0.43
35:2:495:ARG:HE	35:2:495:ARG:HB3	1.67	0.43
37:6:27:PRO:HG3	37:6:85:ARG:HD3	1.99	0.43
37:6:51:GLY:HA3	37:6:56:THR:O	2.19	0.43
40:9:281:TYR:HA	40:9:293:LEU:O	2.17	0.43
41:8:45:LEU:HB3	41:8:49:LYS:NZ	2.34	0.43
1:A:136:ILE:HG12	1:A:228:TRP:CB	2.48	0.43
1:A:414:ARG:NH1	3:C:408:LEU:O	2.49	0.43
1:A:1287:LEU:HA	1:A:1287:LEU:HD12	1.78	0.43
1:A:1527:ASN:OD1	1:A:1527:ASN:N	2.52	0.43
1:A:1575:GLN:HE21	1:A:1575:GLN:HA	1.84	0.43
3:C:724:TRP:HD1	3:C:725:ASP:O	2.02	0.43
3:C:850:LEU:O	3:C:853:ARG:N	2.47	0.43
6:F:92:A:H2'	6:F:93:G:C8	2.54	0.43
8:H:19:G:N2	8:H:20:G:N7	2.67	0.43
9:I:550:TRP:O	9:I:552:ASN:N	2.52	0.43
10:J:242:ILE:H	10:J:242:ILE:HG12	1.59	0.43
11:K:49:SER:O	11:K:53:GLN:HG3	2.19	0.43
16:Q:734:LYS:O	16:Q:778:ILE:HA	2.19	0.43
20:Y:55:VAL:HG12	20:Y:56:PHE:CD2	2.54	0.43
22:1:472:ILE:HA	22:1:472:ILE:HD13	1.58	0.43
22:1:506:ASN:OD1	22:1:506:ASN:N	2.50	0.43
23:3:57:GLU:HG2	23:3:59:PHE:CE1	2.54	0.43
23:3:102:ILE:HD13	23:3:102:ILE:HA	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:579:GLU:HG2	23:3:581:LYS:HB2	2.00	0.43
23:3:623:ASP:OD2	23:3:628:LEU:HD11	2.18	0.43
39:5:5:TYR:O	39:5:9:SER:OG	2.36	0.43
40:9:406:VAL:O	40:9:410:MET:HG3	2.19	0.43
41:8:14:ASP:OD1	41:8:15:ASN:N	2.52	0.43
1:A:67:ARG:CD	1:A:179:ALA:HB2	2.49	0.43
1:A:278:LYS:C	1:A:452:LYS:HZ2	2.22	0.43
1:A:352:PHE:CE1	1:A:359:ILE:HD11	2.54	0.43
1:A:386:PRO:HA	3:C:327:TYR:HE1	1.84	0.43
1:A:405:LEU:HD13	3:C:265:LEU:HD13	2.00	0.43
1:A:532:THR:OG1	1:A:533:LYS:N	2.52	0.43
1:A:544:PHE:CZ	1:A:548:ARG:HD3	2.53	0.43
1:A:574:LEU:O	1:A:578:LEU:HG	2.19	0.43
1:A:1361:GLU:C	1:A:1363:GLN:H	2.22	0.43
1:A:1608:THR:OG1	1:A:1609:VAL:N	2.51	0.43
1:A:1633:ALA:HA	1:A:1637:TRP:CZ2	2.54	0.43
2:B:33:U:H2’	2:B:34:U:H6	1.83	0.43
3:C:191:PRO:HA	3:C:196:LYS:O	2.19	0.43
3:C:284:GLU:O	3:C:288:LEU:HG	2.18	0.43
3:C:377:LEU:O	3:C:381:LEU:HG	2.19	0.43
3:C:920:PRO:HB2	3:C:921:LEU:HD12	2.01	0.43
4:D:1065:ALA:O	4:D:1070:LEU:N	2.45	0.43
5:E:69:VAL:C	5:E:331:ASN:HD22	2.21	0.43
10:J:242:ILE:HD12	10:J:278:LEU:HD13	2.00	0.43
10:J:411:MET:SD	10:J:415:LEU:HD23	2.59	0.43
17:R:148:ARG:CG	17:R:148:ARG:NH2	2.73	0.43
18:T:203:HIS:NE2	18:T:229:LYS:HD2	2.34	0.43
19:X:231:ALA:HB2	20:Y:103:LYS:HZ1	1.84	0.43
22:1:412:TYR:HA	37:6:50:VAL:O	2.18	0.43
22:1:617:ILE:HD13	22:1:617:ILE:HA	1.77	0.43
22:1:871:THR:O	22:1:872:ILE:C	2.58	0.43
22:1:1241:ILE:HD12	22:1:1241:ILE:HG23	1.64	0.43
23:3:854:ALA:C	23:3:856:LYS:HG3	2.38	0.43
37:6:20:ILE:HB	37:6:92:TYR:HB3	2.01	0.43
39:5:71:LYS:O	39:5:73:LEU:N	2.51	0.43
40:9:291:LEU:HD23	40:9:403:GLY:HA3	2.01	0.43
40:9:302:LYS:HG3	40:9:346:TRP:HH2	1.84	0.43
40:9:334:ASP:OD2	40:9:339:GLY:N	2.49	0.43
40:9:364:GLY:O	40:9:399:ARG:HA	2.19	0.43
1:A:155:LYS:HB2	1:A:626:GLY:O	2.19	0.42
1:A:845:ARG:HE	1:A:845:ARG:HB2	1.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1424:GLN:HE22	1:A:1459:ARG:HD2	1.83	0.42
1:A:1664:ILE:HD12	1:A:1664:ILE:HA	1.77	0.42
1:A:1785:VAL:HA	1:A:1806:ALA:N	2.34	0.42
2:B:18:C:O2’	2:B:19:A:O5’	2.35	0.42
2:B:19:A:H1’	2:B:59:G:N2	2.34	0.42
3:C:142:LYS:HB3	3:C:204:ASP:OD1	2.17	0.42
3:C:319:THR:HG22	3:C:320:LEU:N	2.34	0.42
3:C:473:PRO:HB3	3:C:571:ASN:ND2	2.34	0.42
5:E:206:ASP:O	5:E:222:LEU:HG	2.19	0.42
8:H:140:A:H2’	8:H:141:C:H6	1.83	0.42
12:L:73:HIS:HD2	40:9:220:ILE:HB	1.84	0.42
17:R:126:ASN:HD22	18:T:442:ARG:HH11	1.66	0.42
22:1:652:CYS:HB2	22:1:692:HIS:HE1	1.84	0.42
22:1:694:LEU:HD23	22:1:705:SER:OG	2.19	0.42
22:1:759:ALA:O	22:1:763:ASN:HB2	2.19	0.42
22:1:1120:ALA:HB2	22:1:1128:VAL:HG21	2.00	0.42
37:6:105:LYS:HA	37:6:108:GLU:OE2	2.19	0.42
1:A:518:LEU:HD21	1:A:522:PHE:HD1	1.83	0.42
1:A:1581:LEU:HD23	1:A:1746:ARG:CZ	2.50	0.42
2:B:19:A:H2’	2:B:20:G:H5”	2.01	0.42
2:B:63:A:H2’	2:B:64:G:H8	1.84	0.42
3:C:223:ASP:OD2	3:C:441:PRO:HD3	2.19	0.42
3:C:589:LYS:HG3	3:C:630:LEU:CD2	2.47	0.42
6:F:38:G:O6	7:G:9:C:N4	2.51	0.42
12:L:72:LEU:HA	12:L:72:LEU:HD23	1.70	0.42
17:R:315:LYS:HE3	17:R:315:LYS:HB2	1.79	0.42
22:1:133:LEU:HB2	22:1:149:ALA:HB1	2.00	0.42
22:1:413:LYS:HB2	22:1:413:LYS:HE3	1.78	0.42
22:1:490:GLU:O	22:1:494:GLU:HG2	2.19	0.42
22:1:865:ARG:HA	22:1:868:VAL:HG22	2.01	0.42
22:1:1126:PHE:HA	35:2:575:PHE:CE2	2.54	0.42
23:3:604:PHE:HE1	23:3:681:PRO:HA	1.84	0.42
23:3:942:LYS:HG3	23:3:942:LYS:O	2.19	0.42
23:3:999:ARG:NH1	23:3:1024:PHE:CZ	2.87	0.42
35:2:542:GLU:HA	35:2:545:GLU:HB2	2.02	0.42
37:6:66:ASP:CG	37:6:68:PHE:H	2.22	0.42
39:5:50:LEU:HA	39:5:50:LEU:HD12	1.33	0.42
40:9:323:ARG:HB3	40:9:331:GLN:HB3	2.01	0.42
1:A:304:ILE:HB	3:C:923:PRO:HA	2.00	0.42
1:A:428:LYS:HE2	1:A:432:ARG:HD2	2.01	0.42
1:A:546:LEU:CD2	1:A:591:MET:HB3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:LEU:HA	1:A:683:LEU:HD12	1.74	0.42
1:A:814:VAL:HG23	1:A:999:LEU:CD1	2.48	0.42
1:A:841:LEU:HA	1:A:841:LEU:HD23	1.63	0.42
1:A:929:GLU:O	1:A:932:LYS:N	2.52	0.42
1:A:1218:ASN:HB2	1:A:1225:THR:HG21	2.00	0.42
1:A:1663:ASP:OD1	1:A:1664:ILE:N	2.53	0.42
3:C:138:LEU:HD12	3:C:138:LEU:HA	1.80	0.42
3:C:142:LYS:HD2	3:C:205:THR:O	2.19	0.42
3:C:746:VAL:O	3:C:791:ILE:HG13	2.20	0.42
3:C:914:LYS:NZ	3:C:931:ARG:HH12	2.17	0.42
3:C:938:ARG:HH21	3:C:944:SER:H	1.67	0.42
5:E:348:ASP:OD2	5:E:350:ARG:NE	2.47	0.42
6:F:23:U:H3’	6:F:24:A:C8	2.53	0.42
10:J:386:GLU:HB3	10:J:395:ALA:HB2	2.02	0.42
12:L:17:GLU:OE1	12:L:20:LYS:HE2	2.19	0.42
15:P:193:VAL:HG23	15:P:194:PHE:HD2	1.84	0.42
18:T:224:ALA:HA	18:T:248:THR:HA	2.00	0.42
18:T:483:ASP:OD1	18:T:485:THR:OG1	2.36	0.42
22:1:584:ASP:OD1	22:1:585:GLU:N	2.53	0.42
22:1:789:LEU:HA	22:1:789:LEU:HD12	1.66	0.42
22:1:914:PHE:HZ	22:1:932:ILE:HD12	1.83	0.42
22:1:1000:ILE:O	22:1:1004:ILE:HG22	2.19	0.42
22:1:1019:ARG:HH12	22:1:1022:PRO:CG	2.32	0.42
23:3:146:ARG:HG3	23:3:150:ALA:CA	2.45	0.42
23:3:159:GLU:OE2	38:7:14:GLN:HB2	2.19	0.42
23:3:224:TYR:HB3	23:3:261:PHE:CE2	2.55	0.42
23:3:379:LEU:HD22	23:3:383:ASP:OD1	2.19	0.42
23:3:506:LEU:HD12	23:3:506:LEU:HA	1.86	0.42
23:3:715:MET:N	23:3:715:MET:SD	2.92	0.42
1:A:402:ILE:HD13	3:C:268:LYS:HD3	2.01	0.42
1:A:712:HIS:CE1	17:R:250:CYS:HA	2.54	0.42
1:A:1458:GLN:CB	17:R:421:GLY:H	2.32	0.42
1:A:1628:ASP:HB3	1:A:1662:ILE:O	2.19	0.42
3:C:135:CYS:O	3:C:227:LEU:HA	2.19	0.42
3:C:743:ASN:OD1	3:C:784:ILE:HG22	2.20	0.42
11:K:121:TRP:CZ3	11:K:122:LEU:HD23	2.54	0.42
17:R:316:GLU:O	17:R:319:LYS:HG3	2.20	0.42
17:R:323:LYS:HD2	17:R:324:LEU:HD23	2.00	0.42
18:T:334:ALA:H	18:T:349:SER:HA	1.84	0.42
18:T:423:SER:N	18:T:474:GLU:OE2	2.47	0.42
18:T:465:ILE:HG12	18:T:481:GLU:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1:516:LEU:HD12	22:1:516:LEU:HA	1.77	0.42
22:1:578:ILE:HG13	22:1:596:ILE:HD11	2.01	0.42
22:1:645:LEU:HA	22:1:645:LEU:HD12	1.87	0.42
22:1:909:VAL:HG13	22:1:910:MET:H	1.84	0.42
22:1:1115:ALA:O	22:1:1119:VAL:HG23	2.19	0.42
23:3:2:PHE:O	23:3:3:LEU:HD23	2.20	0.42
23:3:22:PHE:CE1	23:3:78:ILE:HG12	2.53	0.42
23:3:121:LEU:HD12	23:3:121:LEU:HA	1.70	0.42
23:3:168:TYR:HD2	23:3:168:TYR:N	2.18	0.42
23:3:441:GLY:HA2	23:3:733:PRO:O	2.18	0.42
23:3:664:TYR:HA	23:3:677:THR:O	2.19	0.42
23:3:870:ASN:HD21	23:3:873:GLN:H	1.67	0.42
23:3:1081:LEU:HD13	23:3:1082:LEU:HB2	2.01	0.42
35:2:587:HIS:CD2	35:2:587:HIS:O	2.73	0.42
40:9:224:THR:H	40:9:224:THR:HG1	1.58	0.42
41:8:51:TRP:CZ2	41:8:104:GLU:HG3	2.54	0.42
41:8:73:ASN:HA	41:8:76:GLU:HG2	2.02	0.42
1:A:66:VAL:CG1	1:A:487:LEU:HD21	2.48	0.42
1:A:121:HIS:HB3	1:A:125:ALA:H	1.83	0.42
1:A:195:LEU:HD13	1:A:204:LEU:HA	2.01	0.42
1:A:318:TYR:CE1	3:C:645:ARG:HD3	2.55	0.42
1:A:531:THR:HG21	6:F:37:C:O2’	2.19	0.42
1:A:685:LEU:HD11	1:A:742:TYR:CD1	2.54	0.42
1:A:864:LEU:HA	1:A:864:LEU:HD23	1.63	0.42
1:A:976:MET:HE2	1:A:976:MET:HB2	1.91	0.42
1:A:978:GLU:HA	1:A:1095:ILE:O	2.19	0.42
1:A:1064:PRO:HG2	1:A:1067:MET:HB2	2.01	0.42
1:A:1627:ALA:HB2	1:A:1696:PRO:HD3	2.00	0.42
3:C:308:CYS:SG	3:C:310:SER:OG	2.66	0.42
3:C:847:TYR:CE1	3:C:857:VAL:HG21	2.54	0.42
5:E:281:VAL:HB	5:E:306:ASP:HB3	2.01	0.42
6:F:58:G:O3’	6:F:59:G:H3’	2.18	0.42
7:G:-2:A:O2’	7:G:-1:C:H5’	2.20	0.42
7:G:-1:C:N4	7:G:0:G:O6	2.52	0.42
10:J:231:PHE:HE2	10:J:251:TRP:CD1	2.37	0.42
10:J:238:ASN:C	10:J:240:THR:H	2.23	0.42
10:J:347:HIS:HA	10:J:350:ILE:HG22	2.01	0.42
12:L:35:ALA:HB2	12:L:43:ALA:HA	2.02	0.42
18:T:239:LYS:HB3	18:T:239:LYS:HE3	1.69	0.42
18:T:301:ASP:C	18:T:317:VAL:HG23	2.40	0.42
18:T:301:ASP:O	18:T:317:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1:656:LYS:HE2	41:8:65:ASP:CB	2.50	0.42
22:1:1149:LYS:O	22:1:1152:SER:N	2.53	0.42
22:1:1197:LEU:HD11	38:7:78:GLN:NE2	2.33	0.42
23:3:126:LYS:HB2	23:3:128:ARG:HH11	1.85	0.42
23:3:673:VAL:HG23	23:3:674:LEU:N	2.34	0.42
23:3:791:HIS:ND1	23:3:930:LEU:HD21	2.34	0.42
39:5:32:LEU:HD13	39:5:32:LEU:HA	1.77	0.42
40:9:285:HIS:O	40:9:429:ASP:HB2	2.20	0.42
40:9:352:ASP:OD2	40:9:374:ASN:N	2.43	0.42
1:A:387:PHE:CE2	3:C:399:LEU:HD23	2.55	0.42
1:A:780:THR:O	1:A:783:TYR:N	2.53	0.42
1:A:1418:ARG:CB	1:A:1462:GLY:HA3	2.50	0.42
1:A:1551:PHE:CD1	1:A:1553:VAL:HG23	2.55	0.42
3:C:643:ASP:O	3:C:647:MET:HG2	2.19	0.42
3:C:660:VAL:HG11	3:C:877:ALA:CB	2.49	0.42
3:C:674:CYS:SG	3:C:819:ALA:HA	2.59	0.42
3:C:685:ILE:HD12	3:C:815:VAL:HG21	2.01	0.42
4:D:530:THR:C	4:D:532:ASN:H	2.23	0.42
5:E:217:ILE:HD11	5:E:234:HIS:CD2	2.55	0.42
7:G:108:U:H5	22:1:828:ARG:NH2	2.17	0.42
9:I:456:LEU:O	9:I:460:THR:CB	2.68	0.42
11:K:363:LYS:N	20:Y:71:LYS:CB	2.83	0.42
12:L:77:LEU:HD23	12:L:77:LEU:HA	1.77	0.42
18:T:191:HIS:CD2	18:T:440:ASP:HB2	2.54	0.42
18:T:308:ARG:HH11	18:T:308:ARG:CG	2.29	0.42
18:T:334:ALA:HB2	18:T:350:HIS:CE1	2.55	0.42
20:Y:26:VAL:HB	22:1:861:ALA:HB2	2.00	0.42
22:1:714:GLU:O	38:7:51:TYR:OH	2.37	0.42
22:1:1170:THR:O	22:1:1173:LEU:N	2.52	0.42
23:3:257:THR:HA	23:3:267:ILE:O	2.20	0.42
23:3:544:ILE:HD11	23:3:547:CYS:HB3	2.01	0.42
23:3:550:ASN:CB	23:3:592:LEU:HG	2.50	0.42
23:3:914:ILE:HD13	23:3:914:ILE:HA	1.84	0.42
23:3:1187:PRO:HA	23:3:1190:GLN:HB2	2.02	0.42
35:2:601:LEU:C	35:2:603:GLU:H	2.23	0.42
37:6:107:GLU:HG3	37:6:108:GLU:N	2.33	0.42
40:9:308:ILE:HD12	40:9:438:TYR:CE2	2.55	0.42
40:9:346:TRP:HZ3	40:9:350:PHE:HB3	1.84	0.42
1:A:148:TRP:HZ3	1:A:612:ILE:HG23	1.85	0.42
1:A:393:LEU:O	3:C:379:LYS:HA	2.20	0.42
1:A:520:TYR:O	1:A:555:LYS:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1197:LEU:HD12	1:A:1197:LEU:HA	1.75	0.42
1:A:1638:ASN:ND2	1:A:1652:MET:HB3	2.35	0.42
6:F:37:C:H4'	6:F:38:G:OP2	2.19	0.42
6:F:43:A:C2	7:G:6:A:N1	2.88	0.42
7:G:9:C:H2'	7:G:10:U:C6	2.55	0.42
11:K:172:PHE:HZ	23:3:1214:ARG:CZ	2.33	0.42
12:L:38:LEU:HD12	12:L:41:LYS:HB2	2.01	0.42
19:X:289:ILE:HG12	19:X:290:ALA:N	2.34	0.42
22:1:489:PRO:O	22:1:492:GLN:HB3	2.19	0.42
22:1:709:ILE:HG23	22:1:709:ILE:HD12	1.78	0.42
22:1:939:ARG:HE	22:1:947:VAL:HB	1.85	0.42
23:3:331:ASP:OD2	23:3:395:LEU:HD12	2.20	0.42
23:3:459:VAL:HB	23:3:757:ILE:HG12	2.01	0.42
23:3:1082:LEU:HD12	23:3:1082:LEU:HA	1.77	0.42
37:6:14:PRO:HA	37:6:15:PRO:HD3	1.92	0.42
37:6:23:ILE:HD13	37:6:89:VAL:HA	2.02	0.42
1:A:68:LYS:HE2	13:N:35:GLU:CB	2.50	0.42
1:A:575:ALA:HA	1:A:630:TRP:HE1	1.85	0.42
1:A:675:GLN:HE21	1:A:675:GLN:HB2	1.49	0.42
1:A:924:GLN:OE1	1:A:1439:ARG:NH2	2.53	0.42
1:A:1460:HIS:CD2	1:A:1460:HIS:N	2.87	0.42
2:B:43:U:H3'	2:B:44:A:H8	1.84	0.42
3:C:692:LEU:HA	3:C:692:LEU:HD23	1.79	0.42
10:J:224:LYS:HD3	10:J:228:ARG:HH22	1.84	0.42
10:J:376:VAL:HB	10:J:406:PHE:CE2	2.55	0.42
11:K:121:TRP:HA	11:K:124:ARG:NH2	2.28	0.42
14:O:236:VAL:O	14:O:269:CYS:HA	2.19	0.42
17:R:386:ARG:HH22	19:X:353:LYS:HB3	1.85	0.42
22:1:614:ARG:NH1	41:8:64:ASP:OD1	2.53	0.42
22:1:692:HIS:CD2	22:1:692:HIS:C	2.92	0.42
22:1:849:ILE:H	22:1:849:ILE:HG12	1.61	0.42
22:1:972:GLY:O	22:1:976:VAL:HG12	2.20	0.42
22:1:982:LEU:HD12	22:1:982:LEU:HA	1.74	0.42
22:1:1145:ASN:ND2	22:1:1183:VAL:HG12	2.35	0.42
23:3:168:TYR:N	23:3:168:TYR:CD2	2.88	0.42
23:3:310:ILE:HG22	23:3:311:PHE:N	2.34	0.42
23:3:515:ALA:HB1	23:3:526:HIS:NE2	2.35	0.42
23:3:999:ARG:HH21	23:3:1041:TYR:HE2	1.68	0.42
23:3:1040:ASP:OD2	35:2:707:PRO:HA	2.19	0.42
23:3:1081:LEU:HB3	23:3:1082:LEU:H	1.65	0.42
23:3:1102:LEU:HA	23:3:1102:LEU:HD23	1.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:5:2:THR:O	39:5:6:THR:HG22	2.20	0.42
40:9:358:LEU:HD22	40:9:399:ARG:HH12	1.84	0.42
41:8:36:LYS:H	41:8:36:LYS:HD2	1.85	0.42
1:A:388:LEU:HD22	1:A:391:THR:OG1	2.20	0.42
1:A:441:VAL:HG22	1:A:444:ARG:NH2	2.35	0.42
1:A:1730:MET:O	1:A:1734:MET:HG2	2.20	0.42
2:B:36:C:H2'	2:B:37:G:C8	2.55	0.42
2:B:69:A:H2'	2:B:69:A:N3	2.35	0.42
3:C:264:ILE:HG23	3:C:378:TYR:CD2	2.54	0.42
3:C:468:CYS:SG	3:C:546:ALA:HB1	2.60	0.42
3:C:480:LYS:HB3	3:C:493:PHE:CD2	2.55	0.42
3:C:907:VAL:HG11	3:C:933:PHE:CE2	2.55	0.42
5:E:235:ALA:HB3	5:E:256:ASP:OD1	2.20	0.42
7:G:10:U:N3	7:G:11:A:C5	2.87	0.42
10:J:294:HIS:HA	10:J:297:ASN:HD22	1.85	0.42
10:J:409:GLU:CD	10:J:410:HIS:ND1	2.74	0.42
18:T:225:ASP:OD2	18:T:227:THR:OG1	2.24	0.42
18:T:394:ASN:HB2	18:T:410:SER:HA	2.02	0.42
22:1:412:TYR:CZ	37:6:61:TYR:HE2	2.38	0.42
22:1:413:LYS:CB	37:6:52:ASN:HD21	2.33	0.42
22:1:672:ALA:HB2	22:1:712:LEU:HD23	2.02	0.42
22:1:752:TYR:O	22:1:755:PRO:HD2	2.20	0.42
22:1:912:ASN:OD1	22:1:957:ARG:NH2	2.50	0.42
23:3:444:VAL:HG22	23:3:765:LEU:HD22	2.01	0.42
23:3:679:LEU:HD12	23:3:679:LEU:HA	1.68	0.42
35:2:585:THR:HB	35:2:589:ASP:CG	2.37	0.42
37:6:68:PHE:HD1	37:6:68:PHE:HA	1.72	0.42
41:8:34:LEU:HD23	41:8:82:SER:HB2	2.02	0.42
41:8:55:ARG:HE	41:8:59:ILE:HD11	1.84	0.42
1:A:82:ARG:NH2	7:G:14:A:OP2	2.53	0.42
1:A:107:PRO:HA	1:A:114:ARG:CZ	2.49	0.42
1:A:114:ARG:HG2	1:A:116:VAL:HG22	2.02	0.42
1:A:136:ILE:HG21	1:A:230:PHE:CZ	2.55	0.42
1:A:941:LYS:HZ2	1:A:943:ALA:CB	2.33	0.42
1:A:1397:ILE:HG12	17:R:405:VAL:N	2.35	0.42
2:B:44:A:H2	7:G:-4:G:O6	2.02	0.42
3:C:66:TYR:HD1	3:C:66:TYR:HA	1.69	0.42
3:C:118:PHE:O	3:C:121:ASP:HB3	2.20	0.42
3:C:262:ARG:O	3:C:266:GLU:HB2	2.20	0.42
3:C:392:LEU:HD23	3:C:392:LEU:HA	1.66	0.42
18:T:233:LEU:O	18:T:233:LEU:HD12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:X:308:TYR:HB3	19:X:324:VAL:HG23	2.02	0.42
22:1:1206:ASP:OD1	22:1:1206:ASP:N	2.52	0.42
23:3:477:SER:OG	23:3:477:SER:O	2.37	0.42
23:3:617:ILE:HG23	23:3:626:GLN:O	2.19	0.42
23:3:791:HIS:HA	23:3:792:PRO:HD3	1.95	0.42
37:6:26:LEU:HA	37:6:26:LEU:HD12	1.73	0.42
37:6:111:LYS:O	37:6:115:GLU:HG3	2.20	0.42
40:9:205:ARG:HE	40:9:205:ARG:HB3	1.61	0.42
41:8:28:LEU:HD12	41:8:28:LEU:HA	1.83	0.42
1:A:318:TYR:HE1	3:C:645:ARG:HD3	1.84	0.41
1:A:872:ASP:HB2	1:A:873:ASN:OD1	2.20	0.41
1:A:954:LYS:HD3	1:A:954:LYS:HA	1.75	0.41
1:A:1035:GLN:H	1:A:1035:GLN:HG2	1.50	0.41
1:A:1072:LEU:HD23	1:A:1072:LEU:HA	1.59	0.41
1:A:1268:ILE:HG12	1:A:1268:ILE:H	1.54	0.41
1:A:1391:LEU:HD22	1:A:1391:LEU:HA	1.90	0.41
1:A:1612:GLU:O	1:A:1614:ILE:HD12	2.20	0.41
5:E:299:LYS:HB2	5:E:335:PHE:CZ	2.55	0.41
6:F:38:G:H2’	6:F:39:A:H8	1.85	0.41
6:F:50:A:H1’	6:F:51:U:H5’	2.01	0.41
6:F:82:A:H4’	8:H:16:U:O4	2.20	0.41
8:H:148:C:N4	8:H:149:A:N6	2.68	0.41
11:K:159:LYS:HZ3	11:K:159:LYS:HG3	1.74	0.41
18:T:274:ASP:HB2	18:T:281:ILE:HD13	2.02	0.41
18:T:297:HIS:CG	18:T:298:PRO:HD2	2.55	0.41
18:T:372:LYS:HB2	18:T:393:ASP:OD2	2.20	0.41
22:1:172:LEU:HD11	37:6:117:TYR:HD2	1.85	0.41
22:1:571:VAL:O	22:1:574:ILE:N	2.52	0.41
22:1:1210:HIS:CE1	35:2:585:THR:HG1	2.38	0.41
22:1:1304:LEU:HA	22:1:1304:LEU:HD23	1.85	0.41
23:3:630:MET:HE3	23:3:630:MET:HB2	1.83	0.41
23:3:804:HIS:HB2	23:3:862:TRP:CZ3	2.55	0.41
37:6:36:TYR:HD2	37:6:45:ILE:HD13	1.83	0.41
1:A:179:ALA:HA	1:A:183:LEU:HB2	2.02	0.41
1:A:363:HIS:CE1	3:C:287:GLY:HA3	2.55	0.41
1:A:728:VAL:HA	1:A:729:PRO:HD3	1.94	0.41
1:A:770:THR:C	1:A:772:CYS:N	2.73	0.41
1:A:832:TYR:HB3	1:A:835:ASP:HB3	2.02	0.41
1:A:951:LEU:HD23	1:A:951:LEU:HA	1.69	0.41
1:A:1237:MET:SD	1:A:1283:GLU:OE1	2.79	0.41
1:A:1495:PHE:HE1	1:A:1748:ARG:HG2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:319:THR:HG22	3:C:320:LEU:H	1.85	0.41
4:D:1223:ILE:HA	4:D:1269:ARG:O	2.19	0.41
5:E:264:VAL:HG13	5:E:272:ARG:NH2	2.35	0.41
8:H:106:G:N2	8:H:107:A:C6	2.88	0.41
15:P:204:GLN:HB3	15:P:206:LYS:HE3	2.01	0.41
17:R:299:ARG:HH12	22:1:448:THR:HA	1.86	0.41
21:Z:612:TYR:O	21:Z:615:SER:N	2.53	0.41
22:1:427:PRO:O	22:1:430:LYS:CB	2.68	0.41
22:1:889:GLU:HG2	22:1:890:GLU:N	2.35	0.41
23:3:195:ASP:O	23:3:197:THR:N	2.53	0.41
23:3:246:SER:O	23:3:258:TYR:OH	2.24	0.41
23:3:444:VAL:CG2	23:3:765:LEU:HD22	2.50	0.41
23:3:485:LEU:HB3	23:3:491:VAL:HG12	2.02	0.41
23:3:736:TYR:CG	23:3:737:GLU:N	2.88	0.41
23:3:806:ALA:HB1	23:3:856:LYS:HD3	2.02	0.41
23:3:993:ILE:O	23:3:993:ILE:HG12	2.20	0.41
35:2:534:GLN:C	35:2:534:GLN:NE2	2.72	0.41
37:6:100:LYS:H	37:6:100:LYS:HG3	1.69	0.41
1:A:441:VAL:HG13	1:A:444:ARG:HH21	1.84	0.41
1:A:693:ILE:HG13	1:A:738:MET:SD	2.60	0.41
1:A:755:HIS:HE1	15:P:220:HIS:ND1	2.16	0.41
1:A:1256:PHE:CE1	1:A:1299:ILE:HG22	2.55	0.41
1:A:1846:ALA:HB1	1:A:2220:PRO:CB	2.50	0.41
3:C:128:LEU:HD23	3:C:197:SER:O	2.21	0.41
3:C:855:GLY:HA2	3:C:874:PHE:O	2.20	0.41
3:C:938:ARG:NH1	3:C:943:LEU:HD23	2.36	0.41
4:D:686:GLU:O	4:D:866:GLU:HA	2.19	0.41
6:F:88:G:N2	8:H:11:G:C4	2.89	0.41
10:J:228:ARG:NH2	10:J:257:GLU:OE2	2.54	0.41
15:P:214:THR:OG1	15:P:215:LEU:N	2.53	0.41
18:T:220:VAL:HG22	18:T:230:ILE:HG13	2.02	0.41
18:T:335:THR:OG1	18:T:336:VAL:N	2.53	0.41
18:T:360:VAL:HG13	18:T:361:ALA:H	1.85	0.41
22:1:1129:LEU:HA	22:1:1129:LEU:HD23	1.61	0.41
22:1:1199:VAL:HG11	22:1:1204:CYS:HB2	2.02	0.41
22:1:1253:GLY:HA3	22:1:1265:TYR:CD1	2.55	0.41
23:3:126:LYS:HB2	23:3:128:ARG:NH1	2.36	0.41
23:3:379:LEU:HD13	23:3:383:ASP:O	2.20	0.41
23:3:477:SER:HB2	23:3:504:PRO:CA	2.48	0.41
23:3:631:GLN:HE21	23:3:632:ALA:C	2.18	0.41
23:3:667:ILE:HB	23:3:675:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:781:LEU:HB3	23:3:801:GLU:OE1	2.20	0.41
35:2:535:GLU:OE2	35:2:535:GLU:CA	2.68	0.41
37:6:13:LEU:O	37:6:13:LEU:HD12	2.20	0.41
40:9:353:GLU:HB3	40:9:355:ARG:NH2	2.35	0.41
40:9:416:ASP:HB3	40:9:419:THR:CG2	2.50	0.41
1:A:141:ILE:HG21	1:A:246:LEU:HD21	2.02	0.41
1:A:636:VAL:HA	1:A:639:PHE:CD2	2.55	0.41
1:A:827:PHE:CG	1:A:828:PRO:HD2	2.55	0.41
1:A:1361:GLU:O	1:A:1363:GLN:N	2.53	0.41
1:A:1381:ASP:OD2	1:A:1414:ARG:NH1	2.52	0.41
1:A:1498:TRP:HB2	1:A:1501:LEU:HD12	2.02	0.41
3:C:94:ILE:HB	18:T:276:GLU:CG	2.51	0.41
3:C:373:ILE:C	3:C:376:PRO:HD2	2.41	0.41
3:C:709:TRP:N	3:C:709:TRP:CD1	2.89	0.41
3:C:772:TRP:CH2	3:C:813:ARG:HD3	2.55	0.41
3:C:788:LYS:NZ	3:C:790:LYS:HE3	2.35	0.41
6:F:84:A:C8	6:F:84:A:H3'	2.55	0.41
7:G:-3:A:N3	7:G:-2:A:C8	2.88	0.41
7:G:99:C:N3	8:H:32:U:O2	2.53	0.41
10:J:417:VAL:O	10:J:421:LYS:HG2	2.21	0.41
11:K:20:GLY:O	11:K:22:GLN:NE2	2.53	0.41
11:K:160:LYS:HA	11:K:163:LEU:HD12	2.01	0.41
12:L:54:LEU:HA	12:L:54:LEU:HD13	1.62	0.41
18:T:264:CYS:SG	18:T:294:LEU:HD22	2.60	0.41
18:T:412:HIS:CG	18:T:437:HIS:CG	3.09	0.41
22:1:413:LYS:HB3	37:6:52:ASN:HD21	1.86	0.41
22:1:694:LEU:HD23	22:1:694:LEU:HA	1.80	0.41
22:1:997:LEU:HA	22:1:997:LEU:HD23	1.80	0.41
23:3:30:ILE:O	23:3:40:LEU:HD12	2.21	0.41
23:3:128:ARG:HH21	23:3:180:PRO:HG3	1.86	0.41
23:3:407:ILE:HB	23:3:1121:THR:O	2.20	0.41
23:3:505:THR:HG21	23:3:508:CYS:HG	1.85	0.41
23:3:709:GLN:HG3	23:3:710:GLU:O	2.20	0.41
37:6:21:LEU:HD13	37:6:64:TYR:CE2	2.55	0.41
38:7:32:ILE:HD11	38:7:71:TYR:HE1	1.84	0.41
1:A:513:LEU:HA	1:A:515:TYR:CE2	2.56	0.41
1:A:557:VAL:HG13	1:A:578:LEU:HD22	2.02	0.41
1:A:941:LYS:HD2	1:A:941:LYS:HA	1.74	0.41
1:A:1637:TRP:HZ3	1:A:1660:TYR:HB2	1.85	0.41
1:A:1721:GLY:O	1:A:1724:PRO:HD2	2.21	0.41
2:B:46:U:H2'	2:B:47:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:82:GLN:HA	3:C:82:GLN:NE2	2.36	0.41
3:C:173:THR:CG2	3:C:177:ARG:HE	2.33	0.41
3:C:522:SER:OG	3:C:523:GLN:N	2.54	0.41
3:C:756:LYS:HA	3:C:759:LEU:HB2	2.01	0.41
3:C:853:ARG:NH1	3:C:883:PHE:HA	2.34	0.41
6:F:44:G:N2	7:G:5:G:N1	2.67	0.41
15:P:205:LYS:HD2	15:P:208:LYS:HG3	2.02	0.41
16:Q:967:PHE:O	16:Q:969:PRO:HD3	2.20	0.41
17:R:386:ARG:HH11	17:R:386:ARG:CB	2.33	0.41
20:Y:44:PRO:HD2	20:Y:47:LEU:HD22	2.02	0.41
22:1:830:TYR:OH	22:1:870:GLU:OE1	2.23	0.41
22:1:871:THR:O	22:1:875:ILE:HD12	2.20	0.41
22:1:970:LEU:O	22:1:973:HIS:HB2	2.20	0.41
22:1:1003:VAL:HG13	22:1:1004:ILE:N	2.36	0.41
22:1:1132:LEU:HA	22:1:1132:LEU:HD23	1.87	0.41
22:1:1227:ILE:HA	22:1:1227:ILE:HD12	1.72	0.41
22:1:1252:GLN:OE1	35:2:499:PRO:CA	2.66	0.41
22:1:1303:ILE:HD13	22:1:1303:ILE:HA	1.72	0.41
23:3:181:MET:HG2	23:3:212:GLU:HB2	2.02	0.41
23:3:273:ARG:HA	23:3:273:ARG:HD3	1.76	0.41
23:3:915:LEU:HD12	23:3:915:LEU:HA	1.56	0.41
23:3:1006:GLN:O	23:3:1006:GLN:HG3	2.21	0.41
35:2:471:ARG:HE	35:2:471:ARG:HB3	1.73	0.41
35:2:538:GLU:N	35:2:538:GLU:OE2	2.53	0.41
35:2:596:GLU:HG2	35:2:597:PHE:CD1	2.56	0.41
38:7:24:GLU:HG2	38:7:66:VAL:HG21	2.03	0.41
40:9:268:GLU:O	40:9:269:ASP:C	2.59	0.41
1:A:261:LYS:NZ	3:C:176:GLU:HG2	2.36	0.41
1:A:282:LEU:HG	2:B:49:A:H5”	2.01	0.41
1:A:589:THR:OG1	1:A:590:GLY:N	2.53	0.41
1:A:602:ILE:HG23	7:G:-5:C:N4	2.36	0.41
1:A:616:PHE:CD1	1:A:621:VAL:HG21	2.55	0.41
1:A:966:TRP:CE3	1:A:1198:PRO:HG3	2.56	0.41
1:A:1232:VAL:HG12	1:A:1237:MET:HG2	2.03	0.41
1:A:1300:LYS:C	1:A:1302:GLY:H	2.22	0.41
1:A:1459:ARG:HD3	1:A:1459:ARG:HA	1.48	0.41
1:A:1610:GLN:O	1:A:1630:LEU:HB2	2.21	0.41
2:B:95:G:H21	2:B:96:A:H5”	1.86	0.41
3:C:129:ILE:HG13	3:C:441:PRO:HD2	2.02	0.41
3:C:259:LYS:HD2	3:C:262:ARG:HH11	1.85	0.41
3:C:623:GLU:HB2	3:C:941:LYS:O	2.21	0.41

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
3:C:821:LEU:HD13	3:C:948:SER:O	2.20	0.41
4:D:1407:LEU:HA	4:D:1426:ILE:O	2.19	0.41
5:E:95:VAL:HG11	5:E:336:HIS:NE2	2.35	0.41
7:G:87:U:H2'	7:G:88:G:O4'	2.21	0.41
7:G:112:U:H2'	7:G:113:U:C6	2.56	0.41
8:H:168:A:H5"	8:H:169:C:C5	2.56	0.41
9:I:342:PRO:C	9:I:344:LEU:H	2.23	0.41
11:K:52:ARG:O	11:K:55:LEU:HB3	2.21	0.41
11:K:145:ASP:HA	11:K:146:PRO:HD3	1.93	0.41
15:P:207:ASP:OD2	15:P:222:LYS:NZ	2.43	0.41
18:T:430:GLY:HA3	18:T:465:ILE:HG21	2.02	0.41
20:Y:36:ALA:O	20:Y:83:CYS:HA	2.21	0.41
20:Y:37:TRP:CE3	20:Y:83:CYS:HB2	2.55	0.41
22:1:968:GLU:OE1	22:1:968:GLU:N	2.51	0.41
22:1:1290:ASP:N	22:1:1290:ASP:OD1	2.51	0.41
23:3:486:SER:OG	23:3:494:VAL:HG11	2.21	0.41
23:3:727:SER:O	23:3:727:SER:OG	2.32	0.41
35:2:453:LYS:HD3	35:2:453:LYS:C	2.41	0.41
37:6:66:ASP:OD2	37:6:68:PHE:HB2	2.21	0.41
1:A:84:ASP:HA	1:A:87:VAL:HB	2.03	0.41
1:A:182:ILE:HG22	1:A:565:ARG:NH2	2.35	0.41
1:A:260:LEU:HB3	1:A:264:PHE:CE2	2.56	0.41
1:A:1131:LYS:O	1:A:1132:LYS:HD2	2.20	0.41
1:A:1210:LYS:C	1:A:1212:GLY:N	2.74	0.41
1:A:1295:ILE:HD11	1:A:1327:MET:HE1	2.03	0.41
1:A:1684:PHE:HB3	1:A:1715:TYR:CD2	2.45	0.41
2:B:23:C:HO2'	2:B:24:G:P	2.44	0.41
3:C:214:GLU:HG3	3:C:480:LYS:HZ3	1.86	0.41
3:C:622:GLU:OE1	3:C:941:LYS:NZ	2.47	0.41
5:E:213:ILE:HG22	5:E:237:SER:OG	2.20	0.41
5:E:343:ILE:HD13	5:E:353:MET:HA	2.02	0.41
6:F:45:A:H4'	6:F:45:A:OP1	2.20	0.41
10:J:266:GLU:OE1	10:J:269:LEU:HD13	2.21	0.41
16:Q:1176:ASP:O	16:Q:1300:GLY:HA2	2.21	0.41
22:1:148:ASN:HB3	37:6:100:LYS:HD2	2.02	0.41
22:1:509:PRO:HB2	22:1:510:PRO:HD3	2.02	0.41
22:1:1028:HIS:HB3	22:1:1031:VAL:CG2	2.51	0.41
22:1:1098:LEU:C	22:1:1100:ASN:N	2.73	0.41
22:1:1272:ILE:O	22:1:1275:GLY:O	2.38	0.41
23:3:34:ARG:CZ	23:3:39:GLU:OE1	2.68	0.41
23:3:260:ASN:CG	23:3:261:PHE:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:423:LEU:HD13	23:3:774:PHE:HE1	1.86	0.41
23:3:843:LEU:HA	23:3:843:LEU:HD12	1.71	0.41
23:3:930:LEU:HD12	23:3:930:LEU:HA	1.72	0.41
36:4:166:TYR:HA	36:4:171:PRO:HA	2.03	0.41
1:A:265:THR:HG22	1:A:269:LEU:HD12	2.02	0.41
1:A:578:LEU:HD12	1:A:630:TRP:NE1	2.36	0.41
1:A:613:TYR:HE1	1:A:627:CYS:HB3	1.85	0.41
1:A:717:TRP:O	1:A:718:ARG:C	2.57	0.41
1:A:997:LEU:HD23	1:A:997:LEU:HA	1.77	0.41
1:A:1210:LYS:O	1:A:1212:GLY:N	2.54	0.41
1:A:1403:LEU:O	1:A:1403:LEU:HD12	2.21	0.41
1:A:1499:GLU:OE1	1:A:1499:GLU:N	2.53	0.41
3:C:73:TYR:HE2	18:T:199:VAL:HG11	1.84	0.41
3:C:814:ARG:HG3	3:C:952:PHE:HD1	1.86	0.41
3:C:823:ALA:O	3:C:825:PRO:HD3	2.21	0.41
3:C:829:GLU:O	3:C:905:GLN:N	2.47	0.41
6:F:39:A:N6	7:G:8:C:N3	2.68	0.41
7:G:99:C:C4	7:G:100:C:N4	2.89	0.41
11:K:44:HIS:O	11:K:50:HIS:HB2	2.21	0.41
11:K:172:PHE:HZ	23:3:1214:ARG:NH2	2.19	0.41
18:T:262:PHE:CD1	18:T:303:LEU:HD11	2.55	0.41
18:T:381:HIS:CD2	18:T:441:TRP:CE2	3.09	0.41
18:T:383:ARG:HG3	18:T:384:HIS:CE1	2.55	0.41
19:X:245:LYS:HE3	19:X:302:GLN:HB2	2.02	0.41
19:X:284:GLY:O	19:X:293:PRO:HA	2.21	0.41
22:1:112:ILE:HG23	22:1:115:ARG:NE	2.35	0.41
22:1:115:ARG:HB2	22:1:585:GLU:OE1	2.21	0.41
22:1:686:LEU:O	22:1:689:ILE:HB	2.21	0.41
22:1:1258:ALA:CB	22:1:1261:VAL:HG13	2.50	0.41
23:3:595:VAL:HG22	23:3:596:PRO:O	2.20	0.41
23:3:1210:ASP:O	23:3:1213:THR:N	2.53	0.41
1:A:67:ARG:HH21	1:A:487:LEU:HD23	1.86	0.41
1:A:141:ILE:HG22	1:A:242:ALA:CB	2.51	0.41
1:A:308:ILE:CG2	1:A:320:TYR:HB3	2.50	0.41
1:A:451:LEU:HD23	1:A:454:TYR:HD2	1.86	0.41
1:A:518:LEU:HD12	1:A:523:ASN:C	2.42	0.41
1:A:574:LEU:HD11	1:A:578:LEU:HD11	2.01	0.41
1:A:590:GLY:O	1:A:593:ARG:HB2	2.21	0.41
1:A:828:PRO:HA	1:A:829:PRO:HD3	1.96	0.41
1:A:839:LEU:HA	1:A:839:LEU:HD12	1.77	0.41
1:A:964:ASP:OD1	1:A:964:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:974:ASN:HB2	1:A:1178:TYR:HB3	2.02	0.41
1:A:1002:ASP:OD1	1:A:1002:ASP:C	2.59	0.41
1:A:1503:TRP:CZ3	1:A:1533:ARG:HD3	2.56	0.41
1:A:1709:TYR:N	1:A:1709:TYR:CD2	2.89	0.41
2:B:16:U:C2	2:B:62:G:N2	2.89	0.41
2:B:49:A:H2'	2:B:50:G:C8	2.56	0.41
3:C:142:LYS:HA	3:C:228:PHE:CE2	2.56	0.41
3:C:211:PHE:HZ	3:C:635:LEU:HG	1.86	0.41
3:C:237:LEU:H	3:C:237:LEU:HD12	1.85	0.41
3:C:350:ASN:HD21	3:C:352:LYS:HE2	1.86	0.41
3:C:412:ILE:H	3:C:412:ILE:HD12	1.86	0.41
5:E:306:ASP:O	5:E:308:PHE:HD2	2.03	0.41
5:E:313:ASP:HB2	5:E:320:LEU:HD11	2.02	0.41
7:G:-4:G:C2	7:G:-3:A:N7	2.89	0.41
7:G:12:G:H4'	7:G:13:C:OP1	2.21	0.41
7:G:14:A:H2'	7:G:15:U:H6	1.86	0.41
10:J:220:LEU:HD11	10:J:224:LYS:HE3	2.01	0.41
10:J:306:LEU:HB3	10:J:309:VAL:HG23	2.03	0.41
11:K:24:LEU:O	11:K:26:TRP:N	2.53	0.41
11:K:70:GLU:OE1	11:K:73:ARG:NE	2.53	0.41
16:Q:877:LEU:N	16:Q:1034:ILE:O	2.54	0.41
17:R:281:ASN:HD21	17:R:283:ASN:ND2	2.18	0.41
18:T:194:TRP:CH2	18:T:491:GLU:HG3	2.56	0.41
18:T:324:HIS:ND1	18:T:362:GLY:HA3	2.35	0.41
18:T:440:ASP:OD2	18:T:443:THR:HG23	2.21	0.41
18:T:496:THR:OG1	18:T:498:GLU:HG3	2.20	0.41
18:T:499:THR:HB	18:T:500:HIS:ND1	2.36	0.41
22:1:118:GLU:HA	22:1:121:LYS:HB2	2.02	0.41
22:1:124:ARG:O	22:1:126:MET:N	2.54	0.41
22:1:130:PRO:HD2	22:1:150:ARG:HD2	2.02	0.41
22:1:686:LEU:HD23	22:1:686:LEU:HA	1.79	0.41
22:1:721:ILE:O	22:1:721:ILE:HG13	2.20	0.41
22:1:815:PHE:HA	22:1:819:TRP:HD1	1.86	0.41
22:1:969:LYS:HE2	22:1:969:LYS:HB2	1.78	0.41
22:1:1144:GLN:O	22:1:1147:VAL:HG13	2.20	0.41
23:3:148:ALA:C	23:3:150:ALA:H	2.23	0.41
23:3:404:LEU:HD23	23:3:407:ILE:HD11	2.03	0.41
23:3:471:ASP:N	23:3:471:ASP:OD1	2.54	0.41
23:3:718:ARG:NH2	23:3:735:SER:HA	2.35	0.41
23:3:817:GLN:HE21	23:3:818:GLN:CA	2.34	0.41
23:3:982:GLU:HG3	23:3:983:ASN:N	2.34	0.41

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
23:3:1049:LYS:HE3	23:3:1049:LYS:HB2	1.56	0.41
23:3:1082:LEU:HG	35:2:496:ASN:HA	2.03	0.41
23:3:1096:HIS:CD2	23:3:1166:TYR:HB2	2.56	0.41
35:2:540:LEU:N	35:2:540:LEU:HD23	2.35	0.41
37:6:46:ARG:N	37:6:65:GLU:HG2	2.36	0.41
38:7:11:CYS:N	38:7:87:LYS:O	2.53	0.41
38:7:46:CYS:N	38:7:85:CYS:SG	2.73	0.41
40:9:310:LEU:HD13	40:9:315:TYR:CD1	2.56	0.41
41:8:23:LYS:C	41:8:27:GLN:HE21	2.24	0.41
41:8:90:THR:HG23	41:8:95:GLY:HA2	2.03	0.41
1:A:545:HIS:O	1:A:549:GLU:HG2	2.21	0.41
1:A:549:GLU:HG3	1:A:594:TYR:CE2	2.54	0.41
1:A:981:PHE:CZ	1:A:1095:ILE:HD11	2.56	0.41
1:A:1412:TRP:CH2	1:A:1423:PHE:HD2	2.39	0.41
1:A:1685:LEU:HD21	1:A:1715:TYR:HE2	1.85	0.41
3:C:141:GLY:O	3:C:145:PHE:CB	2.68	0.41
3:C:550:VAL:HB	3:C:552:ILE:HD11	2.02	0.41
6:F:37:C:H41	7:G:5:G:P	2.43	0.41
6:F:42:C:H2’	6:F:43:A:O4’	2.21	0.41
8:H:38:A:O2’	8:H:39:U:H5’	2.21	0.41
8:H:41:U:H2’	8:H:42:G:O4’	2.21	0.41
9:I:473:SER:O	9:I:475:PRO:HD3	2.21	0.41
11:K:78:GLU:O	11:K:82:ARG:HG3	2.21	0.41
11:K:178:ARG:HD2	11:K:182:GLU:OE1	2.21	0.41
18:T:220:VAL:CG1	18:T:252:VAL:HG21	2.50	0.41
18:T:329:HIS:HD1	18:T:351:ASP:CG	2.16	0.41
22:1:641:ILE:N	22:1:642:PRO:HD2	2.36	0.41
22:1:656:LYS:HE2	41:8:65:ASP:HB2	2.02	0.41
23:3:86:ARG:HH11	23:3:86:ARG:HD2	1.73	0.41
23:3:170:VAL:HG22	23:3:184:CYS:HB2	2.02	0.41
23:3:550:ASN:HB2	23:3:592:LEU:HG	2.03	0.41
23:3:644:GLU:HG2	23:3:645:MET:HB2	2.03	0.41
23:3:791:HIS:HD1	23:3:930:LEU:HD21	1.86	0.41
23:3:1084:GLY:HA3	35:2:495:ARG:HH21	1.86	0.41
39:5:8:HIS:O	39:5:11:LEU:HG	2.21	0.41
40:9:352:ASP:OD2	40:9:370:ASN:ND2	2.54	0.41
41:8:56:VAL:O	41:8:59:ILE:N	2.54	0.41
1:A:156:ARG:HD2	1:A:620:PRO:HG2	2.03	0.40
1:A:245:LEU:HA	1:A:430:TRP:HZ2	1.85	0.40
1:A:417:ARG:HG2	1:A:418:THR:H	1.86	0.40
1:A:1183:PRO:N	1:A:1201:ARG:HH21	2.18	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1307:MET:HB2	2:B:40:U:C4	2.56	0.40
3:C:168:THR:O	3:C:170:ILE:HG12	2.20	0.40
3:C:518:ASP:HB3	3:C:520:GLU:CD	2.41	0.40
3:C:531:TRP:HH2	3:C:553:GLU:HB2	1.85	0.40
3:C:811:THR:O	3:C:815:VAL:HG22	2.21	0.40
3:C:916:ILE:HB	3:C:931:ARG:HG2	2.03	0.40
5:E:115:LEU:HD23	5:E:115:LEU:HA	1.78	0.40
5:E:194:TYR:HD2	5:E:214:ASP:HB3	1.86	0.40
6:F:86:U:C2	8:H:14:C:N4	2.90	0.40
8:H:171:U:H2'	8:H:172:C:C6	2.57	0.40
8:H:172:C:C2	8:H:173:C:C5	3.09	0.40
11:K:73:ARG:O	11:K:77:LEU:HG	2.21	0.40
18:T:371:HIS:CD2	18:T:375:VAL:HG21	2.56	0.40
21:Z:600:ARG:HH22	21:Z:601:LEU:CD1	2.33	0.40
22:1:146:LYS:HB3	22:1:146:LYS:HE3	1.80	0.40
22:1:487:LEU:HD23	22:1:492:GLN:HE21	1.85	0.40
22:1:531:LEU:HD12	22:1:531:LEU:HA	1.59	0.40
22:1:551:LEU:O	22:1:555:VAL:HG12	2.22	0.40
22:1:1210:HIS:CE1	35:2:585:THR:OG1	2.74	0.40
23:3:328:LYS:NZ	23:3:370:GLU:OE1	2.48	0.40
23:3:407:ILE:HG23	23:3:425:VAL:HG13	2.02	0.40
23:3:1016:ARG:HG3	23:3:1017:ASN:H	1.86	0.40
37:6:48:ILE:HG12	37:6:62:VAL:HG12	2.03	0.40
38:7:21:ARG:HH21	38:7:21:ARG:HG2	1.86	0.40
40:9:221:LEU:H	40:9:221:LEU:HG	1.25	0.40
41:8:69:GLU:HG2	41:8:69:GLU:H	1.71	0.40
41:8:89:LEU:HB3	41:8:93:LEU:HD12	2.03	0.40
41:8:106:TRP:O	41:8:110:LEU:HG	2.21	0.40
41:8:123:PHE:HA	41:8:126:LEU:HB3	2.03	0.40
1:A:192:GLN:H	1:A:192:GLN:HG2	1.54	0.40
1:A:260:LEU:H	1:A:260:LEU:HD12	1.86	0.40
1:A:590:GLY:HA2	1:A:592:TYR:CZ	2.56	0.40
1:A:1183:PRO:CA	1:A:1201:ARG:HH21	2.33	0.40
1:A:1426:ASP:O	1:A:1427:ARG:C	2.58	0.40
2:B:39:C:H4'	2:B:40:U:OP1	2.21	0.40
3:C:183:SER:H	3:C:214:GLU:CB	2.34	0.40
3:C:350:ASN:OD1	3:C:352:LYS:HG2	2.21	0.40
3:C:452:THR:O	3:C:578:ARG:N	2.33	0.40
3:C:914:LYS:HA	3:C:931:ARG:HH21	1.86	0.40
5:E:126:SER:HG	5:E:136:TRP:HD1	1.56	0.40
6:F:10:U:H2'	6:F:11:C:O4'	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:60:C:H3'	6:F:60:C:OP2	2.21	0.40
11:K:25:ARG:HD3	11:K:26:TRP:CH2	2.57	0.40
11:K:129:LYS:NZ	11:K:131:ASP:OD2	2.36	0.40
17:R:253:ASN:HB2	17:R:254:TRP:CZ3	2.56	0.40
18:T:292:TYR:HH	18:T:308:ARG:HD3	1.81	0.40
22:1:677:CYS:C	22:1:679:ILE:H	2.24	0.40
22:1:912:ASN:OD1	22:1:957:ARG:NH1	2.50	0.40
22:1:1167:TYR:CD1	35:2:581:LYS:HB2	2.54	0.40
23:3:886:GLU:OE2	23:3:911:LYS:HD3	2.21	0.40
40:9:327:ASN:HB3	40:9:385:ARG:HH11	1.85	0.40
1:A:106:MET:HE1	1:A:557:VAL:HG11	2.02	0.40
1:A:713:LEU:HD13	1:A:739:ILE:HG12	2.03	0.40
1:A:717:TRP:O	1:A:720:TRP:N	2.54	0.40
1:A:769:LYS:HD2	1:A:769:LYS:HA	1.78	0.40
1:A:776:LEU:HD12	1:A:776:LEU:HA	1.80	0.40
1:A:946:GLU:HB3	1:A:950:LEU:HD23	2.02	0.40
1:A:960:ASN:ND2	1:A:1216:LEU:O	2.54	0.40
1:A:1296:GLN:HA	1:A:1299:ILE:CD1	2.51	0.40
1:A:1312:PRO:O	1:A:1312:PRO:CG	2.70	0.40
2:B:103:G:N1	2:B:111:A:C6	2.89	0.40
3:C:495:ARG:CB	3:C:549:TRP:HD1	2.29	0.40
3:C:607:LEU:HD12	3:C:627:HIS:CD2	2.56	0.40
3:C:659:VAL:HG22	3:C:660:VAL:H	1.86	0.40
5:E:174:GLY:HA2	5:E:194:TYR:O	2.21	0.40
6:F:37:C:N4	7:G:5:G:OP2	2.53	0.40
6:F:38:G:OP1	6:F:38:G:C8	2.75	0.40
6:F:41:A:C6	6:F:42:C:C4	3.10	0.40
6:F:83:A:C8	6:F:84:A:C5	3.09	0.40
10:J:216:ASP:O	10:J:220:LEU:HB3	2.20	0.40
10:J:224:LYS:O	10:J:228:ARG:HB2	2.21	0.40
11:K:33:LYS:CB	11:K:44:HIS:HE1	2.34	0.40
11:K:155:LEU:HD23	11:K:158:LYS:HD2	2.03	0.40
11:K:180:GLY:HA3	23:3:690:ARG:NH2	2.37	0.40
12:L:34:ILE:O	12:L:37:LEU:HB2	2.21	0.40
12:L:73:HIS:CD2	40:9:220:ILE:HB	2.57	0.40
17:R:291:LEU:HD23	17:R:291:LEU:HA	1.79	0.40
19:X:229:SER:HB3	20:Y:51:ASP:OD2	2.22	0.40
22:1:171:GLN:O	22:1:174:GLU:N	2.53	0.40
22:1:548:GLU:H	22:1:548:GLU:HG2	1.42	0.40
22:1:642:PRO:HD3	22:1:682:HIS:NE2	2.35	0.40
22:1:1262:ARG:NH1	35:2:483:GLN:NE2	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:14:ILE:HD13	23:3:32:VAL:HG11	2.03	0.40
23:3:149:ALA:HB3	23:3:151:ARG:HD3	2.03	0.40
23:3:356:HIS:HB2	23:3:401:LEU:HB2	2.04	0.40
23:3:412:ILE:HG12	23:3:423:LEU:HG	2.04	0.40
23:3:447:MET:HG2	23:3:750:CYS:HB2	2.03	0.40
23:3:450:SER:HB3	23:3:762:LEU:HD23	2.04	0.40
23:3:535:GLU:HG3	23:3:536:TRP:N	2.36	0.40
23:3:543:THR:O	23:3:559:THR:HG23	2.22	0.40
23:3:791:HIS:HD2	23:3:793:GLU:N	2.18	0.40
23:3:1015:LYS:NZ	23:3:1067:ASP:HB2	2.37	0.40
23:3:1195:GLU:C	23:3:1198:ASP:H	2.25	0.40
39:5:44:MET:HB2	39:5:44:MET:HE2	1.78	0.40
40:9:324:SER:HB3	40:9:415:SER:OG	2.20	0.40
41:8:14:ASP:OD2	41:8:16:ARG:NH2	2.46	0.40
1:A:226:GLN:NE2	1:A:417:ARG:HH21	2.18	0.40
1:A:412:ASN:OD1	1:A:413:LEU:HD23	2.21	0.40
1:A:489:TRP:CZ3	1:A:558:VAL:HG22	2.57	0.40
1:A:541:GLY:HA3	6:F:66:C:P	2.61	0.40
1:A:822:PHE:CD2	1:A:822:PHE:C	2.94	0.40
1:A:826:PRO:O	1:A:826:PRO:CD	2.70	0.40
1:A:1215:ASN:ND2	1:A:1215:ASN:N	2.69	0.40
1:A:1392:LYS:HB2	1:A:1392:LYS:HE2	1.71	0.40
1:A:1404:THR:N	1:A:1407:ASP:OD2	2.54	0.40
1:A:2325:VAL:O	4:D:788:GLY:HA2	2.21	0.40
3:C:289:ILE:O	3:C:292:TYR:N	2.54	0.40
3:C:316:ILE:HD11	3:C:420:CYS:SG	2.62	0.40
3:C:658:PRO:HB2	3:C:881:PHE:CE2	2.57	0.40
4:D:1031:GLU:HA	4:D:1034:LYS:CB	2.51	0.40
5:E:133:VAL:HB	5:E:147:LEU:HD12	2.03	0.40
6:F:46:G:H5'	6:F:47:A:H4'	2.02	0.40
7:G:116:C:C4	20:Y:117:ALA:O	2.75	0.40
8:H:22:U:H5'	8:H:23:A:OP2	2.21	0.40
10:J:286:GLU:HB3	10:J:295:ALA:HB2	2.03	0.40
11:K:280:TRP:C	11:K:282:GLN:H	2.23	0.40
19:X:338:PHE:HA	19:X:342:LYS:O	2.22	0.40
20:Y:22:VAL:HG12	20:Y:26:VAL:HG23	2.03	0.40
22:1:539:LEU:HD23	22:1:577:VAL:HG11	2.02	0.40
22:1:866:LYS:CG	22:1:909:VAL:HG11	2.51	0.40
23:3:78:ILE:HD13	23:3:78:ILE:HG21	1.86	0.40
23:3:268:ARG:CZ	23:3:268:ARG:HB3	2.52	0.40
23:3:272:PRO:HG2	23:3:311:PHE:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:609:LEU:HD11	23:3:615:ARG:HD2	2.02	0.40
23:3:709:GLN:HA	23:3:709:GLN:OE1	2.21	0.40
23:3:833:GLU:O	23:3:836:ALA:N	2.53	0.40
23:3:906:LEU:HD12	23:3:906:LEU:N	2.37	0.40
41:8:39:ASP:HA	41:8:78:LYS:O	2.22	0.40
1:A:111:GLU:OE2	1:A:210:HIS:HA	2.21	0.40
1:A:119:LEU:HD13	1:A:477:LYS:HD3	2.02	0.40
1:A:134:TRP:HB3	1:A:418:THR:CG2	2.52	0.40
1:A:264:PHE:CE1	1:A:455:VAL:HG13	2.56	0.40
1:A:368:GLN:HG2	1:A:369:GLU:H	1.87	0.40
1:A:941:LYS:HG2	1:A:1071:PHE:CE1	2.56	0.40
1:A:1248:LEU:HD23	1:A:1248:LEU:HA	1.81	0.40
1:A:1489:LEU:HD23	1:A:1489:LEU:HA	1.89	0.40
1:A:1490:PHE:CE2	1:A:1498:TRP:HB3	2.57	0.40
1:A:1566:ILE:H	1:A:1566:ILE:HG12	1.52	0.40
1:A:1664:ILE:HD13	1:A:1703:ILE:HG13	2.03	0.40
1:A:1699:THR:HA	1:A:1717:ASN:ND2	2.37	0.40
3:C:219:LEU:HD23	3:C:219:LEU:HA	1.93	0.40
3:C:501:ILE:HB	3:C:544:VAL:CG1	2.52	0.40
3:C:676:ALA:HA	3:C:954:ASP:OD1	2.22	0.40
3:C:772:TRP:CZ2	3:C:813:ARG:HD3	2.56	0.40
5:E:343:ILE:HD13	5:E:343:ILE:HA	1.91	0.40
6:F:70:A:C6	6:F:71:G:N7	2.90	0.40
6:F:86:U:H3	8:H:13:C:H5	1.67	0.40
10:J:222:ASP:O	10:J:226:ARG:HG3	2.21	0.40
22:1:517:ARG:HE	22:1:517:ARG:HB3	1.57	0.40
22:1:774:ILE:O	22:1:777:PHE:HD2	2.04	0.40
22:1:896:ILE:HA	22:1:896:ILE:HD13	1.74	0.40
22:1:954:LEU:O	22:1:958:THR:HG23	2.22	0.40
22:1:986:TYR:HD1	22:1:986:TYR:HA	1.68	0.40
22:1:1051:SER:OG	22:1:1053:ARG:N	2.55	0.40
22:1:1098:LEU:O	22:1:1100:ASN:N	2.55	0.40
22:1:1140:GLU:HB2	22:1:1143:VAL:HG12	2.04	0.40
23:3:534:ASN:OD1	23:3:534:ASN:N	2.55	0.40
23:3:794:SER:O	23:3:795:ASN:HB2	2.21	0.40
23:3:827:ALA:HA	23:3:834:LEU:HD21	2.02	0.40
23:3:861:GLN:HE21	23:3:861:GLN:HB3	1.47	0.40
38:7:54:TYR:CD1	38:7:54:TYR:N	2.89	0.40
40:9:302:LYS:CD	40:9:350:PHE:HB2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2135/2335 (91%)	1880 (88%)	240 (11%)	15 (1%)	22	55
3	C	892/972 (92%)	827 (93%)	65 (7%)	0	100	100
4	D	1720/2136 (80%)	1602 (93%)	114 (7%)	4 (0%)	47	78
5	E	297/357 (83%)	274 (92%)	23 (8%)	0	100	100
9	I	591/855 (69%)	494 (84%)	93 (16%)	4 (1%)	22	55
10	J	245/848 (29%)	226 (92%)	17 (7%)	2 (1%)	19	51
11	K	308/393 (78%)	292 (95%)	14 (4%)	2 (1%)	25	57
12	L	97/802 (12%)	94 (97%)	3 (3%)	0	100	100
13	N	132/144 (92%)	123 (93%)	9 (7%)	0	100	100
14	O	267/420 (64%)	255 (96%)	12 (4%)	0	100	100
15	P	40/229 (18%)	31 (78%)	9 (22%)	0	100	100
16	Q	1319/1485 (89%)	1256 (95%)	62 (5%)	1 (0%)	51	82
17	R	184/536 (34%)	172 (94%)	12 (6%)	0	100	100
18	T	318/514 (62%)	281 (88%)	36 (11%)	1 (0%)	41	72
19	X	152/396 (38%)	142 (93%)	10 (7%)	0	100	100
20	Y	116/322 (36%)	106 (91%)	10 (9%)	0	100	100
21	Z	53/619 (9%)	48 (91%)	5 (9%)	0	100	100
22	1	984/1304 (76%)	872 (89%)	102 (10%)	10 (1%)	15	46
23	3	1168/1217 (96%)	1023 (88%)	141 (12%)	4 (0%)	41	72
24	o	160/255 (63%)	148 (92%)	12 (8%)	0	100	100
25	p	165/225 (73%)	152 (92%)	13 (8%)	0	100	100
26	c	95/118 (80%)	84 (88%)	11 (12%)	0	100	100
26	h	91/118 (77%)	86 (94%)	4 (4%)	1 (1%)	14	44
27	d	72/86 (84%)	66 (92%)	6 (8%)	0	100	100
27	i	70/86 (81%)	65 (93%)	5 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	a	82/240 (34%)	77 (94%)	5 (6%)	0	100	100
28	m	80/240 (33%)	75 (94%)	5 (6%)	0	100	100
29	g	77/126 (61%)	70 (91%)	7 (9%)	0	100	100
29	l	81/126 (64%)	74 (91%)	7 (9%)	0	100	100
30	f	72/76 (95%)	67 (93%)	5 (7%)	0	100	100
30	k	71/76 (93%)	67 (94%)	4 (6%)	0	100	100
31	e	75/92 (82%)	68 (91%)	7 (9%)	0	100	100
31	j	79/92 (86%)	70 (89%)	9 (11%)	0	100	100
32	b	80/119 (67%)	75 (94%)	5 (6%)	0	100	100
32	n	78/119 (66%)	72 (92%)	6 (8%)	0	100	100
33	w	428/501 (85%)	403 (94%)	23 (5%)	2 (0%)	29	61
34	u	183/793 (23%)	175 (96%)	8 (4%)	0	100	100
35	2	225/895 (25%)	205 (91%)	17 (8%)	3 (1%)	12	39
36	4	157/424 (37%)	145 (92%)	12 (8%)	0	100	100
37	6	107/125 (86%)	98 (92%)	9 (8%)	0	100	100
38	7	103/110 (94%)	89 (86%)	14 (14%)	0	100	100
39	5	79/86 (92%)	70 (89%)	9 (11%)	0	100	100
40	9	378/520 (73%)	343 (91%)	34 (9%)	1 (0%)	41	72
41	8	113/904 (12%)	104 (92%)	9 (8%)	0	100	100
42	y	77/301 (26%)	73 (95%)	4 (5%)	0	100	100
43	v	158/464 (34%)	143 (90%)	15 (10%)	0	100	100
All	All	14454/23201 (62%)	13162 (91%)	1242 (9%)	50 (0%)	44	72

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	802	THR
1	A	1553	VAL
22	1	430	LYS
22	1	435	PRO
22	1	437	PRO
22	1	1099	ASN
33	w	498	GLN
35	2	510	TYR
1	A	1549	VAL

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Mol	Chain	Res	Type
4	D	531	ILE
4	D	2098	ALA
9	I	375	ILE
22	1	945	ALA
22	1	1104	GLN
23	3	773	VAL
23	3	1008	SER
33	w	500	LEU
35	2	533	ILE
40	9	269	ASP
1	A	1305	SER
11	K	281	LEU
1	A	366	LYS
1	A	1020	LYS
1	A	1311	PHE
4	D	2099	THR
9	I	207	GLU
18	T	308	ARG
1	A	367	SER
1	A	1362	ASP
1	A	1548	TYR
9	I	85	ARG
11	K	40	GLY
22	1	125	THR
22	1	417	PRO
22	1	717	THR
22	1	973	HIS
23	3	319	GLU
23	3	496	ASP
10	J	241	VAL
1	A	826	PRO
1	A	1308	PRO
1	A	1419	ILE
4	D	1584	ILE
1	A	167	PRO
1	A	942	PRO
9	I	385	VAL
10	J	341	PRO
26	h	103	GLY
35	2	474	VAL
16	Q	489	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1476/2108 (70%)	1265 (86%)	211 (14%)	3	13
3	C	792/866 (92%)	722 (91%)	70 (9%)	10	33
5	E	256/300 (85%)	242 (94%)	14 (6%)	21	51
9	I	23/749 (3%)	23 (100%)	0	100	100
10	J	205/751 (27%)	190 (93%)	15 (7%)	14	43
11	K	164/354 (46%)	139 (85%)	25 (15%)	3	11
12	L	86/709 (12%)	74 (86%)	12 (14%)	3	13
15	P	40/203 (20%)	35 (88%)	5 (12%)	4	17
16	Q	71/1336 (5%)	71 (100%)	0	100	100
17	R	160/459 (35%)	128 (80%)	32 (20%)	1	3
18	T	273/441 (62%)	232 (85%)	41 (15%)	3	12
19	X	139/349 (40%)	128 (92%)	11 (8%)	12	39
20	Y	105/291 (36%)	83 (79%)	22 (21%)	1	3
21	Z	40/545 (7%)	35 (88%)	5 (12%)	4	17
22	1	834/1103 (76%)	707 (85%)	127 (15%)	3	11
23	3	1020/1051 (97%)	831 (82%)	189 (18%)	1	5
24	o	6/218 (3%)	6 (100%)	0	100	100
25	p	8/195 (4%)	8 (100%)	0	100	100
26	h	5/110 (4%)	5 (100%)	0	100	100
27	i	4/74 (5%)	4 (100%)	0	100	100
28	m	4/177 (2%)	4 (100%)	0	100	100
29	l	3/101 (3%)	3 (100%)	0	100	100
30	k	3/66 (4%)	3 (100%)	0	100	100
31	j	1/84 (1%)	1 (100%)	0	100	100
32	n	3/101 (3%)	3 (100%)	0	100	100
33	w	112/446 (25%)	98 (88%)	14 (12%)	4	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	u	10/709 (1%)	10 (100%)	0	100	100
35	2	134/776 (17%)	102 (76%)	32 (24%)	0	2
37	6	97/109 (89%)	86 (89%)	11 (11%)	6	21
38	7	90/95 (95%)	73 (81%)	17 (19%)	1	4
39	5	72/77 (94%)	67 (93%)	5 (7%)	15	45
40	9	223/456 (49%)	197 (88%)	26 (12%)	5	20
41	8	104/831 (12%)	98 (94%)	6 (6%)	20	50
43	v	73/382 (19%)	59 (81%)	14 (19%)	1	4
All	All	6636/16622 (40%)	5732 (86%)	904 (14%)	7	14

All (904) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	VAL
1	A	92	LEU
1	A	123	THR
1	A	150	MET
1	A	176	LEU
1	A	177	ASP
1	A	192	GLN
1	A	193	LEU
1	A	210	HIS
1	A	237	THR
1	A	245	LEU
1	A	256	TYR
1	A	258	PHE
1	A	280	GLU
1	A	310	THR
1	A	311	GLU
1	A	314	ILE
1	A	322	ASN
1	A	325	HIS
1	A	342	THR
1	A	344	ASP
1	A	363	HIS
1	A	383	PHE
1	A	387	PHE
1	A	391	THR
1	A	393	LEU

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Mol	Chain	Res	Type
1	A	409	ARG
1	A	412	ASN
1	A	413	LEU
1	A	417	ARG
1	A	426	LEU
1	A	427	VAL
1	A	430	TRP
1	A	433	GLU
1	A	451	LEU
1	A	452	LYS
1	A	475	SER
1	A	479	THR
1	A	487	LEU
1	A	506	LEU
1	A	524	LEU
1	A	547	CYS
1	A	551	LEU
1	A	555	LYS
1	A	570	ASP
1	A	574	LEU
1	A	591	MET
1	A	596	TYR
1	A	613	TYR
1	A	617	ASN
1	A	621	VAL
1	A	627	CYS
1	A	637	TRP
1	A	642	ARG
1	A	659	GLN
1	A	675	GLN
1	A	693	ILE
1	A	699	GLU
1	A	705	LYS
1	A	708	THR
1	A	709	ILE
1	A	728	VAL
1	A	733	THR
1	A	735	ILE
1	A	738	MET
1	A	739	ILE
1	A	748	ASP
1	A	753	THR

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Mol	Chain	Res	Type
1	A	766	THR
1	A	767	VAL
1	A	770	THR
1	A	771	VAL
1	A	779	LEU
1	A	780	THR
1	A	790	ARG
1	A	793	ASN
1	A	801	ILE
1	A	811	THR
1	A	812	THR
1	A	813	THR
1	A	819	SER
1	A	826	PRO
1	A	848	GLU
1	A	851	SER
1	A	871	TYR
1	A	873	ASN
1	A	879	SER
1	A	894	VAL
1	A	910	ASP
1	A	923	ASP
1	A	946	GLU
1	A	956	CYS
1	A	957	GLN
1	A	963	GLN
1	A	969	SER
1	A	976	MET
1	A	977	LEU
1	A	979	SER
1	A	985	TYR
1	A	990	LEU
1	A	1002	ASP
1	A	1021	ASP
1	A	1022	MET
1	A	1027	SER
1	A	1030	ILE
1	A	1034	LEU
1	A	1048	MET
1	A	1049	ASP
1	A	1051	LEU
1	A	1069	ASN

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Mol	Chain	Res	Type
1	A	1070	ASP
1	A	1074	PHE
1	A	1076	ASP
1	A	1089	CYS
1	A	1092	ILE
1	A	1099	PHE
1	A	1101	PHE
1	A	1105	GLU
1	A	1108	ASP
1	A	1130	ASN
1	A	1133	CYS
1	A	1137	ASP
1	A	1141	ARG
1	A	1147	VAL
1	A	1158	LYS
1	A	1177	VAL
1	A	1181	ASP
1	A	1186	LEU
1	A	1189	MET
1	A	1215	ASN
1	A	1237	MET
1	A	1243	ARG
1	A	1255	THR
1	A	1258	LYS
1	A	1268	ILE
1	A	1284	LEU
1	A	1293	ASN
1	A	1295	ILE
1	A	1297	THR
1	A	1298	ARG
1	A	1299	ILE
1	A	1301	ILE
1	A	1303	LEU
1	A	1304	ASN
1	A	1306	LYS
1	A	1308	PRO
1	A	1310	ARG
1	A	1314	VAL
1	A	1327	MET
1	A	1329	SER
1	A	1332	HIS
1	A	1334	LEU

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Mol	Chain	Res	Type
1	A	1359	HIS
1	A	1363	GLN
1	A	1365	ILE
1	A	1367	ASN
1	A	1368	LEU
1	A	1371	TYR
1	A	1372	ILE
1	A	1376	GLU
1	A	1377	SER
1	A	1380	ILE
1	A	1391	LEU
1	A	1393	ARG
1	A	1402	ARG
1	A	1404	THR
1	A	1405	LEU
1	A	1407	ASP
1	A	1410	ASP
1	A	1416	ILE
1	A	1418	ARG
1	A	1428	HIS
1	A	1438	VAL
1	A	1447	VAL
1	A	1448	LEU
1	A	1458	GLN
1	A	1460	HIS
1	A	1461	ASP
1	A	1471	ARG
1	A	1488	THR
1	A	1493	THR
1	A	1494	TYR
1	A	1502	PHE
1	A	1527	ASN
1	A	1529	ILE
1	A	1531	ASN
1	A	1535	THR
1	A	1539	SER
1	A	1546	ASN
1	A	1547	VAL
1	A	1551	PHE
1	A	1555	LEU
1	A	1557	LEU
1	A	1566	ILE

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Mol	Chain	Res	Type
1	A	1574	ILE
1	A	1575	GLN
1	A	1581	LEU
1	A	1606	ILE
1	A	1608	THR
1	A	1611	LYS
1	A	1614	ILE
1	A	1624	SER
1	A	1650	ASP
1	A	1654	SER
1	A	1655	THR
1	A	1664	ILE
1	A	1681	ARG
1	A	1703	ILE
1	A	1706	ASP
1	A	1737	ASN
1	A	1745	GLU
3	C	59	LEU
3	C	65	TYR
3	C	68	THR
3	C	85	ASP
3	C	126	SER
3	C	129	ILE
3	C	132	VAL
3	C	147	ASP
3	C	148	CYS
3	C	162	ASP
3	C	168	THR
3	C	171	LEU
3	C	202	ILE
3	C	209	VAL
3	C	223	ASP
3	C	245	HIS
3	C	251	LEU
3	C	254	THR
3	C	265	LEU
3	C	306	ASN
3	C	312	SER
3	C	325	LYS
3	C	342	ARG
3	C	394	ARG
3	C	399	LEU

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Mol	Chain	Res	Type
3	C	432	ASP
3	C	433	MET
3	C	460	ASP
3	C	461	LEU
3	C	468	CYS
3	C	476	CYS
3	C	484	THR
3	C	491	HIS
3	C	498	SER
3	C	536	ARG
3	C	543	ARG
3	C	551	LEU
3	C	556	ASP
3	C	562	THR
3	C	584	THR
3	C	587	VAL
3	C	592	VAL
3	C	602	LYS
3	C	609	LYS
3	C	616	SER
3	C	618	THR
3	C	619	THR
3	C	627	HIS
3	C	638	ASP
3	C	639	CYS
3	C	661	THR
3	C	685	ILE
3	C	690	GLU
3	C	707	ILE
3	C	749	THR
3	C	755	ASP
3	C	767	VAL
3	C	779	LEU
3	C	788	LYS
3	C	796	VAL
3	C	824	THR
3	C	850	LEU
3	C	878	ILE
3	C	879	ASP
3	C	884	GLU
3	C	890	HIS
3	C	901	PHE

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Mol	Chain	Res	Type
3	C	902	HIS
3	C	907	VAL
3	C	946	ASP
5	E	62	LEU
5	E	71	CYS
5	E	74	PHE
5	E	86	PHE
5	E	116	HIS
5	E	156	SER
5	E	157	CYS
5	E	168	CYS
5	E	173	ASP
5	E	215	ASN
5	E	236	ASP
5	E	246	GLU
5	E	264	VAL
5	E	304	SER
10	J	252	GLU
10	J	270	ASP
10	J	282	TYR
10	J	305	THR
10	J	306	LEU
10	J	321	GLU
10	J	355	ARG
10	J	363	ARG
10	J	366	TYR
10	J	385	PHE
10	J	404	GLU
10	J	405	PHE
10	J	406	PHE
10	J	419	PHE
10	J	422	PHE
11	K	7	LEU
11	K	8	THR
11	K	19	LYS
11	K	24	LEU
11	K	28	CYS
11	K	35	CYS
11	K	38	GLU
11	K	47	SER
11	K	56	LEU
11	K	63	GLN

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Mol	Chain	Res	Type
11	K	66	ASP
11	K	74	ASN
11	K	77	LEU
11	K	78	GLU
11	K	84	PHE
11	K	93	ILE
11	K	99	ILE
11	K	108	ASN
11	K	141	TYR
11	K	144	ARG
11	K	145	ASP
11	K	165	ASP
11	K	174	GLU
11	K	178	ARG
11	K	181	LEU
12	L	14	THR
12	L	16	ASP
12	L	37	LEU
12	L	38	LEU
12	L	41	LYS
12	L	49	ARG
12	L	54	LEU
12	L	55	ASP
12	L	61	THR
12	L	64	SER
12	L	71	LEU
12	L	77	LEU
15	P	189	ASP
15	P	196	ASN
15	P	202	ASP
15	P	214	THR
15	P	224	MET
17	R	125	MET
17	R	132	LEU
17	R	137	GLU
17	R	138	GLU
17	R	140	ILE
17	R	145	GLU
17	R	148	ARG
17	R	151	LEU
17	R	157	GLN
17	R	231	HIS

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Mol	Chain	Res	Type
17	R	234	SER
17	R	238	THR
17	R	239	VAL
17	R	241	GLU
17	R	256	ASN
17	R	279	HIS
17	R	307	GLN
17	R	319	LYS
17	R	323	LYS
17	R	324	LEU
17	R	332	ARG
17	R	384	GLU
17	R	386	ARG
17	R	388	ILE
17	R	390	GLU
17	R	401	THR
17	R	406	GLN
17	R	408	ASP
17	R	415	SER
17	R	433	TYR
17	R	434	ASP
17	R	438	ARG
18	T	201	SER
18	T	209	CYS
18	T	210	ILE
18	T	223	SER
18	T	225	ASP
18	T	230	ILE
18	T	242	LEU
18	T	263	SER
18	T	267	ASP
18	T	277	TYR
18	T	281	ILE
18	T	282	ARG
18	T	283	HIS
18	T	300	ILE
18	T	307	SER
18	T	309	ASP
18	T	311	THR
18	T	316	ASP
18	T	325	THR
18	T	336	VAL

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Mol	Chain	Res	Type
18	T	349	SER
18	T	350	HIS
18	T	355	ARG
18	T	369	THR
18	T	370	ASN
18	T	373	LYS
18	T	374	SER
18	T	384	HIS
18	T	398	TRP
18	T	400	PHE
18	T	402	ASP
18	T	424	ASP
18	T	426	VAL
18	T	432	ASP
18	T	435	THR
18	T	439	TRP
18	T	443	THR
18	T	459	LEU
18	T	465	ILE
18	T	468	CYS
18	T	499	THR
19	X	232	LEU
19	X	234	GLU
19	X	242	VAL
19	X	261	LEU
19	X	266	ASN
19	X	273	MET
19	X	283	LEU
19	X	289	ILE
19	X	300	SER
19	X	301	LYS
19	X	307	GLN
20	Y	1	MET
20	Y	2	ASN
20	Y	9	LEU
20	Y	13	LEU
20	Y	18	VAL
20	Y	24	ASP
20	Y	34	ASP
20	Y	38	ILE
20	Y	46	GLU
20	Y	51	ASP

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Mol	Chain	Res	Type
20	Y	52	ILE
20	Y	54	CYS
20	Y	69	ARG
20	Y	77	LYS
20	Y	80	CYS
20	Y	85	GLU
20	Y	86	ASP
20	Y	89	SER
20	Y	91	ILE
20	Y	107	ILE
20	Y	108	ARG
20	Y	113	SER
21	Z	574	ASN
21	Z	583	ARG
21	Z	587	VAL
21	Z	598	PHE
21	Z	604	LYS
22	1	91	LEU
22	1	106	GLU
22	1	108	ARG
22	1	116	GLU
22	1	123	ARG
22	1	127	ILE
22	1	128	ILE
22	1	131	GLU
22	1	142	THR
22	1	154	ASP
22	1	160	HIS
22	1	161	LEU
22	1	395	ARG
22	1	451	ARG
22	1	458	ASP
22	1	479	LEU
22	1	483	ASP
22	1	488	SER
22	1	491	GLU
22	1	500	LEU
22	1	502	LEU
22	1	504	ILE
22	1	506	ASN
22	1	520	THR
22	1	524	ARG

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Mol	Chain	Res	Type
22	1	539	LEU
22	1	541	SER
22	1	543	THR
22	1	548	GLU
22	1	551	LEU
22	1	555	VAL
22	1	559	ILE
22	1	582	LEU
22	1	584	ASP
22	1	585	GLU
22	1	596	ILE
22	1	614	ARG
22	1	635	VAL
22	1	637	SER
22	1	673	ILE
22	1	675	MET
22	1	679	ILE
22	1	680	LEU
22	1	690	ILE
22	1	691	GLU
22	1	694	LEU
22	1	705	SER
22	1	714	GLU
22	1	723	SER
22	1	726	SER
22	1	727	VAL
22	1	731	LEU
22	1	733	LYS
22	1	735	ILE
22	1	753	LEU
22	1	758	ASP
22	1	761	TYR
22	1	764	TYR
22	1	765	TYR
22	1	769	VAL
22	1	776	GLU
22	1	784	MET
22	1	795	CYS
22	1	796	CYS
22	1	801	VAL
22	1	808	THR
22	1	810	ILE

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Mol	Chain	Res	Type
22	1	823	MET
22	1	839	GLU
22	1	850	ILE
22	1	853	ILE
22	1	855	ASP
22	1	878	ASN
22	1	883	ASP
22	1	889	GLU
22	1	900	PHE
22	1	905	THR
22	1	914	PHE
22	1	935	THR
22	1	942	ASN
22	1	946	LYS
22	1	950	GLN
22	1	964	THR
22	1	982	LEU
22	1	992	SER
22	1	1013	ILE
22	1	1016	LEU
22	1	1017	LEU
22	1	1021	THR
22	1	1023	ILE
22	1	1059	CYS
22	1	1063	LEU
22	1	1081	PHE
22	1	1084	ILE
22	1	1086	LYS
22	1	1090	PRO
22	1	1092	ASP
22	1	1093	VAL
22	1	1096	THR
22	1	1100	ASN
22	1	1109	ARG
22	1	1112	THR
22	1	1121	GLU
22	1	1135	GLU
22	1	1142	ASN
22	1	1147	VAL
22	1	1152	SER
22	1	1158	ILE
22	1	1160	GLU

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Mol	Chain	Res	Type
22	1	1177	LEU
22	1	1178	MET
22	1	1179	ASP
22	1	1182	LEU
22	1	1184	HIS
22	1	1195	MET
22	1	1223	SER
22	1	1226	VAL
22	1	1239	VAL
22	1	1245	ARG
22	1	1252	GLN
22	1	1267	LYS
22	1	1271	SER
22	1	1277	GLN
22	1	1297	ARG
22	1	1299	GLU
22	1	1303	ILE
22	1	1304	LEU
23	3	6	LEU
23	3	7	THR
23	3	9	GLN
23	3	12	THR
23	3	21	ASN
23	3	25	THR
23	3	27	GLN
23	3	33	SER
23	3	42	ARG
23	3	44	ASP
23	3	54	LEU
23	3	55	THR
23	3	56	VAL
23	3	65	LEU
23	3	68	PHE
23	3	69	ARG
23	3	82	SER
23	3	83	ASP
23	3	95	SER
23	3	123	VAL
23	3	124	ASP
23	3	143	ILE
23	3	146	ARG
23	3	151	ARG

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Mol	Chain	Res	Type
23	3	155	SER
23	3	162	LYS
23	3	164	ASN
23	3	165	THR
23	3	191	GLU
23	3	193	ASP
23	3	205	GLN
23	3	207	THR
23	3	209	THR
23	3	213	LEU
23	3	215	LEU
23	3	219	HIS
23	3	221	VAL
23	3	222	ARG
23	3	225	SER
23	3	226	GLU
23	3	228	LEU
23	3	234	PHE
23	3	237	THR
23	3	246	SER
23	3	259	LYS
23	3	261	PHE
23	3	266	ASP
23	3	268	ARG
23	3	285	MET
23	3	290	SER
23	3	297	SER
23	3	305	THR
23	3	309	ASP
23	3	318	ASP
23	3	320	ASP
23	3	322	VAL
23	3	323	THR
23	3	325	ILE
23	3	328	LYS
23	3	331	ASP
23	3	332	THR
23	3	339	MET
23	3	342	LEU
23	3	344	THR
23	3	347	LEU
23	3	360	GLN

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Mol	Chain	Res	Type
23	3	363	HIS
23	3	368	ASP
23	3	374	SER
23	3	379	LEU
23	3	384	THR
23	3	394	ASN
23	3	395	LEU
23	3	410	CYS
23	3	418	GLU
23	3	433	SER
23	3	439	ARG
23	3	445	SER
23	3	449	VAL
23	3	466	ILE
23	3	482	THR
23	3	483	LEU
23	3	497	SER
23	3	505	THR
23	3	508	CYS
23	3	509	SER
23	3	510	LEU
23	3	511	LEU
23	3	525	ARG
23	3	534	ASN
23	3	547	CYS
23	3	566	PHE
23	3	588	VAL
23	3	589	CYS
23	3	592	LEU
23	3	603	ARG
23	3	604	PHE
23	3	611	ASP
23	3	613	THR
23	3	616	ILE
23	3	624	CYS
23	3	633	LEU
23	3	638	GLU
23	3	664	TYR
23	3	665	LEU
23	3	666	ASN
23	3	674	LEU
23	3	679	LEU

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Mol	Chain	Res	Type
23	3	680	ASP
23	3	683	THR
23	3	686	LEU
23	3	689	THR
23	3	690	ARG
23	3	718	ARG
23	3	724	SER
23	3	729	PHE
23	3	762	LEU
23	3	777	VAL
23	3	791	HIS
23	3	799	ILE
23	3	815	ARG
23	3	817	GLN
23	3	843	LEU
23	3	847	LEU
23	3	851	ILE
23	3	861	GLN
23	3	864	SER
23	3	865	VAL
23	3	867	ARG
23	3	875	ASN
23	3	876	THR
23	3	877	LEU
23	3	886	GLU
23	3	889	PHE
23	3	891	VAL
23	3	897	SER
23	3	899	THR
23	3	902	ASP
23	3	913	LEU
23	3	915	LEU
23	3	931	VAL
23	3	943	THR
23	3	948	VAL
23	3	959	VAL
23	3	963	VAL
23	3	980	LYS
23	3	984	LYS
23	3	991	SER
23	3	993	ILE
23	3	995	THR

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Mol	Chain	Res	Type
23	3	1005	VAL
23	3	1008	SER
23	3	1020	GLN
23	3	1022	ILE
23	3	1028	THR
23	3	1038	LEU
23	3	1041	TYR
23	3	1049	LYS
23	3	1052	ASN
23	3	1057	ARG
23	3	1058	LEU
23	3	1063	ASN
23	3	1081	LEU
23	3	1082	LEU
23	3	1087	GLN
23	3	1088	LYS
23	3	1099	GLU
23	3	1104	LEU
23	3	1105	GLN
23	3	1111	PRO
23	3	1115	GLU
23	3	1120	THR
23	3	1121	THR
23	3	1128	ILE
23	3	1134	SER
23	3	1135	HIS
23	3	1145	GLU
23	3	1148	LEU
23	3	1155	LEU
23	3	1162	SER
23	3	1166	TYR
23	3	1168	PHE
23	3	1181	GLN
23	3	1185	MET
23	3	1197	LEU
23	3	1199	ARG
23	3	1203	GLU
23	3	1214	ARG
23	3	1215	TYR
33	w	381	LYS
33	w	385	LEU
33	w	396	LEU

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Mol	Chain	Res	Type
33	w	469	GLU
33	w	471	TRP
33	w	472	GLN
33	w	477	GLU
33	w	485	ASN
33	w	487	VAL
33	w	488	ASN
33	w	489	LYS
33	w	491	THR
33	w	497	ARG
33	w	500	LEU
35	2	451	LYS
35	2	453	LYS
35	2	454	LEU
35	2	455	ARG
35	2	459	ARG
35	2	467	GLN
35	2	473	ASP
35	2	474	VAL
35	2	486	LYS
35	2	488	LEU
35	2	497	SER
35	2	508	ARG
35	2	514	LYS
35	2	515	ARG
35	2	517	ILE
35	2	525	PRO
35	2	533	ILE
35	2	534	GLN
35	2	535	GLU
35	2	537	ARG
35	2	538	GLU
35	2	541	GLN
35	2	542	GLU
35	2	545	GLU
35	2	566	ILE
35	2	578	TRP
35	2	579	GLN
35	2	581	LYS
35	2	584	LEU
35	2	586	ILE
35	2	587	HIS

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Mol	Chain	Res	Type
35	2	703	ILE
37	6	16	GLU
37	6	31	THR
37	6	37	ASP
37	6	53	THR
37	6	55	GLU
37	6	78	SER
37	6	89	VAL
37	6	102	ASP
37	6	103	THR
37	6	105	LYS
37	6	107	GLU
38	7	7	ASP
38	7	30	CYS
38	7	32	ILE
38	7	33	CYS
38	7	35	SER
38	7	37	VAL
38	7	40	CYS
38	7	46	CYS
38	7	50	ASN
38	7	54	TYR
38	7	60	ILE
38	7	61	CYS
38	7	72	CYS
38	7	77	ILE
38	7	78	GLN
38	7	85	CYS
38	7	88	ILE
39	5	4	ARG
39	5	9	SER
39	5	12	GLU
39	5	14	LEU
39	5	27	THR
40	9	197	LEU
40	9	200	THR
40	9	213	LYS
40	9	221	LEU
40	9	224	THR
40	9	241	TYR
40	9	249	SER
40	9	252	SER

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Mol	Chain	Res	Type
40	9	253	THR
40	9	256	VAL
40	9	260	THR
40	9	261	HIS
40	9	268	GLU
40	9	283	ARG
40	9	298	ASP
40	9	309	ARG
40	9	328	PHE
40	9	336	THR
40	9	346	TRP
40	9	354	PHE
40	9	360	HIS
40	9	367	SER
40	9	389	TYR
40	9	397	PHE
40	9	420	ASP
40	9	453	LEU
41	8	18	SER
41	8	39	ASP
41	8	48	ILE
41	8	82	SER
41	8	90	THR
41	8	105	LEU
43	v	19	SER
43	v	22	SER
43	v	24	ARG
43	v	29	ARG
43	v	32	GLN
43	v	33	LEU
43	v	35	LEU
43	v	37	THR
43	v	38	ILE
43	v	40	ILE
43	v	42	LYS
43	v	82	LEU
43	v	85	ARG
43	v	92	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (138) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	112	GLN
1	A	210	HIS
1	A	221	ASN
1	A	321	ASN
1	A	326	HIS
1	A	328	HIS
1	A	357	ASN
1	A	363	HIS
1	A	400	ASN
1	A	429	ASN
1	A	467	GLN
1	A	502	ASN
1	A	509	HIS
1	A	517	HIS
1	A	521	ASN
1	A	568	ASN
1	A	584	HIS
1	A	675	GLN
1	A	755	HIS
1	A	775	ASN
1	A	1003	HIS
1	A	1023	ASN
1	A	1096	HIS
1	A	1117	HIS
1	A	1124	ASN
1	A	1182	ASN
1	A	1209	HIS
1	A	1215	ASN
1	A	1367	ASN
1	A	1373	GLN
1	A	1424	GLN
1	A	1460	HIS
1	A	1527	ASN
1	A	1563	HIS
1	A	1575	GLN
1	A	1610	GLN
1	A	1665	GLN
1	A	1717	ASN
3	C	137	HIS
3	C	139	HIS
3	C	208	HIS
3	C	335	ASN

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Mol	Chain	Res	Type
3	C	451	HIS
3	C	571	ASN
3	C	706	GLN
3	C	798	GLN
3	C	802	HIS
5	E	150	HIS
5	E	165	GLN
5	E	224	GLN
10	J	250	GLN
10	J	297	ASN
10	J	389	HIS
11	K	44	HIS
11	K	62	GLN
12	L	29	ASN
12	L	30	GLN
15	P	212	ASN
17	R	279	HIS
17	R	283	ASN
17	R	329	GLN
18	T	394	ASN
18	T	407	GLN
18	T	408	ASN
18	T	413	ASN
18	T	451	HIS
19	X	276	HIS
19	X	335	ASN
20	Y	64	ASN
20	Y	114	ASN
22	1	160	HIS
22	1	171	GLN
22	1	492	GLN
22	1	533	ASN
22	1	534	GLN
22	1	547	GLN
22	1	692	HIS
22	1	842	ASN
22	1	878	ASN
22	1	942	ASN
22	1	1007	HIS
22	1	1184	HIS
22	1	1194	HIS
22	1	1210	HIS

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Mol	Chain	Res	Type
22	1	1293	ASN
23	3	5	ASN
23	3	9	GLN
23	3	19	HIS
23	3	103	HIS
23	3	164	ASN
23	3	169	HIS
23	3	203	ASN
23	3	205	GLN
23	3	206	GLN
23	3	219	HIS
23	3	231	HIS
23	3	264	GLN
23	3	304	GLN
23	3	440	HIS
23	3	465	HIS
23	3	636	GLN
23	3	666	ASN
23	3	730	HIS
23	3	775	ASN
23	3	776	GLN
23	3	791	HIS
23	3	796	ASN
23	3	814	GLN
23	3	817	GLN
23	3	861	GLN
23	3	870	ASN
23	3	933	ASN
23	3	985	HIS
23	3	988	ASN
23	3	1020	GLN
23	3	1083	ASN
23	3	1096	HIS
23	3	1192	ASN
33	w	485	ASN
33	w	488	ASN
35	2	458	ASN
35	2	483	GLN
35	2	534	GLN
35	2	572	HIS
35	2	587	HIS
37	6	52	ASN

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Mol	Chain	Res	Type
38	7	14	GLN
39	5	46	HIS
39	5	67	ASN
40	9	379	GLN
40	9	452	GLN
41	8	21	GLN
41	8	27	GLN
41	8	94	ASN
41	8	97	ASN
43	v	32	GLN
43	v	81	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	96/117 (82%)	37 (38%)	3 (3%)
6	F	94/107 (87%)	51 (54%)	8 (8%)
7	G	62/220 (28%)	40 (64%)	10 (16%)
8	H	161/188 (85%)	59 (36%)	4 (2%)
All	All	413/632 (65%)	187 (45%)	25 (6%)

All (187) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	19	A
2	B	20	G
2	B	21	A
2	B	22	U
2	B	23	C
2	B	24	G
2	B	25	C
2	B	28	A
2	B	32	C
2	B	33	U
2	B	35	U
2	B	38	C
2	B	39	C
2	B	40	U
2	B	43	U
2	B	45	C
2	B	47	A

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Mol	Chain	Res	Type
2	B	48	A
2	B	50	G
2	B	57	G
2	B	62	G
2	B	65	G
2	B	71	C
2	B	85	C
2	B	86	C
2	B	87	A
2	B	88	A
2	B	89	U
2	B	90	U
2	B	92	U
2	B	93	U
2	B	94	U
2	B	95	G
2	B	96	A
2	B	97	G
2	B	98	G
2	B	117	A
6	F	5	U
6	F	6	C
6	F	7	G
6	F	9	U
6	F	10	U
6	F	12	G
6	F	16	G
6	F	19	C
6	F	25	C
6	F	26	U
6	F	27	A
6	F	28	A
6	F	29	A
6	F	31	U
6	F	32	U
6	F	33	G
6	F	34	G
6	F	36	A
6	F	37	C
6	F	38	G
6	F	40	U
6	F	41	A

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Mol	Chain	Res	Type
6	F	42	C
6	F	43	A
6	F	44	G
6	F	45	A
6	F	46	G
6	F	47	A
6	F	48	A
6	F	49	G
6	F	50	A
6	F	51	U
6	F	53	A
6	F	54	G
6	F	58	G
6	F	59	G
6	F	60	C
6	F	62	C
6	F	69	A
6	F	73	A
6	F	74	U
6	F	76	A
6	F	77	C
6	F	78	A
6	F	79	C
6	F	80	G
6	F	81	C
6	F	83	A
6	F	85	U
6	F	86	U
6	F	92	A
7	G	-7	U
7	G	-6	C
7	G	-5	C
7	G	-4	G
7	G	-3	A
7	G	-1	C
7	G	1	G
7	G	2	U
7	G	3	A
7	G	4	A
7	G	5	G
7	G	7	G
7	G	12	G

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Mol	Chain	Res	Type
7	G	13	C
7	G	17	U
7	G	18	A
7	G	20	A
7	G	84	U
7	G	85	G
7	G	88	G
7	G	89	U
7	G	90	C
7	G	97	A
7	G	98	U
7	G	99	C
7	G	100	C
7	G	101	U
7	G	102	G
7	G	103	U
7	G	104	C
7	G	105	C
7	G	106	C
7	G	107	U
7	G	109	U
7	G	110	U
7	G	111	U
7	G	112	U
7	G	114	U
7	G	115	C
7	G	116	C
8	H	13	C
8	H	15	U
8	H	18	U
8	H	19	G
8	H	22	U
8	H	23	A
8	H	24	A
8	H	27	U
8	H	28	C
8	H	29	A
8	H	30	A
8	H	31	G
8	H	36	G
8	H	37	U
8	H	44	U

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Mol	Chain	Res	Type
8	H	45	C
8	H	46	U
8	H	47	U
8	H	48	A
8	H	49	U
8	H	53	U
8	H	54	U
8	H	61	C
8	H	63	G
8	H	64	A
8	H	65	U
8	H	83	A
8	H	84	C
8	H	98	G
8	H	100	U
8	H	101	U
8	H	103	U
8	H	104	U
8	H	111	G
8	H	116	A
8	H	117	U
8	H	118	G
8	H	121	A
8	H	122	U
8	H	123	A
8	H	124	G
8	H	125	G
8	H	128	C
8	H	129	U
8	H	130	U
8	H	136	G
8	H	137	U
8	H	146	C
8	H	147	G
8	H	156	U
8	H	157	G
8	H	162	U
8	H	164	C
8	H	166	G
8	H	168	A
8	H	169	C
8	H	177	A

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Mol	Chain	Res	Type
8	H	178	A
8	H	179	C

All (25) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	27	U
2	B	39	C
2	B	94	U
6	F	5	U
6	F	28	A
6	F	37	C
6	F	45	A
6	F	50	A
6	F	59	G
6	F	77	C
6	F	79	C
7	G	12	G
7	G	16	G
7	G	83	A
7	G	84	U
7	G	88	G
7	G	89	U
7	G	101	U
7	G	104	C
7	G	106	C
7	G	108	U
8	H	29	A
8	H	45	C
8	H	46	U
8	H	47	U

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

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

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

RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	SEP	1	129	22	8,9,10	1.13	0	8,12,14	1.45	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
22	SEP	1	129	22	-	1/5/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1	129	SEP	OG-CB-CA	-3.43	104.81	108.14

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1	129	SEP	CB-OG-P-O2P

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1	129	SEP	5	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
45	GTP	C	1500	46	26,34,34	1.14	2 (7%)	32,54,54	1.38	6 (18%)

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
45	GTP	C	1500	46	-	9/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	C	1500	GTP	C5-C6	-3.92	1.39	1.47
45	C	1500	GTP	C2-N3	2.24	1.38	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	C	1500	GTP	C5-C6-N1	3.09	119.40	113.95
45	C	1500	GTP	C8-N7-C5	3.08	108.86	102.99
45	C	1500	GTP	PA-O3A-PB	-2.73	123.47	132.83
45	C	1500	GTP	PB-O3B-PG	-2.65	123.74	132.83
45	C	1500	GTP	C2-N1-C6	-2.64	120.24	125.10
45	C	1500	GTP	O6-C6-C5	-2.14	120.20	124.37

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	C	1500	GTP	O4'-C4'-C5'-O5'
45	C	1500	GTP	C3'-C4'-C5'-O5'
45	C	1500	GTP	PB-O3B-PG-O1G
45	C	1500	GTP	PG-O3B-PB-O2B
45	C	1500	GTP	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
45	C	1500	GTP	PB-O3B-PG-O2G
45	C	1500	GTP	PB-O3B-PG-O3G
45	C	1500	GTP	PG-O3B-PB-O1B
45	C	1500	GTP	PB-O3A-PA-O2A

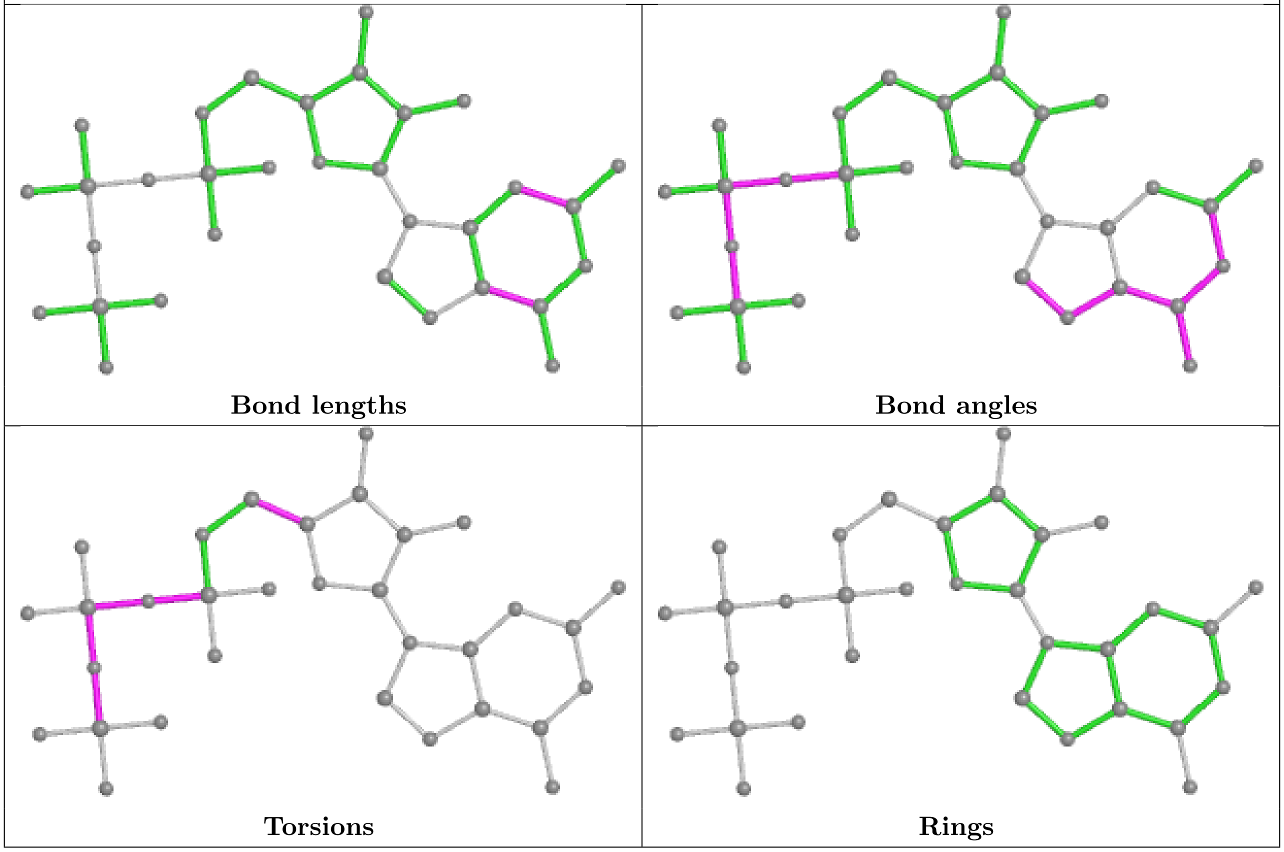
There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	C	1500	GTP	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GTP C 1500



Bond lengths

Bond angles

Torsions

Rings

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.

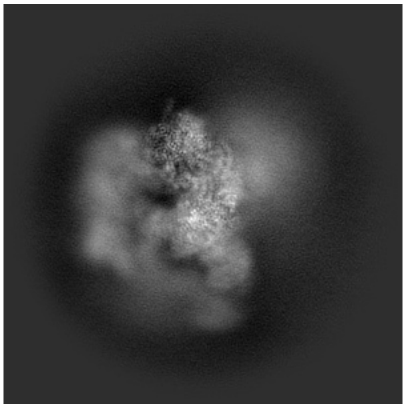
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-35105. These allow visual inspection of the internal detail of the map and identification of artifacts.

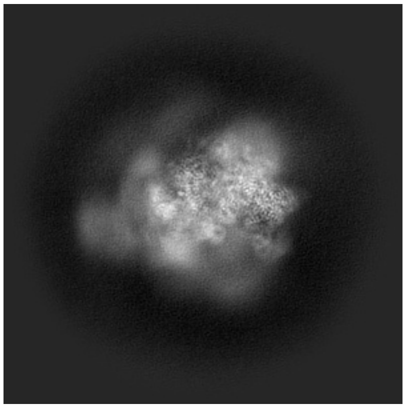
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections ⓘ

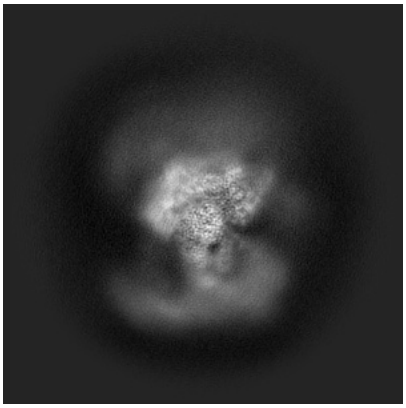
6.1.1 Primary map



X

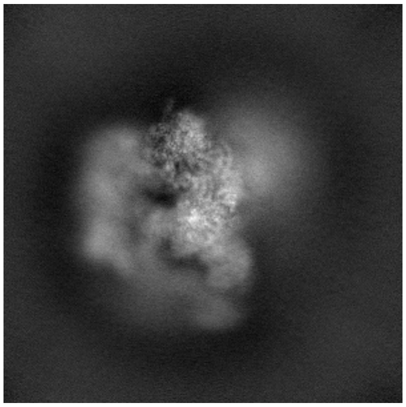


Y

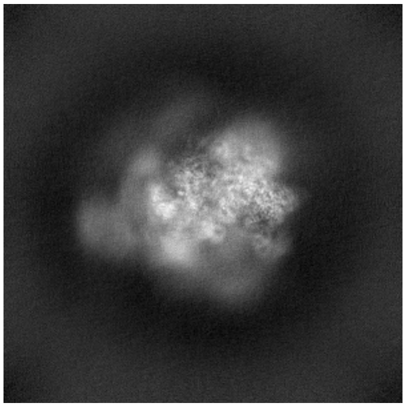


Z

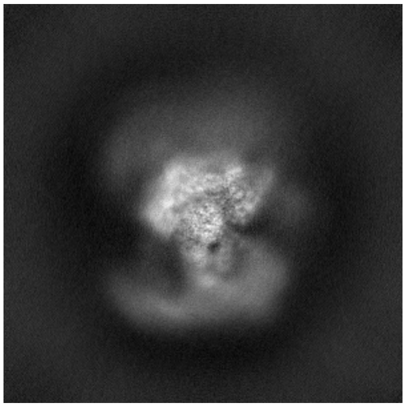
6.1.2 Raw map



X



Y

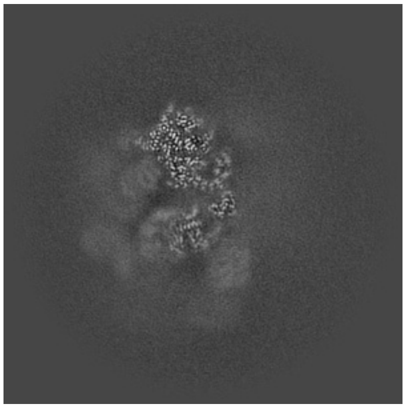


Z

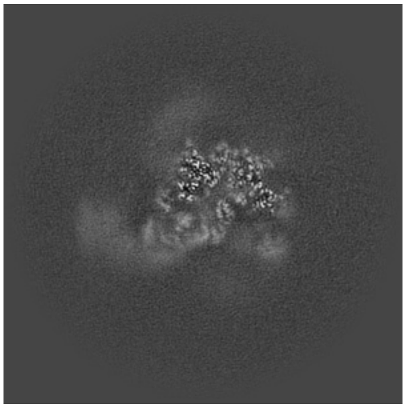
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

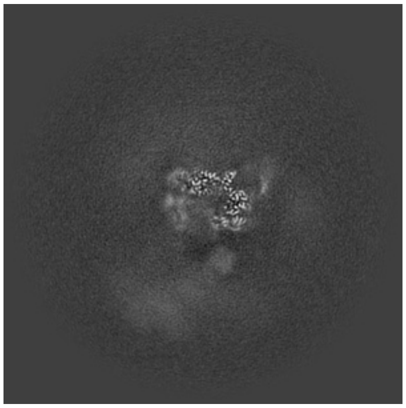
6.2.1 Primary map



X Index: 240

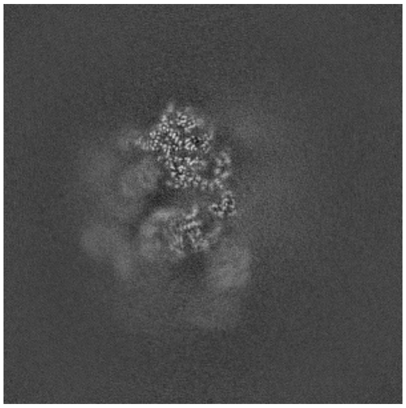


Y Index: 240

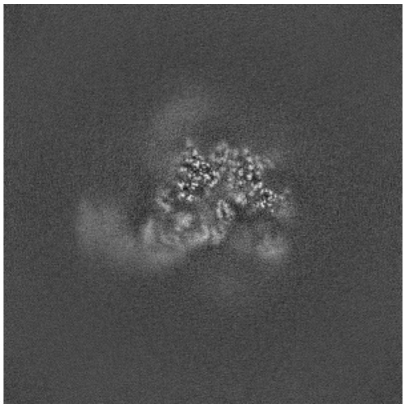


Z Index: 240

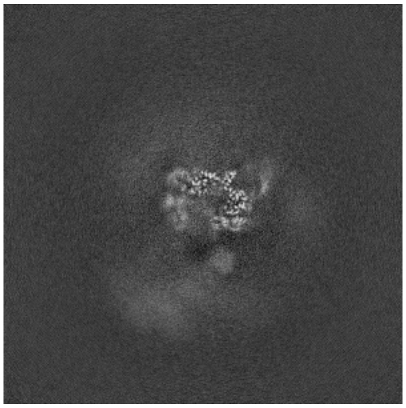
6.2.2 Raw map



X Index: 240



Y Index: 240

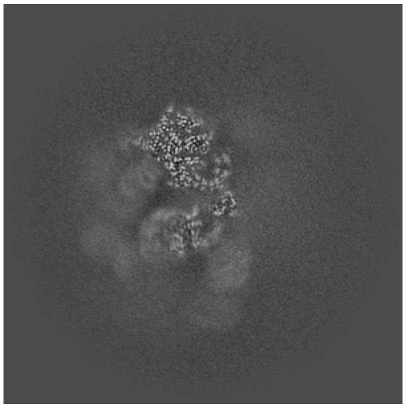


Z Index: 240

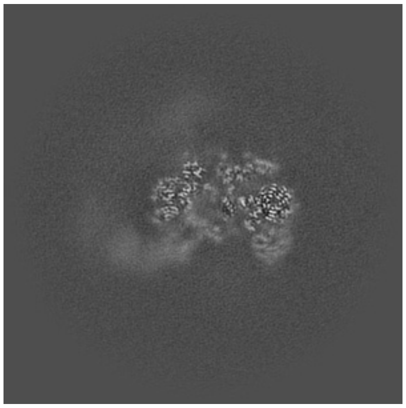
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

6.3.1 Primary map



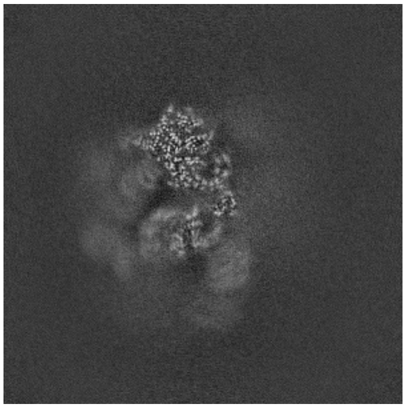
X Index: 239



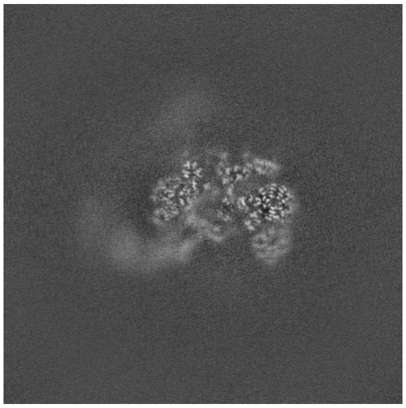
Y Index: 225

Z Index: 222

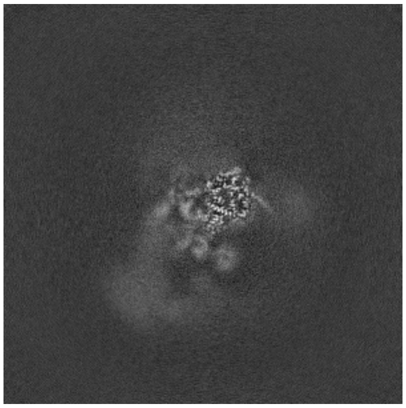
6.3.2 Raw map



X Index: 239



Y Index: 226

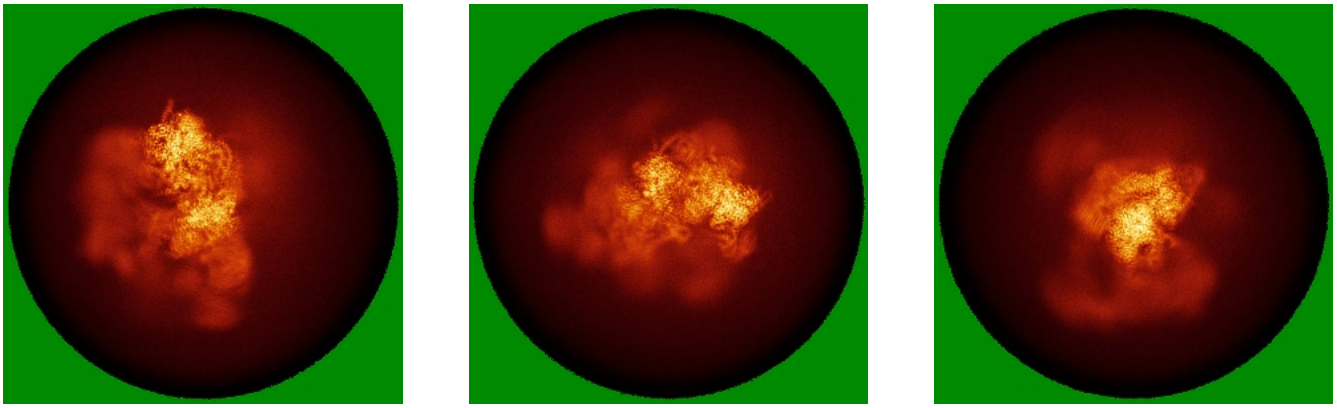


Z Index: 222

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

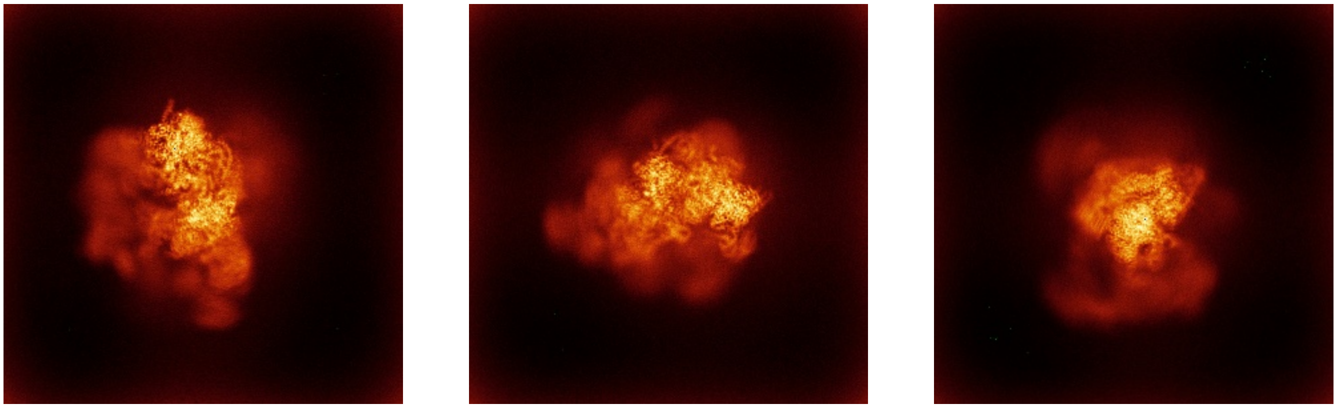
6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

6.4.2 Raw map



X Y Z

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

6.5 Orthogonal surface views

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.19. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

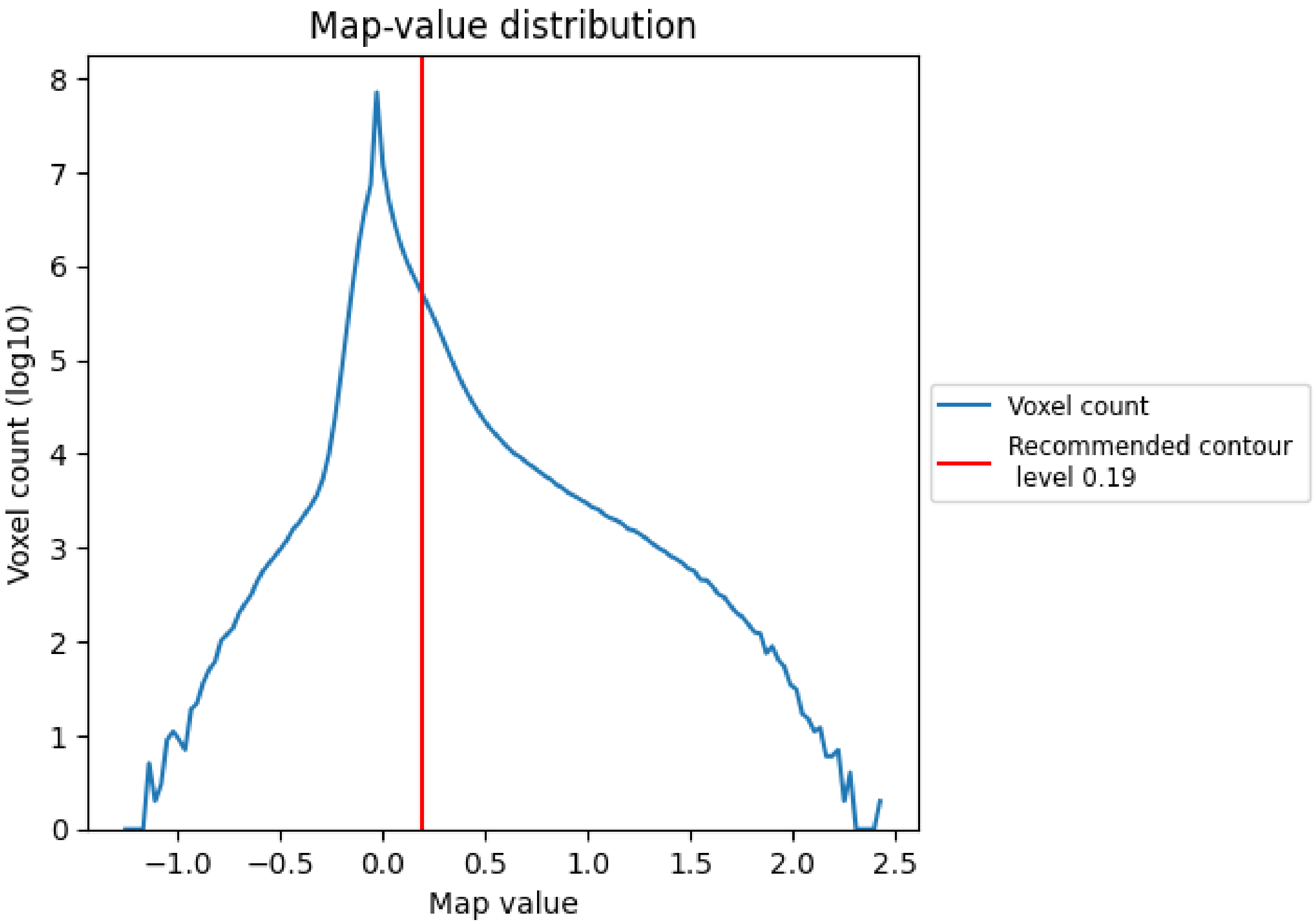
6.6 Mask visualisation

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

7 Map analysis ⓘ

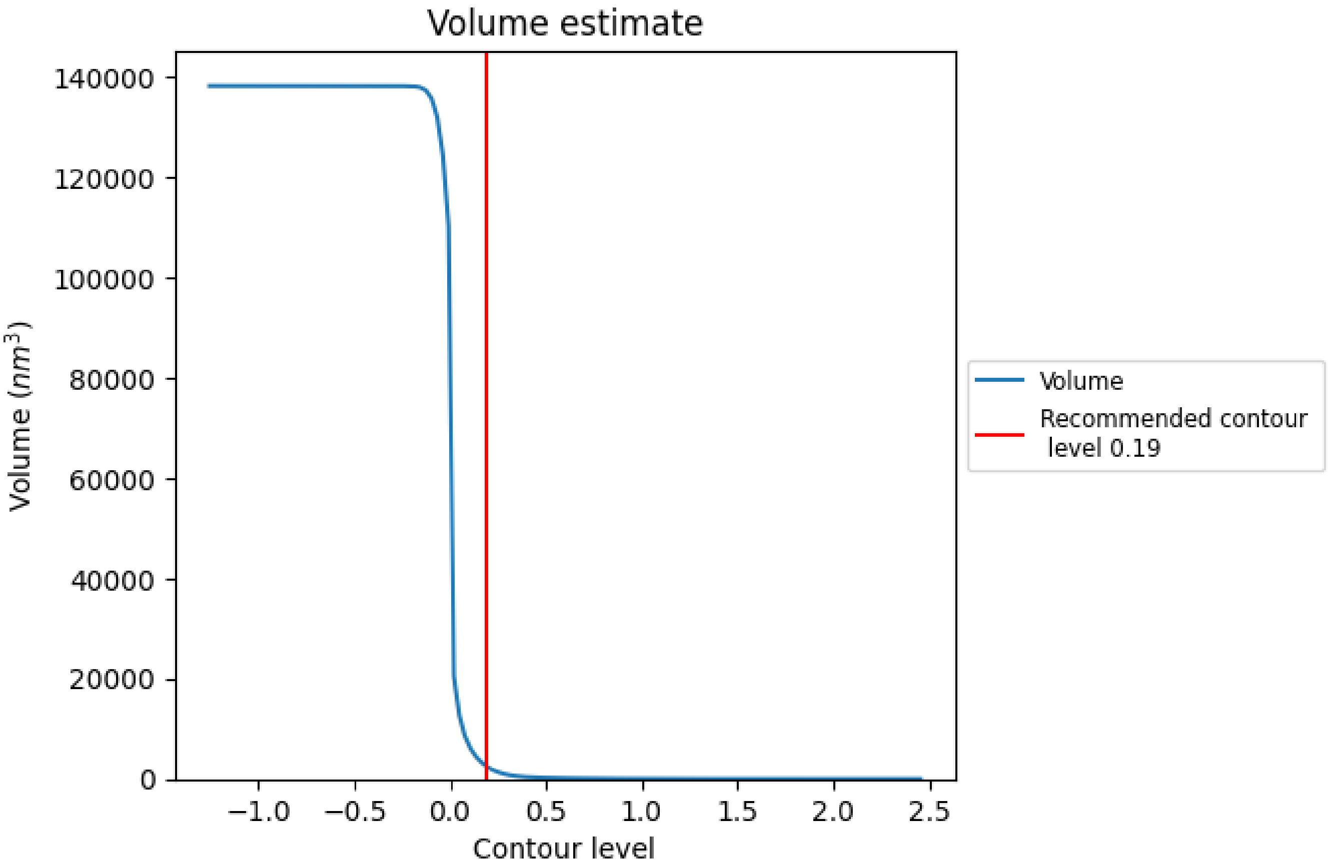
This section contains the results of statistical analysis of the map.

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.

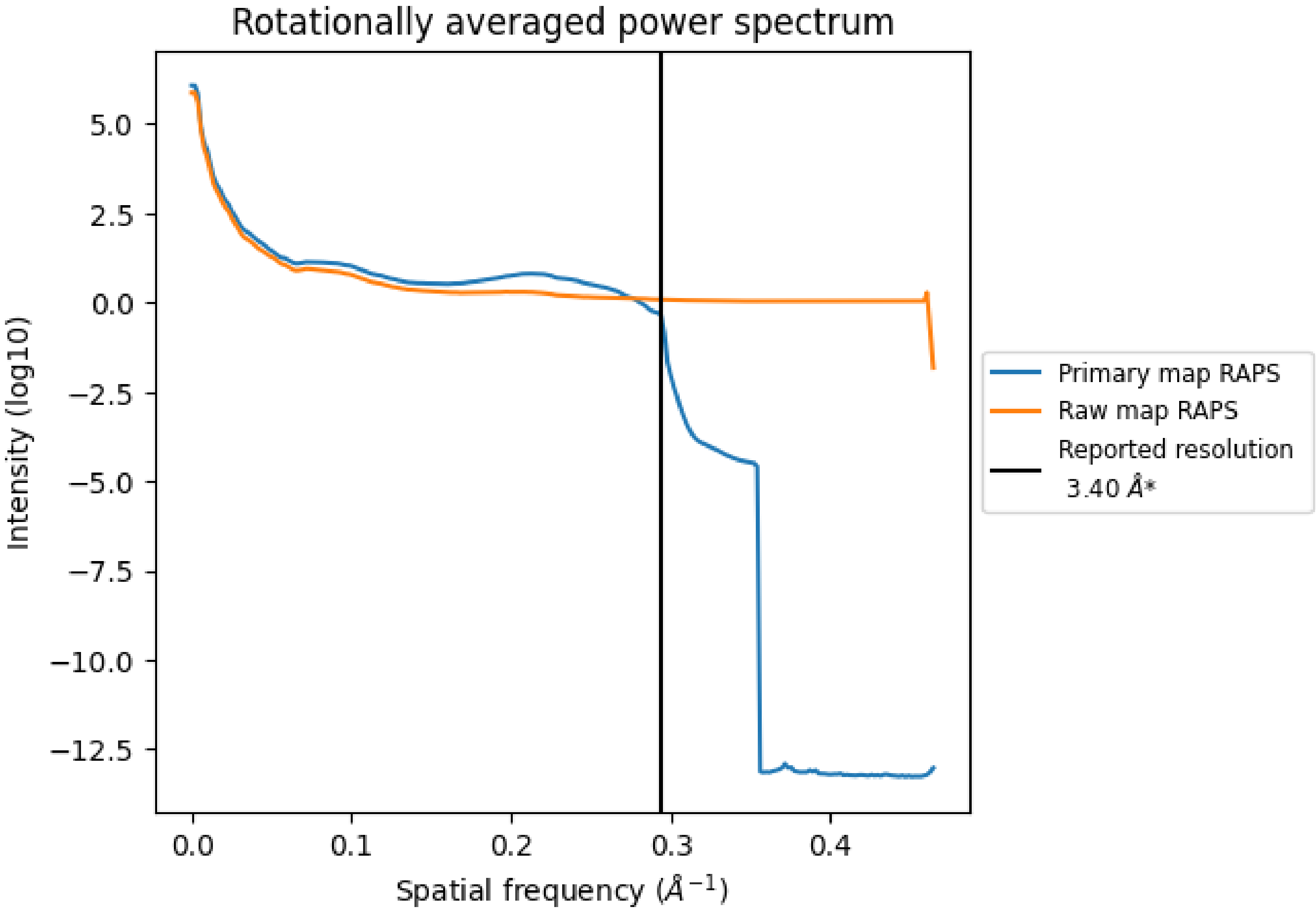
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 2577 nm^3; this corresponds to an approximate mass of 2328 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)

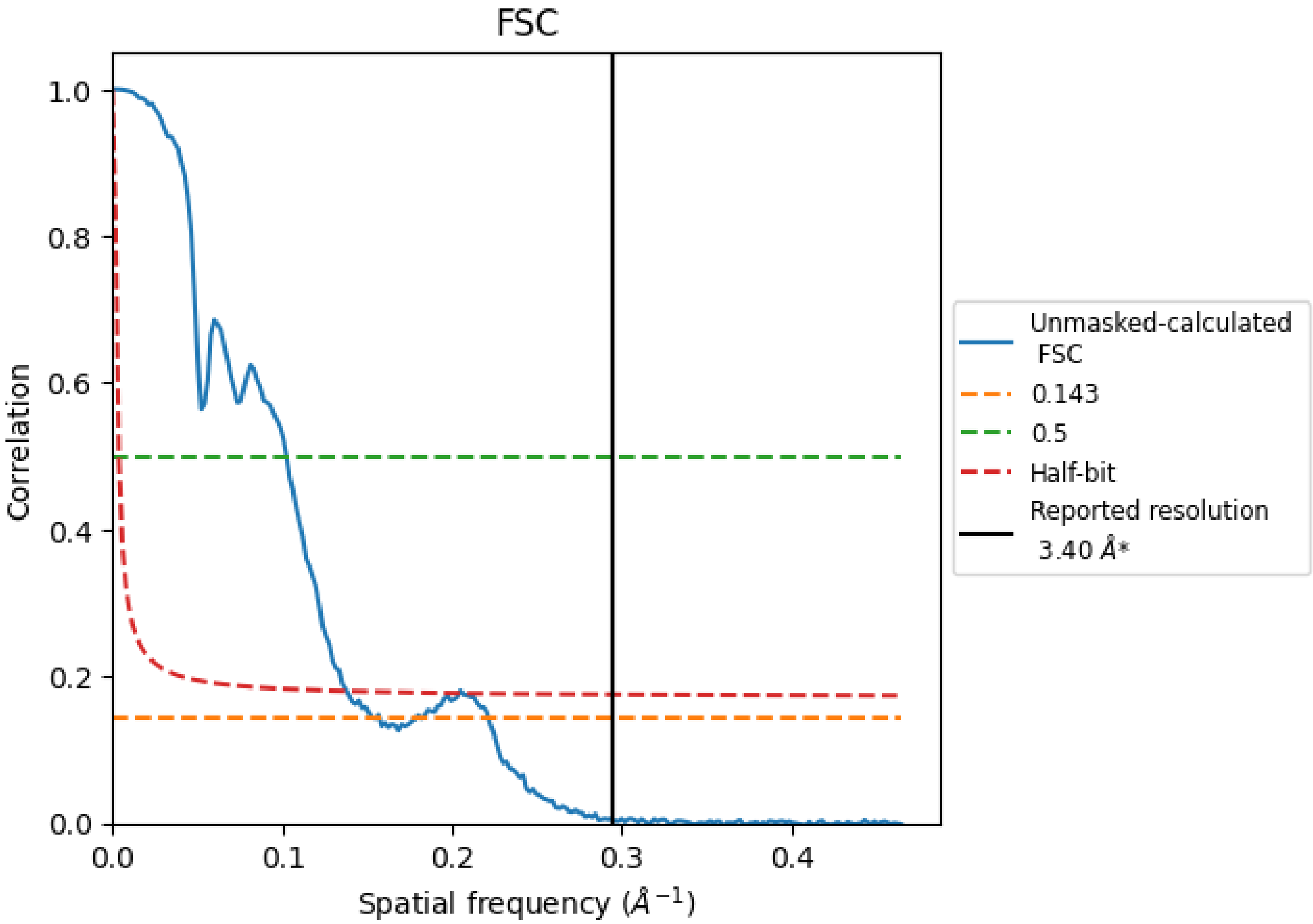


*Reported resolution corresponds to spatial frequency of 0.294 $Å^{-1}$

8 Fourier-Shell correlation ⓘ

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

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.294 $Å^{-1}$

8.2 Resolution estimates ⓘ

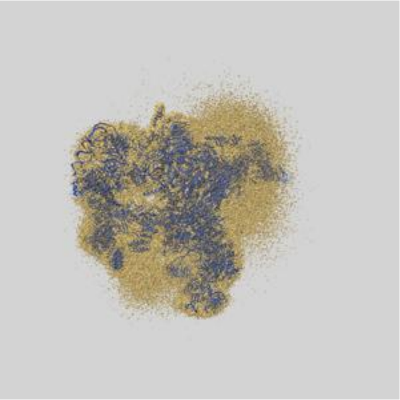
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.48	9.75	7.25

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.48 differs from the reported value 3.4 by more than 10 %

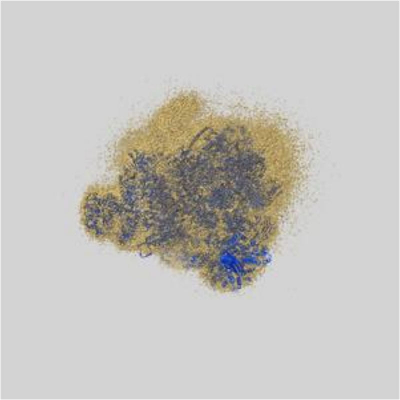
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-35105 and PDB model 8I0P. Per-residue inclusion information can be found in section 3 on page 13.

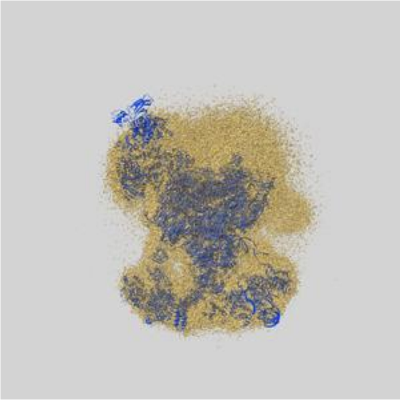
9.1 Map-model overlay ⓘ



X



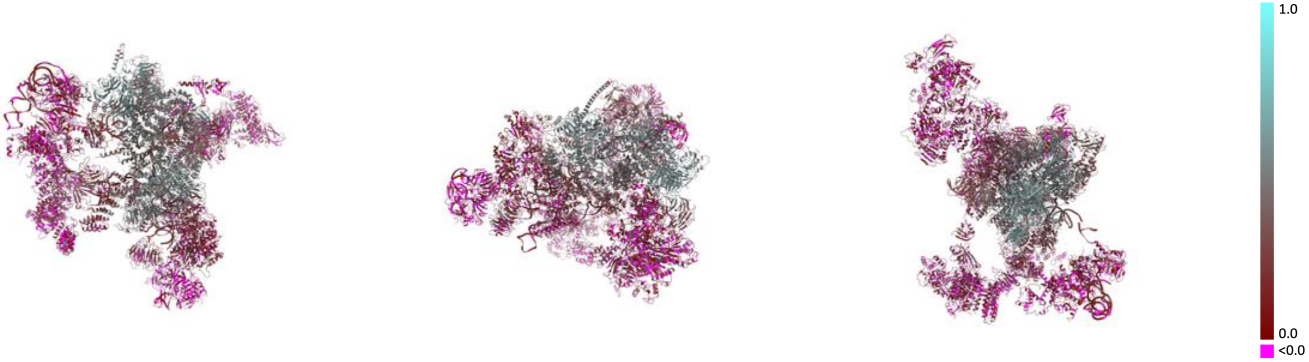
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.19 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.

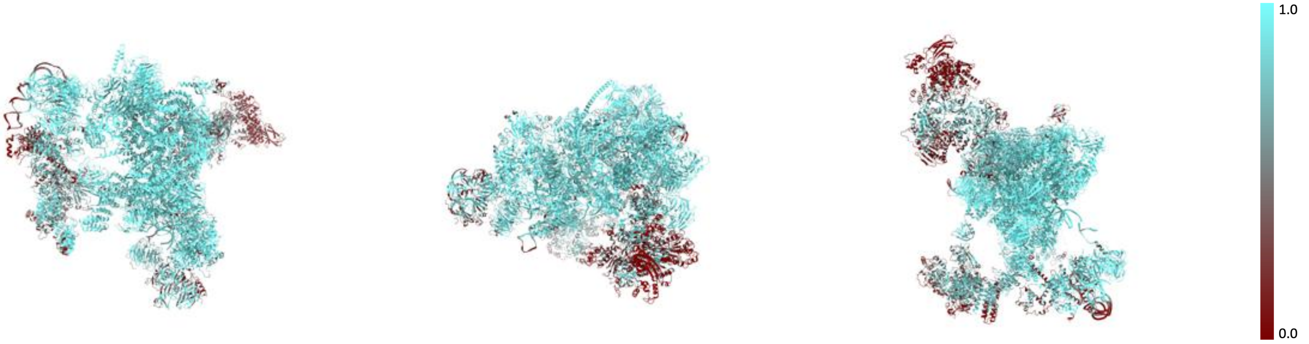
9.2 Q-score mapped to coordinate model ⓘ



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.

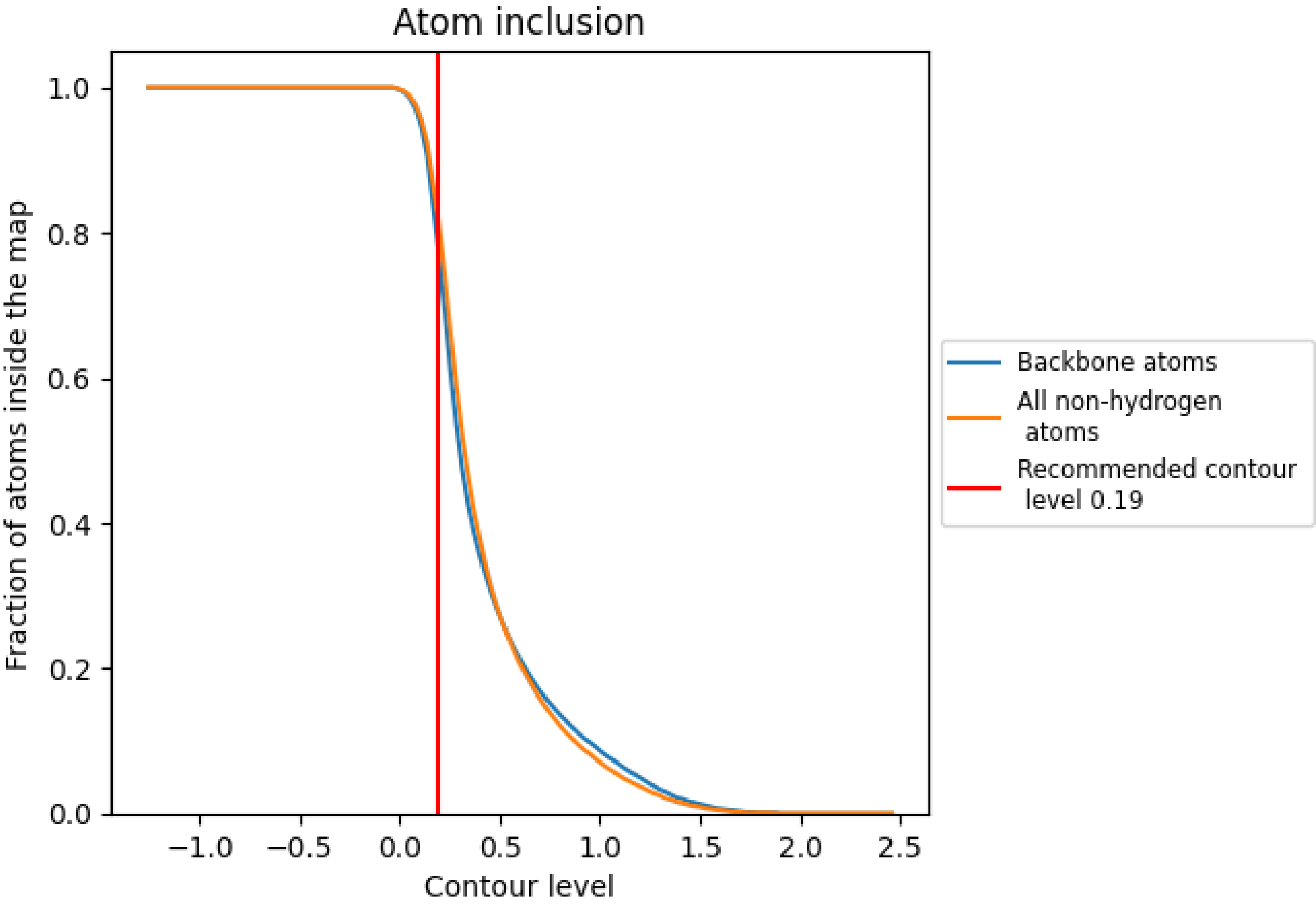
9.3 Atom inclusion mapped to coordinate model ⓘ



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 (0.19).

9.4 Atom inclusion ⓘ



At the recommended contour level, 79% of all backbone atoms, 83% 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 (0.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8270	0.2870
1	0.9710	0.4690
2	0.9300	0.3980
3	0.9870	0.4850
4	0.9420	0.2370
5	0.9340	0.5140
6	0.9910	0.3740
7	0.9520	0.4660
8	0.9720	0.4140
9	0.9100	0.2660
A	0.8960	0.3530
B	0.9040	0.1640
C	0.9010	0.1980
D	0.3650	0.1400
E	0.8420	0.1810
F	0.8960	0.2350
G	0.9640	0.2930
H	0.7850	0.2110
I	0.7100	0.1150
J	0.9590	0.2620
K	0.8650	0.2550
L	0.9840	0.4810
N	0.8340	0.1620
O	0.8730	0.1820
P	0.9520	0.4780
Q	0.5540	0.1340
R	0.9420	0.4120
T	0.9860	0.4700
X	0.9680	0.3540
Y	0.9680	0.4810
Z	0.9670	0.4700
a	0.6700	0.0550
b	0.5760	0.0140
c	0.6260	0.0030
d	0.6420	0.0290

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Chain	Atom inclusion	Q-score
e	🟦 0.6430	🟥 0.0390
f	🟦 0.5850	🟥 0.0300
g	🟦 0.6480	🟪 -0.0220
h	🟦 0.8420	🟥 0.1220
i	🟦 0.8660	🟥 0.1030
j	🟦 0.9280	🟥 0.1720
k	🟦 0.9340	🟥 0.1280
l	🟦 0.8940	🟥 0.1710
m	🟦 0.8860	🟥 0.1450
n	🟦 0.7760	🟥 0.1740
o	🟦 0.8330	🟥 0.1390
p	🟦 0.9010	🟥 0.1850
u	🟦 0.5620	🟥 0.1590
v	🟦 0.7330	🟥 0.2950
w	🟦 0.6850	🟥 0.2220
y	🟦 0.7640	🟥 0.1920
z	🟦 0.9760	🟥 0.3290