Full wwPDB EM Validation Report ⓘ

Jul 31, 2024 – 11:12 AM JST

PDB ID	:	8I0W
EMDB ID	:	EMD-35113
Title	:	The cryo-EM structure of human C complex
Authors	:	Zhan, X.; Lu, Y.; Shi, Y.
Deposited on	:	2023-01-11
Resolution	:	3.40 Å(reported)

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

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

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

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

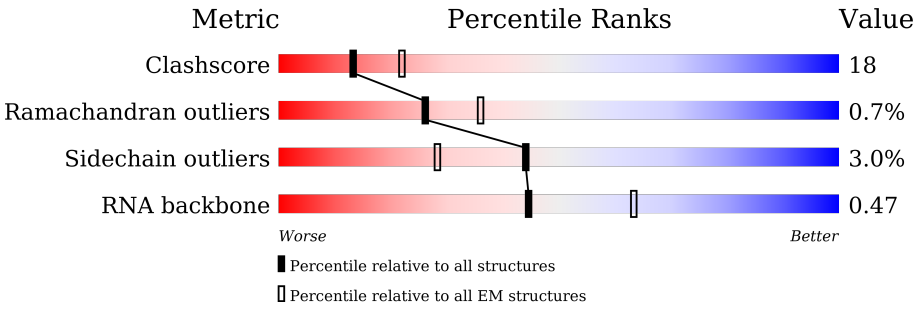
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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	5% 66% 29%
2	B	117	7% 16% 45% 19% 16%
3	C	972	45% 40% 11%
4	D	2136	68% 88% 11%
5	E	357	46% 37% 16%
6	F	107	6% 16% 46% 26% 9%
7	G	46	13% 15% 17% 7% 61%

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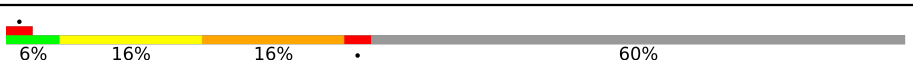
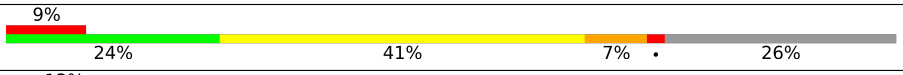
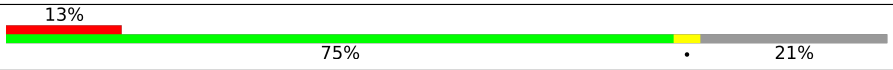
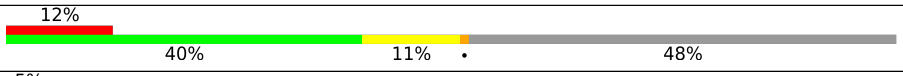
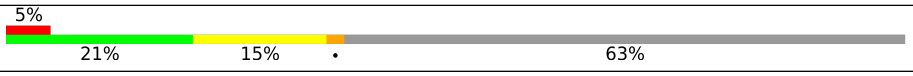
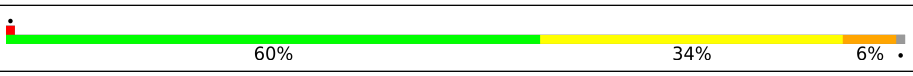
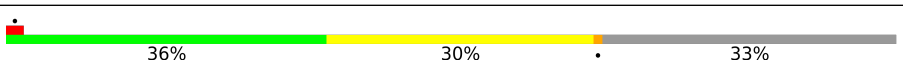
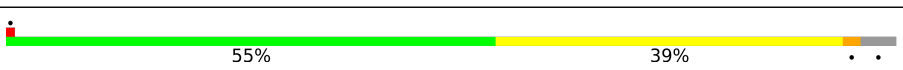
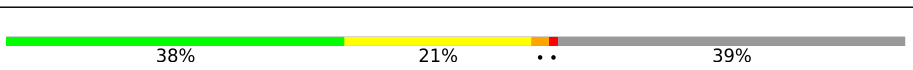
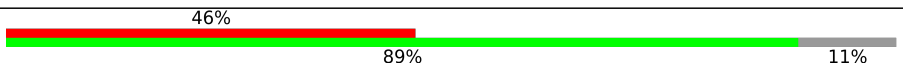
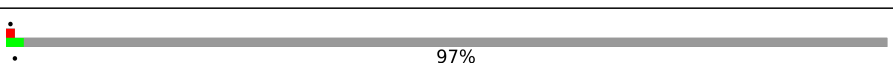
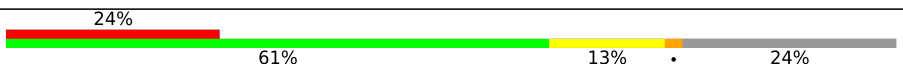
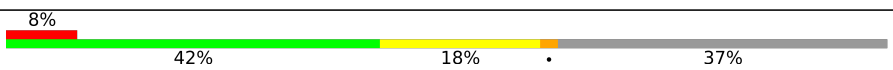
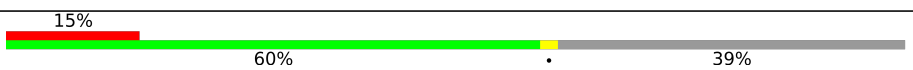
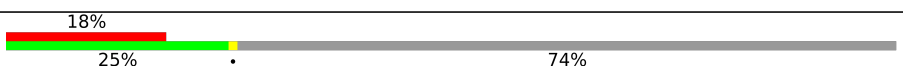
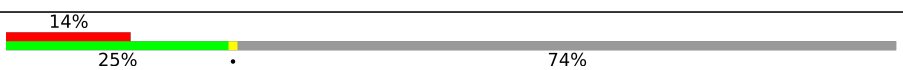
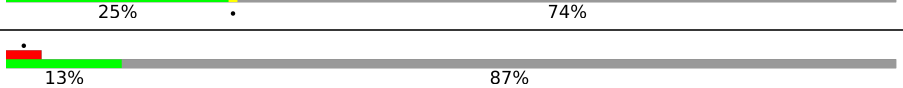
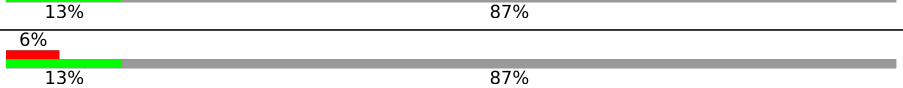
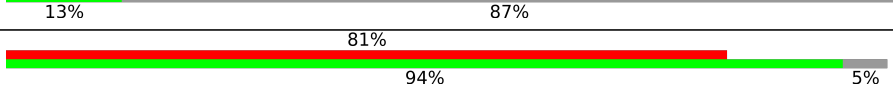
Mol	Chain	Length	Quality of chain
8	6	174	
9	H	188	
10	I	855	
11	J	848	
12	K	225	
13	L	802	
14	M	243	
15	N	144	
16	O	420	
17	P	229	
18	R	536	
19	S	166	
20	T	514	
21	Q	1485	
22	U	2752	
23	V	908	
24	W	579	
25	X	425	
26	Y	323	
27	Z	1227	
28	q	504	
28	r	504	
28	s	504	
28	t	504	
29	u	411	

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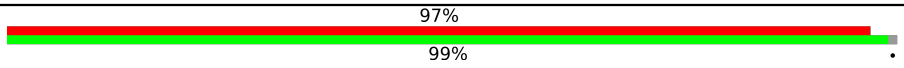
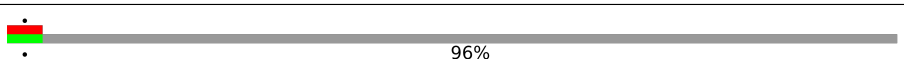
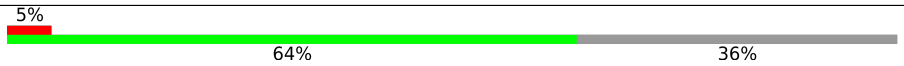
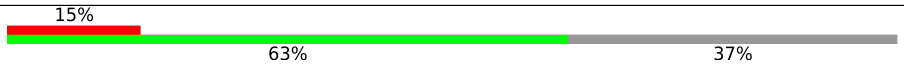
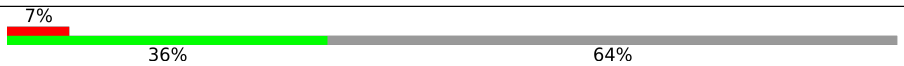
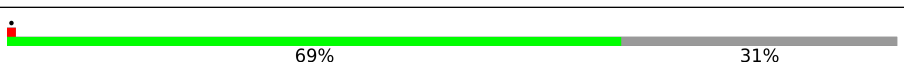
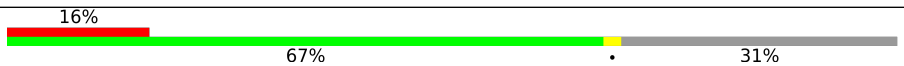
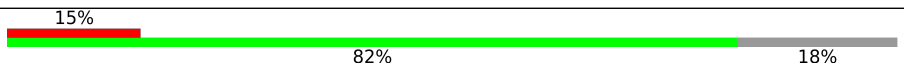
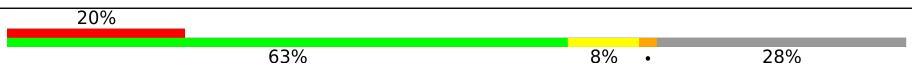
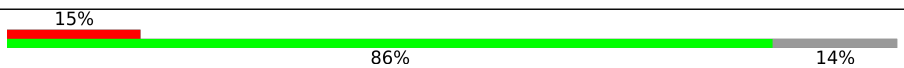
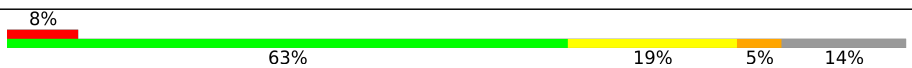
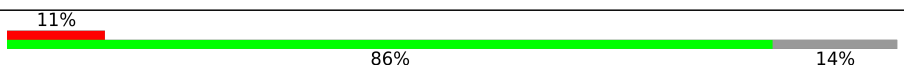
Mol	Chain	Length	Quality of chain
30	v	146	
31	w	174	
32	x	703	
33	g	126	
33	h	126	
34	a	240	
34	i	240	
35	b	119	
35	j	119	
36	c	118	
36	k	118	
37	d	86	
37	m	86	
38	e	92	
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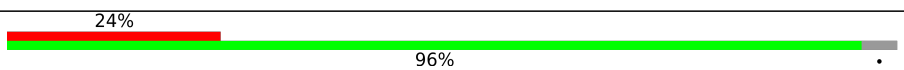
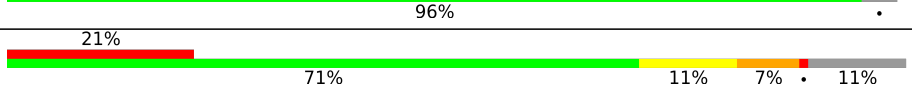
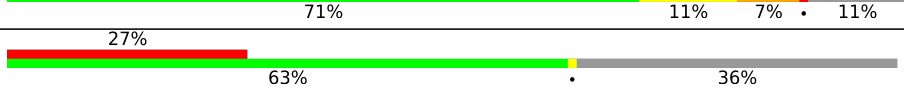
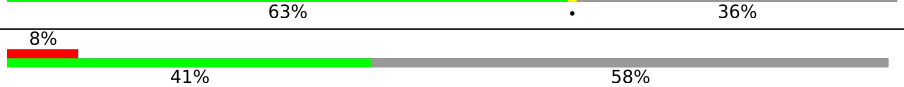
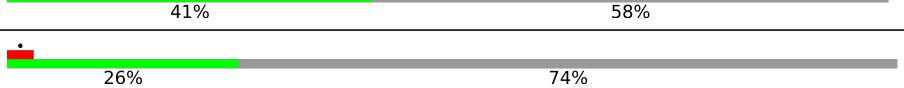
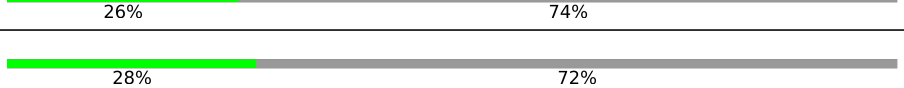
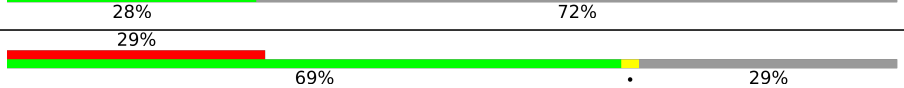
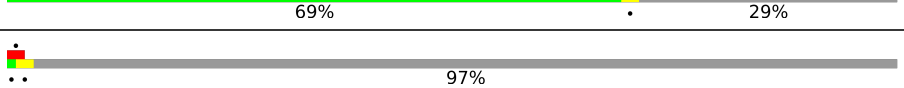
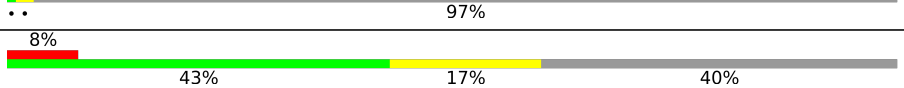
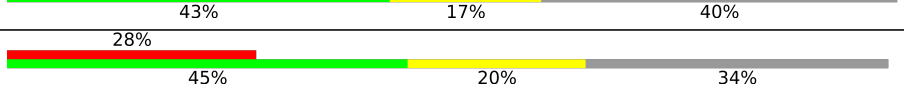
39	f	76	
39	n	76	
40	o	255	
41	p	225	
42	y	301	
43	z	285	
44	3	646	
45	4	450	
46	1	654	
47	2	258	

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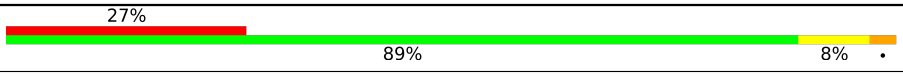
Mol	Chain	Length	Quality of chain
48	5	37	

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 106256 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	2253	17519	11136	3147	3166	70	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	862	6795	4344	1138	1281	32	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	1908	7632	3816	1908	1908	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	97	2075	928	381	669	97	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	18	Total	C	N	O	P	0	0
			383	172	73	121	17		

- Molecule 8 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	6	70	Total	C	N	O	P	0	0
			1256	554	163	469	70		

- Molecule 9 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	139	Total	C	N	O	P	0	0
			2946	1317	507	983	139		

- Molecule 10 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	I	672	Total	C	N	O	0	0
			3387	2043	672	672		

- Molecule 11 is a protein called Crooked neck-like protein 1.

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

- Molecule 12 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	152	Total	C	N	O	S	0	0
			979	611	177	189	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	419	Total	C	N	O	S	0	0
			2885	1809	534	537	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	91	Total	C	N	O	S	0	0
			775	482	146	145	2		

- Molecule 15 is a protein called Protein BUD31 homolog.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	283	Total	C	N	O	S	0	0
			2277	1430	403	424	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	96	Total	C	N	O	S	0	0
			829	508	162	157	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	245	Total	C	N	O	P	S	0	0
			1962	1231	353	364	2	12		

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

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

- Molecule 20 is a protein called Pleiotropic regulator 1.

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

- Molecule 21 is a protein called RNA helicase aquarius.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	Q	1322	Total 5288	C 2644	N 1322	O 1322	0	0

- Molecule 22 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	72	Total 422	C 257	N 82	O 82	S 1	0	0

- Molecule 23 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	452	Total 3410	C 2194	N 590	O 611	S 15	0	0

- Molecule 24 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	440	Total 2615	C 1601	N 487	O 523	S 4	0	0

- Molecule 25 is a protein called Pre-mRNA-splicing factor CWC25 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	X	71	Total 480	C 297	N 95	O 88	0	0

- Molecule 26 is a protein called Coiled-coil domain-containing protein 94.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	204	Total 1426	C 898	N 259	O 261	S 8	0	0

- Molecule 27 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP16.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	Z	754	Total 3727	C 2219	N 754	O 754	0	0

- Molecule 28 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms	AltConf	Trace
28	q	132	Total C N O S 918 581 156 178 3	0	0
28	r	131	Total C N O S 901 572 149 177 3	0	0
28	s	67	Total C N O 268 134 67 67	0	0
28	t	67	Total C N O S 476 300 83 92 1	0	0

- Molecule 29 is a protein called Eukaryotic initiation factor 4A-III.

Mol	Chain	Residues	Atoms	AltConf	Trace
29	u	390	Total C N O S 3126 1974 545 588 19	0	0

- Molecule 30 is a protein called Protein mago nashi homolog.

Mol	Chain	Residues	Atoms	AltConf	Trace
30	v	144	Total C N O S 1196 772 200 221 3	0	0

- Molecule 31 is a protein called RNA-binding protein 8A.

Mol	Chain	Residues	Atoms	AltConf	Trace
31	w	91	Total C N O S 730 463 122 142 3	0	0

- Molecule 32 is a protein called Protein CASC3.

Mol	Chain	Residues	Atoms	AltConf	Trace
32	x	25	Total C N O 216 136 39 41	0	0

- Molecule 33 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms	AltConf	Trace
33	h	80	Total C N O S 621 388 110 117 6	0	0
33	g	81	Total C N O 324 162 81 81	0	0

- Molecule 34 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms	AltConf	Trace
34	i	86	Total C N O S 690 434 126 123 7	0	0
34	a	86	Total C N O 344 172 86 86	0	0

- Molecule 35 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms	AltConf	Trace
35	j	82	Total C N O S 649 413 113 119 4	0	0
35	b	82	Total C N O 328 164 82 82	0	0

- Molecule 36 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms	AltConf	Trace
36	k	85	Total C N O S 688 432 125 126 5	0	0
36	c	97	Total C N O 388 194 97 97	0	0

- Molecule 37 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms	AltConf	Trace
37	m	74	Total C N O S 576 373 95 103 5	0	0
37	d	74	Total C N O 296 148 74 74	0	0

- Molecule 38 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms	AltConf	Trace
38	l	75	Total C N O S 621 392 111 114 4	0	0
38	e	79	Total C N O 316 158 79 79	0	0

- Molecule 39 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms	AltConf	Trace
39	n	68	Total C N O S 533 339 95 93 6	0	0

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Mol	Chain	Residues	Atoms	AltConf	Trace
39	f	73	Total C N O 292 146 73 73	0	0

- Molecule 40 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms	AltConf	Trace
40	o	162	Total C N O S 1277 817 219 238 3	0	0

- Molecule 41 is a protein called U2 small nuclear ribonucleoprotein B".

Mol	Chain	Residues	Atoms	AltConf	Trace
41	p	94	Total C N O S 760 488 135 132 5	0	0

- 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 316 158 79 79	0	0

- Molecule 43 is a protein called Pre-mRNA-splicing factor ISY1 homolog.

Mol	Chain	Residues	Atoms	AltConf	Trace
43	z	80	Total C N O S 546 346 98 101 1	0	0

- Molecule 44 is a protein called Peptidylprolyl isomerase domain and WD repeat-containing protein 1.

Mol	Chain	Residues	Atoms	AltConf	Trace
44	3	460	Total C N O 2301 1381 460 460	0	0

- Molecule 45 is a protein called Corepressor interacting with RBPJ 1.

Mol	Chain	Residues	Atoms	AltConf	Trace
45	4	14	Total C N O S 112 68 21 22 1	0	0

- Molecule 46 is a protein called WD repeat-containing protein 70.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	1	393	Total	C	N	O	S	0	0
			2705	1690	489	510	16		

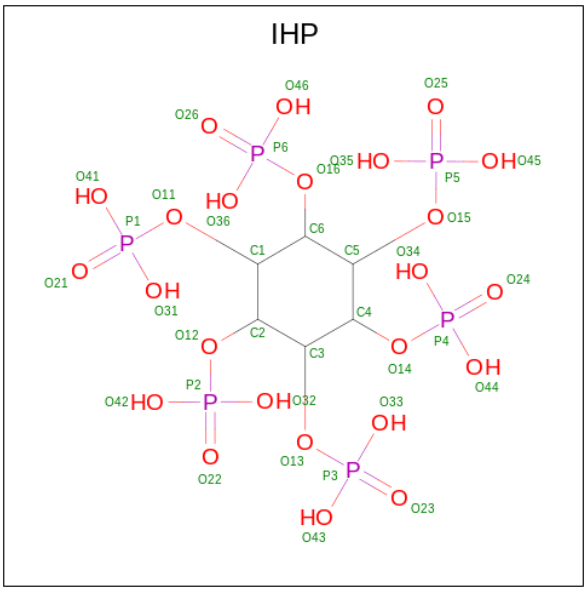
- Molecule 47 is a protein called Protein FRG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	2	169	Total	C	N	O	S	0	0
			1296	814	228	247	7		

- Molecule 48 is a protein called UNK.

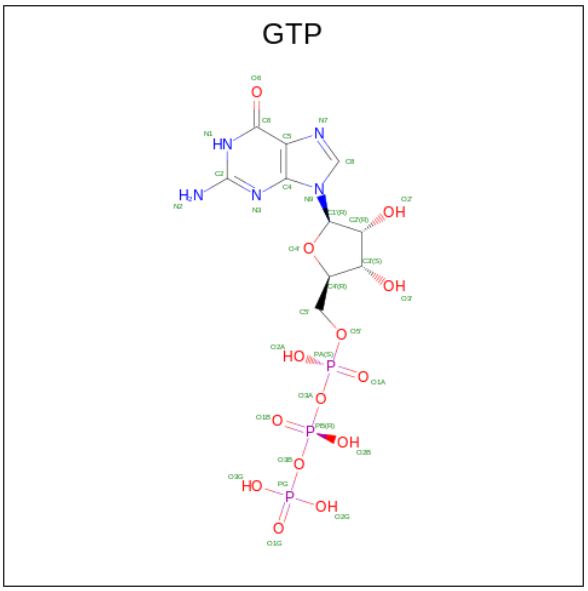
Mol	Chain	Residues	Atoms				AltConf	Trace
48	5	37	Total	C	N	O	0	0
			184	110	37	37		

- Molecule 49 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- Molecule 50 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 51 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
51	C	1	Total	Mg	0
			1	1	
51	F	4	Total	Mg	0
			4	4	

- Molecule 52 is ZINC ION (three-letter code: ZN) (formula: Zn).

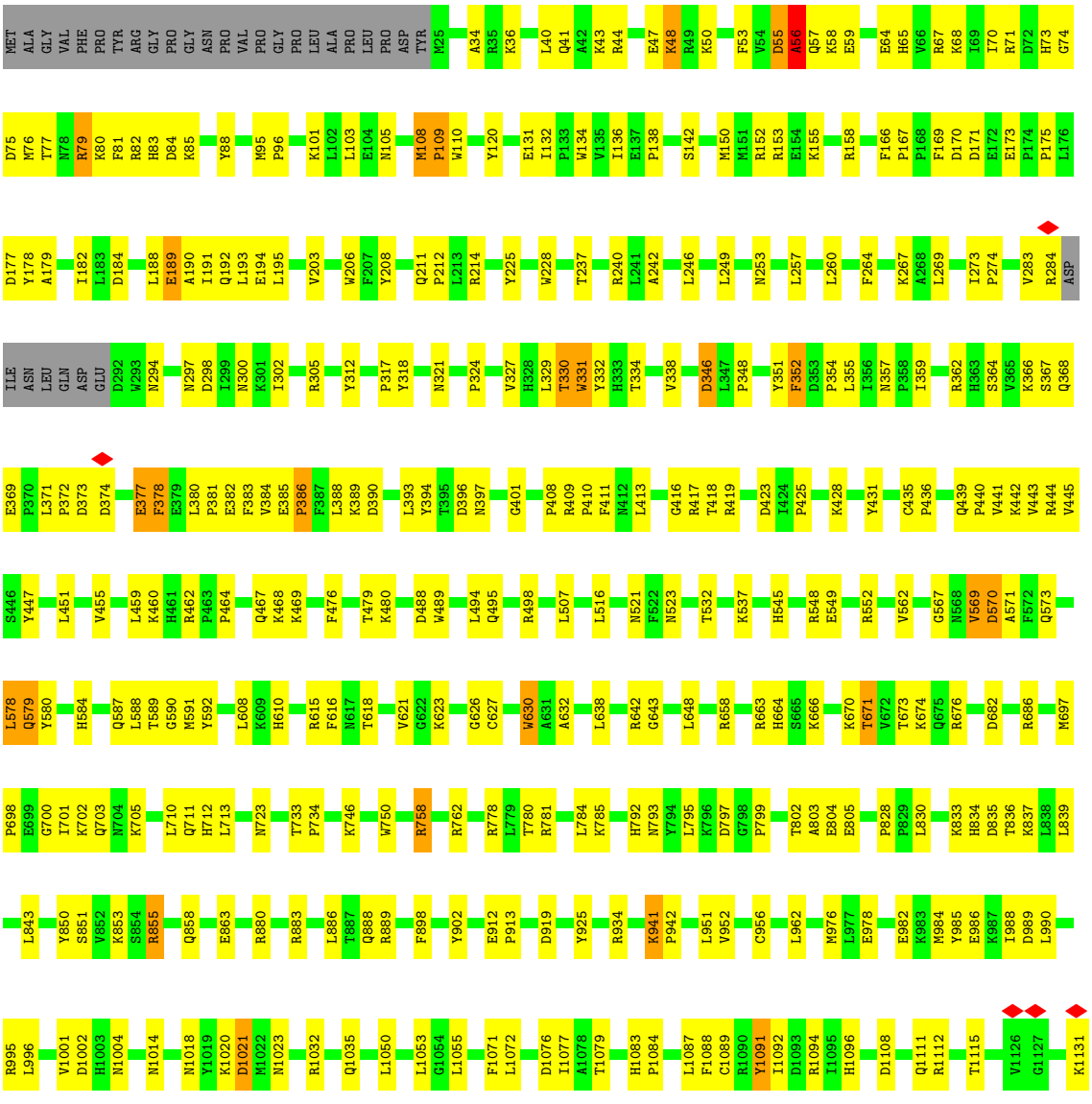
Mol	Chain	Residues	Atoms		AltConf
52	N	3	Total	Zn	0
			3	3	
52	O	3	Total	Zn	0
			3	3	
52	Y	1	Total	Zn	0
			1	1	

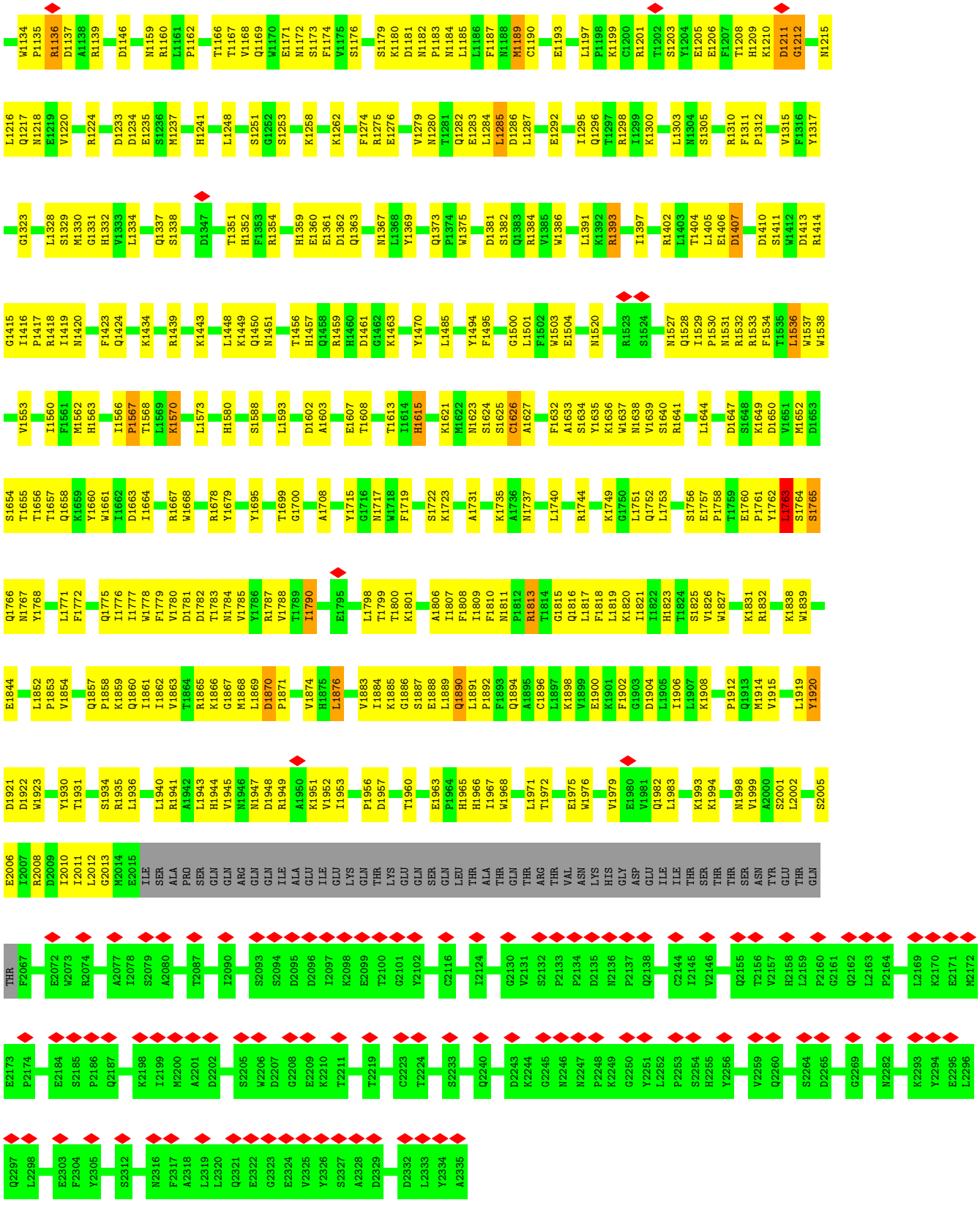
3 Residue-property plots (i)

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

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

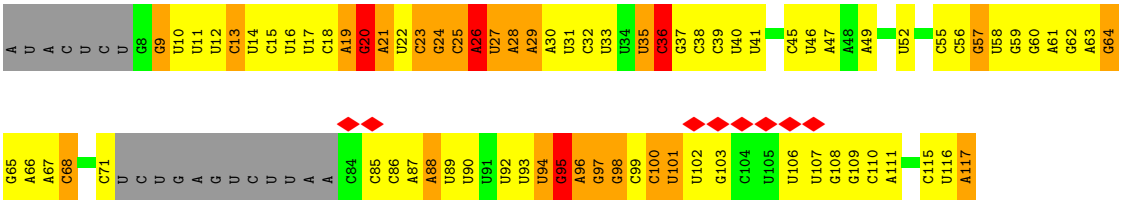
Chain A:





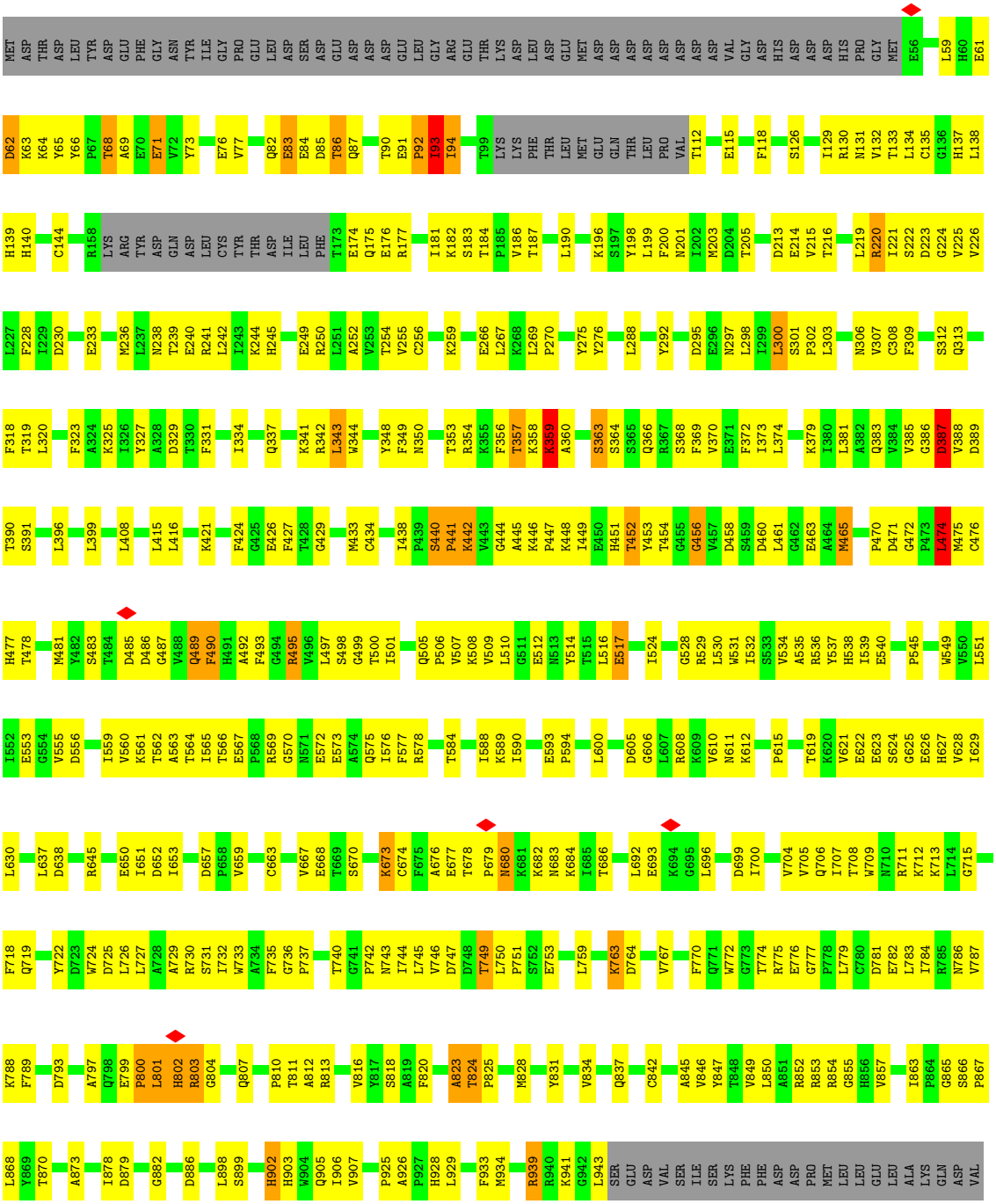
• Molecule 2: U5 snRNA

Chain B:



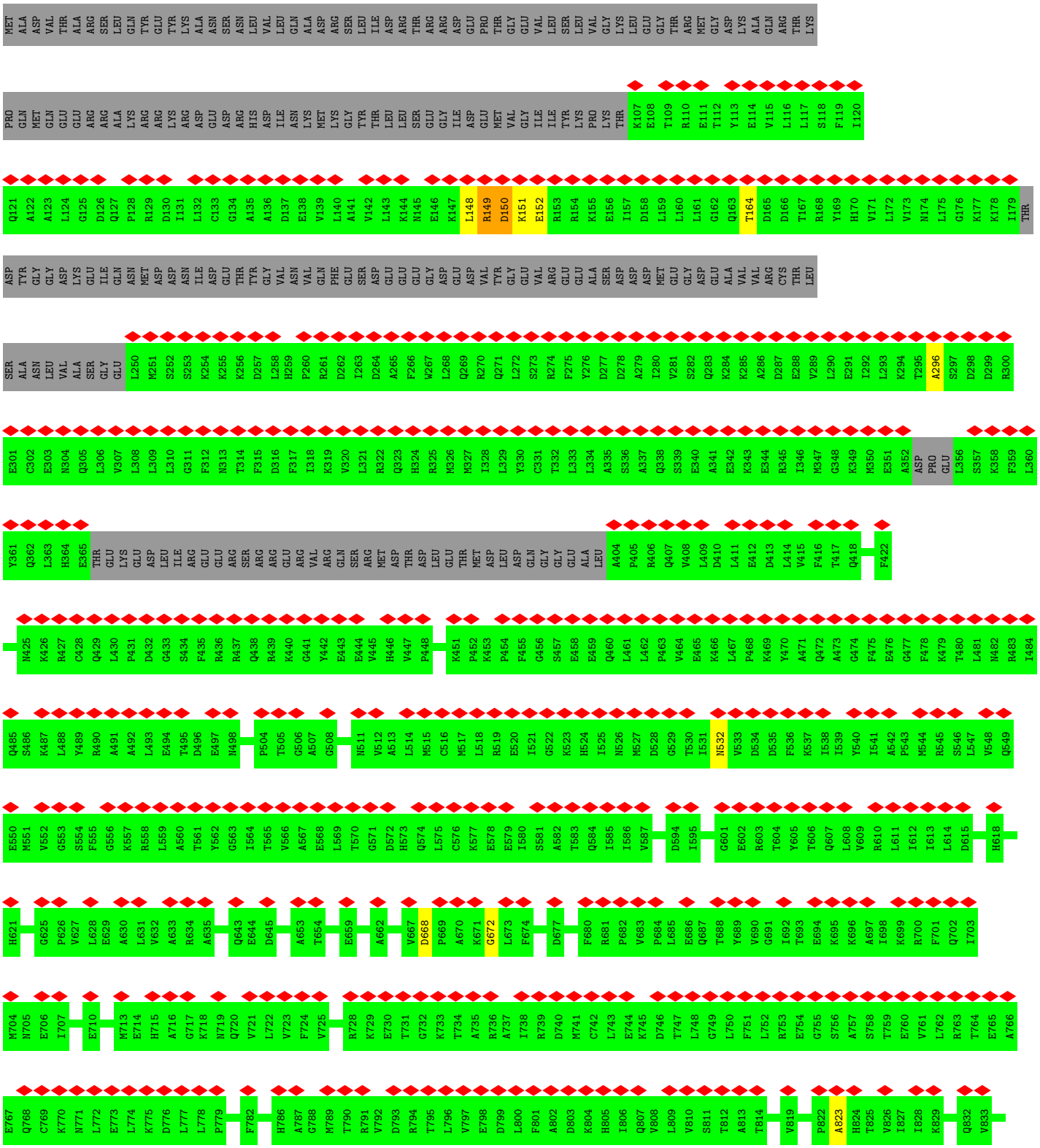
• Molecule 3: 116 kDa U5 small nuclear ribonucleoprotein component

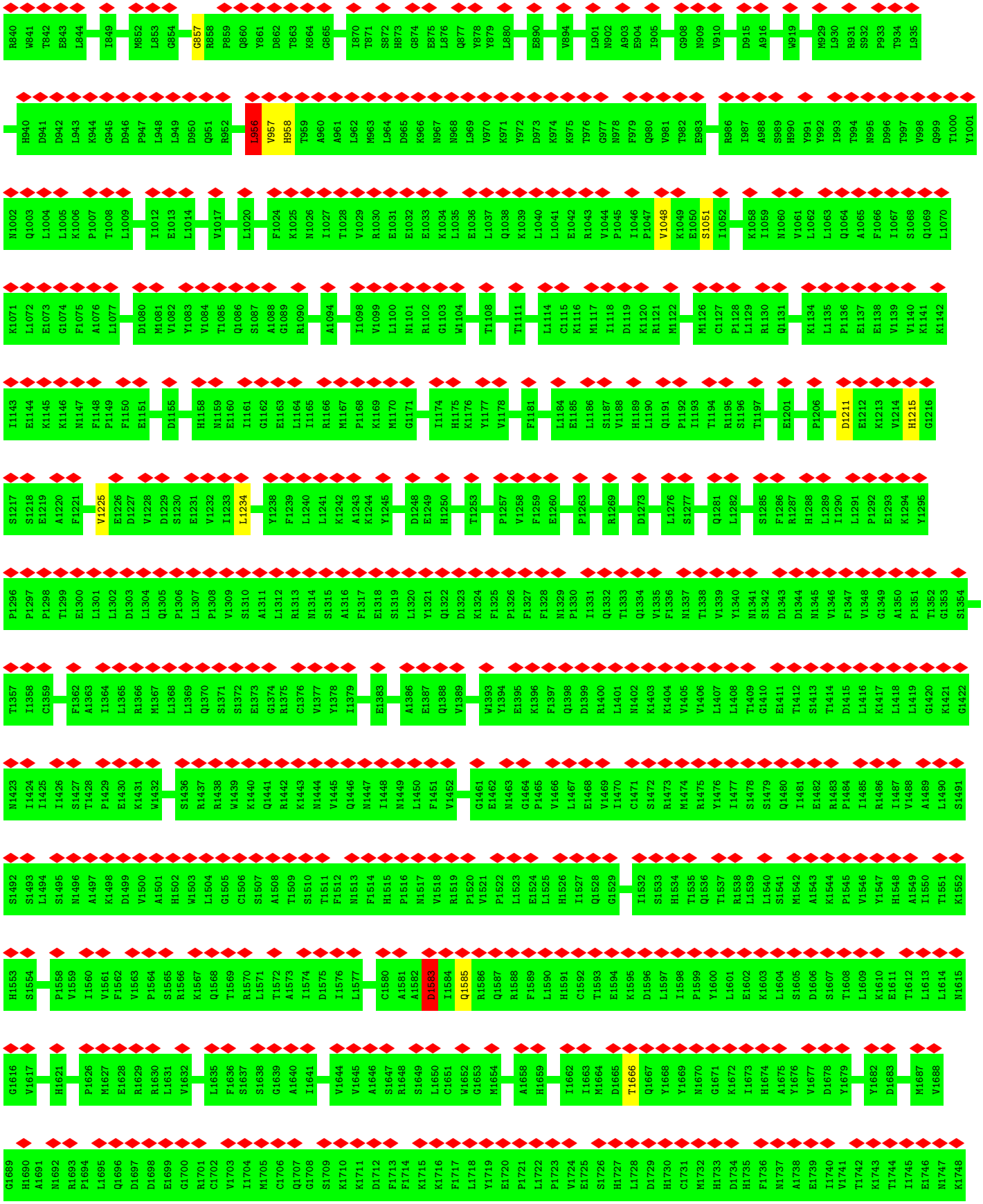
Chain C:

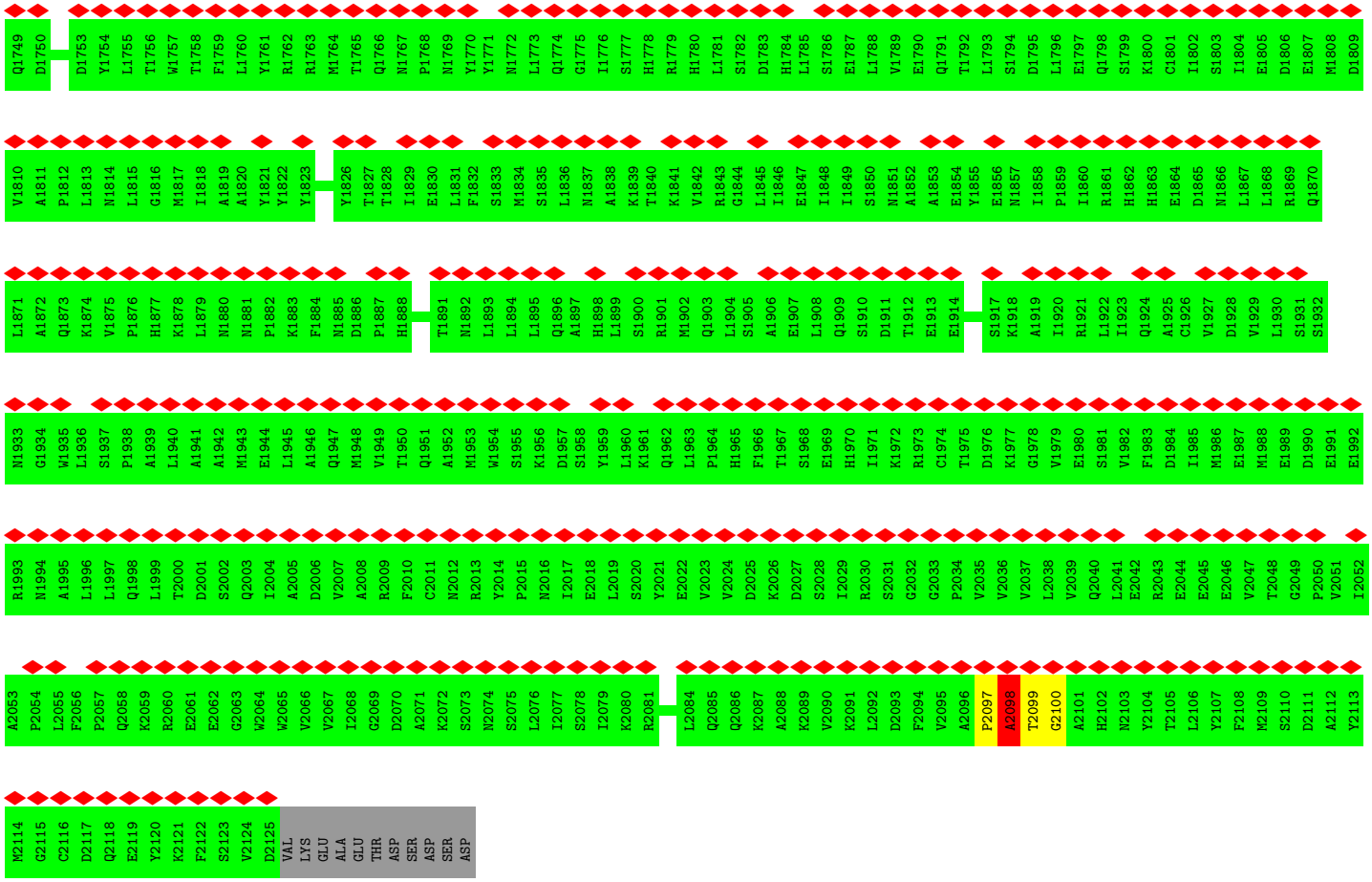


• Molecule 4: U5 small nuclear ribonucleoprotein 200 kDa helicase

Chain D:

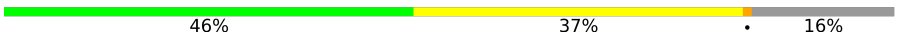


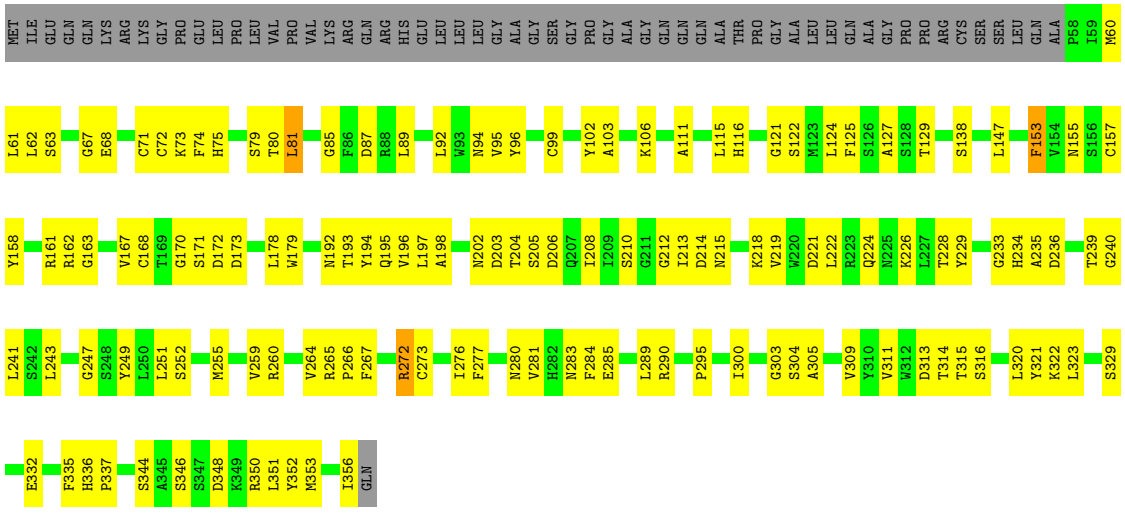

R840 W841 T842 E843 L844 I849 M852 L853 G854 G857 R858 P859 Q860 Y861 D862 T863 K864 G865 I870 T871 S872 H873 G874 E875 L876 Q877 Y878 Y879 L880 E890 V894 L901 N902 A903 E904 I905 G908 N909 V910 D915 A916 W919 M929 L930 R931 S932 P933 T934 L935
H940 D941 D942 L943 K944 G945 D946 P947 L948 L949 D950 Q951 R952 L956 V957 H958 T959 A960 A961 L962 M963 L964 D965 K966 N967 N968 L969 V970 K971 Y972 D973 K974 K975 T976 G977 N978 F979 Q980 V981 T982 E983 R986 I987 A988 S989 H990 Y991 Y992 I993 T994 N995 D996 T997 V998 Q999 T1000 Y1001
N1002 Q1003 L1004 L1005 K1006 P1007 T1008 L1009 I1012 E1013 L1014 V1017 L1020 F1024 K1025 N1026 I1027 T1028 V1029 R1030 E1031 E1032 E1033 K1034 L1035 E1036 L1037 Q1038 K1039 L1040 L1041 E1042 R1043 V1044 P1045 I1046 P1047 V1048 K1049 E1050 S1051 I1052 K1058 I1059 N1060 V1061 L1062 L1063 Q1064 A1065 F1066 I1067 S1068 Q1069 L1070
K1071 L1072 E1073 G1074 F1075 A1076 L1077 D1080 M1081 V1082 Y1083 V1084 T1085 Q1086 S1087 A1088 G1089 R1090 A1094 I1098 V1099 L1100 N1101 R1102 G1103 W1104 T1108 T1111 L1114 C1115 K1116 M1117 I1118 D1119 K1120 R1121 M1122 M1126 C1127 P1128 L1129 R1130 Q1131 K1134 L1135 P1136 E1137 E1138 V1139 V1140 K1141 K1142
I1143 E1144 K1145 K1146 N1147 F1148 P1149 F1150 E1151 D1155 H1158 N1159 E1160 I1161 G1162 E1163 L1164 I1165 R1166 M1167 P1168 K1169 M1170 G1171 I1174 H1175 K1176 Y1177 V1178 F1181 L1184 E1185 L1186 S1187 V1188 H1189 L1190 Q1191 P1192 I1193 T1194 R1195 S1196 T1197 E1201 P1206 D1211 E1212 K1213 V1214 H1215 G1216
S1217 S1218 E1219 A1220 F1221 V1225 E1226 D1227 V1228 D1229 S1230 E1231 V1232 I1233 L1234 Y1238 F1239 L1240 L1241 K1242 A1243 K1244 Y1245 D1248 E1249 H1250 T1253 P1257 V1258 F1259 E1260 P1263 R1269 D1273 L1276 S1277 Q1281 L1282 S1285 F1286 R1287 H1288 L1289 I1290 L1291 P1292 E1293 K1294 Y1295
P1296 P1297 P1298 T1299 E1300 L1301 L1302 D1303 L1304 Q1305 P1306 L1307 P1308 V1309 S1310 A1311 L1312 R1313 N1314 S1315 A1316 F1317 E1318 S1319 L1320 Y1321 Q1322 D1323 K1324 F1325 P1326 F1327 F1328 N1329 P1330 I1331 Q1332 T1333 Q1334 V1335 F1336 N1337 T1338 V1339 Y1340 N1341 S1342 D1343 D1344 N1345 V1346 F1347 V1348 G1349 A1350 P1351 T1352 G1353 S1354
T1357 I1358 C1359 F1362 A1363 I1364 L1365 R1366 M1367 L1368 L1369 Q1370 S1371 S1372 E1373 G1374 R1375 C1376 V1377 Y1378 I1379 E1383 A1386 E1387 Q1388 V1389 W1393 Y1394 E1395 K1396 F1397 Q1398 D1399 R1400 L1401 N1402 K1403 K1404 V1405 V1406 L1407 L1408 T1409 G1410 E1411 T1412 S1413 T1414 D1415 L1416 K1417 L1418 L1419 G1420 K1421 G1422
N1423 I1424 I1425 I1426 S1427 T1428 P1429 E1430 K1431 W1432 S1436 R1437 R1438 W1439 K1440 Q1441 R1442 K1443 N1444 V1445 Q1446 N1447 I1448 N1449 L1450 F1451 V1452 G1461 E1462 N1463 G1464 P1465 V1466 L1467 E1468 V1469 I1470 C1471 S1472 R1473 M1474 R1475 Y1476 I1477 S1478 S1479 Q1480 I1481 E1482 R1483 P1484 I1485 R1486 I1487 V1488 A1489 L1490 S1491
S1492 S1493 L1494 S1495 N1496 A1497 K1498 D1499 V1500 A1501 H1502 W1503 L1504 G1505 C1506 S1507 A1508 T1509 S1510 T1511 F1512 N1513 F1514 H1515 P1516 N1517 V1518 R1519 P1520 V1521 P1522 L1523 E1524 L1525 H1526 I1527 Q1528 G1529 I1532 S1533 H1534 T1535 Q1536 T1537 R1538 L1539 L1540 S1541 M1542 A1543 K1544 P1545 V1546 Y1547 H1548 A1549 I1550 T1551 K1552
H1553 S1554 P1558 V1559 I1560 V1561 F1562 V1563 P1564 S1565 R1566 K1567 Q1568 T1569 R1570 L1571 T1572 A1573 I1574 D1575 I1576 L1577 C1580 A1581 A1582 D1583 I1584 Q1585 R1586 Q1587 R1588 F1589 L1590 H1591 C1592 T1593 E1594 K1595 D1596 L1597 I1598 P1599 Y1600 L1601 E1602 K1603 L1604 S1605 D1606 S1607 T1608 L1609 K1610 E1611 T1612 L1613 L1614 N1615
G1616 V1617 H1621 P1626 M1627 E1628 R1629 R1630 L1631 V1632 L1635 F1636 S1637 S1638 G1639 A1640 I1641 V1644 V1645 A1646 S1647 R1648 S1649 L1650 C1651 W1652 G1653 M1654 A1658 H1659 I1662 I1663 M1664 D1665 T1666 Q1667 Y1668 Y1669 N1670 G1671 K1672 I1673 H1674 A1675 Y1676 V1677 D1678 Y1679 Y1682 D1683 M1687 V1688
G1689 H1690 A1691 N1692 R1693 P1694 L1695 Q1696 D1697 D1698 E1699 G1700 R1701 C1702 V1703 I1704 M1705 C1706 Q1707 G1708 S1709 K1710 K1711 D1712 F1713 F1714 K1715 K1716 F1717 L1718 Y1719 E1720 P1721 L1722 P1723 V1724 E1725 S1726 H1727 L1728 D1729 H1730 C1731 M1732 H1733 D1734 H1735 F1736 N1737 A1738 E1739 I1740 V1741 T1742 K1743 T1744 I1745 E1746 N1747 K1748



• Molecule 5: U5 small nuclear ribonucleoprotein 40 kDa protein

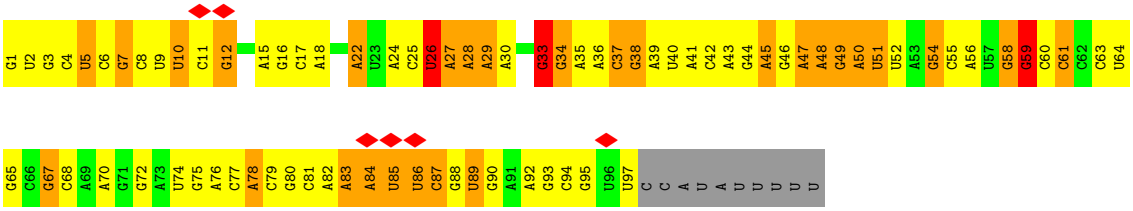
Chain E:





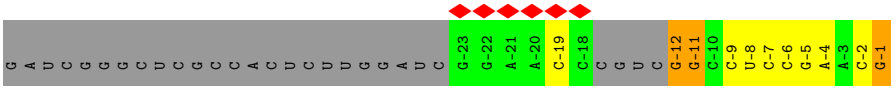
• Molecule 6: U6 snRNA

Chain F:



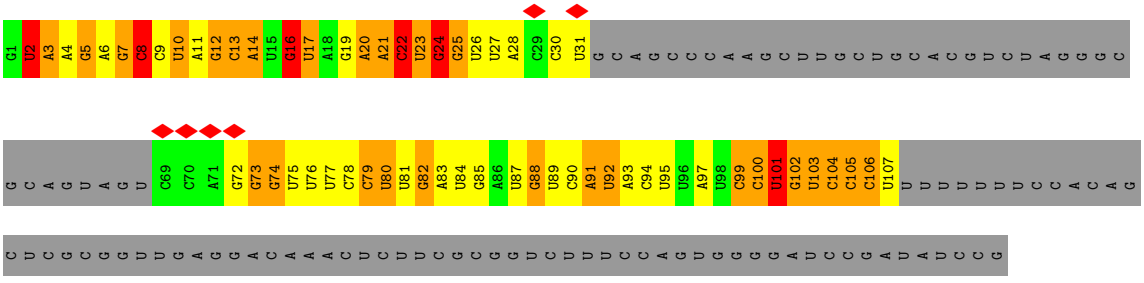
• Molecule 7: pre-mRNA

Chain G:



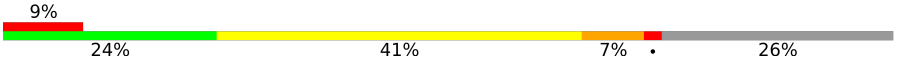
• Molecule 8: pre-mRNA

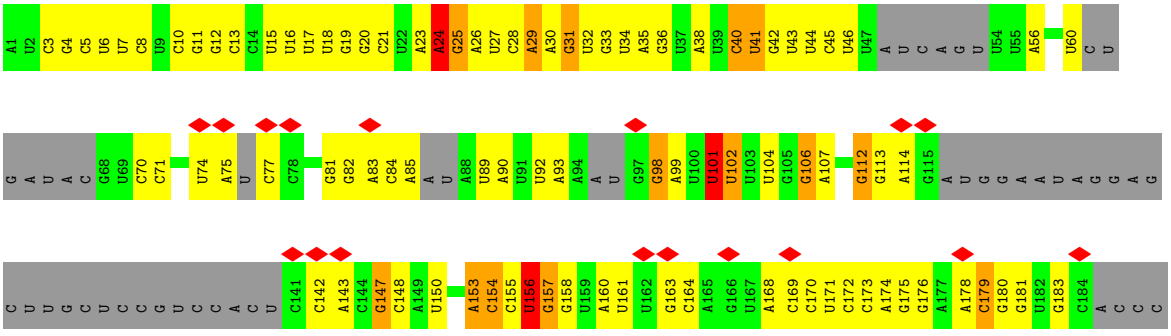
Chain 6:



• Molecule 9: U2 snRNA

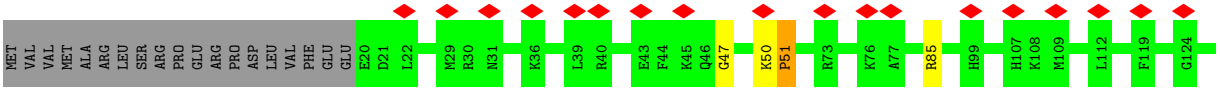
Chain H:

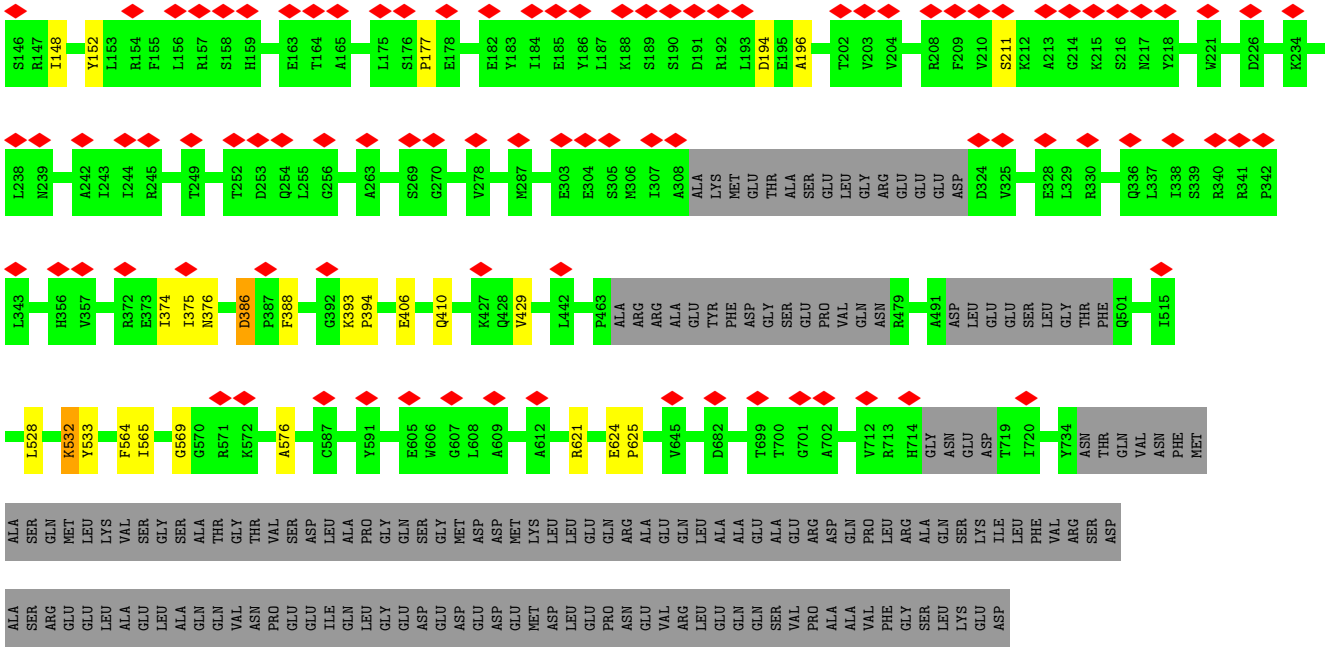




• Molecule 10: Pre-mRNA-splicing factor SYF1

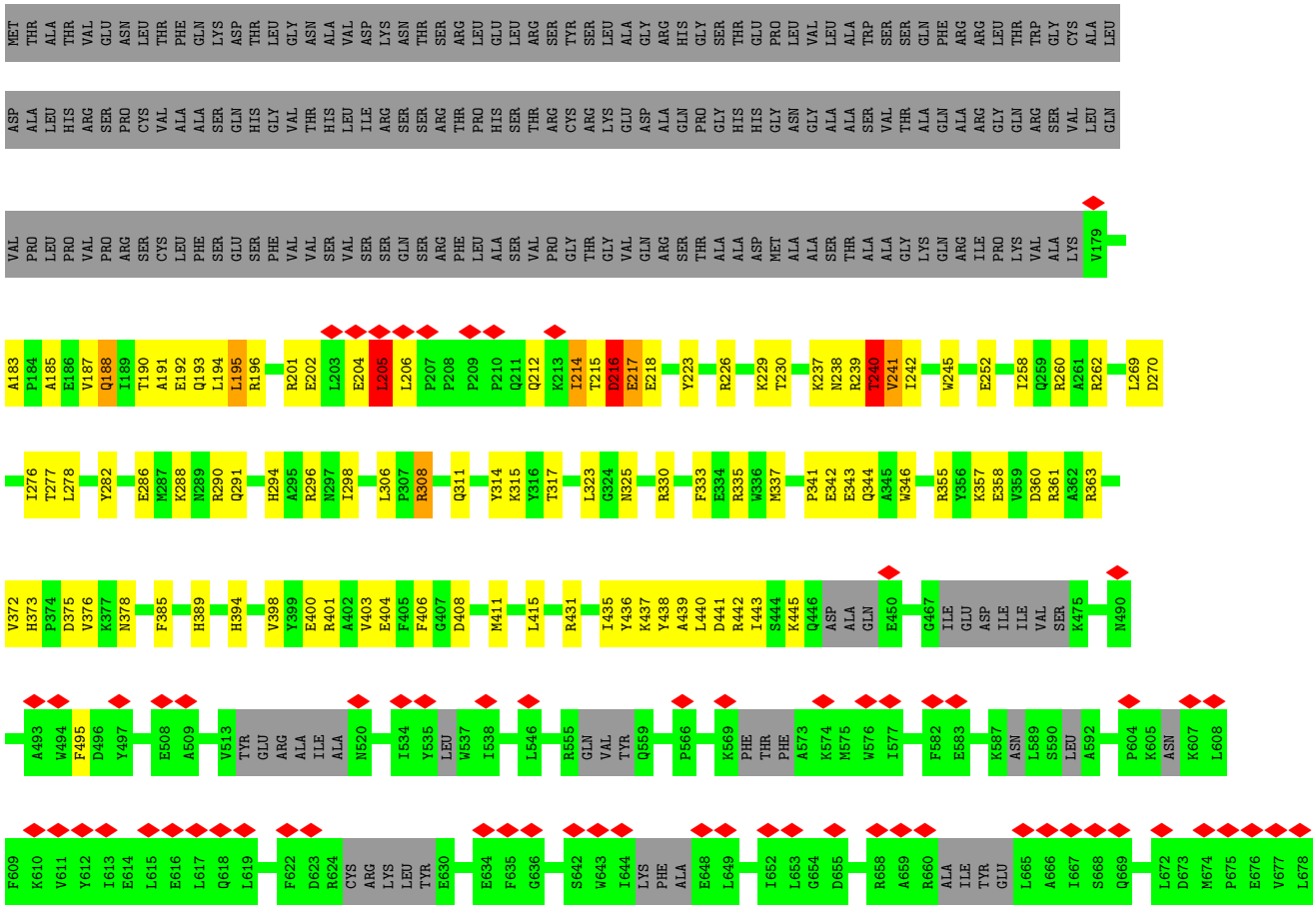
Chain I:

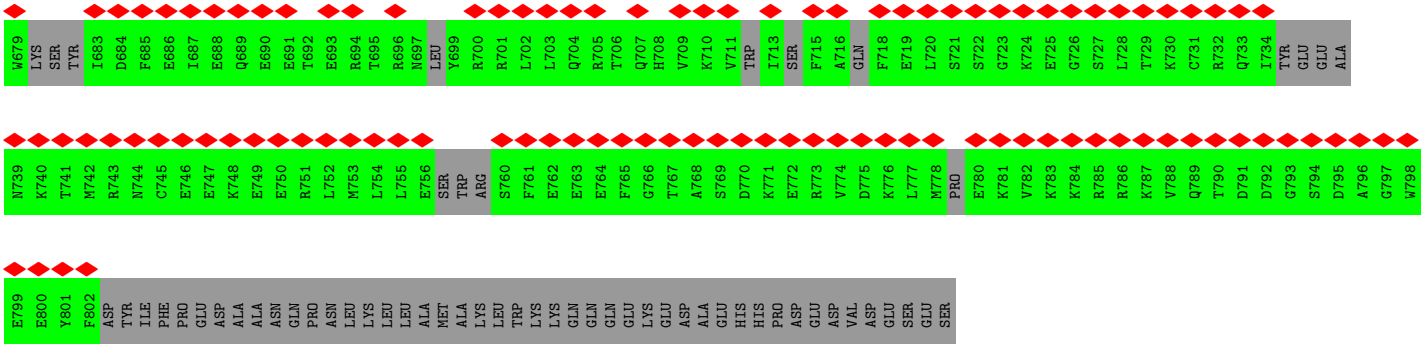




• Molecule 11: Crooked neck-like protein 1

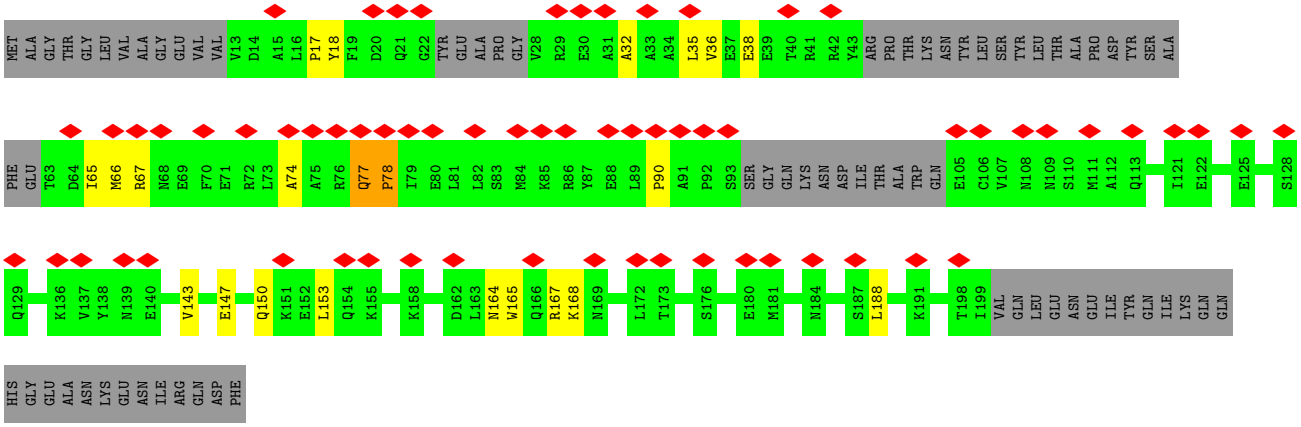
Chain J:





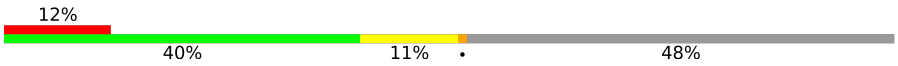
• Molecule 12: Pre-mRNA-splicing factor SPF27

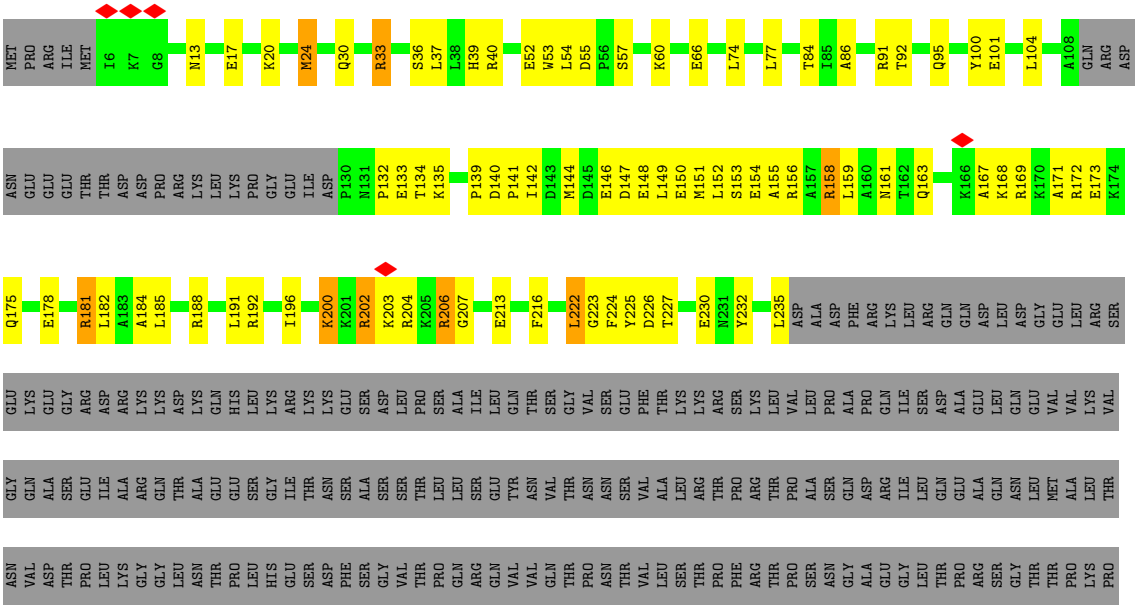
Chain K:

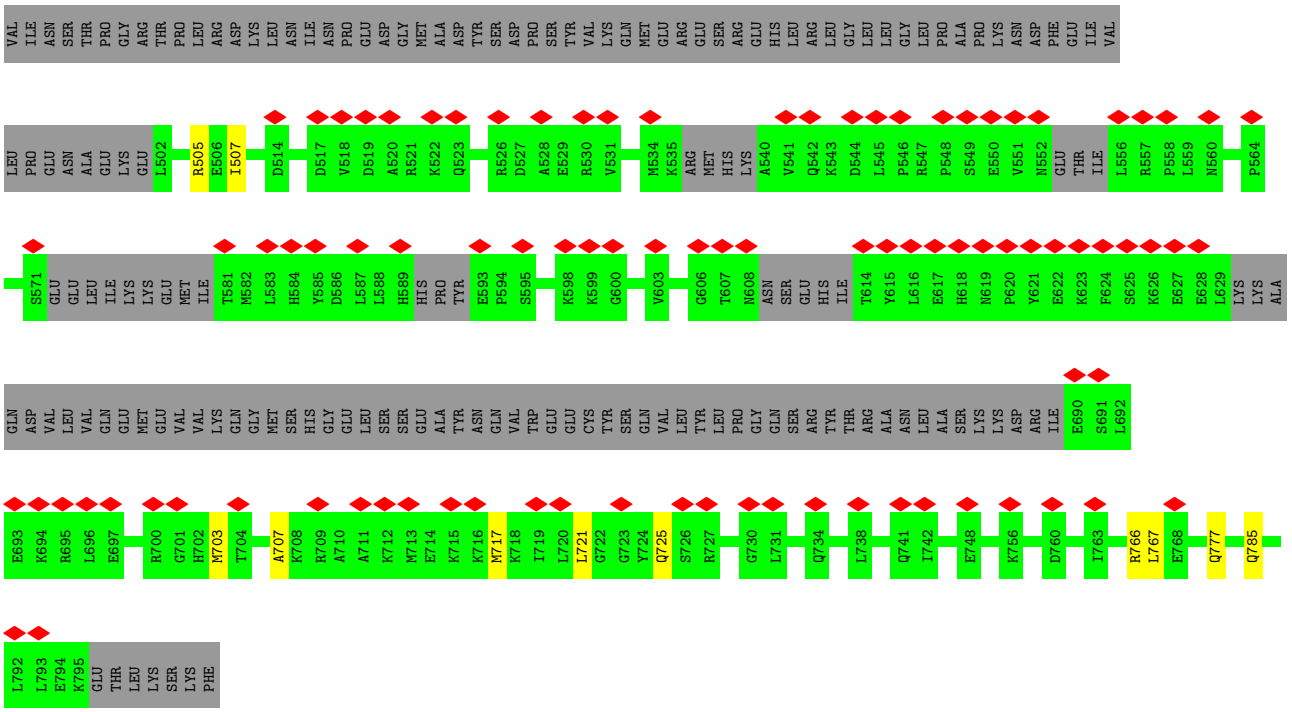


• Molecule 13: Cell division cycle 5-like protein

Chain L:

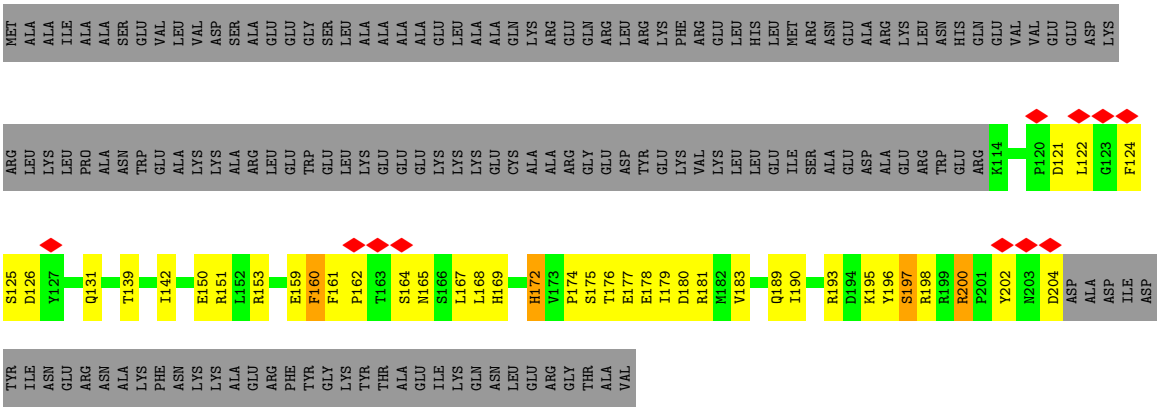






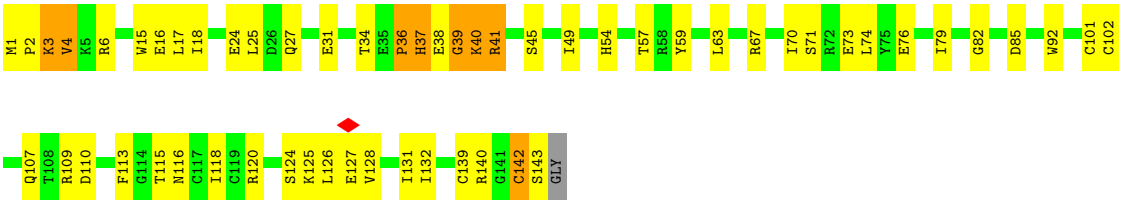
• Molecule 14: Pre-mRNA-splicing factor SYF2

Chain M:



• Molecule 15: Protein BUD31 homolog

Chain N:



• Molecule 16: Pre-mRNA-splicing factor RBM22

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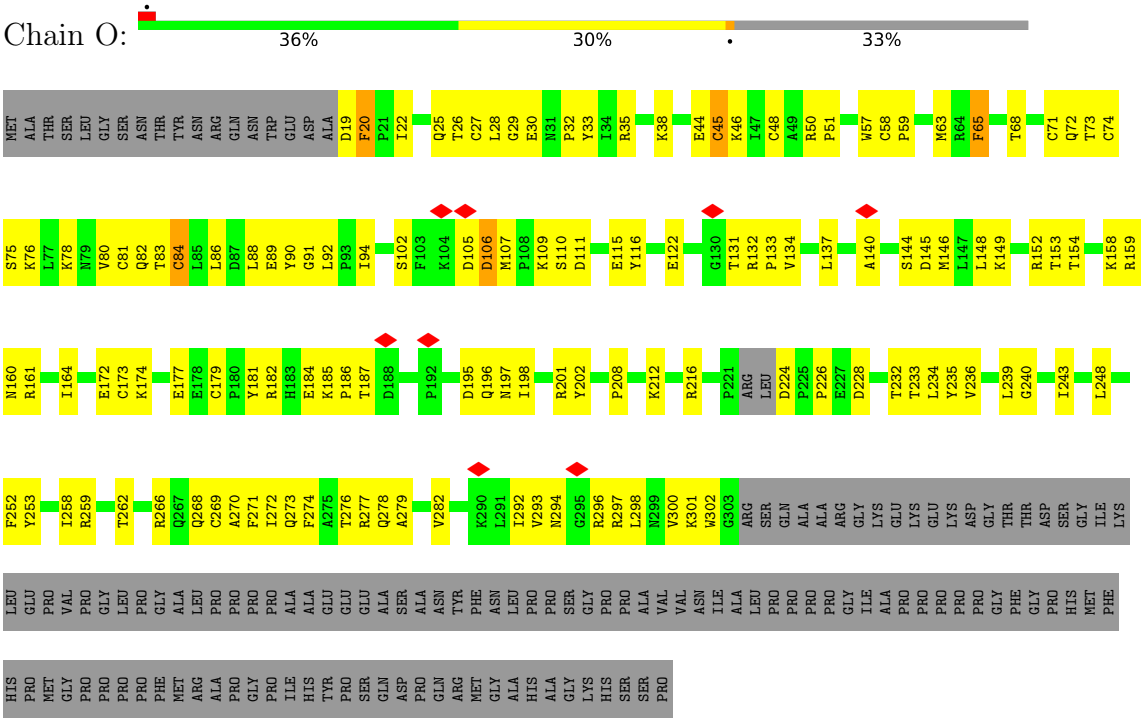
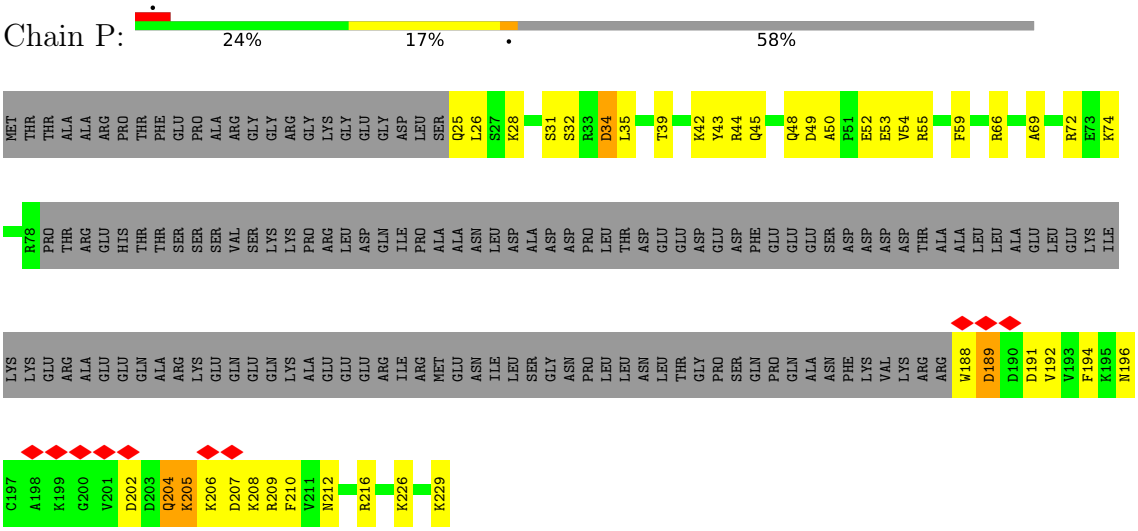


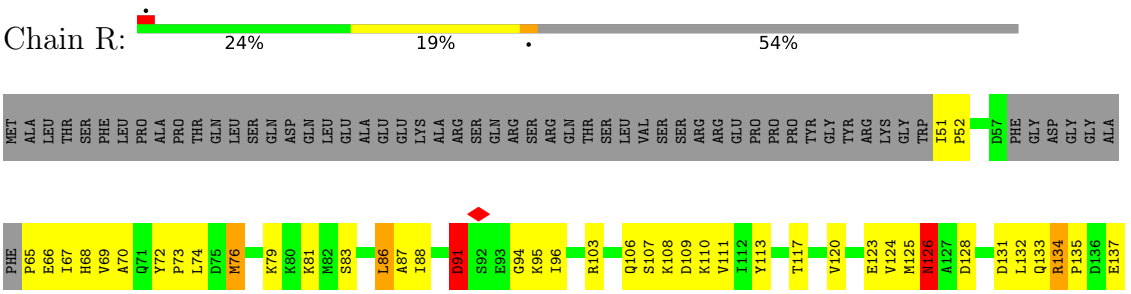
• Molecule 17: Spliceosome-associated protein CWC15 homolog

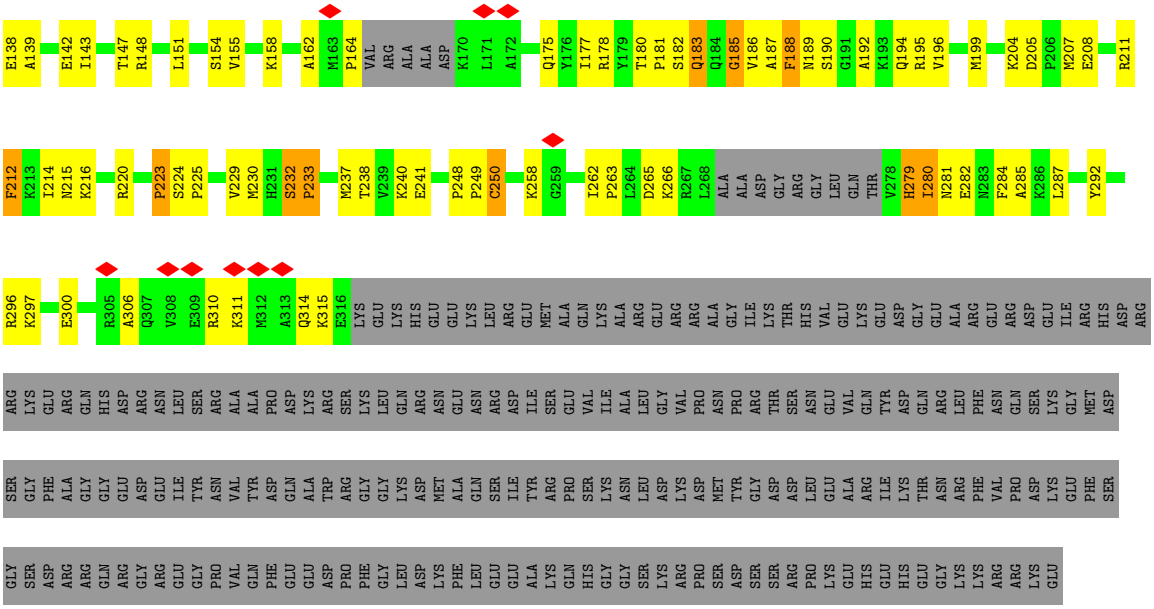
Chain P:



• Molecule 18: SNW domain-containing protein 1

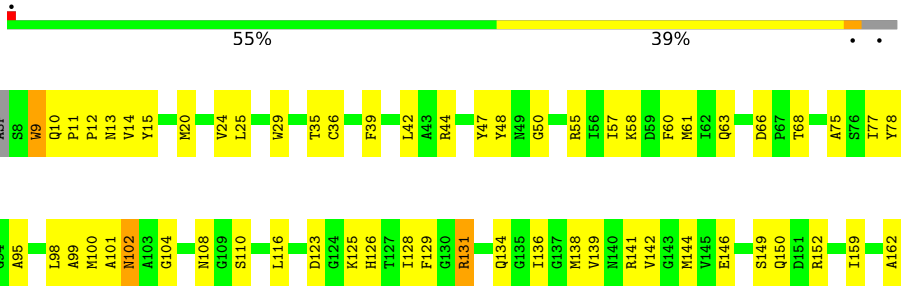
Chain R:





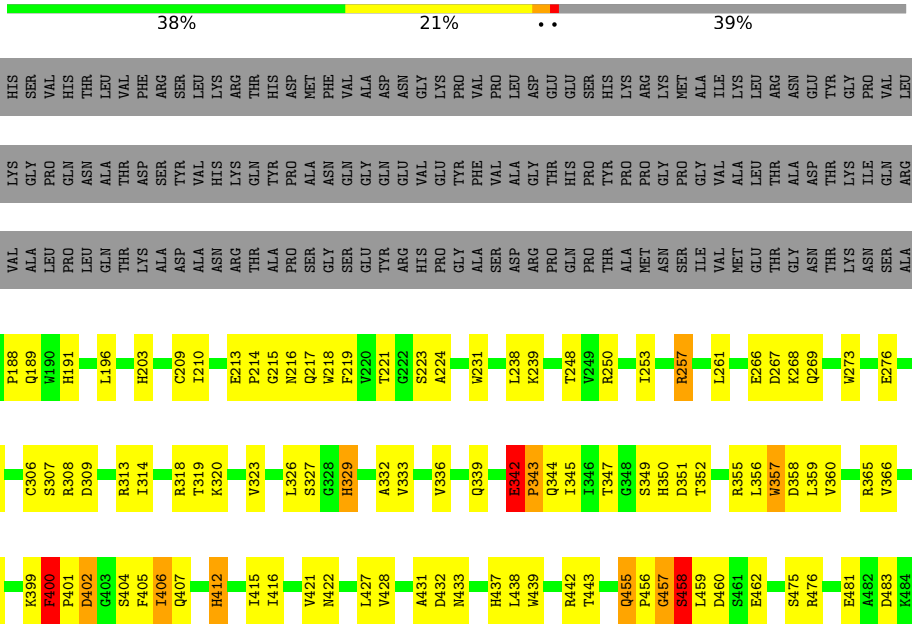
• Molecule 19: Peptidyl-prolyl cis-trans isomerase-like 1

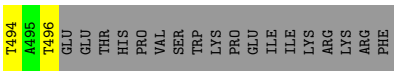
Chain S:



• Molecule 20: Pleiotropic regulator 1

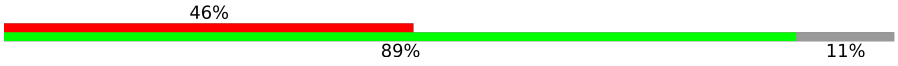
Chain T:

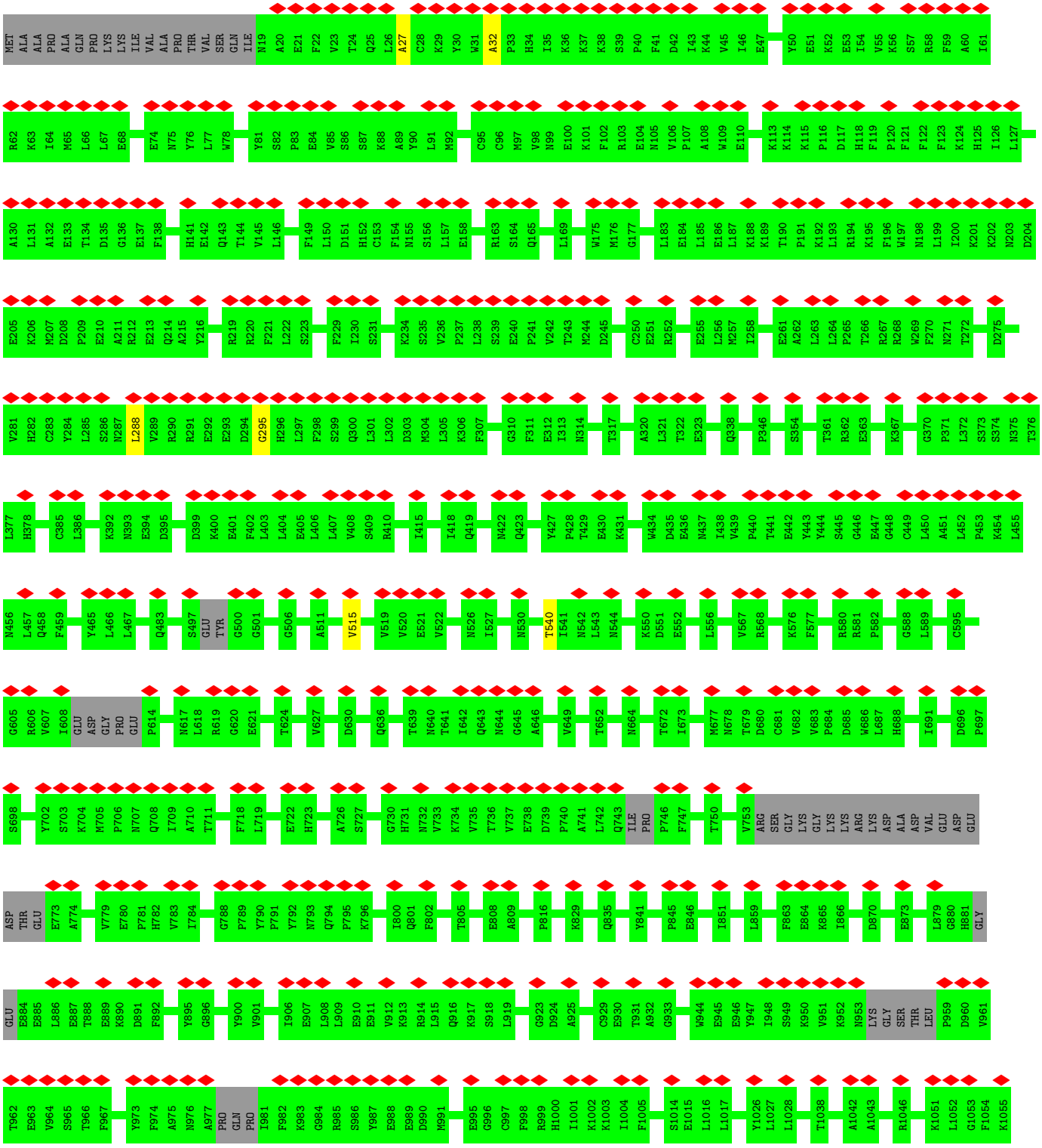


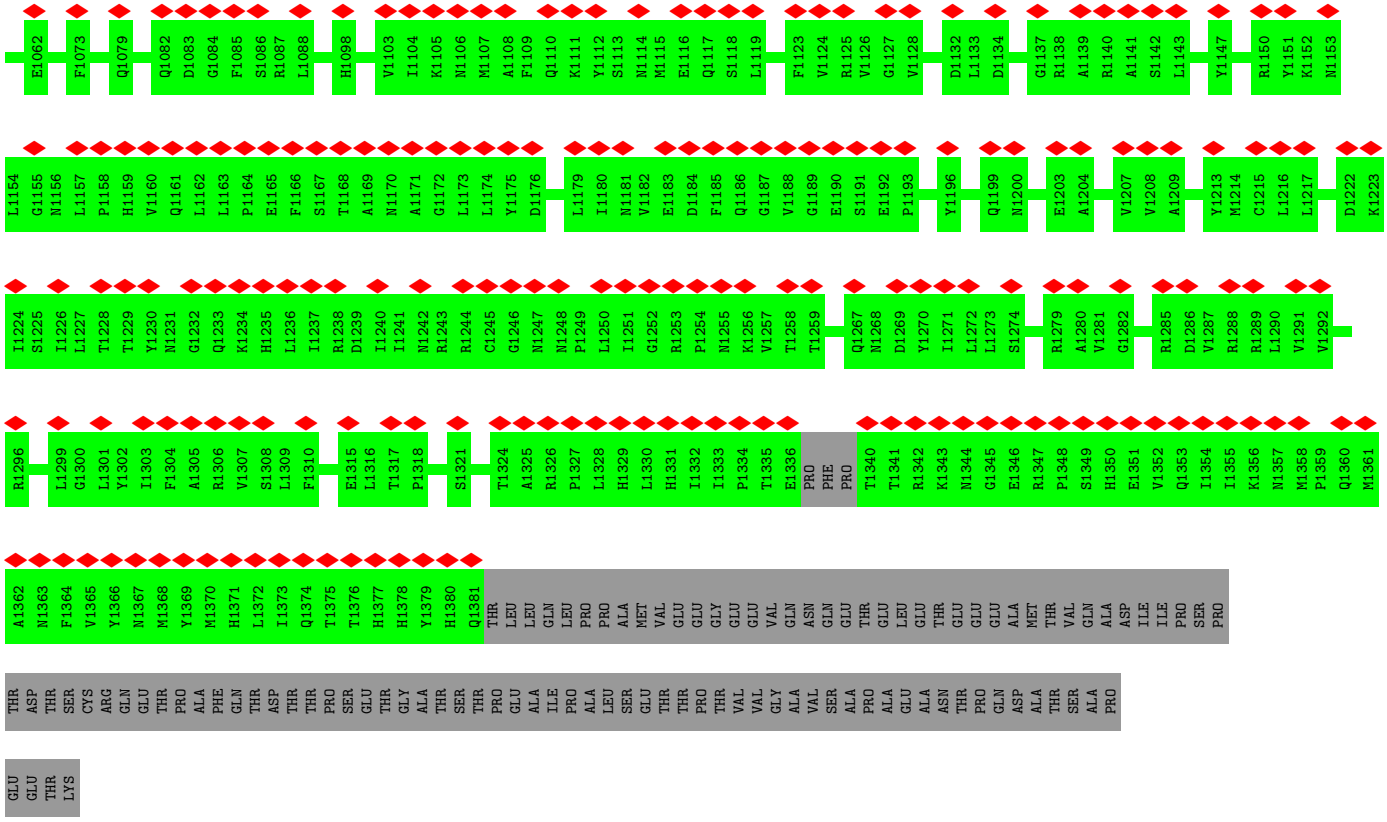


• Molecule 21: RNA helicase aquarius

Chain Q:

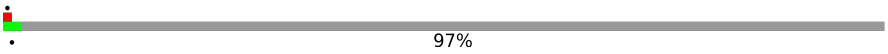


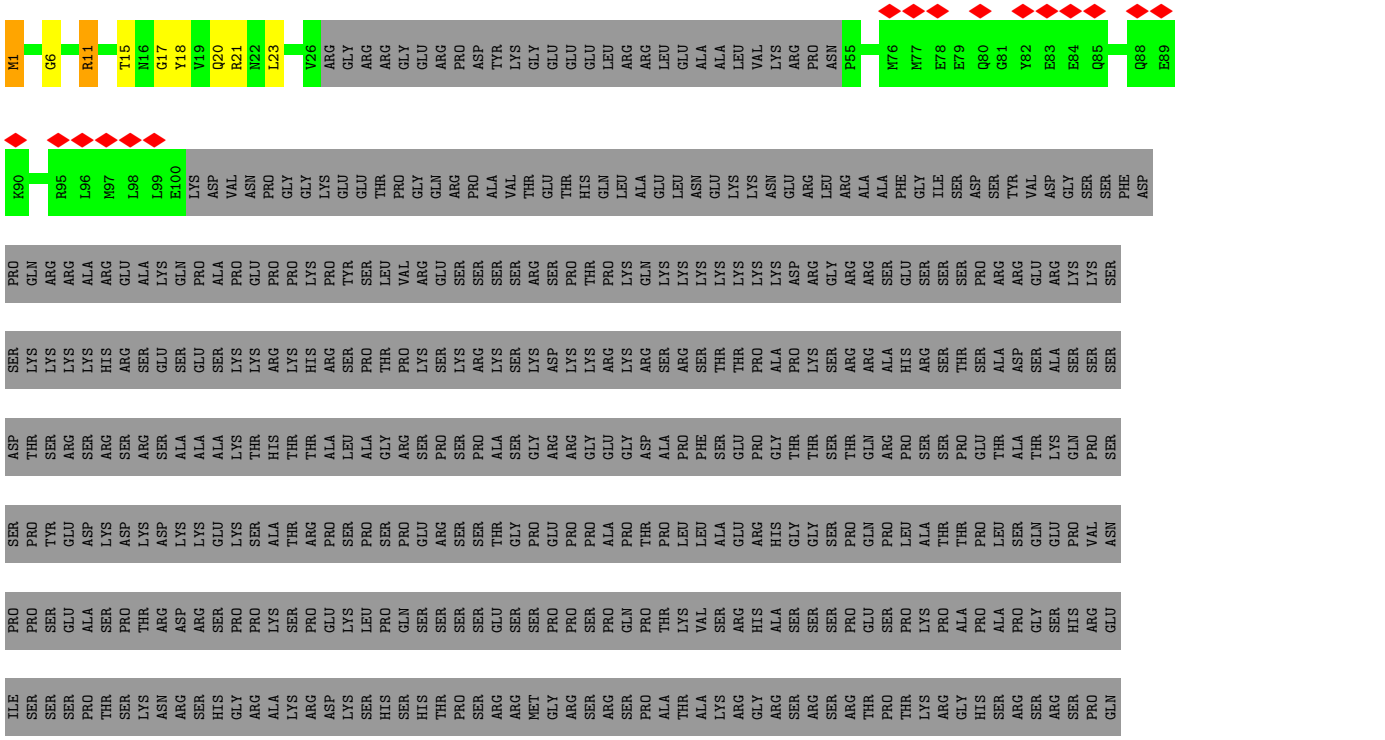


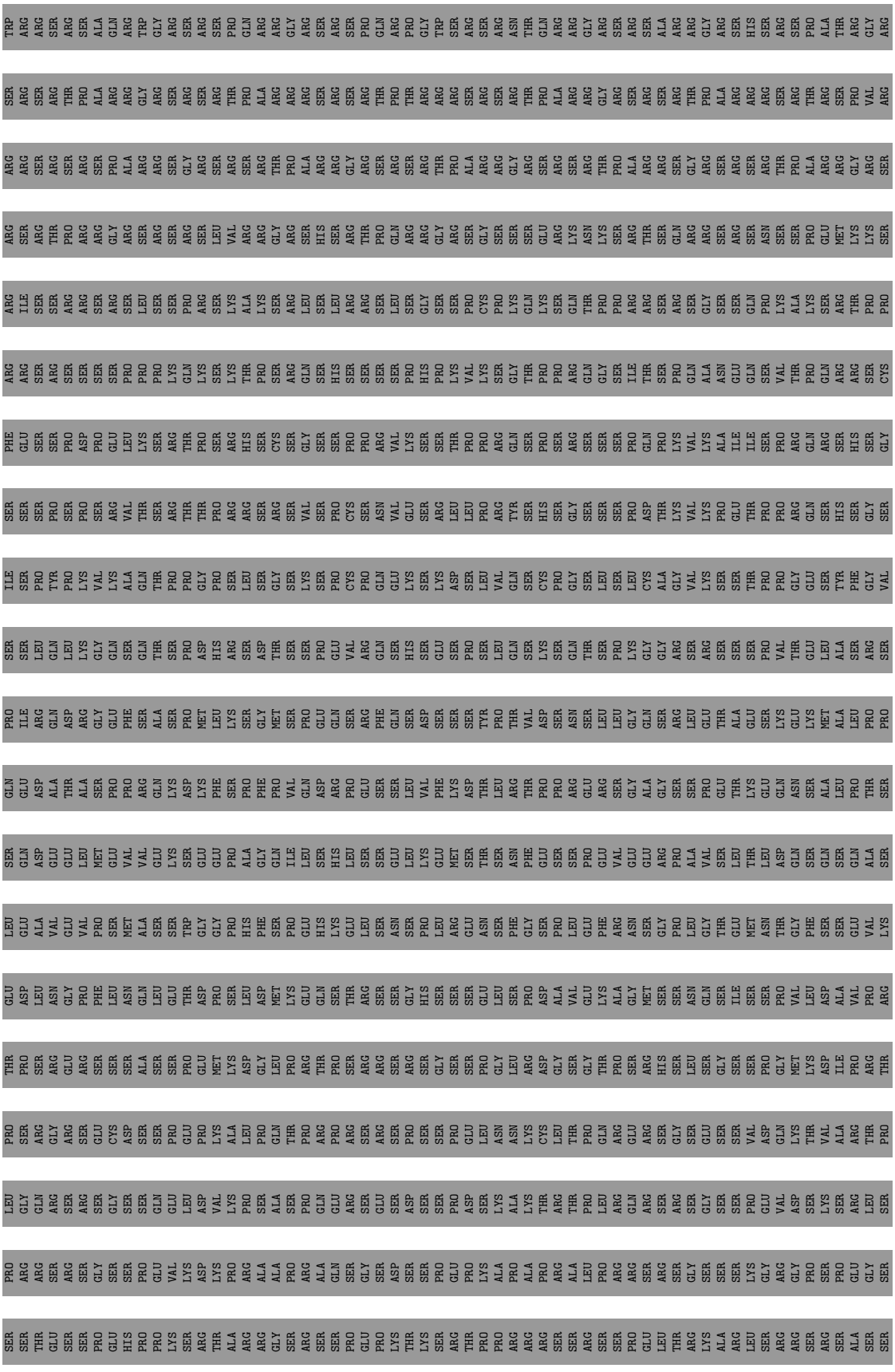


• Molecule 22: Serine/arginine repetitive matrix protein 2

Chain U:







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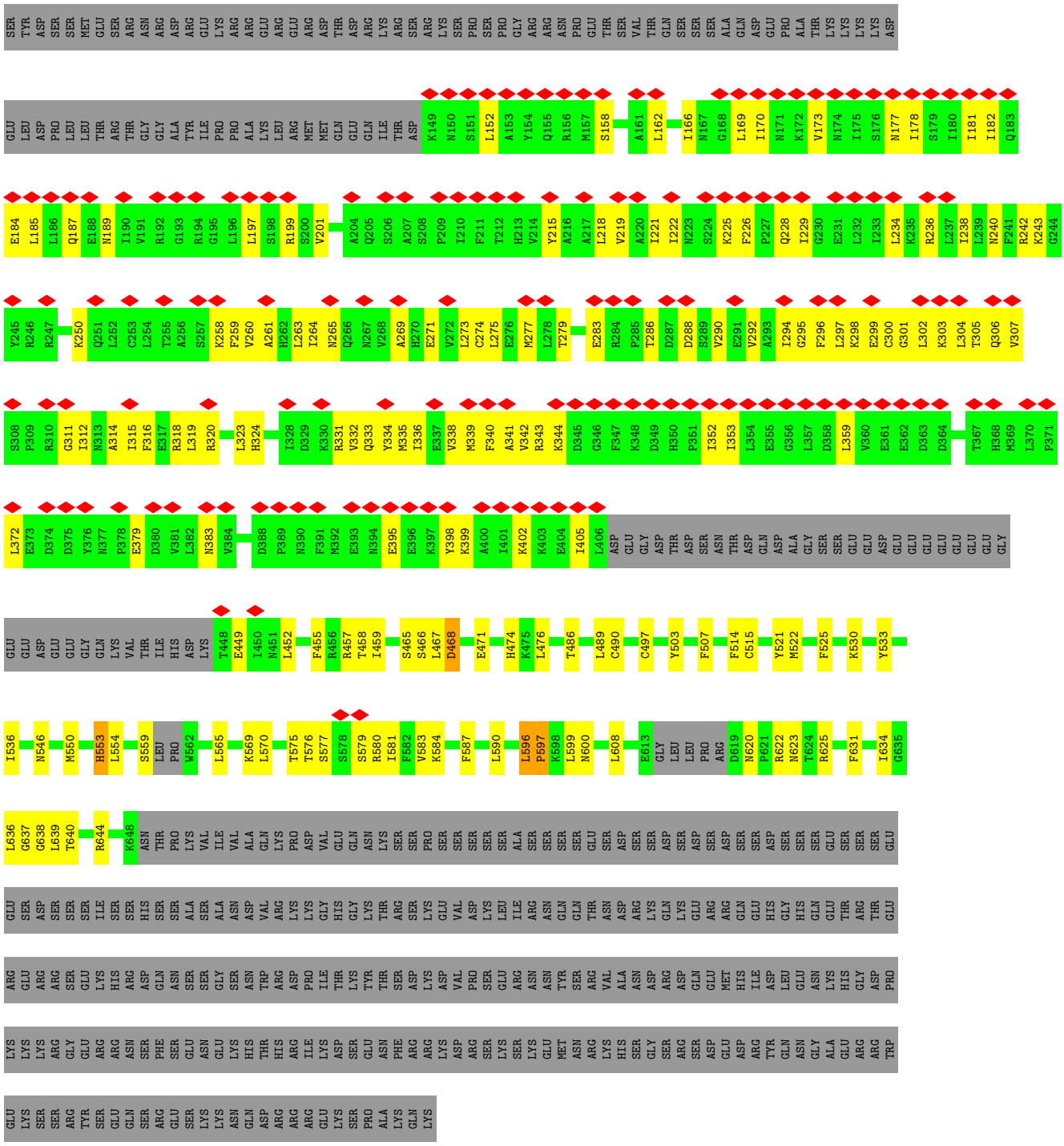
LYS ARG ARG ARG GLU THR PRO SER PRO ARG PRO MET ARG HIS ARG SER SER ARG SER PRO

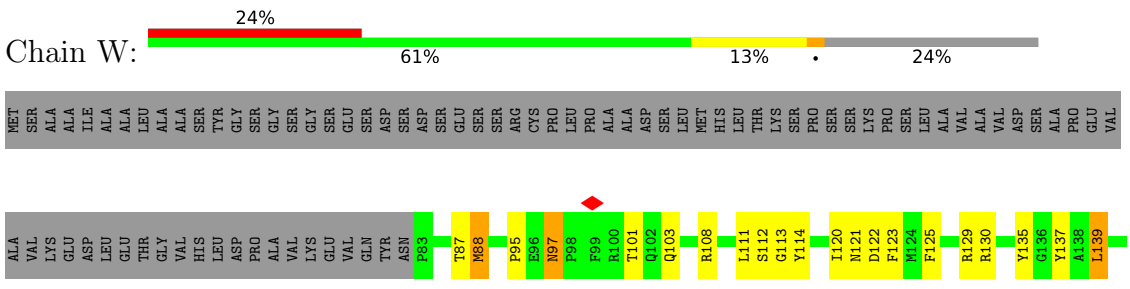
- Molecule 23: Pre-mRNA-splicing factor CWC22 homolog

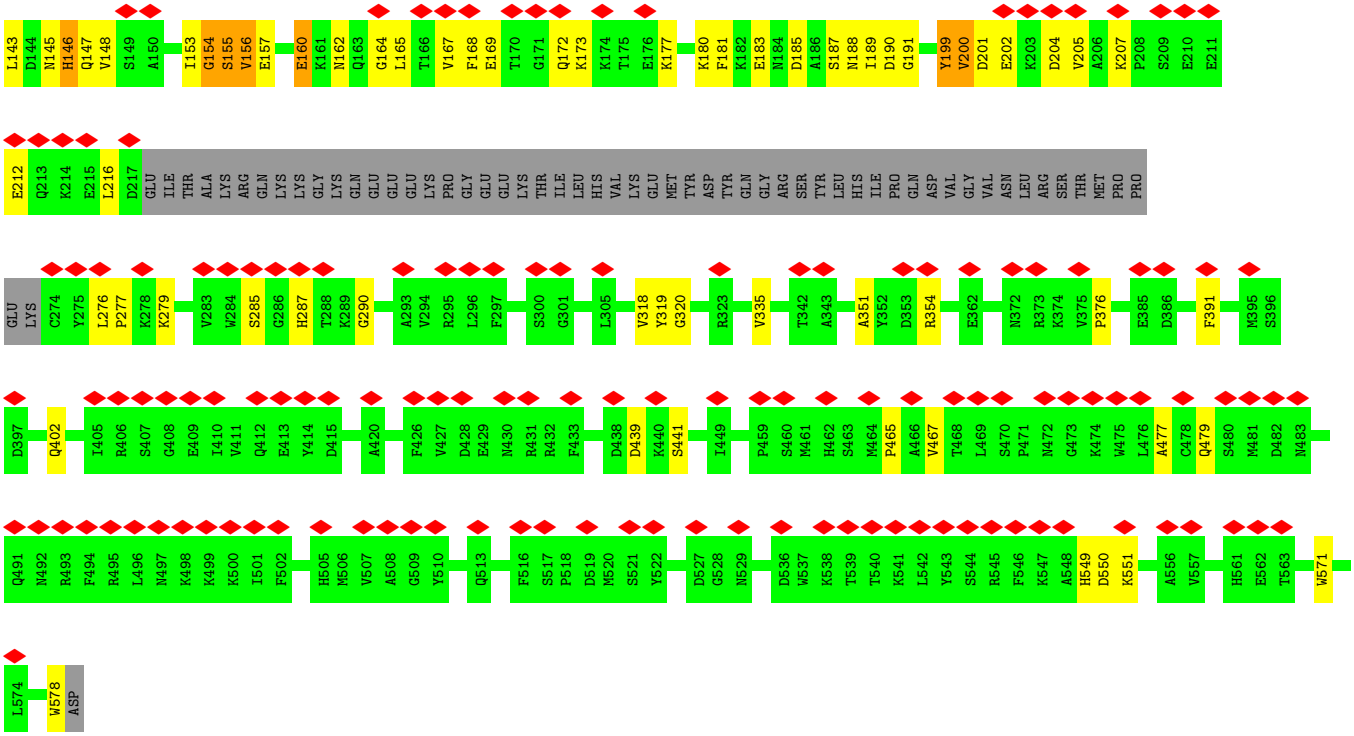
Chain V: 18% | 32% | 18% | 50%

MET LYS SER SER VAL ALA GLN ILE LYS PRO SER SER GLY HIS ASP ARG ARG GLU ASN LEU ASN SER TYR GLN ARG ASN SER SER PRO GLU ASP ARG TYR GLU GLU GLN GLU ARG SER PRO ARG ASP ARG ASP TYR PHE ASP TYR SER ARG SER ASP TYR GLU HIS SER ARG ARG GLY ARG



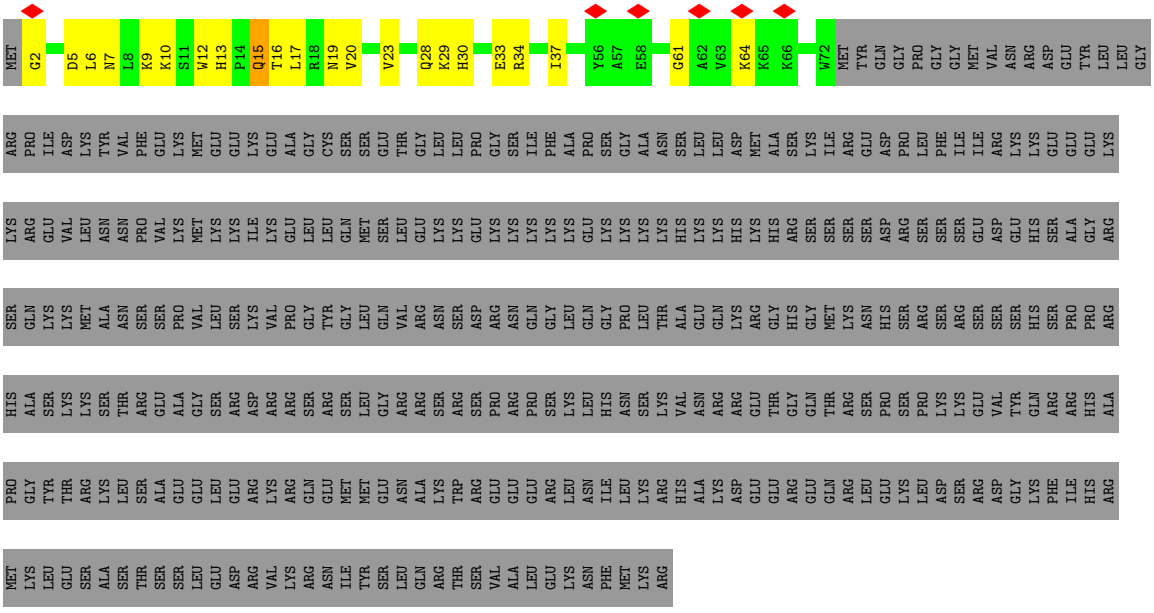
• Molecule 24: Pre-mRNA-processing factor 17





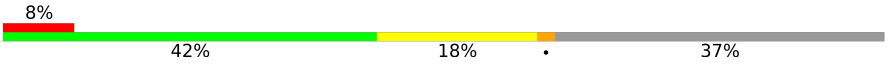
• Molecule 25: Pre-mRNA-splicing factor CWC25 homolog

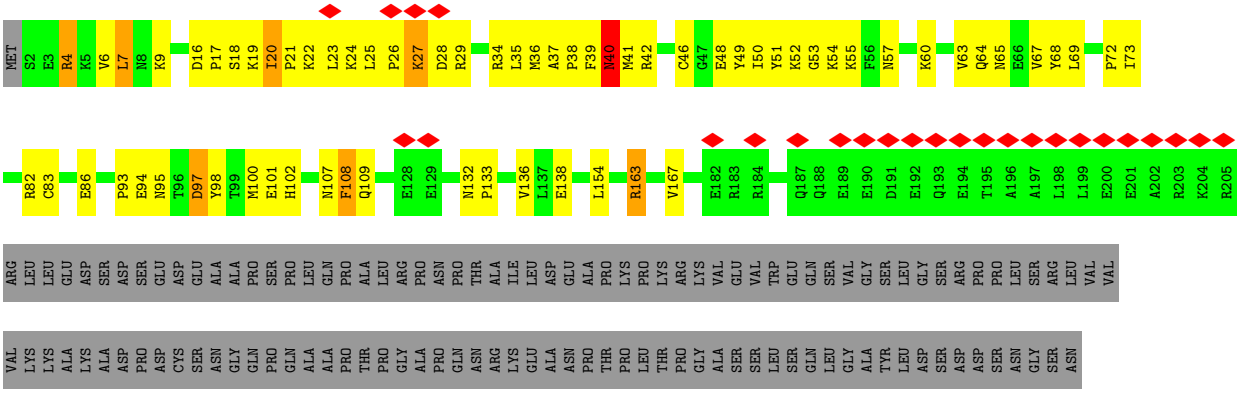
Chain X:



• Molecule 26: Coiled-coil domain-containing protein 94

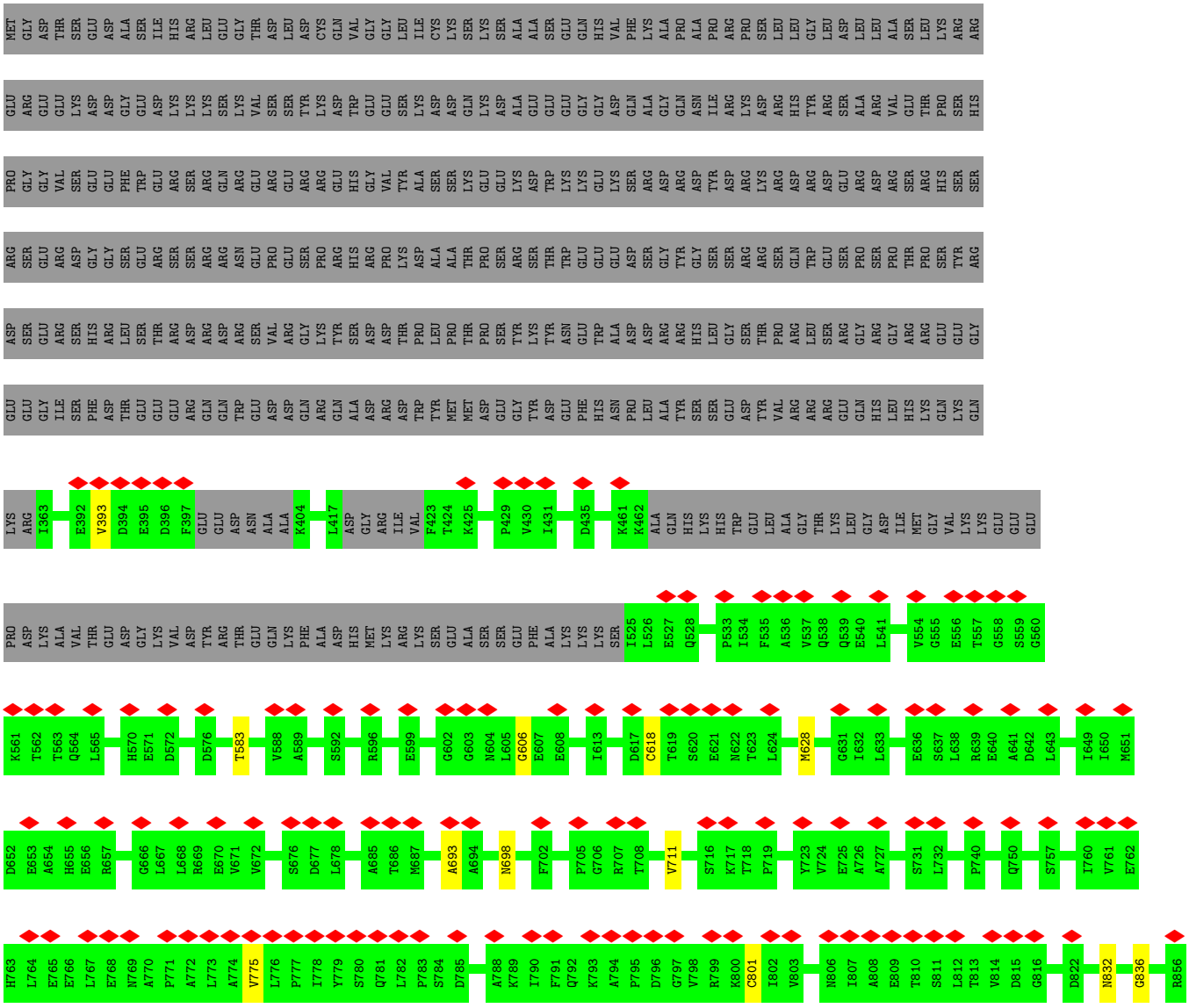
Chain Y:

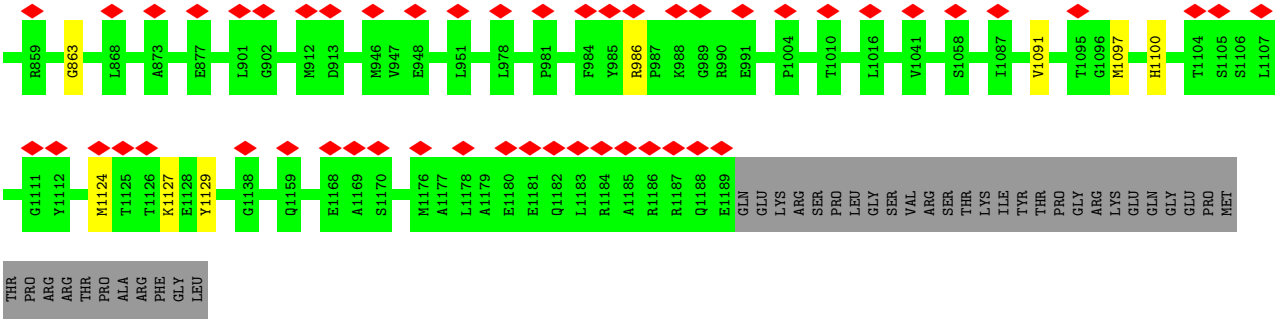




• Molecule 27: Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP16

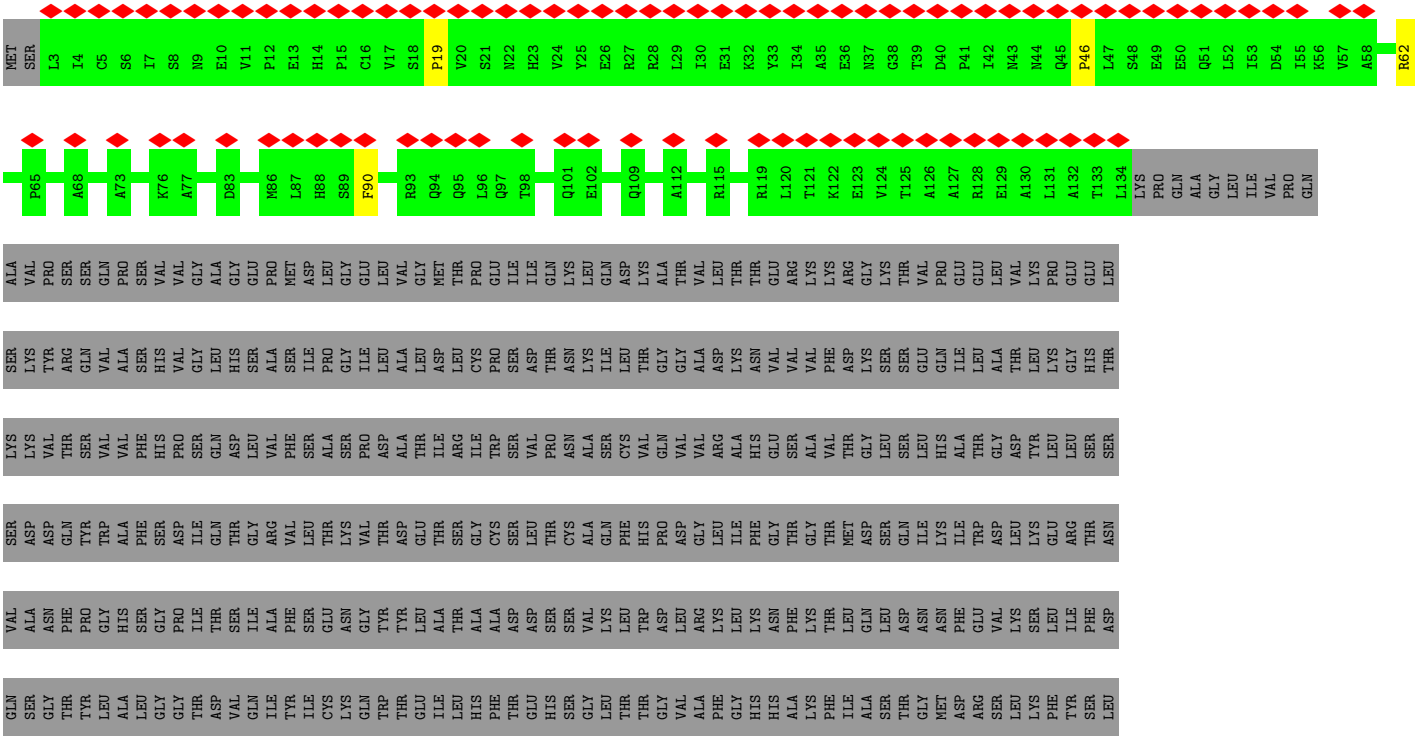
Chain Z:





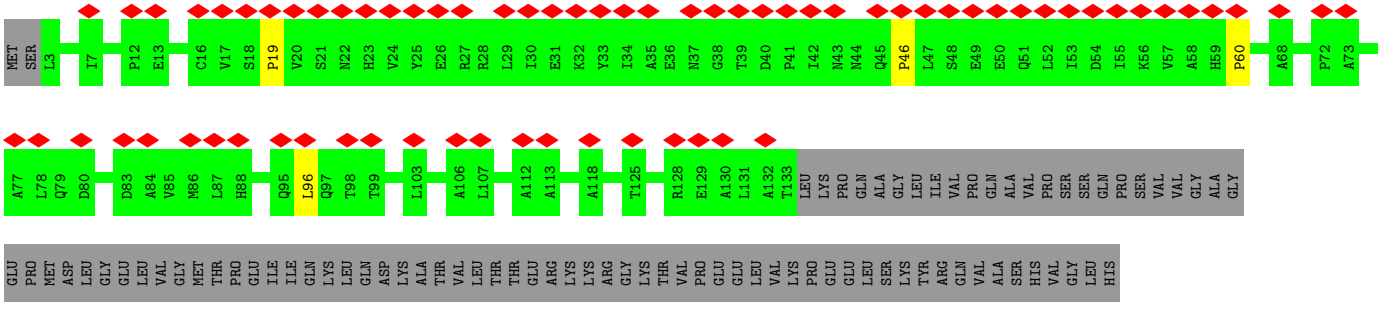
• Molecule 28: Pre-mRNA-processing factor 19

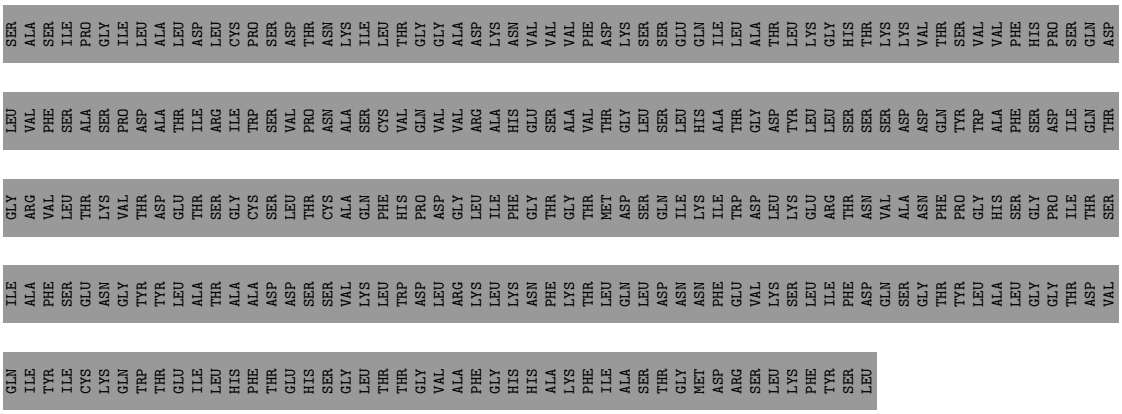
Chain q:



• Molecule 28: Pre-mRNA-processing factor 19

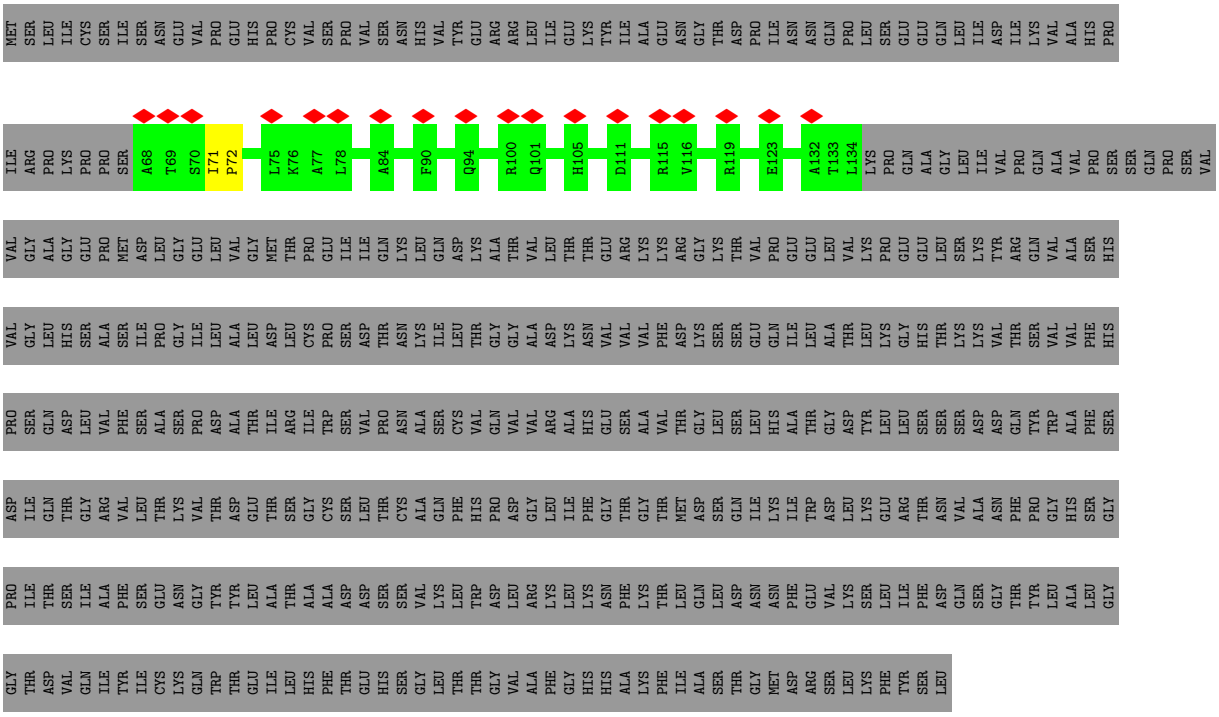
Chain r:





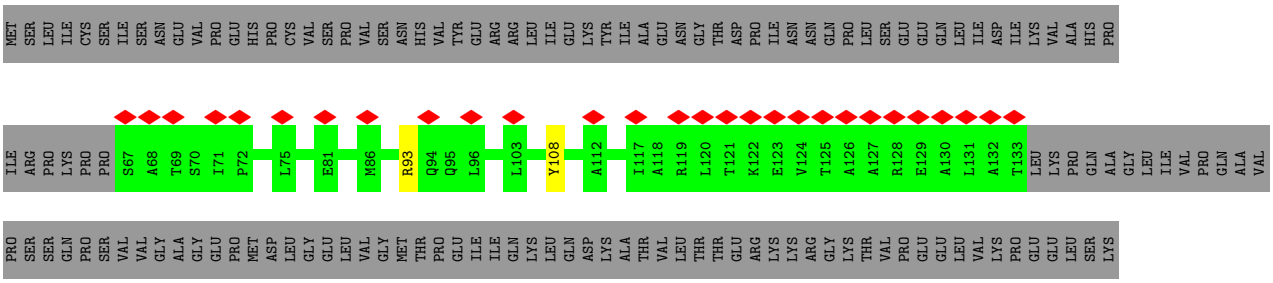
• Molecule 28: Pre-mRNA-processing factor 19

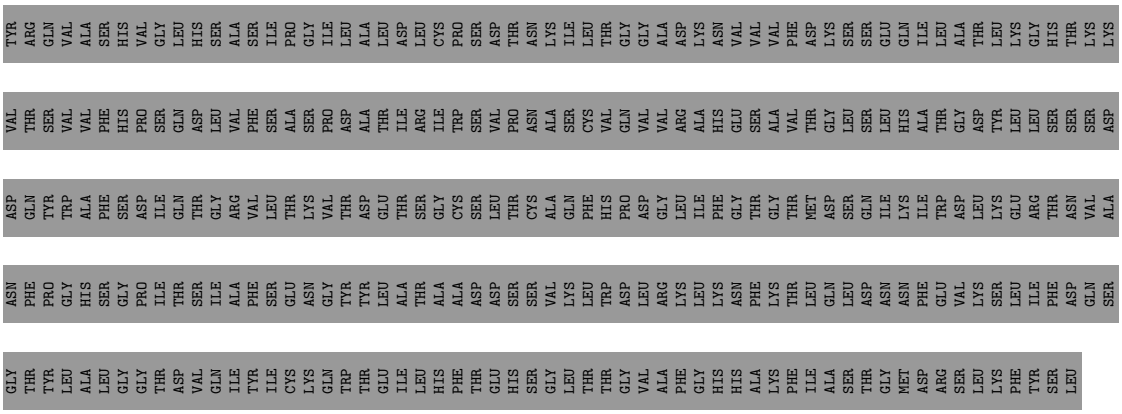
Chain s:



• Molecule 28: Pre-mRNA-processing factor 19

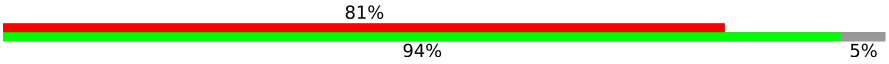
Chain t:

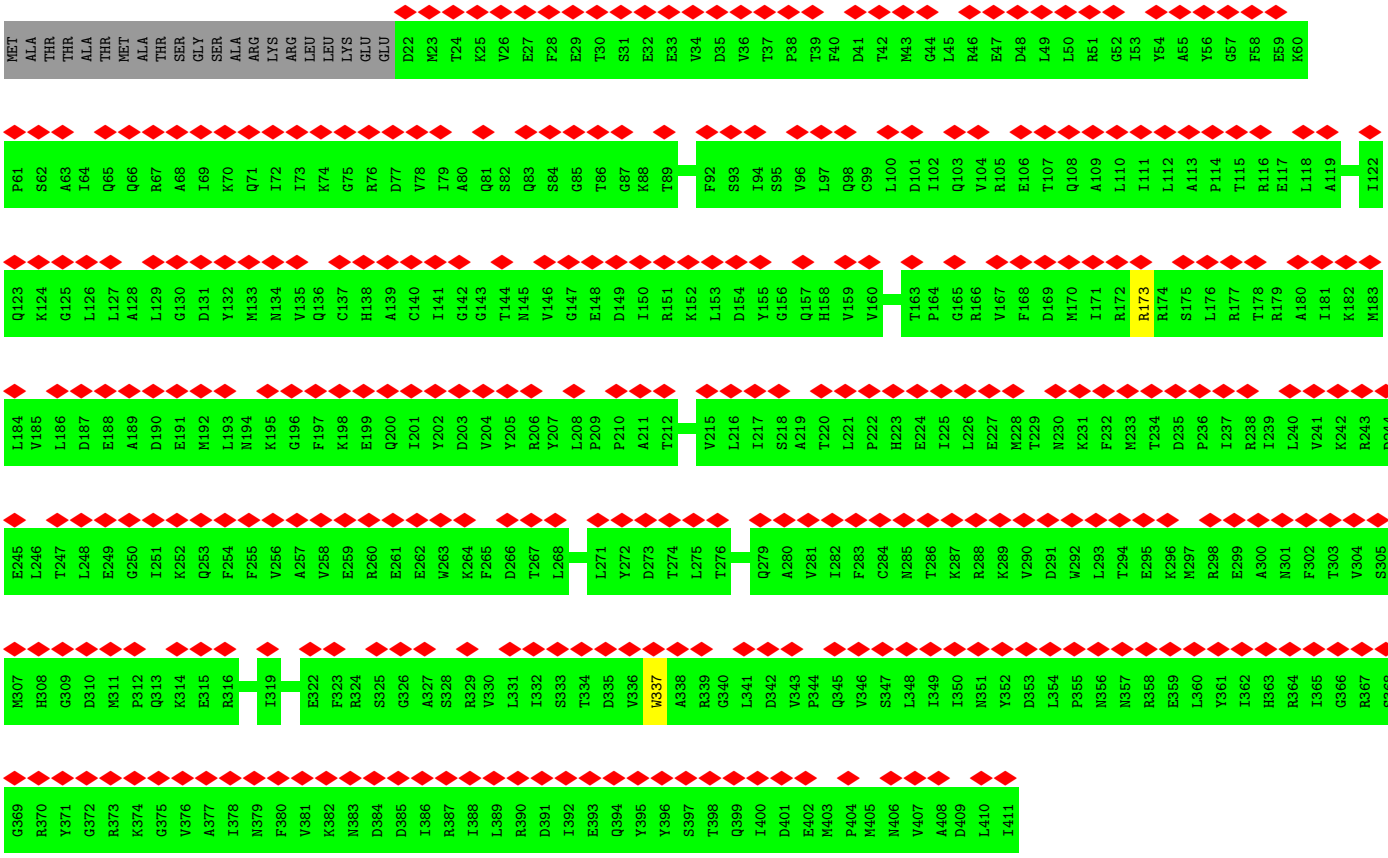




• Molecule 29: Eukaryotic initiation factor 4A-III

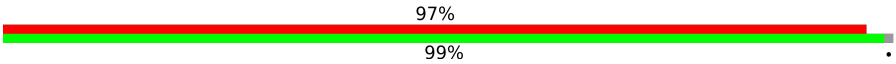
Chain u:

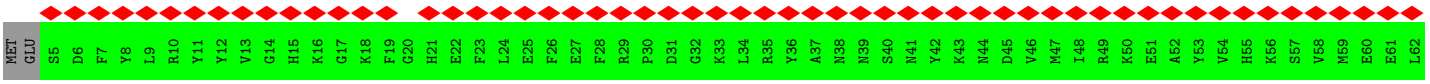


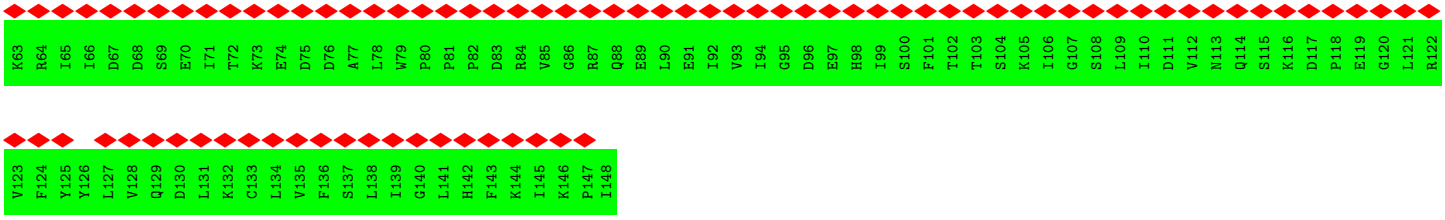


• Molecule 30: Protein mago nashi homolog

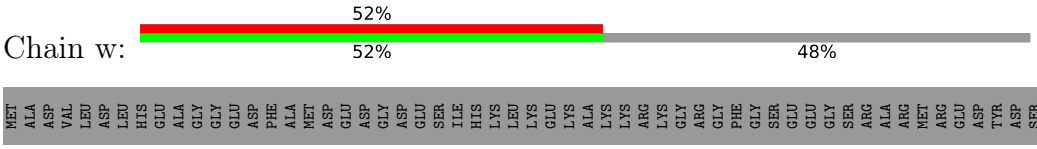
Chain v:



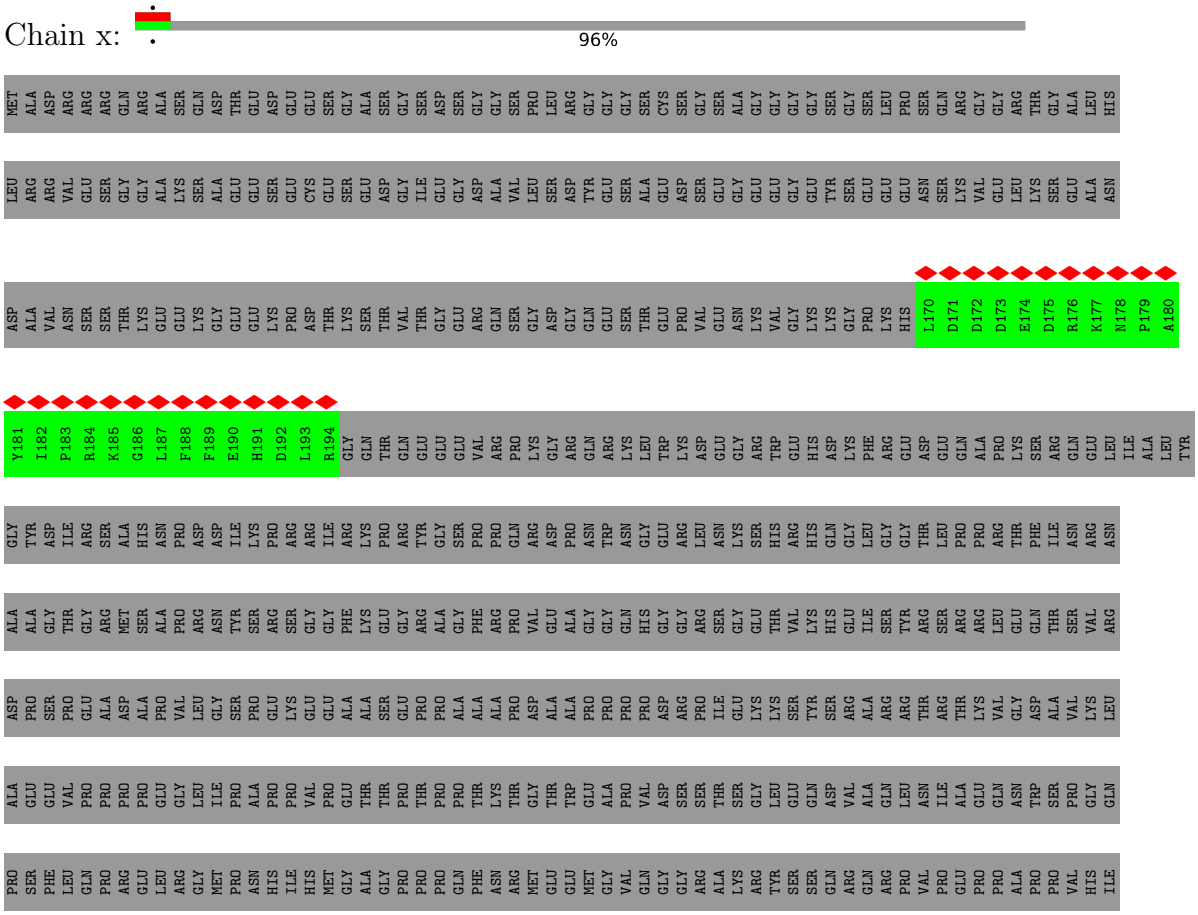


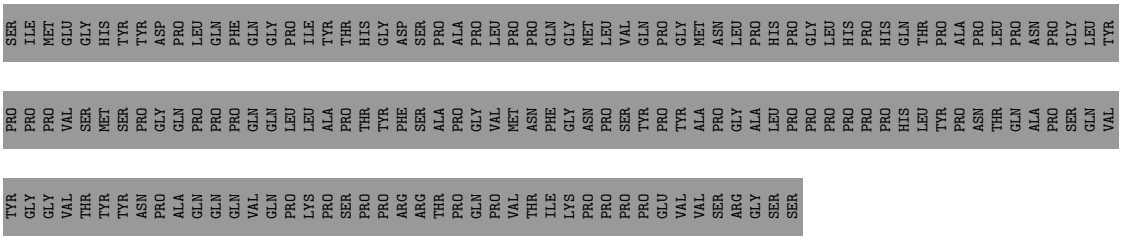


• Molecule 31: RNA-binding protein 8A



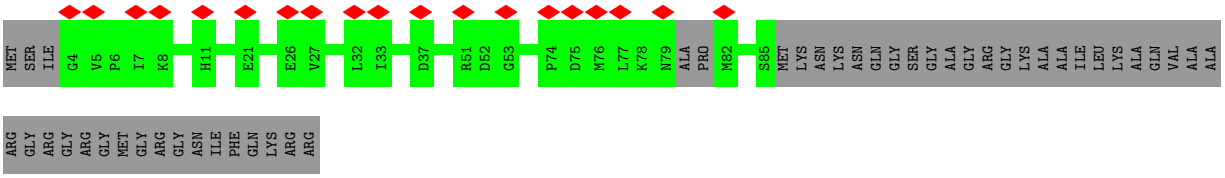
• Molecule 32: Protein CASC3





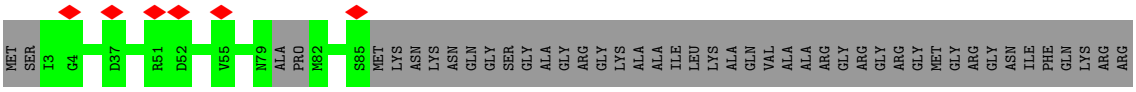
• Molecule 33: Small nuclear ribonucleoprotein Sm D3

Chain h:



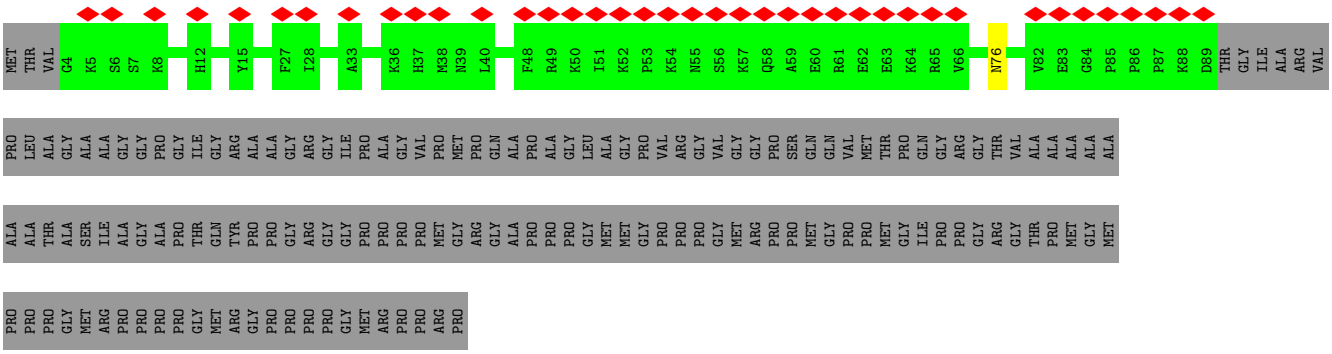
• Molecule 33: Small nuclear ribonucleoprotein Sm D3

Chain g:



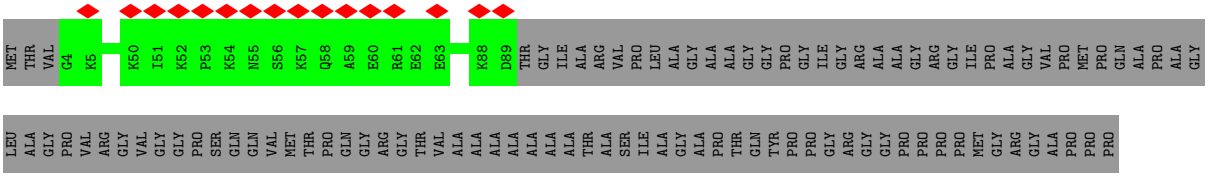
• Molecule 34: Small nuclear ribonucleoprotein-associated proteins B and B'

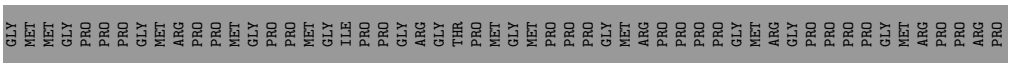
Chain i:



• Molecule 34: Small nuclear ribonucleoprotein-associated proteins B and B'

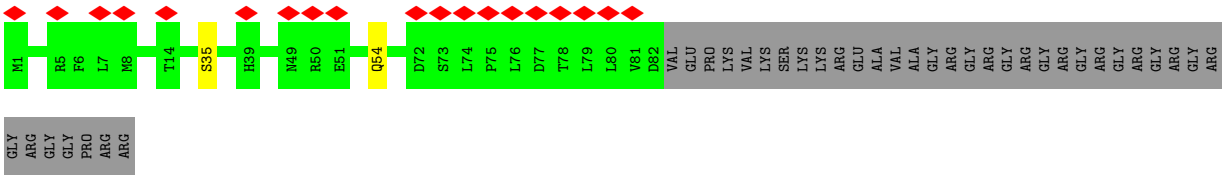
Chain a:





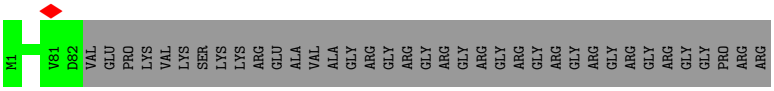
• Molecule 35: Small nuclear ribonucleoprotein Sm D1

Chain j:



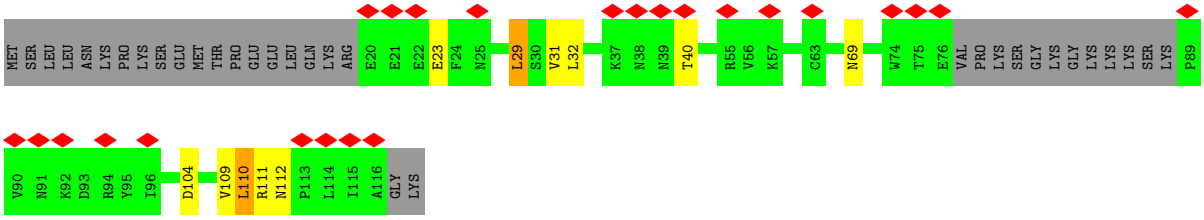
• Molecule 35: Small nuclear ribonucleoprotein Sm D1

Chain b:



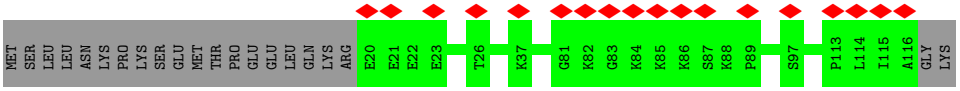
• Molecule 36: Small nuclear ribonucleoprotein Sm D2

Chain k:



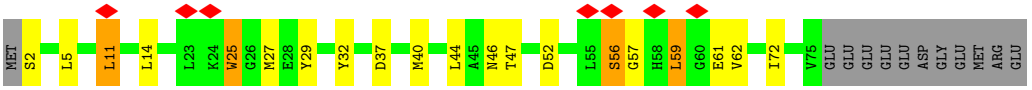
• Molecule 36: Small nuclear ribonucleoprotein Sm D2

Chain c:



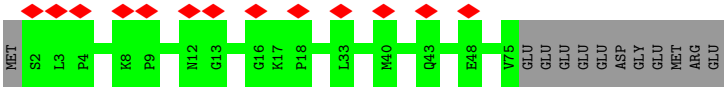
• Molecule 37: Small nuclear ribonucleoprotein F

Chain m:



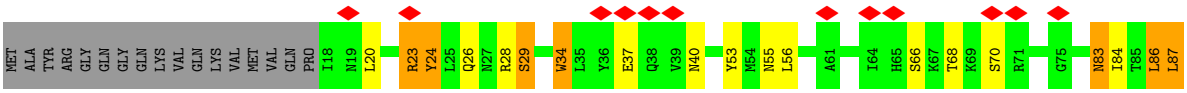
• Molecule 37: Small nuclear ribonucleoprotein F

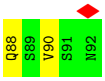
Chain d:



• Molecule 38: Small nuclear ribonucleoprotein E

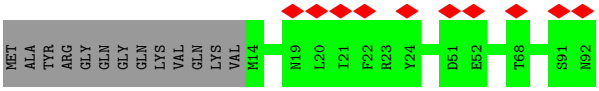
Chain l:





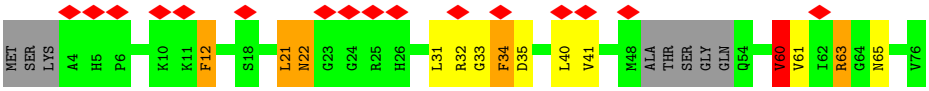
• Molecule 38: Small nuclear ribonucleoprotein E

Chain e:



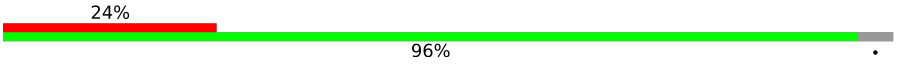
• Molecule 39: Small nuclear ribonucleoprotein G

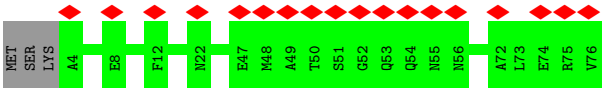
Chain n:



• Molecule 39: Small nuclear ribonucleoprotein G

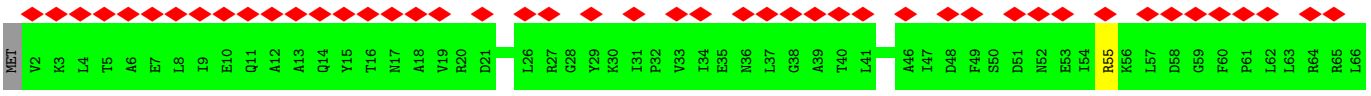
Chain f:

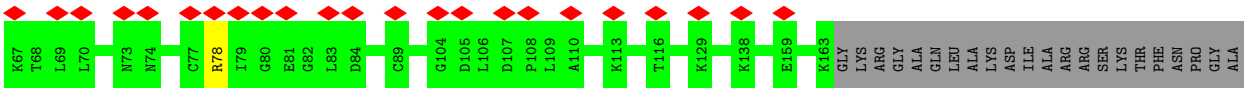




• Molecule 40: U2 small nuclear ribonucleoprotein A'

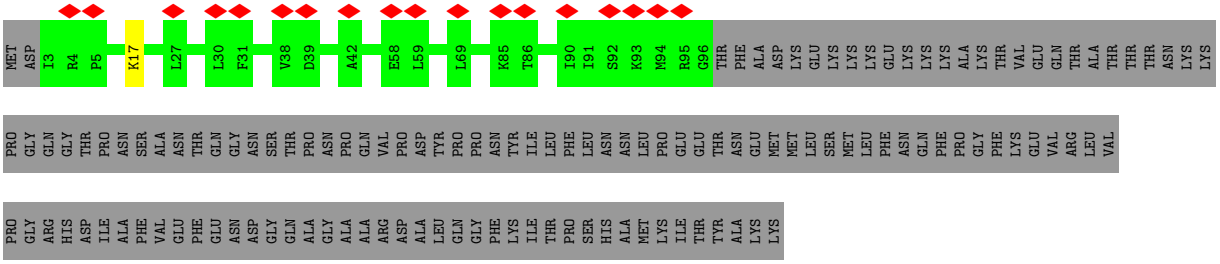
Chain o:





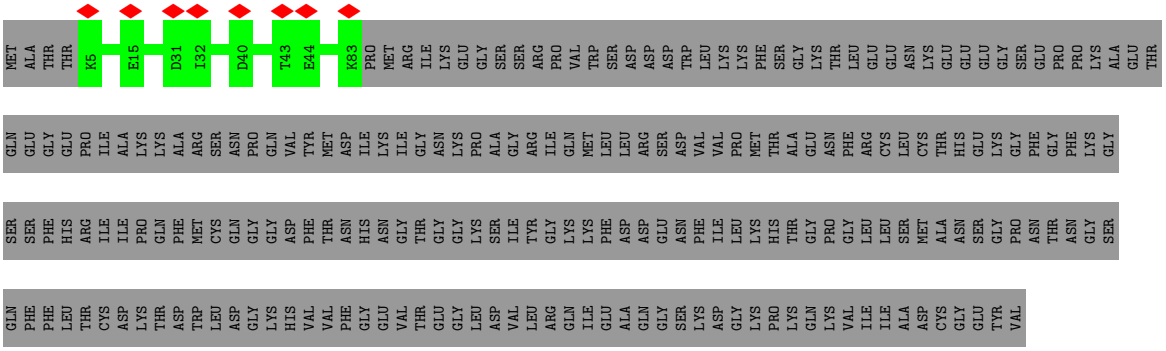
• Molecule 41: U2 small nuclear ribonucleoprotein B"

Chain p:



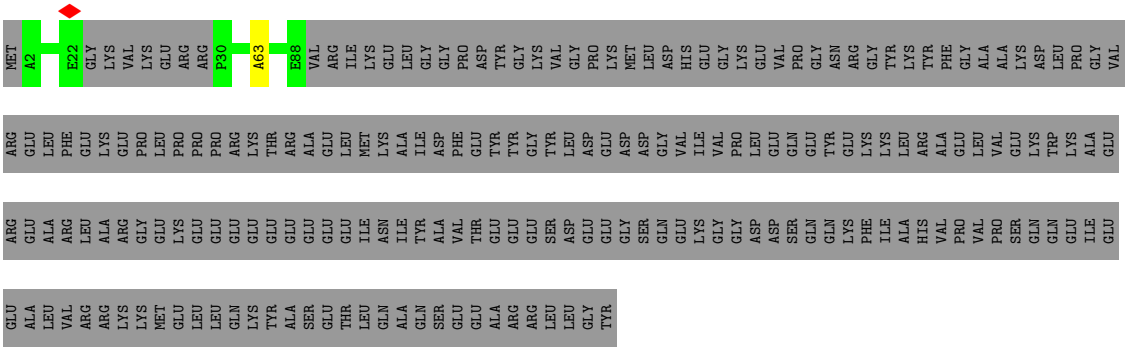
• Molecule 42: Peptidyl-prolyl cis-trans isomerase E

Chain y:



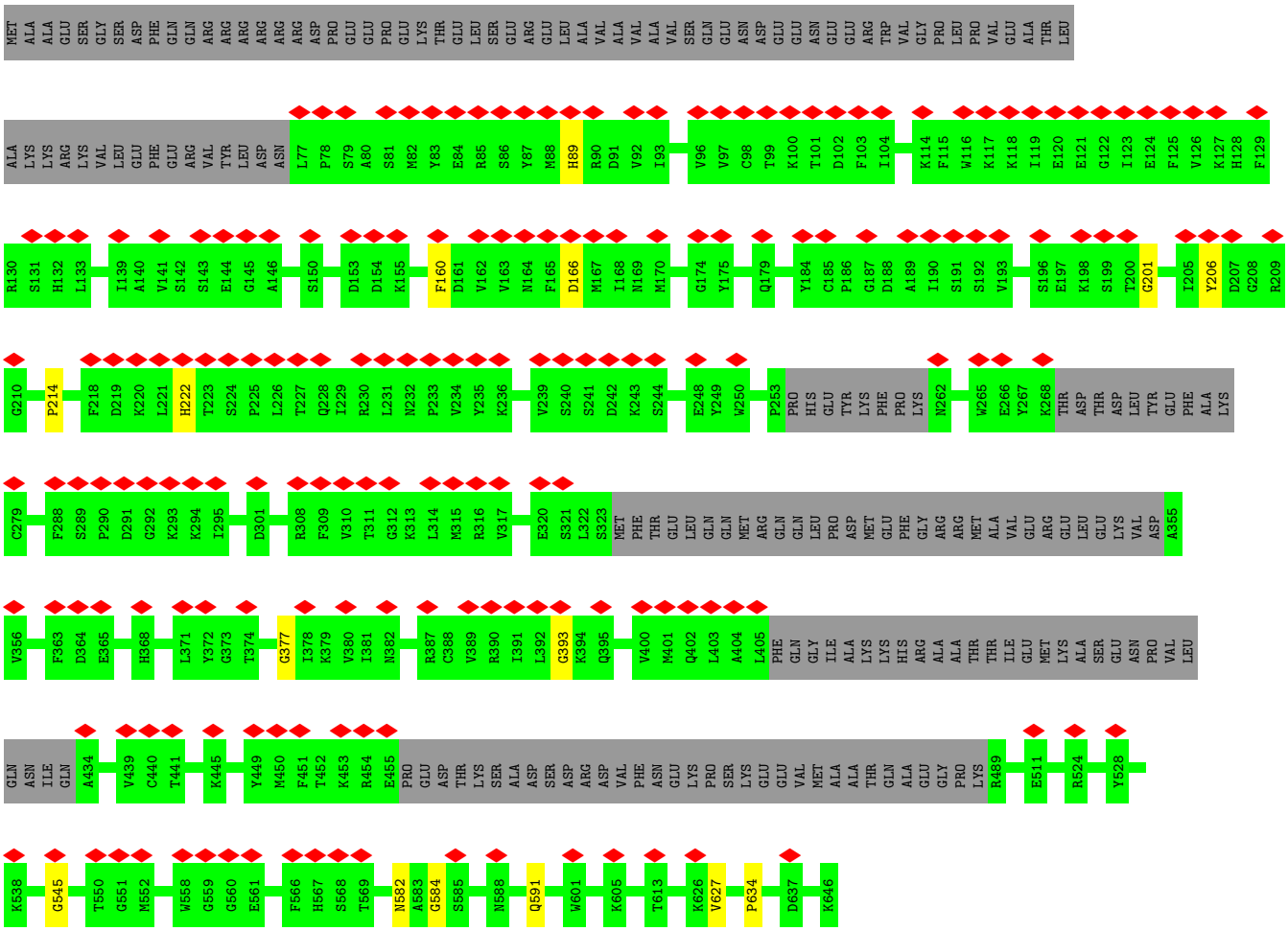
• Molecule 43: Pre-mRNA-splicing factor ISY1 homolog

Chain z:



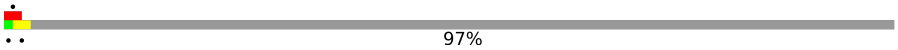
• Molecule 44: Peptidylprolyl isomerase domain and WD repeat-containing protein 1

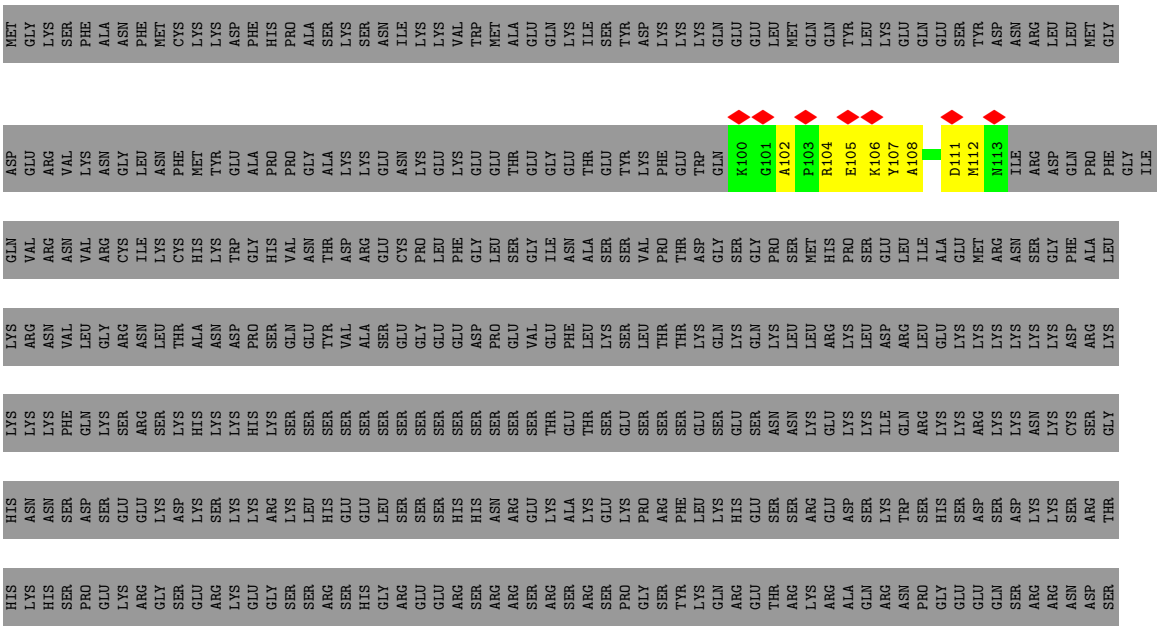
Chain 3:



• Molecule 45: Corepressor interacting with RBPJ 1

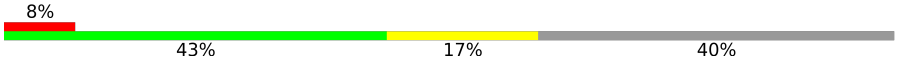
Chain 4:

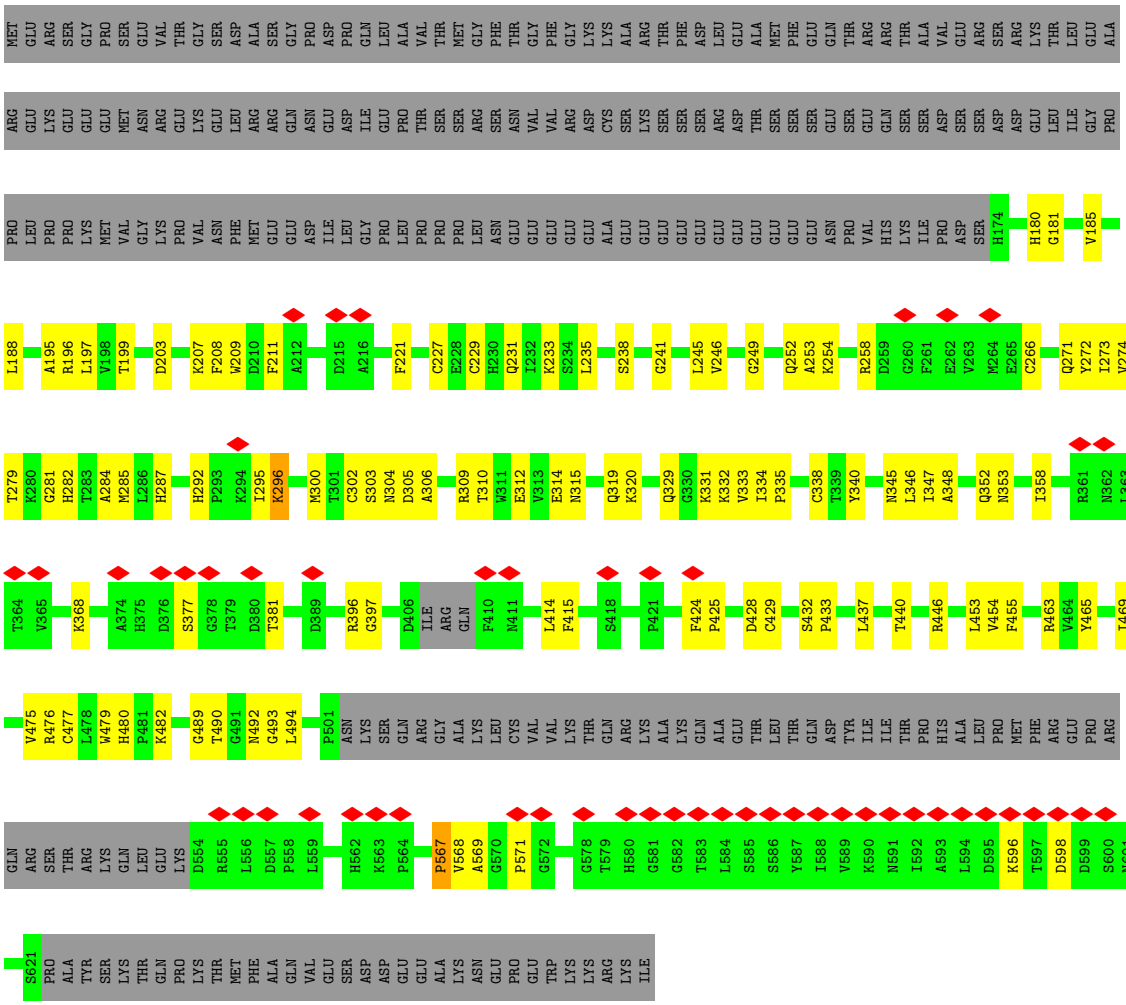




• Molecule 46: WD repeat-containing protein 70

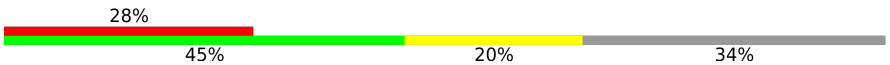
Chain 1:

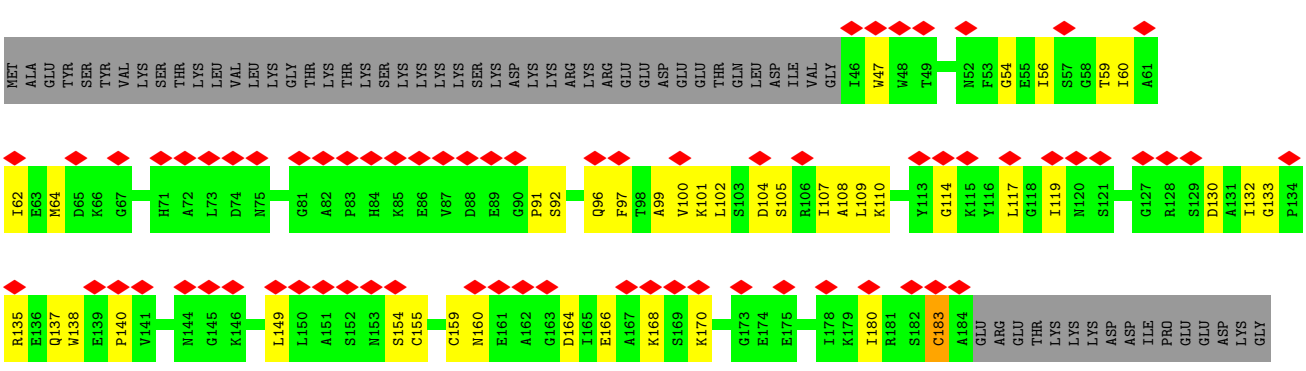


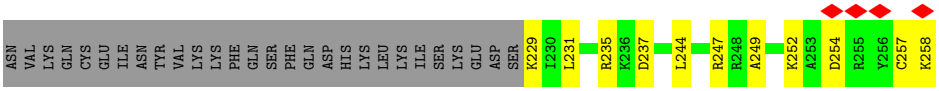


• Molecule 47: Protein FRG1

Chain 2:

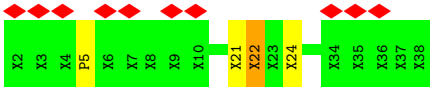






- Molecule 48: UNK

Chain 5:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18223	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	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	2.121	Depositor
Minimum map value	-0.899	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.068	Depositor
Recommended contour level	0.25	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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.76	0/17966	0.67	4/24251 (0.0%)
2	B	1.13	3/2303 (0.1%)	1.23	17/3579 (0.5%)
3	C	0.52	0/6946	0.64	3/9436 (0.0%)
4	D	0.24	0/7628	0.47	0/9528
5	E	0.41	0/2392	0.58	0/3242
6	F	1.27	4/2323 (0.2%)	1.26	7/3619 (0.2%)
7	G	1.13	1/427 (0.2%)	0.96	0/662
8	6	0.83	0/1390	1.27	12/2152 (0.6%)
9	H	0.70	2/3283 (0.1%)	1.08	13/5096 (0.3%)
10	I	0.25	0/3406	0.44	0/4767
11	J	0.58	0/3870	0.57	0/5252
12	K	0.30	0/981	0.50	0/1317
13	L	0.52	0/2914	0.57	0/3929
14	M	0.42	0/791	0.56	0/1058
15	N	0.66	1/1210 (0.1%)	0.65	1/1622 (0.1%)
16	O	0.55	1/2324 (0.0%)	0.60	0/3135
17	P	0.64	0/841	0.62	0/1117
18	R	0.57	0/1976	0.63	0/2651
19	S	0.42	0/1268	0.56	0/1714
20	T	0.94	1/2526 (0.0%)	0.77	0/3443
21	Q	0.24	0/5279	0.46	0/6583
22	U	0.44	0/424	0.54	0/582
23	V	0.33	0/3453	0.50	0/4640
24	W	0.37	0/2651	0.54	0/3647
25	X	0.45	0/486	0.53	0/658
26	Y	0.63	0/1450	0.68	0/1975
27	Z	0.26	0/3723	0.42	0/5180
28	q	0.27	0/929	0.50	0/1260
28	r	0.30	0/912	0.48	0/1239
28	s	0.27	0/267	0.46	0/332
28	t	0.30	0/480	0.48	0/650
29	u	0.30	0/3175	0.51	0/4286

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
30	v	0.29	0/1225	0.51	0/1648
31	w	0.31	0/748	0.51	0/1012
32	x	0.28	0/221	0.48	0/296
33	g	0.24	0/322	0.52	0/399
33	h	0.33	0/627	0.59	0/842
34	a	0.25	0/343	0.54	0/427
34	i	0.29	0/700	0.54	0/933
35	b	0.24	0/327	0.53	0/407
35	j	0.30	0/657	0.56	0/888
36	c	0.23	0/387	0.52	0/482
36	k	0.67	1/696 (0.1%)	1.35	9/935 (1.0%)
37	d	0.25	0/295	0.54	0/367
37	m	0.95	1/588 (0.2%)	1.57	10/795 (1.3%)
38	e	0.23	0/315	0.50	0/392
38	l	2.78	9/628 (1.4%)	1.65	14/842 (1.7%)
39	f	0.24	0/291	0.55	0/362
39	n	1.22	7/539 (1.3%)	1.69	21/718 (2.9%)
40	o	0.29	0/1294	0.54	0/1754
41	p	0.31	0/774	0.50	0/1035
42	y	0.25	0/315	0.51	0/392
43	z	0.32	0/550	0.51	0/736
44	3	0.27	0/2313	0.51	0/3222
45	4	0.61	0/113	0.67	0/148
46	1	0.34	0/2756	0.59	0/3754
47	2	0.34	0/1318	0.53	0/1773
48	5	0.64	0/7	0.76	0/8
All	All	0.61	31/108343 (0.0%)	0.70	111/147169 (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
3	C	0	11
4	D	0	6
5	E	0	1
10	I	0	4
11	J	0	3
12	K	0	1
13	L	0	2

Continued on next page...

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Mol	Chain	#Chirality outliers	#Planarity outliers
14	M	0	1
15	N	0	2
17	P	0	1
18	R	0	5
20	T	0	5
24	W	0	1
25	X	0	1
26	Y	0	3
36	k	0	2
37	m	0	5
38	l	0	3
39	n	0	3
44	3	0	1
46	1	0	2
48	5	0	1
All	All	0	75

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	l	53	TYR	CD2-CE2	33.62	1.89	1.39
38	l	53	TYR	CD1-CE1	31.15	1.86	1.39
38	l	53	TYR	CE2-CZ	25.56	1.71	1.38
38	l	53	TYR	CE1-CZ	24.92	1.71	1.38
38	l	53	TYR	CG-CD1	21.85	1.67	1.39
38	l	53	TYR	CG-CD2	18.05	1.62	1.39
37	m	62	VAL	CB-CG1	-11.39	1.28	1.52
39	n	34	PHE	C-N	8.87	1.54	1.34
39	n	60	VAL	CB-CG1	-8.51	1.34	1.52
38	l	24	TYR	CD2-CE2	-7.59	1.27	1.39
39	n	32	ARG	CB-CG	7.44	1.72	1.52
15	N	101	CYS	CB-SG	-7.34	1.69	1.82
6	F	26	U	O3'-P	6.11	1.68	1.61
7	G	-19	C	C1'-N1	5.99	1.57	1.48
38	l	24	TYR	CD1-CE1	-5.92	1.30	1.39
38	l	34	TRP	CB-CG	-5.81	1.39	1.50
39	n	41	VAL	CB-CG1	-5.72	1.40	1.52
39	n	34	PHE	CB-CG	5.65	1.60	1.51
36	k	110	LEU	CG-CD2	-5.62	1.31	1.51
2	B	26	A	N9-C4	-5.53	1.34	1.37
20	T	357	TRP	CB-CG	-5.47	1.40	1.50
9	H	21	C	N1-C6	-5.38	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	O	84	CYS	CB-SG	-5.37	1.73	1.81
2	B	24	G	N9-C4	-5.29	1.33	1.38
6	F	55	C	N1-C6	-5.21	1.34	1.37
39	n	33	GLY	N-CA	5.17	1.53	1.46
2	B	29	A	N9-C4	-5.16	1.34	1.37
9	H	24	A	N9-C4	-5.13	1.34	1.37
39	n	41	VAL	CB-CG2	5.09	1.63	1.52
6	F	54	G	C5-C4	-5.05	1.34	1.38
6	F	63	C	N1-C6	-5.04	1.34	1.37

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	k	110	LEU	CB-CG-CD2	-25.12	68.30	111.00
37	m	59	LEU	CA-CB-CG	15.66	151.33	115.30
39	n	40	LEU	CA-CB-CG	14.24	148.05	115.30
38	l	86	LEU	CA-CB-CG	13.96	147.40	115.30
38	l	86	LEU	CB-CG-CD1	-12.18	90.29	111.00
37	m	62	VAL	CG1-CB-CG2	-11.91	91.84	110.90
38	l	23	ARG	NE-CZ-NH1	11.72	126.16	120.30
36	k	110	LEU	CA-CB-CG	11.33	141.37	115.30
38	l	86	LEU	CB-CG-CD2	10.67	129.13	111.00
37	m	11	LEU	CA-CB-CG	10.35	139.09	115.30
39	n	34	PHE	C-N-CA	9.94	146.54	121.70
39	n	41	VAL	CG1-CB-CG2	-9.29	96.04	110.90
38	l	20	LEU	CB-CG-CD1	8.81	125.97	111.00
2	B	21	A	O5'-P-OP1	-8.37	98.17	105.70
39	n	60	VAL	CA-CB-CG1	-7.99	98.92	110.90
37	m	29	TYR	CA-CB-CG	7.86	128.33	113.40
39	n	41	VAL	CA-CB-CG2	7.83	122.65	110.90
39	n	21	LEU	CB-CG-CD2	-7.80	97.74	111.00
8	6	2	U	N3-C2-O2	-7.76	116.77	122.20
37	m	11	LEU	CB-CG-CD2	-7.60	98.07	111.00
39	n	31	LEU	CA-CB-CG	7.51	132.57	115.30
37	m	59	LEU	CB-CG-CD2	7.44	123.66	111.00
1	A	1285	LEU	CA-CB-CG	-7.35	98.39	115.30
8	6	82	G	P-O3'-C3'	7.26	128.41	119.70
37	m	44	LEU	CA-CB-CG	7.24	131.96	115.30
2	B	36	C	C2-N1-C1'	7.23	126.76	118.80
38	l	87	LEU	CA-CB-CG	7.21	131.88	115.30
2	B	20	G	O5'-P-OP1	7.15	119.28	110.70
38	l	23	ARG	NE-CZ-NH2	-6.93	116.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	l	20	LEU	CA-CB-CG	-6.71	99.87	115.30
6	F	35	A	N1-C2-N3	6.66	132.63	129.30
36	k	32	LEU	CB-CG-CD2	6.61	122.23	111.00
39	n	32	ARG	CA-C-N	6.58	129.37	116.20
39	n	34	PHE	N-CA-C	6.50	128.55	111.00
37	m	59	LEU	CB-CA-C	-6.45	97.95	110.20
6	F	26	U	P-O3'-C3'	6.42	127.40	119.70
36	k	110	LEU	CD1-CG-CD2	-6.38	91.35	110.50
9	H	98	G	N9-C4-C5	6.38	107.95	105.40
39	n	60	VAL	CB-CA-C	-6.34	99.35	111.40
3	C	343	LEU	CA-CB-CG	-6.34	100.71	115.30
8	6	8	C	C6-N1-C2	-6.33	117.77	120.30
8	6	22	C	C5-C6-N1	6.33	124.16	121.00
8	6	101	U	C5-C6-N1	-6.30	119.55	122.70
2	B	35	U	N3-C2-O2	-6.29	117.80	122.20
2	B	36	C	C6-N1-C1'	-6.26	113.28	120.80
9	H	183	G	N1-C6-O6	6.20	123.62	119.90
2	B	24	G	N3-C4-C5	6.19	131.70	128.60
39	n	35	ASP	CB-CA-C	-6.12	98.16	110.40
8	6	24	G	P-O3'-C3'	6.10	127.03	119.70
36	k	29	LEU	CB-CG-CD1	6.10	121.37	111.00
39	n	21	LEU	CB-CG-CD1	-6.09	100.65	111.00
38	l	53	TYR	CB-CG-CD1	-6.03	117.38	121.00
36	k	110	LEU	CB-CG-CD1	6.01	121.22	111.00
38	l	34	TRP	CA-CB-CG	5.95	125.00	113.70
6	F	33	G	C4-C5-N7	5.90	113.16	110.80
2	B	64	G	C4-N9-C1'	-5.89	118.85	126.50
36	k	109	VAL	CA-CB-CG1	5.88	119.71	110.90
2	B	20	G	C6-C5-N7	-5.85	126.89	130.40
37	m	59	LEU	CD1-CG-CD2	-5.83	93.00	110.50
2	B	35	U	N1-C2-O2	5.76	126.83	122.80
37	m	29	TYR	CB-CG-CD2	5.74	124.44	121.00
39	n	32	ARG	NE-CZ-NH1	5.73	123.17	120.30
2	B	20	G	N3-C4-N9	5.68	129.41	126.00
38	l	26	GLN	C-N-CA	-5.62	107.66	121.70
39	n	31	LEU	CB-CG-CD1	-5.61	101.47	111.00
2	B	101	U	C5-C6-N1	5.59	125.50	122.70
9	H	99	A	O4'-C1'-N9	5.57	112.66	108.20
38	l	56	LEU	CA-CB-CG	5.56	128.08	115.30
9	H	156	U	C5-C6-N1	5.55	125.47	122.70
9	H	98	G	C4-C5-N7	-5.48	108.61	110.80
2	B	68	C	C6-N1-C2	5.47	122.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	6	22	C	C6-N1-C2	-5.47	118.11	120.30
39	n	63	ARG	NE-CZ-NH2	-5.46	117.57	120.30
3	C	474	LEU	CA-CB-CG	5.46	127.85	115.30
2	B	20	G	C5-C6-O6	-5.45	125.33	128.60
38	l	87	LEU	CB-CG-CD2	-5.45	101.74	111.00
36	k	29	LEU	CA-CB-CG	-5.44	102.79	115.30
8	6	24	G	OP1-P-O3'	5.43	117.14	105.20
1	A	1876	LEU	CA-CB-CG	-5.42	102.83	115.30
15	N	40	LYS	C-N-CA	5.42	135.25	121.70
39	n	34	PHE	CB-CA-C	-5.39	99.62	110.40
39	n	60	VAL	N-CA-C	5.37	125.51	111.00
9	H	156	U	C2-N1-C1'	5.36	124.13	117.70
36	k	111	ARG	NE-CZ-NH1	5.36	122.98	120.30
39	n	32	ARG	N-CA-C	5.35	125.43	111.00
1	A	1091	TYR	N-CA-C	-5.34	96.58	111.00
9	H	98	G	N3-C4-N9	-5.31	122.81	126.00
3	C	308	CYS	CA-CB-SG	5.30	123.53	114.00
9	H	183	G	C5-C6-O6	-5.29	125.43	128.60
6	F	33	G	N1-C6-O6	5.28	123.07	119.90
9	H	183	G	C4-C5-N7	5.26	112.90	110.80
8	6	8	C	C5-C6-N1	5.23	123.61	121.00
38	l	28	ARG	CA-CB-CG	5.22	124.89	113.40
2	B	100	C	C5-C6-N1	5.22	123.61	121.00
1	A	578	LEU	CA-CB-CG	-5.21	103.33	115.30
9	H	98	G	C6-C5-N7	5.20	133.52	130.40
9	H	183	G	N9-C4-C5	-5.16	103.33	105.40
39	n	32	ARG	O-C-N	-5.16	114.43	123.20
8	6	16	G	C3'-C2'-C1'	5.12	105.60	101.50
6	F	22	A	O4'-C1'-N9	-5.12	104.11	108.20
39	n	32	ARG	NE-CZ-NH2	-5.12	117.74	120.30
39	n	22	ASN	C-N-CA	-5.07	111.65	122.30
8	6	88	G	N3-C2-N2	-5.07	116.35	119.90
2	B	95	G	C4-N9-C1'	5.04	133.05	126.50
8	6	95	U	C5-C6-N1	-5.03	120.18	122.70
9	H	101	U	O4'-C1'-N1	5.02	112.22	108.20
2	B	20	G	C8-N9-C1'	-5.02	120.47	127.00
9	H	41	U	C5-C6-N1	5.02	125.21	122.70
6	F	59	G	C3'-C2'-C1'	5.01	105.50	101.50
6	F	89	U	C2-N1-C1'	5.01	123.71	117.70
2	B	9	G	C8-N9-C4	5.00	108.40	106.40

There are no chirality outliers.

All (75) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
46	1	567	PRO	Peptide
46	1	598	ASP	Peptide
44	3	89	HIS	Peptide
48	5	22	UNK	Peptide
1	A	1091	TYR	Peptide
1	A	1189	MET	Peptide
1	A	1520	ASN	Peptide
1	A	166	PHE	Peptide
1	A	1763	LEU	Peptide
1	A	1920	TYR	Peptide
1	A	346	ASP	Peptide
1	A	377	GLU	Peptide
1	A	55	ASP	Peptide
1	A	56	ALA	Peptide
1	A	941	LYS	Peptide
3	C	359	LYS	Peptide
3	C	360	ALA	Peptide
3	C	387	ASP	Peptide
3	C	456	GLY	Peptide
3	C	560	VAL	Peptide
3	C	800	PRO	Peptide
3	C	82	GLN	Peptide
3	C	823	ALA	Peptide
3	C	902	HIS	Peptide
3	C	92	PRO	Peptide
3	C	93	ILE	Peptide
4	D	149	ARG	Peptide
4	D	1583	ASP	Peptide
4	D	164	THR	Peptide
4	D	2098	ALA	Peptide
4	D	296	ALA	Peptide
4	D	956	LEU	Peptide
5	E	163	GLY	Peptide
10	I	386	ASP	Peptide
10	I	47	GLY	Peptide
10	I	532	LYS	Peptide
10	I	85	ARG	Peptide
11	J	202	GLU	Peptide
11	J	205	LEU	Peptide
11	J	240	THR	Peptide
12	K	77	GLN	Peptide
13	L	200	LYS	Peptide

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Mol	Chain	Res	Type	Group
13	L	202	ARG	Peptide
14	M	124	PHE	Peptide
15	N	3	LYS	Peptide
15	N	36	PRO	Peptide
17	P	204	GLN	Peptide
18	R	126	ASN	Peptide
18	R	183	GLN	Peptide
18	R	185	GLY	Peptide
18	R	91	ASP	Peptide
18	R	94	GLY	Peptide
20	T	342	GLU	Peptide
20	T	400	PHE	Peptide
20	T	457	GLY	Peptide
20	T	458	SER	Peptide
20	T	494	THR	Peptide
24	W	154	GLY	Peptide
25	X	61	GLY	Peptide
26	Y	19	LYS	Peptide
26	Y	27	LYS	Peptide
26	Y	40	ASN	Peptide
36	k	110	LEU	Peptide
36	k	112	ASN	Peptide
38	l	23	ARG	Peptide
38	l	29	SER	Peptide
38	l	55	ASN	Peptide
37	m	25	TRP	Peptide
37	m	56	SER	Peptide
37	m	57	GLY	Peptide
37	m	59	LEU	Peptide
37	m	61	GLU	Peptide
39	n	12	PHE	Peptide
39	n	21	LEU	Peptide
39	n	60	VAL	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	17519	0	16645	662	0
2	B	2066	0	1047	88	0
3	C	6795	0	6807	349	0
4	D	7632	0	1995	13	0
5	E	2338	0	2275	99	0
6	F	2075	0	1048	113	0
7	G	383	0	200	14	0
8	6	1256	0	637	85	0
9	H	2946	0	1494	106	0
10	I	3387	0	1651	20	0
11	J	3829	0	2907	100	0
12	K	979	0	741	12	0
13	L	2885	0	2427	105	0
14	M	775	0	767	45	0
15	N	1184	0	1189	50	0
16	O	2277	0	2259	130	0
17	P	829	0	814	44	0
18	R	1962	0	2012	121	0
19	S	1236	0	1210	66	0
20	T	2461	0	2420	98	0
21	Q	5288	0	1361	3	0
22	U	422	0	291	10	0
23	V	3410	0	3287	128	0
24	W	2615	0	1751	90	0
25	X	480	0	401	24	0
26	Y	1426	0	1210	70	0
27	Z	3727	0	1676	11	0
28	q	918	0	801	0	0
28	r	901	0	777	0	0
28	s	268	0	65	0	0
28	t	476	0	434	0	0
29	u	3126	0	3167	0	0
30	v	1196	0	1182	0	0
31	w	730	0	690	0	0
32	x	216	0	202	0	0
33	g	324	0	89	0	0
33	h	621	0	623	0	0
34	a	344	0	93	0	0
34	i	690	0	712	0	0
35	b	328	0	89	0	0
35	j	649	0	693	0	0
36	c	388	0	102	0	0
36	k	688	0	709	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	d	296	0	87	0	0
37	m	576	0	589	0	0
38	e	316	0	85	0	0
38	l	621	0	635	0	0
39	f	292	0	83	0	0
39	n	533	0	555	0	0
40	o	1277	0	1297	0	0
41	p	760	0	783	0	0
42	y	316	0	86	0	0
43	z	546	0	454	0	0
44	3	2301	0	1090	7	0
45	4	112	0	109	18	0
46	1	2705	0	2362	90	0
47	2	1296	0	1287	43	0
48	5	184	0	42	4	0
49	A	36	0	6	7	0
50	C	32	0	12	6	0
51	C	1	0	0	0	0
51	F	4	0	0	0	0
52	N	3	0	0	0	0
52	O	3	0	0	0	0
52	Y	1	0	0	0	0
All	All	106256	0	80512	2466	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 18.

All (2466) 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:584:HIS:HE1	49:A:3000:IHP:O26	1.22	1.21
10:I:528:LEU:O	10:I:532:LYS:HA	1.37	1.20
6:F:52:U:HO2'	25:X:2:GLY:N	1.50	1.09
1:A:584:HIS:CE1	49:A:3000:IHP:O26	2.09	1.06
3:C:483:SER:HA	3:C:490:PHE:HB3	1.36	1.03
1:A:1215:ASN:HB3	1:A:1224:ARG:HD2	1.37	1.00
8:6:85:G:H1	9:H:44:U:H3	1.00	0.98
1:A:1463:LYS:NZ	8:6:105:C:OP2	1.98	0.96
10:I:528:LEU:O	10:I:532:LYS:CA	2.14	0.96
6:F:39:A:H61	8:6:8:C:H42	1.12	0.95
14:M:153:ARG:HA	14:M:160:PHE:HE2	1.30	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:38:G:H2'	6:F:39:A:C8	2.04	0.93
3:C:300:LEU:HA	3:C:306:ASN:HD22	1.31	0.93
14:M:165:ASN:HB2	18:R:95:LYS:HA	1.47	0.93
18:R:126:ASN:HD22	18:R:128:ASP:H	0.98	0.92
16:O:26:THR:OG1	16:O:159:ARG:NH2	2.03	0.92
8:6:21:A:N6	16:O:91:GLY:O	2.02	0.92
9:H:150:U:H3	9:H:181:G:H1	1.19	0.91
18:R:106:GLN:HE22	18:R:225:PRO:HD2	1.35	0.91
1:A:1253:SER:HG	9:H:34:U:HO2'	1.07	0.90
15:N:40:LYS:O	15:N:41:ARG:HG3	1.70	0.90
16:O:84:CYS:SG	16:O:159:ARG:NH2	2.45	0.90
1:A:329:LEU:HD23	3:C:177:ARG:HE	1.37	0.90
3:C:387:ASP:O	3:C:389:ASP:N	2.05	0.89
6:F:17:C:H2'	6:F:18:A:H8	1.36	0.89
5:E:72:CYS:N	5:E:332:GLU:OE1	2.05	0.89
3:C:130:ARG:HD3	3:C:438:ILE:HB	1.55	0.88
20:T:399:LYS:HG3	20:T:406:ILE:HD11	1.56	0.88
6:F:26:U:C5	16:O:65:PHE:HD2	1.92	0.88
1:A:1503:TRP:HZ3	1:A:1533:ARG:HE	1.18	0.87
19:S:84:ASP:OD1	19:S:108:ASN:ND2	2.07	0.87
16:O:71:CYS:SG	16:O:73:THR:OG1	2.32	0.87
2:B:64:G:H2'	2:B:65:G:C8	2.09	0.87
3:C:452:THR:HB	3:C:577:PHE:HD2	1.40	0.87
1:A:778:ARG:NH1	9:H:23:A:OP1	2.08	0.86
1:A:1749:LYS:NZ	8:6:91:A:OP1	2.07	0.86
3:C:673:LYS:HG3	3:C:686:THR:HG23	1.56	0.86
13:L:191:LEU:HD22	13:L:196:ILE:HD11	1.57	0.86
2:B:64:G:H2'	2:B:65:G:H8	1.42	0.85
7:G:-2:C:H3'	7:G:-1:G:H5"	1.56	0.85
1:A:1963:GLU:HB3	1:A:1965:HIS:HD2	1.41	0.85
8:6:87:U:O2	9:H:42:G:N2	2.09	0.84
48:5:22:UNK:O	48:5:24:UNK:N	2.11	0.84
1:A:1258:LYS:HG3	1:A:1527:ASN:HD21	1.43	0.84
5:E:260:ARG:NH1	5:E:273:CYS:SG	2.51	0.84
1:A:211:GLN:OE1	1:A:214:ARG:NH1	2.11	0.84
3:C:772:TRP:NE1	3:C:776:GLU:OE2	2.11	0.84
8:6:7:G:H2'	8:6:8:C:H6	1.43	0.83
1:A:1776:ILE:HB	1:A:1858:PRO:HA	1.59	0.83
20:T:250:ARG:NH1	20:T:266:GLU:OE1	2.12	0.83
8:6:7:G:H2'	8:6:8:C:C6	2.14	0.83
12:K:165:TRP:HA	12:K:168:LYS:HD2	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:236:VAL:HG22	16:O:300:VAL:HG22	1.61	0.83
6:F:26:U:H5	16:O:65:PHE:CD2	1.97	0.82
16:O:234:LEU:O	16:O:271:PHE:HA	1.80	0.82
3:C:76:GLU:OE1	3:C:76:GLU:N	2.10	0.82
47:2:160:ASN:HD21	47:2:164:ASP:HB2	1.43	0.82
13:L:161:ASN:ND2	13:L:163:GLN:O	2.13	0.81
14:M:153:ARG:HA	14:M:160:PHE:CE2	2.13	0.81
16:O:30:GLU:O	18:R:190:SER:OG	1.98	0.81
5:E:155:ASN:ND2	5:E:196:VAL:O	2.13	0.81
1:A:663:ARG:NH1	6:F:64:U:OP2	2.12	0.81
1:A:1993:LYS:HG3	1:A:1994:LYS:HD2	1.61	0.81
3:C:448:LYS:O	3:C:452:THR:OG1	1.99	0.81
13:L:172:ARG:HA	13:L:175:GLN:HE21	1.44	0.81
1:A:1180:LYS:HA	1:A:1201:ARG:HH12	1.46	0.81
16:O:133:PRO:HG2	16:O:137:LEU:HB2	1.63	0.81
1:A:1183:PRO:HB3	1:A:1201:ARG:HE	1.44	0.80
10:I:621:ARG:O	10:I:625:PRO:HD2	1.82	0.80
15:N:139:CYS:SG	15:N:140:ARG:N	2.55	0.80
19:S:13:ASN:HA	19:S:25:LEU:O	1.82	0.80
1:A:1211:ASP:OD2	1:A:1369:TYR:OH	1.99	0.80
13:L:149:LEU:HA	13:L:152:LEU:HD12	1.64	0.80
1:A:1330:MET:HG3	1:A:1367:ASN:HD21	1.47	0.80
1:A:1887:SER:OG	1:A:1889:LEU:O	1.99	0.80
6:F:26:U:H5	16:O:65:PHE:HD2	1.25	0.80
16:O:262:THR:HB	16:O:271:PHE:HB2	1.64	0.80
17:P:52:GLU:OE1	17:P:55:ARG:NH2	2.13	0.80
9:H:13:C:H41	14:M:200:ARG:HH12	1.30	0.79
1:A:150:MET:SD	1:A:153:ARG:NH2	2.56	0.79
1:A:1678:ARG:HH21	47:2:249:ALA:HA	1.47	0.79
11:J:360:ASP:HA	11:J:363:ARG:HE	1.47	0.79
3:C:87:GLN:HE22	20:T:239:LYS:HD3	1.46	0.79
3:C:224:GLY:HA3	3:C:438:ILE:HD12	1.64	0.79
1:A:79:ARG:HH11	1:A:82:ARG:HE	1.30	0.79
23:V:169:LEU:HD11	23:V:184:GLU:HG3	1.65	0.79
3:C:453:TYR:CZ	3:C:575:GLN:HB2	2.18	0.79
1:A:79:ARG:NH1	1:A:82:ARG:HE	1.81	0.79
26:Y:68:TYR:HE2	26:Y:94:GLU:HB2	1.48	0.79
1:A:1783:THR:HA	45:4:106:LYS:HE2	1.65	0.78
3:C:507:VAL:HG11	3:C:565:ILE:HG23	1.65	0.78
24:W:162:ASN:HB3	24:W:165:LEU:HD23	1.64	0.78
44:3:201:GLY:HA3	44:3:222:HIS:HA	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:213:GLU:CD	20:T:215:GLY:H	1.86	0.78
20:T:267:ASP:HB3	20:T:269:GLN:HG2	1.66	0.78
9:H:75:A:H61	9:H:77:C:H42	1.32	0.78
1:A:1533:ARG:NH1	1:A:1752:GLN:OE1	2.17	0.78
6:F:39:A:H61	8:6:8:C:N4	1.82	0.78
46:1:490:THR:HG23	46:1:492:ASN:H	1.48	0.77
2:B:46:U:O4	2:B:47:A:N6	2.17	0.77
1:A:1160:ARG:NH1	17:P:189:ASP:OD2	2.16	0.77
23:V:631:PHE:HA	23:V:634:ILE:HG22	1.67	0.77
1:A:663:ARG:NH2	6:F:65:G:N7	2.32	0.77
16:O:243:ILE:HG12	16:O:294:ASN:HD22	1.48	0.77
1:A:1072:LEU:HD22	1:A:1087:LEU:HD22	1.65	0.77
1:A:1310:ARG:NH2	1:A:1563:HIS:O	2.17	0.77
3:C:183:SER:N	3:C:214:GLU:OE1	2.11	0.77
1:A:2005:SER:OG	1:A:2006:GLU:OE2	2.01	0.77
1:A:1831:LYS:HE2	1:A:1832:ARG:HG3	1.66	0.76
8:6:87:U:H3	9:H:42:G:H1	1.24	0.76
19:S:75:ALA:O	19:S:110:SER:OG	2.04	0.76
1:A:1890:GLN:O	45:4:104:ARG:NH2	2.19	0.76
1:A:623:LYS:O	49:A:3000:IHP:O44	2.01	0.76
23:V:294:ILE:HD13	23:V:335:MET:HB3	1.67	0.76
3:C:715:GLY:HA2	3:C:729:ALA:HB1	1.66	0.76
1:A:1863:VAL:HG21	1:A:1868:MET:HB2	1.68	0.76
2:B:12:U:H3	2:B:65:G:H1	1.34	0.76
16:O:276:THR:HG23	16:O:279:ALA:H	1.50	0.76
1:A:300:ASN:O	3:C:939:ARG:NH2	2.19	0.75
1:A:570:ASP:OD1	1:A:571:ALA:N	2.18	0.75
1:A:978:GLU:OE1	1:A:1096:HIS:ND1	2.20	0.75
13:L:36:SER:OG	13:L:158:ARG:NH2	2.19	0.75
19:S:102:ASN:ND2	19:S:104:GLY:O	2.19	0.75
44:3:377:GLY:HA2	44:3:393:GLY:HA2	1.69	0.75
3:C:677:GLU:HA	3:C:683:ASN:O	1.86	0.75
6:F:29:A:N6	8:6:16:G:O2'	2.20	0.75
6:F:58:G:H2'	6:F:59:G:C8	2.20	0.75
9:H:3:C:H2'	9:H:4:G:H8	1.51	0.75
3:C:619:THR:HG22	3:C:629:ILE:HG12	1.69	0.75
3:C:680:ASN:HB3	3:C:807:GLN:HG3	1.68	0.74
3:C:69:ALA:HA	20:T:456:PRO:HG3	1.68	0.74
44:3:206:TYR:HA	44:3:214:PRO:HD2	1.69	0.74
1:A:41:GLN:NE2	1:A:44:ARG:HD3	2.03	0.74
1:A:312:TYR:OH	3:C:886:ASP:OD2	2.05	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:TYR:O	3:C:645:ARG:NH1	2.21	0.74
3:C:678:THR:OG1	3:C:680:ASN:O	2.05	0.74
11:J:325:ASN:HB2	14:M:172:HIS:HD2	1.51	0.74
19:S:15:TYR:HB2	19:S:163:TYR:HB2	1.69	0.74
8:6:8:C:H2'	8:6:9:C:C6	2.23	0.74
23:V:221:ILE:HB	23:V:359:LEU:HD11	1.69	0.74
1:A:184:ASP:OD1	15:N:1:MET:N	2.19	0.74
3:C:682:LYS:HB3	3:C:797:ALA:HB2	1.69	0.74
3:C:707:ILE:HD11	3:C:735:PHE:HB2	1.69	0.74
9:H:84:C:H2'	9:H:85:A:H8	1.52	0.74
11:J:188:GLN:HE22	13:L:140:ASP:H	1.33	0.73
23:V:236:ARG:NH2	23:V:379:GLU:O	2.20	0.73
25:X:34:ARG:HA	25:X:37:ILE:HD12	1.71	0.73
1:A:523:ASN:OD1	1:A:552:ARG:NH2	2.21	0.73
3:C:779:LEU:HD11	3:C:825:PRO:HB2	1.69	0.73
11:J:185:ALA:HA	13:L:142:ILE:HD13	1.70	0.73
19:S:57:ILE:HD13	24:W:97:ASN:HB3	1.69	0.73
3:C:700:ILE:O	3:C:740:THR:OG1	2.06	0.73
1:A:1076:ASP:OD1	1:A:1077:ILE:N	2.22	0.73
3:C:779:LEU:HB3	3:C:934:MET:HE1	1.68	0.73
1:A:396:ASP:OD1	1:A:397:ASN:N	2.22	0.73
3:C:133:THR:HG23	3:C:225:VAL:HG23	1.71	0.73
2:B:97:G:H1	2:B:116:U:H3	1.37	0.73
23:V:189:ASN:ND2	23:V:395:GLU:OE2	2.22	0.72
11:J:188:GLN:HE21	13:L:13:ASN:HD22	1.37	0.72
23:V:503:TYR:HB2	23:V:546:ASN:HA	1.71	0.72
6:F:49:G:N7	13:L:33:ARG:HG3	2.04	0.72
16:O:45:CYS:SG	16:O:48:CYS:N	2.61	0.72
1:A:1588:SER:OG	1:A:1737:ASN:ND2	2.19	0.72
46:1:469:ILE:HG12	46:1:470:THR:HG23	1.72	0.72
1:A:1434:LYS:O	1:A:1439:ARG:NH2	2.13	0.72
13:L:52:GLU:OE2	13:L:134:THR:OG1	2.07	0.72
20:T:188:PRO:HG3	20:T:443:THR:HG21	1.71	0.72
1:A:417:ARG:NH2	2:B:58:U:O3'	2.20	0.72
26:Y:39:PHE:HE2	26:Y:98:TYR:HB2	1.54	0.72
23:V:637:GLY:O	23:V:644:ARG:NH2	2.23	0.71
13:L:134:THR:HB	13:L:135:LYS:NZ	2.04	0.71
16:O:131:THR:HG22	24:W:108:ARG:HH21	1.55	0.71
16:O:240:GLY:HA3	16:O:296:ARG:HH22	1.56	0.71
6:F:39:A:N6	8:6:8:C:H42	1.85	0.71
1:A:1998:ASN:O	1:A:2001:SER:OG	2.09	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:ARG:NH2	6:F:70:A:OP2	2.23	0.71
1:A:1972:THR:N	1:A:1975:GLU:OE1	2.17	0.71
3:C:774:THR:HA	3:C:784:ILE:HD12	1.71	0.71
5:E:219:VAL:HB	5:E:229:TYR:HB2	1.72	0.71
26:Y:68:TYR:HD1	26:Y:69:LEU:H	1.37	0.71
9:H:33:G:N7	25:X:9:LYS:NZ	2.39	0.71
18:R:126:ASN:ND2	18:R:128:ASP:H	1.82	0.71
3:C:300:LEU:HA	3:C:306:ASN:ND2	2.06	0.71
4:D:668:ASP:O	4:D:672:GLY:N	2.23	0.71
18:R:311:LYS:HG2	18:R:315:LYS:HE2	1.72	0.70
1:A:158:ARG:NH2	1:A:570:ASP:OD2	2.24	0.70
22:U:1:MET:SD	22:U:1:MET:N	2.63	0.70
46:1:196:ARG:HH21	46:1:221:PHE:HE2	1.40	0.70
3:C:471:ASP:H	3:C:499:GLY:HA2	1.57	0.70
4:D:956:LEU:O	4:D:958:HIS:N	2.25	0.70
23:V:166:ILE:O	23:V:170:ILE:HG12	1.92	0.70
5:E:60:MET:HB2	5:E:353:MET:HB2	1.73	0.70
23:V:341:ALA:HA	23:V:344:LYS:HE3	1.74	0.70
46:1:425:PRO:HG2	46:1:475:VAL:HG12	1.73	0.70
2:B:100:C:H2'	2:B:101:U:C6	2.27	0.70
6:F:41:A:H2'	6:F:42:C:C6	2.27	0.70
1:A:362:ARG:HD2	23:V:333:GLN:HE22	1.57	0.69
11:J:441:ASP:OD1	11:J:445:LYS:NZ	2.25	0.69
46:1:180:HIS:HB2	46:1:207:LYS:HG3	1.72	0.69
1:A:833:LYS:HE3	1:A:834:HIS:CE1	2.27	0.69
5:E:289:LEU:HD21	5:E:304:SER:HA	1.74	0.69
16:O:27:CYS:SG	16:O:83:THR:OG1	2.50	0.69
19:S:58:LYS:HE2	19:S:144:MET:HG2	1.74	0.69
19:S:90:LEU:HB3	19:S:128:ILE:HB	1.73	0.69
46:1:602:PRO:HA	46:1:605:ALA:HB3	1.75	0.69
1:A:267:LYS:NZ	2:B:49:A:OP1	2.19	0.69
1:A:469:LYS:NZ	2:B:59:G:N7	2.37	0.69
1:A:792:HIS:HE1	18:R:279:HIS:HE1	1.39	0.69
1:A:1963:GLU:HB3	1:A:1965:HIS:CD2	2.27	0.69
23:V:323:LEU:HG	23:V:324:HIS:CD2	2.27	0.69
46:1:333:VAL:HG11	46:1:353:ASN:HB2	1.73	0.69
1:A:305:ARG:HA	1:A:305:ARG:HH11	1.56	0.69
8:6:22:C:O2'	8:6:23:U:OP1	2.10	0.69
14:M:178:GLU:HA	14:M:181:ARG:HD3	1.74	0.69
1:A:1020:LYS:NZ	9:H:26:A:OP1	2.25	0.69
1:A:1276:GLU:OE2	1:A:1375:TRP:N	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:G:H2'	2:B:99:C:C6	2.28	0.69
3:C:706:GLN:HE22	3:C:708:THR:HB	1.56	0.69
3:C:561:LYS:NZ	3:C:611:ASN:O	2.23	0.69
6:F:27:A:OP1	15:N:41:ARG:NH2	2.26	0.69
18:R:306:ALA:O	18:R:310:ARG:HG3	1.92	0.69
25:X:13:HIS:NE2	25:X:15:GLN:HB2	2.08	0.69
46:1:282:HIS:ND1	46:1:303:SER:OG	2.24	0.69
8:6:104:C:OP1	8:6:104:C:H4'	1.93	0.69
3:C:852:ARG:NH2	7:G:-12:G:OP1	2.27	0.68
1:A:982:GLU:HG3	1:A:1169:GLN:HG3	1.75	0.68
1:A:1678:ARG:NH2	47:2:252:LYS:O	2.23	0.68
3:C:230:ASP:HB3	3:C:233:GLU:HB2	1.73	0.68
12:K:188:LEU:HG	13:L:777:GLN:HB3	1.75	0.68
1:A:338:VAL:O	3:C:266:GLU:HG2	1.92	0.68
1:A:189:GLU:OE2	1:A:190:ALA:N	2.27	0.68
2:B:17:U:H3	2:B:60:G:H1	1.40	0.68
11:J:342:GLU:OE2	11:J:344:GLN:N	2.20	0.68
3:C:663:CYS:HB2	3:C:828:MET:HB2	1.75	0.68
1:A:1382:SER:OG	1:A:1416:ILE:N	2.23	0.68
1:A:1405:LEU:HG	1:A:1423:PHE:CE2	2.29	0.68
13:L:146:GLU:OE1	13:L:146:GLU:N	2.26	0.68
24:W:146:HIS:ND1	24:W:146:HIS:O	2.27	0.68
11:J:192:GLU:CD	11:J:192:GLU:H	1.97	0.68
1:A:419:ARG:NH2	1:A:423:ASP:O	2.26	0.67
1:A:1957:ASP:HB3	1:A:1960:THR:HG23	1.75	0.67
7:G:-11:G:OP1	22:U:21:ARG:NE	2.27	0.67
1:A:82:ARG:NH1	8:6:16:G:O6	2.28	0.67
1:A:283:VAL:HG22	1:A:284:ARG:HG3	1.77	0.67
3:C:236:MET:O	3:C:239:THR:OG1	2.11	0.67
3:C:452:THR:HB	3:C:577:PHE:CD2	2.28	0.67
23:V:565:LEU:HD22	23:V:608:LEU:HD13	1.77	0.67
1:A:762:ARG:HH12	17:P:226:LYS:HZ1	1.43	0.67
1:A:67:ARG:HD3	1:A:179:ALA:HB2	1.76	0.67
1:A:171:ASP:OD1	1:A:521:ASN:ND2	2.25	0.67
11:J:311:GLN:HG3	14:M:131:GLN:HG2	1.77	0.67
13:L:188:ARG:HE	13:L:191:LEU:HD12	1.60	0.67
1:A:1275:ARG:NH1	1:A:1373:GLN:O	2.27	0.67
47:2:231:LEU:HD23	47:2:247:ARG:HH21	1.59	0.67
3:C:470:PRO:HB3	3:C:500:THR:HG23	1.77	0.67
6:F:17:C:H2'	6:F:18:A:C8	2.25	0.67
1:A:1948:ASP:HB2	1:A:1949:ARG:HH21	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:60:U:O2'	46:1:258:ARG:NH1	2.28	0.66
24:W:121:ASN:OD1	24:W:123:PHE:N	2.28	0.66
3:C:68:THR:OG1	3:C:71:GLU:HB3	1.94	0.66
23:V:265:ASN:HD22	23:V:352:ILE:HG23	1.60	0.66
1:A:381:PRO:O	1:A:383:PHE:N	2.28	0.66
3:C:624:SER:HB2	3:C:626:GLU:HG2	1.77	0.66
13:L:30:GLN:OE1	13:L:33:ARG:NE	2.29	0.66
16:O:292:ILE:HG12	16:O:297:ARG:HA	1.77	0.66
1:A:369:GLU:OE2	1:A:369:GLU:N	2.28	0.66
1:A:1407:ASP:OD2	1:A:1407:ASP:N	2.23	0.66
6:F:52:U:O2'	25:X:2:GLY:N	2.26	0.66
16:O:185:LYS:HD2	16:O:186:PRO:HD2	1.78	0.66
16:O:235:TYR:HD2	16:O:301:LYS:HB2	1.60	0.66
1:A:1762:TYR:HB3	1:A:1888:GLU:HB2	1.76	0.66
9:H:84:C:H2'	9:H:85:A:C8	2.31	0.66
1:A:1424:GLN:NE2	1:A:1459:ARG:O	2.24	0.66
3:C:853:ARG:NH2	3:C:886:ASP:OD2	2.24	0.66
9:H:89:U:H2'	9:H:90:A:H8	1.61	0.66
26:Y:39:PHE:CE2	26:Y:98:TYR:HB2	2.31	0.66
2:B:99:C:H2'	2:B:100:C:C6	2.31	0.66
3:C:219:LEU:HD12	3:C:245:HIS:CE1	2.30	0.66
9:H:3:C:H2'	9:H:4:G:C8	2.31	0.66
16:O:177:GLU:OE1	16:O:177:GLU:N	2.28	0.66
1:A:460:LYS:NZ	2:B:49:A:OP2	2.29	0.66
18:R:126:ASN:HD22	18:R:128:ASP:N	1.83	0.66
1:A:853:LYS:HE2	8:6:101:U:C5	2.31	0.65
13:L:153:SER:HA	13:L:156:ARG:HD2	1.78	0.65
20:T:210:ILE:HG12	20:T:221:THR:HG22	1.78	0.65
4:D:149:ARG:O	4:D:151:LYS:N	2.30	0.65
1:A:1764:SER:O	1:A:1767:ASN:N	2.28	0.65
1:A:384:VAL:HG12	3:C:331:PHE:CD2	2.31	0.65
1:A:802:THR:HB	1:A:805:GLU:HG3	1.78	0.65
3:C:137:HIS:HB2	3:C:239:THR:HG23	1.79	0.65
9:H:153:A:H2'	9:H:154:C:H5'	1.77	0.65
1:A:1180:LYS:NZ	1:A:1181:ASP:OD2	2.27	0.65
1:A:1352:HIS:CE1	22:U:21:ARG:HG3	2.32	0.65
1:A:1361:GLU:HB2	1:A:1363:GLN:HG2	1.79	0.65
1:A:682:ASP:OD1	1:A:746:LYS:NZ	2.27	0.65
3:C:667:VAL:H	3:C:824:THR:HG23	1.61	0.65
18:R:229:VAL:HG23	18:R:230:MET:H	1.61	0.65
20:T:455:GLN:HG3	20:T:485:THR:HG21	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:GLU:OE1	1:A:64:GLU:N	2.21	0.65
1:A:71:ARG:NH1	1:A:177:ASP:OD2	2.30	0.65
46:1:329:GLN:HE21	46:1:331:LYS:HD3	1.62	0.65
1:A:468:LYS:HD3	1:A:469:LYS:H	1.62	0.65
1:A:799:PRO:HD3	18:R:284:PHE:CD1	2.32	0.65
20:T:345:ILE:HB	20:T:357:TRP:HB2	1.78	0.65
25:X:30:HIS:HA	25:X:33:GLU:OE2	1.97	0.65
8:6:73:G:O2'	8:6:74:G:O5'	2.15	0.65
11:J:311:GLN:OE1	11:J:311:GLN:N	2.25	0.65
47:2:108:ALA:HB2	47:2:132:ILE:HD13	1.79	0.65
13:L:188:ARG:O	13:L:192:ARG:HG2	1.97	0.64
10:I:564:PHE:O	10:I:569:GLY:N	2.29	0.64
11:J:436:TYR:HD1	11:J:437:LYS:HD2	1.61	0.64
17:P:42:LYS:NZ	20:T:276:GLU:HG3	2.12	0.64
1:A:1853:PRO:HG2	47:2:101:LYS:NZ	2.12	0.64
3:C:241:ARG:HH21	3:C:584:THR:HG22	1.61	0.64
9:H:25:G:H2'	9:H:26:A:H8	1.63	0.64
17:P:43:TYR:O	17:P:45:GLN:NE2	2.30	0.64
17:P:204:GLN:O	17:P:206:LYS:N	2.23	0.64
46:1:472:ALA:O	46:1:490:THR:OG1	2.15	0.64
5:E:158:TYR:HB3	5:E:168:CYS:SG	2.37	0.64
18:R:241:GLU:N	18:R:241:GLU:OE1	2.30	0.64
23:V:225:LYS:HG2	23:V:405:ILE:HG12	1.79	0.64
26:Y:38:PRO:HG2	26:Y:39:PHE:CD2	2.32	0.64
2:B:65:G:H2'	2:B:66:A:H8	1.62	0.64
1:A:469:LYS:NZ	2:B:59:G:O6	2.27	0.64
8:6:12:G:H2'	8:6:13:C:C6	2.32	0.64
20:T:347:THR:HG22	20:T:357:TRP:HE1	1.62	0.64
46:1:567:PRO:O	46:1:569:ALA:N	2.27	0.64
3:C:396:LEU:HA	3:C:399:LEU:HD12	1.79	0.64
3:C:670:SER:HA	3:C:823:ALA:HB3	1.78	0.64
3:C:676:ALA:O	3:C:684:LYS:HA	1.98	0.64
8:6:73:G:O2'	8:6:74:G:O4'	2.11	0.64
1:A:1892:PRO:HB3	45:4:104:ARG:HD2	1.80	0.64
11:J:201:ARG:NH2	46:1:596:LYS:O	2.31	0.64
16:O:224:ASP:O	16:O:302:TRP:NE1	2.31	0.64
46:1:480:HIS:HD2	46:1:482:LYS:H	1.46	0.64
1:A:351:TYR:HA	3:C:270:PRO:HG3	1.79	0.63
1:A:462:ARG:HA	1:A:462:ARG:CZ	2.27	0.63
1:A:1761:PRO:O	1:A:1885:LYS:NZ	2.25	0.63
6:F:22:A:H5"	15:N:116:ASN:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:22:ILE:HG23	24:W:112:SER:HB2	1.80	0.63
1:A:40:LEU:O	1:A:44:ARG:HG2	1.97	0.63
1:A:380:LEU:O	3:C:354:ARG:NE	2.25	0.63
16:O:133:PRO:HD2	16:O:137:LEU:HD22	1.80	0.63
1:A:548:ARG:NH1	1:A:549:GLU:OE2	2.32	0.63
1:A:1644:LEU:HD23	1:A:1715:TYR:HD1	1.64	0.63
9:H:114:A:H61	9:H:142:C:H42	1.47	0.63
13:L:74:LEU:HD23	13:L:77:LEU:HD12	1.78	0.63
1:A:47:GLU:O	1:A:50:LYS:HG3	1.98	0.63
6:F:22:A:C6	24:W:130:ARG:HG2	2.33	0.63
8:6:2:U:O4	26:Y:4:ARG:NH2	2.32	0.63
18:R:106:GLN:HG2	18:R:110:LYS:HD2	1.81	0.63
18:R:281:ASN:OD1	18:R:282:GLU:N	2.32	0.63
1:A:1410:ASP:O	1:A:1414:ARG:NH1	2.32	0.63
13:L:717:MET:O	13:L:721:LEU:HB3	1.99	0.63
19:S:102:ASN:OD1	19:S:108:ASN:ND2	2.32	0.63
20:T:213:GLU:OE2	20:T:215:GLY:N	2.30	0.63
1:A:1199:LYS:NZ	1:A:1206:GLU:OE2	2.28	0.63
1:A:1779:PHE:CE1	1:A:1891:LEU:HD12	2.34	0.63
20:T:405:PHE:CG	20:T:405:PHE:O	2.52	0.63
46:1:346:LEU:HD12	46:1:358:ILE:HG22	1.81	0.63
1:A:488:ASP:OD1	1:A:489:TRP:N	2.32	0.63
6:F:42:C:H2'	6:F:43:A:O4'	1.98	0.63
6:F:51:U:OP1	26:Y:54:LYS:HA	1.98	0.63
20:T:339:GLN:NE2	20:T:342:GLU:O	2.31	0.63
1:A:1159:ASN:ND2	17:P:196:ASN:OD1	2.32	0.62
6:F:22:A:OP1	15:N:115:THR:OG1	2.17	0.62
18:R:73:PRO:HB3	19:S:131:ARG:HH22	1.64	0.62
20:T:351:ASP:O	20:T:352:THR:OG1	2.15	0.62
23:V:264:ILE:HG13	23:V:274:CYS:SG	2.39	0.62
1:A:435:CYS:HB2	7:G:-11:G:H22	1.65	0.62
6:F:85:U:H5'	6:F:86:U:C5	2.34	0.62
18:R:125:MET:O	18:R:126:ASN:HB2	1.99	0.62
19:S:57:ILE:HD12	19:S:61:MET:HG3	1.81	0.62
1:A:912:GLU:HG3	1:A:913:PRO:HD2	1.81	0.62
3:C:489:GLN:O	3:C:489:GLN:NE2	2.32	0.62
24:W:137:TYR:HE2	24:W:164:GLY:HA2	1.63	0.62
19:S:44:ARG:HB2	19:S:164:PRO:HG3	1.81	0.62
20:T:432:ASP:OD1	20:T:433:ASN:N	2.33	0.62
1:A:850:TYR:OH	1:A:863:GLU:OE1	2.09	0.62
3:C:731:SER:HB2	3:C:747:ASP:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:ARG:O	1:A:618:THR:OG1	2.13	0.62
1:A:835:ASP:OD1	1:A:836:THR:N	2.33	0.62
3:C:186:VAL:HG22	3:C:535:ALA:HA	1.82	0.62
5:E:322:LYS:NZ	24:W:147:GLN:OE1	2.32	0.62
6:F:39:A:H2'	6:F:40:U:O4'	2.00	0.62
1:A:369:GLU:O	1:A:371:LEU:N	2.28	0.62
13:L:178:GLU:HA	13:L:181:ARG:HG2	1.80	0.62
46:1:208:PHE:HB3	46:1:221:PHE:HD2	1.65	0.62
1:A:108:MET:O	1:A:110:TRP:N	2.32	0.62
1:A:792:HIS:CE1	18:R:279:HIS:HE1	2.16	0.62
1:A:1941:ARG:NH2	1:A:2011:ILE:O	2.32	0.62
3:C:589:LYS:HE3	3:C:628:VAL:HG11	1.81	0.62
8:6:91:A:H2'	8:6:92:U:O4'	1.99	0.62
11:J:361:ARG:HD3	14:M:161:PHE:CD2	2.35	0.62
16:O:197:ASN:OD1	16:O:198:ILE:N	2.33	0.62
22:U:18:TYR:CE2	22:U:20:GLN:HB2	2.34	0.62
25:X:5:ASP:OD1	25:X:7:ASN:N	2.27	0.62
25:X:6:LEU:HD22	26:Y:55:LYS:HE2	1.82	0.62
47:2:102:LEU:HD11	47:2:132:ILE:HG12	1.81	0.62
1:A:855:ARG:HG3	9:H:29:A:C2	2.35	0.62
1:A:1018:ASN:ND2	1:A:1023:ASN:OD1	2.31	0.62
3:C:679:PRO:HD2	3:C:807:GLN:HB3	1.80	0.62
5:E:251:LEU:HD21	5:E:300:ILE:HG23	1.81	0.62
6:F:30:A:H61	8:6:16:G:H1'	1.64	0.62
15:N:2:PRO:HG2	15:N:4:VAL:HA	1.82	0.62
26:Y:108:PHE:HD1	26:Y:109:GLN:H	1.48	0.62
26:Y:63:VAL:HG22	26:Y:73:ILE:O	2.00	0.62
45:4:102:ALA:H	45:4:107:TYR:HD2	1.48	0.62
45:4:112:MET:N	45:4:112:MET:SD	2.72	0.62
1:A:608:LEU:HD13	1:A:632:ALA:HB1	1.81	0.61
5:E:265:ARG:HH11	5:E:267:PHE:H	1.46	0.61
7:G:-5:G:O2'	7:G:-4:A:H5"	1.99	0.61
11:J:216:ASP:HB3	11:J:217:GLU:OE1	2.00	0.61
13:L:13:ASN:ND2	13:L:139:PRO:HA	2.15	0.61
20:T:459:LEU:HB3	20:T:462:GLU:HG3	1.81	0.61
1:A:1173:SER:OG	1:A:1174:PHE:N	2.31	0.61
1:A:1624:SER:OG	1:A:1625:SER:N	2.33	0.61
10:I:386:ASP:O	10:I:388:PHE:N	2.34	0.61
2:B:99:C:H2'	2:B:100:C:H6	1.64	0.61
3:C:474:LEU:HD12	3:C:500:THR:O	2.00	0.61
23:V:260:VAL:O	23:V:264:ILE:HG12	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:216:THR:HG22	3:C:245:HIS:CE1	2.36	0.61
18:R:189:ASN:HD21	18:R:195:ARG:HG3	1.65	0.61
19:S:14:VAL:HG13	19:S:25:LEU:HD13	1.81	0.61
1:A:1233:ASP:OD1	1:A:1235:GLU:N	2.32	0.61
1:A:1456:THR:OG1	1:A:1457:HIS:N	2.33	0.61
13:L:213:GLU:OE2	16:O:110:SER:N	2.33	0.61
1:A:1381:ASP:OD2	1:A:1384:ARG:NH2	2.33	0.61
3:C:510:LEU:HB2	3:C:564:THR:OG1	2.01	0.61
4:D:150:ASP:C	4:D:152:GLU:H	2.04	0.61
8:6:6:A:H2'	8:6:7:G:O4'	2.01	0.61
24:W:285:SER:O	24:W:287:HIS:N	2.30	0.61
1:A:1234:ASP:OD2	1:A:1234:ASP:N	2.32	0.61
1:A:1602:ASP:OD1	1:A:1603:ALA:N	2.32	0.61
3:C:799:GLU:O	3:C:801:LEU:N	2.32	0.61
11:J:188:GLN:NE2	13:L:13:ASN:HD22	1.99	0.61
19:S:39:PHE:HD1	19:S:48:TYR:HH	1.49	0.61
3:C:476:CYS:HB3	3:C:565:ILE:HB	1.82	0.61
9:H:155:C:C2	9:H:176:G:N2	2.69	0.61
47:2:59:THR:HB	47:2:183:CYS:SG	2.41	0.61
3:C:842:CYS:O	3:C:846:VAL:HG23	2.01	0.61
18:R:192:ALA:HB2	24:W:153:ILE:HD13	1.82	0.61
1:A:1410:ASP:OD2	1:A:1411:SER:N	2.34	0.61
1:A:1532:ARG:HB3	1:A:1532:ARG:CZ	2.30	0.61
5:E:206:ASP:O	5:E:222:LEU:HG	2.00	0.61
5:E:239:THR:HB	5:E:289:LEU:H	1.66	0.61
9:H:106:G:H4'	9:H:107:A:O4'	2.01	0.61
23:V:294:ILE:O	23:V:298:LYS:HG2	2.01	0.61
1:A:1162:PRO:HG3	17:P:194:PHE:CZ	2.35	0.60
3:C:86:THR:OG1	3:C:87:GLN:N	2.34	0.60
15:N:54:HIS:CE1	15:N:92:TRP:HZ2	2.18	0.60
18:R:185:GLY:O	18:R:187:ALA:N	2.34	0.60
23:V:449:GLU:HB3	23:V:452:LEU:HB2	1.82	0.60
1:A:985:TYR:HB2	1:A:986:GLU:OE1	2.01	0.60
1:A:1783:THR:HG21	1:A:1894:GLN:HG3	1.83	0.60
1:A:1889:LEU:HD23	1:A:1890:GLN:N	2.15	0.60
8:6:26:U:H3'	16:O:235:TYR:OH	2.01	0.60
13:L:204:ARG:HE	13:L:207:GLY:HA3	1.66	0.60
16:O:259:ARG:HD2	16:O:273:GLN:HG2	1.83	0.60
26:Y:40:ASN:OD1	26:Y:107:ASN:HB2	2.00	0.60
1:A:1765:SER:HA	1:A:1768:TYR:HB3	1.83	0.60
12:K:150:GLN:HA	12:K:153:LEU:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:66:GLU:HG2	18:R:67:ILE:HD13	1.83	0.60
12:K:35:LEU:O	12:K:38:GLU:HG3	2.02	0.60
23:V:277:MET:HG2	23:V:372:LEU:HD22	1.83	0.60
23:V:600:ASN:HA	23:V:639:LEU:HD21	1.83	0.60
1:A:359:ILE:HB	23:V:324:HIS:CE1	2.36	0.60
19:S:125:LYS:HE3	19:S:126:HIS:NE2	2.16	0.60
24:W:97:ASN:ND2	24:W:97:ASN:O	2.33	0.60
26:Y:101:GLU:HB3	26:Y:102:HIS:CD2	2.36	0.60
1:A:1531:ASN:ND2	9:H:35:A:OP1	2.35	0.60
3:C:490:PHE:CZ	3:C:612:LYS:HD2	2.37	0.60
5:E:236:ASP:HB3	5:E:255:MET:HB2	1.84	0.60
16:O:88:LEU:O	18:R:183:GLN:NE2	2.34	0.60
18:R:74:LEU:HB2	19:S:136:ILE:HG12	1.82	0.60
20:T:349:SER:OG	20:T:351:ASP:OD1	2.18	0.60
1:A:712:HIS:CD2	18:R:250:CYS:HB2	2.37	0.60
19:S:60:PHE:CD2	19:S:61:MET:HG2	2.36	0.60
46:1:292:HIS:HB2	46:1:340:TYR:CZ	2.37	0.60
1:A:367:SER:O	1:A:369:GLU:N	2.34	0.60
2:B:27:U:O2'	2:B:28:A:O5'	2.19	0.60
6:F:22:A:C5	24:W:130:ARG:HG2	2.35	0.60
9:H:101:U:H5"	9:H:102:U:H5'	1.84	0.60
11:J:191:ALA:O	11:J:194:LEU:N	2.35	0.60
11:J:252:GLU:OE2	11:J:260:ARG:HB3	2.01	0.60
23:V:279:THR:O	23:V:283:GLU:HG3	2.02	0.60
1:A:1014:ASN:HD21	13:L:84:THR:H	1.48	0.60
3:C:446:LYS:HB3	3:C:447:PRO:HD3	1.84	0.60
16:O:106:ASP:OD1	16:O:107:MET:N	2.29	0.60
1:A:934:ARG:HH22	27:Z:393:VAL:CB	2.15	0.60
5:E:346:SER:OG	5:E:348:ASP:OD1	2.20	0.60
6:F:15:A:H2'	6:F:16:G:H8	1.65	0.60
10:I:406:GLU:HA	10:I:410:GLN:HA	1.83	0.60
3:C:463:GLU:OE1	3:C:463:GLU:N	2.34	0.59
3:C:474:LEU:HD23	3:C:474:LEU:O	2.01	0.59
6:F:26:U:C5	16:O:65:PHE:CD2	2.77	0.59
18:R:132:LEU:HD12	20:T:384:HIS:HB3	1.83	0.59
18:R:147:THR:HG23	20:T:360:VAL:HG12	1.84	0.59
26:Y:40:ASN:HA	26:Y:50:ILE:O	2.02	0.59
1:A:41:GLN:HE22	1:A:44:ARG:HD3	1.67	0.59
3:C:250:ARG:HE	3:C:451:HIS:CD2	2.19	0.59
1:A:700:GLY:HA3	18:R:237:MET:HB2	1.84	0.59
19:S:77:ILE:HG13	19:S:78:TYR:HD1	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:GLU:OE1	1:A:47:GLU:N	2.28	0.59
1:A:428:LYS:HA	1:A:431:TYR:CE2	2.37	0.59
19:S:11:PRO:O	19:S:29:TRP:NE1	2.35	0.59
27:Z:1091:VAL:HA	27:Z:1097:MET:O	2.02	0.59
46:1:249:GLY:HA2	46:1:285:MET:HG3	1.84	0.59
2:B:29:A:H2'	2:B:30:A:H8	1.68	0.59
6:F:40:U:H3	8:6:7:G:H1	1.50	0.59
1:A:385:GLU:HB3	1:A:389:LYS:HD2	1.84	0.59
8:6:12:G:H2'	8:6:13:C:C5	2.37	0.59
9:H:45:C:H2'	9:H:46:U:C6	2.38	0.59
16:O:233:THR:HA	16:O:272:ILE:O	2.02	0.59
20:T:185:MET:HB3	20:T:186:PRO:HD3	1.85	0.59
1:A:1330:MET:HG3	1:A:1367:ASN:ND2	2.15	0.59
1:A:1649:LYS:HB2	47:2:237:ASP:O	2.02	0.59
8:6:13:C:H2'	8:6:14:A:C8	2.38	0.59
16:O:196:GLN:HE21	16:O:208:PRO:HG2	1.66	0.59
3:C:241:ARG:NH2	3:C:584:THR:HG22	2.17	0.59
5:E:243:LEU:HD12	5:E:249:TYR:O	2.02	0.59
44:3:627:VAL:HA	44:3:634:PRO:HA	1.83	0.59
1:A:76:MET:HE1	1:A:88:TYR:CG	2.37	0.59
1:A:1212:GLY:HA3	1:A:1280:ASN:ND2	2.18	0.59
9:H:172:C:H2'	9:H:173:C:H6	1.68	0.59
20:T:257:ARG:NH1	20:T:301:ASP:OD1	2.35	0.59
26:Y:16:ASP:OD1	26:Y:18:SER:N	2.36	0.59
1:A:1762:TYR:O	1:A:1764:SER:N	2.36	0.59
1:A:1889:LEU:HD23	1:A:1890:GLN:H	1.66	0.59
5:E:75:HIS:CE1	5:E:121:GLY:HA3	2.38	0.59
13:L:134:THR:HB	13:L:135:LYS:HZ1	1.67	0.59
18:R:178:ARG:HD3	18:R:194:GLN:HE22	1.68	0.59
26:Y:35:LEU:O	26:Y:55:LYS:HA	2.03	0.59
3:C:216:THR:HG22	3:C:245:HIS:HE1	1.68	0.58
6:F:88:G:H4'	14:M:121:ASP:HB2	1.84	0.58
12:K:17:PRO:HG3	12:K:167:ARG:HH12	1.68	0.58
16:O:89:GLU:OE1	24:W:103:GLN:HB2	2.03	0.58
23:V:575:THR:O	23:V:580:ARG:NH1	2.36	0.58
46:1:282:HIS:CE1	46:1:309:ARG:HD3	2.38	0.58
1:A:188:LEU:HD22	1:A:567:GLY:HA2	1.84	0.58
1:A:1251:SER:O	1:A:1298:ARG:NH2	2.36	0.58
6:F:45:A:H2	26:Y:57:ASN:HD21	1.50	0.58
8:6:21:A:O2'	16:O:216:ARG:NH1	2.36	0.58
11:J:323:LEU:HD13	14:M:174:PRO:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:179:ILE:O	14:M:183:VAL:HG23	2.03	0.58
19:S:50:GLY:N	19:S:159:ILE:O	2.29	0.58
20:T:404:SER:OG	20:T:405:PHE:N	2.32	0.58
46:1:303:SER:OG	46:1:305:ASP:OD1	2.15	0.58
1:A:246:LEU:HD22	1:A:408:PRO:HG2	1.84	0.58
1:A:435:CYS:HB2	7:G:-11:G:N2	2.18	0.58
1:A:1831:LYS:HZ3	1:A:1832:ARG:H	1.51	0.58
3:C:66:TYR:HB3	20:T:456:PRO:O	2.04	0.58
3:C:556:ASP:O	3:C:559:ILE:HG13	2.03	0.58
9:H:112:G:H2'	9:H:113:G:H8	1.68	0.58
13:L:132:PRO:HD2	13:L:133:GLU:OE1	2.02	0.58
16:O:84:CYS:HB3	16:O:86:LEU:HG	1.86	0.58
1:A:1393:ARG:HH11	1:A:1397:ILE:HD11	1.67	0.58
1:A:193:LEU:HD12	1:A:194:GLU:H	1.68	0.58
1:A:1292:GLU:OE2	1:A:1331:GLY:N	2.31	0.58
18:R:151:LEU:O	18:R:155:VAL:HG23	2.04	0.58
9:H:13:C:H41	14:M:200:ARG:NH1	1.98	0.58
18:R:113:TYR:OH	20:T:402:ASP:OD1	2.22	0.58
46:1:347:ILE:O	46:1:358:ILE:HA	2.03	0.58
16:O:144:SER:HA	16:O:148:LEU:HD13	1.85	0.58
16:O:236:VAL:O	16:O:269:CYS:HA	2.04	0.58
3:C:213:ASP:O	3:C:216:THR:OG1	2.11	0.58
6:F:11:C:HO2'	6:F:12:G:H8	1.52	0.58
20:T:457:GLY:O	20:T:458:SER:HB3	2.02	0.58
2:B:97:G:H2'	2:B:98:G:C8	2.38	0.58
7:G:-8:U:H2'	7:G:-7:C:O4'	2.04	0.58
1:A:354:PRO:HG3	23:V:343:ARG:CZ	2.34	0.58
5:E:233:GLY:O	5:E:260:ARG:NH2	2.37	0.58
17:P:229:LYS:O	17:P:229:LYS:NZ	2.32	0.58
19:S:90:LEU:C	19:S:128:ILE:HD12	2.24	0.58
1:A:1633:ALA:HB2	1:A:1637:TRP:CE3	2.39	0.57
3:C:144:CYS:SG	3:C:312:SER:OG	2.60	0.57
9:H:32:U:O5'	25:X:17:LEU:HD12	2.04	0.57
9:H:172:C:H2'	9:H:173:C:C6	2.39	0.57
13:L:223:GLY:HA2	18:R:86:LEU:HD11	1.86	0.57
15:N:16:GLU:N	15:N:16:GLU:OE1	2.36	0.57
20:T:213:GLU:HG3	20:T:218:TRP:CE2	2.39	0.57
1:A:476:PHE:O	1:A:479:THR:OG1	2.22	0.57
1:A:1661:TRP:CD2	1:A:1700:GLY:HA3	2.39	0.57
3:C:73:TYR:HB3	3:C:77:VAL:HG21	1.85	0.57
3:C:500:THR:HG22	3:C:545:PRO:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:179:C:H2'	9:H:180:G:H8	1.67	0.57
46:1:432:SER:HB2	46:1:479:TRP:CD2	2.38	0.57
1:A:1450:GLN:NE2	1:A:1451:ASN:H	2.02	0.57
3:C:454:THR:OG1	3:C:575:GLN:HB3	2.04	0.57
19:S:87:HIS:HB3	19:S:90:LEU:HG	1.86	0.57
27:Z:832:ASN:O	27:Z:836:GLY:N	2.37	0.57
3:C:115:GLU:O	3:C:118:PHE:N	2.36	0.57
20:T:287:HIS:CE1	20:T:313:ARG:HG3	2.39	0.57
1:A:65:HIS:ND1	1:A:120:TYR:OH	2.33	0.57
1:A:1218:ASN:OD1	1:A:1220:VAL:N	2.37	0.57
3:C:850:LEU:O	3:C:855:GLY:N	2.37	0.57
13:L:175:GLN:O	13:L:178:GLU:HG3	2.04	0.57
2:B:40:U:H3	7:G:-1:G:H1	1.52	0.57
3:C:62:ASP:OD1	3:C:62:ASP:N	2.36	0.57
3:C:506:PRO:HB2	3:C:569:ARG:NH1	2.20	0.57
19:S:138:MET:O	19:S:142:VAL:HG23	2.04	0.57
22:U:23:LEU:H	23:V:474:HIS:CD2	2.22	0.57
26:Y:46:CYS:SG	26:Y:83:CYS:HB3	2.45	0.57
1:A:73:HIS:HD2	1:A:81:PHE:CE2	2.22	0.57
1:A:494:LEU:HD21	1:A:562:VAL:HG21	1.87	0.57
1:A:805:GLU:OE1	1:A:1162:PRO:HB3	2.04	0.57
18:R:151:LEU:HD22	20:T:323:VAL:HG11	1.84	0.57
1:A:312:TYR:OH	3:C:853:ARG:NH2	2.37	0.57
1:A:1171:GLU:OE1	1:A:1171:GLU:N	2.33	0.57
5:E:68:GLU:CD	5:E:68:GLU:H	2.08	0.57
5:E:75:HIS:HB2	5:E:80:THR:HG22	1.86	0.57
9:H:41:U:H2'	9:H:42:G:H8	1.69	0.57
10:I:394:PRO:HG2	10:I:429:VAL:HA	1.87	0.57
1:A:1625:SER:OG	1:A:1626:CYS:O	2.23	0.57
1:A:1810:PHE:CE1	1:A:1815:GLY:HA2	2.39	0.57
3:C:686:THR:HB	3:C:793:ASP:HB3	1.87	0.57
5:E:284:PHE:HZ	24:W:120:ILE:HD13	1.70	0.57
6:F:33:G:O2'	6:F:34:G:OP1	2.21	0.57
11:J:346:TRP:CZ2	11:J:372:VAL:HG11	2.40	0.57
46:1:424:PHE:HB2	46:1:425:PRO:HD3	1.86	0.57
47:2:119:ILE:O	47:2:135:ARG:HD2	2.04	0.57
1:A:532:THR:OG1	8:6:2:U:H3'	2.05	0.57
3:C:692:LEU:HD11	3:C:744:ILE:HG13	1.87	0.57
11:J:411:MET:HE2	11:J:415:LEU:HD22	1.87	0.57
18:R:124:VAL:HG13	18:R:125:MET:H	1.70	0.57
1:A:1500:GLY:O	1:A:1756:SER:OG	2.10	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1894:GLN:HE21	1:A:1898:LYS:NZ	2.03	0.56
3:C:801:LEU:O	3:C:803:ARG:N	2.38	0.56
5:E:202:ASN:ND2	5:E:204:THR:OG1	2.38	0.56
10:I:528:LEU:C	10:I:532:LYS:HA	2.22	0.56
11:J:394:HIS:O	11:J:398:VAL:HG23	2.04	0.56
26:Y:41:MET:HG3	26:Y:100:MET:HE1	1.87	0.56
46:1:188:LEU:HD23	46:1:197:LEU:HD21	1.86	0.56
1:A:1820:LYS:HD3	1:A:1914:MET:HE2	1.86	0.56
3:C:138:LEU:HG	3:C:139:HIS:CD2	2.39	0.56
3:C:313:GLN:HB2	50:C:1500:GTP:C6	2.41	0.56
8:6:22:C:H5"	16:O:216:ARG:HD2	1.86	0.56
16:O:248:LEU:O	16:O:252:PHE:HD2	1.87	0.56
20:T:189:GLN:OE1	20:T:191:HIS:NE2	2.35	0.56
20:T:459:LEU:HD12	20:T:460:ASP:H	1.68	0.56
1:A:264:PHE:CE1	1:A:459:LEU:HD13	2.40	0.56
1:A:587:GLN:O	1:A:587:GLN:HG2	2.05	0.56
1:A:1136:ARG:HD2	1:A:1139:ARG:HH21	1.70	0.56
1:A:1567:PRO:HB2	9:H:36:G:OP1	2.05	0.56
3:C:196:LYS:HD3	3:C:198:TYR:OH	2.05	0.56
3:C:221:ILE:HG23	3:C:495:ARG:HB3	1.88	0.56
3:C:320:LEU:HD21	3:C:343:LEU:HB2	1.87	0.56
3:C:379:LYS:O	3:C:383:GLN:HG2	2.04	0.56
3:C:692:LEU:HD21	3:C:788:LYS:HB2	1.87	0.56
9:H:171:U:H2'	9:H:172:C:C6	2.40	0.56
11:J:196:ARG:HH12	46:1:616:SER:CB	2.19	0.56
11:J:308:ARG:HG3	18:R:232:SEP:O	2.05	0.56
13:L:172:ARG:HA	13:L:175:GLN:NE2	2.18	0.56
23:V:515:CYS:HA	23:V:521:TYR:HB2	1.88	0.56
24:W:130:ARG:HH11	24:W:168:PHE:HE1	1.53	0.56
1:A:173:GLU:HG2	46:1:273:ILE:HB	1.87	0.56
1:A:324:PRO:HB2	1:A:327:VAL:HG21	1.86	0.56
3:C:245:HIS:O	3:C:249:GLU:HG2	2.05	0.56
6:F:92:A:H2'	6:F:93:G:H8	1.70	0.56
8:6:13:C:H2'	8:6:14:A:H8	1.71	0.56
11:J:240:THR:OG1	11:J:241:VAL:N	2.38	0.56
11:J:372:VAL:HG13	11:J:373:HIS:CD2	2.41	0.56
1:A:401:GLY:HA3	3:C:386:GLY:HA2	1.88	0.56
1:A:1179:SER:OG	1:A:1180:LYS:N	2.38	0.56
1:A:1279:VAL:HG12	23:V:467:LEU:HD11	1.86	0.56
3:C:902:HIS:ND1	3:C:903:HIS:HB2	2.19	0.56
16:O:293:VAL:HB	16:O:298:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1639:VAL:HG13	1:A:1717:ASN:HB3	1.86	0.56
3:C:606:GLY:O	3:C:610:VAL:HG23	2.05	0.56
6:F:34:G:H1	8:6:12:G:C1'	2.18	0.56
6:F:48:A:O2'	6:F:49:G:OP1	2.18	0.56
13:L:222:LEU:H	13:L:222:LEU:HD22	1.71	0.56
18:R:292:TYR:CZ	26:Y:167:VAL:HG11	2.41	0.56
8:6:2:U:H4'	8:6:3:A:O5'	2.05	0.56
8:6:20:A:H2	16:O:187:THR:HG21	1.71	0.56
1:A:56:ALA:HB3	15:N:109:ARG:HH12	1.71	0.56
1:A:1813:ARG:HB3	1:A:1813:ARG:CZ	2.35	0.56
9:H:60:U:H1'	46:1:258:ARG:HH12	1.69	0.56
10:I:177:PRO:HB3	10:I:211:SER:HA	1.87	0.56
11:J:238:ASN:C	11:J:240:THR:H	2.08	0.56
16:O:26:THR:HG1	16:O:159:ARG:NH2	2.03	0.56
23:V:455:PHE:O	23:V:459:ILE:HG12	2.06	0.56
2:B:31:U:H2'	2:B:32:C:H6	1.71	0.56
8:6:94:C:OP1	26:Y:60:LYS:NZ	2.37	0.56
1:A:1166:THR:OG1	1:A:1167:THR:N	2.39	0.56
1:A:1283:GLU:OE2	1:A:1283:GLU:N	2.28	0.56
1:A:1953:ILE:HG22	1:A:1979:VAL:HG13	1.86	0.56
1:A:1968:TRP:HA	1:A:1968:TRP:CE3	2.41	0.56
5:E:62:LEU:HB2	5:E:351:LEU:HB2	1.88	0.56
1:A:68:LYS:HD3	15:N:49:ILE:HD11	1.88	0.55
1:A:357:ASN:O	3:C:865:GLY:N	2.33	0.55
1:A:1338:SER:OG	1:A:1351:THR:N	2.33	0.55
2:B:23:C:H5	2:B:26:A:N7	2.03	0.55
3:C:131:ASN:ND2	3:C:495:ARG:HH12	2.04	0.55
3:C:510:LEU:HD22	3:C:514:TYR:CE2	2.41	0.55
4:D:1225:VAL:O	4:D:1234:LEU:N	2.39	0.55
24:W:122:ASP:OD2	24:W:123:PHE:N	2.40	0.55
46:1:253:ALA:H	46:1:266:CYS:HB2	1.71	0.55
1:A:750:TRP:CZ2	1:A:778:ARG:HG2	2.42	0.55
1:A:1731:ALA:O	1:A:1735:LYS:HG2	2.06	0.55
8:6:8:C:H2'	8:6:9:C:H6	1.70	0.55
11:J:401:ARG:HA	11:J:404:GLU:OE2	2.06	0.55
16:O:228:ASP:O	16:O:277:ARG:NH2	2.39	0.55
20:T:261:LEU:HB2	20:T:273:TRP:HB2	1.88	0.55
20:T:267:ASP:O	20:T:268:LYS:HB2	2.06	0.55
24:W:439:ASP:O	24:W:441:SER:N	2.39	0.55
1:A:702:LYS:HB2	1:A:705:LYS:HZ2	1.71	0.55
1:A:1900:GLU:OE2	1:A:1951:LYS:NZ	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:770:PHE:HE1	3:C:789:PHE:CD1	2.23	0.55
3:C:803:ARG:O	3:C:807:GLN:HG2	2.06	0.55
5:E:259:VAL:HB	5:E:277:PHE:HB2	1.88	0.55
6:F:59:G:H1	6:F:76:A:H61	1.54	0.55
20:T:314:ILE:HD11	20:T:326:LEU:HD11	1.89	0.55
1:A:1941:ARG:NH1	1:A:2010:ILE:O	2.31	0.55
26:Y:138:GLU:CB	27:Z:1097:MET:HA	2.37	0.55
1:A:203:VAL:HA	1:A:206:TRP:CZ2	2.42	0.55
1:A:1258:LYS:CG	1:A:1527:ASN:HD21	2.18	0.55
8:6:72:G:H5"	8:6:73:G:OP1	2.07	0.55
13:L:144:MET:CB	13:L:149:LEU:HD21	2.36	0.55
1:A:36:LYS:HA	24:W:169:GLU:OE1	2.07	0.55
3:C:183:SER:OG	3:C:203:MET:SD	2.65	0.55
3:C:481:MET:SD	3:C:492:ALA:HA	2.47	0.55
11:J:214:ILE:H	11:J:214:ILE:HD12	1.72	0.55
11:J:406:PHE:HB3	11:J:411:MET:HG2	1.88	0.55
15:N:2:PRO:O	15:N:4:VAL:N	2.39	0.55
16:O:84:CYS:SG	16:O:159:ARG:CZ	2.95	0.55
23:V:290:VAL:HG21	23:V:332:VAL:HG22	1.88	0.55
24:W:335:VAL:HA	24:W:351:ALA:HB2	1.89	0.55
3:C:357:THR:OG1	3:C:358:LYS:O	2.18	0.55
6:F:15:A:H2'	6:F:16:G:C8	2.42	0.55
24:W:290:GLY:HA3	24:W:571:TRP:HA	1.89	0.55
1:A:723:ASN:HB2	1:A:785:LYS:HG2	1.88	0.55
5:E:313:ASP:OD2	5:E:316:SER:OG	2.25	0.55
13:L:163:GLN:HG2	13:L:167:ALA:HB3	1.89	0.55
1:A:1778:TRP:CE2	1:A:1858:PRO:HG3	2.41	0.55
3:C:220:ARG:NH1	3:C:578:ARG:O	2.39	0.55
3:C:812:ALA:O	3:C:816:VAL:HG23	2.07	0.55
9:H:43:U:H2'	9:H:44:U:H6	1.72	0.55
20:T:421:VAL:HG12	20:T:422:ASN:O	2.07	0.55
23:V:302:LEU:HD12	23:V:306:GLN:HE22	1.71	0.55
23:V:334:TYR:O	23:V:338:VAL:HG23	2.06	0.55
26:Y:95:ASN:O	26:Y:97:ASP:N	2.39	0.55
1:A:253:ASN:OD1	1:A:334:THR:OG1	2.24	0.55
1:A:670:LYS:O	20:T:268:LYS:NZ	2.36	0.55
1:A:1615:HIS:CE1	46:1:271:GLN:HG2	2.42	0.55
1:A:1935:ARG:HD3	1:A:1976:TRP:CZ3	2.42	0.55
3:C:196:LYS:HD3	3:C:198:TYR:CZ	2.42	0.55
3:C:529:ARG:H	3:C:553:GLU:HB3	1.70	0.55
3:C:555:VAL:HG11	3:C:565:ILE:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:134:THR:HB	13:L:135:LYS:HZ2	1.72	0.55
1:A:1532:ARG:HA	1:A:1568:THR:HG21	1.89	0.54
1:A:1787:ARG:HB3	45:4:112:MET:HE1	1.88	0.54
3:C:567:GLU:OE2	3:C:570:GLY:HA3	2.07	0.54
6:F:47:A:H4'	6:F:48:A:OP1	2.07	0.54
8:6:4:A:H2'	8:6:5:G:O4'	2.07	0.54
11:J:242:ILE:HA	11:J:245:TRP:HD1	1.71	0.54
16:O:81:CYS:SG	16:O:84:CYS:N	2.70	0.54
17:P:32:SER:O	17:P:35:LEU:HD12	2.06	0.54
18:R:180:THR:HB	24:W:114:TYR:HB3	1.89	0.54
20:T:442:ARG:HB3	20:T:443:THR:HG23	1.89	0.54
3:C:534:VAL:HB	3:C:537:TYR:HB2	1.88	0.54
3:C:779:LEU:HD13	3:C:934:MET:HE1	1.89	0.54
3:C:781:ASP:HB3	3:C:941:LYS:NZ	2.22	0.54
5:E:344:SER:OG	5:E:352:TYR:HB2	2.07	0.54
6:F:45:A:C4	26:Y:34:ARG:NH2	2.75	0.54
16:O:89:GLU:HG3	16:O:90:TYR:CE1	2.42	0.54
27:Z:693:ALA:O	27:Z:698:ASN:N	2.41	0.54
44:3:545:GLY:HA3	44:3:591:GLN:HA	1.89	0.54
1:A:671:THR:O	1:A:676:ARG:NH1	2.41	0.54
1:A:703:GLN:H	1:A:703:GLN:CD	2.10	0.54
1:A:1020:LYS:HB3	9:H:24:A:C5	2.41	0.54
6:F:22:A:OP2	24:W:130:ARG:NH2	2.35	0.54
20:T:343:PRO:HG2	20:T:356:LEU:HD23	1.89	0.54
26:Y:86:GLU:CD	26:Y:86:GLU:H	2.10	0.54
1:A:853:LYS:HD2	1:A:855:ARG:O	2.08	0.54
1:A:1361:GLU:C	1:A:1363:GLN:H	2.10	0.54
5:E:311:VAL:HB	5:E:321:TYR:HB2	1.88	0.54
18:R:123:GLU:O	18:R:125:MET:HG3	2.07	0.54
2:B:98:G:H2'	2:B:99:C:H6	1.71	0.54
11:J:192:GLU:OE1	11:J:192:GLU:N	2.32	0.54
16:O:234:LEU:HB2	16:O:272:ILE:HB	1.89	0.54
1:A:1668:TRP:CD2	1:A:1708:ALA:HB2	2.43	0.54
2:B:20:G:H4'	2:B:20:G:OP1	2.06	0.54
3:C:134:LEU:CD2	3:C:226:VAL:HB	2.37	0.54
3:C:244:LYS:HB2	3:C:292:TYR:CE2	2.43	0.54
3:C:390:THR:OG1	3:C:391:SER:N	2.41	0.54
5:E:67:GLY:N	5:E:87:ASP:OD2	2.37	0.54
6:F:40:U:H2'	6:F:41:A:H8	1.72	0.54
11:J:290:ARG:NH2	14:M:179:ILE:HD11	2.23	0.54
16:O:30:GLU:OE1	16:O:30:GLU:N	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:315:ILE:O	23:V:319:LEU:HG	2.07	0.54
3:C:440:SER:O	3:C:442:LYS:N	2.40	0.54
3:C:528:GLY:N	3:C:553:GLU:O	2.40	0.54
5:E:61:LEU:HD23	5:E:61:LEU:H	1.72	0.54
5:E:321:TYR:OH	5:E:356:ILE:HG23	2.08	0.54
23:V:199:ARG:HB2	23:V:383:ASN:HD21	1.72	0.54
23:V:301:GLY:O	23:V:305:THR:HG23	2.07	0.54
26:Y:68:TYR:CE2	26:Y:94:GLU:HB2	2.38	0.54
46:1:446:ARG:HH12	46:1:472:ALA:HB2	1.73	0.54
3:C:605:ASP:HA	3:C:608:ARG:NH1	2.22	0.54
13:L:100:TYR:CE2	13:L:104:LEU:HD11	2.43	0.54
19:S:57:ILE:HG21	24:W:97:ASN:HB2	1.88	0.54
46:1:282:HIS:HA	46:1:309:ARG:HH12	1.72	0.54
47:2:138:TRP:HB3	47:2:149:LEU:HD22	1.90	0.54
1:A:195:LEU:HD11	1:A:208:TYR:HE2	1.73	0.54
1:A:1286:ASP:OD1	1:A:1286:ASP:N	2.38	0.54
1:A:1494:TYR:HB3	1:A:1744:ARG:HD3	1.90	0.54
8:6:9:C:H2'	8:6:10:U:C6	2.43	0.54
13:L:223:GLY:O	13:L:225:TYR:N	2.41	0.54
18:R:180:THR:N	24:W:114:TYR:O	2.38	0.54
18:R:262:ILE:HG13	18:R:263:PRO:HD2	1.90	0.54
20:T:306:CYS:SG	20:T:336:VAL:HB	2.48	0.54
1:A:142:SER:HA	1:A:242:ALA:HB2	1.89	0.54
46:1:414:LEU:HG	46:1:415:PHE:H	1.73	0.54
1:A:1210:LYS:O	1:A:1212:GLY:N	2.41	0.53
3:C:847:TYR:CE1	3:C:857:VAL:HG21	2.42	0.53
6:F:2:U:H2'	6:F:3:G:H8	1.73	0.53
16:O:240:GLY:HA3	16:O:296:ARG:HH12	1.71	0.53
19:S:123:ASP:OD1	19:S:123:ASP:N	2.40	0.53
23:V:301:GLY:HA2	23:V:304:LEU:HD12	1.90	0.53
1:A:1404:THR:HG23	1:A:1406:GLU:H	1.73	0.53
1:A:1661:TRP:CE2	1:A:1700:GLY:HA3	2.44	0.53
3:C:222:SER:OG	3:C:223:ASP:N	2.39	0.53
3:C:801:LEU:O	3:C:804:GLY:N	2.41	0.53
5:E:171:SER:OG	5:E:173:ASP:OD1	2.25	0.53
19:S:77:ILE:HG13	19:S:78:TYR:CD1	2.41	0.53
20:T:475:SER:OG	20:T:476:ARG:NH1	2.41	0.53
24:W:185:ASP:OD2	24:W:187:SER:OG	2.26	0.53
25:X:29:LYS:O	25:X:33:GLU:HG3	2.08	0.53
1:A:1359:HIS:HB3	1:A:1363:GLN:HB2	1.90	0.53
6:F:94:C:H2'	6:F:95:G:H8	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:98:G:H5'	9:H:104:U:OP2	2.08	0.53
20:T:350:HIS:HA	20:T:374:SER:HB3	1.90	0.53
21:Q:27:ALA:O	21:Q:32:ALA:N	2.32	0.53
25:X:13:HIS:CD2	25:X:15:GLN:HB2	2.44	0.53
1:A:283:VAL:HG13	1:A:284:ARG:H	1.74	0.53
1:A:1262:LYS:HE2	8:6:102:G:OP1	2.08	0.53
1:A:1782:ASP:O	1:A:1785:VAL:HG12	2.08	0.53
12:K:17:PRO:HG3	12:K:167:ARG:NH1	2.24	0.53
1:A:354:PRO:O	23:V:344:LYS:HG2	2.09	0.53
1:A:1135:PRO:HB2	1:A:1137:ASP:OD1	2.09	0.53
3:C:650:GLU:OE1	3:C:650:GLU:N	2.27	0.53
5:E:336:HIS:CG	5:E:337:PRO:HD2	2.44	0.53
6:F:34:G:H5'	13:L:203:LYS:HE2	1.91	0.53
6:F:78:A:O3'	11:J:237:LYS:NZ	2.31	0.53
23:V:271:GLU:O	23:V:275:LEU:HG	2.09	0.53
23:V:497:CYS:HB3	23:V:507:PHE:CG	2.43	0.53
47:2:64:MET:HG2	47:2:159:CYS:SG	2.48	0.53
2:B:65:G:H2'	2:B:66:A:C8	2.42	0.53
5:E:67:GLY:H	5:E:87:ASP:CG	2.11	0.53
5:E:172:ASP:O	5:E:195:GLN:HG3	2.08	0.53
8:6:22:C:HO2'	8:6:23:U:P	2.32	0.53
16:O:232:THR:HG22	16:O:277:ARG:HA	1.91	0.53
18:R:205:ASP:OD1	18:R:207:MET:N	2.37	0.53
24:W:155:SER:O	24:W:157:GLU:N	2.41	0.53
1:A:1870:ASP:HB2	1:A:1871:PRO:HD3	1.90	0.53
1:A:1943:LEU:HA	1:A:1947:ASN:HA	1.90	0.53
6:F:2:U:H2'	6:F:3:G:C8	2.44	0.53
9:H:34:U:C2	9:H:35:A:C8	2.96	0.53
15:N:120:ARG:HH11	15:N:142:CYS:HB2	1.74	0.53
23:V:352:ILE:HG22	23:V:353:ILE:HG13	1.89	0.53
47:2:56:ILE:O	47:2:101:LYS:HE3	2.08	0.53
1:A:300:ASN:C	3:C:939:ARG:HH21	2.10	0.53
1:A:1189:MET:HG2	1:A:1190:CYS:H	1.74	0.53
14:M:160:PHE:HB3	14:M:161:PHE:CD1	2.44	0.53
18:R:208:GLU:OE2	18:R:211:ARG:NH2	2.42	0.53
23:V:238:ILE:HG23	23:V:372:LEU:HD12	1.90	0.53
23:V:316:PHE:CE2	23:V:343:ARG:HD3	2.44	0.53
25:X:30:HIS:ND1	25:X:33:GLU:OE2	2.41	0.53
1:A:1503:TRP:HZ3	1:A:1533:ARG:NE	1.98	0.53
5:E:92:LEU:HD12	5:E:103:ALA:HB3	1.91	0.53
5:E:153:PHE:HB2	5:E:172:ASP:OD2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:333:PHE:O	11:J:337:MET:HG2	2.09	0.53
11:J:439:ALA:O	11:J:443:ILE:HG12	2.09	0.53
14:M:175:SER:N	14:M:178:GLU:OE2	2.42	0.53
16:O:78:LYS:HG3	16:O:202:TYR:CZ	2.43	0.53
16:O:224:ASP:OD2	16:O:224:ASP:N	2.41	0.53
20:T:412:HIS:HE1	20:T:431:ALA:HB2	1.74	0.53
23:V:332:VAL:O	23:V:336:ILE:HG13	2.08	0.53
26:Y:37:ALA:O	26:Y:52:LYS:O	2.26	0.53
1:A:799:PRO:HD3	18:R:284:PHE:CE1	2.43	0.53
1:A:1283:GLU:H	1:A:1283:GLU:CD	2.09	0.53
1:A:1413:ASP:O	1:A:1418:ARG:NH1	2.42	0.53
1:A:1763:LEU:HD22	1:A:1889:LEU:HD13	1.91	0.53
1:A:1853:PRO:HG2	47:2:101:LYS:HZ2	1.73	0.53
1:A:1999:VAL:HA	1:A:2002:LEU:HG	1.90	0.53
5:E:265:ARG:HG2	5:E:266:PRO:HD2	1.91	0.53
6:F:87:C:OP2	14:M:193:ARG:HA	2.09	0.53
9:H:4:G:H2'	9:H:5:C:C6	2.44	0.53
9:H:74:U:H2'	9:H:75:A:H8	1.73	0.53
13:L:101:GLU:OE1	26:Y:163:ARG:NH2	2.38	0.53
14:M:168:LEU:HG	19:S:141:ARG:HH12	1.73	0.53
18:R:185:GLY:O	18:R:188:PHE:N	2.37	0.53
22:U:23:LEU:H	23:V:474:HIS:HD2	1.55	0.53
1:A:569:VAL:O	1:A:570:ASP:HB2	2.09	0.52
3:C:223:ASP:OD1	3:C:495:ARG:NH2	2.42	0.52
3:C:777:GLY:HA3	3:C:782:GLU:O	2.09	0.52
8:6:104:C:HO2'	8:6:105:C:P	2.31	0.52
16:O:235:TYR:HD1	16:O:271:PHE:HE1	1.57	0.52
23:V:178:ILE:O	23:V:182:ILE:HG12	2.09	0.52
23:V:316:PHE:CZ	23:V:343:ARG:HD3	2.44	0.52
23:V:340:PHE:O	23:V:344:LYS:HG3	2.08	0.52
1:A:57:GLN:O	1:A:59:GLU:N	2.42	0.52
1:A:1839:TRP:HH2	1:A:1874:VAL:HG21	1.73	0.52
1:A:1923:TRP:CZ3	1:A:1935:ARG:HD2	2.45	0.52
3:C:387:ASP:OD2	3:C:390:THR:OG1	2.26	0.52
3:C:588:ILE:O	3:C:630:LEU:HA	2.09	0.52
3:C:820:PHE:CE1	3:C:825:PRO:HB3	2.45	0.52
8:6:6:A:N6	8:6:7:G:O6	2.41	0.52
13:L:152:LEU:HB3	13:L:156:ARG:NH1	2.25	0.52
13:L:206:ARG:H	13:L:206:ARG:HD3	1.75	0.52
16:O:131:THR:HG23	24:W:111:LEU:H	1.75	0.52
1:A:79:ARG:HH11	1:A:82:ARG:NE	2.04	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:ARG:HA	1:A:362:ARG:NE	2.25	0.52
8:6:5:G:H3'	8:6:6:A:H2	1.74	0.52
8:6:19:G:C6	8:6:20:A:N6	2.77	0.52
13:L:55:ASP:OD1	13:L:57:SER:OG	2.18	0.52
15:N:143:SER:O	15:N:143:SER:OG	2.27	0.52
1:A:976:MET:HG2	1:A:1187:PHE:HB3	1.91	0.52
1:A:1094:ARG:NH1	1:A:1094:ARG:HB2	2.24	0.52
1:A:1411:SER:HA	1:A:1414:ARG:HE	1.74	0.52
1:A:1902:PHE:O	1:A:1906:ILE:HG12	2.10	0.52
4:D:2098:ALA:O	4:D:2100:GLY:N	2.42	0.52
15:N:38:GLU:O	15:N:40:LYS:N	2.43	0.52
16:O:19:ASP:OD1	16:O:20:PHE:N	2.42	0.52
23:V:312:ILE:HA	23:V:315:ILE:HD12	1.91	0.52
24:W:153:ILE:O	24:W:153:ILE:HG13	2.09	0.52
44:3:582:ASN:O	44:3:584:GLY:N	2.41	0.52
1:A:1189:MET:CG	1:A:1190:CYS:H	2.22	0.52
1:A:1790:ILE:CG2	1:A:1798:LEU:HB3	2.40	0.52
3:C:233:GLU:CD	3:C:837:GLN:HE22	2.12	0.52
3:C:929:LEU:HB3	3:C:933:PHE:CZ	2.44	0.52
4:D:668:ASP:O	4:D:672:GLY:CA	2.57	0.52
10:I:533:TYR:HA	13:L:505:ARG:CB	2.39	0.52
13:L:146:GLU:HG2	13:L:147:ASP:N	2.23	0.52
1:A:373:ASP:OD1	1:A:374:ASP:N	2.42	0.52
1:A:1809:ILE:O	1:A:1817:LEU:HD12	2.10	0.52
1:A:1820:LYS:NZ	1:A:1844:GLU:OE1	2.37	0.52
1:A:1949:ARG:NH1	1:A:1952:VAL:HG21	2.25	0.52
3:C:679:PRO:HD3	3:C:811:THR:OG1	2.08	0.52
3:C:831:TYR:N	3:C:903:HIS:O	2.38	0.52
6:F:39:A:C6	6:F:40:U:C4	2.98	0.52
9:H:29:A:C2	9:H:31:G:C6	2.97	0.52
1:A:436:PRO:HB2	1:A:439:GLN:HG3	1.91	0.52
1:A:1783:THR:HA	45:4:106:LYS:CE	2.37	0.52
3:C:132:VAL:HA	3:C:224:GLY:O	2.10	0.52
6:F:26:U:O2	6:F:26:U:H2'	2.09	0.52
8:6:104:C:O2'	8:6:105:C:O5'	2.27	0.52
9:H:43:U:H2'	9:H:44:U:C6	2.45	0.52
13:L:178:GLU:HA	13:L:181:ARG:CG	2.40	0.52
23:V:219:VAL:HA	23:V:222:ILE:HG12	1.90	0.52
46:1:252:GLN:HG2	46:1:266:CYS:O	2.09	0.52
5:E:197:LEU:HG	5:E:212:GLY:HA2	1.91	0.52
6:F:59:G:H1	6:F:76:A:N6	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:29:GLY:O	18:R:195:ARG:NH1	2.43	0.52
18:R:263:PRO:HB2	18:R:266:LYS:HG2	1.90	0.52
23:V:577:SER:HA	23:V:580:ARG:HD2	1.91	0.52
1:A:941:LYS:HG3	1:A:1071:PHE:CE1	2.45	0.52
1:A:1772:PHE:CD2	1:A:1813:ARG:HG2	2.44	0.52
1:A:1780:VAL:HG22	1:A:1809:ILE:HD12	1.91	0.52
2:B:97:G:N2	2:B:117:A:H62	2.08	0.52
9:H:81:G:H2'	9:H:82:G:H8	1.74	0.52
15:N:15:TRP:CE3	15:N:18:ILE:HD11	2.45	0.52
19:S:55:ARG:HB2	19:S:63:GLN:HB3	1.91	0.52
19:S:150:GLN:O	19:S:152:ARG:HG3	2.10	0.52
1:A:1292:GLU:OE2	1:A:1330:MET:N	2.39	0.52
5:E:94:ASN:OD1	5:E:96:TYR:N	2.41	0.52
5:E:241:LEU:HA	5:E:251:LEU:O	2.10	0.52
9:H:25:G:C2	9:H:26:A:C8	2.98	0.52
19:S:57:ILE:HD12	19:S:61:MET:CG	2.40	0.52
24:W:188:ASN:ND2	24:W:191:GLY:HA3	2.25	0.52
46:1:396:ARG:NH2	46:1:440:THR:OG1	2.43	0.52
4:D:1048:VAL:O	4:D:1051:SER:N	2.24	0.51
14:M:126:ASP:OD2	14:M:126:ASP:N	2.40	0.51
15:N:38:GLU:C	15:N:40:LYS:H	2.12	0.51
26:Y:132:ASN:O	26:Y:136:VAL:HG23	2.10	0.51
1:A:136:ILE:HG22	1:A:138:PRO:HD2	1.91	0.51
1:A:712:HIS:CG	18:R:250:CYS:HB2	2.44	0.51
1:A:758:ARG:HH11	1:A:902:TYR:HA	1.75	0.51
1:A:1607:GLU:OE2	1:A:1634:SER:HA	2.10	0.51
2:B:31:U:H2'	2:B:32:C:C6	2.44	0.51
13:L:92:THR:HB	13:L:95:GLN:HG3	1.93	0.51
18:R:132:LEU:HD23	18:R:132:LEU:H	1.76	0.51
23:V:182:ILE:HG13	23:V:221:ILE:HG21	1.91	0.51
24:W:199:TYR:HB3	24:W:202:GLU:HG2	1.91	0.51
47:2:155:CYS:SG	47:2:170:LYS:HD3	2.50	0.51
1:A:385:GLU:OE1	1:A:386:PRO:HD2	2.10	0.51
1:A:1002:ASP:OD1	1:A:1004:ASN:N	2.33	0.51
1:A:1668:TRP:CE2	1:A:1708:ALA:HB2	2.45	0.51
1:A:1790:ILE:HA	1:A:1799:THR:O	2.10	0.51
2:B:40:U:H6	2:B:40:U:O5'	1.93	0.51
3:C:176:GLU:OE1	3:C:176:GLU:N	2.37	0.51
3:C:323:PHE:CD1	3:C:373:ILE:HG12	2.44	0.51
3:C:863:ILE:HD12	3:C:868:LEU:HB2	1.93	0.51
8:6:24:G:O2'	8:6:25:G:OP1	2.20	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:36:PRO:O	15:N:38:GLU:N	2.43	0.51
16:O:20:PHE:CD1	18:R:177:ILE:HD11	2.45	0.51
24:W:391:PHE:O	24:W:402:GLN:HA	2.11	0.51
1:A:79:ARG:O	1:A:82:ARG:HG3	2.10	0.51
1:A:1655:THR:OG1	1:A:1656:THR:N	2.43	0.51
5:E:295:PRO:HD3	5:E:335:PHE:HB3	1.91	0.51
6:F:10:U:H2'	6:F:11:C:O4'	2.09	0.51
6:F:41:A:H61	8:6:6:A:N6	2.08	0.51
9:H:7:U:H2'	9:H:8:C:C6	2.46	0.51
11:J:357:LYS:N	11:J:357:LYS:HD2	2.24	0.51
13:L:224:PHE:H	18:R:86:LEU:HD12	1.75	0.51
20:T:295:ASP:OD1	20:T:296:LEU:N	2.42	0.51
23:V:515:CYS:SG	23:V:525:PHE:CG	3.03	0.51
47:2:62:ILE:HD12	47:2:180:ILE:HG12	1.93	0.51
1:A:348:PRO:HB3	1:A:394:TYR:CZ	2.46	0.51
1:A:762:ARG:NH1	17:P:226:LYS:HZ1	2.09	0.51
1:A:1337:GLN:OE1	1:A:1354:ARG:NH1	2.43	0.51
1:A:2013:GLY:HA2	45:4:104:ARG:HH21	1.74	0.51
8:6:93:A:C6	9:H:38:A:N1	2.79	0.51
10:I:374:ILE:O	10:I:376:ASN:N	2.43	0.51
15:N:57:THR:HG22	15:N:85:ASP:H	1.76	0.51
16:O:196:GLN:OE1	16:O:201:ARG:HD2	2.11	0.51
1:A:698:PRO:HG2	1:A:701:ILE:HD11	1.92	0.51
1:A:1810:PHE:CE1	1:A:1919:LEU:HD12	2.46	0.51
3:C:478:THR:OG1	3:C:563:ALA:HB3	2.11	0.51
3:C:673:LYS:HG3	3:C:686:THR:CG2	2.34	0.51
8:6:87:U:N3	9:H:42:G:N1	2.37	0.51
11:J:205:LEU:HG	11:J:206:LEU:H	1.76	0.51
23:V:305:THR:HG22	23:V:312:ILE:HD13	1.92	0.51
1:A:1084:PRO:HG2	17:P:188:TRP:CE3	2.46	0.51
1:A:1778:TRP:HB2	1:A:1861:ILE:HD12	1.91	0.51
3:C:471:ASP:OD1	3:C:472:GLY:N	2.43	0.51
9:H:168:A:H5'	9:H:169:C:OP2	2.11	0.51
18:R:117:THR:O	18:R:120:VAL:HG12	2.09	0.51
24:W:465:PRO:HD2	24:W:479:GLN:O	2.10	0.51
26:Y:68:TYR:CD2	26:Y:93:PRO:HG2	2.46	0.51
3:C:507:VAL:CG1	3:C:565:ILE:HG23	2.40	0.51
6:F:94:C:H2'	6:F:95:G:C8	2.45	0.51
8:6:21:A:O2'	8:6:22:C:O5'	2.28	0.51
1:A:919:ASP:HB3	1:A:1035:GLN:HB2	1.93	0.51
1:A:1809:ILE:HB	1:A:1818:PHE:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:U:C4	2:B:47:A:N7	2.79	0.51
2:B:115:C:H2'	2:B:116:U:O4'	2.11	0.51
3:C:470:PRO:HB3	3:C:500:THR:CG2	2.40	0.51
3:C:564:THR:HG21	3:C:577:PHE:H	1.76	0.51
3:C:572:GLU:HG3	3:C:573:GLU:H	1.76	0.51
13:L:168:LYS:O	13:L:172:ARG:HG3	2.10	0.51
17:P:42:LYS:HZ2	20:T:276:GLU:HG3	1.75	0.51
23:V:297:LEU:HB3	23:V:339:MET:CE	2.40	0.51
26:Y:23:LEU:O	26:Y:25:LEU:N	2.44	0.51
1:A:1160:ARG:HD3	17:P:192:VAL:HG11	1.92	0.51
3:C:83:GLU:OE1	3:C:83:GLU:N	2.42	0.51
3:C:434:CYS:HA	3:C:438:ILE:HG12	1.93	0.51
5:E:94:ASN:O	5:E:99:CYS:HA	2.10	0.51
9:H:174:A:H2'	9:H:175:G:C8	2.46	0.51
17:P:50:ALA:HB3	17:P:53:GLU:HG2	1.92	0.51
24:W:156:VAL:HG12	24:W:160:GLU:OE1	2.11	0.51
45:4:102:ALA:N	45:4:107:TYR:HD2	2.08	0.51
1:A:781:ARG:HH22	1:A:1021:ASP:HB2	1.75	0.50
1:A:1258:LYS:HG3	1:A:1527:ASN:ND2	2.20	0.50
1:A:1337:GLN:NE2	22:U:6:GLY:H	2.09	0.50
1:A:1649:LYS:HD2	47:2:237:ASP:HB2	1.93	0.50
3:C:742:PRO:HB2	3:C:786:ASN:H	1.76	0.50
3:C:801:LEU:C	3:C:803:ARG:N	2.63	0.50
6:F:92:A:H2'	6:F:93:G:C8	2.46	0.50
8:6:88:G:H22	9:H:41:U:H3	1.59	0.50
17:P:69:ALA:HA	17:P:72:ARG:NH1	2.26	0.50
18:R:220:ARG:HB3	18:R:220:ARG:CZ	2.41	0.50
23:V:240:ASN:HA	23:V:243:LYS:HD3	1.92	0.50
27:Z:711:VAL:HA	27:Z:863:GLY:O	2.11	0.50
1:A:36:LYS:O	1:A:40:LEU:HG	2.11	0.50
1:A:1503:TRP:O	1:A:1504:GLU:HG3	2.11	0.50
1:A:1979:VAL:O	1:A:1983:LEU:HG	2.11	0.50
9:H:13:C:N3	14:M:197:SER:OG	2.39	0.50
9:H:147:G:H2'	9:H:148:C:C6	2.46	0.50
15:N:79:ILE:O	15:N:82:GLY:N	2.34	0.50
16:O:32:PRO:HG3	24:W:153:ILE:HD11	1.93	0.50
19:S:57:ILE:HB	19:S:60:PHE:HB3	1.94	0.50
23:V:273:LEU:O	23:V:277:MET:HG3	2.11	0.50
25:X:16:THR:HG23	25:X:19:ASN:H	1.76	0.50
47:2:154:SER:O	47:2:154:SER:OG	2.28	0.50
1:A:425:PRO:HG3	2:B:26:A:H5'	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1663:ASP:OD1	1:A:1664:ILE:N	2.44	0.50
11:J:188:GLN:HA	11:J:188:GLN:OE1	2.10	0.50
11:J:238:ASN:O	11:J:240:THR:N	2.32	0.50
17:P:206:LYS:O	17:P:209:ARG:HB2	2.11	0.50
46:1:284:ALA:HB1	46:1:304:ASN:HB3	1.93	0.50
1:A:298:ASP:O	1:A:302:ILE:HG12	2.11	0.50
1:A:380:LEU:HD23	1:A:384:VAL:HG23	1.93	0.50
1:A:984:MET:O	1:A:988:ILE:HG13	2.12	0.50
1:A:1352:HIS:ND1	22:U:21:ARG:HA	2.26	0.50
2:B:61:A:H2'	2:B:62:G:H8	1.77	0.50
6:F:67:G:H8	6:F:67:G:OP2	1.94	0.50
11:J:438:TYR:HE2	11:J:442:ARG:NH1	2.09	0.50
19:S:36:CYS:HA	19:S:129:PHE:CZ	2.47	0.50
23:V:173:VAL:HG21	23:V:218:LEU:HD12	1.92	0.50
46:1:246:VAL:HG23	46:1:254:LYS:HB3	1.94	0.50
1:A:58:LYS:HA	15:N:107:GLN:NE2	2.26	0.50
1:A:1821:ILE:HG12	1:A:1906:ILE:HG22	1.92	0.50
3:C:670:SER:HA	3:C:823:ALA:CB	2.41	0.50
11:J:217:GLU:HG2	11:J:218:GLU:OE1	2.11	0.50
14:M:153:ARG:CA	14:M:160:PHE:HE2	2.15	0.50
18:R:79:LYS:HG3	18:R:81:LYS:NZ	2.27	0.50
18:R:154:SER:O	18:R:158:LYS:HD3	2.12	0.50
47:2:100:VAL:CG2	47:2:108:ALA:HB3	2.42	0.50
1:A:537:LYS:HD2	6:F:37:C:N4	2.27	0.50
2:B:107:U:H2'	2:B:108:G:O4'	2.11	0.50
3:C:719:GLN:OE1	3:C:726:LEU:HD13	2.12	0.50
9:H:25:G:N3	9:H:26:A:C8	2.80	0.50
12:K:32:ALA:O	12:K:36:VAL:HG23	2.12	0.50
13:L:172:ARG:NH1	26:Y:82:ARG:HA	2.25	0.50
1:A:1608:THR:HG22	1:A:1632:PHE:HB2	1.93	0.50
1:A:1667:ARG:HD2	1:A:1679:TYR:CE2	2.47	0.50
3:C:275:TYR:HD1	3:C:369:PHE:CD2	2.30	0.50
3:C:800:PRO:O	3:C:801:LEU:O	2.29	0.50
4:D:148:LEU:O	4:D:150:ASP:N	2.42	0.50
5:E:73:LYS:O	5:E:81:LEU:HD13	2.12	0.50
18:R:74:LEU:HD13	19:S:136:ILE:HB	1.94	0.50
18:R:154:SER:OG	18:R:158:LYS:NZ	2.31	0.50
19:S:11:PRO:HB3	19:S:166:GLY:HA3	1.92	0.50
1:A:58:LYS:HE2	15:N:110:ASP:OD1	2.12	0.50
1:A:436:PRO:HB2	1:A:439:GLN:CG	2.42	0.50
1:A:1870:ASP:O	1:A:1874:VAL:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:514:TYR:HB3	3:C:576:ILE:HD11	1.94	0.50
6:F:43:A:O2'	6:F:44:G:H5'	2.12	0.50
13:L:153:SER:O	13:L:156:ARG:HB2	2.11	0.50
16:O:145:ASP:OD2	16:O:146:MET:N	2.42	0.50
16:O:185:LYS:NZ	16:O:186:PRO:O	2.44	0.50
19:S:81:GLN:HA	19:S:108:ASN:O	2.12	0.50
20:T:329:HIS:HE2	20:T:347:THR:HG23	1.77	0.50
20:T:481:GLU:OE2	20:T:487:LYS:HD2	2.11	0.50
24:W:181:PHE:HD1	24:W:200:VAL:HG12	1.76	0.50
24:W:212:GLU:OE2	24:W:216:LEU:HD11	2.11	0.50
1:A:84:ASP:OD1	1:A:84:ASP:N	2.42	0.50
1:A:834:HIS:O	1:A:837:LYS:N	2.44	0.50
1:A:1137:ASP:OD1	1:A:1137:ASP:N	2.44	0.50
2:B:17:U:H2'	2:B:18:C:H6	1.77	0.50
6:F:4:C:H2'	6:F:5:U:H6	1.77	0.50
6:F:58:G:O2'	6:F:59:G:OP1	2.26	0.50
7:G:-12:G:O2'	7:G:-11:G:O5'	2.25	0.50
9:H:5:C:H2'	9:H:6:U:H6	1.77	0.50
16:O:68:THR:HA	16:O:83:THR:HG22	1.94	0.50
24:W:172:GLN:HE21	24:W:173:LYS:NZ	2.09	0.50
46:1:281:GLY:O	46:1:309:ARG:NH1	2.44	0.50
46:1:480:HIS:HD2	46:1:482:LYS:N	2.09	0.50
47:2:229:LYS:NZ	47:2:235:ARG:HH22	2.09	0.50
1:A:642:ARG:HG2	1:A:642:ARG:O	2.12	0.49
1:A:780:THR:HG22	1:A:898:PHE:CD1	2.47	0.49
2:B:17:U:H2'	2:B:18:C:C6	2.47	0.49
3:C:370:VAL:HA	3:C:374:LEU:HB2	1.94	0.49
11:J:431:ARG:O	11:J:435:ILE:HG12	2.12	0.49
17:P:210:PHE:HD2	20:T:455:GLN:HE22	1.60	0.49
18:R:65:PRO:HB2	19:S:90:LEU:HA	1.94	0.49
46:1:428:ASP:OD1	46:1:429:CYS:N	2.45	0.49
1:A:269:LEU:HD22	1:A:321:ASN:HD21	1.77	0.49
3:C:490:PHE:CE1	3:C:612:LYS:HD2	2.47	0.49
6:F:59:G:N2	6:F:76:A:N1	2.55	0.49
9:H:174:A:H2'	9:H:175:G:H8	1.77	0.49
11:J:286:GLU:HG3	11:J:298:ILE:HD12	1.95	0.49
13:L:37:LEU:HD11	13:L:158:ARG:HG3	1.93	0.49
17:P:188:TRP:CE3	17:P:189:ASP:HB2	2.46	0.49
18:R:113:TYR:OH	20:T:402:ASP:O	2.16	0.49
20:T:248:THR:HB	20:T:266:GLU:HG2	1.93	0.49
1:A:1892:PRO:O	1:A:1940:LEU:HD23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:280:ASN:ND2	5:E:303:GLY:O	2.45	0.49
14:M:165:ASN:HB2	18:R:95:LYS:CA	2.32	0.49
16:O:131:THR:HG22	24:W:108:ARG:NH2	2.26	0.49
19:S:39:PHE:HB3	19:S:129:PHE:HZ	1.77	0.49
19:S:42:LEU:HD22	19:S:47:TYR:CG	2.48	0.49
23:V:189:ASN:HA	23:V:398:TYR:CE2	2.47	0.49
23:V:258:LYS:HG3	23:V:299:GLU:HG3	1.93	0.49
1:A:1537:TRP:CE3	1:A:1751:LEU:HD13	2.47	0.49
1:A:1949:ARG:HH12	1:A:1952:VAL:HG21	1.78	0.49
3:C:349:PHE:HB2	3:C:356:PHE:CD1	2.47	0.49
3:C:699:ASP:OD2	3:C:722:TYR:OH	2.27	0.49
5:E:193:THR:HG23	5:E:194:TYR:CG	2.48	0.49
9:H:4:G:H2'	9:H:5:C:H6	1.77	0.49
13:L:172:ARG:CA	13:L:175:GLN:HE21	2.20	0.49
1:A:1625:SER:OG	1:A:1663:ASP:OD2	2.19	0.49
1:A:1831:LYS:HG3	1:A:1832:ARG:H	1.77	0.49
3:C:878:ILE:HG13	3:C:879:ASP:H	1.77	0.49
13:L:505:ARG:C	13:L:507:ILE:H	2.16	0.49
13:L:721:LEU:O	13:L:725:GLN:N	2.39	0.49
20:T:219:PHE:CE2	20:T:231:TRP:HB2	2.47	0.49
27:Z:1100:HIS:O	27:Z:1129:TYR:HA	2.13	0.49
46:1:285:MET:O	46:1:304:ASN:N	2.35	0.49
46:1:287:HIS:HB2	46:1:302:CYS:SG	2.53	0.49
1:A:109:PRO:HD3	1:A:630:TRP:CZ2	2.48	0.49
1:A:579:GLN:HG3	1:A:580:TYR:N	2.23	0.49
1:A:658:ARG:NH2	6:F:65:G:OP2	2.45	0.49
1:A:1334:LEU:HB2	23:V:471:GLU:OE2	2.13	0.49
1:A:1790:ILE:HD11	45:4:111:ASP:CG	2.33	0.49
3:C:453:TYR:CE2	3:C:575:GLN:HB2	2.46	0.49
8:6:103:U:H2'	8:6:104:C:O4'	2.11	0.49
23:V:177:ASN:O	23:V:181:ILE:HG12	2.13	0.49
23:V:234:LEU:HD22	23:V:269:ALA:HB2	1.95	0.49
1:A:1217:GLN:HB2	1:A:1224:ARG:CZ	2.42	0.49
1:A:1615:HIS:CG	46:1:271:GLN:HE21	2.30	0.49
3:C:349:PHE:HB2	3:C:356:PHE:CE1	2.48	0.49
3:C:350:ASN:HB3	3:C:353:THR:HG23	1.94	0.49
3:C:745:LEU:HD23	3:C:767:VAL:HG22	1.93	0.49
11:J:270:ASP:OD2	18:R:223:PRO:HD2	2.13	0.49
13:L:149:LEU:HD23	13:L:152:LEU:HD12	1.95	0.49
16:O:76:LYS:HA	24:W:111:LEU:HD21	1.95	0.49
16:O:240:GLY:HA3	16:O:296:ARG:NH2	2.23	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:329:HIS:CE1	20:T:355:ARG:HG3	2.48	0.49
24:W:156:VAL:O	24:W:160:GLU:HG2	2.12	0.49
46:1:352:GLN:O	46:1:377:SER:HA	2.12	0.49
1:A:1312:PRO:HB3	1:A:1360:GLU:CD	2.33	0.49
1:A:1580:HIS:CE1	26:Y:17:PRO:HG3	2.48	0.49
1:A:1892:PRO:HB3	45:4:104:ARG:CD	2.42	0.49
1:A:2013:GLY:HA2	45:4:104:ARG:NH2	2.28	0.49
5:E:127:ALA:HB2	5:E:157:CYS:HB3	1.95	0.49
11:J:258:ILE:HG23	13:L:232:TYR:CD2	2.47	0.49
11:J:408:ASP:OD2	11:J:408:ASP:N	2.44	0.49
26:Y:27:LYS:O	26:Y:28:ASP:HB2	2.12	0.49
46:1:396:ARG:HB2	46:1:429:CYS:SG	2.53	0.49
1:A:134:TRP:HB3	1:A:418:THR:HG21	1.93	0.49
1:A:283:VAL:HG13	1:A:284:ARG:N	2.28	0.49
1:A:673:THR:HG22	1:A:674:LYS:H	1.77	0.49
1:A:1276:GLU:O	1:A:1279:VAL:HG22	2.13	0.49
1:A:1762:TYR:HB3	1:A:1888:GLU:CB	2.42	0.49
1:A:1860:GLN:O	1:A:1861:ILE:HD13	2.13	0.49
2:B:101:U:H2'	2:B:102:U:C6	2.48	0.49
5:E:79:SER:O	5:E:95:VAL:HG22	2.13	0.49
10:I:528:LEU:O	10:I:532:LYS:CB	2.61	0.49
15:N:37:HIS:CG	15:N:37:HIS:O	2.65	0.49
16:O:240:GLY:H	16:O:268:GLN:HB3	1.78	0.49
19:S:39:PHE:HB3	19:S:129:PHE:CZ	2.47	0.49
23:V:457:ARG:HH21	23:V:457:ARG:HG3	1.77	0.49
3:C:845:ALA:O	3:C:849:VAL:HG23	2.13	0.49
12:K:18:TYR:CD2	12:K:168:LYS:HA	2.48	0.49
16:O:172:GLU:O	16:O:174:LYS:HG3	2.12	0.49
20:T:213:GLU:HG2	20:T:214:PRO:HD2	1.95	0.49
23:V:466:SER:HB2	23:V:471:GLU:HB3	1.95	0.49
24:W:212:GLU:HG2	24:W:216:LEU:HG	1.94	0.49
1:A:68:LYS:NZ	15:N:45:SER:OG	2.46	0.48
3:C:135:CYS:HB2	3:C:242:LEU:HD13	1.94	0.48
3:C:507:VAL:HG13	3:C:566:THR:O	2.13	0.48
3:C:705:VAL:HG22	3:C:705:VAL:O	2.12	0.48
11:J:195:LEU:HD12	11:J:195:LEU:H	1.78	0.48
17:P:50:ALA:O	17:P:54:VAL:HG23	2.13	0.48
23:V:169:LEU:HD13	23:V:185:LEU:HG	1.95	0.48
23:V:187:GLN:HA	23:V:402:LYS:HD2	1.95	0.48
1:A:1209:HIS:CD2	1:A:1210:LYS:HG2	2.48	0.48
1:A:1303:LEU:HD12	1:A:1311:PHE:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1615:HIS:CD2	46:1:271:GLN:HE21	2.31	0.48
3:C:461:LEU:O	3:C:465:MET:HG2	2.13	0.48
3:C:925:PRO:HD2	3:C:928:HIS:NE2	2.28	0.48
5:E:283:ASN:ND2	5:E:305:ALA:HB1	2.28	0.48
9:H:34:U:H2'	9:H:35:A:H8	1.78	0.48
14:M:168:LEU:HB3	18:R:96:ILE:HD11	1.95	0.48
16:O:81:CYS:SG	16:O:83:THR:N	2.79	0.48
16:O:131:THR:HG22	24:W:108:ARG:HE	1.79	0.48
17:P:39:THR:O	20:T:318:ARG:HD3	2.13	0.48
17:P:59:PHE:HB3	20:T:216:ASN:HD22	1.78	0.48
17:P:202:ASP:OD2	17:P:202:ASP:N	2.44	0.48
24:W:181:PHE:CD1	24:W:200:VAL:HG12	2.48	0.48
47:2:110:LYS:HE2	47:2:114:GLY:HA2	1.95	0.48
1:A:70:ILE:HD13	1:A:495:GLN:HG3	1.96	0.48
1:A:1758:PRO:O	48:5:5:PRO:HG2	2.13	0.48
3:C:775:ARG:HA	3:C:783:LEU:HD13	1.95	0.48
5:E:234:HIS:CE1	5:E:260:ARG:HG3	2.47	0.48
18:R:73:PRO:HB2	18:R:74:LEU:HD12	1.93	0.48
18:R:282:GLU:O	18:R:285:ALA:N	2.36	0.48
24:W:154:GLY:C	24:W:156:VAL:N	2.67	0.48
24:W:189:ILE:HG22	24:W:190:ASP:OD1	2.13	0.48
25:X:12:TRP:CZ2	26:Y:35:LEU:HD21	2.49	0.48
26:Y:42:ARG:HG3	26:Y:49:TYR:CE1	2.48	0.48
46:1:332:LYS:HB3	46:1:332:LYS:HE2	1.64	0.48
1:A:468:LYS:HD3	1:A:469:LYS:N	2.25	0.48
1:A:1775:GLN:HG2	1:A:1859:LYS:CB	2.43	0.48
1:A:1904:ASP:O	1:A:1908:LYS:HG2	2.13	0.48
3:C:508:LYS:HB3	3:C:566:THR:HG23	1.94	0.48
3:C:651:ILE:O	3:C:653:ILE:HG13	2.13	0.48
46:1:292:HIS:CE1	46:1:295:ILE:HD12	2.47	0.48
2:B:62:G:H2'	2:B:63:A:H8	1.79	0.48
3:C:174:GLU:OE2	3:C:182:LYS:N	2.46	0.48
3:C:205:THR:HB	3:C:215:VAL:HG22	1.96	0.48
8:6:21:A:H4'	8:6:22:C:OP1	2.12	0.48
9:H:10:C:H2'	9:H:11:G:H8	1.79	0.48
15:N:54:HIS:CE1	15:N:92:TRP:CZ2	3.00	0.48
18:R:238:THR:HG22	18:R:240:LYS:H	1.78	0.48
23:V:173:VAL:HB	23:V:181:ILE:HG21	1.96	0.48
24:W:279:LYS:O	24:W:578:TRP:HA	2.13	0.48
1:A:1562:MET:HE1	1:A:1566:ILE:H	1.79	0.48
3:C:309:PHE:HB2	3:C:318:PHE:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:570:GLY:O	3:C:572:GLU:N	2.38	0.48
5:E:155:ASN:N	5:E:170:GLY:O	2.47	0.48
13:L:146:GLU:O	13:L:149:LEU:N	2.46	0.48
16:O:158:LYS:HG3	16:O:161:ARG:HD2	1.95	0.48
23:V:338:VAL:O	23:V:342:VAL:HG23	2.13	0.48
24:W:183:GLU:HG2	24:W:188:ASN:HD21	1.79	0.48
46:1:302:CYS:HB3	46:1:338:CYS:SG	2.53	0.48
47:2:108:ALA:CB	47:2:132:ILE:HD13	2.42	0.48
1:A:355:LEU:O	3:C:867:PRO:HB3	2.13	0.48
1:A:803:ALA:HB2	18:R:287:LEU:HA	1.94	0.48
1:A:1167:THR:OG1	1:A:1168:VAL:N	2.46	0.48
1:A:1787:ARG:HB3	45:4:112:MET:CE	2.44	0.48
3:C:348:TYR:CD1	3:C:359:LYS:HB3	2.48	0.48
3:C:824:THR:HG23	3:C:824:THR:O	2.13	0.48
8:6:79:C:O2'	8:6:80:U:OP1	2.28	0.48
1:A:152:ARG:NH1	1:A:616:PHE:O	2.47	0.48
1:A:155:LYS:HD2	1:A:626:GLY:O	2.14	0.48
1:A:828:PRO:HG3	1:A:925:TYR:CE2	2.49	0.48
1:A:1234:ASP:HA	1:A:1237:MET:HE2	1.96	0.48
3:C:929:LEU:HB3	3:C:933:PHE:CE2	2.48	0.48
5:E:284:PHE:HB3	24:W:139:LEU:HD13	1.95	0.48
9:H:168:A:H3'	9:H:169:C:H6	1.79	0.48
9:H:179:C:H2'	9:H:180:G:C8	2.48	0.48
11:J:215:THR:O	11:J:216:ASP:HB2	2.14	0.48
16:O:33:TYR:HD1	24:W:125:PHE:CE1	2.32	0.48
16:O:236:VAL:HB	16:O:270:ALA:HB3	1.96	0.48
19:S:15:TYR:O	19:S:162:ALA:HA	2.14	0.48
23:V:215:TYR:O	23:V:219:VAL:HG23	2.14	0.48
46:1:273:ILE:HD11	46:1:279:THR:HB	1.95	0.48
46:1:432:SER:OG	46:1:433:PRO:HD3	2.14	0.48
47:2:54:GLY:O	47:2:101:LYS:NZ	2.46	0.48
2:B:101:U:H2'	2:B:102:U:H6	1.78	0.48
8:6:17:U:O2	16:O:46:LYS:NZ	2.43	0.48
9:H:156:U:N3	9:H:157:G:N7	2.62	0.48
11:J:229:LYS:HG3	11:J:230:THR:N	2.28	0.48
12:K:143:VAL:O	12:K:147:GLU:HG2	2.14	0.48
16:O:72:GLN:O	16:O:75:SER:OG	2.28	0.48
18:R:88:ILE:H	18:R:88:ILE:HD12	1.79	0.48
19:S:42:LEU:HD22	19:S:47:TYR:CD1	2.49	0.48
26:Y:20:ILE:HG23	26:Y:21:PRO:HD2	1.95	0.48
1:A:56:ALA:HB3	15:N:109:ARG:NH1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:PRO:HA	3:C:327:TYR:OH	2.14	0.48
1:A:388:LEU:O	3:C:379:LYS:NZ	2.38	0.48
1:A:439:GLN:HB3	1:A:443:VAL:CG2	2.44	0.48
1:A:462:ARG:HA	1:A:462:ARG:NE	2.29	0.48
1:A:1775:GLN:HG2	1:A:1859:LYS:HB2	1.95	0.48
1:A:1788:VAL:HG23	1:A:1801:LYS:C	2.35	0.48
3:C:201:ASN:HB3	3:C:549:TRP:CE3	2.48	0.48
16:O:81:CYS:SG	16:O:83:THR:OG1	2.71	0.48
24:W:145:ASN:OD1	24:W:146:HIS:N	2.43	0.48
25:X:12:TRP:HZ2	26:Y:35:LEU:HD21	1.78	0.48
26:Y:39:PHE:O	26:Y:40:ASN:ND2	2.47	0.48
26:Y:163:ARG:HA	26:Y:163:ARG:HD3	1.60	0.48
46:1:199:THR:OG1	46:1:207:LYS:HB2	2.13	0.48
1:A:1241:HIS:ND1	1:A:1287:LEU:HD11	2.29	0.47
1:A:1667:ARG:HD2	1:A:1679:TYR:CD2	2.49	0.47
1:A:1763:LEU:O	1:A:1763:LEU:HD23	2.14	0.47
11:J:190:THR:O	11:J:193:GLN:HB2	2.14	0.47
13:L:37:LEU:HA	13:L:37:LEU:HD12	1.57	0.47
16:O:258:ILE:HG12	16:O:274:PHE:CE1	2.49	0.47
17:P:212:ASN:HB2	20:T:455:GLN:OE1	2.13	0.47
18:R:91:ASP:OD2	18:R:91:ASP:N	2.36	0.47
25:X:28:GLN:HA	25:X:28:GLN:OE1	2.14	0.47
47:2:92:SER:O	47:2:96:GLN:HG3	2.14	0.47
47:2:160:ASN:ND2	47:2:164:ASP:HB2	2.21	0.47
1:A:260:LEU:HD23	1:A:455:VAL:HG22	1.96	0.47
2:B:110:C:H2'	2:B:111:A:C8	2.49	0.47
3:C:529:ARG:HB3	3:C:540:GLU:OE1	2.15	0.47
3:C:593:GLU:HG3	3:C:594:PRO:HD2	1.95	0.47
11:J:330:ARG:HG2	11:J:361:ARG:HH21	1.78	0.47
23:V:152:LEU:H	23:V:152:LEU:HD12	1.77	0.47
1:A:578:LEU:HD23	1:A:578:LEU:HA	1.53	0.47
3:C:749:THR:O	3:C:753:GLU:N	2.43	0.47
3:C:834:VAL:HG22	3:C:899:SER:HB3	1.97	0.47
5:E:147:LEU:HD22	5:E:179:TRP:CE3	2.49	0.47
5:E:215:ASN:ND2	5:E:235:ALA:O	2.47	0.47
9:H:168:A:H5"	9:H:169:C:H5	1.80	0.47
15:N:113:PHE:CZ	16:O:35:ARG:HB3	2.49	0.47
22:U:15:THR:OG1	22:U:17:GLY:N	2.40	0.47
26:Y:46:CYS:C	26:Y:48:GLU:H	2.17	0.47
1:A:1332:HIS:ND1	1:A:1359:HIS:CE1	2.82	0.47
1:A:1537:TRP:HE3	1:A:1751:LEU:HD13	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:U:HO2'	2:B:28:A:P	2.37	0.47
2:B:61:A:H2'	2:B:62:G:C8	2.50	0.47
3:C:65:TYR:CD2	17:P:216:ARG:HD3	2.50	0.47
3:C:348:TYR:CE1	3:C:359:LYS:HB3	2.49	0.47
3:C:534:VAL:HG12	3:C:535:ALA:H	1.79	0.47
9:H:156:U:C2	9:H:157:G:C8	3.03	0.47
15:N:70:ILE:HG23	15:N:74:LEU:HD23	1.96	0.47
16:O:73:THR:OG1	16:O:74:CYS:N	2.47	0.47
20:T:318:ARG:HE	20:T:319:THR:CG2	2.28	0.47
24:W:467:VAL:HA	24:W:477:ALA:O	2.13	0.47
26:Y:38:PRO:HG2	26:Y:39:PHE:CE2	2.50	0.47
1:A:384:VAL:HA	3:C:331:PHE:CE2	2.49	0.47
1:A:888:GLN:O	1:A:889:ARG:HD3	2.15	0.47
1:A:1553:VAL:HG11	26:Y:7:LEU:HD12	1.97	0.47
1:A:1777:ILE:HG12	1:A:1860:GLN:HB2	1.96	0.47
1:A:1863:VAL:HG22	1:A:1865:ARG:H	1.79	0.47
1:A:1943:LEU:O	1:A:1947:ASN:HB2	2.14	0.47
3:C:59:LEU:HB3	3:C:61:GLU:HG2	1.97	0.47
3:C:693:GLU:H	3:C:696:LEU:HD12	1.78	0.47
6:F:48:A:H1'	13:L:33:ARG:CZ	2.44	0.47
11:J:436:TYR:CD1	11:J:437:LYS:HD2	2.46	0.47
18:R:123:GLU:OE2	18:R:123:GLU:N	2.42	0.47
18:R:138:GLU:O	18:R:142:GLU:HG2	2.13	0.47
23:V:250:LYS:HD3	23:V:288:ASP:CG	2.35	0.47
46:1:235:LEU:HA	46:1:245:LEU:O	2.14	0.47
1:A:1382:SER:HA	1:A:1415:GLY:HA2	1.96	0.47
3:C:126:SER:O	3:C:126:SER:OG	2.30	0.47
3:C:561:LYS:HD3	3:C:615:PRO:O	2.15	0.47
9:H:25:G:C2	9:H:26:A:N7	2.83	0.47
11:J:294:HIS:HE1	13:L:230:GLU:HB2	1.79	0.47
16:O:50:ARG:NH1	16:O:122:GLU:OE1	2.47	0.47
18:R:76:MET:HG2	19:S:95:ALA:CB	2.44	0.47
23:V:550:MET:O	23:V:554:LEU:HG	2.15	0.47
24:W:204:ASP:CG	24:W:205:VAL:N	2.68	0.47
1:A:312:TYR:CZ	3:C:882:GLY:HA3	2.49	0.47
1:A:982:GLU:OE1	1:A:1172:ASN:HB2	2.15	0.47
1:A:1134:TRP:O	1:A:1139:ARG:NH1	2.48	0.47
1:A:1870:ASP:OD2	1:A:1870:ASP:N	2.48	0.47
1:A:1941:ARG:O	1:A:1945:VAL:HG22	2.14	0.47
3:C:225:VAL:HG12	3:C:252:ALA:O	2.14	0.47
3:C:323:PHE:CE2	3:C:424:PHE:HE1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:325:LYS:HG2	3:C:329:ASP:OD1	2.14	0.47
3:C:343:LEU:HA	3:C:368:SER:OG	2.15	0.47
5:E:260:ARG:HD3	5:E:276:ILE:HG12	1.96	0.47
9:H:6:U:H2'	9:H:7:U:H6	1.80	0.47
9:H:156:U:C4	9:H:157:G:N7	2.83	0.47
9:H:160:A:H2'	9:H:161:U:C6	2.50	0.47
16:O:35:ARG:HD3	24:W:129:ARG:NE	2.29	0.47
18:R:134:ARG:NH2	20:T:339:GLN:OE1	2.48	0.47
19:S:14:VAL:HA	19:S:163:TYR:O	2.15	0.47
23:V:515:CYS:SG	23:V:522:MET:HA	2.54	0.47
1:A:839:LEU:O	1:A:843:LEU:HG	2.14	0.47
1:A:1638:ASN:HB3	1:A:1652:MET:O	2.15	0.47
1:A:1819:LEU:HB3	1:A:1915:VAL:HG13	1.97	0.47
1:A:1823:HIS:HB3	1:A:1912:PRO:HG3	1.95	0.47
1:A:1826:VAL:HG23	1:A:1827:TRP:CE3	2.50	0.47
5:E:158:TYR:OH	5:E:161:ARG:NH1	2.48	0.47
6:F:38:G:H2'	6:F:39:A:H8	1.74	0.47
6:F:83:A:O2'	6:F:84:A:OP2	2.30	0.47
9:H:156:U:C2	9:H:175:G:C2	3.03	0.47
14:M:162:PRO:HB3	14:M:167:LEU:HB2	1.97	0.47
15:N:120:ARG:NH1	15:N:142:CYS:HB2	2.29	0.47
16:O:51:PRO:HB3	18:R:212:PHE:CZ	2.50	0.47
16:O:278:GLN:O	16:O:282:VAL:HG23	2.15	0.47
18:R:111:VAL:CG1	20:T:366:VAL:HG22	2.45	0.47
20:T:213:GLU:HG3	20:T:218:TRP:CZ2	2.50	0.47
26:Y:28:ASP:OD1	26:Y:29:ARG:N	2.48	0.47
26:Y:67:VAL:HG12	26:Y:72:PRO:HA	1.96	0.47
1:A:43:LYS:NZ	24:W:168:PHE:HB3	2.29	0.47
1:A:372:PRO:HG3	3:C:341:LYS:O	2.15	0.47
1:A:1771:LEU:HD21	1:A:1930:TYR:HA	1.97	0.47
3:C:240:GLU:HG2	3:C:288:LEU:HD13	1.95	0.47
5:E:111:ALA:O	5:E:129:THR:HG23	2.15	0.47
16:O:226:PRO:HG3	16:O:302:TRP:CH2	2.50	0.47
23:V:577:SER:HA	23:V:580:ARG:HH11	1.80	0.47
26:Y:94:GLU:OE2	26:Y:95:ASN:HB2	2.15	0.47
47:2:54:GLY:HA2	47:2:101:LYS:HZ3	1.80	0.47
1:A:1650:ASP:OD2	1:A:1723:LYS:NZ	2.34	0.47
1:A:1783:THR:HG23	45:4:106:LYS:HZ3	1.79	0.47
3:C:461:LEU:HA	3:C:461:LEU:HD23	1.61	0.47
3:C:831:TYR:CE1	3:C:905:GLN:HB3	2.50	0.47
6:F:40:U:H3	8:6:7:G:H22	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:6:7:G:C4	8:6:8:C:C5	3.03	0.47
8:6:19:G:C2	8:6:20:A:C6	3.03	0.47
8:6:19:G:H2'	8:6:20:A:C8	2.49	0.47
9:H:34:U:H2'	9:H:35:A:C8	2.50	0.47
13:L:203:LYS:HD2	13:L:203:LYS:HA	1.51	0.47
16:O:239:LEU:HG	16:O:240:GLY:O	2.16	0.47
19:S:99:ALA:HA	19:S:129:PHE:H	1.80	0.47
20:T:415:ILE:HD12	20:T:432:ASP:OD2	2.14	0.47
23:V:303:LYS:HA	23:V:303:LYS:HD2	1.79	0.47
23:V:305:THR:OG1	23:V:306:GLN:NE2	2.47	0.47
24:W:177:LYS:HE3	24:W:177:LYS:HB3	1.65	0.47
1:A:64:GLU:H	1:A:64:GLU:CD	2.07	0.46
1:A:1076:ASP:O	1:A:1079:THR:OG1	2.25	0.46
1:A:1208:THR:HG21	23:V:553:HIS:CD2	2.50	0.46
1:A:1212:GLY:HA3	1:A:1280:ASN:HD21	1.80	0.46
5:E:313:ASP:HB2	5:E:320:LEU:HD21	1.96	0.46
8:6:87:U:O2	9:H:42:G:C2	2.67	0.46
16:O:80:VAL:HG12	16:O:94:ILE:HD11	1.97	0.46
24:W:180:LYS:HD3	24:W:199:TYR:CE2	2.50	0.46
24:W:204:ASP:CG	24:W:205:VAL:H	2.18	0.46
1:A:1300:LYS:HB3	1:A:1305:SER:O	2.15	0.46
3:C:524:ILE:HD12	3:C:569:ARG:HH22	1.80	0.46
3:C:693:GLU:N	3:C:696:LEU:HD12	2.30	0.46
6:F:16:G:C6	6:F:17:C:C4	3.04	0.46
9:H:156:U:C2	9:H:175:G:N2	2.83	0.46
17:P:205:LYS:HB3	17:P:208:LYS:HG2	1.96	0.46
19:S:9:TRP:C	19:S:11:PRO:HD3	2.36	0.46
23:V:182:ILE:HG21	23:V:221:ILE:HG12	1.98	0.46
23:V:306:GLN:OE1	23:V:352:ILE:HD11	2.15	0.46
24:W:204:ASP:OD2	24:W:205:VAL:HG23	2.16	0.46
46:1:295:ILE:HG22	46:1:296:LYS:O	2.15	0.46
1:A:48:LYS:HE3	1:A:48:LYS:HB3	1.77	0.46
1:A:191:ILE:CG1	1:A:571:ALA:HB1	2.45	0.46
1:A:191:ILE:O	1:A:191:ILE:HG22	2.14	0.46
1:A:312:TYR:HH	3:C:886:ASP:CG	2.12	0.46
1:A:951:LEU:HA	1:A:951:LEU:HD23	1.58	0.46
1:A:1891:LEU:HD23	1:A:1891:LEU:HA	1.68	0.46
2:B:55:C:H2'	2:B:56:C:H6	1.81	0.46
3:C:926:ALA:HA	3:C:929:LEU:HG	1.97	0.46
13:L:53:TRP:CE2	13:L:60:LYS:HE2	2.50	0.46
17:P:25:GLN:HG2	17:P:25:GLN:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:67:ILE:HG22	18:R:69:VAL:HG23	1.97	0.46
20:T:405:PHE:O	20:T:407:GLN:N	2.48	0.46
27:Z:1124:MET:HA	27:Z:1127:LYS:O	2.15	0.46
1:A:131:GLU:OE2	1:A:132:ILE:N	2.45	0.46
1:A:643:GLY:HA3	2:B:28:A:O2'	2.14	0.46
1:A:1931:THR:O	1:A:1934:SER:OG	2.30	0.46
2:B:88:A:H4'	2:B:94:U:O4	2.15	0.46
3:C:813:ARG:NH1	3:C:813:ARG:HB2	2.30	0.46
6:F:88:G:O6	14:M:198:ARG:HD3	2.14	0.46
9:H:29:A:H2	9:H:31:G:C6	2.33	0.46
24:W:318:VAL:C	24:W:320:GLY:H	2.18	0.46
26:Y:68:TYR:CD1	26:Y:69:LEU:HG	2.50	0.46
46:1:314:GLU:N	46:1:314:GLU:OE1	2.49	0.46
1:A:195:LEU:HD11	1:A:208:TYR:CE2	2.50	0.46
1:A:702:LYS:O	1:A:705:LYS:NZ	2.31	0.46
3:C:623:GLU:C	3:C:625:GLY:H	2.18	0.46
5:E:264:VAL:HA	5:E:272:ARG:HH21	1.79	0.46
12:K:74:ALA:O	12:K:78:PRO:HA	2.16	0.46
19:S:125:LYS:HE3	19:S:126:HIS:CE1	2.50	0.46
1:A:549:GLU:HB3	1:A:591:MET:HG2	1.98	0.46
3:C:137:HIS:HD2	3:C:238:ASN:H	1.63	0.46
5:E:281:VAL:N	5:E:304:SER:OG	2.47	0.46
6:F:41:A:H2'	6:F:42:C:H6	1.78	0.46
6:F:48:A:N3	13:L:33:ARG:NH2	2.53	0.46
8:6:6:A:C5	8:6:7:G:N7	2.83	0.46
11:J:223:TYR:HA	11:J:226:ARG:CZ	2.46	0.46
11:J:288:LYS:HD2	14:M:190:ILE:HD11	1.97	0.46
13:L:66:GLU:H	13:L:66:GLU:CD	2.19	0.46
16:O:38:LYS:HB2	18:R:199:MET:HE1	1.98	0.46
25:X:34:ARG:HA	25:X:37:ILE:CD1	2.43	0.46
47:2:166:GLU:HB2	47:2:168:LYS:HD3	1.98	0.46
1:A:302:ILE:HD12	3:C:657:ASP:OD1	2.16	0.46
1:A:464:PRO:HG2	2:B:20:G:H2'	1.97	0.46
1:A:1660:TYR:OH	1:A:1717:ASN:O	2.24	0.46
3:C:259:LYS:HG2	50:C:1500:GTP:C2	2.51	0.46
8:6:21:A:H5'	8:6:21:A:H8	1.81	0.46
9:H:161:U:O2	9:H:163:G:N2	2.47	0.46
11:J:296:ARG:HD2	13:L:225:TYR:CZ	2.51	0.46
11:J:325:ASN:CB	14:M:172:HIS:HD2	2.24	0.46
15:N:120:ARG:HD2	15:N:142:CYS:SG	2.55	0.46
17:P:26:LEU:HD12	17:P:26:LEU:HA	1.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:14:VAL:HG12	19:S:25:LEU:HB2	1.97	0.46
24:W:188:ASN:OD1	24:W:188:ASN:N	2.48	0.46
46:1:203:ASP:OD1	46:1:203:ASP:N	2.46	0.46
46:1:469:ILE:HG23	46:1:470:THR:H	1.81	0.46
1:A:1084:PRO:HG2	17:P:188:TRP:CD2	2.51	0.46
1:A:1495:PHE:CD2	1:A:1501:LEU:HD11	2.51	0.46
12:K:65:ILE:O	12:K:67:ARG:N	2.48	0.46
13:L:39:HIS:H	13:L:151:MET:HE1	1.81	0.46
16:O:158:LYS:HG3	16:O:161:ARG:CD	2.46	0.46
24:W:146:HIS:HB3	24:W:148:VAL:O	2.15	0.46
47:2:101:LYS:HG2	47:2:107:ILE:CD1	2.45	0.46
1:A:377:GLU:O	1:A:378:PHE:HB2	2.16	0.46
1:A:469:LYS:NZ	2:B:59:G:C6	2.84	0.46
1:A:658:ARG:NH1	6:F:67:G:OP1	2.49	0.46
3:C:724:TRP:HD1	3:C:729:ALA:HB2	1.79	0.46
5:E:266:PRO:HG2	13:L:785:GLN:HB2	1.97	0.46
18:R:178:ARG:NH1	24:W:143:LEU:HD21	2.31	0.46
23:V:297:LEU:HB3	23:V:339:MET:HE3	1.98	0.46
25:X:16:THR:O	25:X:20:VAL:HG23	2.16	0.46
1:A:359:ILE:HB	23:V:324:HIS:NE2	2.31	0.46
1:A:1014:ASN:HD21	13:L:84:THR:N	2.13	0.46
1:A:1083:HIS:NE2	17:P:189:ASP:OD1	2.43	0.46
1:A:1258:LYS:HE2	8:6:102:G:C6	2.51	0.46
3:C:182:LYS:HA	3:C:214:GLU:OE2	2.16	0.46
3:C:556:ASP:OD1	3:C:556:ASP:N	2.33	0.46
3:C:567:GLU:O	3:C:567:GLU:HG3	2.16	0.46
3:C:590:ILE:HD11	3:C:637:LEU:HD13	1.98	0.46
6:F:2:U:C2	6:F:3:G:C8	3.03	0.46
9:H:112:G:H2'	9:H:113:G:C8	2.48	0.46
13:L:154:GLU:HG3	13:L:155:ALA:N	2.30	0.46
18:R:79:LYS:HG3	18:R:81:LYS:HZ3	1.81	0.46
1:A:705:LYS:H	1:A:705:LYS:HD2	1.80	0.45
1:A:762:ARG:HH22	17:P:226:LYS:NZ	2.13	0.45
1:A:1621:LYS:HE3	1:A:1623:ASN:HD21	1.80	0.45
1:A:1790:ILE:HG21	1:A:1798:LEU:HB3	1.98	0.45
2:B:23:C:C5	2:B:26:A:N7	2.83	0.45
3:C:415:LEU:HD12	3:C:415:LEU:HA	1.54	0.45
3:C:657:ASP:OD2	3:C:657:ASP:N	2.49	0.45
5:E:322:LYS:HB3	24:W:88:MET:HE2	1.97	0.45
8:6:6:A:N6	8:6:7:G:C6	2.84	0.45
9:H:153:A:C5	9:H:154:C:C6	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:258:ILE:HG12	13:L:232:TYR:CE2	2.51	0.45
16:O:174:LYS:HA	24:W:205:VAL:HG13	1.97	0.45
1:A:182:ILE:HD11	1:A:562:VAL:HG13	1.98	0.45
1:A:381:PRO:HD2	3:C:334:ILE:HG22	1.98	0.45
1:A:989:ASP:OD1	1:A:990:LEU:N	2.49	0.45
1:A:1274:PHE:O	1:A:1275:ARG:HB2	2.16	0.45
2:B:30:A:O2'	2:B:31:U:H5'	2.16	0.45
3:C:732:ILE:HA	3:C:746:VAL:HG22	1.98	0.45
5:E:116:HIS:O	5:E:124:LEU:HD12	2.16	0.45
5:E:285:GLU:OE1	24:W:121:ASN:HB3	2.17	0.45
11:J:343:GLU:OE1	11:J:373:HIS:ND1	2.49	0.45
18:R:280:ILE:HD12	18:R:281:ASN:N	2.32	0.45
23:V:311:GLY:O	23:V:315:ILE:HG13	2.16	0.45
26:Y:39:PHE:HE1	26:Y:100:MET:CE	2.29	0.45
46:1:185:VAL:O	46:1:475:VAL:HG21	2.16	0.45
1:A:81:PHE:O	1:A:83:HIS:N	2.49	0.45
1:A:1808:PHE:CZ	1:A:1817:LEU:HD13	2.51	0.45
1:A:1953:ILE:O	1:A:1956:PRO:HD3	2.15	0.45
3:C:175:GLN:NE2	3:C:536:ARG:HH12	2.14	0.45
3:C:711:ARG:NH2	3:C:730:ARG:O	2.49	0.45
5:E:81:LEU:O	5:E:92:LEU:HA	2.16	0.45
5:E:167:VAL:O	5:E:178:LEU:HD12	2.16	0.45
15:N:124:SER:O	15:N:127:GLU:HG2	2.16	0.45
17:P:229:LYS:HD2	17:P:229:LYS:HA	1.68	0.45
24:W:135:TYR:OH	24:W:165:LEU:HD11	2.15	0.45
1:A:1503:TRP:CE2	1:A:1753:LEU:HD21	2.51	0.45
2:B:32:C:O2'	2:B:33:U:H5'	2.16	0.45
2:B:100:C:H2'	2:B:101:U:C5	2.50	0.45
3:C:396:LEU:HA	3:C:396:LEU:HD12	1.83	0.45
5:E:192:ASN:OD1	5:E:218:LYS:NZ	2.45	0.45
8:6:88:G:C2	8:6:89:U:C4	3.04	0.45
9:H:6:U:H2'	9:H:7:U:C6	2.51	0.45
9:H:45:C:H2'	9:H:46:U:H6	1.80	0.45
9:H:89:U:H2'	9:H:90:A:C8	2.46	0.45
20:T:412:HIS:HB2	20:T:437:HIS:CE1	2.51	0.45
23:V:554:LEU:O	23:V:559:SER:N	2.49	0.45
44:3:160:PHE:HA	44:3:166:ASP:O	2.16	0.45
1:A:352:PHE:HB3	23:V:320:ARG:NH2	2.31	0.45
1:A:549:GLU:OE1	1:A:552:ARG:NH1	2.49	0.45
1:A:995:ARG:HA	1:A:995:ARG:HD2	1.87	0.45
1:A:1896:CYS:HB2	1:A:1940:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:A:3000:IHP:O24	49:A:3000:IHP:H3	2.16	0.45
2:B:24:G:O4'	2:B:57:G:N2	2.50	0.45
2:B:88:A:H2'	2:B:88:A:N3	2.32	0.45
3:C:733:TRP:CE2	3:C:763:LYS:HG3	2.51	0.45
5:E:92:LEU:HB3	5:E:102:TYR:CZ	2.52	0.45
5:E:193:THR:HG23	5:E:194:TYR:CD2	2.52	0.45
5:E:206:ASP:C	5:E:222:LEU:HG	2.37	0.45
6:F:86:U:O2'	6:F:87:C:O5'	2.30	0.45
7:G:-12:G:H4'	7:G:-11:G:OP1	2.16	0.45
15:N:25:LEU:HD23	15:N:25:LEU:HA	1.81	0.45
19:S:98:LEU:O	19:S:129:PHE:N	2.48	0.45
20:T:352:THR:HG22	20:T:373:LYS:C	2.37	0.45
23:V:294:ILE:HG13	23:V:295:GLY:N	2.30	0.45
24:W:167:VAL:HG23	24:W:168:PHE:CD1	2.52	0.45
46:1:454:VAL:CG2	46:1:463:ARG:HG3	2.47	0.45
46:1:490:THR:HG22	46:1:494:LEU:HB2	1.98	0.45
1:A:1112:ARG:O	1:A:1115:THR:HB	2.16	0.45
1:A:1253:SER:O	1:A:1253:SER:OG	2.35	0.45
1:A:1285:LEU:HA	1:A:1285:LEU:HD23	1.64	0.45
1:A:1337:GLN:OE1	1:A:1354:ARG:HD3	2.16	0.45
1:A:1418:ARG:O	1:A:1420:ASN:N	2.49	0.45
1:A:1527:ASN:HD22	8:6:102:G:N2	2.15	0.45
1:A:1784:ASN:OD1	1:A:1806:ALA:HB3	2.17	0.45
1:A:2006:GLU:OE2	1:A:2006:GLU:N	2.49	0.45
2:B:62:G:C2	2:B:63:A:C4	3.05	0.45
3:C:177:ARG:NH2	3:C:638:ASP:OD2	2.45	0.45
3:C:183:SER:OG	3:C:184:THR:N	2.50	0.45
3:C:497:LEU:HD13	3:C:577:PHE:CZ	2.51	0.45
3:C:509:VAL:O	3:C:510:LEU:HD23	2.16	0.45
11:J:204:GLU:HG3	11:J:204:GLU:O	2.17	0.45
11:J:278:LEU:HA	11:J:278:LEU:HD12	1.74	0.45
20:T:188:PRO:HG3	20:T:443:THR:CG2	2.43	0.45
23:V:242:ARG:NH1	23:V:372:LEU:O	2.50	0.45
25:X:13:HIS:ND1	26:Y:98:TYR:OH	2.49	0.45
47:2:132:ILE:HG23	47:2:132:ILE:O	2.17	0.45
47:2:133:GLY:O	47:2:137:GLN:HG3	2.17	0.45
1:A:386:PRO:HD3	3:C:372:PHE:CE1	2.52	0.45
1:A:758:ARG:O	1:A:758:ARG:HG3	2.15	0.45
1:A:1831:LYS:HZ3	1:A:1832:ARG:N	2.12	0.45
1:A:1852:LEU:HD12	1:A:1853:PRO:HD2	1.97	0.45
3:C:847:TYR:CD1	3:C:857:VAL:HG21	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:823:ALA:O	4:D:857:GLY:N	2.37	0.45
6:F:17:C:C2	6:F:18:A:C8	3.04	0.45
6:F:30:A:N6	8:6:16:G:H1'	2.30	0.45
11:J:291:GLN:HA	13:L:230:GLU:OE2	2.17	0.45
13:L:213:GLU:OE1	16:O:109:LYS:N	2.44	0.45
15:N:131:ILE:O	15:N:132:ILE:HD13	2.16	0.45
46:1:185:VAL:HG11	46:1:489:GLY:HA3	1.99	0.45
46:1:231:GLN:HE22	46:1:233:LYS:NZ	2.15	0.45
47:2:100:VAL:HG23	47:2:108:ALA:HB3	1.99	0.45
1:A:733:THR:OG1	1:A:734:PRO:HD3	2.16	0.45
1:A:1298:ARG:HD2	1:A:1298:ARG:HA	1.68	0.45
2:B:66:A:H2'	2:B:67:A:H8	1.82	0.45
2:B:108:G:H3'	2:B:109:G:H8	1.81	0.45
6:F:5:U:H3'	6:F:7:G:H5'	1.99	0.45
7:G:-1:G:O3'	26:Y:4:ARG:HD2	2.17	0.45
17:P:191:ASP:N	17:P:191:ASP:OD1	2.50	0.45
23:V:261:ALA:HB2	23:V:296:PHE:CE1	2.52	0.45
47:2:258:LYS:HA	47:2:258:LYS:HD3	1.83	0.45
1:A:441:VAL:O	1:A:445:VAL:HG23	2.16	0.45
1:A:1055:LEU:HA	1:A:1055:LEU:HD23	1.77	0.45
2:B:59:G:C4	2:B:60:G:C8	3.05	0.45
11:J:360:ASP:O	11:J:363:ARG:HG2	2.17	0.45
15:N:63:LEU:HD23	15:N:67:ARG:HD2	1.99	0.45
19:S:99:ALA:HA	19:S:129:PHE:HB2	1.99	0.45
23:V:303:LYS:O	23:V:307:VAL:HG22	2.17	0.45
24:W:189:ILE:C	24:W:191:GLY:H	2.20	0.45
46:1:480:HIS:CD2	46:1:482:LYS:H	2.31	0.45
1:A:443:VAL:O	1:A:447:TYR:HD2	1.99	0.45
1:A:793:ASN:O	1:A:797:ASP:HB2	2.17	0.45
1:A:1201:ARG:O	1:A:1203:SER:N	2.48	0.45
3:C:449:ILE:HG22	3:C:456:GLY:O	2.17	0.45
3:C:524:ILE:HD12	3:C:569:ARG:NH2	2.32	0.45
5:E:281:VAL:O	5:E:304:SER:OG	2.35	0.45
15:N:27:GLN:NE2	15:N:31:GLU:OE2	2.50	0.45
16:O:90:TYR:O	16:O:92:LEU:HG	2.17	0.45
18:R:214:ILE:O	18:R:216:LYS:N	2.49	0.45
46:1:195:ALA:HB1	46:1:211:PHE:HD2	1.82	0.45
46:1:300:MET:SD	46:1:347:ILE:HD13	2.57	0.45
46:1:381:THR:HA	46:1:397:GLY:HA2	1.99	0.45
1:A:249:LEU:HA	1:A:249:LEU:HD13	1.83	0.44
1:A:762:ARG:HH22	17:P:226:LYS:HZ3	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:996:LEU:HD23	1:A:996:LEU:HA	1.74	0.44
1:A:1766:GLN:CD	1:A:1766:GLN:H	2.20	0.44
2:B:29:A:H2'	2:B:30:A:C8	2.49	0.44
2:B:62:G:H2'	2:B:63:A:C8	2.51	0.44
3:C:233:GLU:OE2	3:C:837:GLN:NE2	2.43	0.44
3:C:474:LEU:HD13	3:C:505:GLN:HE22	1.82	0.44
3:C:668:GLU:N	3:C:824:THR:HG21	2.32	0.44
3:C:736:GLY:HA3	3:C:737:PRO:HD3	1.89	0.44
8:6:5:G:H3'	8:6:6:A:C2	2.51	0.44
11:J:191:ALA:N	13:L:17:GLU:OE1	2.50	0.44
18:R:139:ALA:O	18:R:143:ILE:HG12	2.17	0.44
18:R:229:VAL:HG23	18:R:230:MET:N	2.30	0.44
19:S:101:ALA:HB1	24:W:95:PRO:HD3	1.99	0.44
26:Y:94:GLU:OE2	26:Y:95:ASN:N	2.50	0.44
1:A:284:ARG:HD2	1:A:284:ARG:O	2.17	0.44
1:A:1295:ILE:HG13	1:A:1296:GLN:N	2.32	0.44
1:A:1922:ASP:OD2	1:A:1966:HIS:NE2	2.51	0.44
2:B:12:U:H2'	2:B:13:C:H6	1.82	0.44
5:E:124:LEU:HD12	5:E:124:LEU:HA	1.71	0.44
9:H:5:C:H2'	9:H:6:U:C6	2.52	0.44
9:H:25:G:H2'	9:H:26:A:C8	2.48	0.44
16:O:26:THR:OG1	16:O:27:CYS:N	2.50	0.44
18:R:87:ALA:HB1	19:S:20:MET:HE1	1.98	0.44
20:T:405:PHE:O	20:T:406:ILE:C	2.56	0.44
24:W:199:TYR:O	24:W:201:ASP:N	2.49	0.44
24:W:354:ARG:HA	24:W:376:PRO:HD3	2.00	0.44
26:Y:35:LEU:HA	26:Y:35:LEU:HD23	1.51	0.44
47:2:97:PHE:CE2	47:2:117:LEU:HD21	2.52	0.44
1:A:393:LEU:HD12	1:A:393:LEU:HA	1.69	0.44
1:A:1284:LEU:HA	1:A:1284:LEU:HD23	1.57	0.44
1:A:1416:ILE:HD13	1:A:1416:ILE:HA	1.80	0.44
2:B:15:C:H2'	2:B:16:U:H6	1.82	0.44
3:C:259:LYS:CG	50:C:1500:GTP:C6	3.00	0.44
3:C:674:CYS:HB2	3:C:818:SER:HB3	1.99	0.44
6:F:50:A:HO2'	6:F:51:U:P	2.38	0.44
16:O:212:LYS:HE3	16:O:212:LYS:HB3	1.84	0.44
20:T:455:GLN:HG3	20:T:485:THR:CG2	2.44	0.44
1:A:73:HIS:O	1:A:74:GLY:C	2.55	0.44
1:A:257:LEU:HD23	1:A:257:LEU:HA	1.82	0.44
1:A:467:GLN:NE2	2:B:20:G:H2'	2.32	0.44
1:A:830:LEU:H	1:A:830:LEU:HG	1.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:883:ARG:HG3	1:A:883:ARG:NH1	2.32	0.44
1:A:1501:LEU:HD12	1:A:1753:LEU:HD13	1.98	0.44
3:C:878:ILE:HG13	3:C:879:ASP:N	2.33	0.44
11:J:276:ILE:HG13	11:J:277:THR:N	2.33	0.44
13:L:202:ARG:O	13:L:203:LYS:HD3	2.17	0.44
18:R:310:ARG:O	18:R:314:GLN:HG2	2.17	0.44
24:W:137:TYR:CE2	24:W:164:GLY:HA2	2.50	0.44
46:1:348:ALA:HA	46:1:358:ILE:HD13	1.98	0.44
48:5:22:UNK:C	48:5:24:UNK:N	2.78	0.44
1:A:178:TYR:HB2	1:A:494:LEU:HD12	2.00	0.44
1:A:378:PHE:HB2	3:C:342:ARG:NH1	2.33	0.44
1:A:1032:ARG:H	1:A:1032:ARG:HD2	1.82	0.44
1:A:1275:ARG:C	1:A:1276:GLU:HG3	2.38	0.44
1:A:1536:LEU:HA	1:A:1536:LEU:HD23	1.57	0.44
1:A:1560:ILE:HD13	1:A:1573:LEU:HD13	2.00	0.44
1:A:1639:VAL:CG1	1:A:1717:ASN:HB3	2.48	0.44
1:A:1923:TRP:CE3	1:A:1935:ARG:HD2	2.52	0.44
1:A:1957:ASP:O	1:A:1960:THR:OG1	2.13	0.44
3:C:323:PHE:CE1	3:C:373:ILE:HG12	2.53	0.44
5:E:115:LEU:HA	5:E:125:PHE:O	2.18	0.44
6:F:34:G:H22	8:6:12:G:C2'	2.31	0.44
8:6:84:U:H2'	8:6:85:G:H8	1.82	0.44
11:J:196:ARG:NE	46:1:612:ALA:HB1	2.33	0.44
16:O:179:CYS:SG	16:O:181:TYR:HB2	2.58	0.44
20:T:287:HIS:CE1	20:T:307:SER:HG	2.36	0.44
46:1:345:ASN:N	46:1:345:ASN:OD1	2.51	0.44
47:2:109:LEU:HD23	47:2:138:TRP:CD1	2.52	0.44
1:A:312:TYR:HH	3:C:853:ARG:NH2	2.15	0.44
1:A:1869:LEU:HA	1:A:1869:LEU:HD23	1.72	0.44
1:A:1968:TRP:HA	1:A:1968:TRP:HE3	1.82	0.44
1:A:1971:LEU:HB3	1:A:1975:GLU:HB2	2.00	0.44
3:C:215:VAL:HG11	3:C:242:LEU:HD22	2.00	0.44
3:C:531:TRP:CZ3	3:C:540:GLU:HB2	2.53	0.44
3:C:589:LYS:HG3	3:C:628:VAL:HG13	2.00	0.44
3:C:799:GLU:HG3	3:C:801:LEU:CD2	2.47	0.44
7:G:-1:G:H8	7:G:-1:G:OP1	2.01	0.44
13:L:101:GLU:CD	26:Y:163:ARG:HH21	2.20	0.44
14:M:160:PHE:C	14:M:161:PHE:HD1	2.21	0.44
16:O:146:MET:O	16:O:149:LYS:N	2.51	0.44
23:V:226:PHE:HB3	23:V:229:ILE:HG12	1.99	0.44
1:A:76:MET:HE1	1:A:88:TYR:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:TRP:O	1:A:331:TRP:HE3	2.01	0.44
1:A:588:LEU:HA	1:A:588:LEU:HD23	1.67	0.44
1:A:686:ARG:NH2	1:A:710:LEU:HB3	2.33	0.44
1:A:1224:ARG:HD3	1:A:1224:ARG:HA	1.63	0.44
1:A:1317:TYR:CE1	1:A:1329:SER:HB3	2.52	0.44
1:A:1790:ILE:HG23	1:A:1800:THR:HG22	2.00	0.44
2:B:106:U:H2'	2:B:107:U:C6	2.53	0.44
3:C:77:VAL:HG11	20:T:196:LEU:HD23	2.00	0.44
3:C:337:GLN:O	3:C:341:LYS:HG3	2.18	0.44
3:C:383:GLN:O	3:C:387:ASP:HB2	2.18	0.44
3:C:725:ASP:OD1	3:C:727:LEU:N	2.50	0.44
3:C:730:ARG:N	3:C:730:ARG:HD2	2.32	0.44
6:F:24:A:C5	16:O:65:PHE:HE2	2.36	0.44
10:I:50:LYS:CB	10:I:51:PRO:HD3	2.47	0.44
11:J:411:MET:HE1	11:J:415:LEU:HB3	1.99	0.44
13:L:703:MET:O	13:L:707:ALA:HB3	2.17	0.44
16:O:253:TYR:HB2	18:R:68:HIS:O	2.18	0.44
18:R:132:LEU:O	18:R:133:GLN:HG2	2.16	0.44
19:S:99:ALA:HB2	19:S:128:ILE:HA	1.99	0.44
23:V:158:SER:O	23:V:162:LEU:HG	2.18	0.44
23:V:314:ALA:O	23:V:318:ARG:HG2	2.18	0.44
23:V:622:ARG:HA	23:V:625:ARG:HH11	1.83	0.44
1:A:75:ASP:O	1:A:77:THR:N	2.41	0.44
1:A:76:MET:HE3	1:A:76:MET:HB2	1.55	0.44
1:A:1323:GLY:HA2	1:A:1529:ILE:HD11	2.00	0.44
1:A:1528:GLN:O	1:A:1530:PRO:HD3	2.18	0.44
1:A:1763:LEU:HB2	1:A:1887:SER:HA	2.00	0.44
3:C:63:LYS:HG3	3:C:65:TYR:CE1	2.53	0.44
3:C:199:LEU:HD12	3:C:199:LEU:HA	1.79	0.44
5:E:265:ARG:H	5:E:272:ARG:HH21	1.64	0.44
6:F:11:C:O2'	6:F:12:G:H8	2.00	0.44
8:6:2:U:O2	8:6:2:U:O4'	2.34	0.44
10:I:406:GLU:HA	10:I:410:GLN:CA	2.47	0.44
11:J:206:LEU:HD11	13:L:171:ALA:HB1	2.00	0.44
18:R:180:THR:HA	18:R:181:PRO:HD3	1.80	0.44
20:T:385:TYR:CE2	20:T:401:PRO:HD3	2.52	0.44
24:W:135:TYR:CZ	24:W:165:LEU:HD11	2.53	0.44
1:A:53:PHE:CE2	1:A:55:ASP:HB3	2.53	0.44
1:A:332:TYR:C	1:A:332:TYR:CD1	2.91	0.44
1:A:357:ASN:HB2	3:C:863:ILE:O	2.18	0.44
1:A:702:LYS:HB2	1:A:705:LYS:NZ	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:366:GLN:OE1	3:C:370:VAL:HG21	2.17	0.44
3:C:709:TRP:HB3	3:C:713:LYS:HB2	1.98	0.44
9:H:70:C:H2'	9:H:71:C:C6	2.53	0.44
13:L:40:ARG:HG3	26:Y:109:GLN:HE22	1.82	0.44
13:L:154:GLU:HB3	26:Y:49:TYR:HE2	1.83	0.44
18:R:103:ARG:HD3	18:R:108:LYS:HA	2.00	0.44
19:S:149:SER:OG	19:S:150:GLN:NE2	2.42	0.44
47:2:101:LYS:HG2	47:2:107:ILE:HD12	2.00	0.44
1:A:103:LEU:O	1:A:105:ASN:N	2.51	0.43
1:A:409:ARG:HD2	2:B:25:C:O2'	2.18	0.43
4:D:1583:ASP:O	4:D:1585:GLN:N	2.51	0.43
14:M:150:GLU:OE2	14:M:153:ARG:HD3	2.18	0.43
15:N:126:LEU:O	15:N:128:VAL:HG23	2.18	0.43
19:S:57:ILE:HG21	24:W:97:ASN:CB	2.48	0.43
19:S:66:ASP:OD1	19:S:68:THR:OG1	2.33	0.43
20:T:203:HIS:CE1	20:T:223:SER:OG	2.71	0.43
20:T:307:SER:OG	20:T:309:ASP:OD1	2.36	0.43
24:W:205:VAL:HG12	24:W:207:LYS:HD2	2.00	0.43
46:1:329:GLN:O	46:1:329:GLN:HG2	2.18	0.43
1:A:697:MET:HG3	1:A:701:ILE:HD12	1.99	0.43
1:A:956:CYS:HB3	1:A:1216:LEU:HD11	2.00	0.43
1:A:1131:LYS:NZ	1:A:1193:GLU:OE1	2.41	0.43
1:A:1898:LYS:HD3	1:A:1898:LYS:N	2.33	0.43
1:A:1919:LEU:HD23	1:A:1967:ILE:HD13	1.99	0.43
1:A:1965:HIS:O	1:A:1966:HIS:ND1	2.38	0.43
3:C:85:ASP:HB3	20:T:238:LEU:HG	1.99	0.43
3:C:267:LEU:HB3	3:C:269:LEU:HG	1.99	0.43
3:C:589:LYS:HB3	3:C:659:VAL:O	2.17	0.43
4:D:148:LEU:C	4:D:150:ASP:N	2.72	0.43
5:E:68:GLU:O	5:E:85:GLY:HA3	2.18	0.43
5:E:224:GLN:O	5:E:226:LYS:HG3	2.18	0.43
9:H:7:U:H2'	9:H:8:C:H6	1.80	0.43
9:H:169:C:H2'	9:H:170:C:C6	2.54	0.43
13:L:86:ALA:HB1	13:L:91:ARG:O	2.18	0.43
14:M:121:ASP:O	14:M:122:LEU:HD13	2.18	0.43
16:O:111:ASP:O	16:O:115:GLU:HG3	2.18	0.43
18:R:211:ARG:HB2	18:R:211:ARG:NH1	2.33	0.43
19:S:42:LEU:HB3	19:S:47:TYR:HB3	2.00	0.43
23:V:530:LYS:HA	23:V:533:TYR:CZ	2.53	0.43
1:A:833:LYS:HE3	1:A:834:HIS:HE1	1.81	0.43
1:A:1418:ARG:HD3	1:A:1418:ARG:HA	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1876:LEU:HA	1:A:1876:LEU:HD23	1.75	0.43
3:C:69:ALA:HA	20:T:456:PRO:CG	2.42	0.43
3:C:255:VAL:O	3:C:307:VAL:HA	2.18	0.43
3:C:512:GLU:HG2	3:C:562:THR:HB	2.01	0.43
3:C:750:LEU:HB3	3:C:751:PRO:HD3	2.01	0.43
3:C:763:LYS:HD2	3:C:764:ASP:OD1	2.18	0.43
6:F:45:A:C8	8:6:3:A:C2	3.07	0.43
8:6:99:C:H5"	8:6:100:C:OP2	2.19	0.43
9:H:40:C:H2'	9:H:41:U:C6	2.52	0.43
14:M:160:PHE:C	14:M:162:PRO:HD3	2.38	0.43
17:P:31:SER:N	17:P:34:ASP:OD2	2.51	0.43
17:P:44:ARG:NH1	17:P:49:ASP:HB3	2.34	0.43
23:V:331:ARG:HG2	23:V:335:MET:HE2	2.00	0.43
25:X:19:ASN:O	25:X:23:VAL:HG23	2.19	0.43
26:Y:97:ASP:C	26:Y:97:ASP:OD2	2.56	0.43
1:A:410:PRO:HG2	1:A:411:PHE:CD2	2.53	0.43
1:A:710:LEU:HD23	1:A:710:LEU:HA	1.77	0.43
1:A:797:ASP:OD1	3:C:63:LYS:HE3	2.19	0.43
1:A:1050:LEU:HA	1:A:1050:LEU:HD23	1.66	0.43
1:A:1495:PHE:CE2	1:A:1501:LEU:HD11	2.53	0.43
1:A:1953:ILE:HD13	1:A:1982:GLN:HB3	1.99	0.43
2:B:66:A:H2'	2:B:67:A:C8	2.53	0.43
3:C:594:PRO:HG3	3:C:600:LEU:HA	1.99	0.43
5:E:314:THR:HG23	5:E:315:THR:HG23	1.99	0.43
6:F:34:G:C5'	13:L:203:LYS:HE2	2.48	0.43
6:F:58:G:C6	6:F:78:A:N1	2.86	0.43
6:F:89:U:C4	9:H:10:C:N3	2.86	0.43
8:6:105:C:H4'	8:6:106:C:OP1	2.16	0.43
10:I:148:ILE:O	10:I:152:TYR:N	2.44	0.43
16:O:90:TYR:HB3	16:O:92:LEU:HD12	2.00	0.43
18:R:66:GLU:O	18:R:68:HIS:HD2	2.00	0.43
20:T:196:LEU:HD12	20:T:196:LEU:HA	1.74	0.43
23:V:620:ASN:HB3	23:V:623:ASN:HB2	2.01	0.43
26:Y:68:TYR:HD1	26:Y:69:LEU:HG	1.84	0.43
46:1:310:THR:OG1	46:1:320:LYS:HB2	2.18	0.43
1:A:175:PRO:HG2	1:A:498:ARG:NH2	2.33	0.43
1:A:952:VAL:HG22	1:A:1189:MET:HB3	1.99	0.43
1:A:1146:ASP:OD2	1:A:1182:ASN:ND2	2.52	0.43
1:A:1570:LYS:NZ	26:Y:6:VAL:O	2.51	0.43
1:A:1637:TRP:O	1:A:1656:THR:HA	2.18	0.43
1:A:1866:LYS:HG3	1:A:1867:GLY:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:1:G:H2'	6:F:2:U:C6	2.54	0.43
6:F:49:G:H2'	6:F:50:A:H8	1.82	0.43
6:F:97:U:O5'	6:F:97:U:H6	2.01	0.43
9:H:24:A:HO2'	9:H:25:G:P	2.41	0.43
10:I:565:ILE:HA	10:I:569:GLY:HA3	1.99	0.43
11:J:212:GLN:HE21	13:L:182:LEU:HD13	1.84	0.43
17:P:207:ASP:OD2	17:P:208:LYS:HE2	2.18	0.43
19:S:57:ILE:O	19:S:116:LEU:HD12	2.19	0.43
20:T:308:ARG:HG3	20:T:332:ALA:HB2	2.01	0.43
23:V:476:LEU:HA	23:V:476:LEU:HD23	1.71	0.43
26:Y:39:PHE:HE1	26:Y:100:MET:HE3	1.84	0.43
1:A:409:ARG:HG2	1:A:409:ARG:HH11	1.84	0.43
1:A:469:LYS:NZ	2:B:59:G:C5	2.86	0.43
1:A:1922:ASP:OD2	1:A:1966:HIS:CE1	2.71	0.43
2:B:36:C:C2	2:B:37:G:C8	3.06	0.43
7:G:-2:C:C3'	7:G:-1:G:H5"	2.39	0.43
8:6:7:G:O2'	8:6:8:C:H5'	2.19	0.43
9:H:92:U:H2'	9:H:93:A:C8	2.54	0.43
11:J:314:TYR:O	11:J:317:THR:OG1	2.31	0.43
13:L:148:GLU:O	13:L:151:MET:HB2	2.19	0.43
15:N:116:ASN:OD1	15:N:116:ASN:N	2.51	0.43
16:O:32:PRO:HG2	16:O:33:TYR:CD2	2.53	0.43
18:R:279:HIS:ND1	18:R:279:HIS:N	2.66	0.43
20:T:427:LEU:O	20:T:439:TRP:HD1	2.00	0.43
23:V:199:ARG:HD3	23:V:383:ASN:ND2	2.34	0.43
23:V:228:GLN:HG2	23:V:229:ILE:HD13	1.99	0.43
23:V:302:LEU:CD1	23:V:306:GLN:HE22	2.32	0.43
24:W:154:GLY:C	24:W:156:VAL:H	2.22	0.43
1:A:228:TRP:CD1	1:A:416:GLY:O	2.72	0.43
1:A:589:THR:OG1	1:A:590:GLY:N	2.51	0.43
1:A:784:LEU:HD23	1:A:784:LEU:HA	1.80	0.43
1:A:883:ARG:HG3	1:A:883:ARG:HH11	1.83	0.43
1:A:1386:TRP:HE1	1:A:1417:PRO:HD2	1.84	0.43
3:C:134:LEU:HD23	3:C:226:VAL:HB	2.01	0.43
3:C:733:TRP:CH2	3:C:759:LEU:HD11	2.53	0.43
8:6:84:U:H2'	8:6:85:G:C8	2.53	0.43
11:J:252:GLU:OE1	11:J:260:ARG:HD3	2.19	0.43
11:J:315:LYS:NZ	14:M:189:GLN:HE22	2.17	0.43
11:J:411:MET:HB3	11:J:411:MET:HE3	1.83	0.43
14:M:202:TYR:OH	14:M:204:ASP:OD1	2.31	0.43
16:O:115:GLU:HG3	16:O:115:GLU:H	1.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:66:ARG:NH1	17:P:66:ARG:HB2	2.34	0.43
18:R:66:GLU:CD	18:R:66:GLU:H	2.20	0.43
18:R:189:ASN:OD1	18:R:195:ARG:NE	2.52	0.43
21:Q:515:VAL:N	21:Q:540:THR:O	2.48	0.43
46:1:238:SER:OG	46:1:241:GLY:N	2.51	0.43
1:A:638:LEU:HA	1:A:638:LEU:HD23	1.63	0.43
1:A:1203:SER:C	1:A:1205:GLU:H	2.21	0.43
3:C:129:ILE:HG22	3:C:199:LEU:HB3	2.01	0.43
5:E:162:ARG:NH2	5:E:203:ASP:O	2.52	0.43
6:F:42:C:H2'	6:F:43:A:C8	2.54	0.43
14:M:181:ARG:H	14:M:181:ARG:HG3	1.60	0.43
16:O:25:GLN:HE22	18:R:195:ARG:HH21	1.67	0.43
18:R:214:ILE:HG13	18:R:215:ASN:N	2.32	0.43
23:V:636:LEU:O	23:V:638:GLY:N	2.52	0.43
1:A:170:ASP:OD1	1:A:1621:LYS:NZ	2.47	0.43
1:A:440:PRO:O	1:A:443:VAL:HG22	2.18	0.43
1:A:590:GLY:HA2	1:A:592:TYR:CE2	2.53	0.43
1:A:962:LEU:HD23	1:A:962:LEU:HA	1.84	0.43
1:A:1404:THR:C	1:A:1406:GLU:H	2.22	0.43
1:A:1607:GLU:HB2	1:A:1633:ALA:O	2.19	0.43
3:C:343:LEU:HA	3:C:343:LEU:HD23	1.66	0.43
3:C:366:GLN:HB3	3:C:370:VAL:HB	2.01	0.43
3:C:374:LEU:HA	3:C:374:LEU:HD23	1.68	0.43
5:E:74:PHE:CD2	5:E:337:PRO:HD3	2.53	0.43
5:E:95:VAL:HG23	5:E:96:TYR:CD2	2.53	0.43
6:F:16:G:H2'	6:F:17:C:C6	2.53	0.43
8:6:87:U:C2	9:H:42:G:N1	2.77	0.43
11:J:206:LEU:HD23	11:J:206:LEU:HA	1.75	0.43
11:J:258:ILE:HG12	13:L:232:TYR:CZ	2.54	0.43
15:N:125:LYS:N	15:N:125:LYS:HD3	2.33	0.43
16:O:102:SER:OG	16:O:105:ASP:OD1	2.37	0.43
16:O:240:GLY:HA3	16:O:296:ARG:NH1	2.34	0.43
18:R:134:ARG:O	18:R:135:PRO:C	2.57	0.43
18:R:182:SER:OG	24:W:113:GLY:HA2	2.19	0.43
20:T:296:LEU:HD23	20:T:296:LEU:HA	1.80	0.43
26:Y:68:TYR:O	26:Y:69:LEU:C	2.56	0.43
1:A:1740:LEU:O	1:A:1744:ARG:HG3	2.19	0.43
1:A:1771:LEU:HD12	1:A:1772:PHE:N	2.34	0.43
1:A:1965:HIS:C	1:A:1966:HIS:HD1	2.21	0.43
2:B:10:U:H2'	2:B:11:U:C6	2.54	0.43
3:C:174:GLU:OE2	3:C:181:ILE:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:183:ALA:O	13:L:141:PRO:HA	2.19	0.43
11:J:201:ARG:HD2	11:J:201:ARG:O	2.19	0.43
11:J:325:ASN:HB2	14:M:172:HIS:CD2	2.41	0.43
13:L:184:ALA:O	13:L:188:ARG:HG2	2.19	0.43
14:M:200:ARG:HD2	14:M:200:ARG:N	2.33	0.43
46:1:381:THR:HB	46:1:396:ARG:O	2.19	0.43
1:A:1975:GLU:O	1:A:1979:VAL:HG23	2.19	0.42
2:B:40:U:H2'	2:B:41:U:H6	1.83	0.42
3:C:381:LEU:O	3:C:385:VAL:HG22	2.19	0.42
3:C:678:THR:HG21	3:C:683:ASN:HD22	1.84	0.42
3:C:726:LEU:O	3:C:730:ARG:HG2	2.19	0.42
3:C:789:PHE:CE2	3:C:816:VAL:HG13	2.54	0.42
8:6:73:G:O2'	8:6:74:G:P	2.77	0.42
11:J:262:ARG:NE	11:J:286:GLU:OE2	2.39	0.42
11:J:355:ARG:NH2	14:M:139:THR:HG23	2.34	0.42
11:J:385:PHE:CE1	11:J:389:HIS:CD2	3.07	0.42
11:J:400:GLU:O	11:J:403:VAL:HG22	2.19	0.42
13:L:224:PHE:H	18:R:86:LEU:CD1	2.30	0.42
16:O:44:GLU:HA	16:O:50:ARG:O	2.19	0.42
16:O:45:CYS:HB2	16:O:71:CYS:N	2.34	0.42
23:V:596:LEU:HD13	23:V:599:LEU:HD23	2.01	0.42
26:Y:37:ALA:O	26:Y:53:GLY:HA2	2.18	0.42
46:1:455:PHE:O	46:1:463:ARG:HA	2.19	0.42
47:2:108:ALA:HB2	47:2:132:ILE:CD1	2.47	0.42
1:A:80:LYS:HZ3	15:N:37:HIS:CD2	2.36	0.42
1:A:516:LEU:HA	1:A:516:LEU:HD23	1.79	0.42
1:A:673:THR:HG22	1:A:674:LYS:N	2.34	0.42
1:A:750:TRP:CE2	1:A:778:ARG:HG2	2.54	0.42
1:A:1854:VAL:HA	1:A:1857:GLN:HB2	2.01	0.42
2:B:55:C:H2'	2:B:56:C:C6	2.54	0.42
3:C:132:VAL:HG21	3:C:226:VAL:HG23	2.02	0.42
3:C:303:LEU:HD21	3:C:344:TRP:HB3	2.00	0.42
3:C:454:THR:HG23	3:C:576:ILE:O	2.19	0.42
5:E:122:SER:HA	5:E:138:SER:OG	2.19	0.42
6:F:28:A:O2'	15:N:39:GLY:HA2	2.19	0.42
6:F:59:G:O2'	6:F:61:C:P	2.77	0.42
11:J:335:ARG:HA	14:M:164:SER:OG	2.19	0.42
13:L:163:GLN:OE1	13:L:168:LYS:N	2.53	0.42
13:L:185:LEU:HA	13:L:185:LEU:HD12	1.71	0.42
15:N:4:VAL:O	15:N:6:ARG:NH1	2.52	0.42
23:V:238:ILE:CG2	23:V:372:LEU:HD12	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1248:LEU:HA	1:A:1248:LEU:HD23	1.69	0.42
1:A:1639:VAL:O	1:A:1654:SER:HB3	2.19	0.42
1:A:1965:HIS:ND1	47:2:130:ASP:OD1	2.52	0.42
1:A:2008:ARG:O	1:A:2012:LEU:HB3	2.19	0.42
3:C:87:GLN:HG3	3:C:91:GLU:HG2	2.01	0.42
3:C:140:HIS:CE1	3:C:230:ASP:H	2.37	0.42
3:C:190:LEU:HA	3:C:190:LEU:HD23	1.70	0.42
3:C:259:LYS:HG2	50:C:1500:GTP:C6	2.54	0.42
6:F:49:G:O2'	6:F:50:A:H5'	2.18	0.42
6:F:77:C:C2'	6:F:78:A:H5'	2.49	0.42
9:H:12:G:N2	14:M:196:TYR:CZ	2.87	0.42
9:H:171:U:H2'	9:H:172:C:H6	1.84	0.42
13:L:149:LEU:O	13:L:152:LEU:HB2	2.19	0.42
16:O:185:LYS:HD2	16:O:185:LYS:HA	1.93	0.42
17:P:206:LYS:HA	17:P:209:ARG:HD2	2.01	0.42
18:R:232:SEP:OG	18:R:233:PRO:HD2	2.19	0.42
19:S:146:GLU:O	19:S:146:GLU:HG2	2.18	0.42
20:T:347:THR:CG2	20:T:357:TRP:HE1	2.30	0.42
23:V:486:THR:HA	23:V:489:LEU:HB3	2.01	0.42
27:Z:775:VAL:HA	27:Z:801:CYS:O	2.20	0.42
1:A:711:GLN:OE1	9:H:18:U:H5"	2.19	0.42
1:A:858:GLN:HB2	9:H:29:A:OP1	2.19	0.42
1:A:912:GLU:HG3	1:A:913:PRO:CD	2.48	0.42
1:A:1184:ASN:OD1	1:A:1197:LEU:HD13	2.19	0.42
1:A:1627:ALA:HB2	1:A:1695:TYR:HD1	1.85	0.42
2:B:47:A:C1'	22:U:11:ARG:HH21	2.33	0.42
3:C:531:TRP:HB2	3:C:551:LEU:HB2	2.01	0.42
3:C:823:ALA:O	3:C:824:THR:HG22	2.18	0.42
6:F:8:C:N4	6:F:9:U:C2	2.87	0.42
24:W:276:LEU:HA	24:W:277:PRO:HD3	1.87	0.42
46:1:197:LEU:HB3	46:1:209:TRP:HB2	1.99	0.42
1:A:101:LYS:HD3	1:A:101:LYS:HA	1.87	0.42
1:A:357:ASN:ND2	3:C:866:SER:O	2.53	0.42
1:A:579:GLN:HG2	1:A:627:CYS:O	2.20	0.42
1:A:1944:HIS:CG	45:4:104:ARG:HB2	2.54	0.42
3:C:213:ASP:OD1	3:C:213:ASP:N	2.50	0.42
3:C:807:GLN:O	3:C:810:PRO:HD2	2.18	0.42
6:F:95:G:C6	9:H:4:G:C6	3.08	0.42
13:L:40:ARG:HG3	26:Y:109:GLN:NE2	2.35	0.42
15:N:59:TYR:CZ	15:N:63:LEU:HD11	2.54	0.42
16:O:63:MET:SD	16:O:160:ASN:HB2	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:132:ARG:CZ	16:O:137:LEU:HD23	2.49	0.42
16:O:253:TYR:HE1	19:S:93:THR:HG1	1.62	0.42
18:R:76:MET:HG2	19:S:95:ALA:HB2	2.01	0.42
19:S:24:VAL:HB	19:S:134:GLN:HB3	2.00	0.42
20:T:215:GLY:O	20:T:217:GLN:HG2	2.19	0.42
20:T:261:LEU:HD23	20:T:261:LEU:HA	1.89	0.42
23:V:584:LYS:HA	23:V:634:ILE:HD12	2.01	0.42
46:1:181:GLY:O	46:1:493:GLY:HA3	2.19	0.42
1:A:75:ASP:C	1:A:77:THR:H	2.21	0.42
1:A:237:THR:HG23	1:A:240:ARG:NH1	2.35	0.42
1:A:1391:LEU:HD12	1:A:1391:LEU:HA	1.80	0.42
1:A:1783:THR:HG21	1:A:1894:GLN:CG	2.50	0.42
2:B:30:A:H2'	2:B:31:U:H6	1.83	0.42
3:C:64:LYS:H	3:C:64:LYS:HG2	1.65	0.42
3:C:213:ASP:OD2	3:C:615:PRO:HD2	2.19	0.42
3:C:906:ILE:HG22	3:C:907:VAL:O	2.20	0.42
5:E:221:ASP:HB2	5:E:228:THR:OG1	2.20	0.42
10:I:393:LYS:N	10:I:394:PRO:HD3	2.34	0.42
16:O:58:CYS:HA	16:O:59:PRO:HD3	1.82	0.42
18:R:73:PRO:HB3	19:S:131:ARG:NH2	2.32	0.42
18:R:178:ARG:HD3	18:R:194:GLN:NE2	2.33	0.42
18:R:296:ARG:O	18:R:300:GLU:HG2	2.20	0.42
20:T:250:ARG:HD2	20:T:250:ARG:HA	1.78	0.42
20:T:428:VAL:HG22	20:T:438:LEU:HD22	2.01	0.42
23:V:457:ARG:HG3	23:V:457:ARG:NH2	2.35	0.42
1:A:385:GLU:OE1	1:A:389:LYS:HD2	2.20	0.42
1:A:507:LEU:HA	1:A:507:LEU:HD12	1.79	0.42
1:A:941:LYS:HA	1:A:941:LYS:HD2	1.77	0.42
1:A:1282:GLN:O	1:A:1285:LEU:N	2.51	0.42
3:C:501:ILE:HG22	3:C:530:LEU:HD11	2.02	0.42
5:E:208:ILE:HG13	5:E:222:LEU:HD21	2.01	0.42
5:E:289:LEU:HD12	5:E:289:LEU:HA	1.70	0.42
9:H:25:G:C2	9:H:26:A:C5	3.08	0.42
9:H:157:G:O6	9:H:174:A:N6	2.53	0.42
11:J:188:GLN:HE21	13:L:13:ASN:ND2	2.13	0.42
11:J:376:VAL:HG23	11:J:415:LEU:HB2	2.00	0.42
16:O:137:LEU:HD12	16:O:140:ALA:HB3	2.02	0.42
16:O:164:ILE:HD12	16:O:182:ARG:O	2.20	0.42
18:R:124:VAL:HG13	18:R:125:MET:N	2.33	0.42
20:T:390:GLY:HA3	20:T:416:ILE:HD11	2.02	0.42
1:A:95:MET:N	1:A:96:PRO:HD2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1534:PHE:CE1	1:A:1538:TRP:CD1	3.08	0.42
1:A:1719:PHE:O	1:A:1722:SER:OG	2.19	0.42
1:A:1763:LEU:HD12	1:A:1887:SER:HB2	2.02	0.42
1:A:1816:GLN:NE2	1:A:1817:LEU:O	2.52	0.42
1:A:1920:TYR:CE1	1:A:1936:LEU:HD22	2.55	0.42
2:B:12:U:H2'	2:B:13:C:C6	2.54	0.42
3:C:259:LYS:HG2	50:C:1500:GTP:N1	2.34	0.42
3:C:621:VAL:HG22	3:C:627:HIS:ND1	2.35	0.42
5:E:63:SER:OG	5:E:350:ARG:HG2	2.19	0.42
5:E:243:LEU:HD21	5:E:247:GLY:HA2	2.01	0.42
6:F:26:U:O2	6:F:26:U:C2'	2.67	0.42
6:F:75:G:N1	6:F:76:A:C5	2.88	0.42
6:F:89:U:C2	6:F:90:G:C8	3.08	0.42
11:J:194:LEU:HA	11:J:194:LEU:HD23	1.73	0.42
13:L:54:LEU:HD12	13:L:54:LEU:HA	1.73	0.42
19:S:98:LEU:CD2	19:S:129:PHE:HD2	2.33	0.42
23:V:173:VAL:HA	23:V:181:ILE:HG13	2.00	0.42
23:V:288:ASP:O	23:V:292:VAL:HG23	2.19	0.42
23:V:341:ALA:CA	23:V:344:LYS:HE3	2.47	0.42
23:V:533:TYR:HA	23:V:536:ILE:HG23	2.01	0.42
1:A:317:PRO:HB2	1:A:327:VAL:HG11	2.01	0.42
1:A:664:HIS:NE2	1:A:666:LYS:HD3	2.35	0.42
1:A:1108:ASP:HA	1:A:1111:GLN:OE1	2.18	0.42
1:A:1839:TRP:CZ3	1:A:1871:PRO:HA	2.55	0.42
49:A:3000:IHP:O12	49:A:3000:IHP:P1	2.78	0.42
3:C:138:LEU:HG	3:C:139:HIS:CG	2.54	0.42
3:C:652:ASP:N	3:C:652:ASP:OD1	2.53	0.42
5:E:204:THR:O	5:E:205:SER:OG	2.31	0.42
5:E:240:GLY:O	5:E:252:SER:HA	2.19	0.42
6:F:42:C:C4	6:F:43:A:C5	3.07	0.42
8:6:89:U:H2'	8:6:90:C:O4'	2.20	0.42
13:L:24:MET:HE2	13:L:24:MET:HB2	1.83	0.42
15:N:24:GLU:HG3	24:W:189:ILE:HG13	2.02	0.42
23:V:631:PHE:HB2	23:V:640:THR:HG21	2.02	0.42
1:A:439:GLN:O	1:A:444:ARG:NH1	2.53	0.42
1:A:440:PRO:HG2	1:A:443:VAL:HG13	2.01	0.42
1:A:569:VAL:HG12	1:A:573:GLN:OE1	2.20	0.42
1:A:1404:THR:O	1:A:1405:LEU:HB2	2.20	0.42
1:A:1788:VAL:HG13	45:4:111:ASP:OD1	2.20	0.42
3:C:134:LEU:HD22	3:C:228:PHE:HE1	1.85	0.42
3:C:327:TYR:OH	3:C:372:PHE:HD1	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:863:ILE:HG12	3:C:870:THR:HG23	2.02	0.42
5:E:178:LEU:HD12	5:E:178:LEU:HA	1.86	0.42
9:H:56:A:N1	9:H:93:A:C6	2.88	0.42
11:J:269:LEU:HD23	11:J:269:LEU:HA	1.67	0.42
13:L:151:MET:HA	13:L:154:GLU:HG2	2.00	0.42
14:M:159:GLU:OE1	14:M:169:HIS:HB2	2.20	0.42
16:O:131:THR:CG2	24:W:108:ARG:HE	2.33	0.42
17:P:74:LYS:HE2	17:P:74:LYS:HB2	1.72	0.42
17:P:206:LYS:HA	17:P:209:ARG:CD	2.50	0.42
18:R:107:SER:OG	18:R:109:ASP:OD1	2.37	0.42
20:T:371:HIS:CE1	20:T:396:LYS:HD2	2.55	0.42
23:V:234:LEU:HD23	23:V:263:LEU:HD13	2.02	0.42
26:Y:98:TYR:CD1	26:Y:98:TYR:N	2.88	0.42
45:4:106:LYS:HZ2	45:4:108:ALA:CA	2.32	0.42
46:1:358:ILE:HB	46:1:368:LYS:HB2	2.01	0.42
1:A:1210:LYS:HE2	1:A:1280:ASN:OD1	2.20	0.41
1:A:1485:LEU:HD23	1:A:1485:LEU:HA	1.80	0.41
1:A:1635:TYR:O	1:A:1636:LYS:HG3	2.20	0.41
1:A:1760:GLU:HB3	1:A:1885:LYS:HZ1	1.85	0.41
49:A:3000:IHP:O24	49:A:3000:IHP:P3	2.78	0.41
2:B:67:A:O2'	2:B:68:C:H5'	2.19	0.41
3:C:93:ILE:HG22	3:C:94:ILE:H	1.85	0.41
3:C:319:THR:HG23	3:C:429:GLY:HA3	2.02	0.41
3:C:389:ASP:OD1	3:C:390:THR:N	2.53	0.41
3:C:718:PHE:HB3	3:C:724:TRP:CB	2.49	0.41
10:I:621:ARG:O	10:I:624:GLU:N	2.52	0.41
15:N:17:LEU:HD12	15:N:18:ILE:HG23	2.02	0.41
16:O:25:GLN:HB2	18:R:183:GLN:OE1	2.20	0.41
18:R:248:PRO:HA	18:R:249:PRO:HD3	1.97	0.41
20:T:209:CYS:O	20:T:221:THR:HA	2.20	0.41
20:T:358:ASP:OD1	20:T:365:ARG:HD2	2.20	0.41
23:V:290:VAL:HG23	23:V:335:MET:HE3	2.01	0.41
26:Y:25:LEU:HA	26:Y:26:PRO:HD3	1.88	0.41
46:1:440:THR:HA	46:1:477:CYS:SG	2.60	0.41
1:A:451:LEU:HD23	1:A:451:LEU:HA	1.61	0.41
1:A:1448:LEU:HA	1:A:1448:LEU:HD12	1.62	0.41
1:A:1634:SER:OG	1:A:1635:TYR:N	2.53	0.41
1:A:1890:GLN:HG2	45:4:105:GLU:OE1	2.19	0.41
2:B:100:C:H2'	2:B:101:U:H6	1.82	0.41
3:C:64:LYS:HE3	17:P:209:ARG:HH22	1.85	0.41
3:C:90:THR:O	3:C:92:PRO:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:295:ASP:OD1	3:C:297:ASN:ND2	2.53	0.41
5:E:277:PHE:N	5:E:277:PHE:CD1	2.87	0.41
8:6:19:G:N1	8:6:20:A:N6	2.68	0.41
8:6:21:A:C2	16:O:152:ARG:HB2	2.55	0.41
9:H:12:G:N7	14:M:200:ARG:NH2	2.67	0.41
23:V:300:CYS:SG	23:V:304:LEU:HD11	2.60	0.41
27:Z:583:THR:HA	27:Z:628:MET:O	2.18	0.41
1:A:75:ASP:HB3	1:A:77:THR:HG23	2.02	0.41
1:A:294:ASN:HB2	1:A:297:ASN:HD22	1.84	0.41
1:A:1303:LEU:HD12	1:A:1311:PHE:CE1	2.55	0.41
1:A:1661:TRP:CD1	1:A:1699:THR:O	2.73	0.41
3:C:531:TRP:CE3	3:C:538:HIS:HB3	2.54	0.41
5:E:162:ARG:HE	5:E:162:ARG:HB2	1.54	0.41
11:J:185:ALA:HA	13:L:142:ILE:CD1	2.45	0.41
11:J:306:LEU:HD23	18:R:229:VAL:HG21	2.02	0.41
13:L:169:ARG:O	13:L:173:GLU:HG2	2.20	0.41
18:R:265:ASP:N	18:R:265:ASP:OD1	2.51	0.41
19:S:90:LEU:O	19:S:91:LYS:HD3	2.20	0.41
20:T:344:GLN:OE1	20:T:359:LEU:HB3	2.20	0.41
26:Y:36:MET:HG2	26:Y:53:GLY:HA3	2.02	0.41
47:2:244:LEU:HD23	47:2:244:LEU:HA	1.86	0.41
48:5:21:UNK:O	48:5:22:UNK:C	2.68	0.41
1:A:59:GLU:HA	1:A:59:GLU:OE2	2.21	0.41
1:A:169:PHE:HE1	46:1:274:VAL:HG21	1.85	0.41
1:A:459:LEU:HD12	1:A:459:LEU:HA	1.82	0.41
1:A:713:LEU:HA	1:A:713:LEU:HD12	1.85	0.41
1:A:804:GLU:OE2	1:A:805:GLU:N	2.53	0.41
1:A:1776:ILE:CB	1:A:1858:PRO:HA	2.42	0.41
3:C:408:LEU:HD12	3:C:408:LEU:HA	1.78	0.41
5:E:75:HIS:HB2	5:E:80:THR:CG2	2.50	0.41
5:E:214:ASP:OD1	5:E:214:ASP:N	2.42	0.41
6:F:93:G:H2'	6:F:94:C:H6	1.85	0.41
10:I:565:ILE:CB	10:I:576:ALA:HB1	2.50	0.41
16:O:59:PRO:HD2	16:O:63:MET:HB2	2.03	0.41
16:O:76:LYS:HG2	24:W:111:LEU:CD2	2.51	0.41
17:P:44:ARG:HH11	17:P:49:ASP:HB3	1.85	0.41
24:W:199:TYR:O	24:W:200:VAL:C	2.59	0.41
26:Y:27:LYS:NZ	26:Y:64:GLN:HE21	2.18	0.41
1:A:298:ASP:OD1	1:A:300:ASN:N	2.54	0.41
1:A:312:TYR:N	1:A:312:TYR:CD1	2.87	0.41
1:A:1863:VAL:CG1	1:A:1886:GLY:HA2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:G:H2'	2:B:98:G:H8	1.82	0.41
3:C:854:ARG:NH1	3:C:879:ASP:OD2	2.53	0.41
9:H:82:G:H2'	9:H:83:A:H8	1.86	0.41
13:L:159:LEU:HD23	13:L:159:LEU:HA	1.91	0.41
18:R:132:LEU:O	18:R:132:LEU:HG	2.21	0.41
20:T:329:HIS:NE2	20:T:355:ARG:HG3	2.36	0.41
23:V:166:ILE:HG23	23:V:197:LEU:HD12	2.02	0.41
23:V:197:LEU:O	23:V:201:VAL:HG23	2.20	0.41
23:V:221:ILE:HD11	23:V:225:LYS:HE2	2.03	0.41
23:V:569:LYS:HG2	23:V:570:LEU:N	2.35	0.41
23:V:577:SER:O	23:V:581:ILE:HG12	2.20	0.41
27:Z:606:GLY:HA2	27:Z:618:CYS:O	2.20	0.41
46:1:246:VAL:CG2	46:1:254:LYS:HB3	2.50	0.41
47:2:105:SER:O	47:2:140:PRO:HD2	2.20	0.41
1:A:1640:SER:OG	1:A:1641:ARG:N	2.54	0.41
3:C:129:ILE:HA	3:C:199:LEU:O	2.20	0.41
3:C:213:ASP:HB2	3:C:615:PRO:HB2	2.01	0.41
3:C:487:GLY:HA3	3:C:489:GLN:OE1	2.21	0.41
3:C:731:SER:OG	3:C:746:VAL:HG13	2.20	0.41
4:D:1211:ASP:O	4:D:1215:HIS:N	2.52	0.41
5:E:71:CYS:SG	5:E:115:LEU:HG	2.60	0.41
6:F:22:A:O4'	15:N:118:ILE:HG22	2.19	0.41
6:F:45:A:N7	8:6:3:A:C4	2.89	0.41
6:F:64:U:H2'	6:F:65:G:O4'	2.20	0.41
7:G:-12:G:HO2'	7:G:-11:G:C5'	2.32	0.41
9:H:81:G:H2'	9:H:82:G:C8	2.55	0.41
11:J:294:HIS:CE1	13:L:227:THR:OG1	2.74	0.41
11:J:440:LEU:HG	11:J:445:LYS:CE	2.50	0.41
12:K:164:ASN:HB3	12:K:168:LYS:NZ	2.35	0.41
20:T:253:ILE:HD13	20:T:253:ILE:HA	1.94	0.41
23:V:286:THR:O	23:V:290:VAL:HG13	2.20	0.41
23:V:467:LEU:O	23:V:468:ASP:HB2	2.20	0.41
23:V:640:THR:O	23:V:644:ARG:HG3	2.20	0.41
24:W:185:ASP:N	24:W:185:ASP:OD1	2.53	0.41
1:A:191:ILE:HG13	1:A:571:ALA:HB1	2.02	0.41
1:A:212:PRO:HD2	1:A:225:TYR:OH	2.20	0.41
1:A:1176:SER:OG	1:A:1185:LEU:HD12	2.21	0.41
1:A:1197:LEU:HA	1:A:1197:LEU:HD12	1.83	0.41
1:A:1418:ARG:HB2	1:A:1461:ASP:O	2.21	0.41
1:A:1633:ALA:HB2	1:A:1637:TRP:CZ3	2.56	0.41
1:A:1823:HIS:ND1	1:A:1825:SER:OG	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:U:H2'	2:B:11:U:H6	1.85	0.41
2:B:19:A:C2	2:B:59:G:C4	3.09	0.41
2:B:95:G:H21	2:B:96:A:H5"	1.86	0.41
3:C:64:LYS:NZ	17:P:209:ARG:HH12	2.18	0.41
3:C:416:LEU:HD23	3:C:416:LEU:HA	1.93	0.41
5:E:89:LEU:CD2	5:E:106:LYS:HG2	2.51	0.41
5:E:309:VAL:HB	5:E:323:LEU:HB2	2.03	0.41
10:I:194:ASP:C	10:I:196:ALA:H	2.24	0.41
13:L:767:LEU:HD23	13:L:767:LEU:HA	1.90	0.41
14:M:179:ILE:HG13	14:M:180:ASP:N	2.35	0.41
16:O:35:ARG:HD3	24:W:129:ARG:HE	1.85	0.41
16:O:78:LYS:HE3	16:O:94:ILE:HG21	2.02	0.41
18:R:51:ILE:N	18:R:52:PRO:CD	2.83	0.41
18:R:137:GLU:HG2	18:R:138:GLU:N	2.36	0.41
20:T:224:ALA:HA	20:T:248:THR:HG23	2.02	0.41
20:T:366:VAL:HG21	20:T:402:ASP:HA	2.02	0.41
23:V:577:SER:CA	23:V:580:ARG:HH11	2.33	0.41
25:X:33:GLU:O	25:X:37:ILE:HG13	2.20	0.41
26:Y:9:LYS:HE2	26:Y:9:LYS:HB2	1.82	0.41
1:A:84:ASP:O	1:A:88:TYR:HB2	2.21	0.41
1:A:1053:LEU:HD21	1:A:1088:PHE:CD1	2.56	0.41
1:A:1334:LEU:HB2	23:V:471:GLU:CD	2.41	0.41
1:A:1781:ASP:HB3	1:A:1808:PHE:HB3	2.03	0.41
1:A:1921:ASP:HB3	1:A:1966:HIS:CG	2.56	0.41
1:A:1943:LEU:HA	1:A:1943:LEU:HD23	1.94	0.41
3:C:441:PRO:HA	3:C:444:GLY:HA3	2.02	0.41
6:F:3:G:O2'	6:F:4:C:H5'	2.21	0.41
9:H:174:A:C2	9:H:175:G:C4	3.09	0.41
15:N:73:GLU:O	15:N:76:GLU:HG3	2.21	0.41
18:R:204:LYS:HB2	18:R:204:LYS:HE3	1.86	0.41
20:T:288:LEU:HD23	20:T:288:LEU:HA	1.83	0.41
20:T:483:ASP:O	20:T:485:THR:HG23	2.20	0.41
24:W:87:THR:OG1	24:W:88:MET:N	2.54	0.41
25:X:13:HIS:CE1	26:Y:98:TYR:HH	2.38	0.41
26:Y:86:GLU:OE2	26:Y:86:GLU:N	2.46	0.41
46:1:312:GLU:HB2	46:1:315:ASN:OD1	2.20	0.41
46:1:319:GLN:N	46:1:319:GLN:OE1	2.53	0.41
46:1:440:THR:O	46:1:453:LEU:HD12	2.21	0.41
47:2:104:ASP:OD2	47:2:104:ASP:N	2.54	0.41
1:A:338:VAL:O	1:A:338:VAL:HG13	2.21	0.41
1:A:750:TRP:CD1	1:A:778:ARG:NH2	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1275:ARG:O	1:A:1369:TYR:HE1	2.02	0.41
1:A:1593:LEU:HD23	1:A:1593:LEU:HA	1.69	0.41
1:A:1647:ASP:O	1:A:1723:LYS:NZ	2.39	0.41
1:A:1762:TYR:CB	1:A:1888:GLU:HB2	2.49	0.41
1:A:1862:ILE:CG2	1:A:1887:SER:HB2	2.51	0.41
2:B:14:U:H2'	2:B:15:C:H6	1.85	0.41
2:B:19:A:C6	2:B:59:G:C6	3.08	0.41
2:B:63:A:C4	2:B:64:G:C8	3.08	0.41
2:B:103:G:N1	2:B:111:A:C6	2.89	0.41
3:C:187:THR:HA	3:C:200:PHE:O	2.21	0.41
3:C:445:ALA:O	3:C:449:ILE:HG13	2.20	0.41
3:C:445:ALA:O	3:C:449:ILE:N	2.38	0.41
3:C:493:PHE:CZ	3:C:549:TRP:HB3	2.56	0.41
3:C:743:ASN:HA	3:C:787:VAL:O	2.20	0.41
3:C:801:LEU:O	3:C:802:HIS:C	2.58	0.41
6:F:40:U:H2'	6:F:41:A:C8	2.54	0.41
9:H:142:C:N4	9:H:143:A:N6	2.69	0.41
9:H:157:G:H5'	9:H:158:G:OP2	2.21	0.41
11:J:439:ALA:HA	11:J:442:ARG:HB3	2.01	0.41
13:L:226:ASP:OD1	18:R:83:SER:HB3	2.21	0.41
14:M:176:THR:O	14:M:179:ILE:N	2.54	0.41
15:N:63:LEU:HD23	15:N:63:LEU:HA	1.90	0.41
18:R:126:ASN:ND2	18:R:128:ASP:O	2.53	0.41
18:R:196:VAL:HG11	24:W:120:ILE:HD12	2.03	0.41
18:R:238:THR:HB	18:R:241:GLU:OE1	2.21	0.41
20:T:284:TYR:CE2	20:T:320:LYS:HA	2.56	0.41
23:V:261:ALA:HB2	23:V:296:PHE:CD1	2.56	0.41
23:V:399:LYS:N	23:V:399:LYS:HD3	2.35	0.41
23:V:600:ASN:HA	23:V:639:LEU:HD11	2.02	0.41
24:W:549:HIS:C	24:W:551:LYS:H	2.24	0.41
46:1:282:HIS:NE2	46:1:309:ARG:HB2	2.36	0.41
46:1:302:CYS:HB2	46:1:335:PRO:HG2	2.03	0.41
47:2:60:ILE:HG12	47:2:99:ALA:HB2	2.02	0.41
1:A:712:HIS:CE1	18:R:250:CYS:HB2	2.55	0.41
1:A:863:GLU:HG3	1:A:913:PRO:HB3	2.03	0.41
1:A:880:ARG:HH11	1:A:880:ARG:HD3	1.77	0.41
1:A:1189:MET:CG	1:A:1190:CYS:N	2.84	0.41
1:A:1757:GLU:HA	1:A:1757:GLU:OE2	2.21	0.41
1:A:1781:ASP:OD1	1:A:1783:THR:OG1	2.30	0.41
1:A:1863:VAL:HG22	1:A:1865:ARG:N	2.36	0.41
1:A:1963:GLU:OE1	1:A:1965:HIS:CD2	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:U:O2	2:B:60:G:N2	2.41	0.41
2:B:37:G:C2	2:B:46:U:C2	3.08	0.41
3:C:440:SER:O	3:C:441:PRO:C	2.59	0.41
3:C:485:ASP:OD1	3:C:486:ASP:N	2.54	0.41
5:E:198:ALA:O	5:E:210:SER:HA	2.21	0.41
5:E:305:ALA:HA	5:E:329:SER:OG	2.21	0.41
6:F:72:G:C6	6:F:75:G:C8	3.08	0.41
6:F:93:G:H2'	6:F:94:C:C6	2.55	0.41
11:J:212:GLN:NE2	13:L:182:LEU:HD13	2.36	0.41
11:J:411:MET:CE	11:J:415:LEU:HB3	2.51	0.41
18:R:148:ARG:HH11	18:R:148:ARG:HG3	1.86	0.41
20:T:185:MET:CB	20:T:186:PRO:HD3	2.49	0.41
25:X:6:LEU:HD11	25:X:10:LYS:HE2	2.02	0.41
1:A:260:LEU:HD23	1:A:260:LEU:HA	1.93	0.40
1:A:273:ILE:O	1:A:274:PRO:C	2.60	0.40
1:A:442:LYS:HD2	1:A:610:HIS:NE2	2.37	0.40
1:A:723:ASN:OD1	1:A:785:LYS:HE3	2.21	0.40
1:A:843:LEU:HD23	1:A:843:LEU:HA	1.81	0.40
1:A:1361:GLU:C	1:A:1363:GLN:N	2.74	0.40
1:A:1621:LYS:HD3	46:1:272:TYR:CZ	2.56	0.40
1:A:1644:LEU:N	1:A:1647:ASP:OD2	2.41	0.40
1:A:1811:ASN:O	1:A:1815:GLY:N	2.44	0.40
49:A:3000:IHP:P6	49:A:3000:IHP:O25	2.79	0.40
3:C:323:PHE:HE2	3:C:424:PHE:HE1	1.69	0.40
3:C:516:LEU:HD12	3:C:517:GLU:HG3	2.03	0.40
11:J:296:ARG:HD2	13:L:225:TYR:CE2	2.56	0.40
11:J:308:ARG:HA	11:J:308:ARG:HD2	1.64	0.40
11:J:440:LEU:O	11:J:445:LYS:HD2	2.21	0.40
13:L:150:GLU:OE1	13:L:150:GLU:HA	2.21	0.40
15:N:15:TRP:HE3	15:N:74:LEU:HD11	1.87	0.40
16:O:57:TRP:O	16:O:65:PHE:HA	2.21	0.40
18:R:142:GLU:OE1	18:R:142:GLU:N	2.54	0.40
21:Q:288:LEU:O	21:Q:295:GLY:HA3	2.20	0.40
23:V:583:VAL:O	23:V:587:PHE:HD2	2.03	0.40
24:W:180:LYS:HG2	24:W:199:TYR:HA	2.04	0.40
25:X:29:LYS:HE3	25:X:33:GLU:OE1	2.21	0.40
26:Y:132:ASN:N	26:Y:133:PRO:HD2	2.36	0.40
46:1:227:CYS:O	46:1:229:CYS:N	2.54	0.40
1:A:34:ALA:HA	5:E:213:ILE:CD1	2.52	0.40
1:A:348:PRO:HB3	1:A:394:TYR:CE1	2.57	0.40
1:A:648:LEU:HA	1:A:648:LEU:HD23	1.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:886:LEU:HA	1:A:886:LEU:HD23	1.74	0.40
1:A:1001:VAL:HG23	1:A:1002:ASP:O	2.22	0.40
1:A:1621:LYS:HD3	46:1:272:TYR:CE1	2.55	0.40
1:A:1807:ILE:O	1:A:1819:LEU:HD12	2.21	0.40
2:B:97:G:C2	2:B:98:G:C5	3.09	0.40
3:C:276:TYR:HD1	3:C:276:TYR:HA	1.77	0.40
3:C:363:SER:O	3:C:364:SER:OG	2.26	0.40
6:F:17:C:C2	6:F:18:A:N7	2.89	0.40
11:J:187:VAL:O	11:J:188:GLN:HG2	2.21	0.40
11:J:375:ASP:HB3	11:J:378:ASN:ND2	2.37	0.40
13:L:100:TYR:O	13:L:104:LEU:HG	2.21	0.40
14:M:177:GLU:HA	14:M:180:ASP:OD2	2.21	0.40
15:N:70:ILE:HG22	15:N:71:SER:O	2.20	0.40
16:O:28:LEU:HB3	18:R:195:ARG:NH2	2.36	0.40
16:O:160:ASN:OD1	16:O:160:ASN:N	2.53	0.40
18:R:91:ASP:OD2	18:R:95:LYS:HG2	2.21	0.40
19:S:35:THR:C	19:S:129:PHE:HE1	2.24	0.40
20:T:333:VAL:HA	20:T:349:SER:HB2	2.03	0.40
1:A:83:HIS:C	1:A:85:LYS:N	2.73	0.40
1:A:480:LYS:CB	15:N:110:ASP:HA	2.51	0.40
1:A:545:HIS:ND1	1:A:548:ARG:NH2	2.69	0.40
1:A:1443:LYS:HD3	1:A:1443:LYS:HA	1.66	0.40
1:A:1657:THR:OG1	1:A:1658:GLN:N	2.55	0.40
1:A:1883:VAL:O	1:A:1884:ILE:HD13	2.21	0.40
3:C:898:LEU:HD23	3:C:898:LEU:HA	1.73	0.40
6:F:76:A:H2'	6:F:77:C:O4'	2.21	0.40
9:H:27:U:O2'	9:H:28:C:H5'	2.22	0.40
9:H:157:G:C6	9:H:174:A:C6	3.09	0.40
11:J:282:TYR:CZ	11:J:298:ILE:HD11	2.57	0.40
14:M:150:GLU:HA	14:M:153:ARG:HB3	2.04	0.40
16:O:153:THR:OG1	16:O:154:THR:HG23	2.21	0.40
24:W:121:ASN:OD1	24:W:121:ASN:C	2.60	0.40
47:2:47:TRP:CD1	47:2:91:PRO:HD2	2.56	0.40
1:A:795:LEU:HA	1:A:795:LEU:HD23	1.68	0.40
1:A:835:ASP:OD1	1:A:835:ASP:N	2.53	0.40
1:A:1328:LEU:HD23	1:A:1470:TYR:CE2	2.57	0.40
1:A:1562:MET:CE	1:A:1566:ILE:H	2.35	0.40
1:A:1808:PHE:CE1	1:A:1817:LEU:HD13	2.56	0.40
2:B:9:G:H2'	2:B:10:U:H6	1.86	0.40
3:C:301:SER:OG	3:C:302:PRO:HD2	2.22	0.40
3:C:444:GLY:O	3:C:447:PRO:HD2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:510:LEU:HB3	3:C:514:TYR:HD2	1.86	0.40
3:C:531:TRP:HA	3:C:539:ILE:O	2.22	0.40
3:C:749:THR:O	3:C:753:GLU:HB2	2.22	0.40
3:C:857:VAL:HA	3:C:873:ALA:CB	2.51	0.40
6:F:1:G:C6	6:F:2:U:C4	3.10	0.40
9:H:74:U:H2'	9:H:75:A:C8	2.55	0.40
13:L:216:PHE:HB3	16:O:116:TYR:CE2	2.56	0.40
16:O:72:GLN:HA	16:O:82:GLN:HE21	1.85	0.40
16:O:80:VAL:CG1	16:O:94:ILE:HD11	2.51	0.40
16:O:164:ILE:HD11	16:O:184:GLU:H	1.85	0.40
19:S:136:ILE:HA	19:S:139:VAL:HG12	2.04	0.40
26:Y:154:LEU:HA	26:Y:154:LEU:HD23	1.84	0.40
46:1:306:ALA:HA	46:1:334:ILE:HA	2.04	0.40
1:A:701:ILE:HG22	1:A:705:LYS:NZ	2.36	0.40
1:A:1762:TYR:C	1:A:1764:SER:H	2.23	0.40
2:B:62:G:N1	2:B:63:A:C5	2.90	0.40
2:B:108:G:H3'	2:B:109:G:C8	2.56	0.40
3:C:254:THR:HB	3:C:433:MET:HE3	2.03	0.40
3:C:313:GLN:HB2	50:C:1500:GTP:C5	2.57	0.40
3:C:474:LEU:HA	3:C:498:SER:O	2.22	0.40
3:C:532:ILE:HD13	3:C:532:ILE:HA	1.87	0.40
3:C:589:LYS:HG3	3:C:628:VAL:CG1	2.51	0.40
3:C:622:GLU:O	3:C:625:GLY:N	2.55	0.40
3:C:668:GLU:H	3:C:824:THR:CG2	2.34	0.40
3:C:863:ILE:CG1	3:C:870:THR:HG23	2.51	0.40
5:E:147:LEU:HD22	5:E:179:TRP:HE3	1.86	0.40
5:E:336:HIS:CD2	5:E:337:PRO:HD2	2.57	0.40
6:F:16:G:C2	6:F:17:C:C2	3.10	0.40
8:6:28:A:H4'	16:O:266:ARG:HD2	2.02	0.40
14:M:139:THR:O	14:M:142:ILE:HG22	2.21	0.40
18:R:162:ALA:O	18:R:164:PRO:HD3	2.20	0.40
20:T:343:PRO:HD3	20:T:401:PRO:HB3	2.02	0.40
23:V:576:THR:O	23:V:579:SER:N	2.54	0.40
46:1:428:ASP:HB2	46:1:476:ARG:HD3	2.02	0.40
46:1:437:LEU:HD21	46:1:455:PHE:HD2	1.86	0.40
47:2:254:ASP:HB2	47:2:257:CYS:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	2247/2335 (96%)	2098 (93%)	127 (6%)	22 (1%)	15 46
3	C	856/972 (88%)	783 (92%)	61 (7%)	12 (1%)	11 37
4	D	1900/2136 (89%)	1838 (97%)	53 (3%)	9 (0%)	29 61
5	E	297/357 (83%)	281 (95%)	16 (5%)	0	100 100
10	I	662/855 (77%)	585 (88%)	75 (11%)	2 (0%)	41 72
11	J	530/848 (62%)	502 (95%)	20 (4%)	8 (2%)	10 36
12	K	144/225 (64%)	136 (94%)	5 (4%)	3 (2%)	7 30
13	L	401/802 (50%)	381 (95%)	19 (5%)	1 (0%)	47 78
14	M	89/243 (37%)	79 (89%)	9 (10%)	1 (1%)	14 44
15	N	141/144 (98%)	121 (86%)	15 (11%)	5 (4%)	3 21
16	O	279/420 (66%)	250 (90%)	25 (9%)	4 (1%)	11 37
17	P	92/229 (40%)	84 (91%)	6 (6%)	2 (2%)	6 29
18	R	235/536 (44%)	205 (87%)	25 (11%)	5 (2%)	7 30
19	S	157/166 (95%)	148 (94%)	8 (5%)	1 (1%)	25 57
20	T	311/514 (60%)	279 (90%)	24 (8%)	8 (3%)	5 26
21	Q	1304/1485 (88%)	1280 (98%)	24 (2%)	0	100 100
22	U	68/2752 (2%)	63 (93%)	5 (7%)	0	100 100
23	V	444/908 (49%)	430 (97%)	12 (3%)	2 (0%)	29 61
24	W	436/579 (75%)	397 (91%)	34 (8%)	5 (1%)	14 44
25	X	69/425 (16%)	62 (90%)	6 (9%)	1 (1%)	11 37
26	Y	202/323 (62%)	181 (90%)	19 (9%)	2 (1%)	15 46
27	Z	746/1227 (61%)	730 (98%)	15 (2%)	1 (0%)	51 82
28	q	130/504 (26%)	123 (95%)	7 (5%)	0	100 100
28	r	129/504 (26%)	123 (95%)	6 (5%)	0	100 100
28	s	65/504 (13%)	61 (94%)	2 (3%)	2 (3%)	4 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	t	65/504 (13%)	64 (98%)	1 (2%)	0	100	100
29	u	388/411 (94%)	379 (98%)	9 (2%)	0	100	100
30	v	142/146 (97%)	140 (99%)	2 (1%)	0	100	100
31	w	89/174 (51%)	88 (99%)	1 (1%)	0	100	100
32	x	23/703 (3%)	23 (100%)	0	0	100	100
33	g	77/126 (61%)	70 (91%)	7 (9%)	0	100	100
33	h	76/126 (60%)	74 (97%)	2 (3%)	0	100	100
34	a	84/240 (35%)	78 (93%)	6 (7%)	0	100	100
34	i	84/240 (35%)	82 (98%)	2 (2%)	0	100	100
35	b	80/119 (67%)	76 (95%)	4 (5%)	0	100	100
35	j	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
36	c	95/118 (80%)	84 (88%)	11 (12%)	0	100	100
36	k	81/118 (69%)	74 (91%)	6 (7%)	1 (1%)	13	41
37	d	72/86 (84%)	66 (92%)	6 (8%)	0	100	100
37	m	72/86 (84%)	64 (89%)	6 (8%)	2 (3%)	5	24
38	e	77/92 (84%)	70 (91%)	7 (9%)	0	100	100
38	l	73/92 (79%)	63 (86%)	7 (10%)	3 (4%)	3	18
39	f	71/76 (93%)	66 (93%)	5 (7%)	0	100	100
39	n	64/76 (84%)	53 (83%)	8 (12%)	3 (5%)	2	15
40	o	160/255 (63%)	152 (95%)	8 (5%)	0	100	100
41	p	92/225 (41%)	92 (100%)	0	0	100	100
42	y	77/301 (26%)	76 (99%)	1 (1%)	0	100	100
43	z	76/285 (27%)	70 (92%)	5 (7%)	1 (1%)	12	39
44	3	448/646 (69%)	419 (94%)	29 (6%)	0	100	100
45	4	12/450 (3%)	9 (75%)	3 (25%)	0	100	100
46	1	387/654 (59%)	320 (83%)	64 (16%)	3 (1%)	19	51
47	2	165/258 (64%)	159 (96%)	6 (4%)	0	100	100
48	5	1/37 (3%)	0	1 (100%)	0	100	100
All	All	15145/26756 (57%)	14208 (94%)	828 (6%)	109 (1%)	26	55

All (109) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	GLU
3	C	388	VAL
3	C	801	LEU
3	C	802	HIS
3	C	824	THR
4	D	956	LEU
4	D	957	VAL
11	J	216	ASP
15	N	3	LYS
15	N	37	HIS
18	R	233	PRO
20	T	186	PRO
20	T	406	ILE
20	T	458	SER
36	k	29	LEU
37	m	46	ASN
38	l	37	GLU
39	n	22	ASN
39	n	65	ASN
1	A	330	THR
1	A	368	GLN
1	A	382	GLU
1	A	1763	LEU
3	C	94	ILE
4	D	1583	ASP
4	D	2097	PRO
4	D	2099	THR
11	J	188	GLN
11	J	205	LEU
11	J	217	GLU
11	J	241	VAL
11	J	358	GLU
12	K	66	MET
13	L	200	LYS
15	N	39	GLY
15	N	41	ARG
17	P	205	LYS
18	R	126	ASN
18	R	186	VAL
20	T	329	HIS
23	V	596	LEU
23	V	597	PRO
24	W	155	SER

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Mol	Chain	Res	Type
24	W	156	VAL
28	s	72	PRO
39	n	12	PHE
43	z	63	ALA
46	1	568	VAL
1	A	109	PRO
1	A	167	PRO
1	A	570	ASP
1	A	1211	ASP
1	A	1362	ASP
3	C	363	SER
3	C	441	PRO
11	J	495	PHE
17	P	48	GLN
18	R	223	PRO
20	T	327	SER
24	W	550	ASP
25	X	64	LYS
26	Y	24	LYS
1	A	346	ASP
1	A	364	SER
1	A	366	LYS
3	C	426	GLU
4	D	532	ASN
4	D	1666	THR
4	D	2098	ALA
12	K	78	PRO
14	M	195	LYS
24	W	319	TYR
26	Y	97	ASP
38	l	84	ILE
1	A	56	ALA
1	A	1092	ILE
3	C	83	GLU
3	C	440	SER
3	C	803	ARG
4	D	150	ASP
11	J	341	PRO
16	O	20	PHE
16	O	173	CYS
18	R	70	ALA
20	T	343	PRO

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Mol	Chain	Res	Type
20	T	400	PHE
28	s	71	ILE
37	m	40	MET
1	A	192	GLN
1	A	378	PHE
16	O	106	ASP
38	l	83	ASN
46	1	571	PRO
46	1	616	SER
10	I	51	PRO
10	I	375	ILE
15	N	4	VAL
16	O	134	VAL
24	W	200	VAL
1	A	942	PRO
1	A	1212	GLY
3	C	93	ILE
19	S	12	PRO
1	A	108	MET
1	A	1419	ILE
12	K	77	GLN
20	T	342	GLU
27	Z	986	ARG
1	A	1567	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1778/2108 (84%)	1743 (98%)	35 (2%)	55 77
3	C	760/866 (88%)	725 (95%)	35 (5%)	27 57
5	E	256/300 (85%)	252 (98%)	4 (2%)	62 81
10	I	24/749 (3%)	24 (100%)	0	100 100
11	J	241/751 (32%)	235 (98%)	6 (2%)	47 72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
12	K	51/196 (26%)	50 (98%)	1 (2%)	55 77
13	L	193/709 (27%)	184 (95%)	9 (5%)	26 57
14	M	85/209 (41%)	79 (93%)	6 (7%)	14 44
15	N	130/130 (100%)	127 (98%)	3 (2%)	50 74
16	O	253/361 (70%)	250 (99%)	3 (1%)	71 85
17	P	90/203 (44%)	87 (97%)	3 (3%)	38 66
18	R	210/457 (46%)	196 (93%)	14 (7%)	16 46
19	S	129/134 (96%)	124 (96%)	5 (4%)	32 61
20	T	269/441 (61%)	262 (97%)	7 (3%)	46 72
22	U	21/2432 (1%)	19 (90%)	2 (10%)	8 29
23	V	324/838 (39%)	315 (97%)	9 (3%)	43 70
24	W	125/502 (25%)	118 (94%)	7 (6%)	21 51
25	X	33/381 (9%)	32 (97%)	1 (3%)	41 68
26	Y	114/289 (39%)	105 (92%)	9 (8%)	12 39
28	q	76/435 (18%)	72 (95%)	4 (5%)	22 52
28	r	75/435 (17%)	71 (95%)	4 (5%)	22 52
28	t	40/435 (9%)	38 (95%)	2 (5%)	24 54
29	u	344/361 (95%)	342 (99%)	2 (1%)	86 94
30	v	132/134 (98%)	132 (100%)	0	100 100
31	w	76/143 (53%)	76 (100%)	0	100 100
32	x	23/581 (4%)	23 (100%)	0	100 100
33	h	68/101 (67%)	68 (100%)	0	100 100
34	i	77/177 (44%)	76 (99%)	1 (1%)	69 84
35	j	77/101 (76%)	75 (97%)	2 (3%)	46 72
36	k	80/110 (73%)	75 (94%)	5 (6%)	18 47
37	m	63/74 (85%)	51 (81%)	12 (19%)	1 4
38	l	70/84 (83%)	58 (83%)	12 (17%)	2 8
39	n	59/66 (89%)	55 (93%)	4 (7%)	16 45
40	o	138/218 (63%)	136 (99%)	2 (1%)	67 83
41	p	82/195 (42%)	81 (99%)	1 (1%)	71 85
43	z	33/240 (14%)	33 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
44	3	18/572 (3%)	18 (100%)	0	100 100
45	4	11/411 (3%)	11 (100%)	0	100 100
46	1	234/572 (41%)	232 (99%)	2 (1%)	78 90
47	2	135/223 (60%)	134 (99%)	1 (1%)	84 92
48	5	1/1 (100%)	1 (100%)	0	100 100
All	All	6998/17725 (40%)	6785 (97%)	213 (3%)	44 68

All (213) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LYS
1	A	79	ARG
1	A	330	THR
1	A	331	TRP
1	A	352	PHE
1	A	386	PRO
1	A	390	ASP
1	A	413	LEU
1	A	569	VAL
1	A	579	GLN
1	A	621	VAL
1	A	630	TRP
1	A	671	THR
1	A	758	ARG
1	A	851	SER
1	A	855	ARG
1	A	1021	ASP
1	A	1089	CYS
1	A	1136	ARG
1	A	1315	VAL
1	A	1393	ARG
1	A	1402	ARG
1	A	1407	ASP
1	A	1449	LYS
1	A	1536	LEU
1	A	1570	LYS
1	A	1613	THR
1	A	1615	HIS
1	A	1626	CYS
1	A	1765	SER

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Mol	Chain	Res	Type
1	A	1790	ILE
1	A	1813	ARG
1	A	1838	LYS
1	A	1870	ASP
1	A	1890	GLN
3	C	62	ASP
3	C	68	THR
3	C	71	GLU
3	C	84	GLU
3	C	86	THR
3	C	112	THR
3	C	220	ARG
3	C	256	CYS
3	C	298	LEU
3	C	300	LEU
3	C	357	THR
3	C	359	LYS
3	C	387	ASP
3	C	421	LYS
3	C	427	PHE
3	C	442	LYS
3	C	452	THR
3	C	458	ASP
3	C	460	ASP
3	C	465	MET
3	C	474	LEU
3	C	475	MET
3	C	477	HIS
3	C	489	GLN
3	C	490	PHE
3	C	495	ARG
3	C	517	GLU
3	C	673	LYS
3	C	680	ASN
3	C	704	VAL
3	C	712	LYS
3	C	749	THR
3	C	763	LYS
3	C	939	ARG
3	C	943	LEU
5	E	81	LEU
5	E	153	PHE

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Mol	Chain	Res	Type
5	E	272	ARG
5	E	290	ARG
11	J	195	LEU
11	J	214	ILE
11	J	216	ASP
11	J	239	ARG
11	J	240	THR
11	J	308	ARG
12	K	90	PRO
13	L	20	LYS
13	L	24	MET
13	L	33	ARG
13	L	158	ARG
13	L	181	ARG
13	L	206	ARG
13	L	222	LEU
13	L	235	LEU
13	L	766	ARG
14	M	125	SER
14	M	151	ARG
14	M	160	PHE
14	M	172	HIS
14	M	197	SER
14	M	200	ARG
15	N	34	THR
15	N	102	CYS
15	N	142	CYS
16	O	45	CYS
16	O	65	PHE
16	O	195	ASP
17	P	28	LYS
17	P	34	ASP
17	P	189	ASP
18	R	72	TYR
18	R	76	MET
18	R	86	LEU
18	R	91	ASP
18	R	131	ASP
18	R	134	ARG
18	R	175	GLN
18	R	188	PHE
18	R	212	PHE

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Mol	Chain	Res	Type
18	R	250	CYS
18	R	258	LYS
18	R	279	HIS
18	R	280	ILE
18	R	297	LYS
19	S	9	TRP
19	S	10	GLN
19	S	100	MET
19	S	102	ASN
19	S	131	ARG
20	T	257	ARG
20	T	282	ARG
20	T	400	PHE
20	T	402	ASP
20	T	412	HIS
20	T	455	GLN
20	T	496	THR
22	U	1	MET
22	U	11	ARG
23	V	259	PHE
23	V	458	THR
23	V	465	SER
23	V	468	ASP
23	V	490	CYS
23	V	514	PHE
23	V	553	HIS
23	V	590	LEU
23	V	597	PRO
24	W	88	MET
24	W	97	ASN
24	W	101	THR
24	W	139	LEU
24	W	146	HIS
24	W	160	GLU
24	W	199	TYR
25	X	15	GLN
26	Y	4	ARG
26	Y	7	LEU
26	Y	20	ILE
26	Y	22	LYS
26	Y	40	ASN
26	Y	51	TYR

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Mol	Chain	Res	Type
26	Y	65	ASN
26	Y	108	PHE
26	Y	163	ARG
28	q	19	PRO
28	q	46	PRO
28	q	62	ARG
28	q	90	PHE
28	r	19	PRO
28	r	46	PRO
28	r	60	PRO
28	r	96	LEU
28	t	93	ARG
28	t	108	TYR
29	u	173	ARG
29	u	337	TRP
34	i	76	ASN
35	j	35	SER
35	j	54	GLN
36	k	23	GLU
36	k	31	VAL
36	k	40	THR
36	k	69	ASN
36	k	104	ASP
37	m	2	SER
37	m	5	LEU
37	m	11	LEU
37	m	14	LEU
37	m	25	TRP
37	m	27	MET
37	m	32	TYR
37	m	37	ASP
37	m	47	THR
37	m	52	ASP
37	m	56	SER
37	m	72	ILE
38	l	24	TYR
38	l	29	SER
38	l	34	TRP
38	l	40	ASN
38	l	66	SER
38	l	68	THR
38	l	70	SER

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Mol	Chain	Res	Type
38	l	83	ASN
38	l	86	LEU
38	l	87	LEU
38	l	88	GLN
38	l	90	VAL
39	n	34	PHE
39	n	60	VAL
39	n	61	VAL
39	n	63	ARG
40	o	55	ARG
40	o	78	ARG
41	p	17	LYS
46	1	296	LYS
46	1	465	TYR
47	2	183	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	73	HIS
1	A	97	HIS
1	A	181	ASN
1	A	192	GLN
1	A	297	ASN
1	A	321	ASN
1	A	439	GLN
1	A	584	HIS
1	A	587	GLN
1	A	601	GLN
1	A	675	GLN
1	A	723	ASN
1	A	775	ASN
1	A	792	HIS
1	A	1003	HIS
1	A	1004	ASN
1	A	1014	ASN
1	A	1293	ASN
1	A	1296	GLN
1	A	1359	HIS
1	A	1450	GLN
1	A	1460	HIS

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Mol	Chain	Res	Type
1	A	1563	HIS
1	A	1615	HIS
1	A	1717	ASN
1	A	1766	GLN
1	A	1816	GLN
1	A	1875	HIS
1	A	1894	GLN
1	A	1944	HIS
1	A	1965	HIS
3	C	87	GLN
3	C	175	GLN
3	C	245	HIS
3	C	306	ASN
3	C	437	HIS
3	C	451	HIS
3	C	491	HIS
3	C	583	ASN
3	C	892	GLN
5	E	101	ASN
5	E	165	GLN
11	J	188	GLN
11	J	212	GLN
11	J	389	HIS
12	K	164	ASN
13	L	39	HIS
13	L	175	GLN
14	M	134	GLN
14	M	172	HIS
14	M	189	GLN
15	N	27	GLN
15	N	54	HIS
15	N	99	ASN
15	N	136	HIS
16	O	25	GLN
16	O	82	GLN
16	O	196	GLN
16	O	254	GLN
16	O	267	GLN
16	O	294	ASN
18	R	68	HIS
18	R	106	GLN
18	R	126	ASN

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Mol	Chain	Res	Type
18	R	194	GLN
18	R	279	HIS
19	S	150	GLN
20	T	217	GLN
20	T	269	GLN
20	T	413	ASN
20	T	417	ASN
20	T	446	ASN
20	T	451	HIS
20	T	455	GLN
23	V	174	ASN
23	V	183	GLN
23	V	262	HIS
23	V	306	GLN
24	W	97	ASN
24	W	119	HIS
24	W	162	ASN
24	W	172	GLN
25	X	41	GLN
26	Y	57	ASN
26	Y	64	GLN
26	Y	102	HIS
28	r	79	GLN
29	u	285	ASN
29	u	345	GLN
29	u	356	ASN
30	v	41	ASN
30	v	98	HIS
30	v	114	GLN
31	w	67	GLN
31	w	105	ASN
31	w	137	GLN
32	x	178	ASN
33	h	23	ASN
34	i	22	GLN
34	i	76	ASN
35	j	39	HIS
35	j	64	ASN
36	k	62	HIS
36	k	69	ASN
36	k	112	ASN
37	m	58	HIS

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Mol	Chain	Res	Type
38	l	19	ASN
38	l	83	ASN
38	l	88	GLN
39	n	65	ASN
40	o	130	HIS
41	p	7	HIS
46	1	231	GLN
46	1	236	GLN
46	1	271	GLN
46	1	278	ASN
46	1	329	GLN
46	1	480	HIS
47	2	52	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	96/117 (82%)	31 (32%)	3 (3%)
6	F	96/107 (89%)	38 (39%)	12 (12%)
7	G	17/46 (36%)	4 (23%)	1 (5%)
8	6	68/174 (39%)	43 (63%)	5 (7%)
9	H	132/188 (70%)	23 (17%)	1 (0%)
All	All	409/632 (64%)	139 (33%)	22 (5%)

All (139) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	13	C
2	B	19	A
2	B	20	G
2	B	21	A
2	B	22	U
2	B	23	C
2	B	25	C
2	B	26	A
2	B	28	A
2	B	35	U
2	B	36	C
2	B	38	C
2	B	39	C
2	B	45	C

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Mol	Chain	Res	Type
2	B	52	U
2	B	57	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	6	C
6	F	7	G
6	F	10	U
6	F	12	G
6	F	25	C
6	F	26	U
6	F	27	A
6	F	28	A
6	F	29	A
6	F	33	G
6	F	34	G
6	F	36	A
6	F	37	C
6	F	38	G
6	F	45	A
6	F	46	G
6	F	48	A
6	F	49	G
6	F	51	U
6	F	54	G
6	F	56	A
6	F	58	G
6	F	59	G
6	F	60	C
6	F	61	C

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Mol	Chain	Res	Type
6	F	67	G
6	F	68	C
6	F	74	U
6	F	78	A
6	F	79	C
6	F	80	G
6	F	81	C
6	F	82	A
6	F	83	A
6	F	84	A
6	F	85	U
6	F	86	U
6	F	87	C
7	G	-11	G
7	G	-9	C
7	G	-6	C
7	G	-1	G
8	6	2	U
8	6	3	A
8	6	5	G
8	6	7	G
8	6	8	C
8	6	10	U
8	6	11	A
8	6	12	G
8	6	13	C
8	6	14	A
8	6	16	G
8	6	17	U
8	6	21	A
8	6	22	C
8	6	23	U
8	6	24	G
8	6	25	G
8	6	27	U
8	6	30	C
8	6	31	U
8	6	73	G
8	6	74	G
8	6	75	U
8	6	76	U
8	6	77	U

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Mol	Chain	Res	Type
8	6	78	C
8	6	79	C
8	6	80	U
8	6	81	U
8	6	82	G
8	6	83	A
8	6	91	A
8	6	92	U
8	6	97	A
8	6	99	C
8	6	100	C
8	6	101	U
8	6	102	G
8	6	103	U
8	6	104	C
8	6	105	C
8	6	106	C
8	6	107	U
9	H	15	U
9	H	16	U
9	H	17	U
9	H	19	G
9	H	20	G
9	H	24	A
9	H	25	G
9	H	29	A
9	H	30	A
9	H	31	G
9	H	40	C
9	H	101	U
9	H	102	U
9	H	106	G
9	H	112	G
9	H	147	G
9	H	153	A
9	H	154	C
9	H	156	U
9	H	157	G
9	H	164	C
9	H	178	A
9	H	179	C

All (22) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	20	G
2	B	27	U
2	B	94	U
6	F	5	U
6	F	25	C
6	F	26	U
6	F	33	G
6	F	47	A
6	F	48	A
6	F	50	A
6	F	58	G
6	F	59	G
6	F	81	C
6	F	84	A
6	F	86	U
7	G	-12	G
8	6	16	G
8	6	20	A
8	6	21	A
8	6	22	C
8	6	105	C
9	H	15	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	SEP	R	232	18	8,9,10	1.50	1 (12%)	8,12,14	2.25	2 (25%)
18	SEP	R	224	18	8,9,10	1.39	1 (12%)	8,12,14	1.78	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	SEP	R	232	18	-	4/5/8/10	-
18	SEP	R	224	18	-	3/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	232	SEP	P-O1P	3.25	1.61	1.50
18	R	224	SEP	P-O1P	3.04	1.60	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	R	224	SEP	P-OG-CB	-4.49	105.92	118.30
18	R	232	SEP	P-OG-CB	-4.35	106.32	118.30
18	R	232	SEP	OG-CB-CA	4.28	112.31	108.14

There are no chirality outliers.

All (7) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	R	232	SEP	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 12 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
50	GTP	C	1500	51	26,34,34	1.45	3 (11%)	32,54,54	2.00	6 (18%)
49	IHP	A	3000	-	36,36,36	1.07	0	54,60,60	1.82	11 (20%)

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
50	GTP	C	1500	51	-	6/18/38/38	0/3/3/3
49	IHP	A	3000	-	-	7/30/54/54	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	C	1500	GTP	C5-C6	-4.74	1.37	1.47
50	C	1500	GTP	C5-C4	-2.20	1.37	1.43
50	C	1500	GTP	O4'-C4'	-2.06	1.40	1.45

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	C	1500	GTP	PA-O3A-PB	-6.58	110.23	132.83
49	A	3000	IHP	C6-C5-C4	4.97	121.29	110.41
50	C	1500	GTP	PB-O3B-PG	-4.61	117.00	132.83
49	A	3000	IHP	C6-C1-C2	4.07	119.31	110.41
49	A	3000	IHP	C3-C2-C1	3.76	118.64	110.41
49	A	3000	IHP	C5-C6-C1	3.55	118.18	110.41
50	C	1500	GTP	C2-N1-C6	-3.45	118.75	125.10
49	A	3000	IHP	C4-C3-C2	3.44	117.94	110.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	C	1500	GTP	C5-C6-N1	3.40	119.96	113.95
50	C	1500	GTP	C8-N7-C5	3.06	108.82	102.99
50	C	1500	GTP	C3'-C2'-C1'	2.75	105.11	100.98
49	A	3000	IHP	O11-C1-C2	2.54	114.67	108.69
49	A	3000	IHP	C5-C4-C3	2.47	115.82	110.41
49	A	3000	IHP	O45-P5-O25	2.31	119.74	110.68
49	A	3000	IHP	O43-P3-O33	2.26	116.27	107.64
49	A	3000	IHP	O12-P2-O22	-2.16	101.07	109.39
49	A	3000	IHP	O42-P2-O32	2.01	115.33	107.64

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
49	A	3000	IHP	C2-C1-O11-P1
49	A	3000	IHP	C2-O12-P2-O22
49	A	3000	IHP	C6-O16-P6-O26
50	C	1500	GTP	PB-O3B-PG-O3G
50	C	1500	GTP	C5'-O5'-PA-O3A
50	C	1500	GTP	C5'-O5'-PA-O1A
50	C	1500	GTP	C5'-O5'-PA-O2A
50	C	1500	GTP	C3'-C4'-C5'-O5'
50	C	1500	GTP	O4'-C4'-C5'-O5'
49	A	3000	IHP	C3-C4-O14-P4
49	A	3000	IHP	C1-O11-P1-O21
49	A	3000	IHP	C1-O11-P1-O41
49	A	3000	IHP	C4-O14-P4-O34

There are no ring outliers.

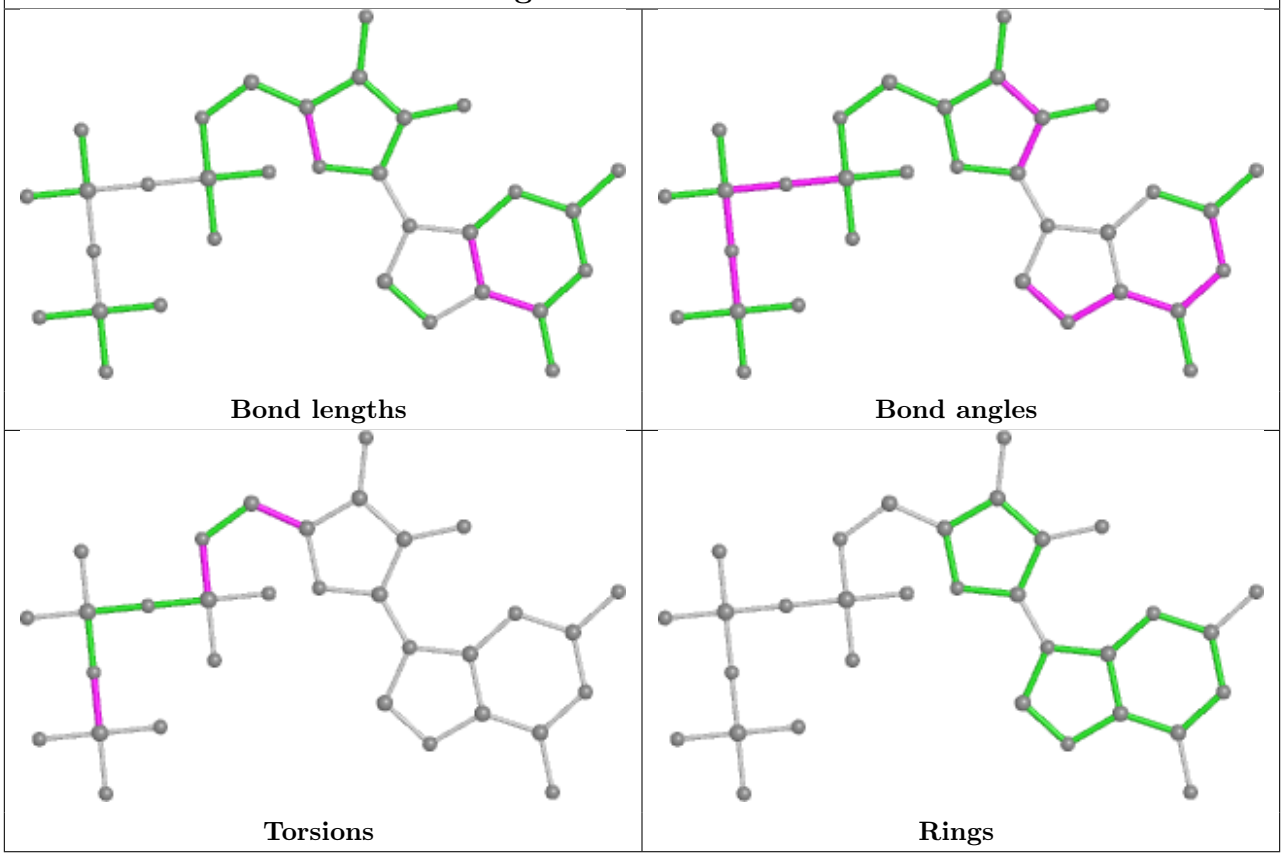
2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	C	1500	GTP	6	0
49	A	3000	IHP	7	0

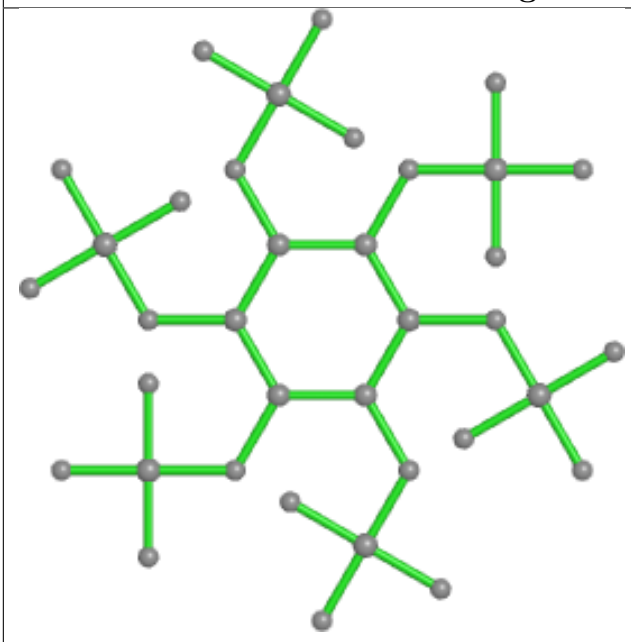
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

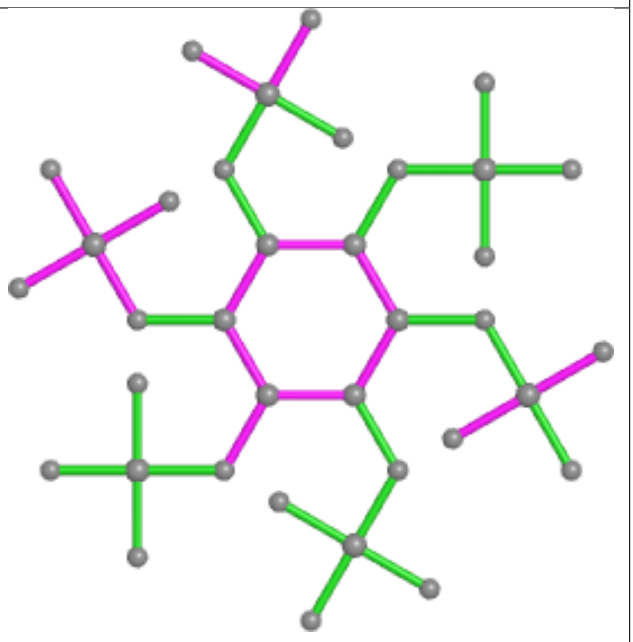
Ligand GTP C 1500



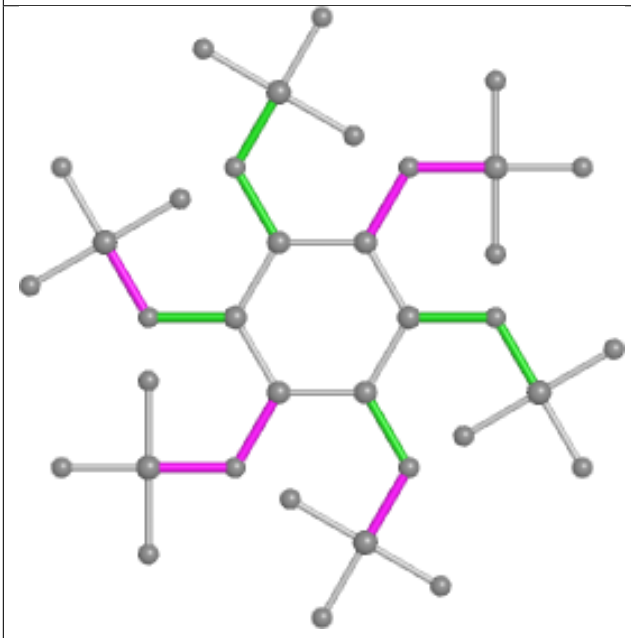
Ligand IHP A 3000



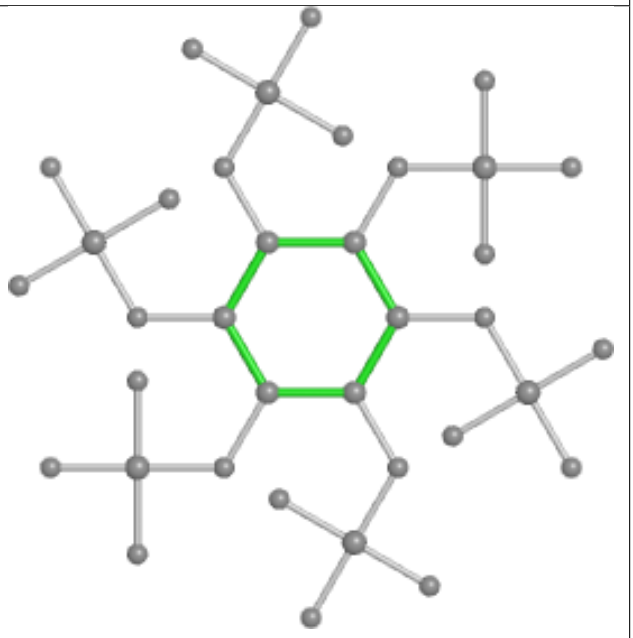
Bond lengths



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.

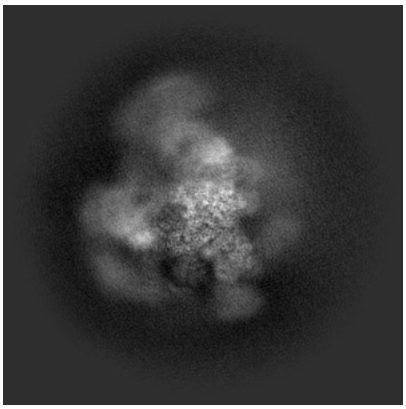
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35113. These allow visual inspection of the internal detail of the map and identification of artifacts.

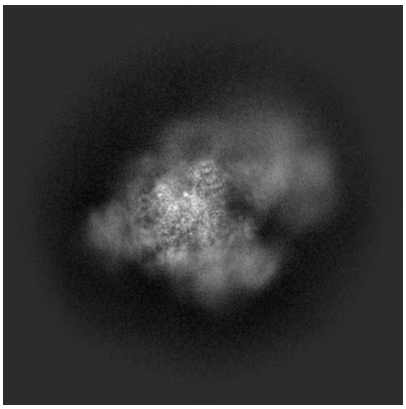
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

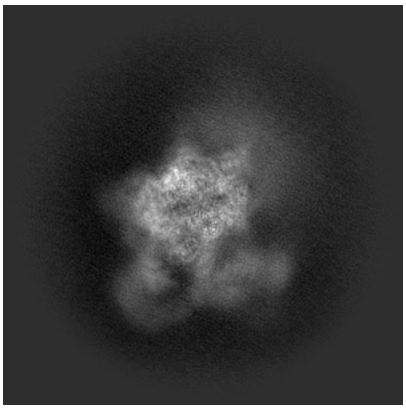
6.1.1 Primary map



X

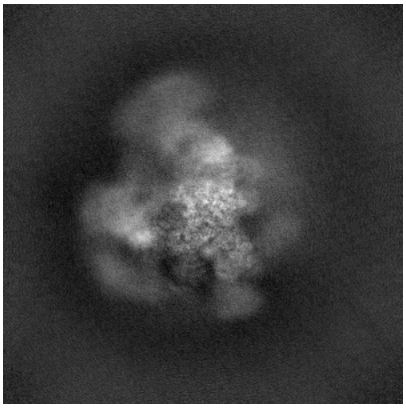


Y

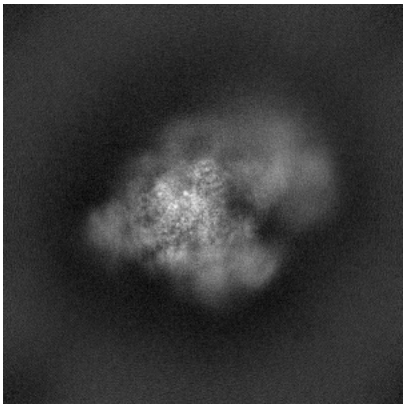


Z

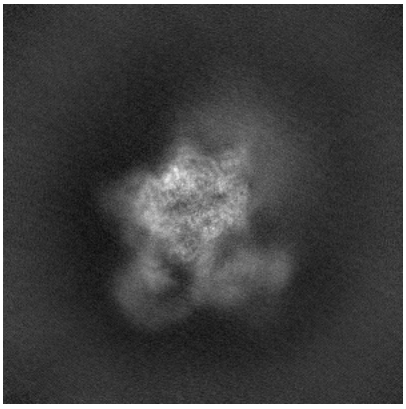
6.1.2 Raw map



X



Y

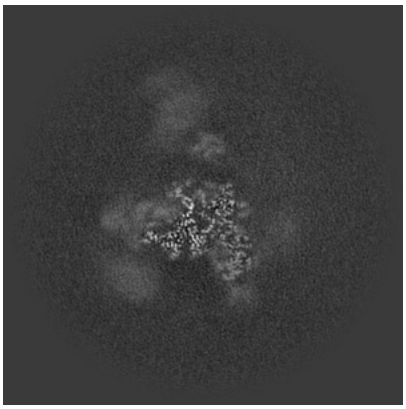


Z

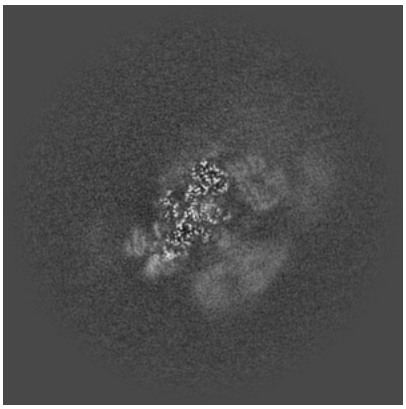
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

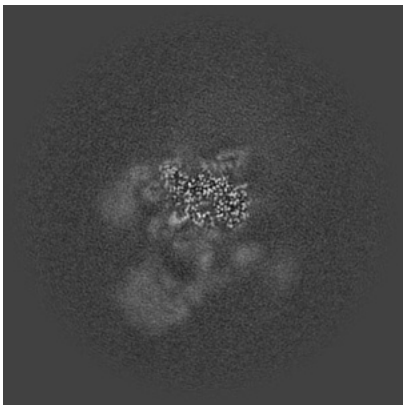
6.2.1 Primary map



X Index: 240

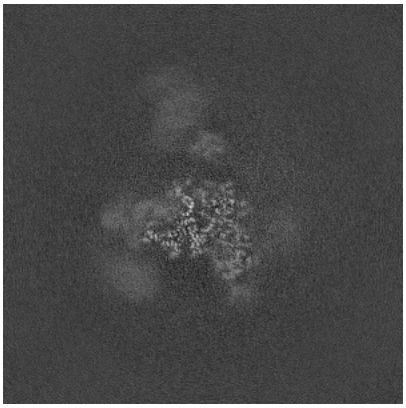


Y Index: 240

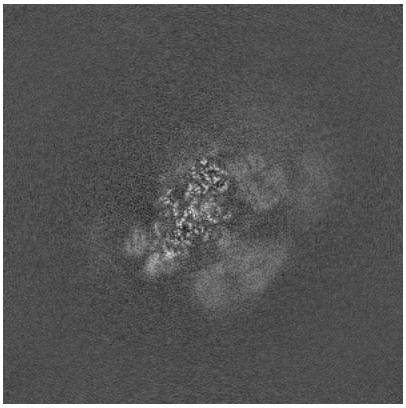


Z Index: 240

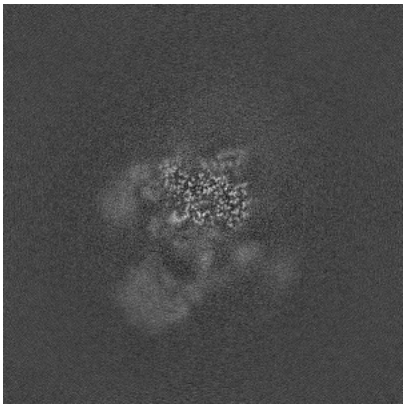
6.2.2 Raw map



X Index: 240



Y Index: 240

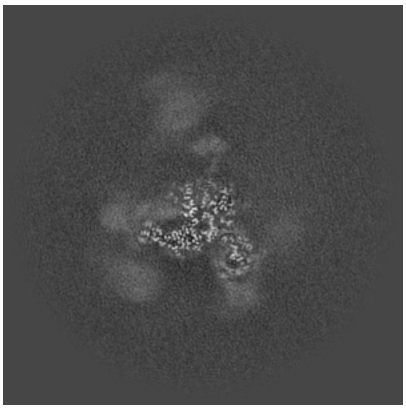


Z Index: 240

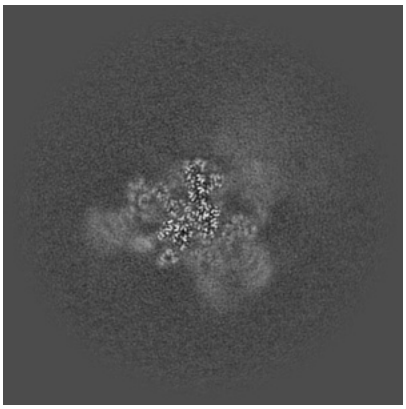
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

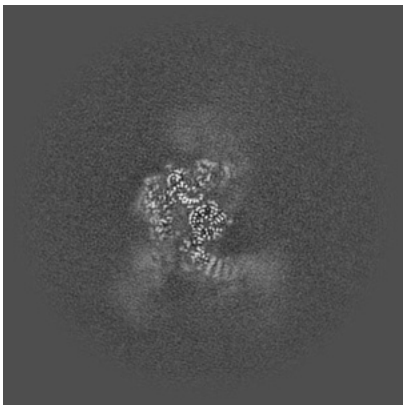
6.3.1 Primary map



X Index: 236

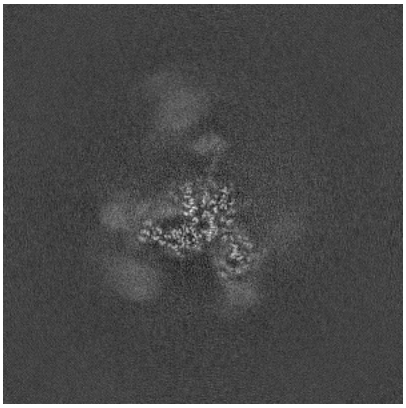


Y Index: 262

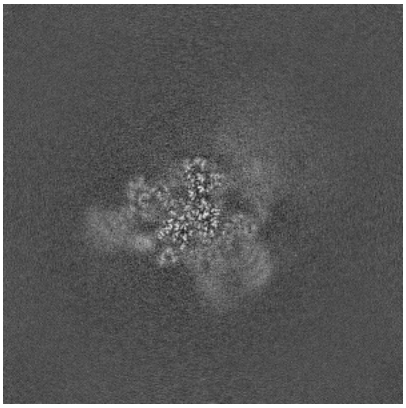


Z Index: 200

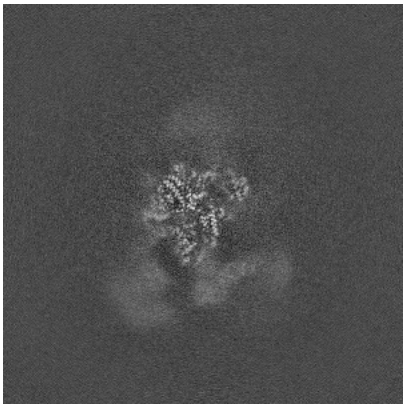
6.3.2 Raw map



X Index: 236



Y Index: 262

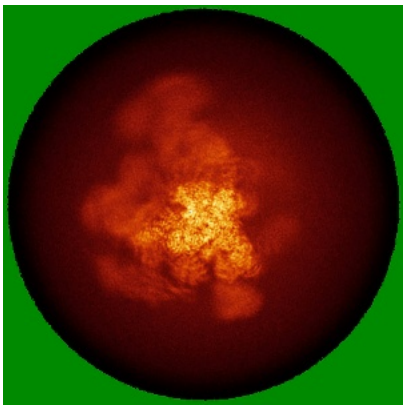


Z Index: 218

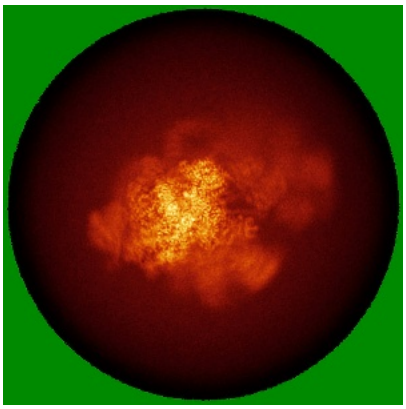
The images above show the largest variance slices of the map in three orthogonal directions.

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

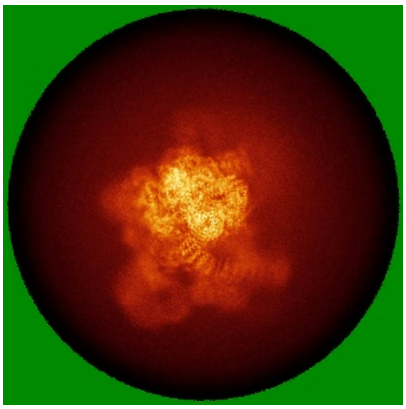
6.4.1 Primary map



X

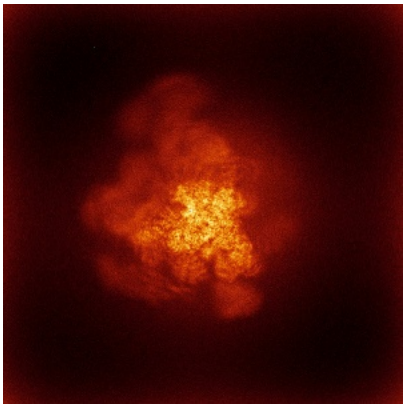


Y

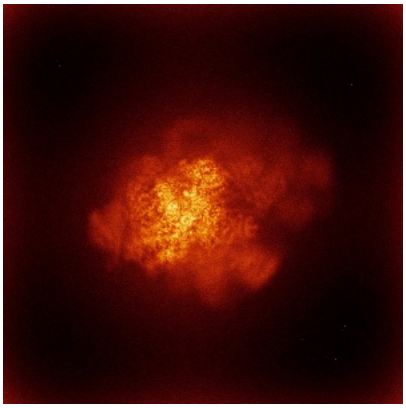


Z

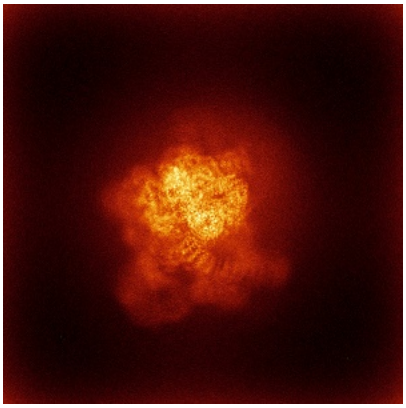
6.4.2 Raw map



X



Y



Z

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

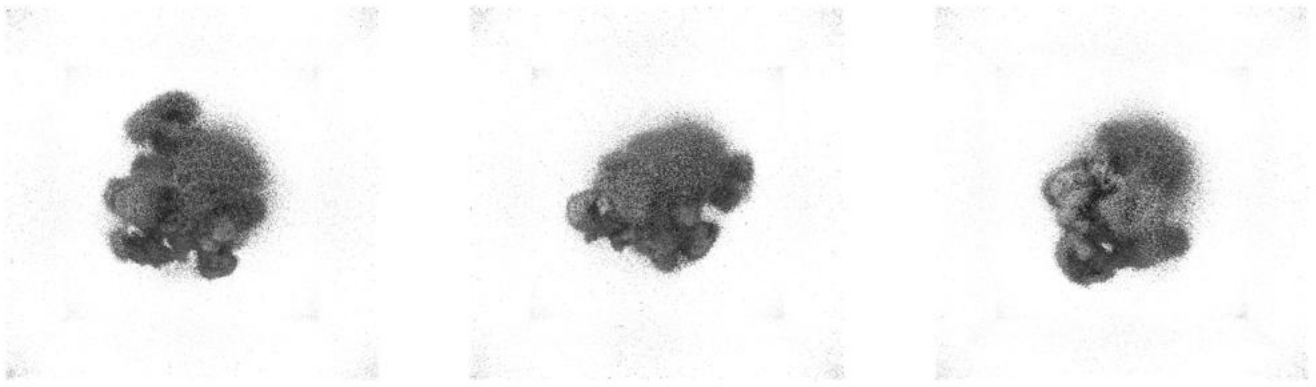
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

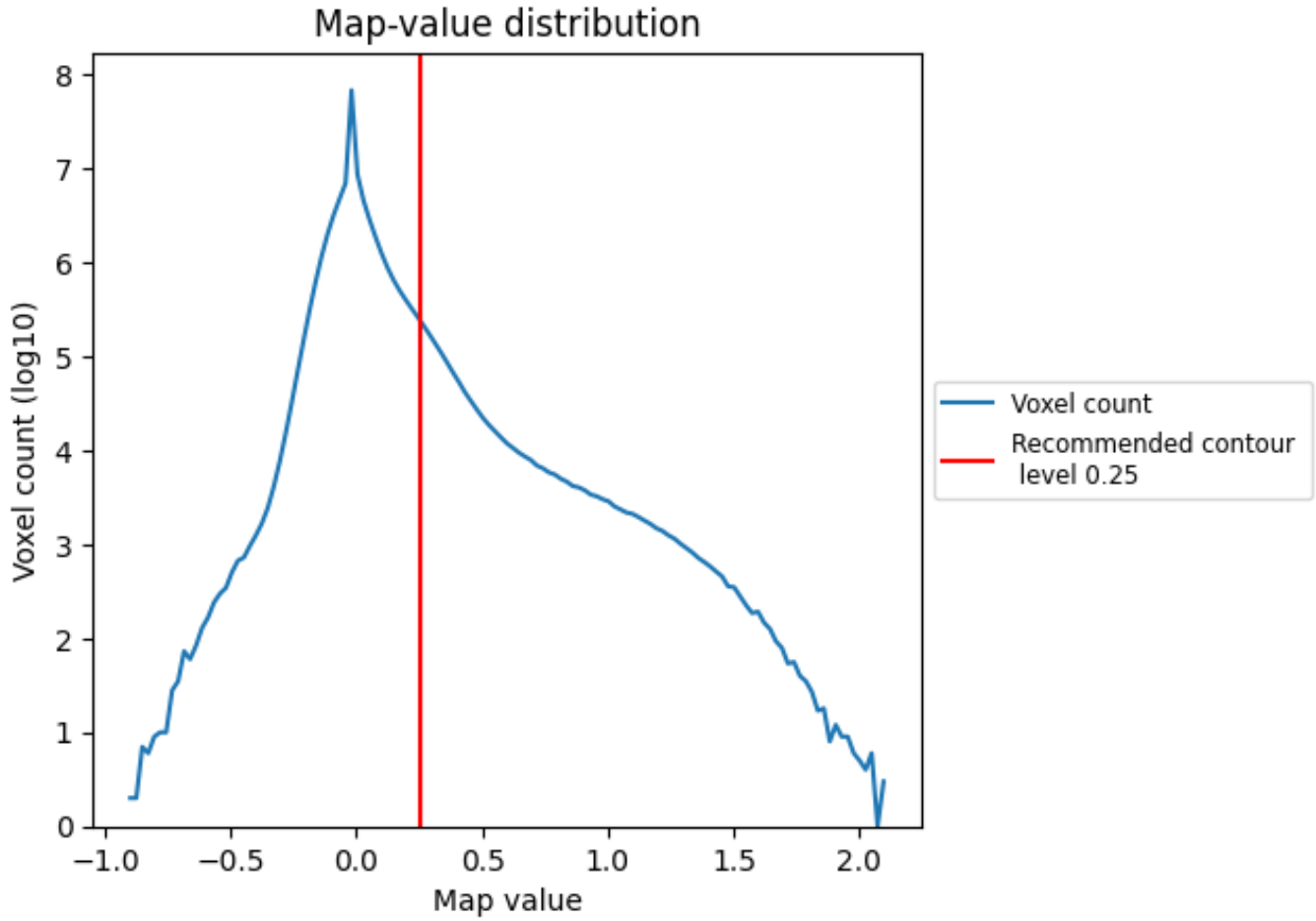
6.6 Mask visualisation (i)

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

7 Map analysis

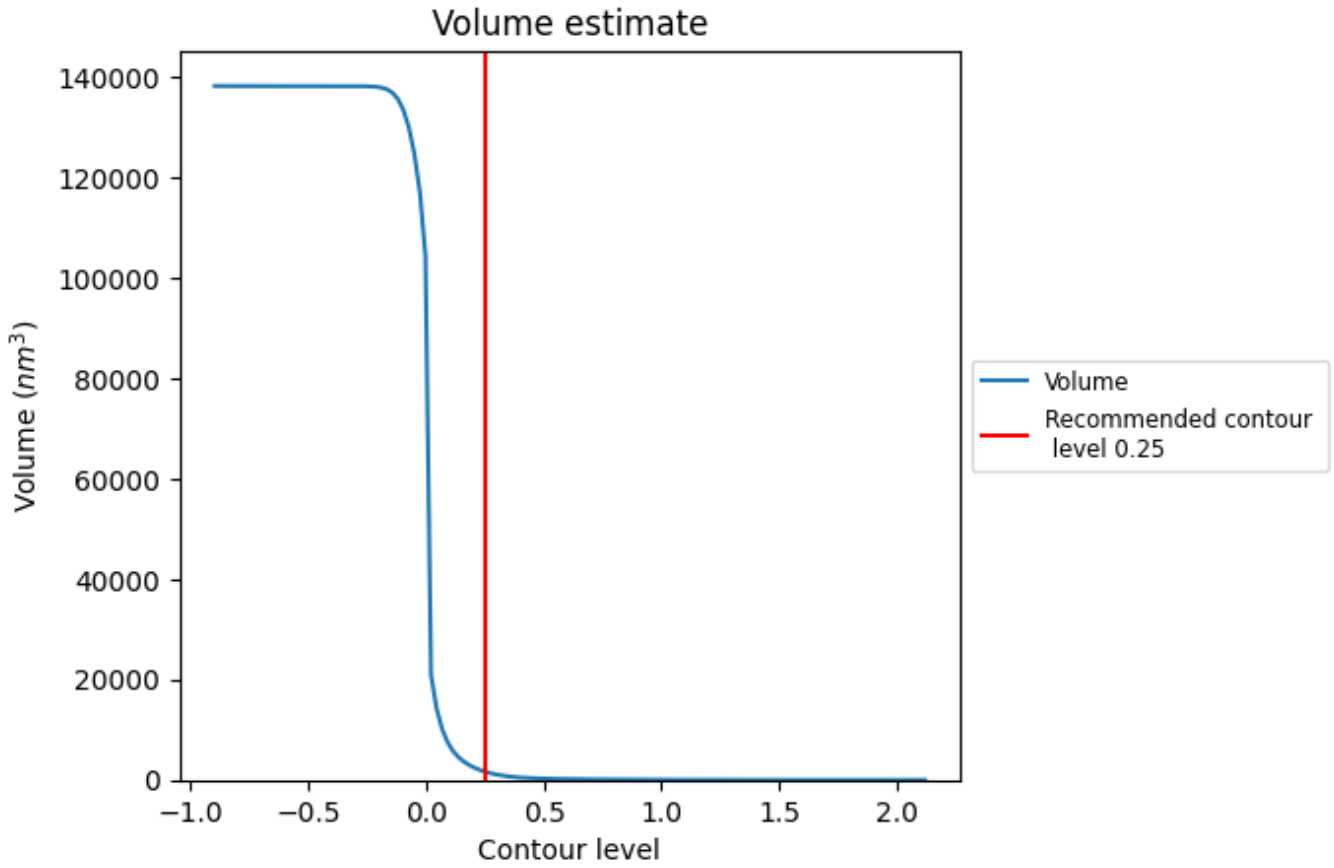
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

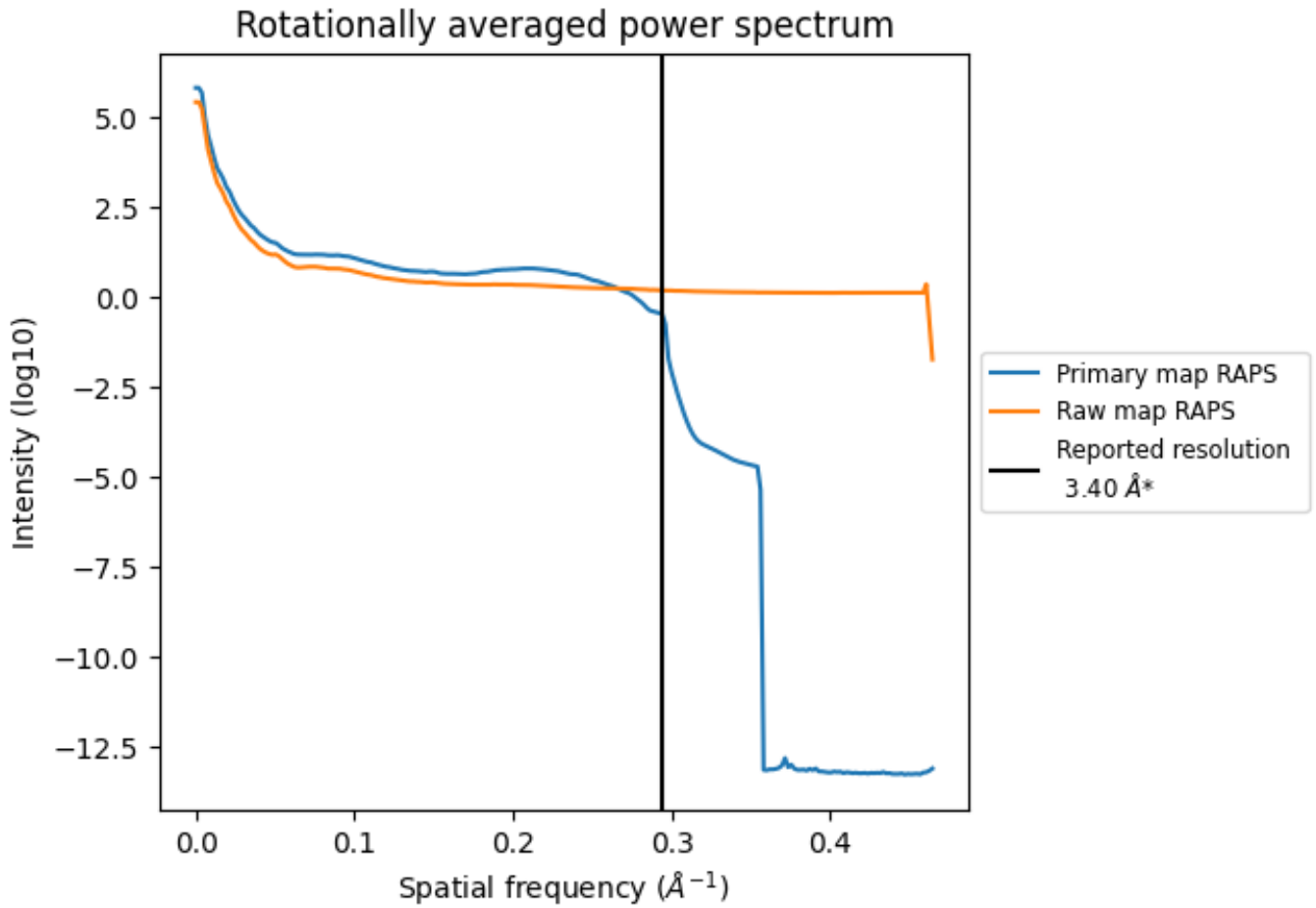
7.2 Volume estimate



The volume at the recommended contour level is 1654 nm^3; this corresponds to an approximate mass of 1495 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)

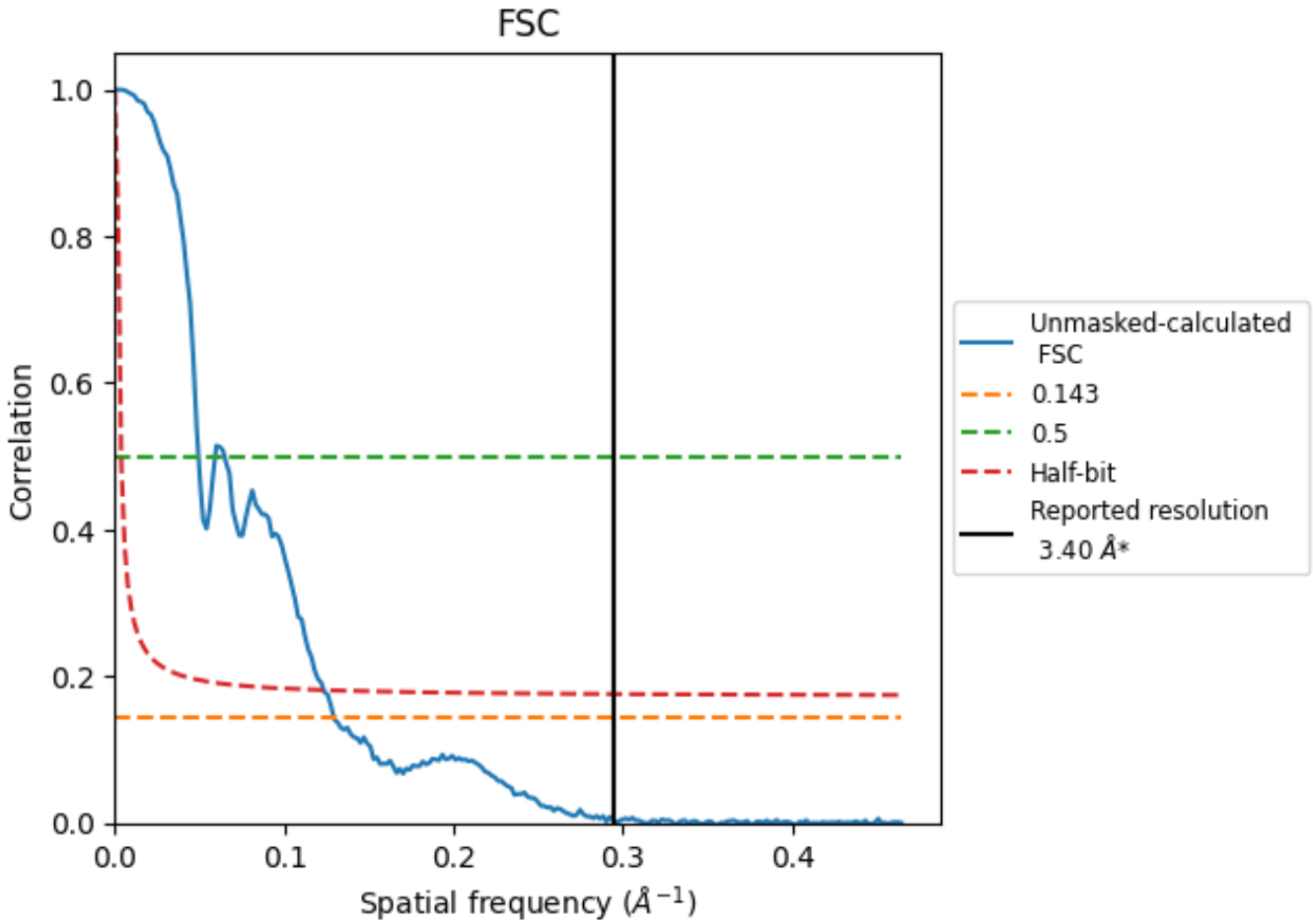


*Reported resolution corresponds to spatial frequency of 0.294 $Å^{-1}$

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 (i)

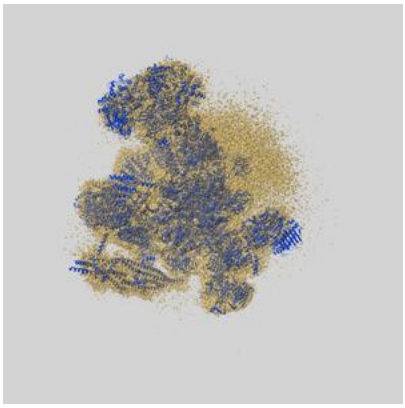
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.73	20.24	8.10

*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 7.73 differs from the reported value 3.4 by more than 10 %

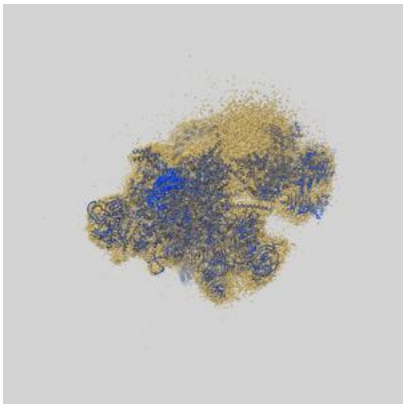
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35113 and PDB model 8I0W. Per-residue inclusion information can be found in section 3 on page 15.

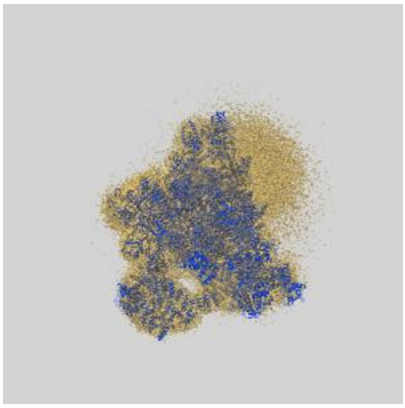
9.1 Map-model overlay



X



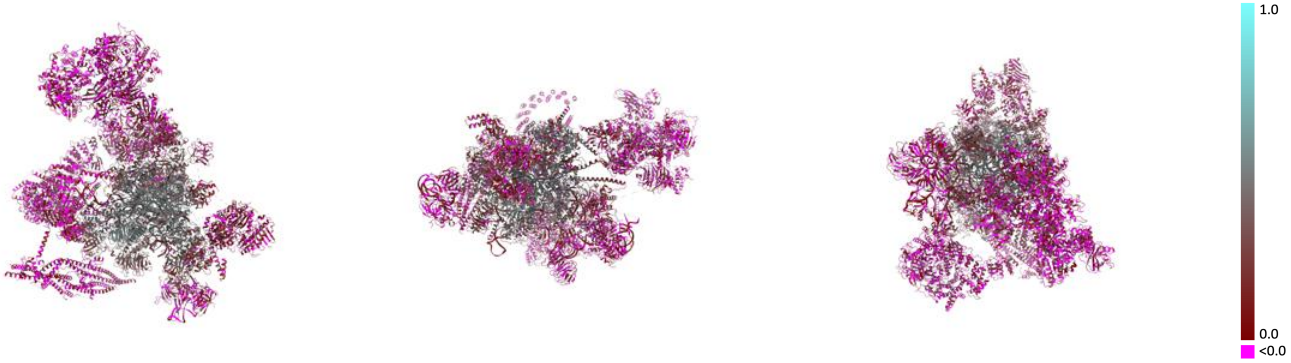
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 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.

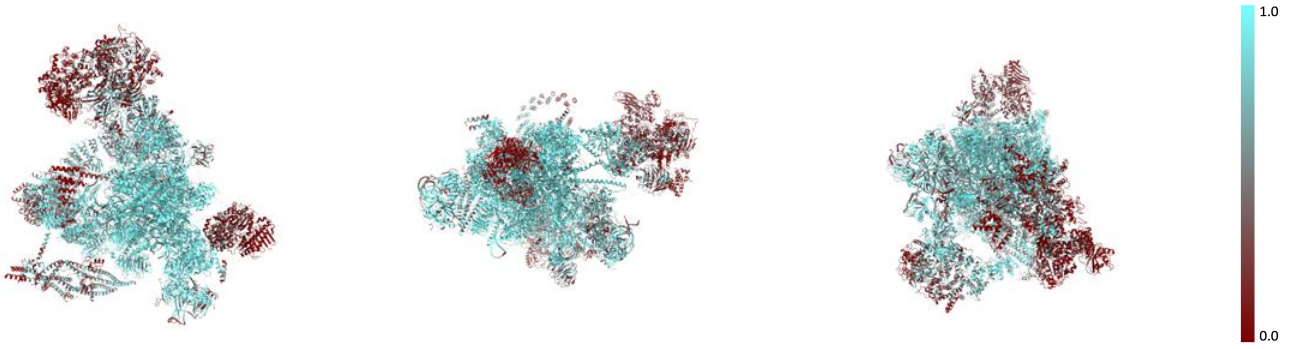
9.2 Q-score mapped to coordinate model



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.

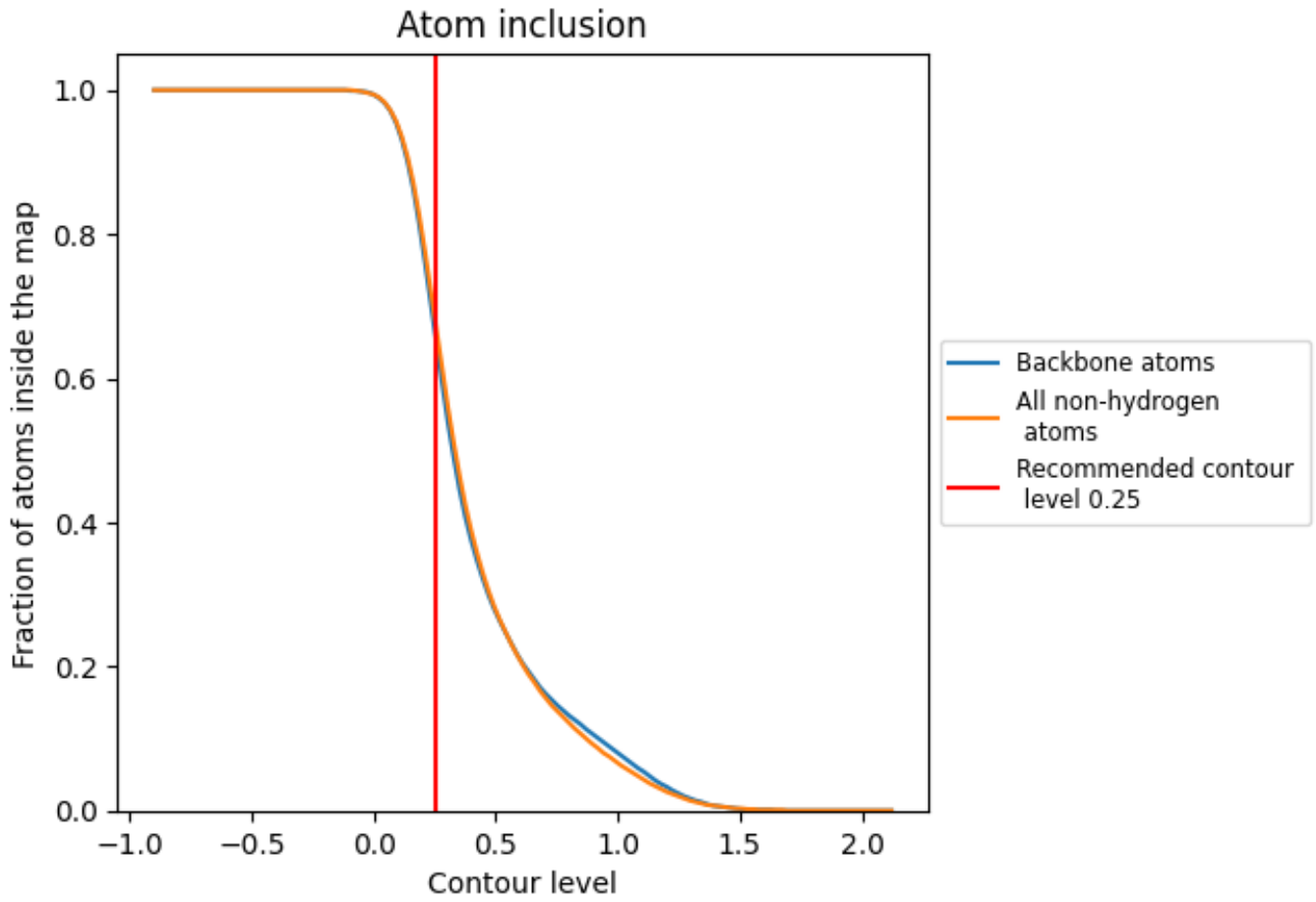
9.3 Atom inclusion mapped to coordinate model



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 (0.25).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 68% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6840	0.2310
1	0.7650	0.2030
2	0.4860	0.1790
3	0.5550	0.0900
4	0.4770	0.1300
5	0.7070	0.3070
6	0.8500	0.2460
A	0.8970	0.4280
B	0.8620	0.2550
C	0.9070	0.3610
D	0.1970	0.0360
E	0.9250	0.2880
F	0.8900	0.3270
G	0.6580	0.3060
H	0.7390	0.1200
I	0.7980	0.1070
J	0.7170	0.2580
K	0.5170	0.0640
L	0.7310	0.2630
M	0.7730	0.2440
N	0.9240	0.4300
O	0.8530	0.3150
P	0.8360	0.3900
Q	0.3980	0.0480
R	0.8710	0.3850
S	0.8950	0.2700
T	0.9720	0.5180
U	0.7280	0.2950
V	0.5520	0.1830
W	0.6510	0.1820
X	0.8570	0.3260
Y	0.8390	0.3640
Z	0.7080	0.1440
a	0.7530	0.0930
b	0.8840	0.1120

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Chain	Atom inclusion	Q-score
c	0.7630	0.0580
d	0.7130	0.0330
e	0.7660	0.1150
f	0.6710	0.0530
g	0.8300	0.1580
h	0.5970	0.0860
i	0.4440	0.0620
j	0.6200	0.1210
k	0.6260	0.0720
l	0.6980	0.0900
m	0.7700	0.0630
n	0.6110	0.0300
o	0.4800	0.0920
p	0.6940	0.0770
q	0.2690	0.0640
r	0.4390	0.0700
s	0.5860	-0.0050
t	0.4720	0.0260
u	0.1910	0.1160
v	0.0310	0.0980
w	0.0360	0.0930
x	0.0380	0.0740
y	0.7280	0.1030
z	0.8960	0.3010