Full wwPDB EM Validation Report ⓘ

Nov 3, 2024 – 01:09 PM JST

PDB ID	:	5Z56
EMDB ID	:	EMD-6889
Title	:	cryo-EM structure of a human activated spliceosome (mature Bact) at 5.1 angstrom.
Authors	:	Zhang, X.; Yan, C.; Zhan, X.; Li, L.; Lei, J.; Shi, Y.
Deposited on	:	2018-01-17
Resolution	:	5.10 Å(reported)

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

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

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

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

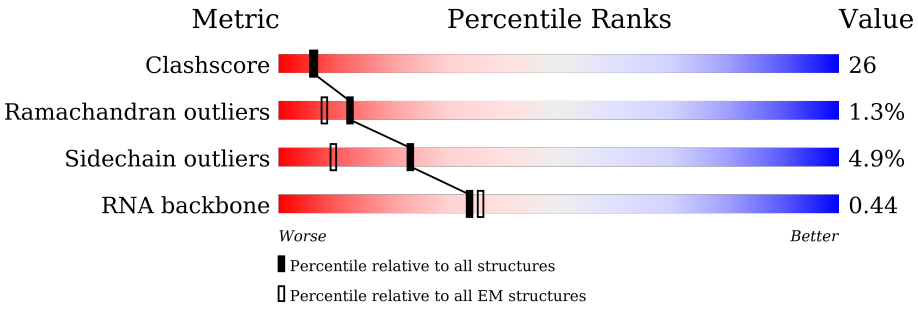
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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

The reported resolution of this entry is 5.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	A	2335	21% 55% 36%
2	B	117	18% 29% 26% 14% 28%
3	C	972	10% 49% 31% 7% 12%
4	D	2136	75% 79% 19%
5	E	357	26% 58% 22% 16%
6	a	126	62% 64% 36%
6	h	126	63% 63% 37%

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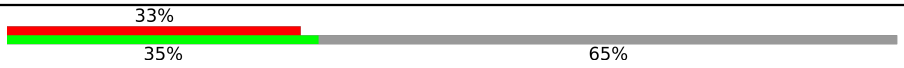
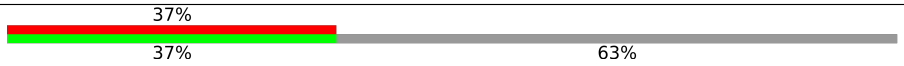
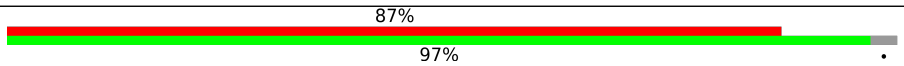
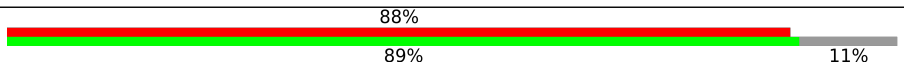
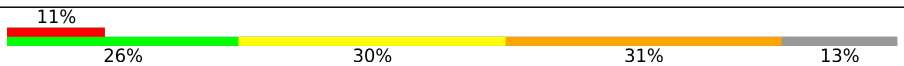
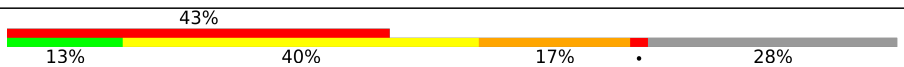
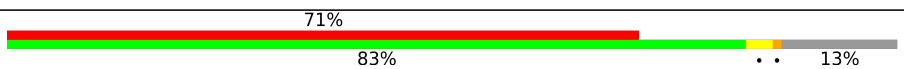
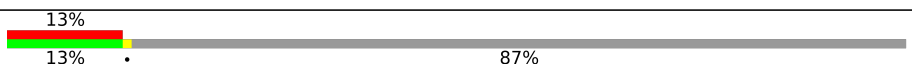
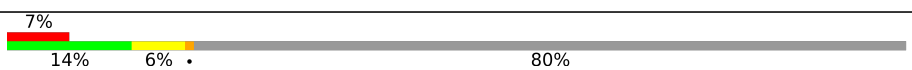
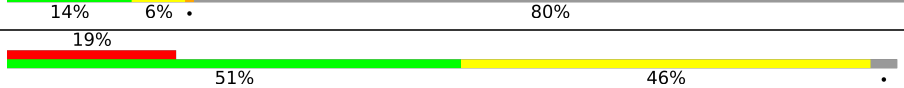
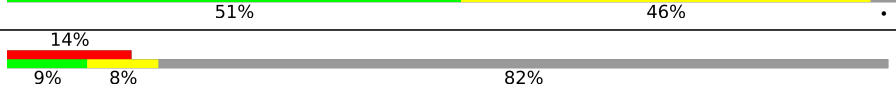
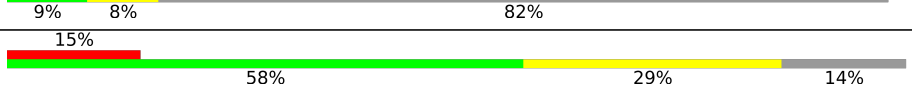
Mol	Chain	Length	Quality of chain
7	b	231	
7	i	231	
8	c	119	
8	j	119	
9	d	118	
9	k	118	
10	f	86	
10	m	86	
11	e	92	
11	l	92	
12	g	76	
12	n	76	
13	F	107	
14	G	274	
15	H	188	
16	o	255	
17	p	225	
18	w	501	
19	u	793	
20	v	464	
21	1	1304	
22	2	895	
23	3	1217	
24	4	424	
25	5	125	

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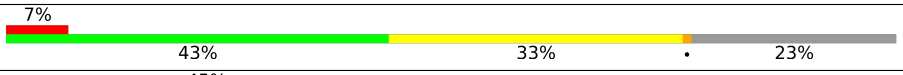
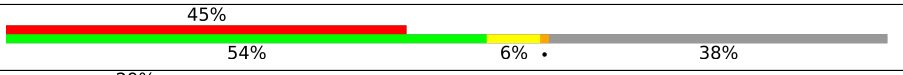
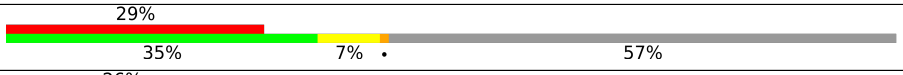
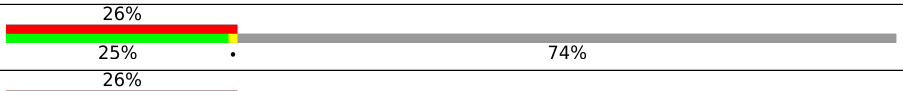
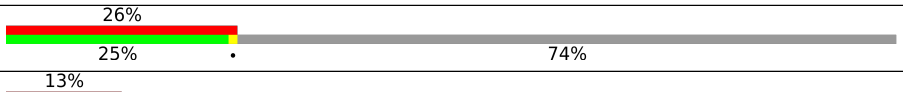
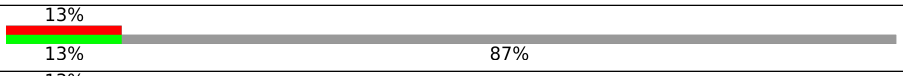
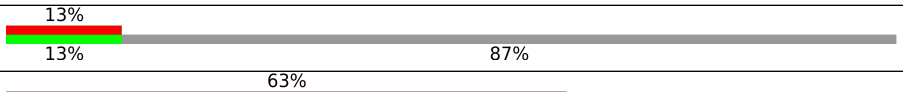
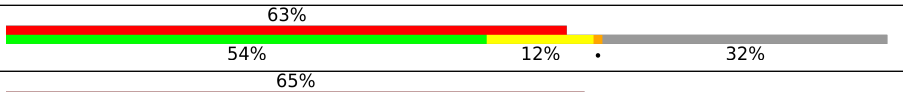
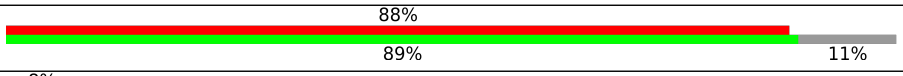
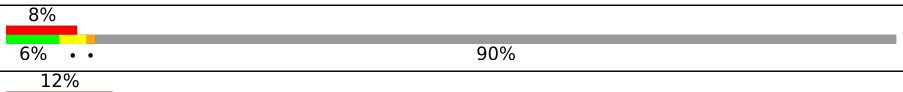
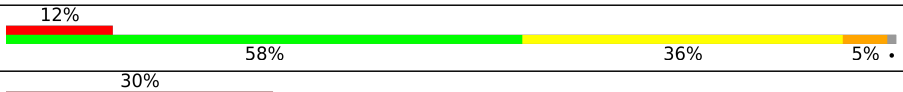
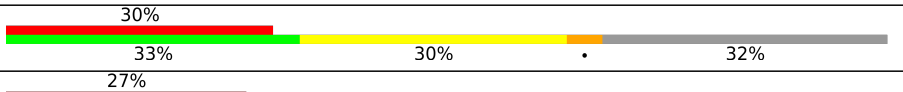
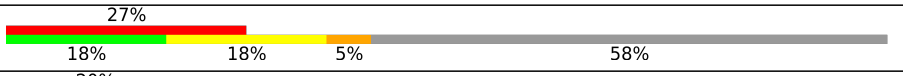
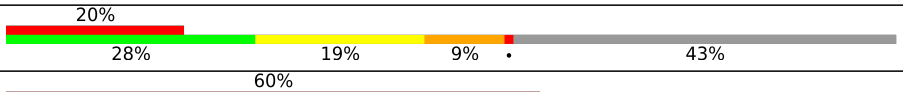
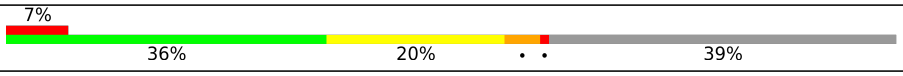
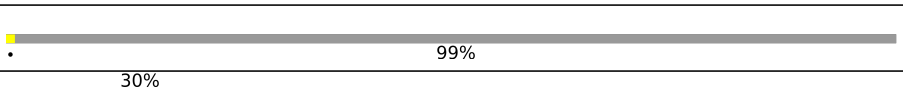
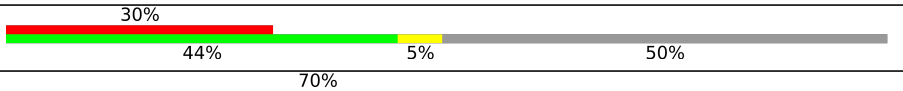
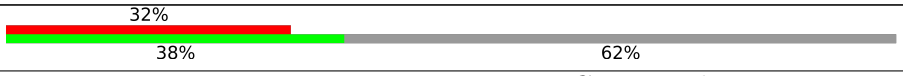
Mol	Chain	Length	Quality of chain
26	6	110	
27	7	86	
28	J	848	
29	L	802	
30	q	504	
30	r	504	
30	s	504	
30	t	504	
31	K	225	
32	I	855	
33	Q	1485	
34	M	343	
35	N	144	
36	O	420	
37	P	229	
38	R	540	
39	S	166	
40	T	514	
41	U	2752	
42	V	908	
43	W	579	
44	X	396	
45	Y	322	
46	Z	619	
47	z	472	

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Mol	Chain	Length	Quality of chain
48	x	1041	56% 55% 44%
49	y	301	74% 77% 23%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
50	IHP	A	3000	-	-	X	-
51	GTP	C	1500	-	-	X	-
53	ZN	O	502	-	-	X	-

2 Entry composition (i)

There are 53 unique types of molecules in this entry. The entry contains 117278 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	2232	18450	11885	3217	3269	79	0	0

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	84	1768	792	295	597	84	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	860	6716	4294	1120	1270	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	1722	8528	5084	1722	1722	0	0

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

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

- Molecule 6 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	a	81	399	237	81	81	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
6	h	80	Total 393	C 233	N 80	O 80	0	0

- Molecule 7 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	b	82	Total 405	C 241	N 82	O 82	0	0
7	i	86	Total 422	C 250	N 86	O 86	0	0

- Molecule 8 is a protein called Small nuclear ribonucleoprotein Sm D1.

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

- Molecule 9 is a protein called Small nuclear ribonucleoprotein Sm D2.

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

- Molecule 10 is a protein called Small nuclear ribonucleoprotein F.

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

- Molecule 11 is a protein called Small nuclear ribonucleoprotein E.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	g	74	Total 363	C 215	N 74	O 74	0	0
12	n	68	Total 334	C 198	N 68	O 68	0	0

- Molecule 13 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	93	Total 1988	C 889	N 363	O 643	P 93	0	0

- Molecule 14 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	77	Total 1545	C 689	N 240	O 539	P 77	0	0

- Molecule 15 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	136	Total 2886	C 1289	N 499	O 962	P 136	0	0

- Molecule 16 is a protein called U2 small nuclear ribonucleoprotein A'.

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

- Molecule 17 is a protein called U2 small nuclear ribonucleoprotein B".

Mol	Chain	Residues	Atoms				AltConf	Trace
17	p	165	Total 813	C 483	N 165	O 165	0	0

- Molecule 18 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	w	437	Total 2369	C 1448	N 460	O 458	S 3	0	0

- Molecule 19 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	u	106	Total	C	N	O	0	0
			530	318	106	106		

- Molecule 20 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	v	167	Total	C	N	O	S	0	0
			946	571	193	180	2		

- Molecule 21 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	1	1038	Total	C	N	O	S	0	0
			7702	4900	1347	1415	40		

- Molecule 22 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	2	183	Total	C	N	O	S	0	0
			1252	809	213	226	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	3	1177	Total	C	N	O	S	0	0
			9220	5854	1566	1755	45		

- Molecule 24 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	4	78	Total	C	N	O	0	0
			527	345	83	99		

- Molecule 25 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	5	108	Total	C	N	O	S	0	0
			807	512	142	150	3		

- Molecule 26 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	6	85	Total	C	N	O	S	0	0
			645	396	114	122	13		

- Molecule 27 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	7	66	Total	C	N	O	S	0	0
			540	343	94	98	5		

- Molecule 28 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	J	522	Total	C	N	O	S	0	0
			3463	2156	653	648	6		

- Molecule 29 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	L	342	Total	C	N	O	S	0	0
			2260	1430	406	420	4		

- Molecule 30 is a protein called Pre-mRNA-processing factor 19.

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

- Molecule 31 is a protein called Pre-mRNA-splicing factor SPF27.

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

- Molecule 32 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	I	564	Total 2778	C 1650	N 564	O 564	0	0

- Molecule 33 is a protein called Intron-binding protein aquarius.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	Q	1317	Total 6528	C 3894	N 1317	O 1317	0	0

- Molecule 34 is a protein called RING finger protein 113A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	M	36	Total 267	C 167	N 45	O 52	S 3	0	0

- Molecule 35 is a protein called Protein BUD31 homolog.

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

- Molecule 36 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	O	285	Total 2273	C 1428	N 401	O 424	S 20	0	0

- Molecule 37 is a protein called Spliceosome-associated protein CWC15 homolog.

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

- Molecule 38 is a protein called Skip.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	R	309	Total 2316	C 1456	N 413	O 435	S 12	0	0

- Molecule 39 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

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

- Molecule 40 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	T	313	Total	C	N	O	S	0	0
			2457	1552	447	450	8		

- Molecule 41 is a protein called Serine/arginine repetitive matrix protein 2.

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

- Molecule 42 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	V	452	Total	C	N	O	0	0
			2243	1339	452	452		

- Molecule 43 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	W	481	Total	C	N	O	0	0
			2374	1412	481	481		

- Molecule 44 is a protein called Smad nuclear-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	X	159	Total	C	N	O	S	0	0
			1021	649	173	198	1		

- Molecule 45 is a protein called RNA-binding motif protein, X-linked 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Y	105	Total	C	N	O	S	0	0
			743	470	127	144	2		

- Molecule 46 is a protein called BUD13 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	Z	113	Total	C	N	O	0	0
			755	474	147	134		

- Molecule 47 is a protein called Peptidyl-prolyl cis-trans isomerase CWC27 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	z	177	Total	C	N	O	S	1	0
			1381	869	241	266	5		

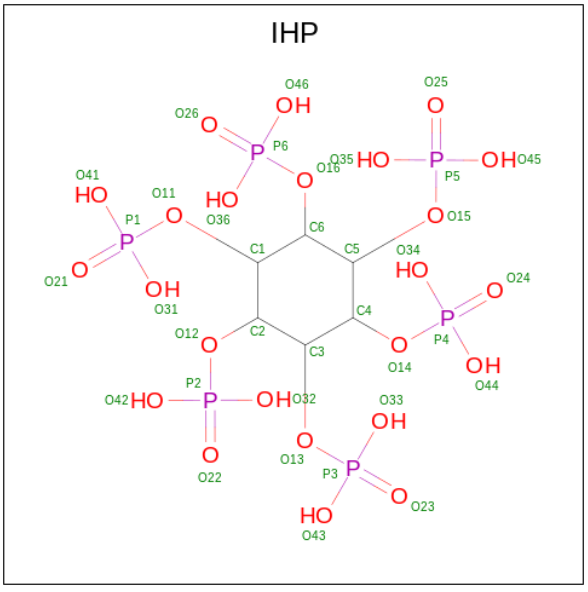
- Molecule 48 is a protein called Putative pre-mRNA-splicing factor ATP-dependent RNA helicase DHX16.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	x	584	Total	C	N	O	0	0
			2887	1718	584	585		

- Molecule 49 is a protein called Peptidyl-prolyl cis-trans isomerase E.

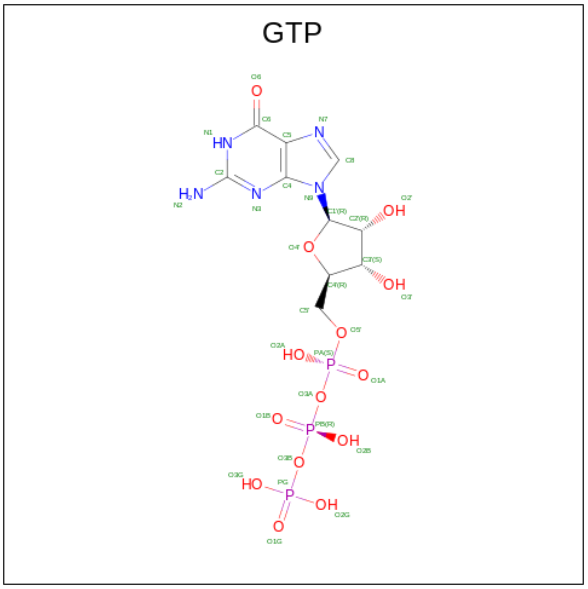
Mol	Chain	Residues	Atoms				AltConf	Trace
49	y	232	Total	C	N	O	0	0
			1133	669	232	232		

- Molecule 50 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- Molecule 51 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
52	C	1	Total	Mg	0
			1	1	
52	F	5	Total	Mg	0
			5	5	

- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
53	v	1	Total	Zn	0
			1	1	
53	6	3	Total	Zn	0
			3	3	
53	M	1	Total	Zn	0
			1	1	
53	N	3	Total	Zn	0
			3	3	
53	O	3	Total	Zn	0
			3	3	

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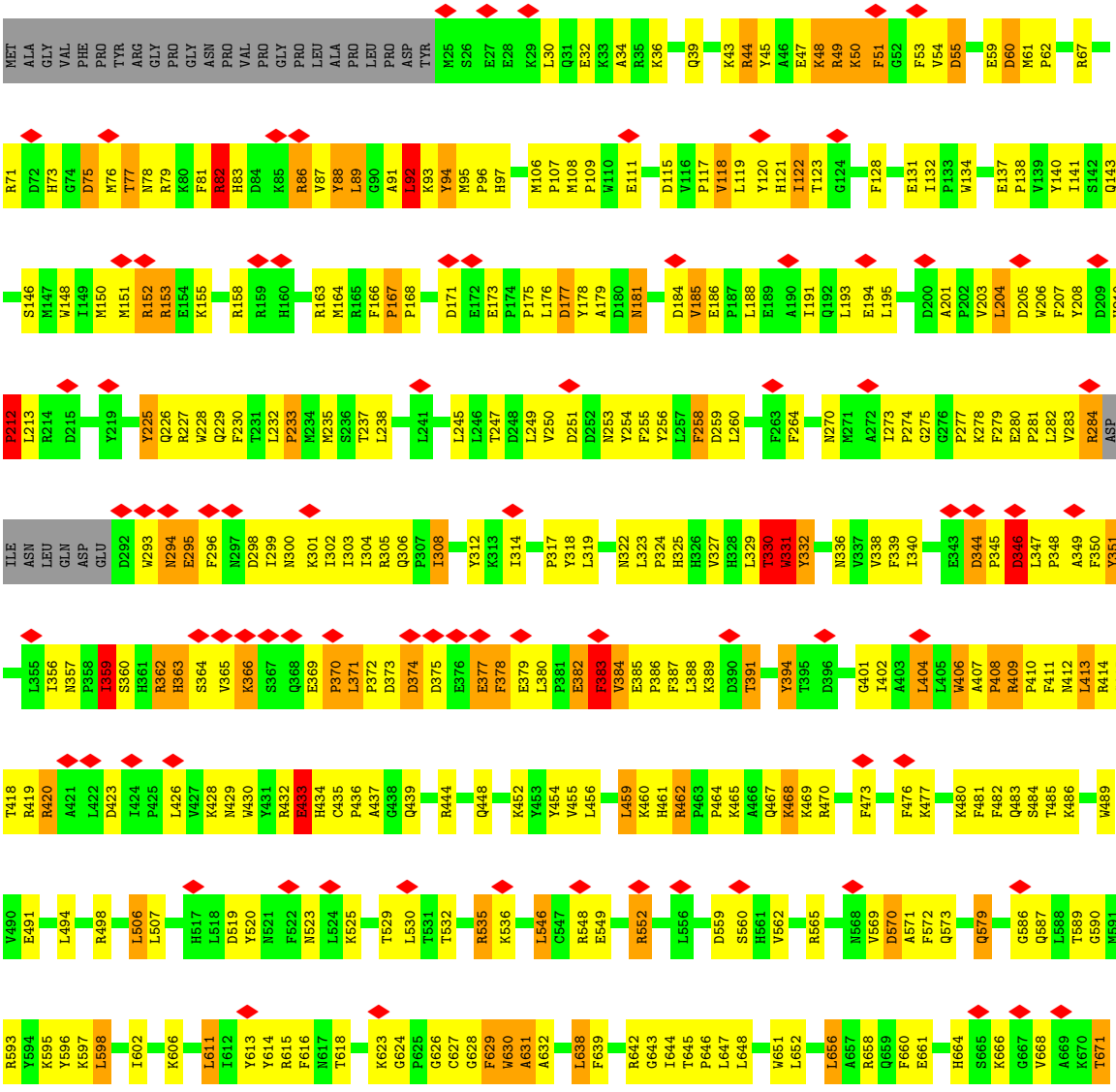
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
53	W	2	2	2	0

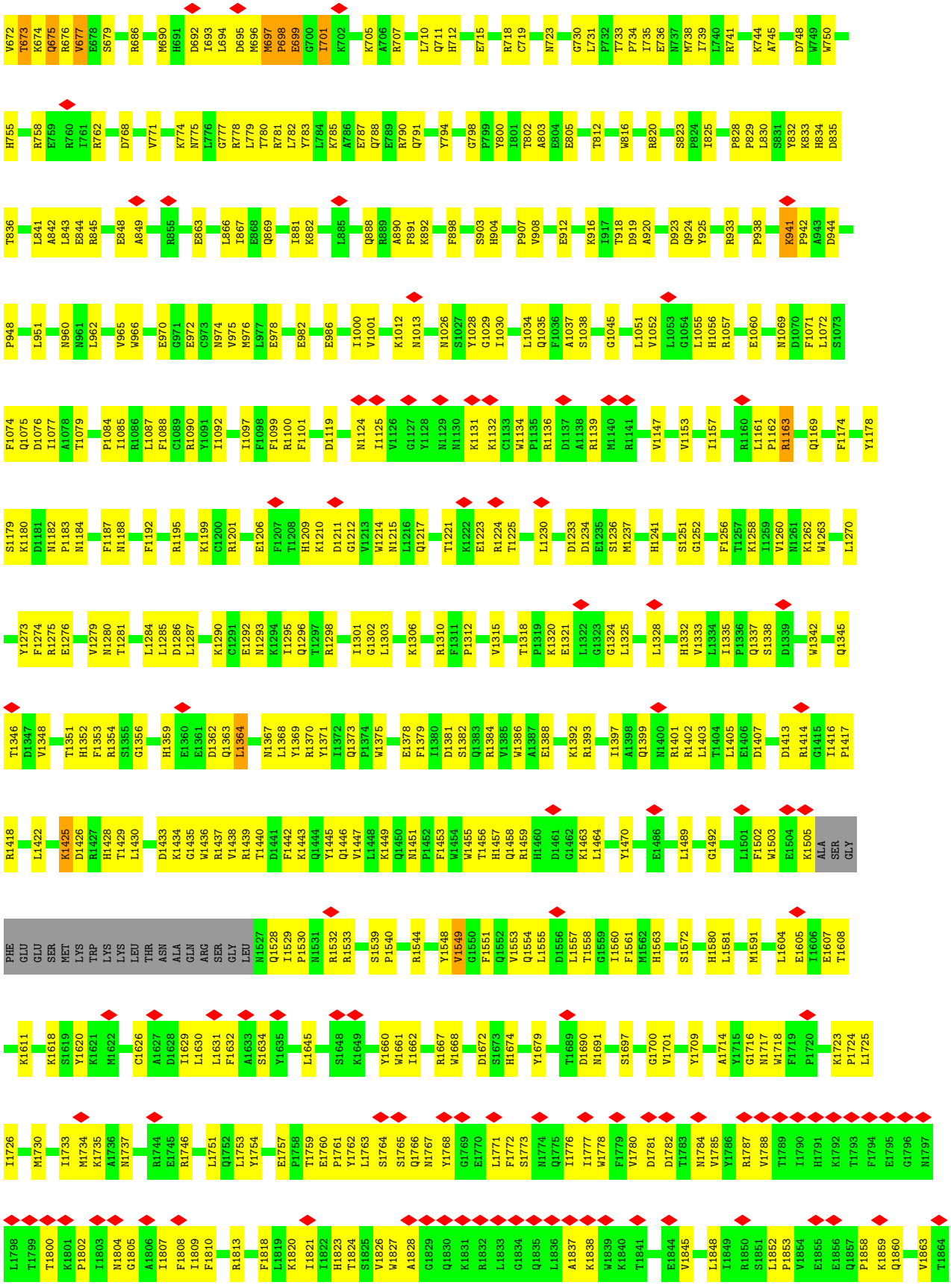
3 Residue-property plots (i)

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

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

Chain A:

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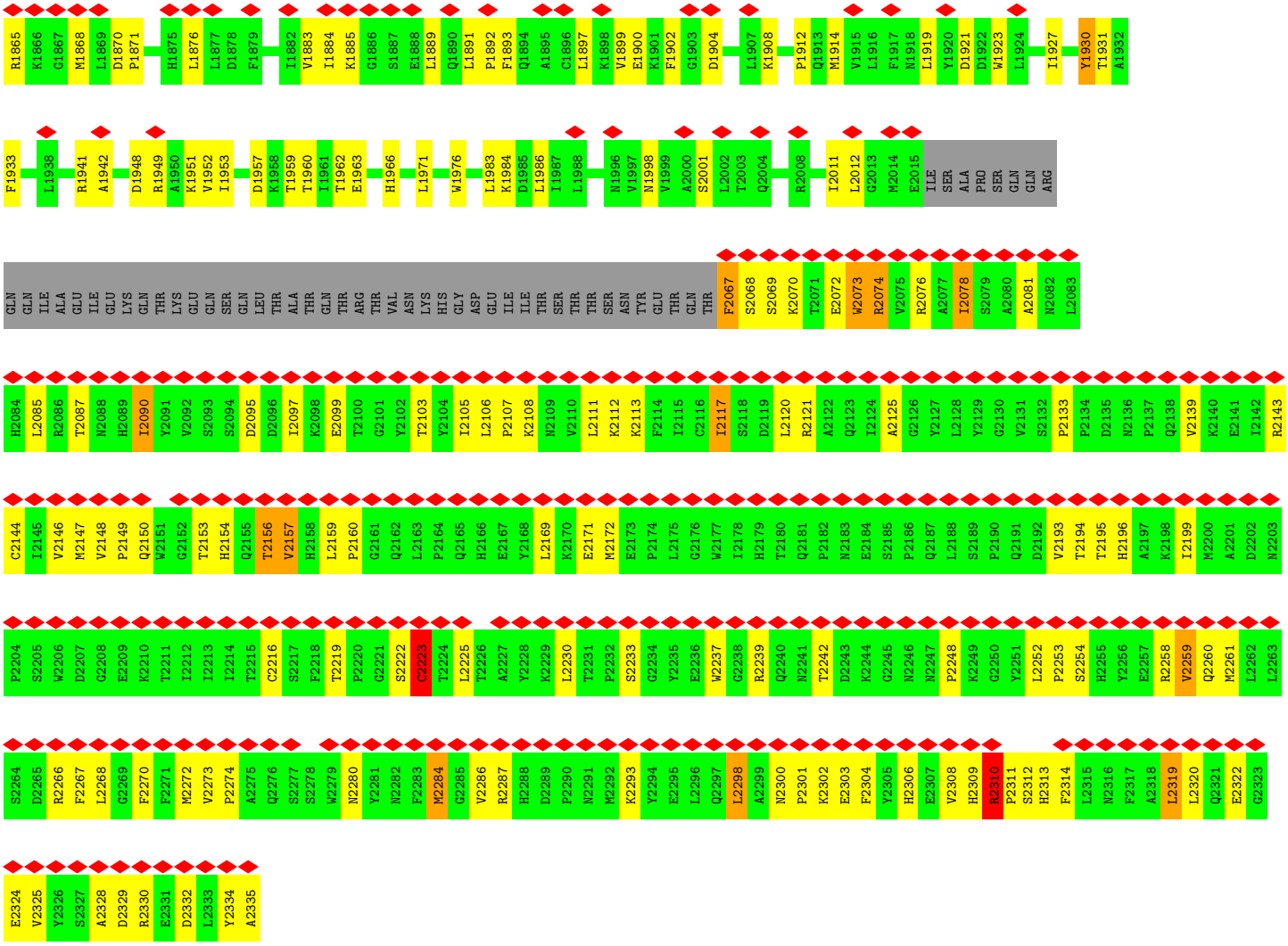
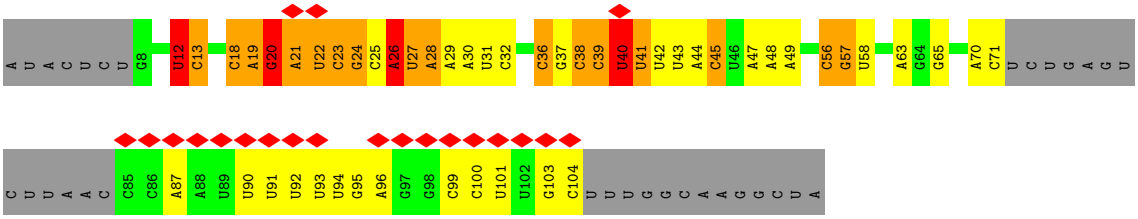
H755 R758 E759 R760 I761 R762 D768 V771 K774 W775 L776 G777 R778 L779 T780 R781 L782 Y783 L784 K785 A786 E787 Q788 E789 R790 Q791 Y794 G798 P799 Y800 I801 T802 A803 E804 E805 T812 W816 R820 S823 P824 I825 P828 P829 L830 S831 Y832 K833 H834 D835
T836 L841 A842 L843 E844 R845 E848 A849 R855 E863 L866 I867 E868 Q869 I881 K882 L885 Q888 R889 A890 F891 K892 F898 S903 H904 P907 V908 E912 K916 I917 T918 D919 A920 D923 Q924 Y925 R933 P938 K941 P942 A943 D944
P948 L951 N960 N961 L962 V965 W966 E970 G971 E972 C973 N974 V975 M976 L977 E978 E982 E986 I1000 V1001 K1012 N1013 N1026 S1027 Y1028 G1029 I1030 L1034 Q1035 F1036 A1037 S1038 G1045 L1051 V1052 L1053 G1054 L1055 H1056 R1057 E1060 N1069 D1070 F1071 L1072 S1073
F1074 Q1075 D1076 I1077 A1078 T1079 P1084 I1085 R1086 L1087 F1088 C1089 R1090 Y1091 I1092 I1097 F1098 F1099 R1100 F1101 D1119 N1124 I1125 V1126 G1127 Y1128 N1129 N1130 K1131 K1132 C1133 W1134 P1135 R1136 D1137 A1138 R1139 M1140 R1141 V1147 V1153 I1157 R1160 L1161 P1162 R1163 Q1169 F1174 Y1178
S1179 K1180 D1181 N1182 P1183 N1184 F1187 N1188 F1192 R1195 K1199 C1200 R1201 E1206 F1207 T1208 H1209 K1210 D1211 G1212 V1213 W1214 N1215 L1216 Q1217 T1221 K1222 E1223 R1224 T1225 L1230 D1233 D1234 E1235 S1236 M1237 H1241 S1251 G1252 F1256 T1257 K1258 I1259 V1260 N1261 K1262 W1263 L1270
Y1273 F1274 R1275 E1276 V1279 N1280 T1281 L1284 L1285 D1286 L1287 K1290 C1291 E1292 N1293 K1294 I1295 Q1296 T1297 R1298 I1301 G1302 L1303 K1306 R1310 F1311 P1312 V1315 T1318 P1319 K1320 E1321 L1322 G1323 G1324 L1325 L1328 H1332 V1333 L1334 I1335 P1336 Q1337 S1338 D1339 W1342 Q1345
T1346 D1347 V1348 T1351 H1352 F1353 R1354 S1355 G1356 H1359 E1360 E1361 D1362 Q1363 L1364 N1367 L1368 Y1369 R1370 Y1371 I1372 Q1373 P1374 W1375 E1378 F1379 I1380 D1381 S1382 Q1383 R1384 V1385 W1386 A1387 E1388 K1392 R1393 I1397 A1398 Q1399 N1400 R1401 R1402 L1403 T1404 L1405 E1406 D1407 D1413 R1414 G1415 I1416 P1417
R1418 L1422 K1425 D1426 R1427 H1428 T1429 L1430 D1433 K1434 G1435 W1436 R1437 V1438 R1439 T1440 D1441 F1442 K1443 Q1444 Y1445 Q1446 V1447 L1448 K1449 Q1450 N1451 P1452 F1453 W1454 W1455 T1456 H1457 Q1458 R1459 H1460 D1461 G1462 K1463 L1464 Y1470 E1486 L1489 G1492 L1501 F1502 W1503 E1504 K1505 ALA SER GLY
PHE GLU GLU SER MET LYS TRP LYS LYS LEU THR ASN ALA GLN ARG SER GLY LEU N1527 Q1528 I1529 P1530 N1531 R1532 R1533 S1539 P1540 R1544 Y1548 V1549 G1550 F1551 Q1552 V1553 Q1554 L1555 D1556 L1557 T1558 G1559 I1560 F1561 M1562 H1563 S1572 H1580 L1581 M1591 L1604 E1605 I1606 E1607 T1608
K1611 K1618 S1619 Y1620 K1621 M1622 C1626 A1627 D1628 I1629 L1630 L1631 F1632 A1633 S1634 Y1635 L1645 S1648 K1649 Y1660 W1661 I1662 R1667 W1668 D1672 S1673 H1674 Y1679 T1689 D1690 N1691 S1697 G1700 V1701 Y1709 A1714 Y1715 G1716 N1717 W1718 F1719 P1720 K1723 P1724 L1725
I1726 M1730 I1733 M1734 K1735 A1736 N1737 R1744 E1745 R1746 L1751 Q1752 L1753 Y1754 E1757 P1758 T1759 E1760 P1761 Y1762 L1763 S1764 S1765 Q1766 N1767 Y1768 G1769 E1770 L1771 F1772 S1773 N1774 Q1775 I1776 I1777 W1778 F1779 V1780 D1781 D1782 T1783 N1784 V1785 Y1786 R1787 V1788 T1789 I1790 H1791 K1792 T1793 F1794 E1795 G1796 N1797
L1798 T1799 T1800 K1801 P1802 I1803 N1804 G1805 A1806 I1807 F1808 I1809 F1810 R1813 F1818 L1819 K1820 I1821 I1822 H1823 T1824 S1825 V1826 W1827 A1828 G1829 Q1830 K1831 R1832 L1833 G1834 Q1835 L1836 A1837 K1838 W1839 K1840 T1841 E1844 V1845 L1848 I1849 R1850 S1851 L1852 P1853 V1854 E1855 E1856 Q1857 P1858 K1859 Q1860 V1863 T1864



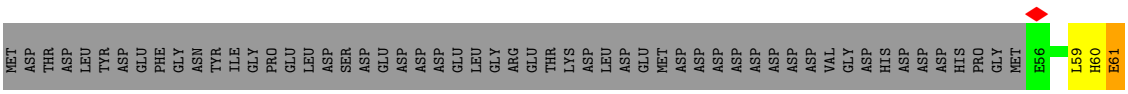
• Molecule 2: U5 snRNA

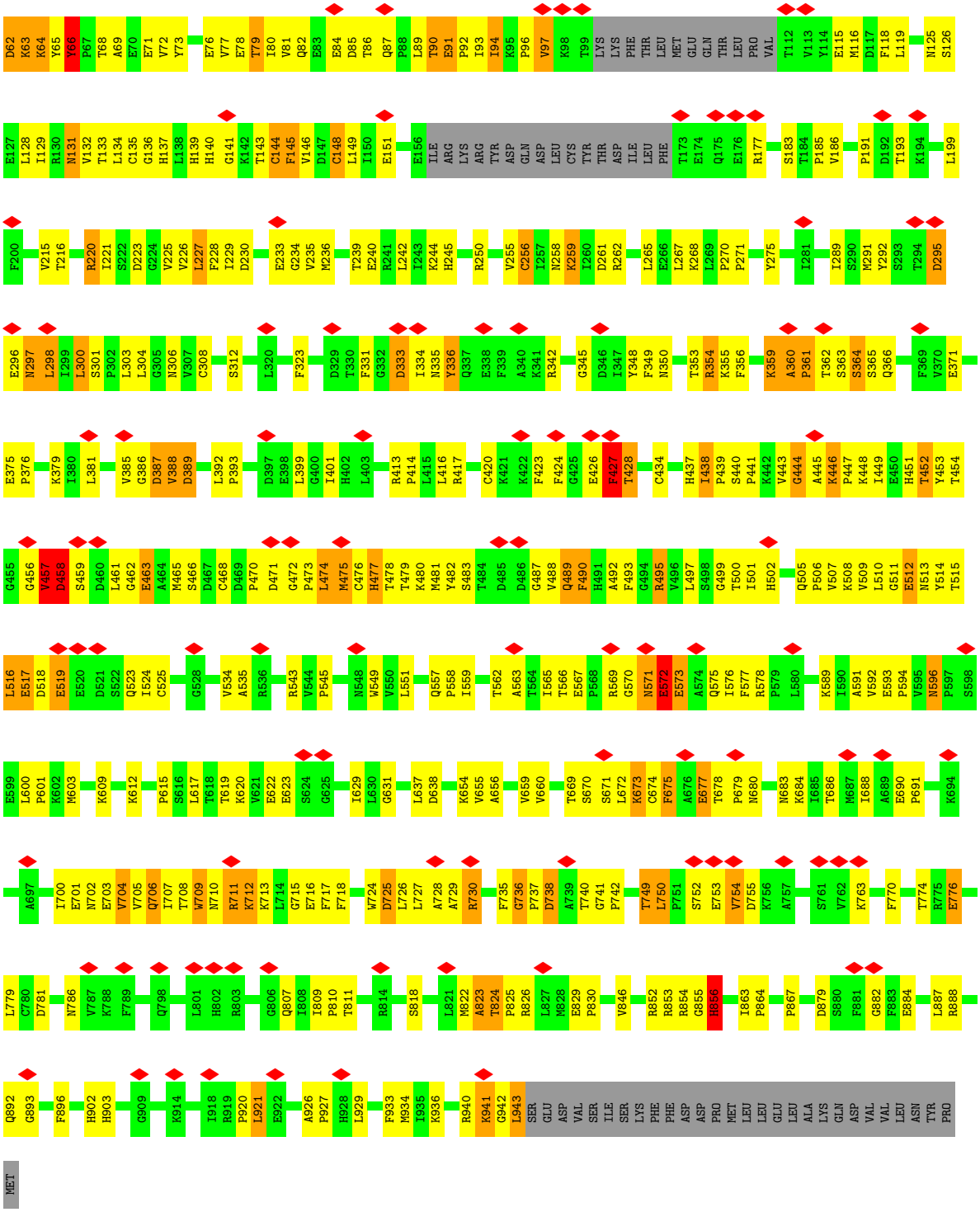
Chain B:



• Molecule 3: 116 kDa U5 small nuclear ribonucleoprotein component

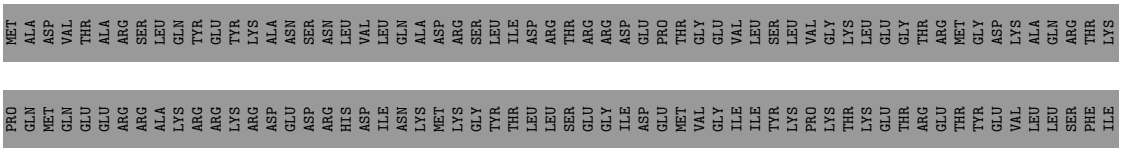
Chain C:

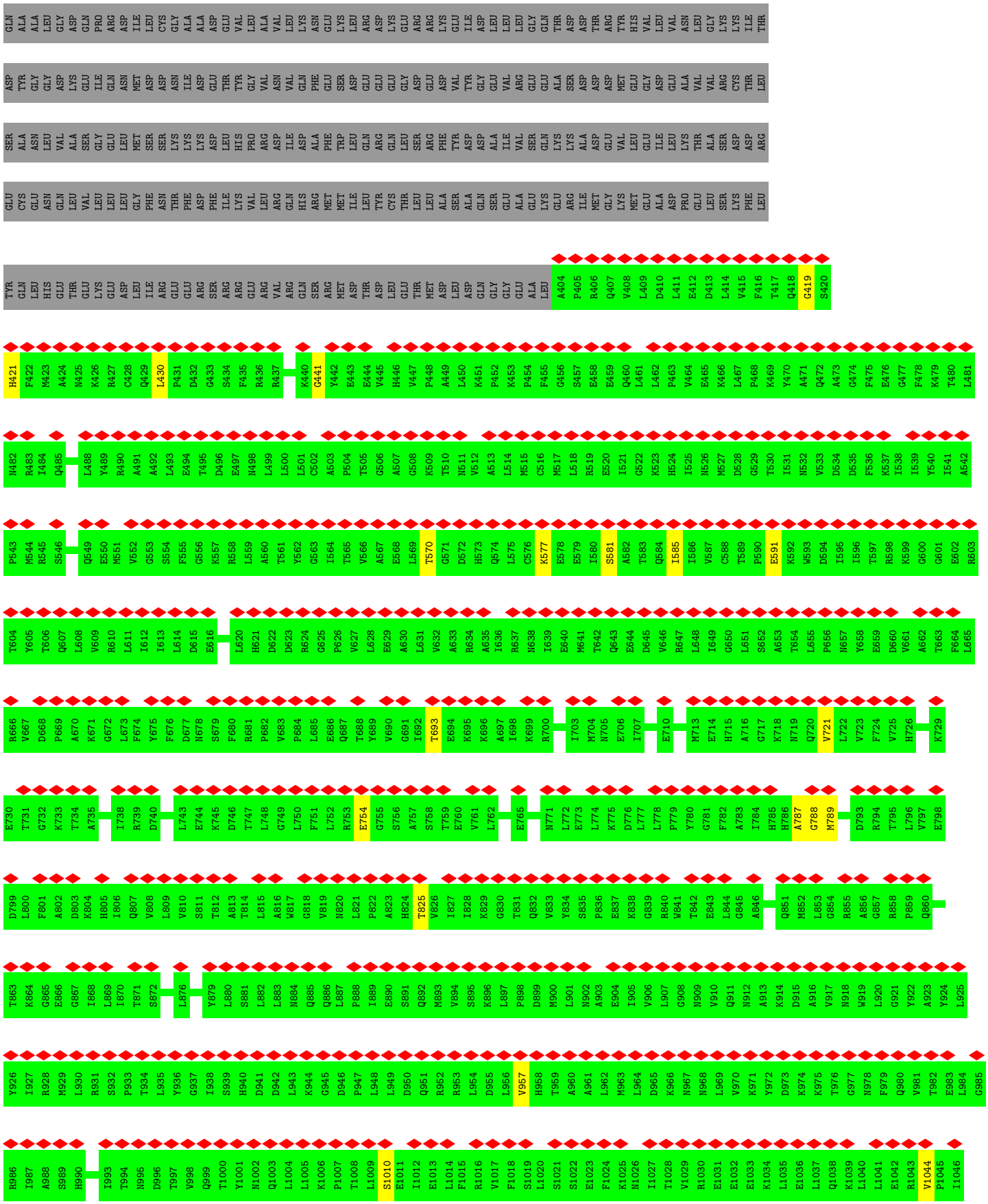




• Molecule 4: U5 small nuclear ribonucleoprotein 200 kDa helicase

Chain D:

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ASP TYR GLY GLY ASP LYS GLU ILE GLN ASN MET ASP ASP ASN ILE ASP GLU GLU THR TYR GLY VAL ASN VAL GLN PHE GLU GLU GLU GLY ASP GLU ASP VAL TYR GLY GLU VAL ALA ASP ASP ASP MET GLU GLY ASP GLU ALA VAL LEU LYS THR ALA SER ASP ASP LEU
SER ALA ASN LEU VAL ALA SER GLY GLU LEU MET SER SER LYS LYS LYS ASP LEU HIS PRO ARG ASP ILE ASP ALA ILE ALA PHE TRP LEU GLN ARG GLN LEU SER ARG PHE TYR ASP LEU ASP ALA GLN SER GLU ALA VAL SER GLN LYS LYS ALA ASP PRO GLU LEU SER LYS PHE LEU
GLU CYS GLU ASN GLN LEU VAL LEU LEU LEU GLY PHE ASN THR PHE ASP PHE ILE LYS VAL LEU ARG GLN HIS ARG MET MET ILE LEU TYR CYS THR LEU LEU ALA SER ALA GLN SER GLU ALA GLU LYS GLU ARG ILE MET GLY LYS MET GLU ALA ASP PRO GLU LEU SER LYS PHE LEU
TYR GLN LEU HIS GLU THR GLU LYS GLU ASP LEU ILE ARG GLU GLU ARG SER ARG ARG GLU ARG VAL ARG GLN SER ARG MET ASP THR ASP LEU GLU THR MET ASP LEU ASP GLN GLY GLY GLU ALA LEU A404 P405 R406 Q407 V408 L409 D410 L411 E412 D413 L414 V415 F416 T417 Q418 G419 S420
H421 F422 M423 A424 N425 K426 R427 C428 Q429 L430 P431 D432 G433 S434 F435 R436 R437 K440 G441 Y442 E443 E444 V445 H446 V447 P448 A449 L450 K451 P452 K453 P454 F455 G456 S457 E458 E459 Q460 L461 L462 P463 V464 E465 K466 L467 P468 K469 Y470 A471 Q472 A473 G474 F475 E476 G477 F478 K479 T480 L481
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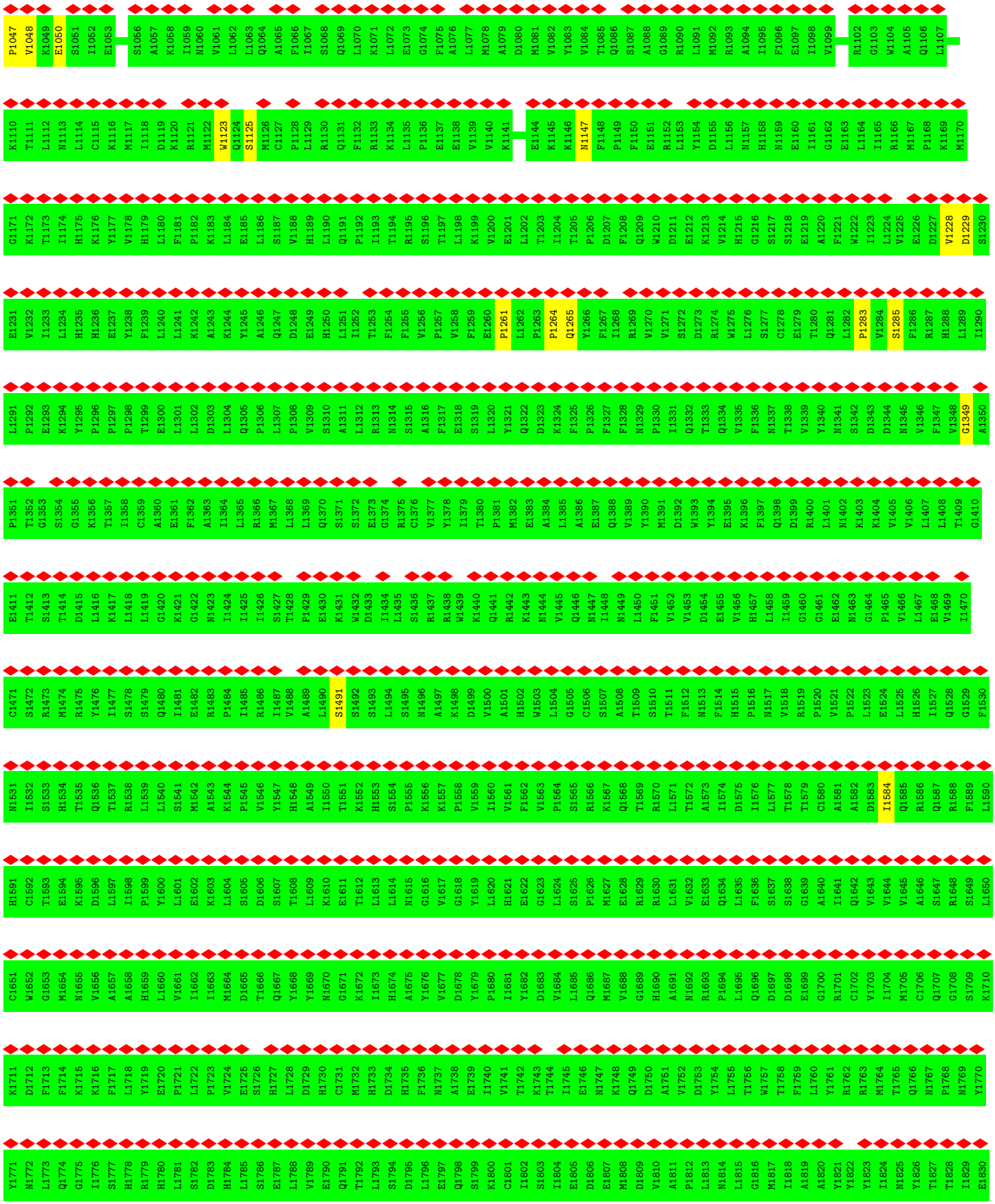
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G1171 K1172 T1173 I1174 H1175 K1176 Y1177 V1178 H1179 L1180 F1181 P1182 K1183 L1184 E1185 L1186 S1187 V1188 H1189 L1190 Q1191 P1192 I1193 T1194 R1195 S1196 T1197 L1198 K1199 V1200 E1201 L1202 T1203 I1204 T1205 P1206 D1207 F1208 Q1209 W1210 D1211 E1212 K1213 V1214 H1215 G1216 S1217 S1218 E1219 A1220 F1221 W1222 I1223 L1224 V1225 E1226 D1227 V1228 D1229 S1230
E1231 V1232 I1233 L1234 H1235 H1236 E1237 Y1238 F1239 L1240 L1241 F1181 P1182 K1242 A1243 K1244 Y1245 A1246 Q1247 D1248 E1249 H1250 L1251 I1252 T1253 F1254 F1255 V1256 P1257 V1258 F1259 E1260 P1261 L1262 P1263 P1264 Q1265 Y1266 F1267 I1268 R1269 V1270 V1271 S1272 D1273 R1274 W1275 L1276 S1277 C1278 E1279 T1280 Q1281 L1282 P1283 V1284 S1285 F1286 R1287 H1288 L1289 I1290
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P1351 T1352 G1353 S1354 G1355 K1356 T1357 I1358 C1359 A1360 E1361 F1362 A1363 I1364 L1365 R1366 M1367 L1368 L1369 Q1370 S1371 S1372 E1373 G1374 R1375 C1376 V1377 Y1378 I1379 T1380 P1381 M1382 E1383 A1384 L1385 A1386 E1387 Q1388 V1389 Y1390 M1391 D1392 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 D1433 I1434 L1435 S1436 R1437 R1438 W1439 K1440 Q1441 R1442 K1443 N1444 V1445 Q1446 N1447 I1448 N1449 L1450 F1451 V1452 V1453 D1454 E1455 V1456 H1457 L1458 I1459 G1460 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 F1530
N1531 I1532 S1533 H1534 T1535 Q1536 T1537 R1538 L1539 L1540 S1541 M1542 A1543 K1544 P1545 V1546 Y1547 H1548 A1549 I1550 T1551 K1552 H1553 S1554 P1555 K1556 K1557 P1558 V1559 I1560 V1561 F1562 V1563 P1564 S1565 R1566 K1567 Q1568 T1569 R1570 L1571 T1572 A1573 I1574 D1575 I1576 L1577 T1578 T1579 C1580 A1581 A1582 D1583 I1584 Q1585 R1586 Q1587 R1588 F1589 L1590
H1591 C1592 T1593 E1594 K1595 D1596 L1597 I1598 P1599 Y1600 L1601 E1602 K1603 L1604 S1605 D1606 S1607 T1608 L1609 K1610 E1611 T1612 L1613 L1614 N1615 G1616 V1617 G1618 Y1619 L1620 H1621 E1622 G1623 L1624 S1625 P1626 M1627 E1628 R1629 R1630 L1631 V1632 E1633 Q1634 L1635 F1636 S1637 S1638 G1639 A1640 I1641 Q1642 V1643 V1644 V1645 A1646 S1647 R1648 S1649 L1650
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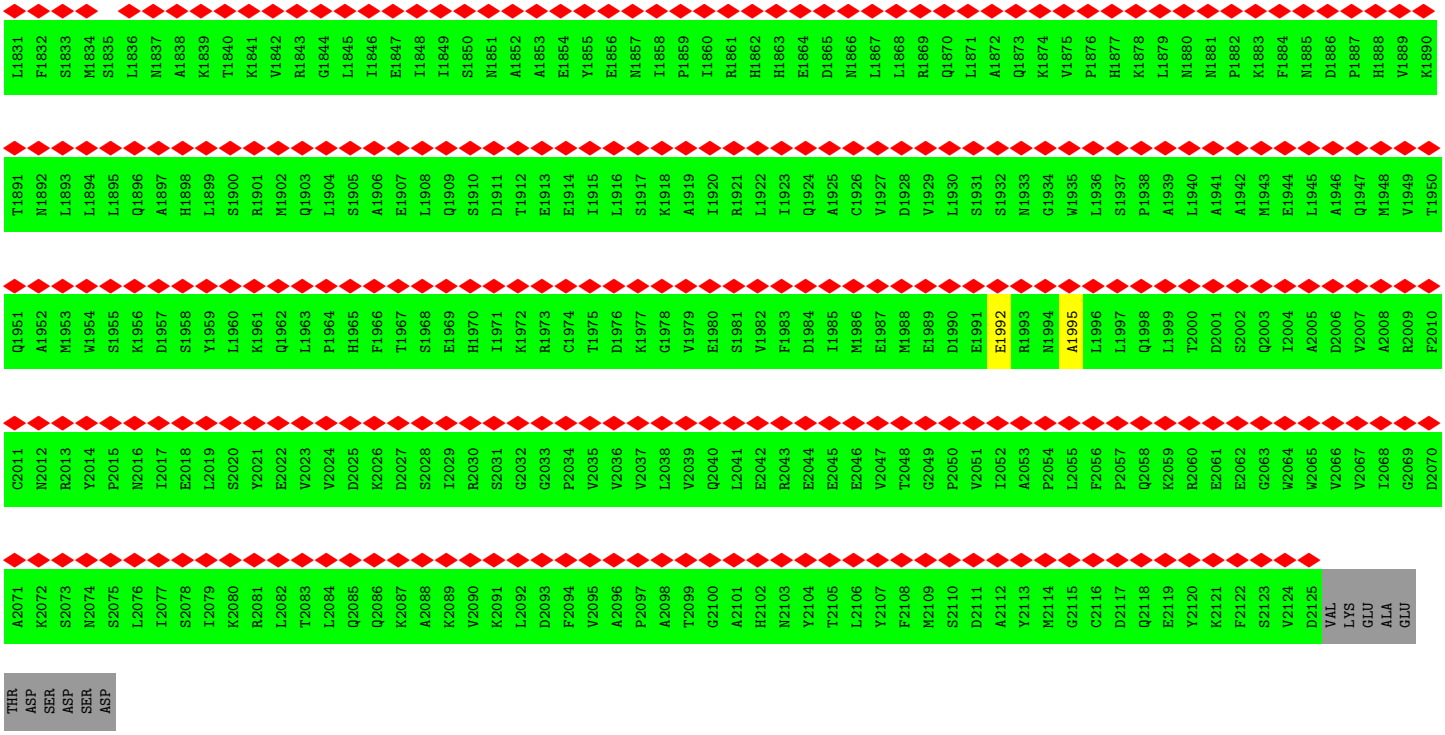
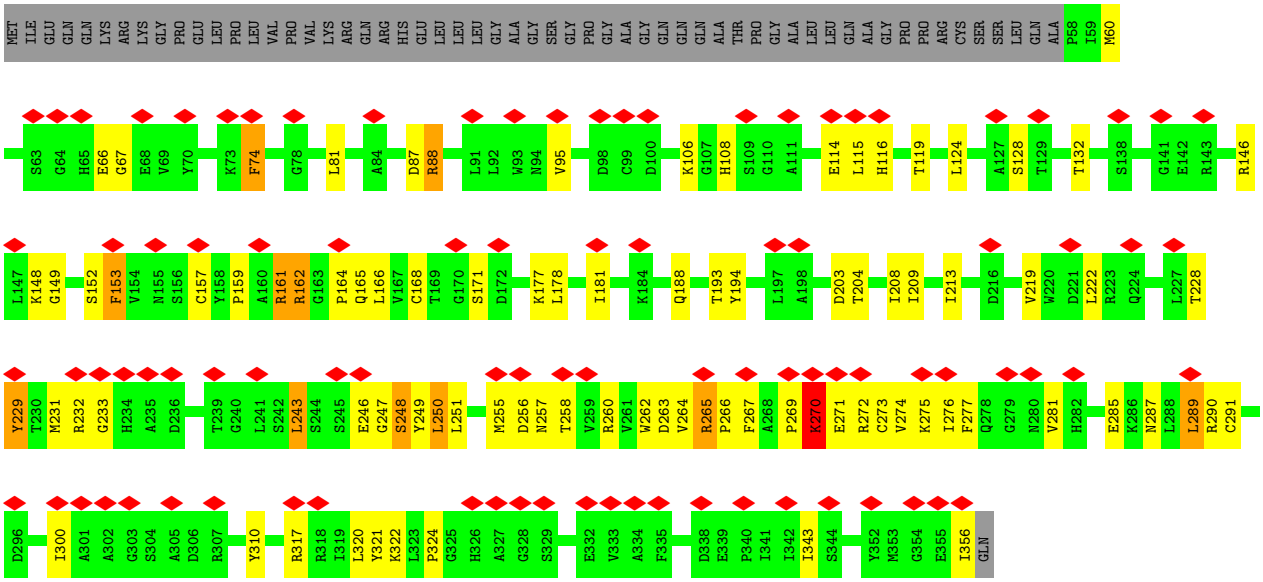
K1711 D1712 F1713 F1714 K1715 K1716 F1717 L1718 Y1719 E1720 P1721 L1722 P1723 V1724 E1725 S1726 H1727 L1728 D1729 H1730 C1731 M1732 H1733 D1734 H1735 F1736 N1737 A1738 E1739 I1740 V1741 T1742 K1743 T1744 I1745 E1746 N1747 K1748 Q1749 D1750 A1751 V1752 D1753 Y1754 L1755 T1756 W1757 T1758 F1759 L1760 Y1761 R1762 R1763 M1764 T1765 Q1766 N1767 P1768 N1769 Y1770
Y1771 N1772 L1773 Q1774 G1775 I1776 S1777 H1778 R1779 H1780 L1781 S1782 D1783 H1784 L1785 S1786 E1787 L1788 V1789 E1790 Q1791 T1792 L1793 S1794 D1795 L1796 E1797 Q1798 S1799 K1800 C1801 I1802 S1803 I1804 E1805 D1806 E1807 M1808 D1809 V1810 A1811 P1812 L1813 N1814 L1815 G1816 M1817 I1818 A1819 A1820 Y1821 Y1822 Y1823 I1824 N1825 Y1826 T1827 T1828 I1829 E1830



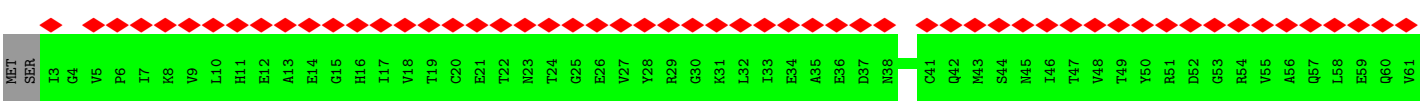
• Molecule 5: U5 small nuclear ribonucleoprotein 40 kDa protein

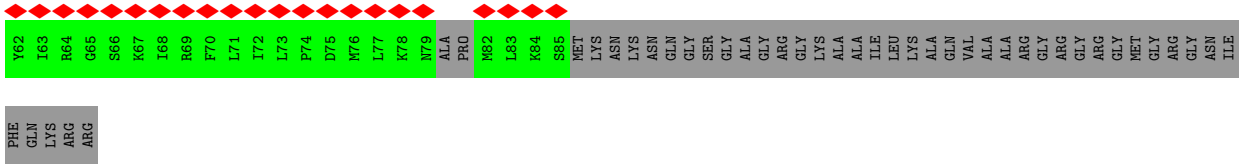
Chain E:



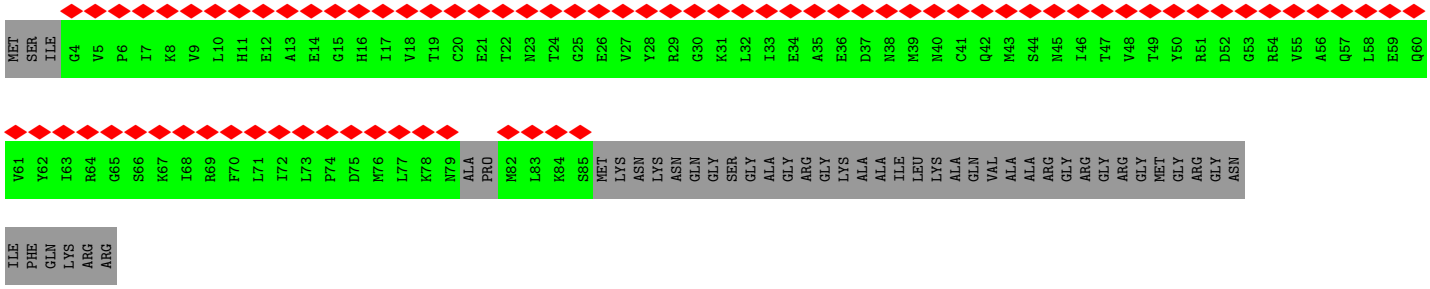
• Molecule 6: Small nuclear ribonucleoprotein Sm D3

Chain a:

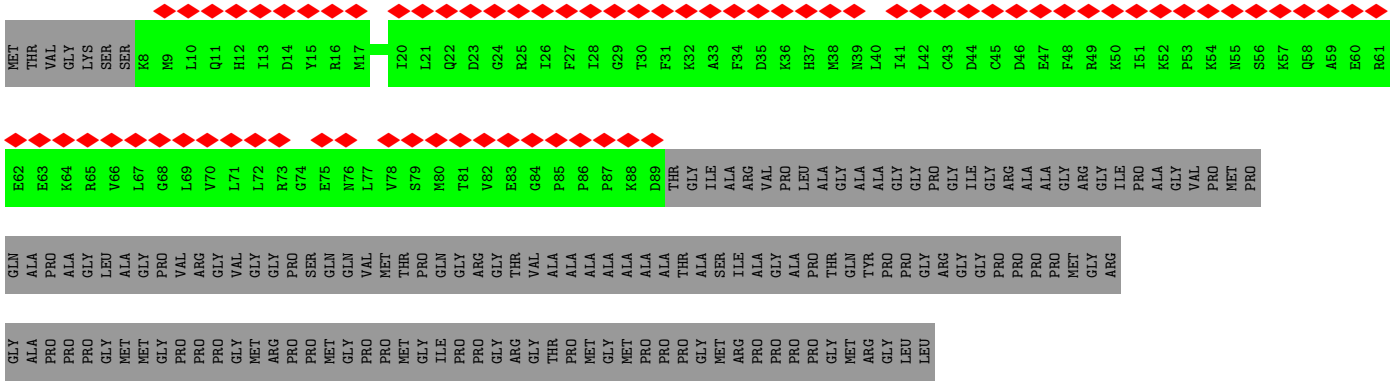




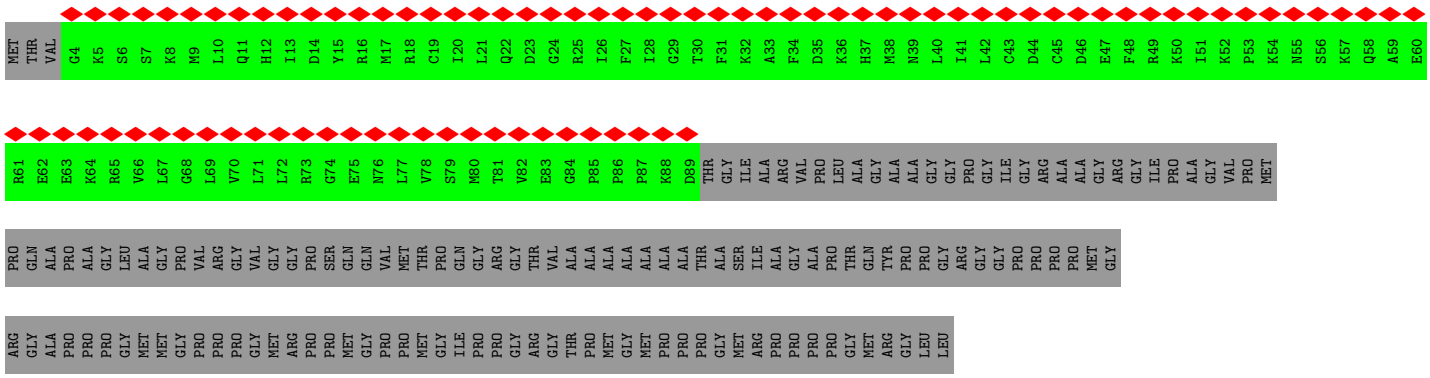
• Molecule 6: Small nuclear ribonucleoprotein Sm D3



• Molecule 7: Small nuclear ribonucleoprotein-associated proteins B and B'

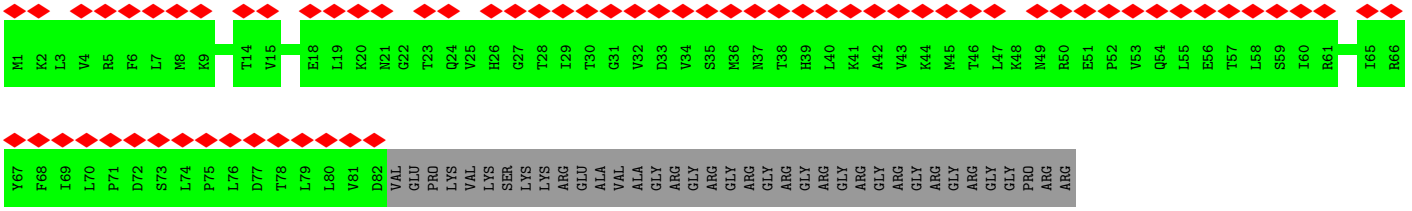


• Molecule 7: Small nuclear ribonucleoprotein-associated proteins B and B'



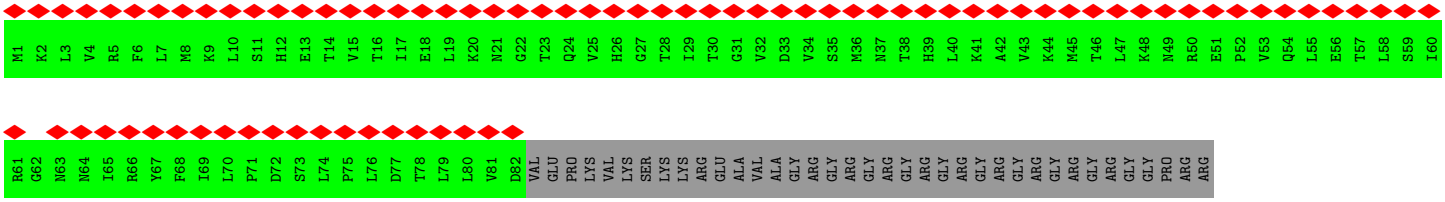
• Molecule 8: Small nuclear ribonucleoprotein Sm D1

Chain c:



• Molecule 8: Small nuclear ribonucleoprotein Sm D1

Chain j:



• Molecule 9: Small nuclear ribonucleoprotein Sm D2

Chain d:

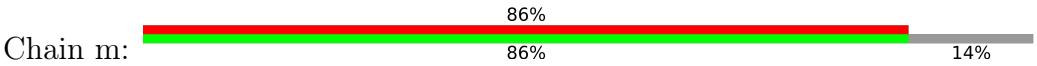
• Molecule 9: Small nuclear ribonucleoprotein Sm D2

Chain k:

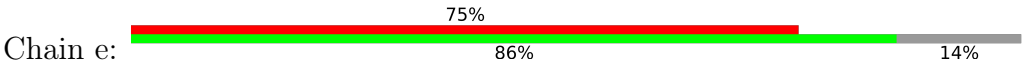
• Molecule 10: Small nuclear ribonucleoprotein F

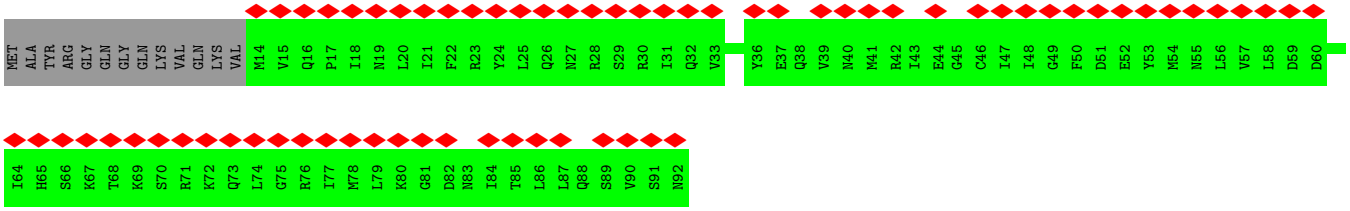
Chain f:

• Molecule 10: Small nuclear ribonucleoprotein F

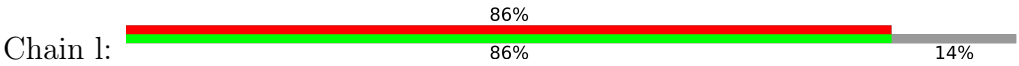


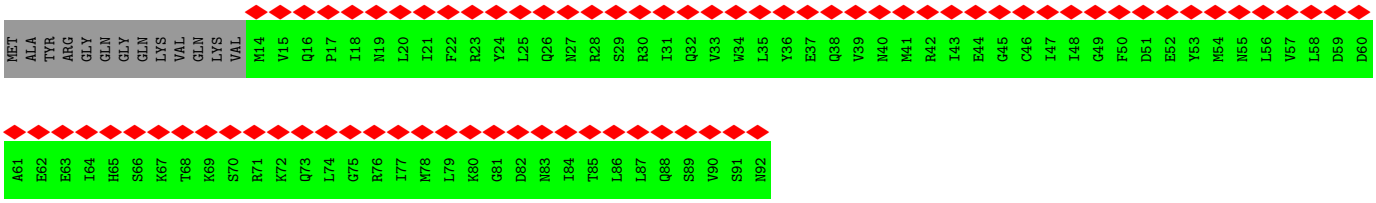
• Molecule 11: Small nuclear ribonucleoprotein E



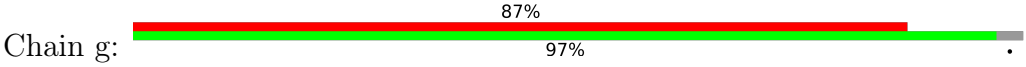


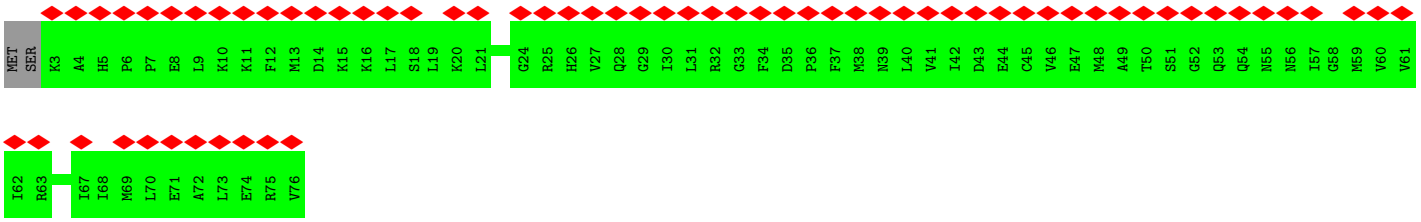
• Molecule 11: Small nuclear ribonucleoprotein E





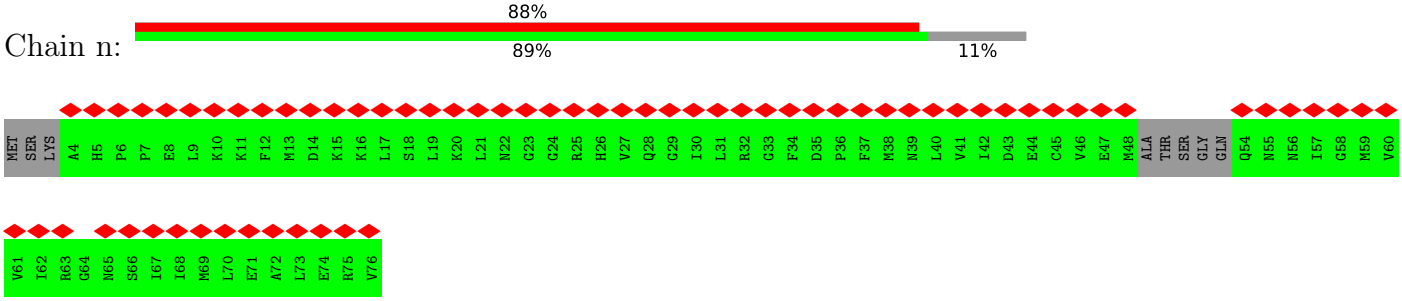
• Molecule 12: Small nuclear ribonucleoprotein G





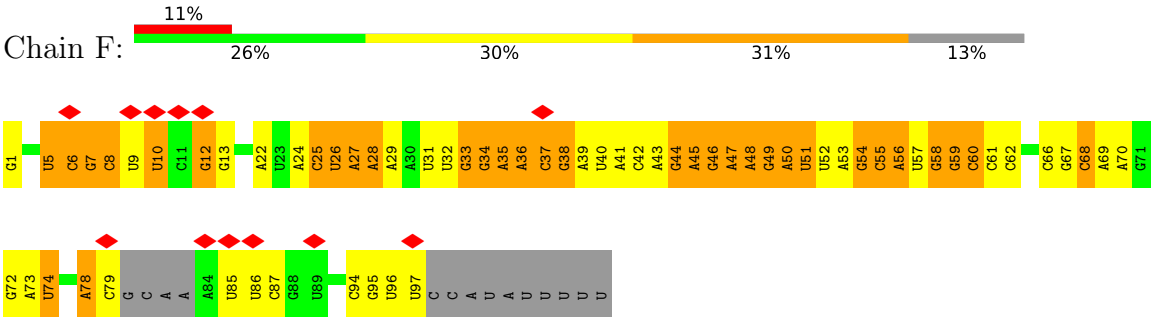
• Molecule 12: Small nuclear ribonucleoprotein G

Chain n:



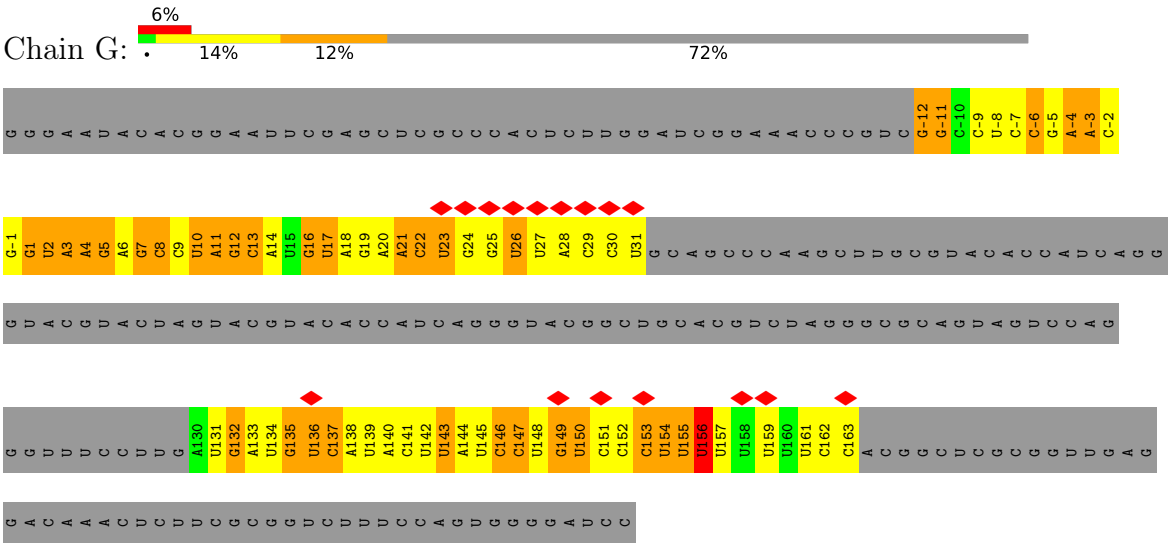
• Molecule 13: U6 snRNA

Chain F:



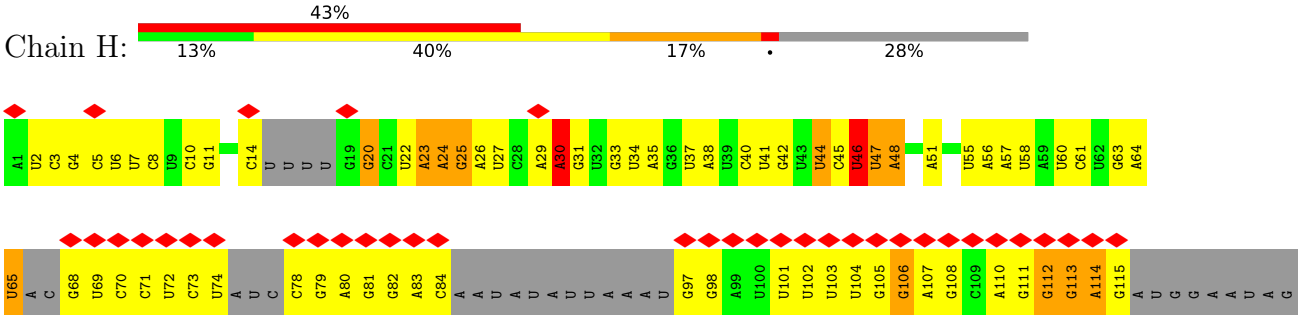
• Molecule 14: pre-mRNA

Chain G:



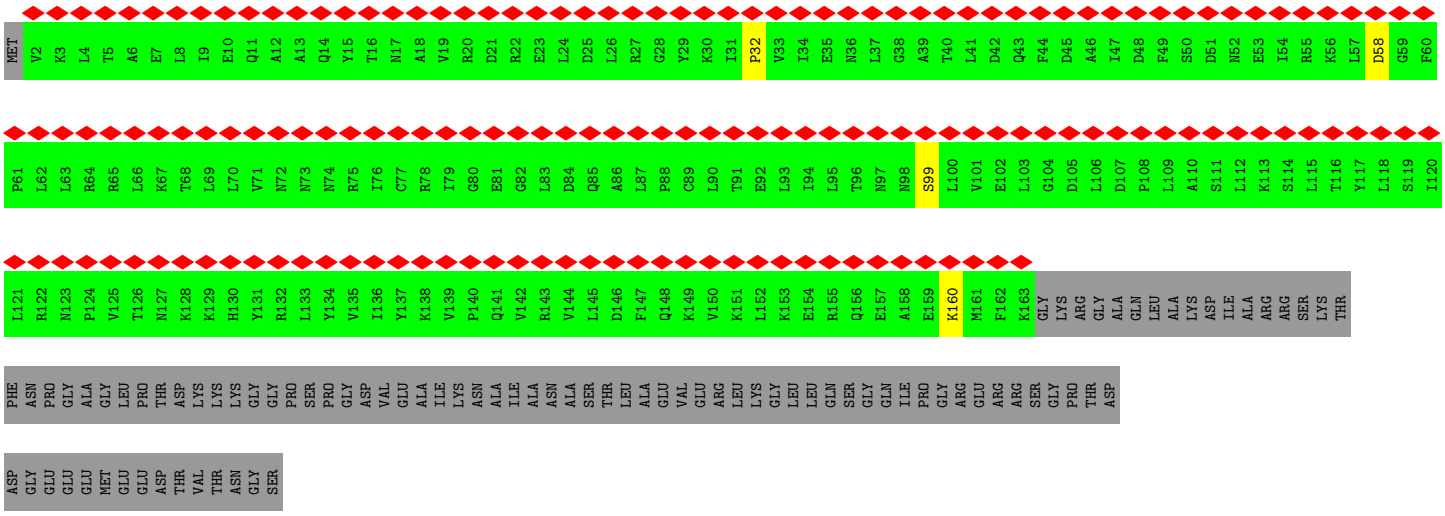
• Molecule 15: U2 snRNA

Chain H:



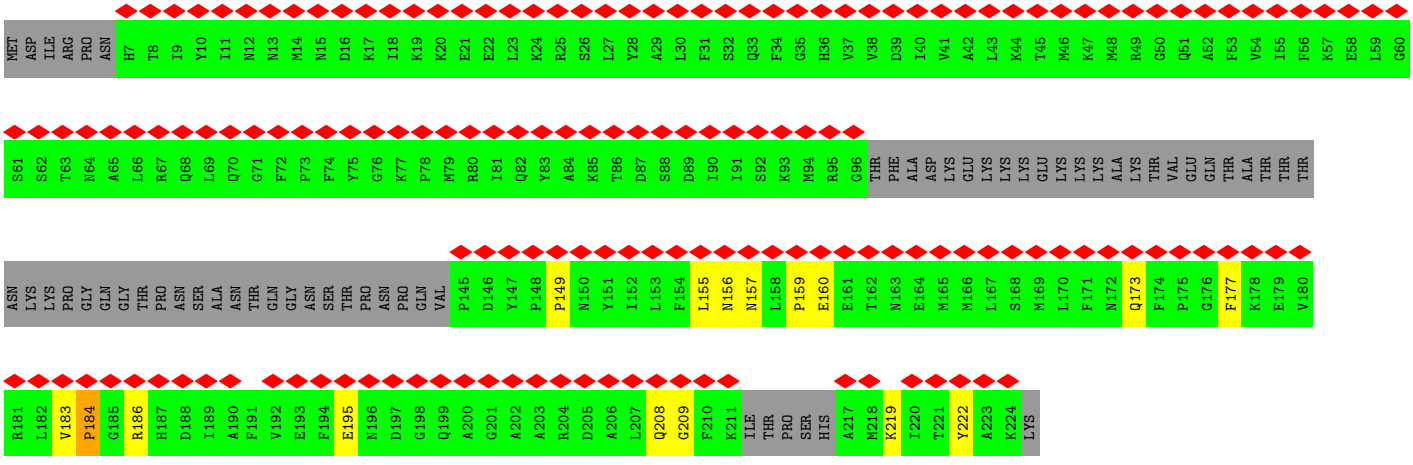
• Molecule 16: U2 small nuclear ribonucleoprotein A'

Chain o:



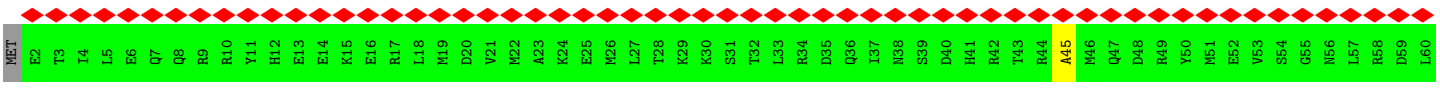
• Molecule 17: U2 small nuclear ribonucleoprotein B"

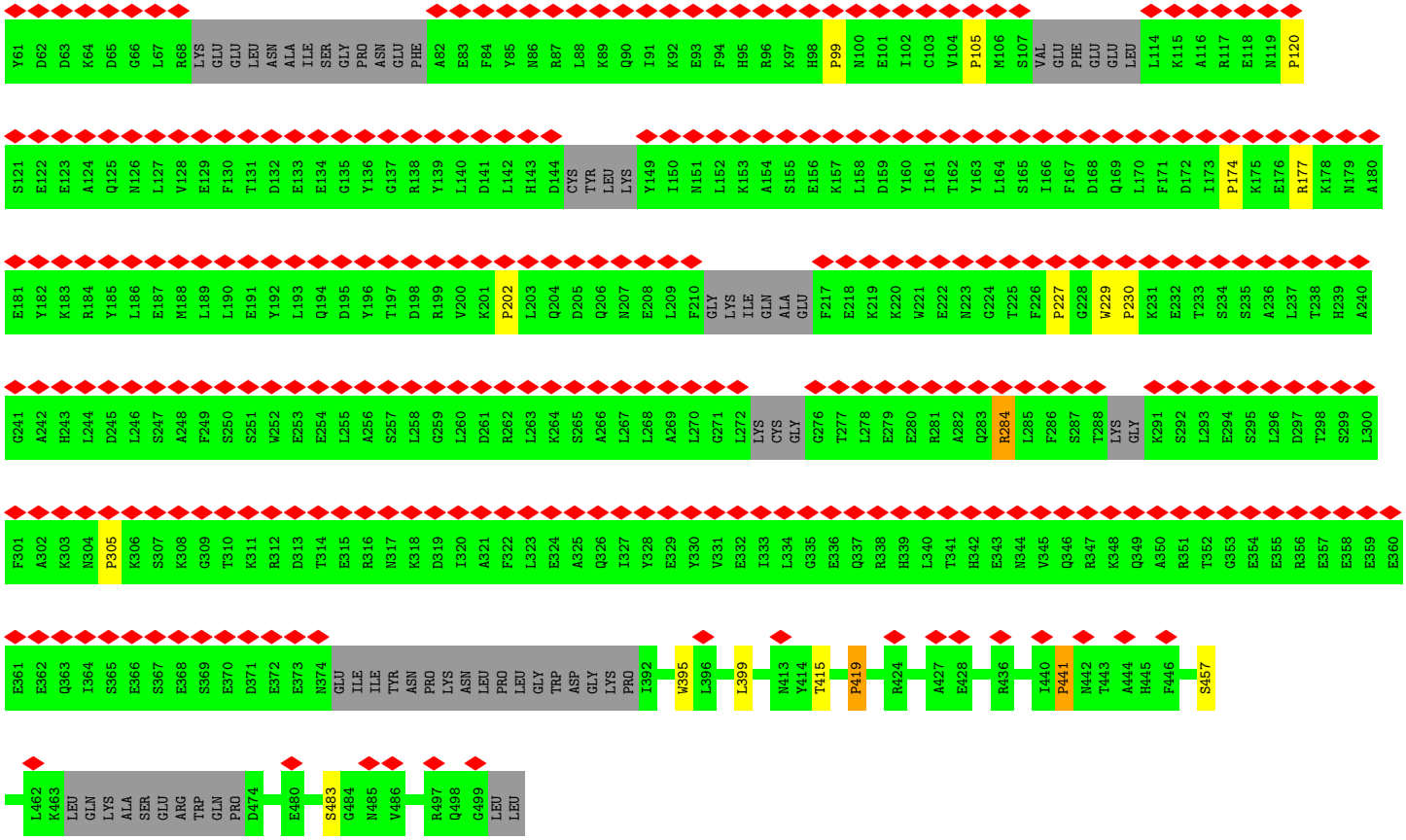
Chain p:



• Molecule 18: Splicing factor 3A subunit 3

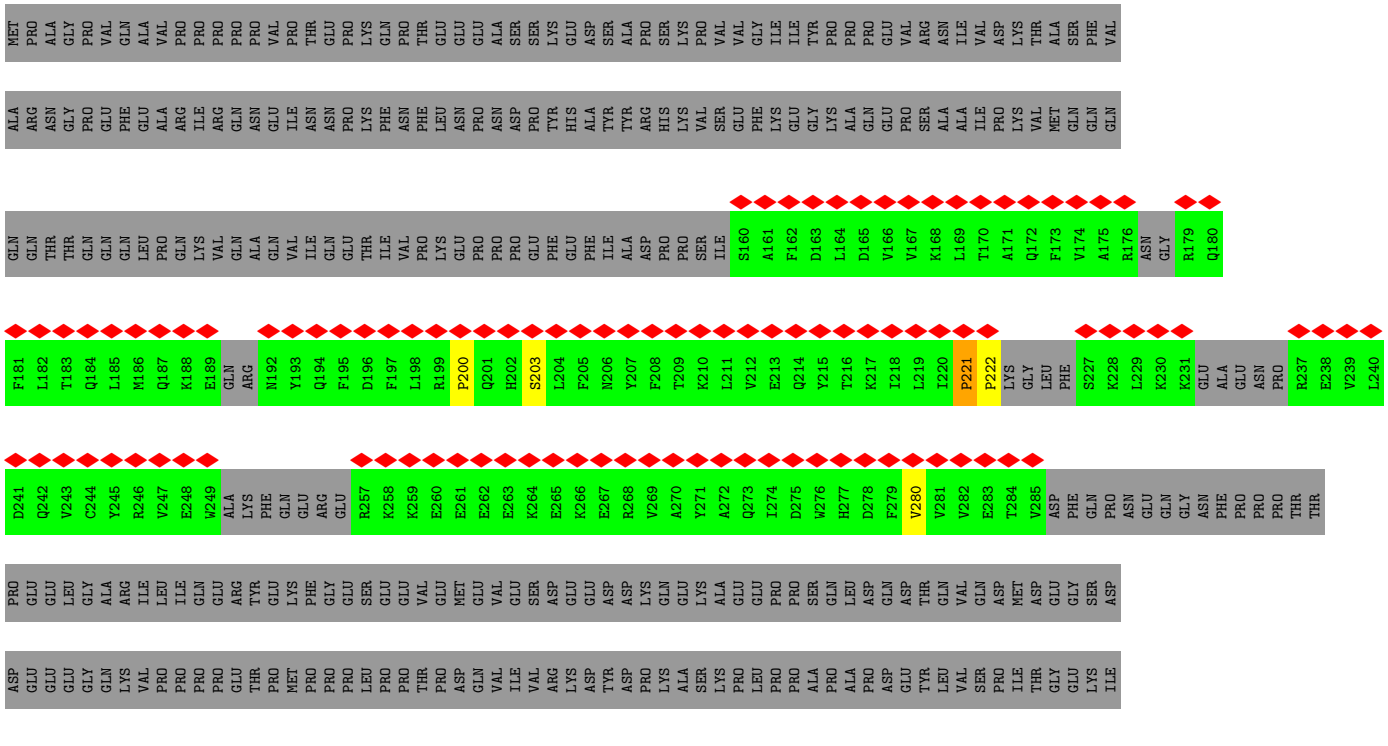
Chain w:





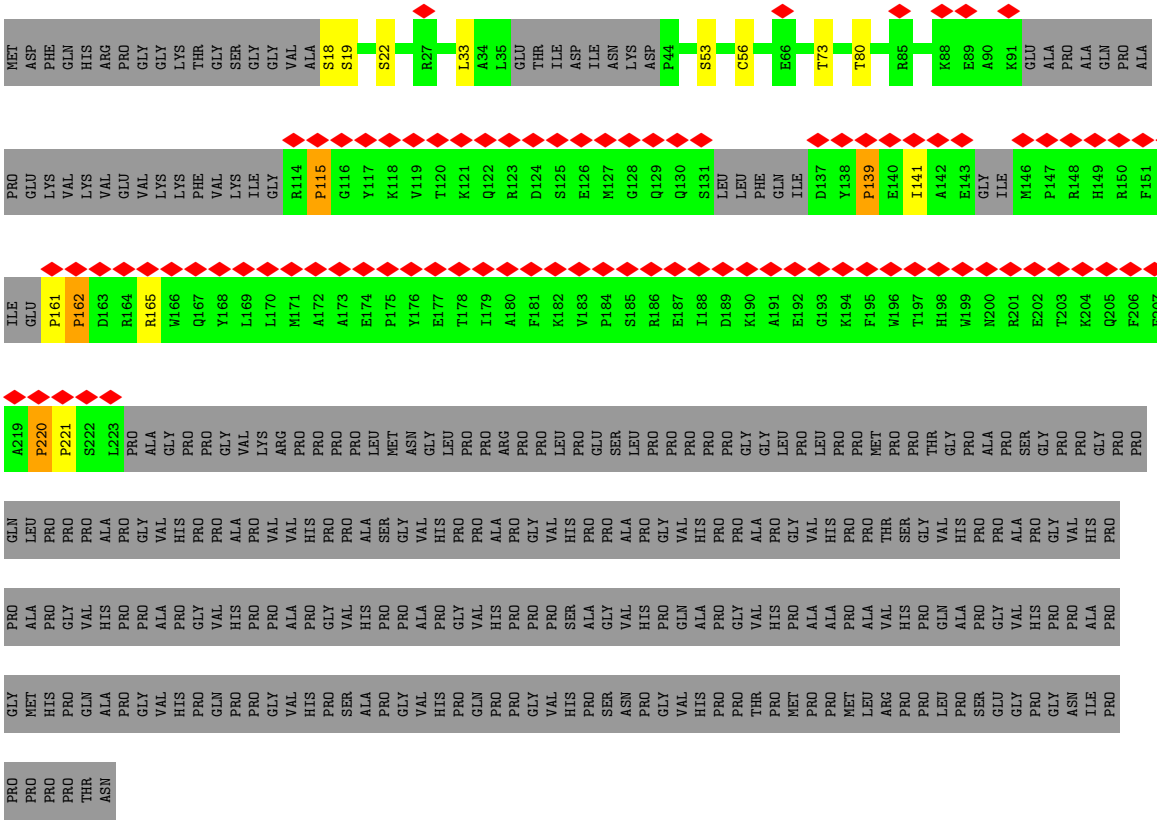
• Molecule 19: Splicing factor 3A subunit 1

Chain u:



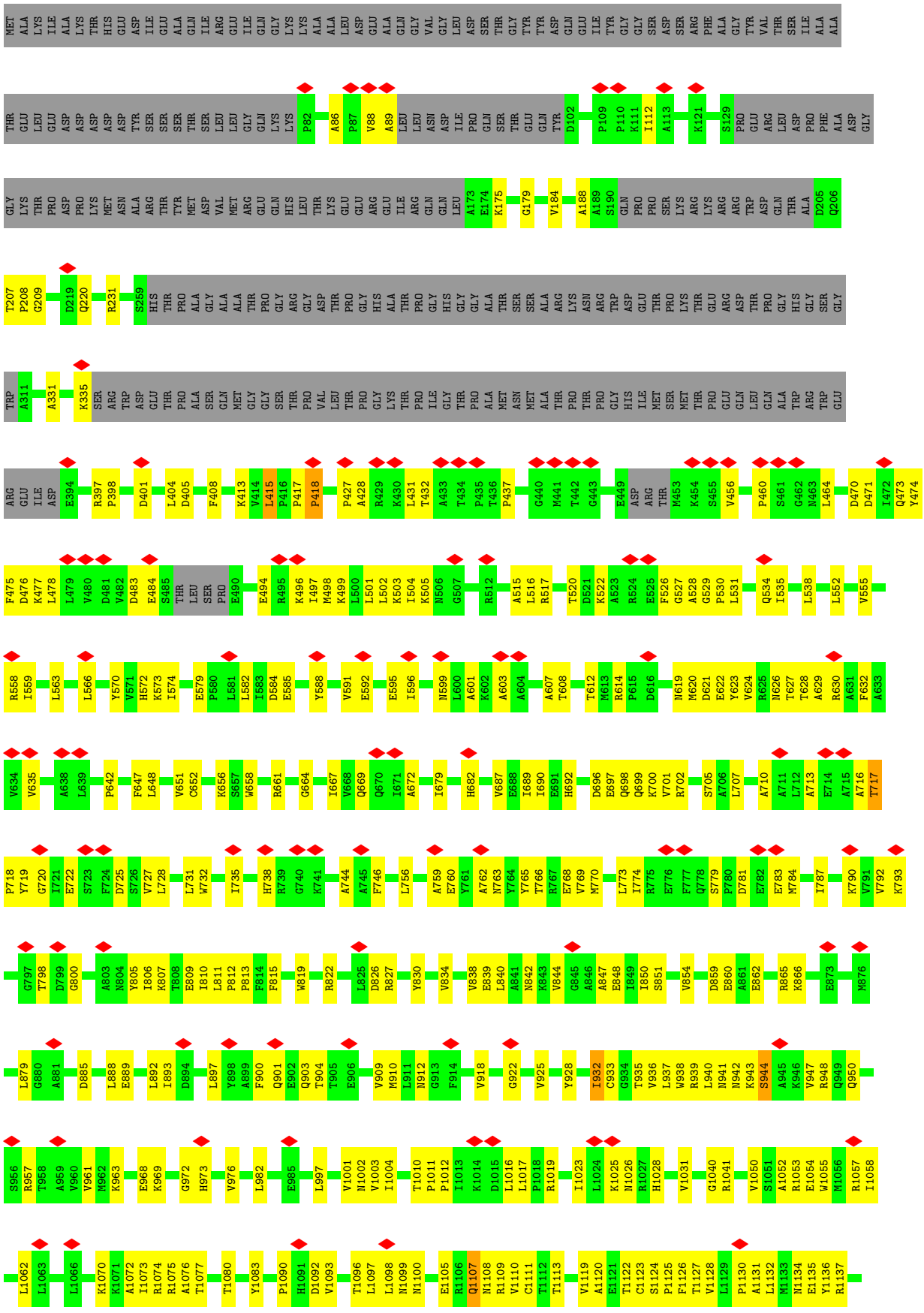
• Molecule 20: Splicing factor 3A subunit 2

Chain v:



• Molecule 21: Splicing factor 3B subunit 1

Chain 1: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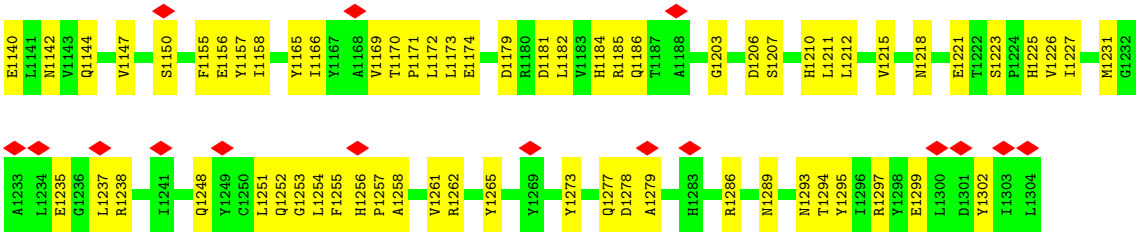
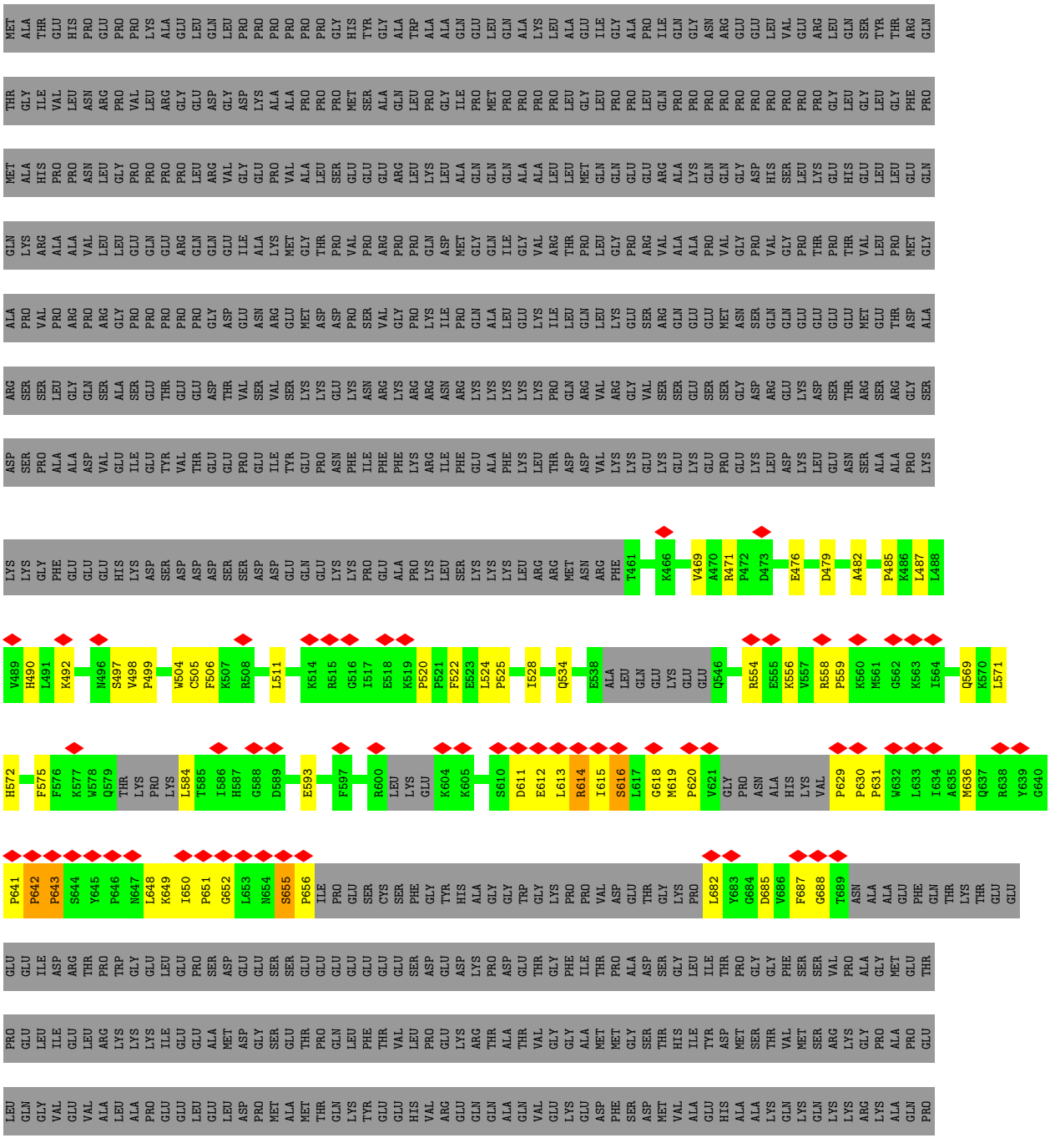
THR GLU LEU GLU ASP ASP ASP ASP ASP TYR SER SER SER THR SER LEU LEU GLY GLN LYS LYS P82 A86 P87 V88 A89 LEU LEU ASN ASP ILE PRO GLN SER THR GLU GLN TYR D102 P109 P110 K111 I112 A113 K121 S129 PRO GLU ARG LEU ASP PRO PHE ALA ASP GLY
GLY LYS THR PRO ASP PRO LYS MET ASN ALA ARG THR TYR MET ASP VAL MET ARG GLU GLN HIS LEU THR LYS GLU GLU ARG GLU ILE ARG GLN GLN LEU A173 E174 K175 G179 V184 A188 A189 S190 GLN PRO PRO SER LYS ARG LYS ARG ARG TRP ASP GLN THR ALA D205 Q206
T207 P208 C209 D219 Q220 R231 S259 HIS THR PRO ALA GLY ALA ALA THR PRO GLY ARG GLY ASP THR PRO GLY HIS ALA THR PRO GLY HIS GLY GLY ALA THR SER SER ALA ARG LYS ASN ARG TRP ASP GLU THR PRO LYS THR GLU ARG ASP THR PRO GLY GLY ALA ALA PRO GLY GLY SER GLY
TRP A311 A331 K335 SER ARG TRP ASP GLU THR PRO ALA SER GLN MET GLY GLY SER THR PRO VAL LEU THR PRO GLY LYS THR PRO ILE GLY THR PRO ALA MET ASN MET ALA THR PRO THR PRO GLY HIS ILE MET SER MET THR PRO GLU GLN LEU GLN ALA TRP ARG TRP GLU
ARG GLU ILE ASP E394 R397 P398 D401 L404 D405 F408 K413 V414 L415 P416 P417 P418 P427 A428 R429 K430 L431 T432 A433 T434 P435 T436 P437 G440 M441 T442 G443 E449 ASP ARG THR M453 K454 S455 V456 P460 S461 G462 N463 L464 D470 D471 I472 Q473 Y474
F475 D476 K477 L478 L479 V480 D481 V482 D483 E484 S485 THR LEU SER PRO E490 E494 R495 K496 I497 M498 K499 L500 L501 L502 K503 I504 K505 N506 G507 R512 A515 L516 R517 T520 D521 K522 A523 R524 E525 F526 G527 A528 G529 P530 L531 Q534 I535 L538 L552 V555
R558 I559 L563 L566 Y570 V571 H572 K573 I574 E579 P580 L581 L582 I583 D584 E585 Y588 V591 E592 E595 I596 N599 L600 A601 K602 A603 A604 A607 T608 T612 K613 R614 P615 D616 N619 M620 D621 E622 Y623 V624 R625 N626 T627 T628 A629 R630 A631 F632 A633
V634 V635 A638 L639 P642 F647 L648 V651 C652 K656 S657 W658 R661 G664 I667 V668 Q669 Q670 I671 A672 I679 H682 V687 E688 I689 I690 E691 H692 D696 E697 Q698 Q699 K700 V701 R702 S705 A706 L707 A710 A711 L712 A713 E714 A715 A716 T717
P718 Y719 G720 I721 E722 S723 F724 D725 S726 V727 L728 L731 W732 I735 H738 R739 G740 K741 A744 A745 F746 L756 A759 E760 Y761 A762 N763 Y764 Y765 T766 R767 E768 V769 M770 L773 I774 R775 E776 F777 Q778 S779 P780 D781 E782 E783 M784 I787 K790 V791 V792 K793
G797 T798 D799 G800 A803 N804 Y805 I806 K807 T808 E809 I810 L811 P812 P813 F814 F815 W819 R822 L825 D826 R827 Y830 V834 V838 E839 L840 A841 N842 K843 V844 G845 A846 A847 E848 I849 I850 S851 V854 D859 E860 A861 E862 R865 K866 E873 M876
L879 G880 A881 D885 L888 E889 L892 I893 D894 L897 Y898 A899 F900 Q901 E902 Q903 T904 Y905 E906 V909 M910 L911 N912 G913 F914 V918 G922 V925 Y928 I932 C933 G934 T935 V936 L937 W938 R939 L940 N941 N942 K943 S944 A945 K946 V947 R948 Q949 Q950
S956 R957 T958 A959 V960 V961 M962 K963 E968 K969 G972 H973 V976 L982 E985 L997 V1001 N1002 V1003 I1004 T1010 P1011 P1012 I1013 K1014 D1015 L1016 L1017 P1018 R1019 I1023 L1024 K1025 N1026 R1027 H1028 V1031 G1040 R1041 V1050 S1051 A1052 R1053 E1054 W1055 M1056 R1057 I1058
L1062 L1063 L1066 K1070 K1071 A1072 I1073 R1074 R1075 A1076 T1077 T1080 Y1083 P1090 H1091 D1092 V1093 T1096 L1097 L1098 N1099 N1100 E1105 R1106 Q1107 N1108 R1109 V1110 C1111 T1112 T1113 V1119 A1120 E1121 T1122 C1123 S1124 P1125 F1126 T1127 V1128 L1129 P1130 A1131 L1132 M1133 N1134 E1135 Y1136 R1137



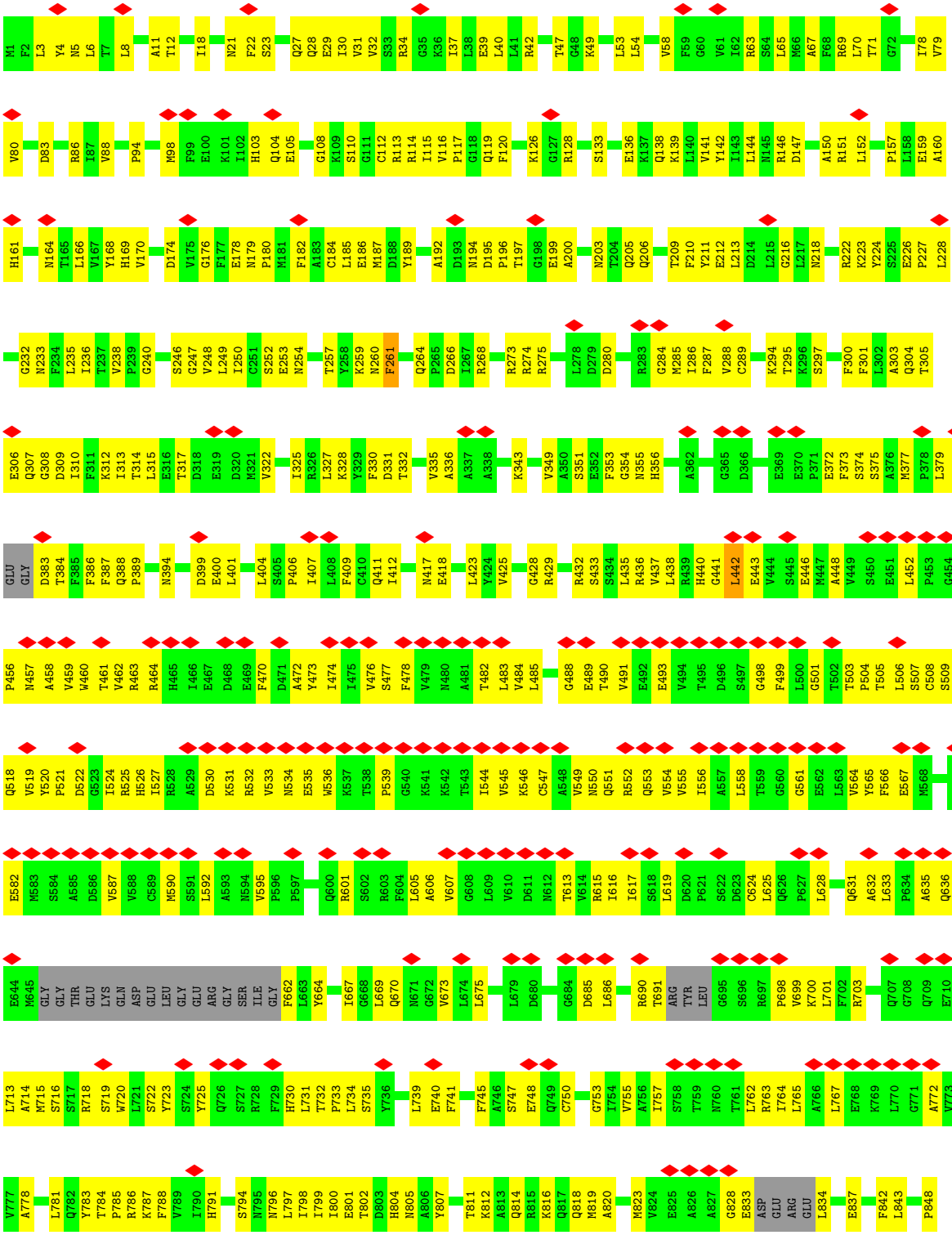
• Molecule 22: Splicing factor 3B subunit 2

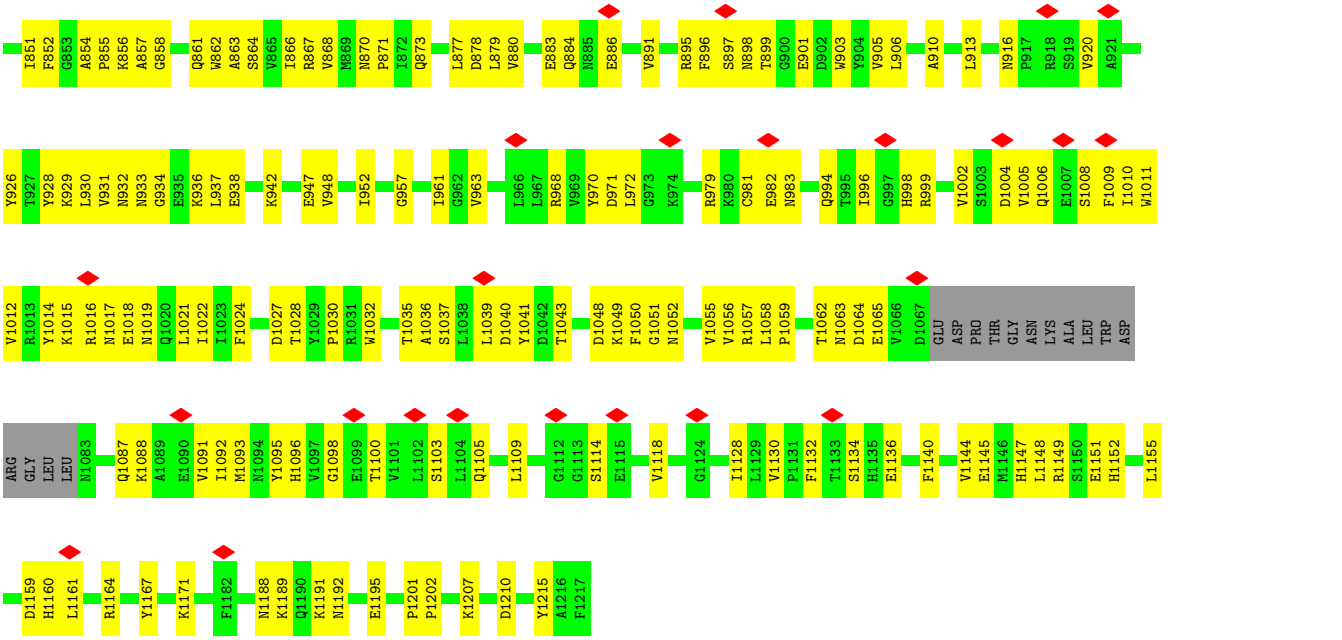
Chain 2:



• Molecule 23: Splicing factor 3B subunit 3

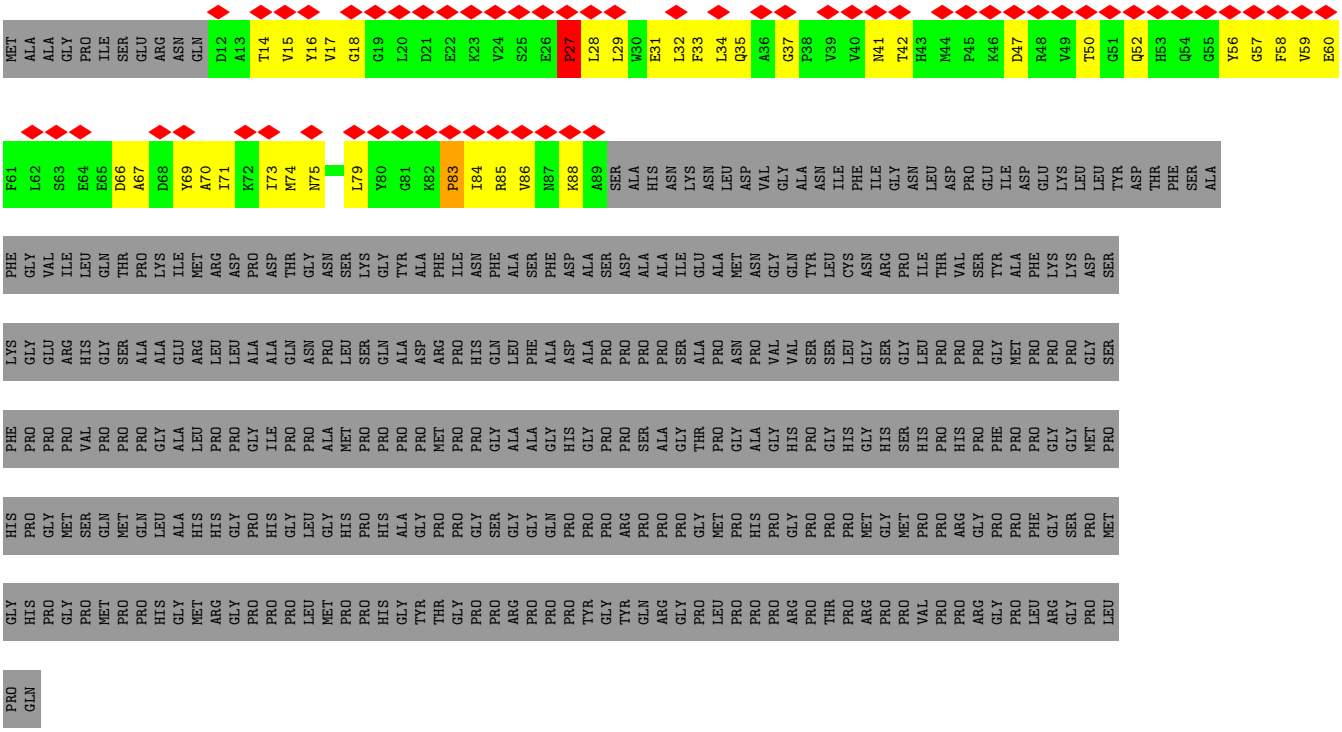
Chain 3:





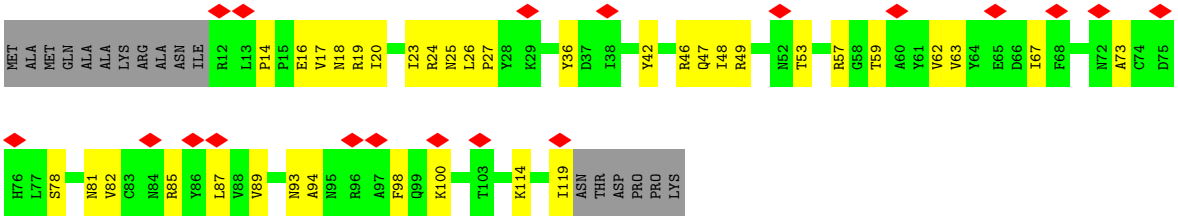
• Molecule 24: Splicing factor 3B subunit 4

Chain 4:



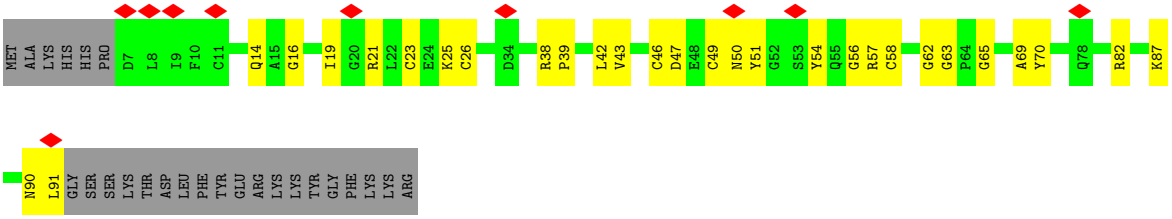
• Molecule 25: Splicing factor 3B subunit 6

Chain 5:



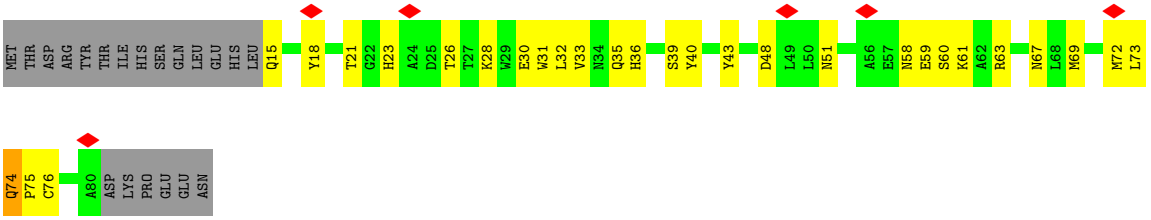
• Molecule 26: PHD finger-like domain-containing protein 5A

Chain 6:



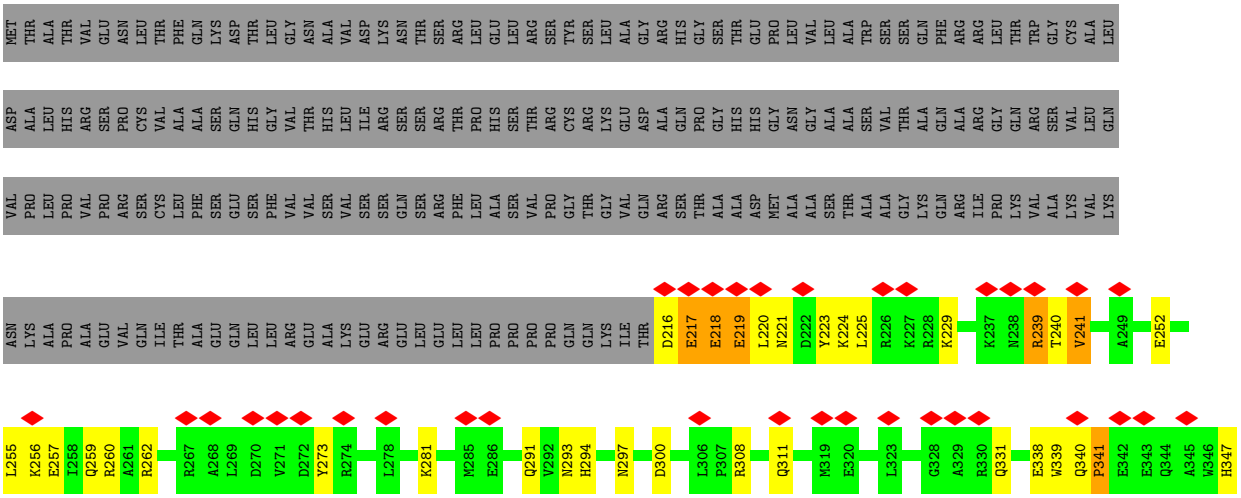
• Molecule 27: Splicing factor 3B subunit 5

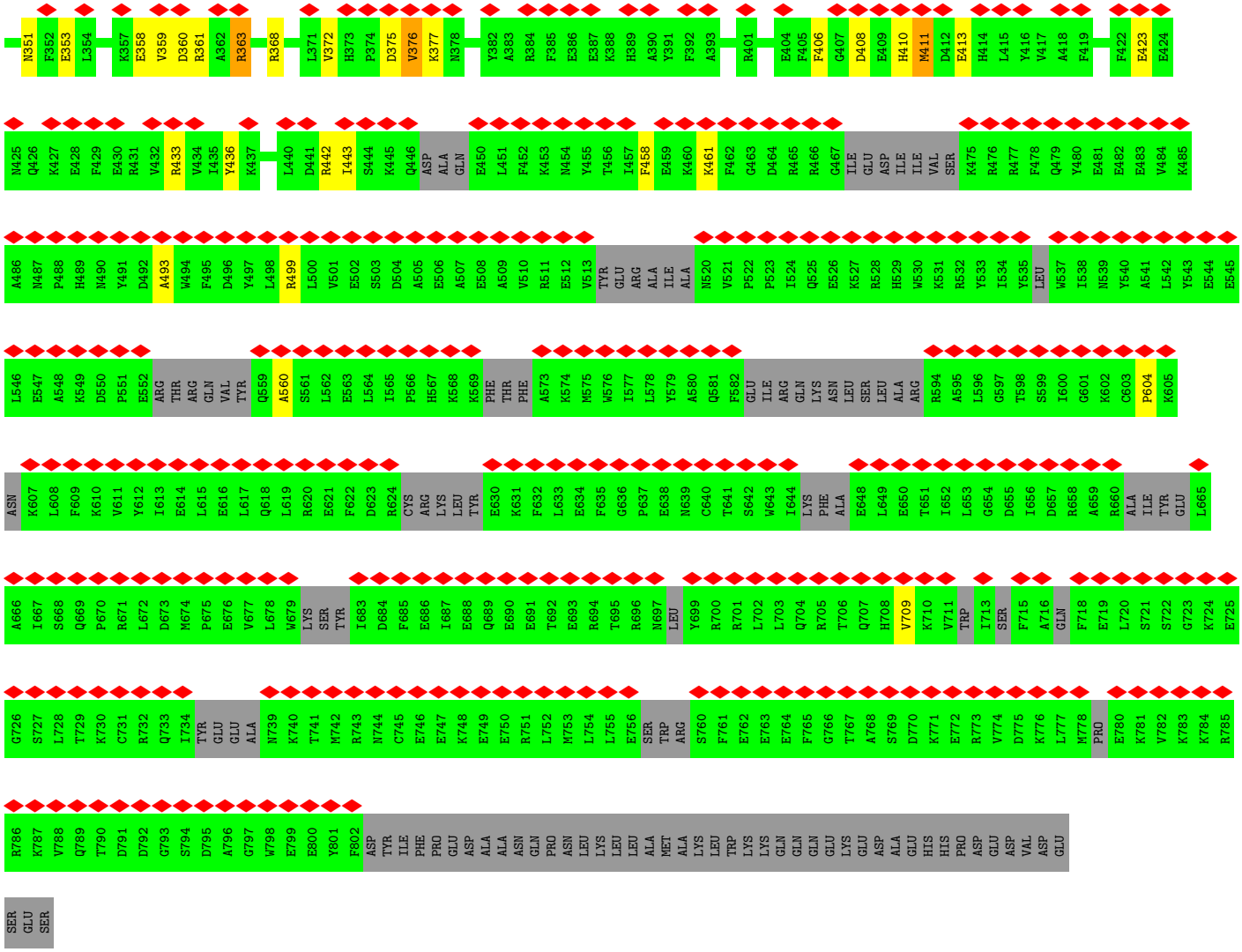
Chain 7:



• Molecule 28: Crooked neck-like protein 1

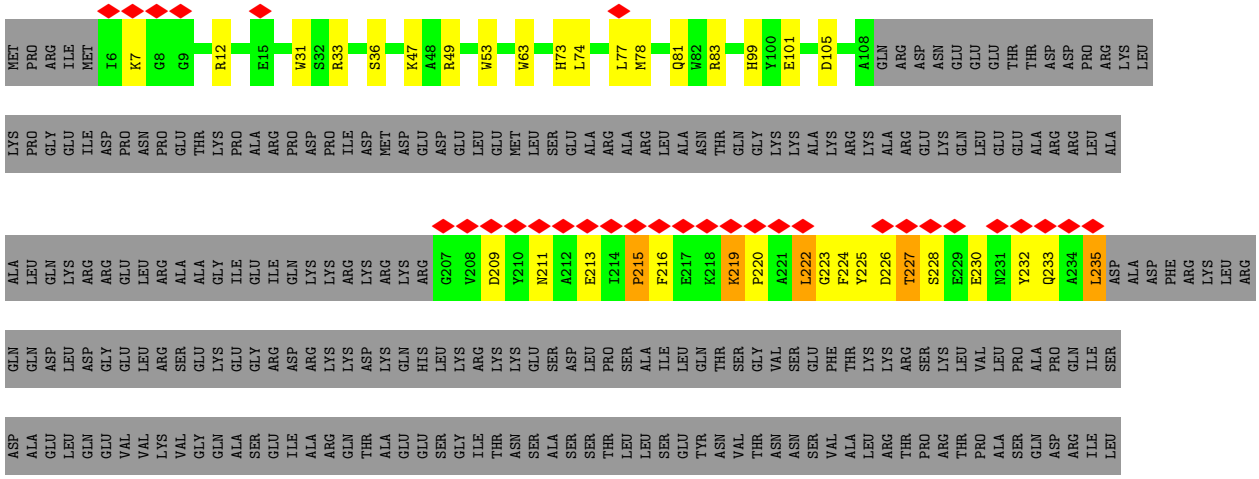
Chain J:

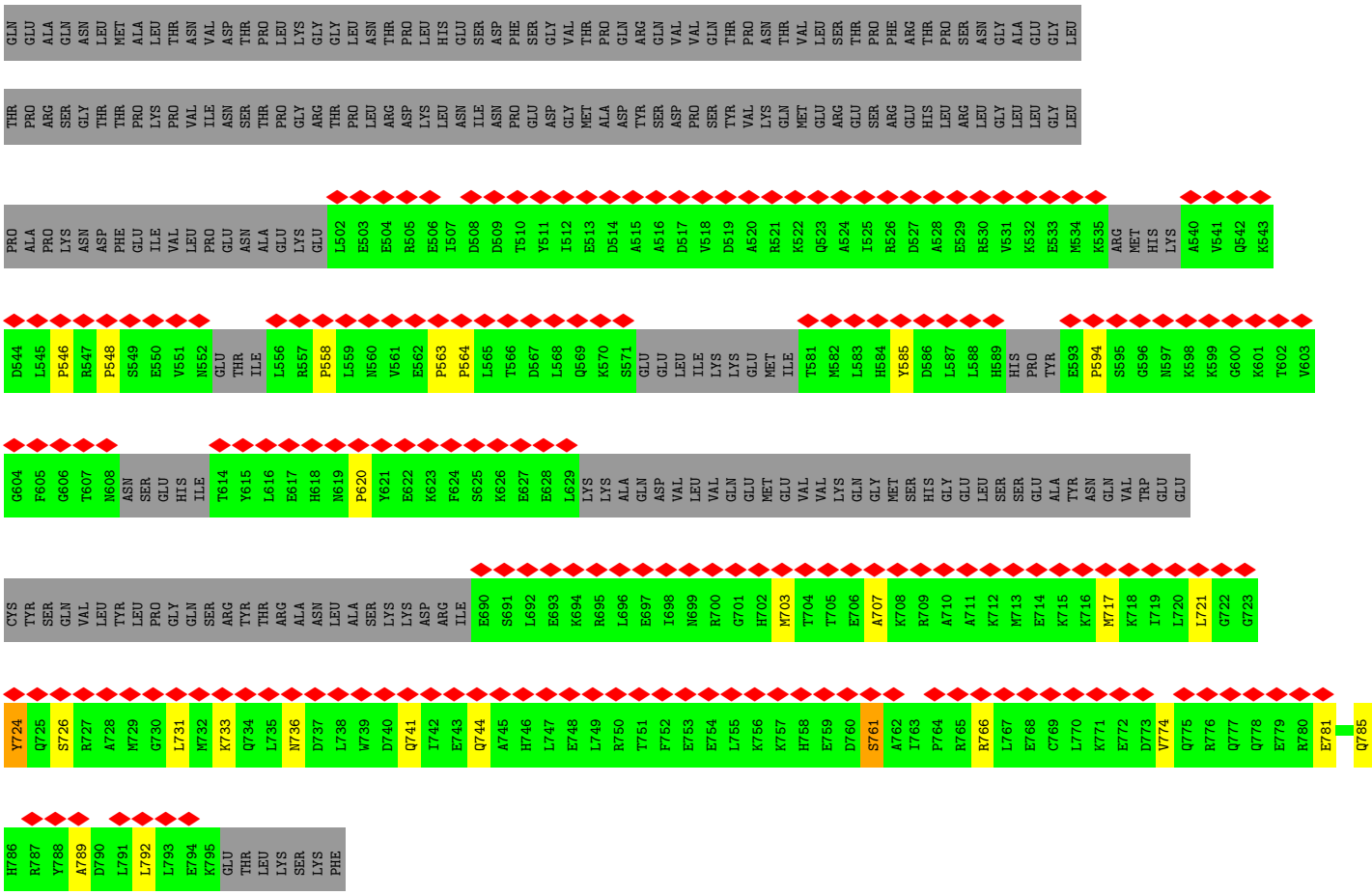




• Molecule 29: Cell division cycle 5-like protein

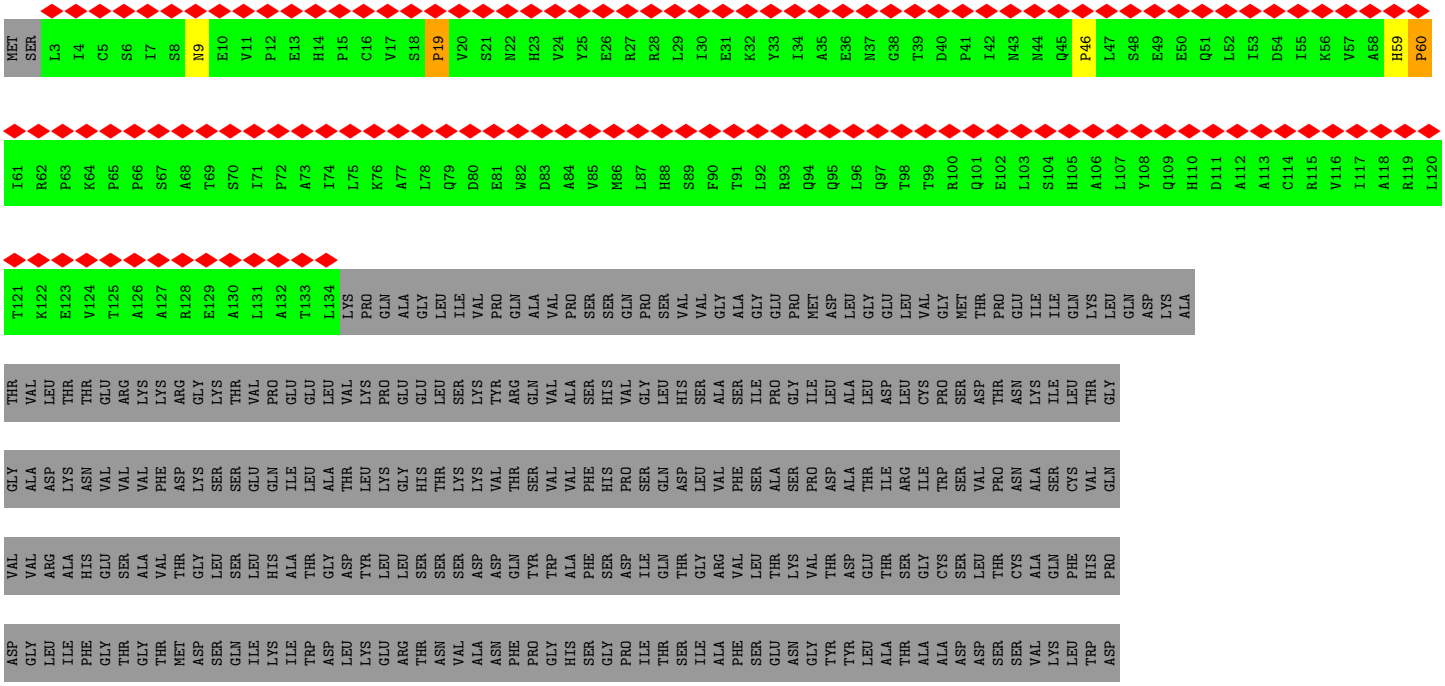
Chain L:

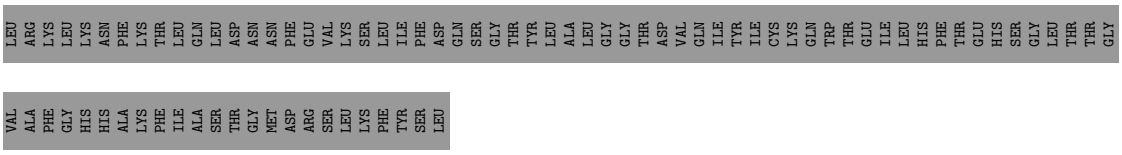




• Molecule 30: Pre-mRNA-processing factor 19

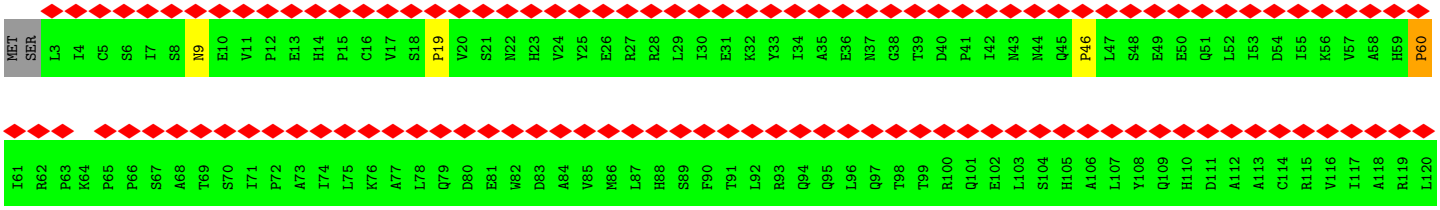
Chain q:





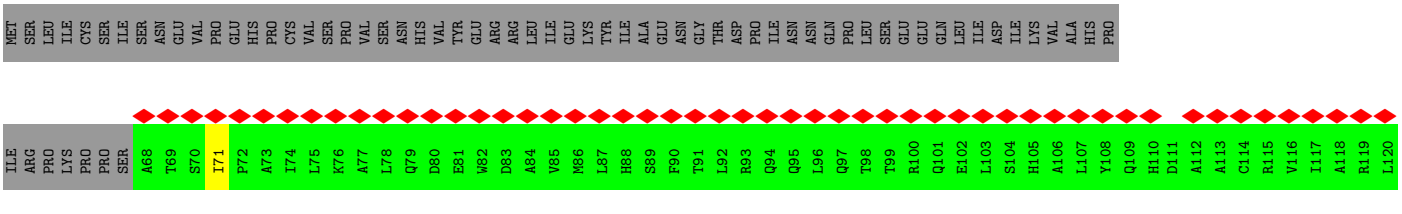
• Molecule 30: Pre-mRNA-processing factor 19

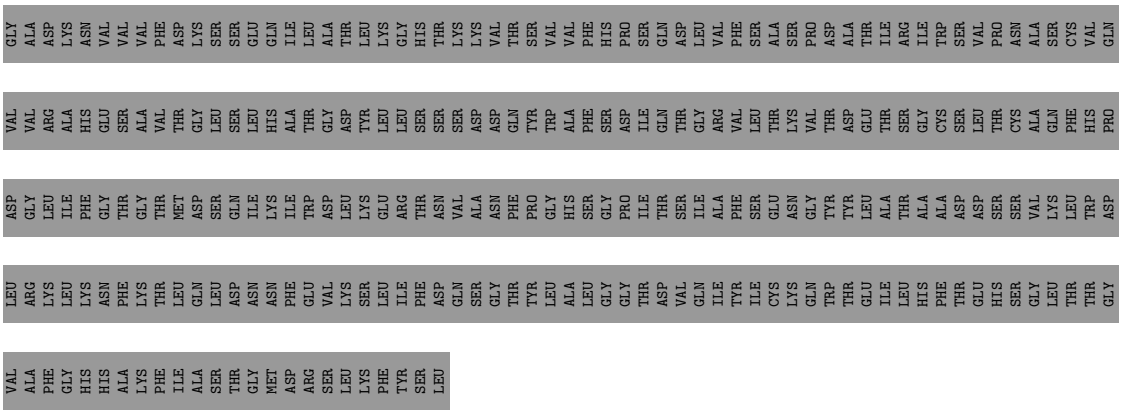
Chain r:



• Molecule 30: Pre-mRNA-processing factor 19

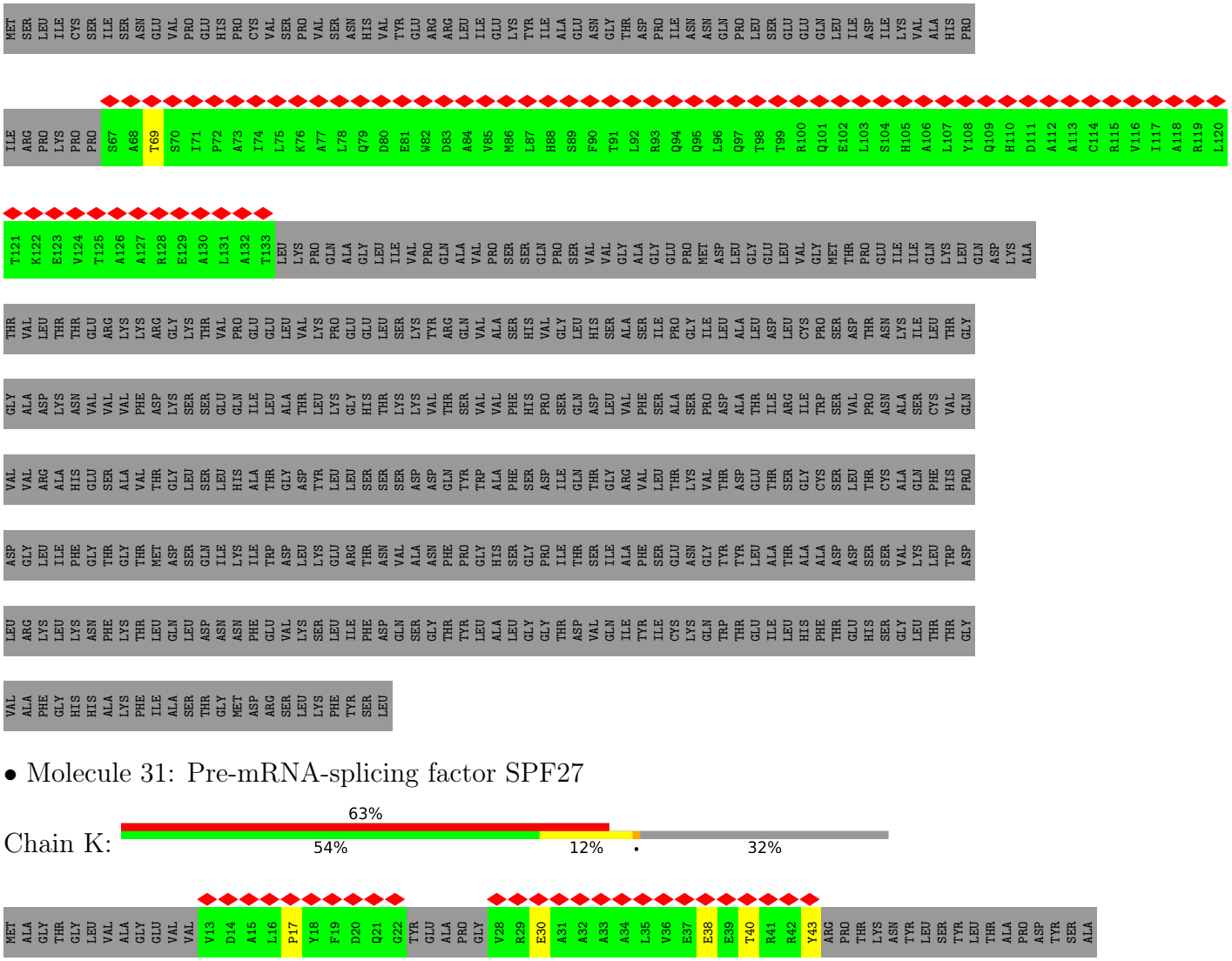
Chain s:





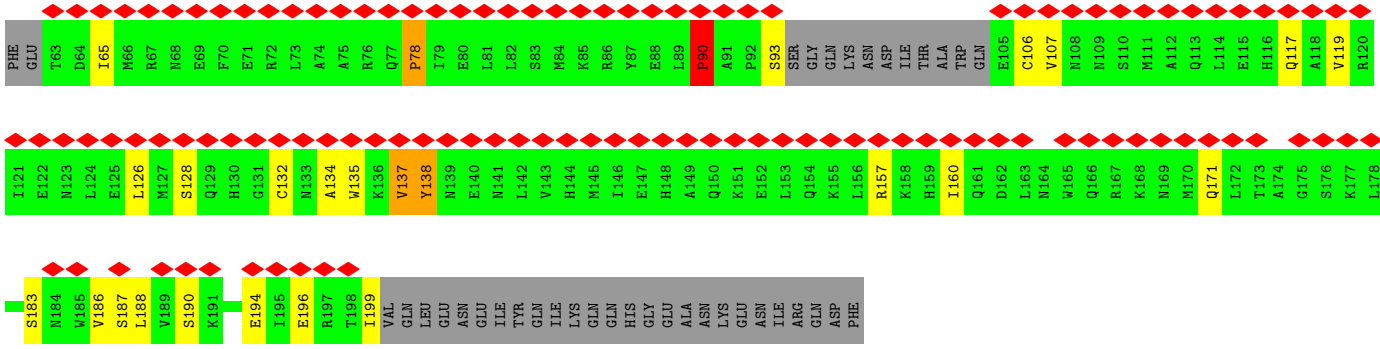
• Molecule 30: Pre-mRNA-processing factor 19

Chain t:



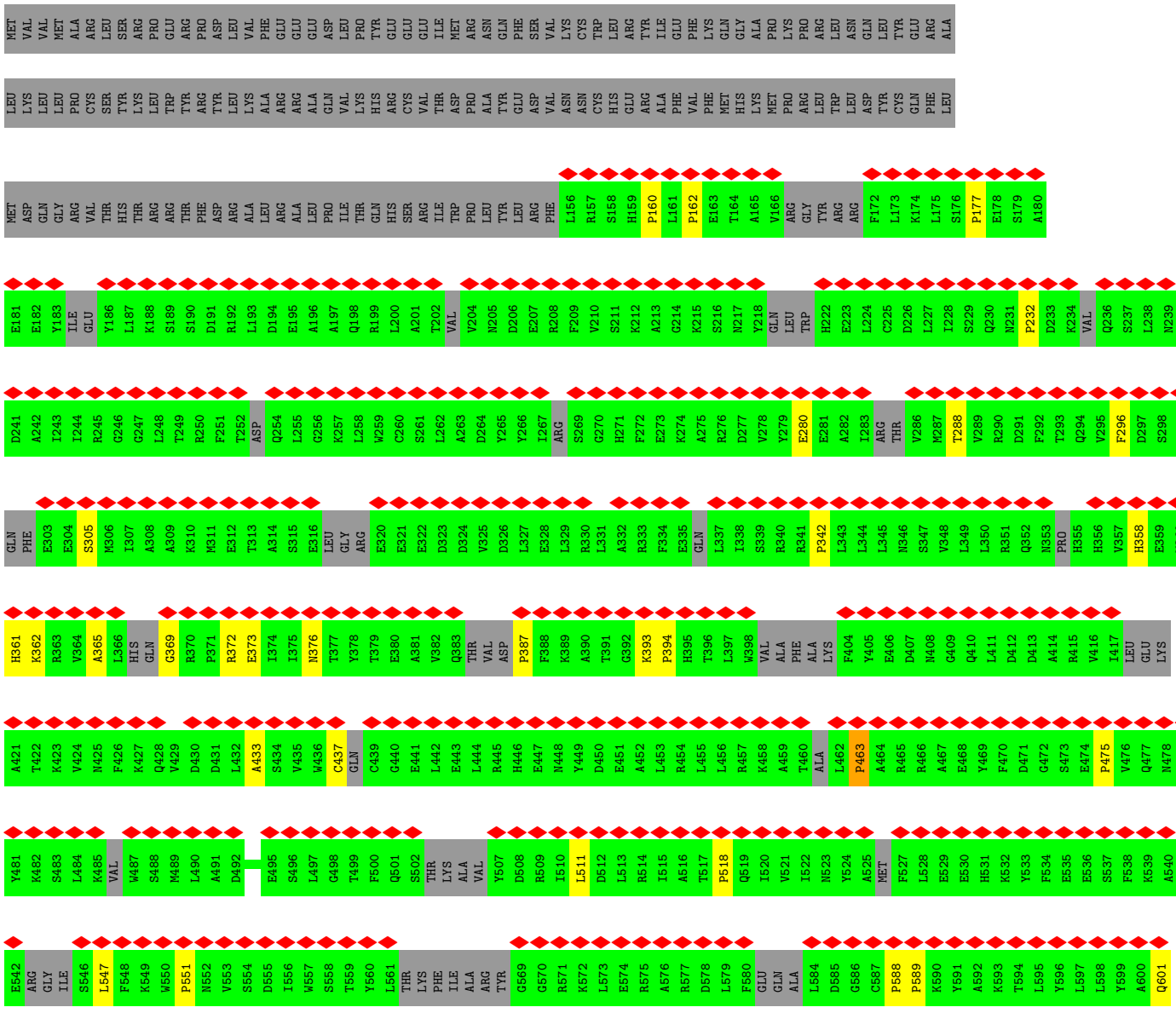
• Molecule 31: Pre-mRNA-splicing factor SPF27

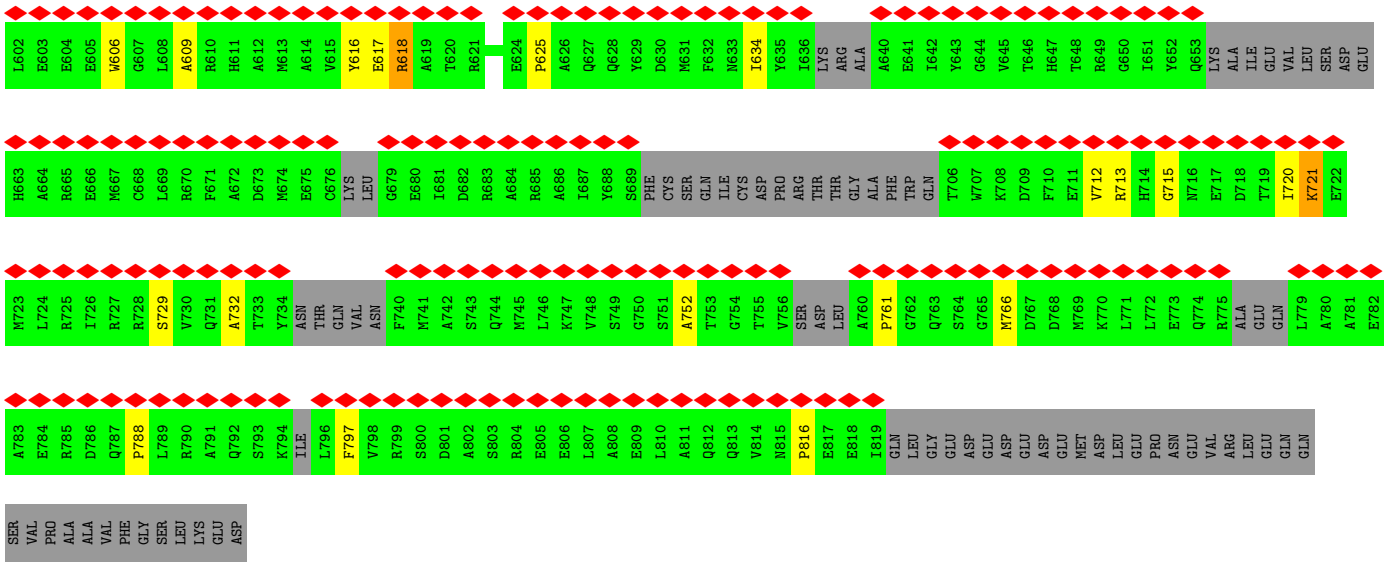
Chain K:



• Molecule 32: Pre-mRNA-splicing factor SYF1

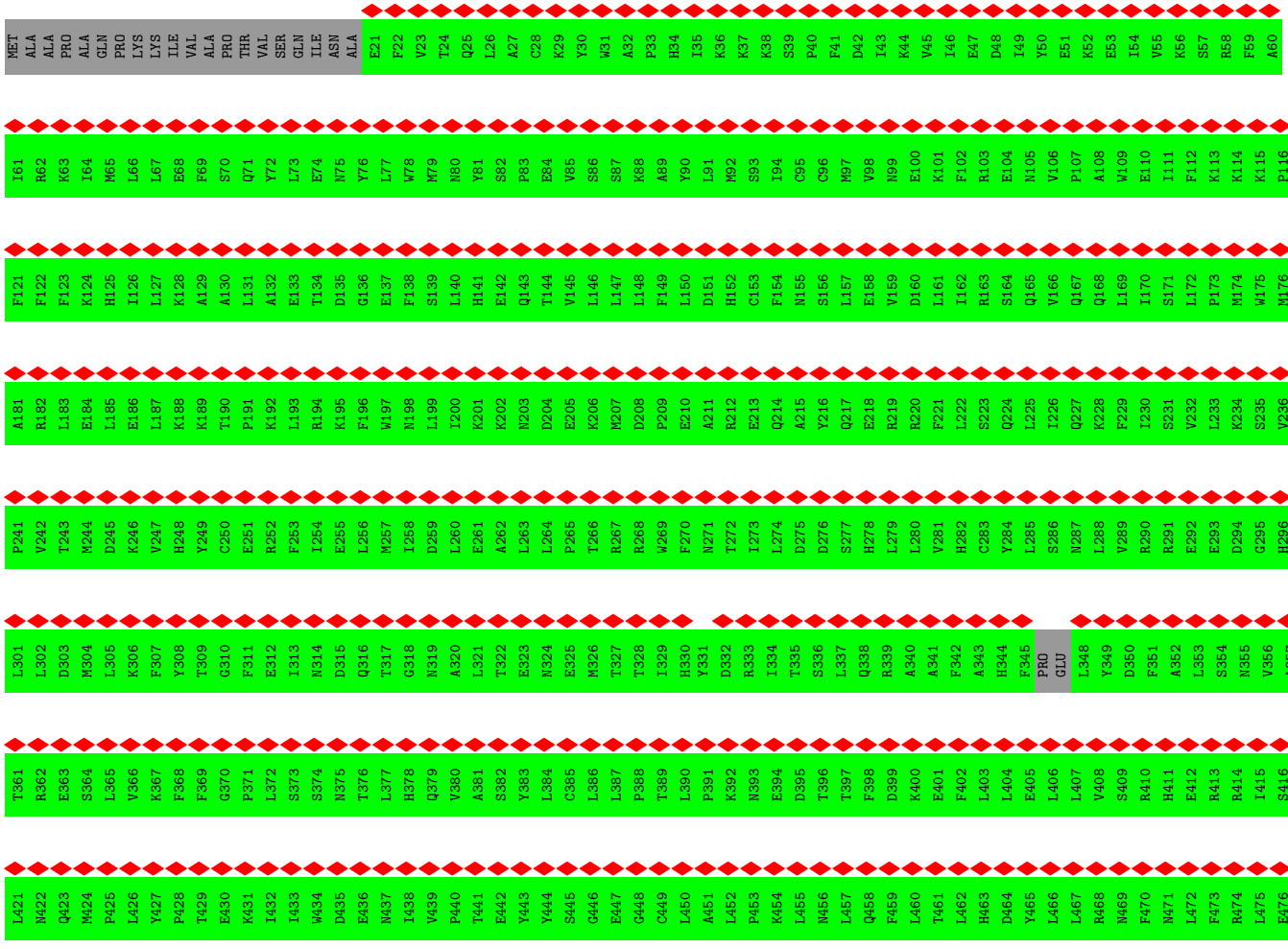
Chain I:

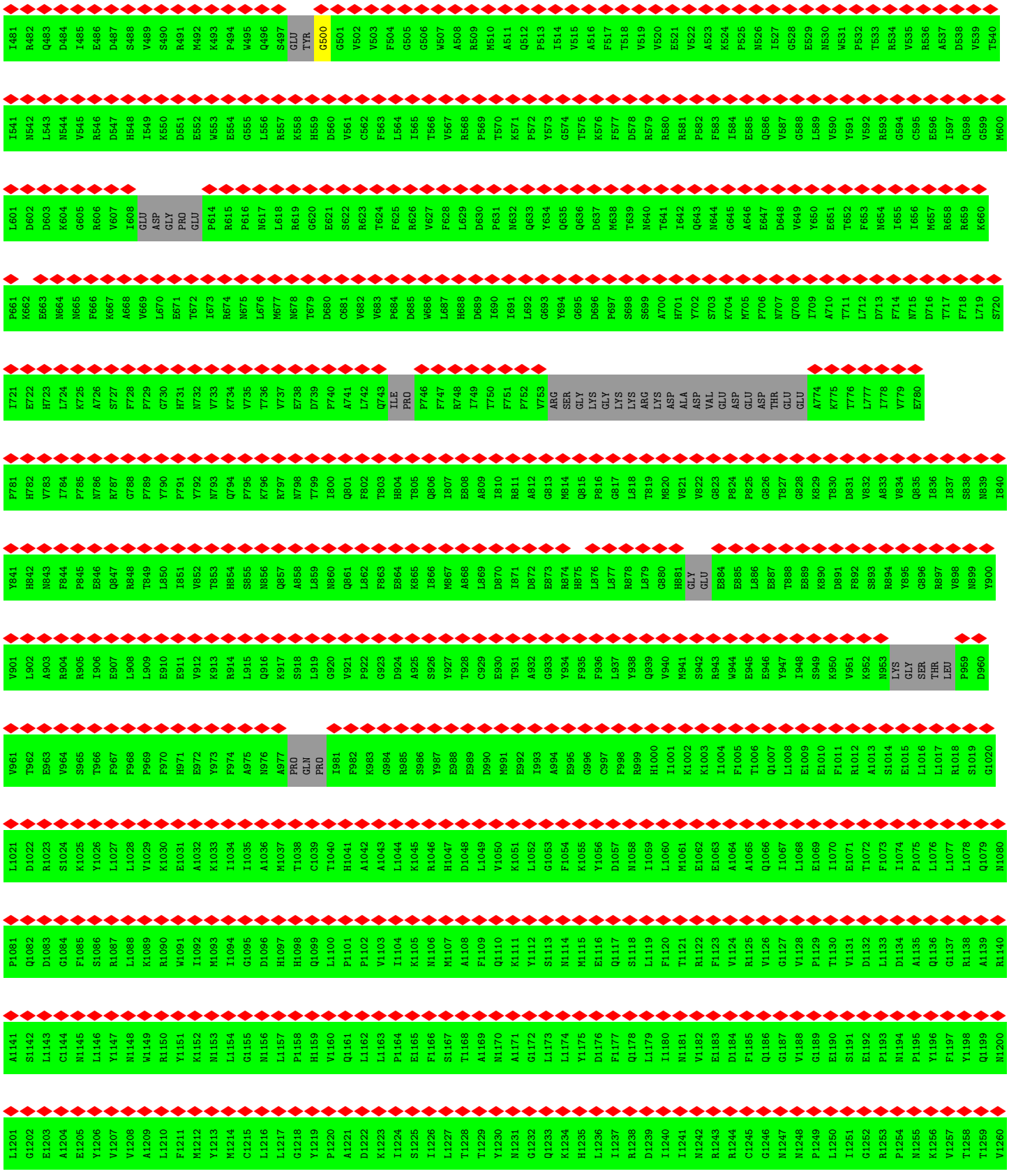




• Molecule 33: Intron-binding protein aquarius

Chain Q:

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I541 N542 L543 N544 V545 R546 D547 H548 I549 K550 D551 E552 W553 E554 G555 L556 R557 K558 H559 D560 V561 C562 F563 L564 I565 T566 V567 R568 P569 T570 K571 P572 Y573 G574 T575 K576 F577 D578 R579 R580 R581 P582 F583 I584 E585 Q586 V587 G588 L589 V590 Y591 V592 R593 G594 C595 E596 I597 Q598 G599 M600
L601 D602 D603 K604 G605 R606 V607 I608 GLU ASP GLY PRO GLU P614 R615 P616 N617 L618 R619 G620 E621 S622 R623 T624 F625 R626 V627 F628 L629 D630 P631 N632 Q633 Y634 Q635 Q636 D637 M638 T639 N640 T641 I642 Q643 N644 G645 A646 E647 D648 V649 Y650 E651 T652 F653 N654 I655 I656 M657 R658 R659 K660
P661 K662 E663 N664 M665 F666 K667 A668 V669 L670 E671 T672 I673 R674 N675 L676 M677 N678 T679 D680 C681 V682 V683 P684 D685 W686 L687 H688 D689 I690 I691 L692 G693 Y694 G695 D696 P697 S698 S699 A700 H701 Y702 S703 K704 M705 P706 N707 Q708 I709 A710 T711 L712 D713 F714 N715 D716 T717 F718 L719 S720
I721 E722 H723 L724 K725 A726 S727 F728 P729 G730 H731 N732 V733 K734 V735 T736 V737 E738 D739 P740 A741 L742 Q743 ILE PRO P746 F747 R748 I749 T750 F751 P752 V753 ARG SER GLY LYS GLY LYS LYS ARG LYS ASP ALA ASP VAL GLU ASP GLU ASP THR GLU GLU A774 K775 T776 L777 I778 V779 E780
P781 H782 V783 I784 P785 N786 R787 G788 P789 Y790 P791 Y792 N793 Q794 P795 K796 R797 N798 T799 I800 Q801 F802 T803 H804 T805 Q806 I807 E808 A809 I810 R811 A812 G813 M814 Q815 P816 G817 L818 T819 M820 V821 V822 G823 P824 P825 G826 T827 G828 K829 T830 D831 V832 A833 V834 Q835 I836 I837 S838 N839 I840
Y841 H842 N843 F844 P845 E846 Q847 R848 T849 L850 I851 V852 T853 H854 S855 N856 Q857 A858 L859 N860 Q861 L862 F863 E864 K865 I866 M867 A868 L869 D870 I871 D872 E873 R874 H875 L876 L877 R878 L879 G880 H881 GLY GLU E884 E885 L886 E887 T888 E889 K890 D891 F892 S893 R894 Y895 G896 R897 V898 N899 Y900
V901 L902 A903 R904 R905 I906 E907 L908 L909 E910 E911 V912 K913 R914 L915 Q916 K917 S918 L919 G920 V921 P922 G923 D924 A925 S926 Y927 T928 C929 E930 T931 A932 G933 Y934 F935 F936 L937 Y938 Q939 V940 M941 S942 R943 W944 E945 E946 Y947 I948 S949 K950 V951 K952 N953 LYS GLY SER THR LEU P959 D960
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P1081 Q1082 D1083 G1084 F1085 S1086 R1087 L1088 K1089 R1090 W1091 I1092 M1093 I1094 G1095 D1096 H1097 H1098 Q1099 L1100 P1101 P1102 V1103 I1104 K1105 N1106 M1107 A1108 F1109 Q1110 K1111 Y1112 S1113 N1114 M1115 E1116 Q1117 S1118 L1119 F1120 T1121 R1122 F1123 V1124 R1125 V1126 G1127 V1128 P1129 T1130 V1131 D1132 L1133 D1134 A1135 Q1136 G1137 R1138 A1139 R1140
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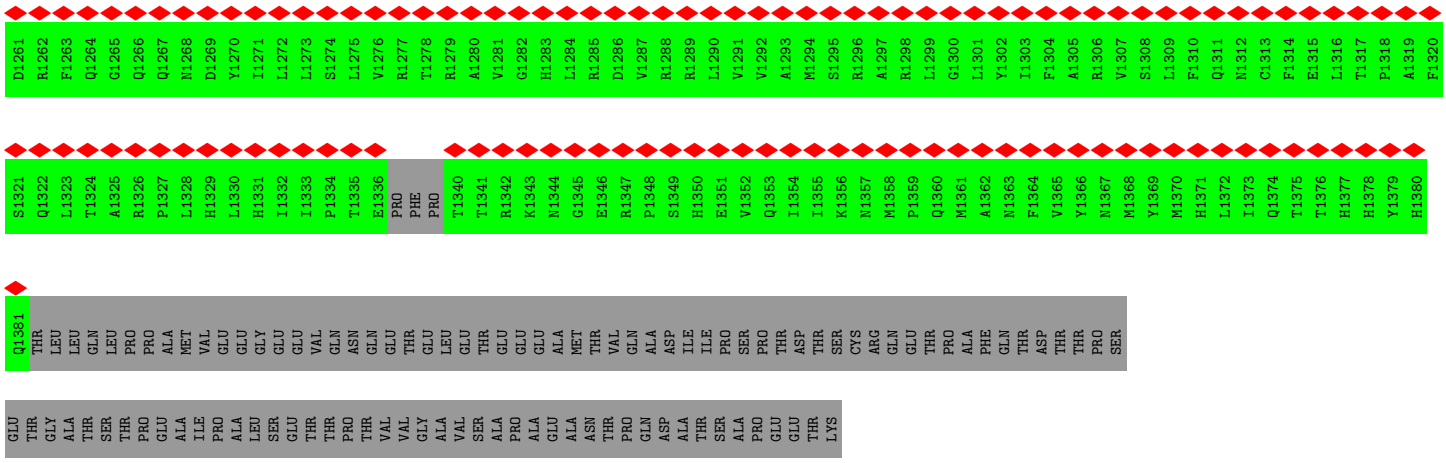
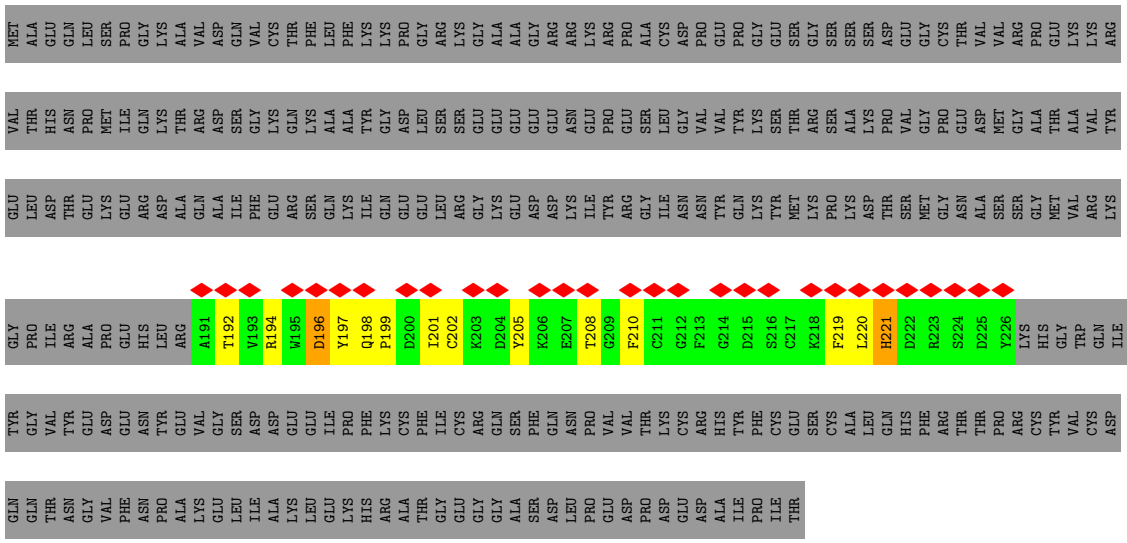
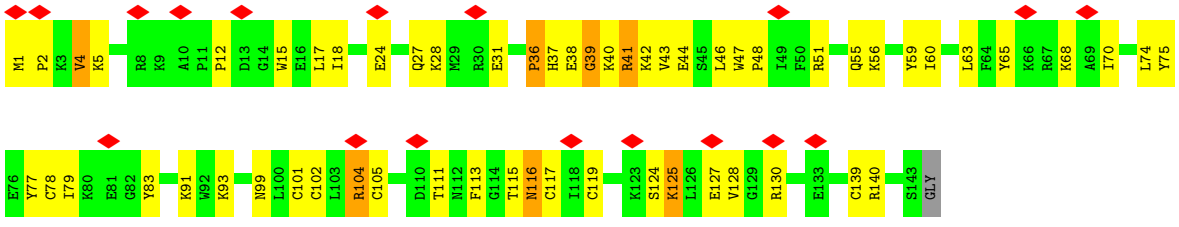


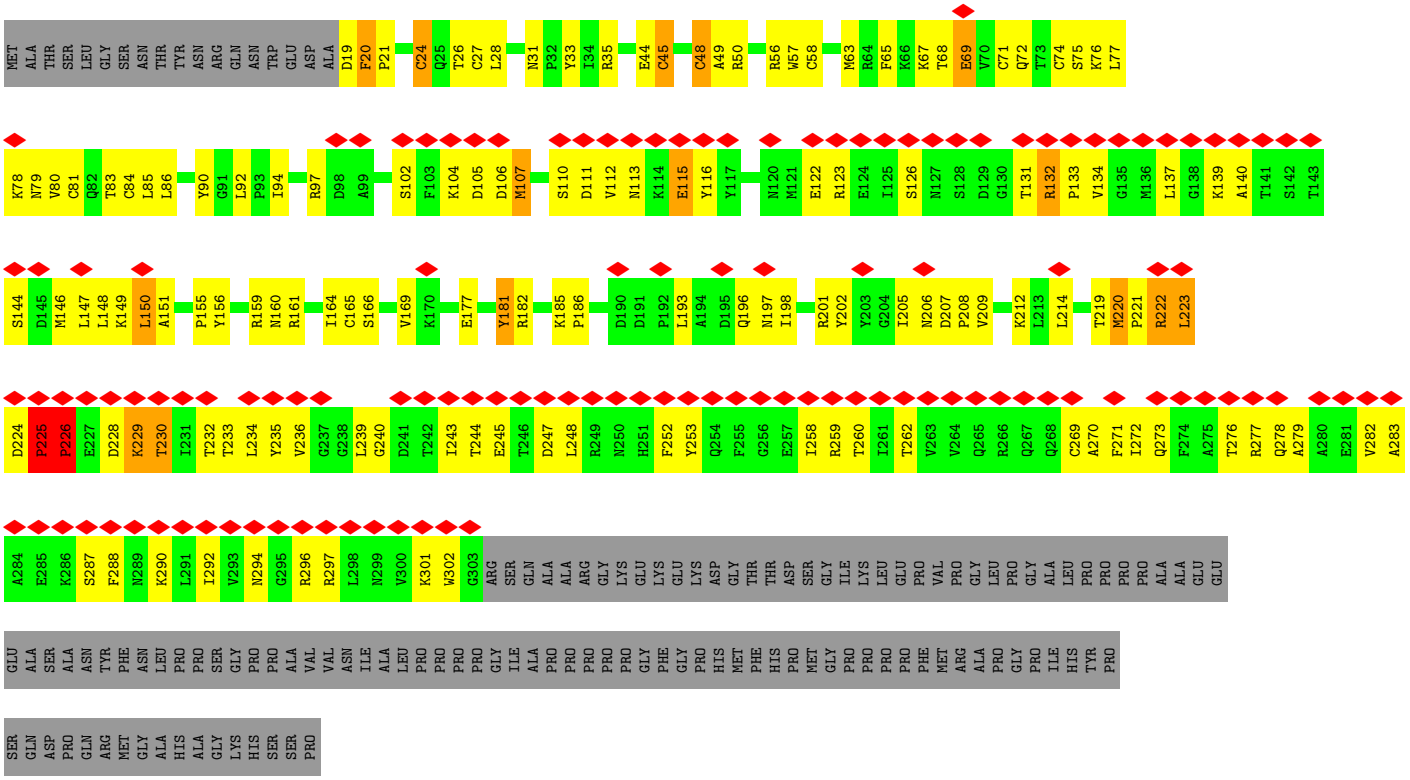
• Molecule 34: RING finger protein 113A



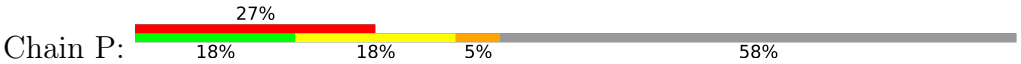
• Molecule 35: Protein BUD31 homolog

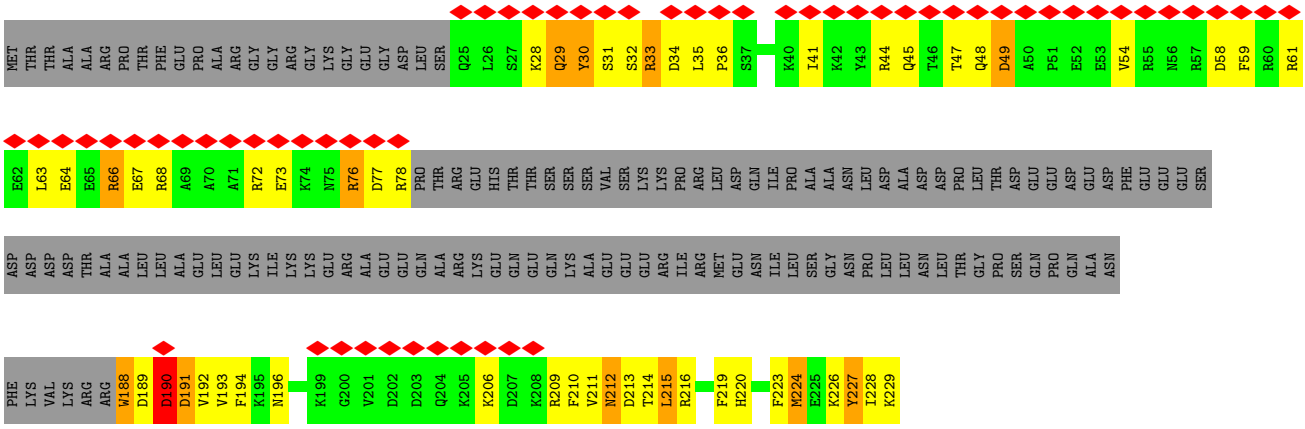


• Molecule 36: Pre-mRNA-splicing factor RBM22

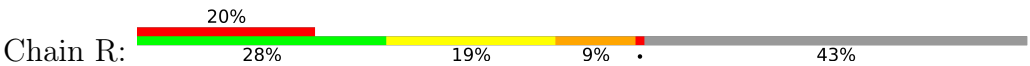


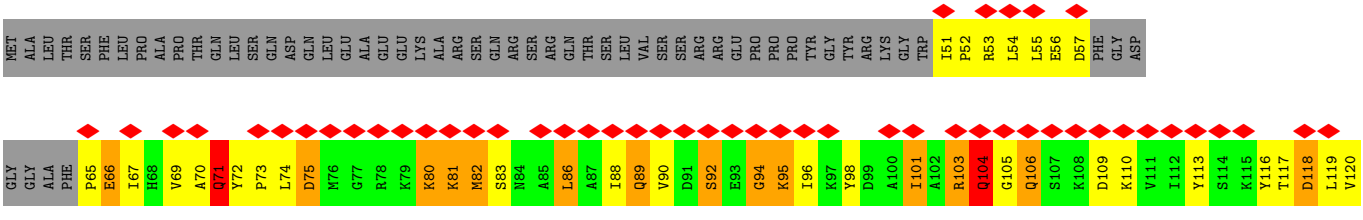
• Molecule 37: Spliceosome-associated protein CWC15 homolog

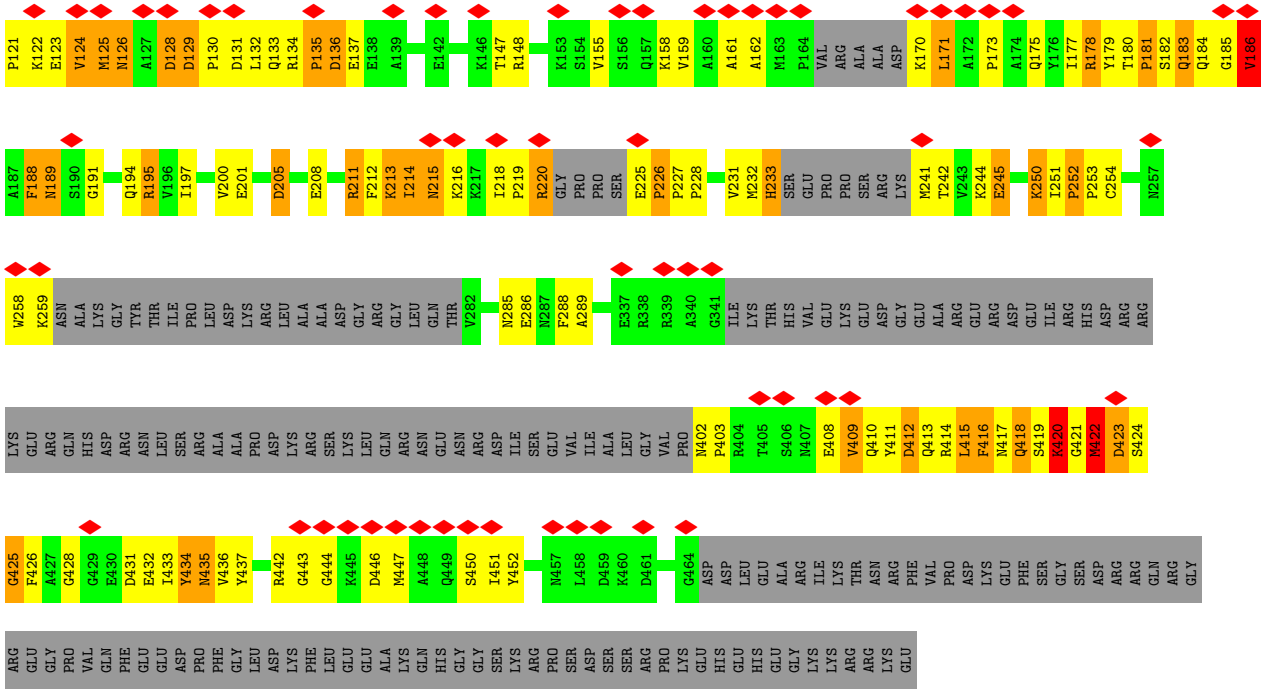




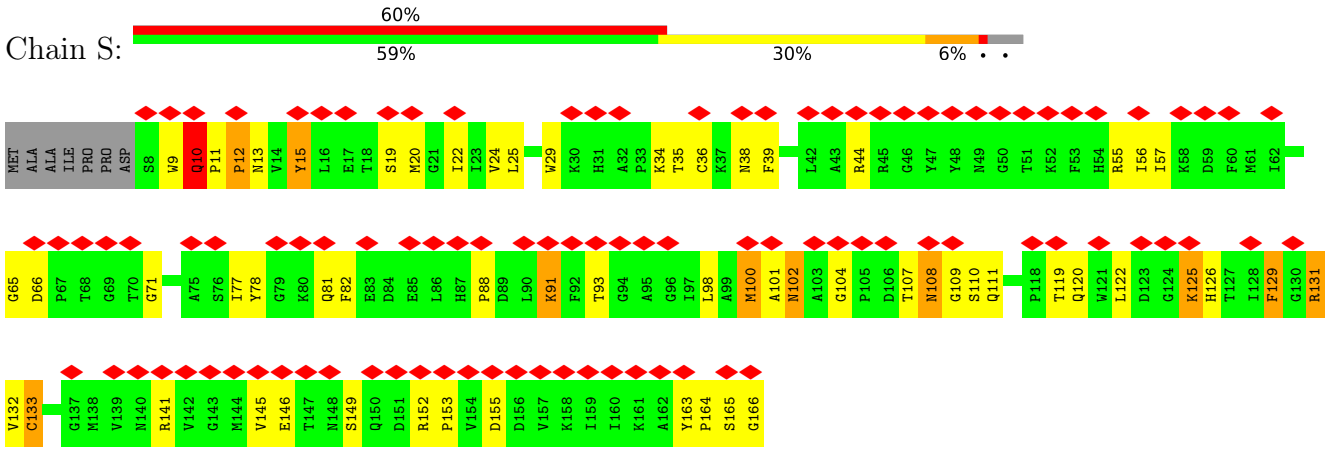
• Molecule 38: Skip



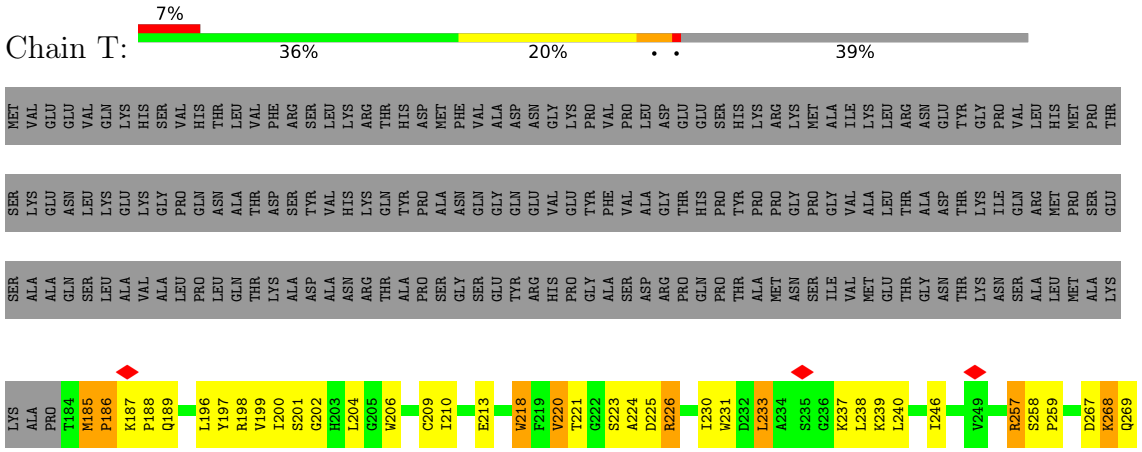


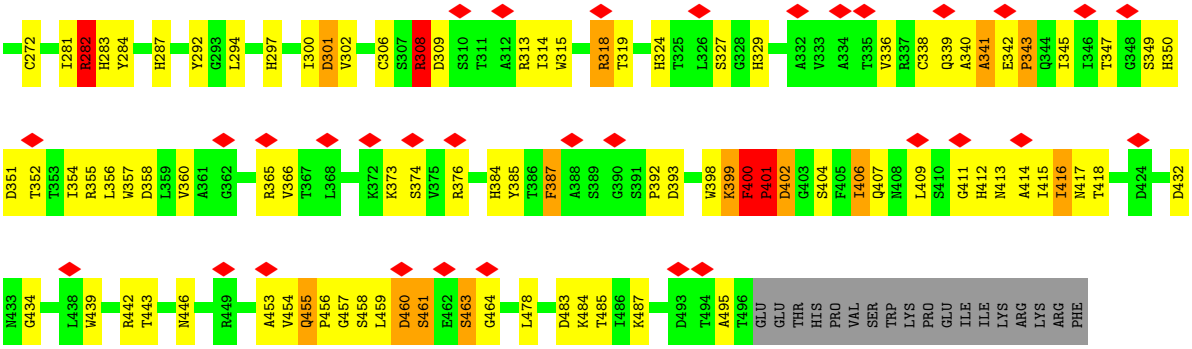


• Molecule 39: Peptidyl-prolyl cis-trans isomerase-like 1



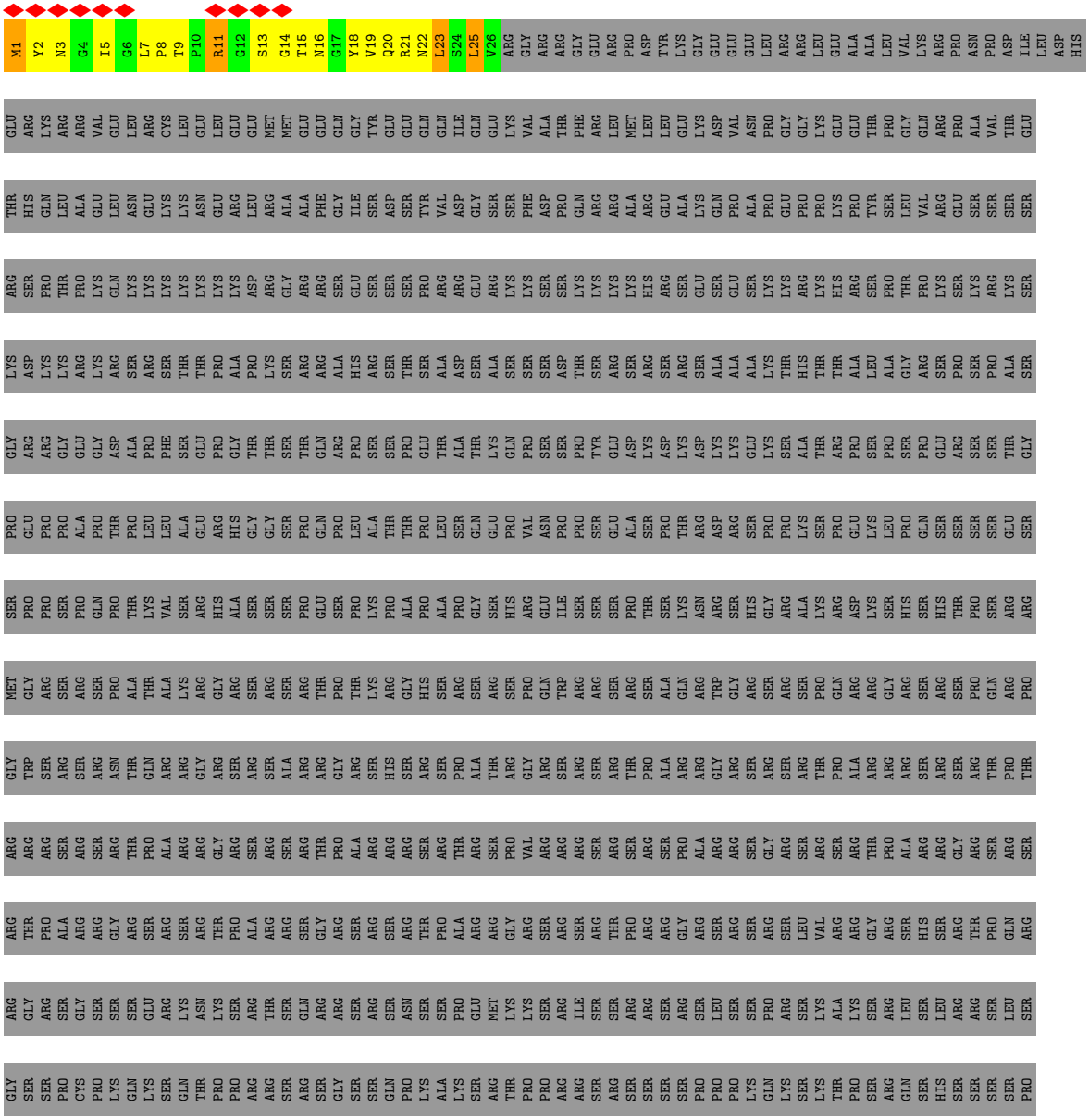
• Molecule 40: Pleiotropic regulator 1





• Molecule 41: Serine/arginine repetitive matrix protein 2

Chain U: 99%



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SER SER THR PRO PRO ARG GLN SER PRO SER ARG SER SER SER PRO GLN PRO LYS VAL LYS ALA ILE ILE SER PRO ARG GLN ARG SER HIS SER GLY SER SER SER PRO SER PRO SER ARG VAL THR SER ARG THR THR PRO ARG ARG SER ARG SER VAL SER PRO CYS SER ASN VAL GLU

SER ARG LEU LEU PRO ARG TYR SER HIS SER GLY SER SER SER PRO ASP THR LYS VAL LYS PRO GLU THR PRO PRO ARG GLN SER HIS SER GLY SER ILE SER PRO TYR PRO LYS VAL LYS ALA GLN THR PRO PRO GLY PRO SER LEU SER GLY SER LYS SER PRO CYS PRO GLN GLU LYS

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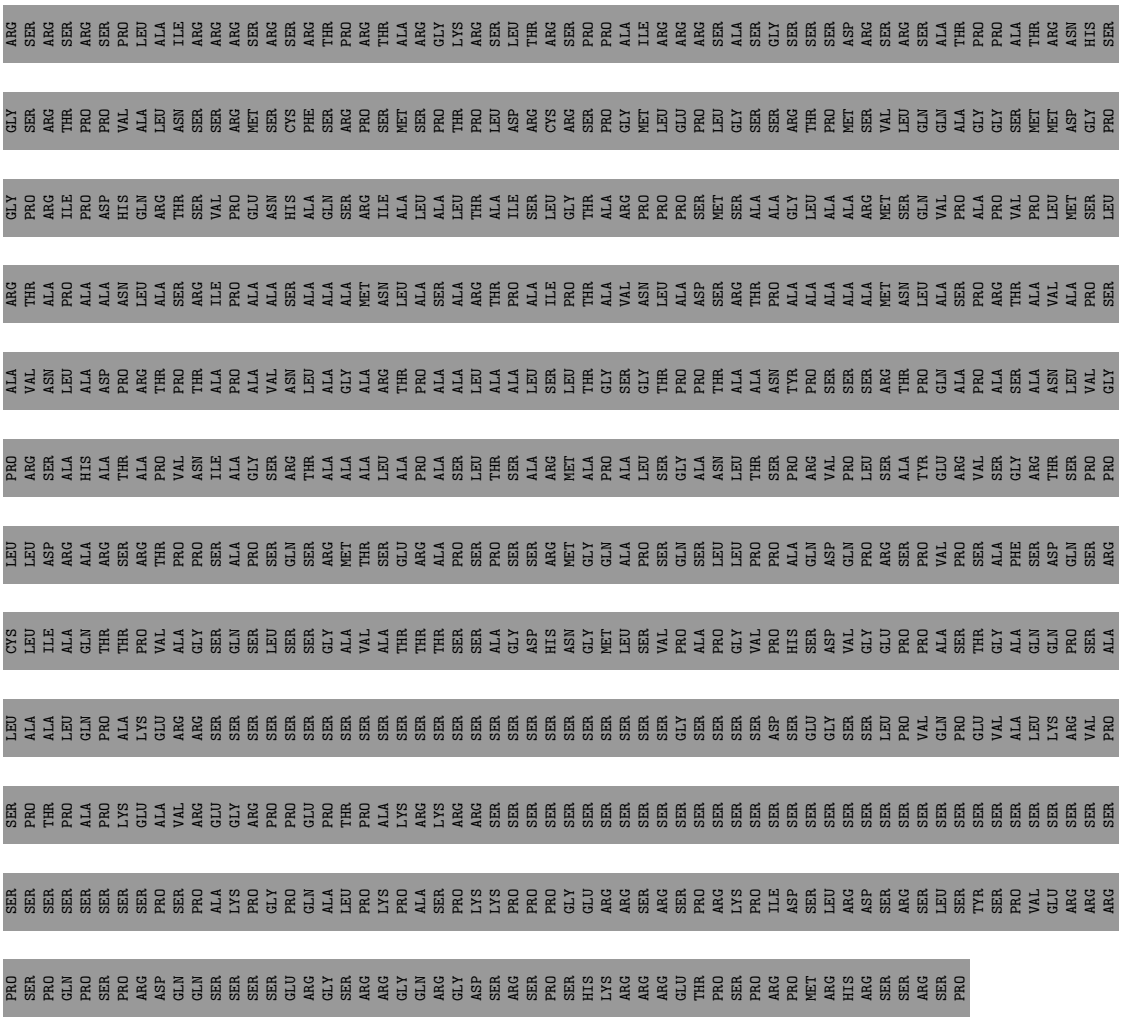
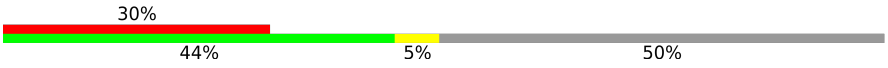
ARG ARG SER ARG SER ARG THR PRO PRO VAL THR ARG ARG SER ARG SER ARG THR PRO THR THR ARG ARG SER ARG SER ARG THR PRO PRO VAL THR ARG ARG SER SER ARG SER ARG THR PRO PRO VAL THR ARG ARG SER ARG SER SER ARG THR SER PRO ILE THR ARG ARG

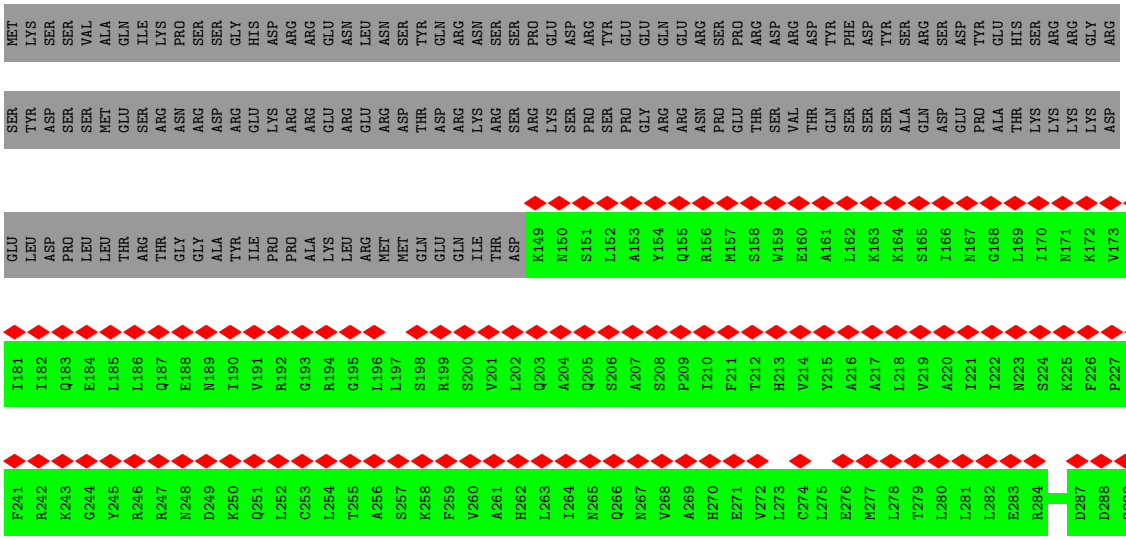
ARG SER ARG SER ARG THR SER PRO VAL THR ARG ARG SER ARG SER ARG THR SER PRO VAL THR ARG ARG SER ARG SER ARG THR SER PRO VAL THR ARG ARG SER SER ARG SER ARG THR PRO PRO ALA ILE ARG ARG SER ARG SER ARG THR PRO LEU LEU PRO ARG LYS

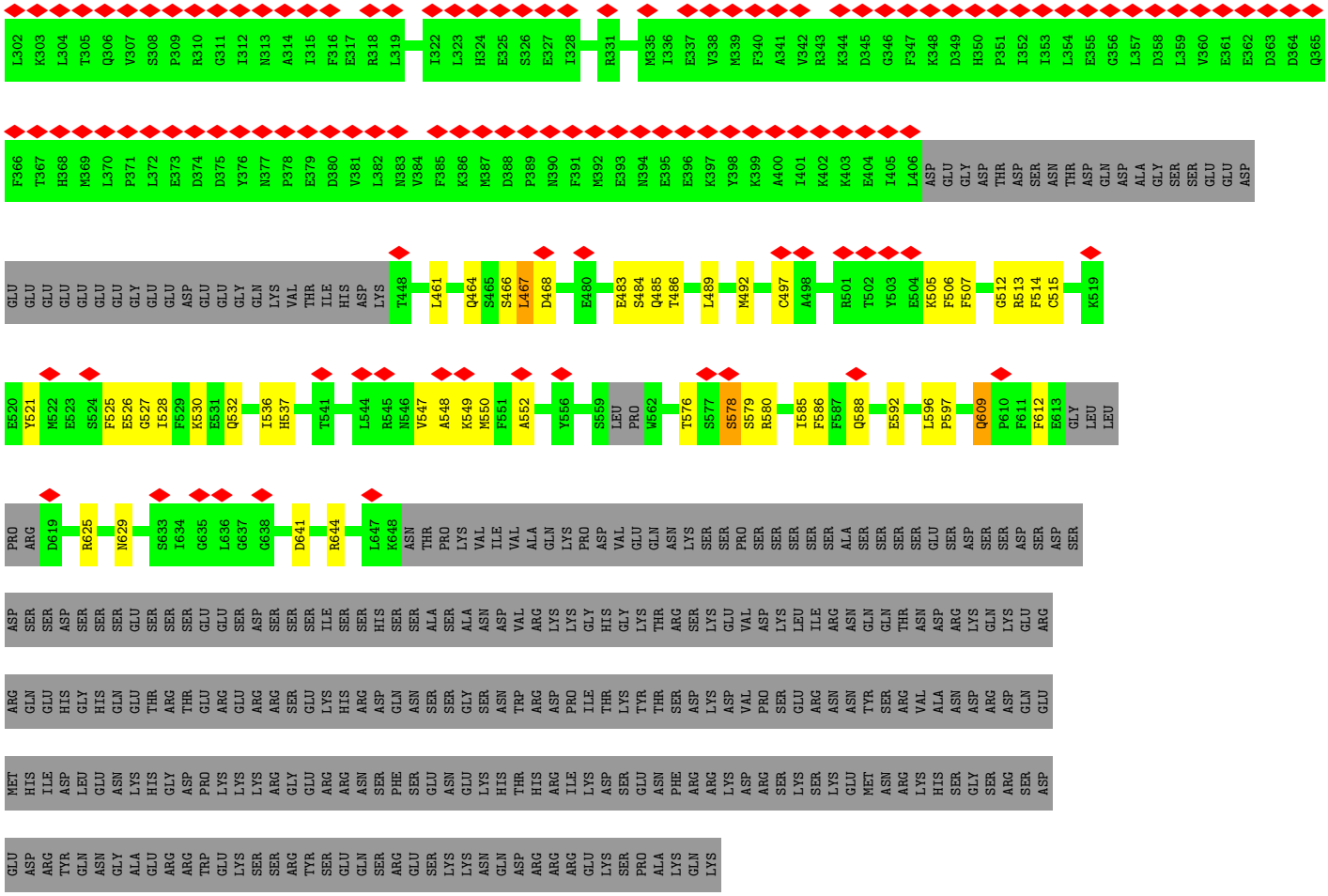


• Molecule 42: Pre-mRNA-splicing factor CWC22 homolog

Chain V:

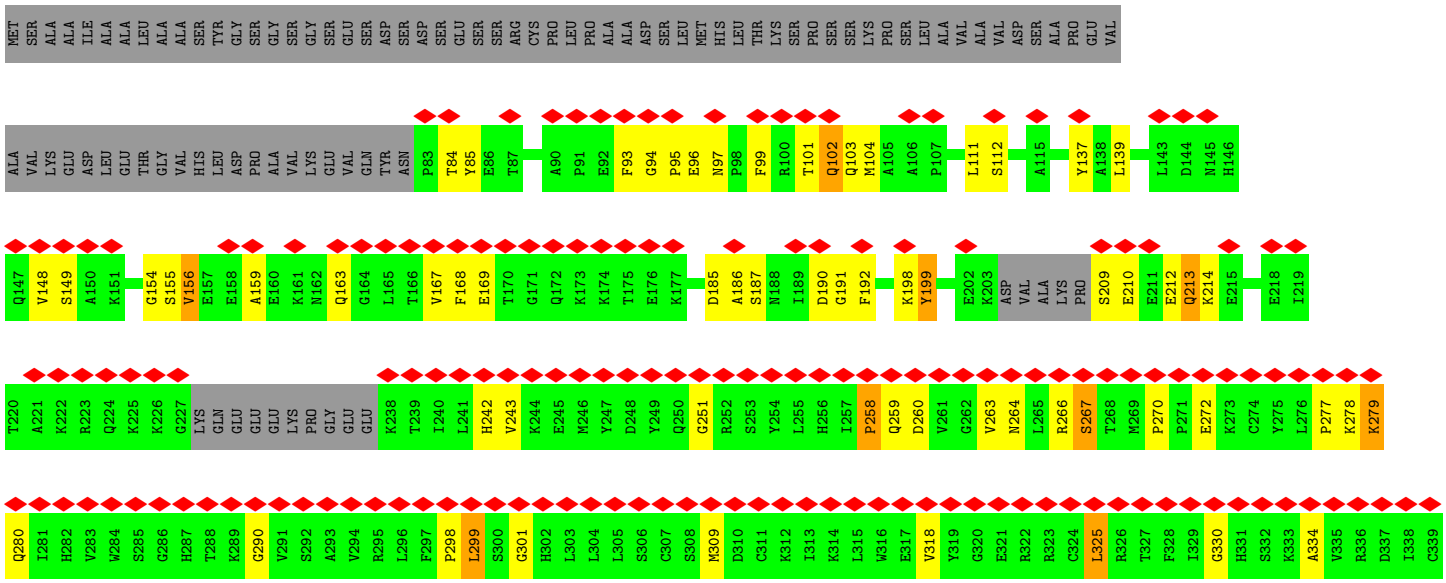


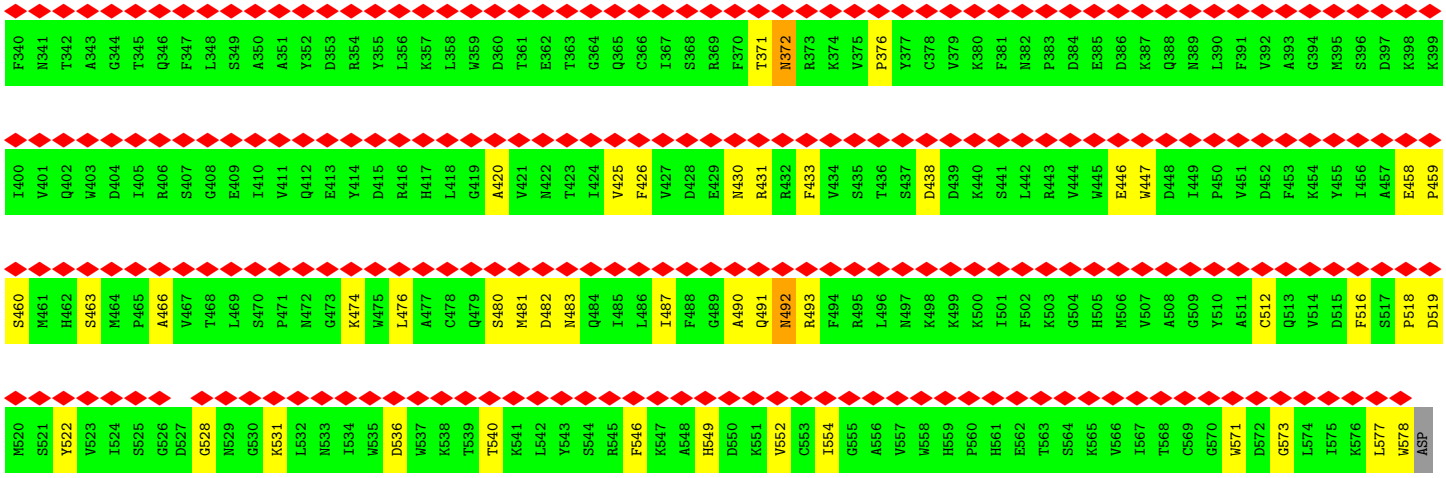




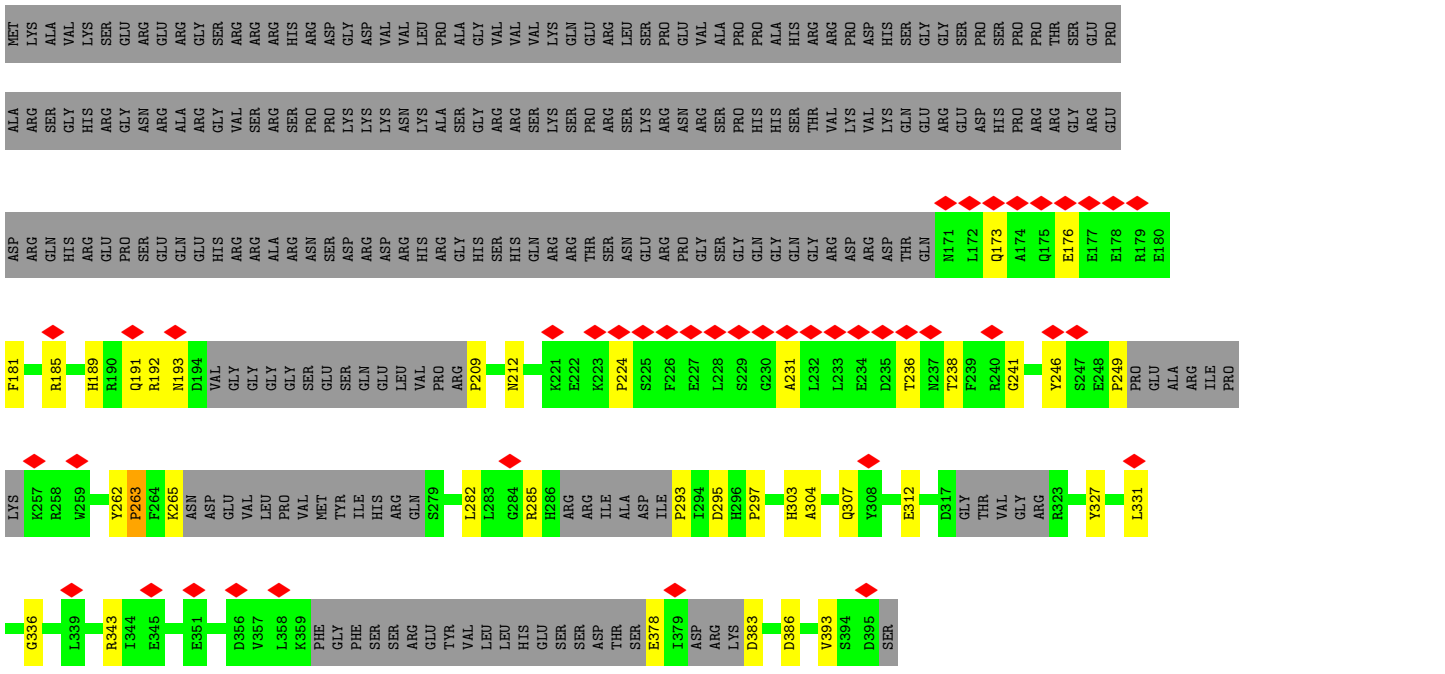
• Molecule 43: Pre-mRNA-processing factor 17

Chain W:

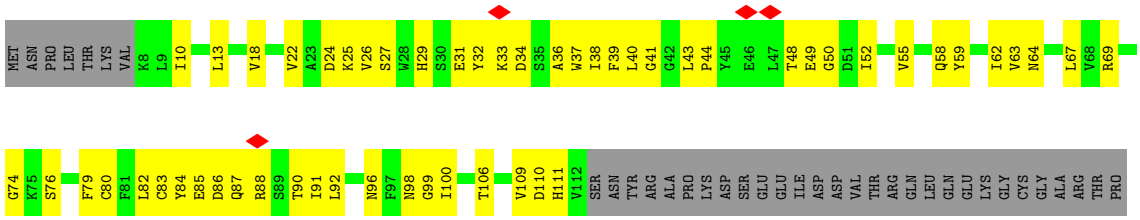


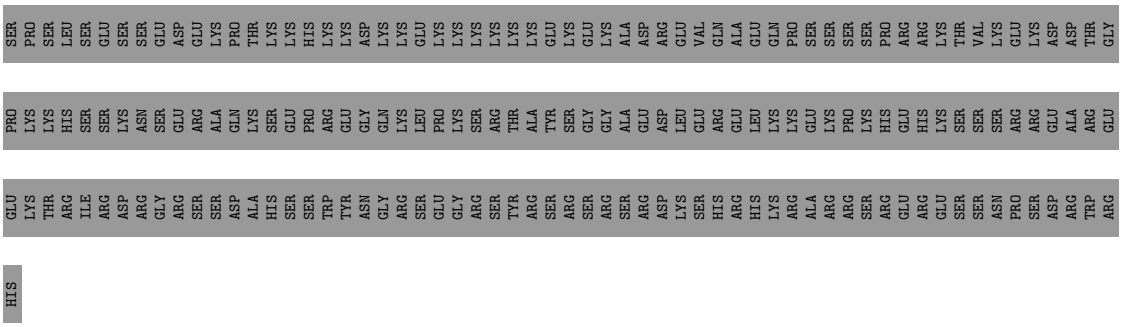


• Molecule 44: Smad nuclear-interacting protein 1



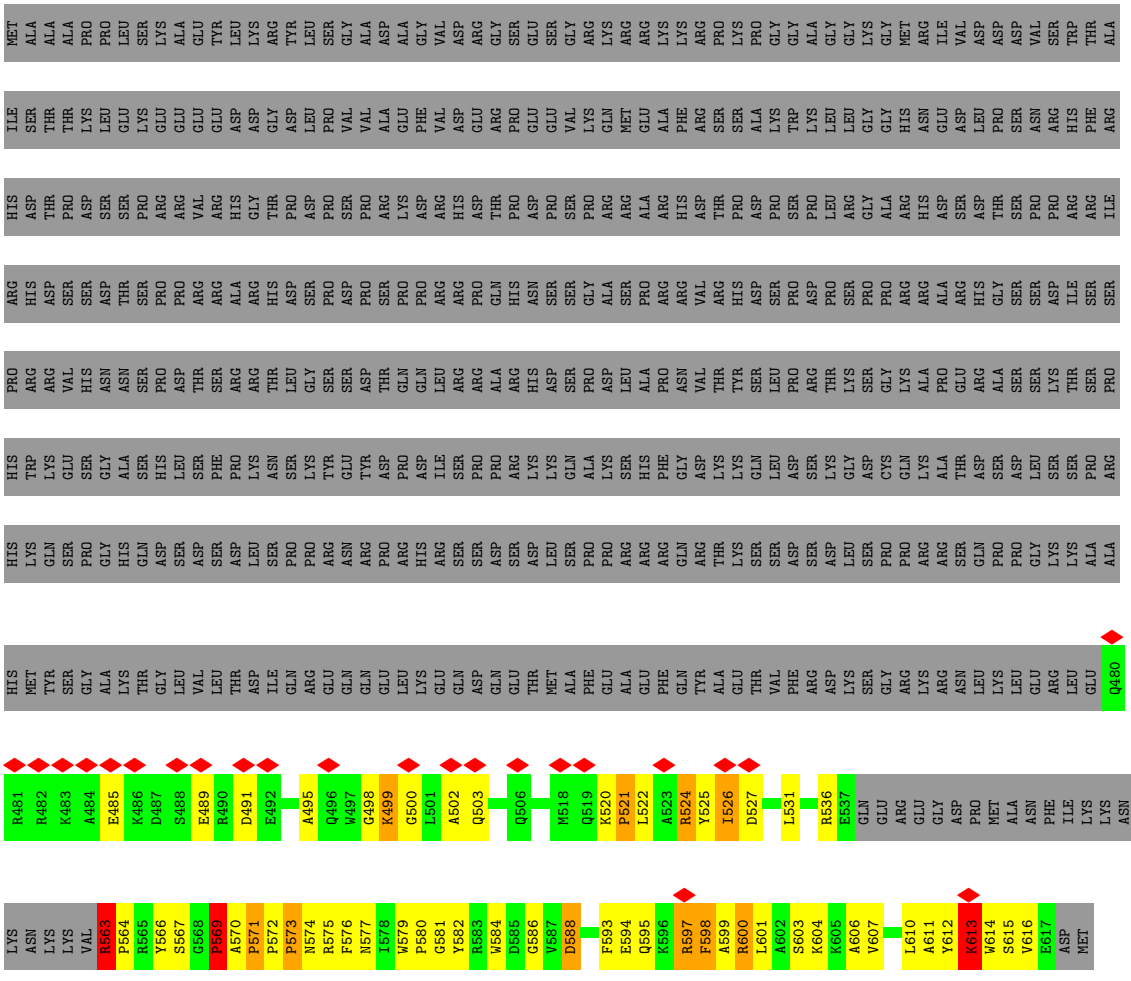
• Molecule 45: RNA-binding motif protein, X-linked 2





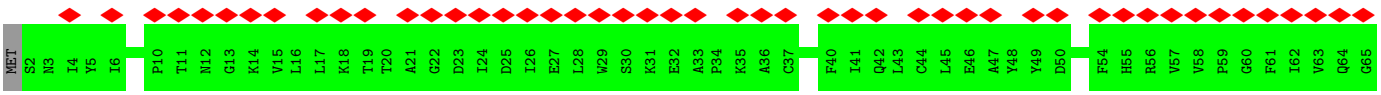
• Molecule 46: BUD13 homolog

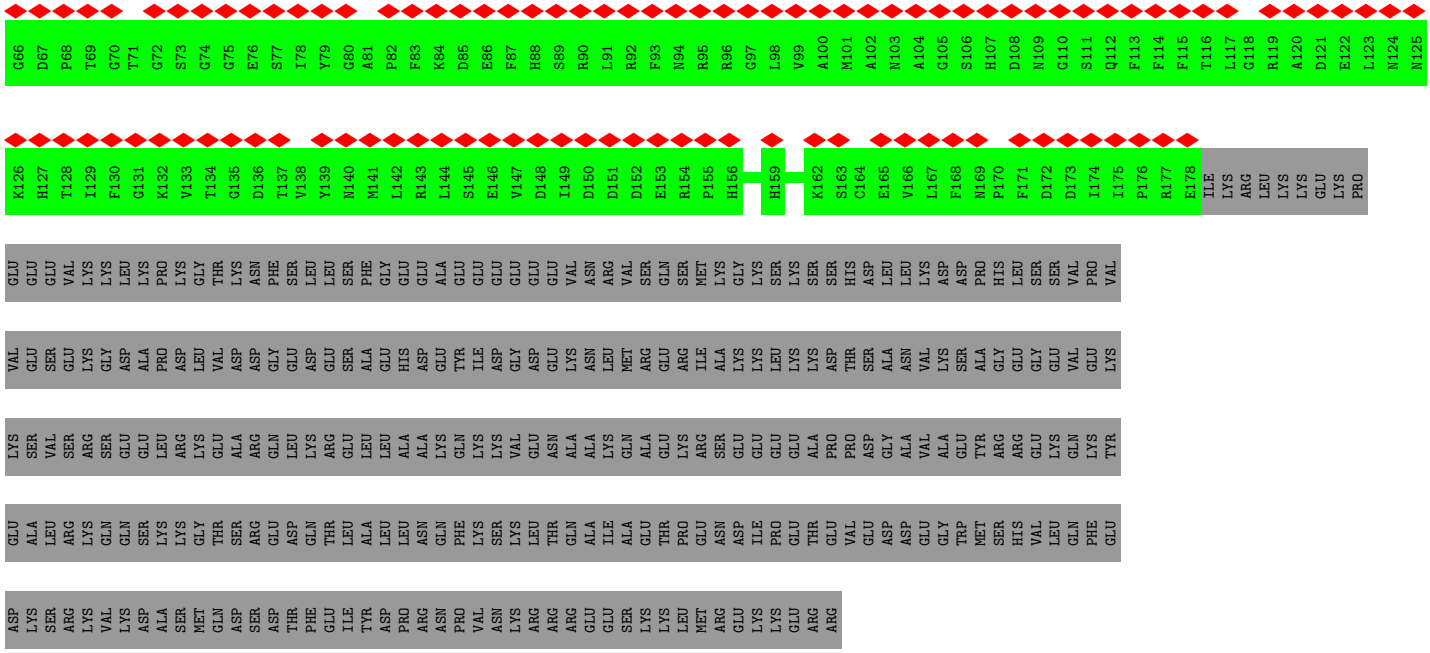
Chain Z:



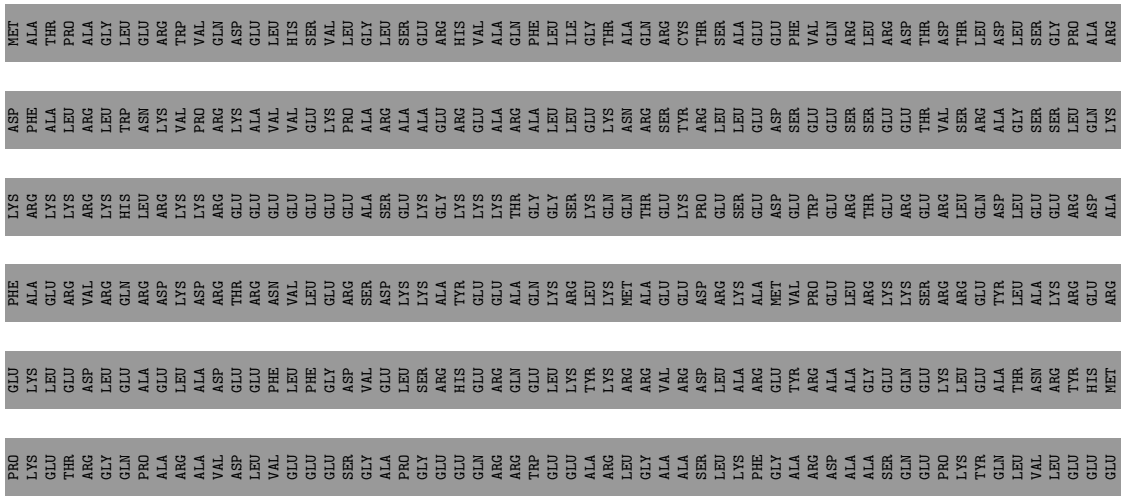
• Molecule 47: Peptidyl-prolyl cis-trans isomerase CWC27 homolog

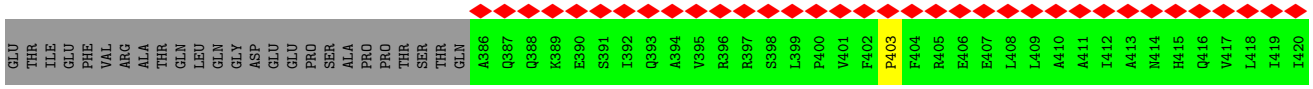
Chain z:

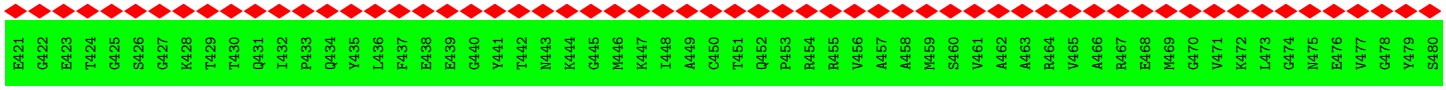


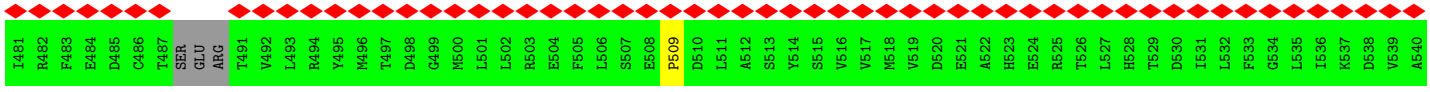


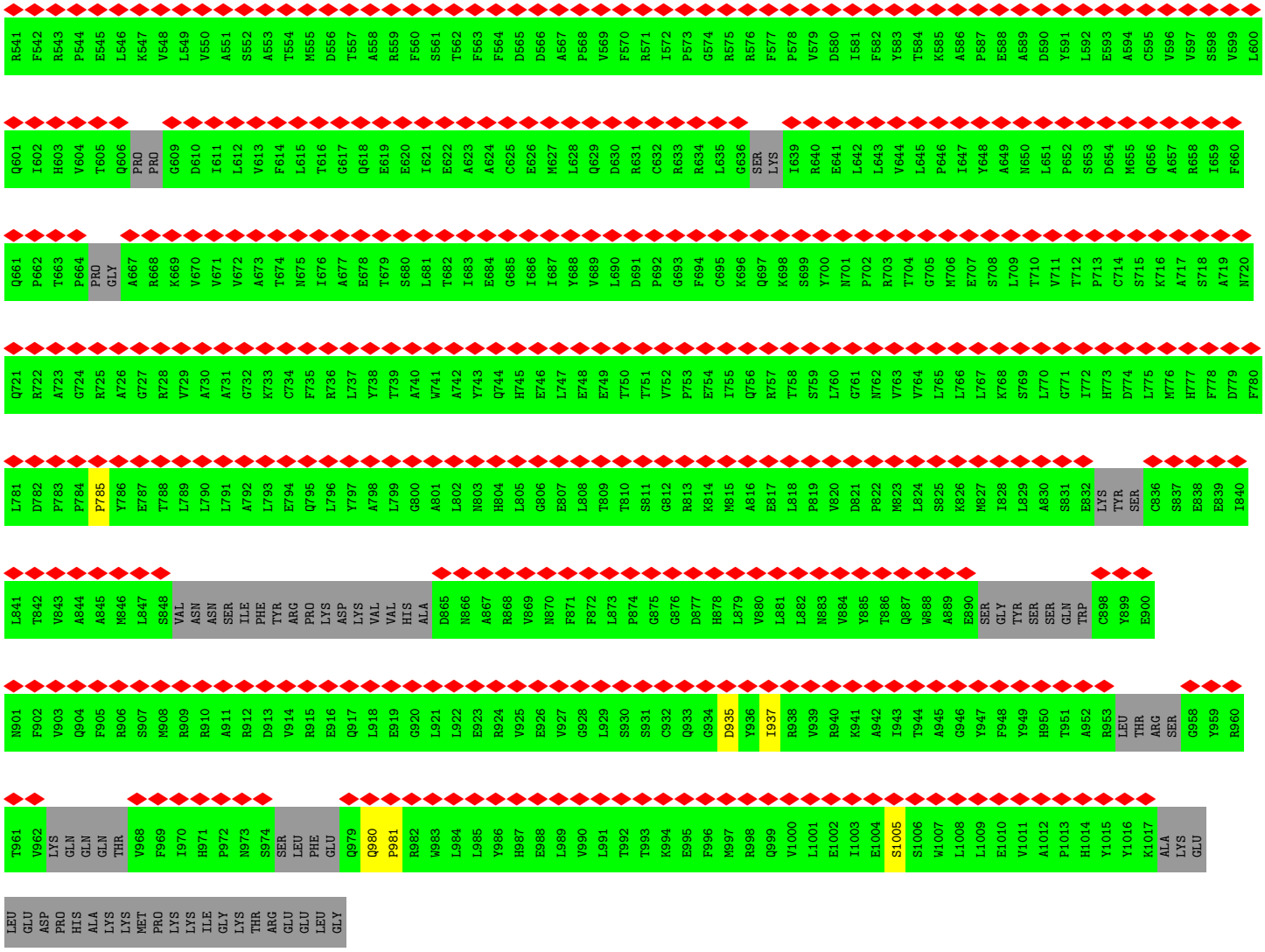
• Molecule 48: Putative pre-mRNA-splicing factor ATP-dependent RNA helicase DHX16





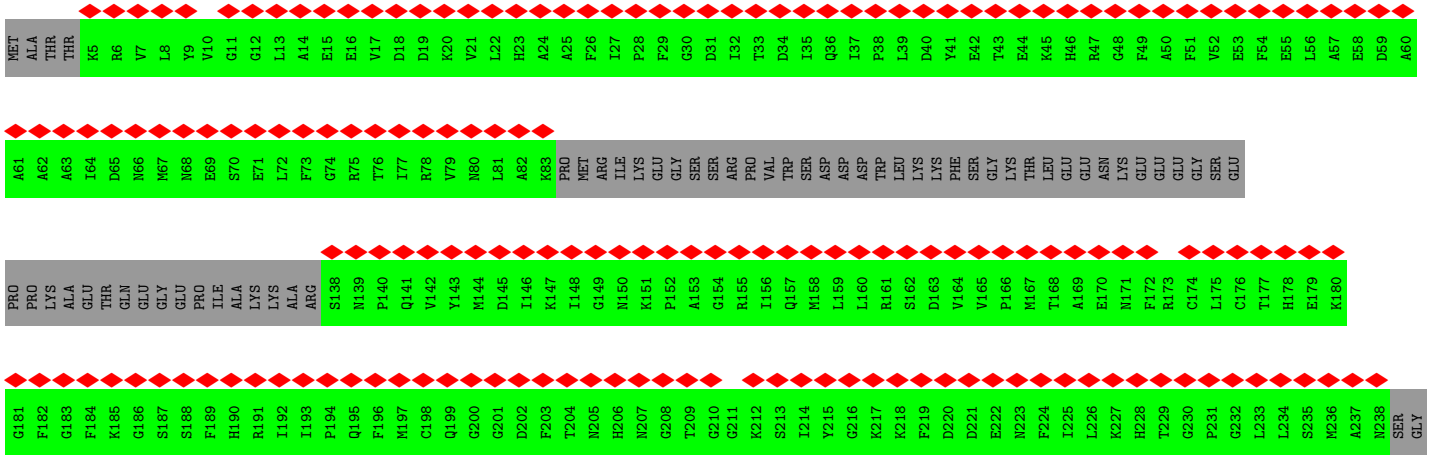


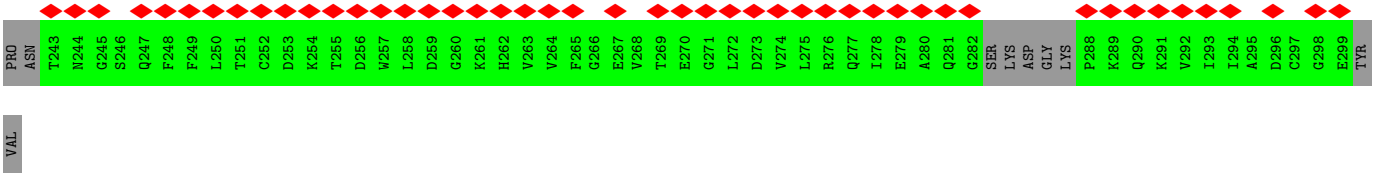




• Molecule 49: Peptidyl-prolyl cis-trans isomerase E

Chain y:




PRO
ASN
T243
N244
G245
S246
Q247
F248
F249
L250
T251
C252
D253
K254
T255
D256
W257
L258
D259
G260
K261
H262
V263
V264
F265
G266
E267
V268
T269
E270
G271
L272
D273
V274
L275
R276
Q277
I278
E279
A280
Q281
G282
SER
LYS
ASP
GLY
LYS
P288
K289
Q290
K291
V292
I293
I294
A295
D296
C297
G298
E299
TYR
VAL

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	27405	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 ($e^-/Å^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.168	Depositor
Minimum map value	-0.080	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0374	Depositor
Map size (Å)	535.2, 535.2, 535.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.338, 1.338, 1.338	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.68	9/18964 (0.0%)	0.77	25/25741 (0.1%)
2	B	0.75	2/1970 (0.1%)	0.91	7/3060 (0.2%)
3	C	0.79	1/6864 (0.0%)	0.96	10/9334 (0.1%)
4	D	0.33	0/8527	0.59	0/11887
5	E	0.64	0/2392	0.79	0/3242
6	a	0.47	0/397	0.61	0/549
6	h	0.46	0/391	0.61	0/540
7	b	0.49	0/404	0.72	0/561
7	i	0.50	0/421	0.73	0/583
8	c	0.57	0/405	0.73	0/563
8	j	0.57	0/405	0.73	0/563
9	d	0.68	0/479	0.84	0/666
9	k	0.70	0/420	0.85	0/583
10	f	0.75	0/360	0.81	0/497
10	m	0.75	0/360	0.81	0/497
11	e	0.65	0/390	0.80	0/542
11	l	0.64	0/390	0.80	0/542
12	g	0.54	0/362	0.71	0/501
12	n	0.54	0/332	0.72	0/458
13	F	0.39	0/2224	0.86	0/3462
14	G	0.35	0/1717	0.95	1/2664 (0.0%)
15	H	0.59	7/3217 (0.2%)	1.06	18/4997 (0.4%)
16	o	0.61	0/803	1.41	2/1119 (0.2%)
17	p	1.01	1/810 (0.1%)	1.46	4/1122 (0.4%)
18	w	0.53	5/2376 (0.2%)	0.67	13/3269 (0.4%)
19	u	0.23	0/524	0.62	4/724 (0.6%)
20	v	0.73	4/945 (0.4%)	0.83	10/1280 (0.8%)
21	1	0.33	0/7826	0.51	0/10617
22	2	0.52	3/1277 (0.2%)	0.73	7/1724 (0.4%)
23	3	0.32	0/9408	0.53	0/12767
24	4	0.83	2/535 (0.4%)	0.98	4/724 (0.6%)
25	5	0.29	0/823	0.48	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
26	6	0.29	0/653	0.48	0/877
27	7	0.31	0/556	0.45	0/751
28	J	0.62	0/3500	0.73	0/4750
29	L	0.52	3/2283 (0.1%)	0.58	8/3088 (0.3%)
30	q	0.35	0/658	0.58	3/919 (0.3%)
30	r	0.32	0/653	0.59	3/912 (0.3%)
30	s	0.26	0/334	0.37	0/466
30	t	0.30	0/334	0.38	0/466
31	K	1.28	14/981 (1.4%)	0.69	5/1317 (0.4%)
32	I	0.39	0/2745	0.56	17/3765 (0.5%)
33	Q	0.21	0/6518	0.42	0/9075
34	M	0.29	0/272	0.48	0/363
35	N	0.88	1/1210 (0.1%)	1.00	3/1622 (0.2%)
36	O	0.80	3/2321 (0.1%)	0.94	6/3135 (0.2%)
37	P	0.83	1/841 (0.1%)	1.01	2/1117 (0.2%)
38	R	0.66	4/2353 (0.2%)	0.87	8/3167 (0.3%)
39	S	0.59	0/1268	0.80	1/1714 (0.1%)
40	T	1.05	1/2522 (0.0%)	1.11	4/3438 (0.1%)
41	U	1.03	0/196	1.09	1/265 (0.4%)
42	V	0.54	0/2239	0.67	1/3118 (0.0%)
43	W	0.55	0/2371	0.77	4/3296 (0.1%)
44	X	0.27	0/1020	0.48	0/1360
45	Y	0.31	0/753	0.48	0/1014
46	Z	0.57	2/772 (0.3%)	0.79	7/1056 (0.7%)
47	z	0.29	0/1414	0.51	0/1916
48	x	0.35	0/2876	0.53	3/3988 (0.1%)
49	y	0.35	0/1129	0.61	0/1558
All	All	0.57	63/119490 (0.1%)	0.74	181/165014 (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	6
3	C	0	3
4	D	0	1
9	d	0	1
9	k	0	1
21	1	0	9
22	2	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
23	3	0	4
27	7	0	1
34	M	0	1
35	N	0	1
38	R	0	1
40	T	0	2
44	X	0	1
All	All	0	33

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	K	106	CYS	CB-SG	-23.13	1.43	1.82
31	K	132	CYS	CB-SG	-17.48	1.52	1.82
29	L	761	SER	CB-OG	8.91	1.53	1.42
31	K	128	SER	CB-OG	8.42	1.53	1.42
31	K	183	SER	CB-OG	8.28	1.53	1.42
18	w	457	SER	CB-OG	8.21	1.52	1.42
36	O	181	TYR	CE1-CZ	-8.11	1.28	1.38
29	L	726	SER	CB-OG	8.08	1.52	1.42
31	K	190	SER	CB-OG	8.01	1.52	1.42
31	K	187	SER	CB-OG	7.96	1.52	1.42
18	w	483	SER	CB-OG	7.46	1.51	1.42
15	H	142	C	C1'-N1	7.35	1.59	1.48
22	2	655	SER	CB-OG	7.35	1.51	1.42
35	N	102	CYS	CB-SG	-7.30	1.69	1.82
1	A	406	TRP	CB-CG	-7.06	1.37	1.50
20	v	19	SER	CB-OG	6.99	1.51	1.42
2	B	103	G	C1'-N9	-6.95	1.37	1.46
15	H	150	U	C1'-N1	6.76	1.58	1.48
1	A	2223	CYS	CB-SG	-6.76	1.70	1.82
37	P	227	TYR	CG-CD2	-6.70	1.30	1.39
1	A	476	PHE	CG-CD2	6.66	1.48	1.38
20	v	53	SER	CB-OG	6.65	1.50	1.42
29	L	724	TYR	CB-CG	-6.58	1.41	1.51
15	H	97	G	C1'-N9	-6.48	1.37	1.46
20	v	22	SER	CB-OG	6.46	1.50	1.42
15	H	151	C	C1'-N1	6.44	1.58	1.48
15	H	184	C	C1'-N1	6.37	1.58	1.48
31	K	43	TYR	CB-CG	-6.33	1.42	1.51
31	K	138	TYR	CB-CG	-6.33	1.42	1.51
15	H	141	C	C1'-N1	6.31	1.58	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	K	93	SER	CB-OG	6.29	1.50	1.42
24	4	50	THR	CB-OG1	5.94	1.55	1.43
18	w	395	TRP	CZ3-CH2	5.86	1.49	1.40
24	4	42	THR	CB-OG1	5.85	1.54	1.43
40	T	218	TRP	CB-CG	-5.71	1.40	1.50
20	v	80	THR	CB-OG1	5.66	1.54	1.43
31	K	40	THR	CB-OG1	5.61	1.54	1.43
2	B	56	C	O3'-P	-5.45	1.54	1.61
1	A	212	PRO	N-CA	-5.43	1.38	1.47
46	Z	569	PRO	N-CD	5.43	1.55	1.47
22	2	620	PRO	N-CD	5.41	1.55	1.47
18	w	284	ARG	CA-CB	-5.37	1.42	1.53
1	A	94	TYR	CB-CG	-5.33	1.43	1.51
36	O	225	PRO	N-CD	5.33	1.55	1.47
31	K	30	GLU	CB-CG	-5.25	1.42	1.52
22	2	643	PRO	N-CD	5.24	1.55	1.47
36	O	226	PRO	N-CD	5.22	1.55	1.47
17	p	156	ASN	C-N	-5.21	1.22	1.34
18	w	415	THR	CB-OG1	5.21	1.53	1.43
38	R	130	PRO	N-CD	5.18	1.55	1.47
31	K	137	VAL	CB-CG1	-5.18	1.42	1.52
31	K	119	VAL	CB-CG2	-5.15	1.42	1.52
46	Z	521	PRO	N-CD	5.15	1.55	1.47
15	H	110	A	C1'-N9	-5.13	1.39	1.46
1	A	140	TYR	CG-CD2	-5.13	1.32	1.39
1	A	351	TYR	CB-CG	-5.11	1.44	1.51
1	A	225	TYR	CB-CG	-5.09	1.44	1.51
31	K	186	VAL	CA-CB	-5.08	1.44	1.54
38	R	253	PRO	N-CD	5.05	1.54	1.47
3	C	145	PHE	CB-CG	-5.04	1.42	1.51
38	R	252	PRO	N-CD	5.04	1.54	1.47
1	A	406	TRP	CG-CD2	-5.03	1.35	1.43
38	R	227	PRO	N-CD	5.03	1.54	1.47

All (181) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	4	83	PRO	CA-CB-CG	10.19	124.17	104.80
22	2	636	MET	CG-SD-CE	9.28	115.05	100.20
38	R	226	PRO	CA-N-CD	-8.88	99.07	111.50
31	K	90	PRO	CA-CB-CG	8.66	121.26	104.80
46	Z	569	PRO	CA-N-CD	-8.56	99.52	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	Z	573	PRO	CA-N-CD	-8.45	99.67	111.50
36	O	225	PRO	CA-N-CD	-8.17	100.07	111.50
1	A	404	LEU	CB-CG-CD1	8.13	124.83	111.00
36	O	226	PRO	CA-N-CD	-8.07	100.21	111.50
36	O	35	ARG	NE-CZ-NH2	-7.69	116.45	120.30
1	A	552	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	A	153	ARG	NE-CZ-NH2	-7.36	116.62	120.30
2	B	20	G	N9-C1'-C2'	7.29	123.48	114.00
43	W	278	LYS	CB-CA-C	-7.29	95.82	110.40
15	H	113	G	OP2-P-O3'	7.25	121.15	105.20
15	H	141	C	OP2-P-O3'	7.24	121.14	105.20
15	H	114	A	OP2-P-O3'	7.22	121.09	105.20
3	C	144	CYS	N-CA-CB	7.20	123.56	110.60
15	H	150	U	OP2-P-O3'	7.19	121.01	105.20
38	R	180	THR	C-N-CD	-7.16	104.85	120.60
18	w	441	PRO	N-CA-CB	7.16	111.89	103.30
19	u	222	PRO	N-CA-CB	7.14	111.87	103.30
1	A	611	LEU	CB-CG-CD1	-7.10	98.92	111.00
20	v	161	PRO	N-CA-CB	7.07	111.78	103.30
22	2	656	PRO	N-CA-CB	6.88	111.56	103.30
1	A	565	ARG	NE-CZ-NH2	-6.88	116.86	120.30
15	H	155	C	P-O3'-C3'	6.78	127.84	119.70
15	H	141	C	O3'-P-O5'	-6.77	91.14	104.00
15	H	150	U	O3'-P-O5'	-6.77	91.14	104.00
2	B	104	C	C2'-C3'-O3'	-6.77	94.61	109.50
2	B	26	A	O5'-P-OP2	6.74	118.78	110.70
15	H	113	G	O3'-P-O5'	-6.73	91.21	104.00
15	H	114	A	O3'-P-O5'	-6.72	91.23	104.00
15	H	30	A	O5'-P-OP1	-6.71	99.66	105.70
20	v	115	PRO	N-CA-CB	6.65	111.28	103.30
3	C	420	CYS	CA-CB-SG	-6.63	102.07	114.00
2	B	12	U	N1-C1'-C2'	-6.62	104.72	112.00
37	P	215	LEU	CB-CG-CD1	-6.61	99.76	111.00
30	q	46	PRO	N-CA-CB	6.59	111.21	103.30
31	K	90	PRO	N-CA-CB	6.57	111.19	103.30
43	W	279	LYS	N-CA-C	-6.57	93.26	111.00
20	v	139	PRO	N-CA-CB	6.54	111.15	103.30
24	4	27	PRO	N-CA-CB	6.50	111.10	103.30
1	A	598	LEU	CB-CG-CD2	-6.50	99.96	111.00
30	q	60	PRO	N-CA-CB	6.48	111.08	103.30
30	r	46	PRO	N-CA-CB	6.48	111.08	103.30
37	P	215	LEU	CB-CG-CD2	6.47	122.00	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	W	251	GLY	N-CA-C	-6.47	96.93	113.10
18	w	120	PRO	N-CA-CB	6.47	111.06	103.30
18	w	227	PRO	N-CA-CB	6.47	111.06	103.30
31	K	78	PRO	N-CA-CB	6.42	111.00	103.30
35	N	101	CYS	CB-CA-C	-6.41	97.58	110.40
3	C	921	LEU	CB-CG-CD1	6.41	121.89	111.00
48	x	403	PRO	N-CA-CB	6.35	110.92	103.30
19	u	200	PRO	N-CA-CB	6.31	110.87	103.30
32	I	475	PRO	N-CA-CB	6.31	110.87	103.30
39	S	152	ARG	NE-CZ-NH2	-6.31	117.15	120.30
38	R	205	ASP	CB-CG-OD2	6.30	123.97	118.30
1	A	476	PHE	CB-CG-CD1	6.30	125.21	120.80
36	O	181	TYR	CG-CD2-CE2	-6.28	116.28	121.30
20	v	218	PRO	N-CA-CB	6.28	110.83	103.30
46	Z	570	ALA	C-N-CD	6.25	141.52	128.40
18	w	105	PRO	N-CA-CB	6.24	110.79	103.30
32	I	551	PRO	N-CA-CB	6.24	110.78	103.30
31	K	107	VAL	CA-CB-CG1	6.23	120.25	110.90
18	w	305	PRO	N-CA-CB	6.23	110.77	103.30
32	I	589	PRO	N-CA-CB	6.23	110.77	103.30
1	A	153	ARG	NE-CZ-NH1	6.22	123.41	120.30
22	2	641	PRO	N-CA-CB	6.21	110.76	103.30
18	w	174	PRO	N-CA-CB	6.21	110.75	103.30
1	A	506	LEU	CB-CG-CD1	-6.20	100.45	111.00
32	I	162	PRO	N-CA-CB	6.20	110.73	103.30
40	T	220	VAL	CB-CA-C	-6.18	99.65	111.40
40	T	282	ARG	NE-CZ-NH2	-6.18	117.21	120.30
19	u	221	PRO	N-CA-CB	6.17	110.70	103.30
32	I	232	PRO	N-CA-CB	6.16	110.69	103.30
48	x	509	PRO	N-CA-CB	6.14	110.66	103.30
29	L	558	PRO	N-CA-CB	6.12	110.64	103.30
17	p	184	PRO	N-CA-CB	6.10	110.62	103.30
32	I	177	PRO	N-CA-CB	6.10	110.61	103.30
29	L	546	PRO	N-CA-CB	6.09	110.60	103.30
18	w	202	PRO	N-CA-CB	6.04	110.55	103.30
20	v	221	PRO	N-CA-CB	6.04	110.55	103.30
32	I	788	PRO	N-CA-CB	6.03	110.54	103.30
32	I	816	PRO	N-CA-CB	6.01	110.51	103.30
17	p	155	LEU	N-CA-CB	5.99	122.37	110.40
14	G	156	U	C2-N1-C1'	5.97	124.87	117.70
20	v	162	PRO	N-CA-CB	5.96	110.45	103.30
18	w	99	PRO	N-CA-CB	5.96	110.45	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	I	160	PRO	N-CA-CB	5.95	110.44	103.30
32	I	394	PRO	N-CA-CB	5.95	110.44	103.30
38	R	252	PRO	C-N-CD	5.93	140.85	128.40
29	L	563	PRO	N-CA-CB	5.89	110.37	103.30
32	I	387	PRO	N-CA-CB	5.87	110.35	103.30
18	w	230	PRO	N-CA-CB	5.86	110.33	103.30
38	R	226	PRO	C-N-CD	5.86	140.71	128.40
17	p	219	LYS	O-C-N	5.86	132.07	122.70
20	v	220	PRO	N-CA-CB	5.86	110.33	103.30
18	w	419	PRO	N-CA-CB	5.85	110.32	103.30
20	v	217	PRO	N-CA-CB	5.84	110.31	103.30
15	H	172	C	P-O3'-C3'	5.84	126.71	119.70
32	I	342	PRO	N-CA-CB	5.84	110.30	103.30
29	L	564	PRO	N-CA-CB	5.83	110.30	103.30
30	q	19	PRO	N-CA-CB	5.83	110.29	103.30
3	C	148	CYS	CB-CA-C	5.82	122.04	110.40
3	C	446	LYS	C-N-CD	5.81	140.61	128.40
29	L	594	PRO	N-CA-CB	5.81	110.28	103.30
32	I	518	PRO	N-CA-CB	5.81	110.28	103.30
30	r	19	PRO	N-CA-CB	5.79	110.25	103.30
15	H	156	U	P-O3'-C3'	-5.77	112.78	119.70
29	L	548	PRO	N-CA-CB	5.77	110.22	103.30
29	L	620	PRO	N-CA-CB	5.77	110.23	103.30
22	2	629	PRO	N-CA-CB	5.77	110.22	103.30
46	Z	563	ARG	C-N-CD	5.76	140.49	128.40
32	I	588	PRO	N-CA-CB	5.75	110.20	103.30
36	O	48	CYS	CA-CB-SG	5.70	124.27	114.00
1	A	565	ARG	NE-CZ-NH1	5.69	123.15	120.30
22	2	642	PRO	C-N-CD	5.65	140.27	128.40
24	4	27	PRO	CA-CB-CG	5.64	115.51	104.80
1	A	1364	LEU	CA-CB-CG	5.63	128.25	115.30
1	A	332	TYR	N-CA-C	-5.61	95.85	111.00
46	Z	520	LYS	C-N-CD	5.61	140.18	128.40
32	I	463	PRO	N-CA-CB	5.58	110.00	103.30
31	K	93	SER	N-CA-CB	-5.58	102.14	110.50
32	I	761	PRO	N-CA-CB	5.58	109.99	103.30
15	H	46	U	P-O3'-C3'	5.57	126.39	119.70
48	x	785	PRO	N-CA-CB	5.56	109.97	103.30
29	L	774	VAL	CA-CB-CG2	5.54	119.20	110.90
16	o	58	ASP	N-CA-CB	-5.52	100.66	110.60
35	N	104	ARG	NE-CZ-NH2	-5.49	117.55	120.30
20	v	73	THR	CA-CB-OG1	5.48	120.50	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	118	VAL	CB-CA-C	-5.47	101.01	111.40
15	H	157	G	O4'-C1'-N9	-5.47	103.83	108.20
3	C	146	VAL	CA-CB-CG2	-5.46	102.70	110.90
30	r	60	PRO	N-CA-CB	5.46	109.85	103.30
32	I	625	PRO	N-CA-CB	5.45	109.84	103.30
1	A	656	LEU	CB-CG-CD1	-5.45	101.74	111.00
18	w	399	LEU	CB-CG-CD1	-5.42	101.78	111.00
3	C	91	GLU	C-N-CD	-5.42	108.68	120.60
1	A	2310	ARG	CG-CD-NE	5.41	123.16	111.80
41	U	19	VAL	CB-CA-C	-5.41	101.13	111.40
35	N	102	CYS	CB-CA-C	-5.40	99.59	110.40
1	A	420	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	251	ASP	CB-CG-OD1	5.39	123.15	118.30
22	2	651	PRO	N-CA-CB	5.39	109.77	103.30
40	T	308	ARG	NE-CZ-NH2	-5.36	117.62	120.30
22	2	619	MET	C-N-CD	5.36	139.66	128.40
15	H	106	G	O5'-P-OP1	5.34	117.10	110.70
15	H	156	U	OP2-P-O3'	5.33	116.93	105.20
1	A	92	LEU	CB-CG-CD1	-5.31	101.97	111.00
2	B	40	U	N1-C1'-C2'	5.31	120.90	114.00
38	R	178	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	314	ILE	CA-CB-CG1	-5.28	100.96	111.00
1	A	656	LEU	CA-CB-CG	-5.28	103.16	115.30
2	B	37	G	O5'-P-OP2	-5.26	100.97	105.70
24	4	50	THR	CA-CB-OG1	5.25	120.02	109.00
3	C	921	LEU	CB-CG-CD2	-5.24	102.09	111.00
17	p	149	PRO	N-CA-CB	5.23	109.58	103.30
1	A	656	LEU	CB-CG-CD2	5.21	119.86	111.00
46	Z	588	ASP	CB-CG-OD2	5.20	122.98	118.30
3	C	776	GLU	N-CA-C	5.19	125.02	111.00
38	R	178	ARG	NE-CZ-NH1	5.19	122.90	120.30
46	Z	527	ASP	CB-CG-OD2	5.19	122.97	118.30
19	u	203	SER	N-CA-CB	-5.18	102.73	110.50
36	O	24	CYS	CA-CB-SG	5.17	123.31	114.00
1	A	330	THR	CA-CB-CG2	-5.17	105.16	112.40
1	A	647	LEU	CB-CG-CD1	-5.14	102.26	111.00
15	H	157	G	P-O5'-C5'	-5.13	112.69	120.90
42	V	467	LEU	CB-CA-C	-5.13	100.45	110.20
1	A	638	LEU	CA-CB-CG	-5.11	103.54	115.30
43	W	279	LYS	N-CA-CB	5.10	119.77	110.60
18	w	399	LEU	CD1-CG-CD2	5.09	125.76	110.50
2	B	20	G	O4'-C1'-N9	5.09	112.27	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	H	156	U	C4'-C3'-C2'	5.08	107.68	102.60
1	A	677	VAL	CB-CA-C	-5.07	101.78	111.40
40	T	233	LEU	CB-CG-CD1	-5.06	102.40	111.00
18	w	45	ALA	N-CA-CB	-5.04	103.04	110.10
38	R	101	ILE	CB-CA-C	-5.04	101.53	111.60
16	o	99	SER	N-CA-CB	-5.03	102.96	110.50
20	v	33	LEU	CB-CG-CD1	-5.02	102.47	111.00
3	C	220	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	1	1028	HIS	Peptide
21	1	1105	GLU	Peptide
21	1	1107	GLN	Peptide
21	1	220	GLN	Peptide
21	1	415	LEU	Peptide
21	1	418	PRO	Peptide
21	1	460	PRO	Peptide
21	1	717	THR	Peptide
21	1	943	LYS	Peptide
22	2	558	ARG	Peptide
23	3	261	PHE	Peptide
23	3	530	ASP	Peptide
23	3	552	ARG	Peptide
23	3	916	ASN	Peptide
27	7	74	GLN	Peptide
1	A	166	PHE	Peptide
1	A	346	ASP	Peptide
1	A	408	PRO	Peptide
1	A	433	GLU	Peptide
1	A	697	MET	Peptide
1	A	941	LYS	Peptide
3	C	622	GLU	Peptide
3	C	736	GLY	Peptide
3	C	823	ALA	Peptide
4	D	430	LEU	Peptide
34	M	196	ASP	Peptide
35	N	36	PRO	Peptide
38	R	94	GLY	Peptide
40	T	400	PHE	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
44	X	193	ASN	Peptide
9	d	112	ASN	Peptide
9	k	112	ASN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	18450	0	18276	1482	0
2	B	1768	0	897	120	0
3	C	6716	0	6691	892	0
4	D	8528	0	3745	69	0
5	E	2338	0	2272	153	0
6	a	399	0	173	0	0
6	h	393	0	170	0	0
7	b	405	0	170	0	0
7	i	422	0	177	0	0
8	c	406	0	170	0	0
8	j	406	0	170	0	0
9	d	480	0	200	0	0
9	k	422	0	175	0	0
10	f	361	0	158	0	0
10	m	361	0	158	0	0
11	e	391	0	163	0	0
11	l	391	0	163	0	0
12	g	363	0	160	0	0
12	n	334	0	143	0	0
13	F	1988	0	1005	186	0
14	G	1545	0	786	190	0
15	H	2886	0	1463	239	0
16	o	804	0	350	0	0
17	p	813	0	365	0	0
18	w	2369	0	1298	0	0
19	u	530	0	218	0	0
20	v	946	0	594	0	0
21	1	7702	0	7389	291	0
22	2	1252	0	1040	57	0
23	3	9220	0	9139	481	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	4	527	0	438	40	0
25	5	807	0	729	26	0
26	6	645	0	628	21	0
27	7	540	0	509	25	0
28	J	3463	0	2544	102	0
29	L	2260	0	1776	92	0
30	q	659	0	296	0	0
30	r	654	0	294	0	0
30	s	335	0	168	0	0
30	t	335	0	168	0	0
31	K	979	0	739	11	0
32	I	2778	0	1238	21	0
33	Q	6528	0	2814	6	0
34	M	267	0	225	29	0
35	N	1184	0	1190	75	0
36	O	2273	0	2244	225	0
37	P	829	0	814	192	0
38	R	2316	0	2189	420	0
39	S	1236	0	1210	135	0
40	T	2457	0	2416	251	0
41	U	193	0	196	40	0
42	V	2243	0	971	48	0
43	W	2374	0	1051	108	0
44	X	1021	0	738	19	0
45	Y	743	0	613	67	0
46	Z	755	0	591	154	0
47	z	1381	0	1298	0	0
48	x	2887	0	1310	0	0
49	y	1133	0	519	0	0
50	A	36	0	6	10	0
51	C	32	0	12	11	0
52	C	1	0	0	0	0
52	F	5	0	0	0	0
53	6	3	0	0	0	0
53	M	1	0	0	0	0
53	N	3	0	0	0	0
53	O	3	0	0	3	0
53	W	2	0	0	0	0
53	v	1	0	0	0	0
All	All	117278	0	87812	4995	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 26.

All (4995) 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)
45:Y:37:TRP:CH2	46:Z:498:GLY:HA2	1.23	1.65
1:A:2270:PHE:HB3	4:D:1264:PRO:CB	1.34	1.57
1:A:2270:PHE:CG	4:D:1264:PRO:CB	1.89	1.56
3:C:149:LEU:HD13	3:C:427:PHE:CD2	1.38	1.54
3:C:77:VAL:HG11	40:T:196:LEU:CG	1.39	1.52
45:Y:37:TRP:CH2	46:Z:498:GLY:CA	1.93	1.51
1:A:2270:PHE:CB	4:D:1264:PRO:CB	1.86	1.50
46:Z:564:PRO:HB2	46:Z:582:TYR:CG	1.45	1.49
37:P:193:VAL:HG23	37:P:194:PHE:CD2	1.46	1.47
38:R:442:ARG:HH11	38:R:443:GLY:C	1.17	1.45
1:A:844:GLU:CB	38:R:422:MET:CE	1.94	1.45
37:P:193:VAL:CG2	37:P:194:PHE:HD2	1.28	1.45
23:3:440:HIS:CE1	23:3:733:PRO:HD3	1.50	1.43
36:O:149:LYS:HD2	36:O:290:LYS:CE	1.49	1.43
38:R:414:ARG:NH1	46:Z:598:PHE:CZ	1.86	1.43
39:S:57:ILE:HD13	43:W:97:ASN:CB	1.44	1.42
14:G:21:A:H2	36:O:212:LYS:CB	1.30	1.42
1:A:2270:PHE:CD1	4:D:1264:PRO:CB	2.03	1.41
3:C:705:VAL:HG23	3:C:717:PHE:CD2	1.55	1.41
1:A:384:VAL:HG12	3:C:331:PHE:CE2	1.56	1.40
3:C:79:THR:CG2	40:T:199:VAL:HB	1.51	1.40
1:A:73:HIS:HD2	1:A:81:PHE:CE2	1.37	1.40
28:J:293:ASN:CB	29:L:225:TYR:CB	1.98	1.39
3:C:79:THR:HG23	40:T:199:VAL:CB	1.49	1.39
5:E:260:ARG:NH1	5:E:273:CYS:SG	1.95	1.39
1:A:299:ILE:CG1	1:A:1342:TRP:HZ3	1.34	1.39
28:J:339:TRP:HA	38:R:116:TYR:CE2	1.58	1.38
3:C:387:ASP:O	3:C:388:VAL:HG12	1.20	1.37
38:R:442:ARG:CD	38:R:443:GLY:H	1.37	1.37
1:A:380:LEU:CB	3:C:354:ARG:HG3	1.54	1.36
3:C:77:VAL:HG12	40:T:196:LEU:C	1.46	1.36
38:R:92:SER:CA	39:S:19:SER:HB2	1.55	1.36
1:A:762:ARG:HH22	37:P:226:LYS:NZ	1.19	1.35
29:L:216:PHE:CD1	36:O:113:ASN:CA	2.08	1.35
28:J:339:TRP:HA	38:R:116:TYR:CD2	1.60	1.35
38:R:414:ARG:NH1	46:Z:598:PHE:CE2	1.93	1.35
3:C:77:VAL:CG1	40:T:196:LEU:C	1.94	1.35
3:C:149:LEU:CD1	3:C:427:PHE:CD2	2.08	1.34
38:R:442:ARG:HD3	38:R:443:GLY:N	1.05	1.34
38:R:414:ARG:NE	46:Z:598:PHE:CZ	1.95	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:452:THR:CG2	3:C:577:PHE:HD2	1.40	1.34
39:S:39:PHE:CB	39:S:129:PHE:CZ	2.10	1.34
1:A:1962:THR:CG2	46:Z:524:ARG:HB2	1.57	1.33
1:A:121:HIS:NE2	1:A:481:PHE:HB3	1.42	1.33
3:C:145:PHE:CA	3:C:312:SER:HB2	1.57	1.31
39:S:57:ILE:CD1	43:W:97:ASN:CB	2.08	1.31
38:R:414:ARG:CZ	46:Z:598:PHE:CZ	2.14	1.31
3:C:670:SER:HA	3:C:823:ALA:CB	1.60	1.31
1:A:73:HIS:CD2	1:A:81:PHE:CZ	2.20	1.30
1:A:299:ILE:HG13	1:A:1342:TRP:CZ3	1.67	1.30
37:P:212:ASN:O	40:T:458:SER:HA	1.30	1.30
1:A:264:PHE:CZ	1:A:459:LEU:HD13	1.66	1.30
1:A:844:GLU:CB	38:R:422:MET:HE3	1.54	1.30
1:A:1342:TRP:CD2	3:C:921:LEU:HD13	1.65	1.30
32:I:280:GLU:CB	32:I:288:THR:CB	2.08	1.29
1:A:296:PHE:CG	3:C:656:ALA:HB2	1.66	1.29
37:P:211:VAL:HG13	40:T:457:GLY:CA	1.62	1.29
14:G:-9:C:C4	41:U:18:TYR:CE1	2.20	1.29
32:I:280:GLU:C	32:I:288:THR:CB	2.00	1.28
1:A:73:HIS:CD2	1:A:81:PHE:CE2	2.20	1.28
3:C:77:VAL:CG1	40:T:196:LEU:HG	1.63	1.28
3:C:705:VAL:CG2	3:C:717:PHE:CE2	2.15	1.28
1:A:1342:TRP:CE3	3:C:921:LEU:HD13	1.69	1.28
1:A:1364:LEU:CD1	42:V:461:LEU:CB	2.11	1.28
38:R:92:SER:HA	39:S:19:SER:CB	1.61	1.28
23:3:440:HIS:CE1	23:3:733:PRO:CD	2.14	1.27
1:A:2268:LEU:HD23	4:D:1261:PRO:O	1.21	1.27
1:A:2268:LEU:HD22	4:D:1261:PRO:CB	1.65	1.26
3:C:78:GLU:O	40:T:198:ARG:HA	1.35	1.26
3:C:145:PHE:HA	3:C:312:SER:CB	1.65	1.26
14:G:-9:C:C5	41:U:18:TYR:CE1	2.23	1.26
37:P:211:VAL:CG1	40:T:457:GLY:HA3	1.65	1.26
37:P:193:VAL:CG2	37:P:194:PHE:CD2	2.09	1.26
5:E:146:ARG:NH1	5:E:148:LYS:CE	1.98	1.25
38:R:414:ARG:CZ	46:Z:598:PHE:HZ	1.47	1.25
1:A:299:ILE:CG1	1:A:1342:TRP:CZ3	2.18	1.25
39:S:131:ARG:HD3	39:S:132:VAL:O	1.09	1.25
39:S:39:PHE:CG	39:S:129:PHE:HE2	1.53	1.25
1:A:2113:LYS:HE3	4:D:1229:ASP:O	1.33	1.25
1:A:299:ILE:CD1	3:C:921:LEU:HB2	1.67	1.24
1:A:380:LEU:HD22	3:C:354:ARG:O	1.24	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:THR:HG22	34:M:199:PRO:CD	1.66	1.24
24:4:14:THR:HA	24:4:59:VAL:O	1.32	1.24
38:R:442:ARG:HD2	38:R:444:GLY:N	1.50	1.24
39:S:39:PHE:HB2	39:S:129:PHE:CZ	1.66	1.24
3:C:679:PRO:HB2	3:C:807:GLN:OE1	1.25	1.24
3:C:84:GLU:O	40:T:238:LEU:HD23	1.34	1.24
14:G:21:A:C2	36:O:212:LYS:CB	2.21	1.23
1:A:380:LEU:HB2	3:C:354:ARG:CG	1.67	1.23
45:Y:37:TRP:CZ3	46:Z:498:GLY:CA	2.20	1.23
45:Y:37:TRP:CZ3	46:Z:498:GLY:HA2	1.73	1.23
1:A:121:HIS:CE1	1:A:481:PHE:HB3	1.73	1.23
3:C:140:HIS:CG	3:C:230:ASP:HB2	1.74	1.22
23:3:440:HIS:NE2	23:3:733:PRO:CD	2.03	1.22
1:A:1342:TRP:CD2	3:C:921:LEU:CD1	2.22	1.22
38:R:225:GLU:HB2	38:R:226:PRO:CD	1.68	1.22
1:A:762:ARG:HH22	37:P:226:LYS:CE	1.51	1.22
3:C:78:GLU:HG2	3:C:80:ILE:CD1	1.69	1.22
3:C:145:PHE:CA	3:C:312:SER:CB	2.18	1.22
28:J:256:LYS:O	29:L:232:TYR:CD2	1.93	1.22
3:C:77:VAL:HG13	40:T:196:LEU:O	1.40	1.21
3:C:497:LEU:HD13	3:C:577:PHE:CZ	1.76	1.21
13:F:28:A:O2'	35:N:39:GLY:HA2	1.40	1.21
45:Y:18:VAL:CB	46:Z:600:ARG:HH21	1.53	1.21
1:A:2325:VAL:HG13	4:D:788:GLY:O	1.40	1.21
36:O:149:LYS:HD2	36:O:290:LYS:NZ	1.53	1.21
1:A:1320:LYS:HE2	38:R:434:TYR:CE1	1.76	1.21
3:C:137:HIS:CD2	3:C:236:MET:HB2	1.75	1.21
38:R:442:ARG:CD	38:R:443:GLY:N	1.95	1.20
39:S:39:PHE:CB	39:S:129:PHE:HZ	1.46	1.20
1:A:2298:LEU:HB3	4:D:1283:PRO:CB	1.71	1.20
23:3:699:VAL:HA	23:3:715:MET:O	1.40	1.20
1:A:227:ARG:HA	1:A:416:GLY:O	1.39	1.20
1:A:755:HIS:ND1	37:P:223:PHE:CG	2.10	1.19
3:C:705:VAL:HG23	3:C:717:PHE:CE2	1.75	1.19
5:E:146:ARG:NH1	5:E:148:LYS:HE3	1.53	1.19
39:S:39:PHE:CG	39:S:129:PHE:CE2	2.30	1.19
1:A:380:LEU:HB3	3:C:354:ARG:NH1	1.58	1.19
32:I:280:GLU:O	32:I:288:THR:CB	1.90	1.19
1:A:380:LEU:O	3:C:354:ARG:HG2	1.37	1.18
13:F:68:C:N4	37:P:33:ARG:HB3	1.55	1.18
1:A:402:ILE:HG21	3:C:268:LYS:NZ	1.55	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:L:209:ASP:OD2	36:O:111:ASP:HB2	1.39	1.18
1:A:695:ASP:HB3	40:T:374:SER:OG	1.40	1.18
1:A:299:ILE:HD11	3:C:921:LEU:CB	1.75	1.17
1:A:1290:LYS:HE2	41:U:13:SER:CA	1.74	1.17
1:A:2268:LEU:CD2	4:D:1261:PRO:O	1.91	1.17
3:C:149:LEU:HD13	3:C:427:PHE:CG	1.79	1.17
1:A:705:LYS:CB	38:R:251:ILE:HD12	1.72	1.17
2:B:42:U:N3	14:G:-3:A:H2	1.42	1.17
3:C:140:HIS:CG	3:C:230:ASP:CB	2.27	1.17
1:A:696:MET:CB	40:T:415:ILE:CD1	2.22	1.17
3:C:465:MET:HE1	3:C:475:MET:HG3	1.26	1.17
3:C:77:VAL:CG1	40:T:196:LEU:O	1.89	1.16
1:A:86:ARG:HH22	38:R:211:ARG:CG	1.57	1.16
1:A:417:ARG:HH22	2:B:58:U:H5"	1.03	1.16
1:A:1290:LYS:CE	41:U:13:SER:HA	1.75	1.16
3:C:78:GLU:CG	3:C:80:ILE:HD11	1.72	1.16
3:C:221:ILE:HD11	3:C:479:THR:OG1	1.46	1.16
1:A:758:ARG:HB3	37:P:227:TYR:CE2	1.79	1.16
3:C:679:PRO:CB	3:C:807:GLN:OE1	1.95	1.15
1:A:338:VAL:CG2	3:C:867:PRO:HG3	1.74	1.15
1:A:1900:GLU:OE1	46:Z:522:LEU:HB2	1.47	1.15
1:A:755:HIS:CE1	37:P:223:PHE:CG	2.35	1.14
39:S:131:ARG:CD	39:S:132:VAL:O	1.95	1.14
1:A:1262:LYS:HG2	38:R:431:ASP:CB	1.77	1.14
3:C:670:SER:HA	3:C:823:ALA:HB1	1.27	1.14
5:E:74:PHE:CE1	5:E:81:LEU:HD21	1.82	1.14
24:4:28:LEU:O	24:4:32:LEU:HB2	1.48	1.14
32:I:373:GLU:CA	32:I:393:LYS:CB	2.26	1.14
38:R:101:ILE:O	38:R:104:GLN:HG3	1.48	1.14
38:R:225:GLU:CB	38:R:226:PRO:HD3	1.77	1.14
1:A:305:ARG:CB	3:C:879:ASP:OD1	1.94	1.14
1:A:1405:LEU:HB3	38:R:415:LEU:HD23	1.29	1.14
15:H:156:U:H6	15:H:156:U:H5"	1.10	1.14
45:Y:18:VAL:CB	46:Z:600:ARG:NH2	2.10	1.14
1:A:1405:LEU:HB3	38:R:415:LEU:CD2	1.78	1.14
1:A:2298:LEU:O	4:D:1283:PRO:CB	1.95	1.14
3:C:77:VAL:HG12	40:T:197:TYR:N	1.61	1.14
38:R:442:ARG:NH1	38:R:443:GLY:C	2.00	1.14
1:A:1342:TRP:CE2	3:C:921:LEU:CD1	2.31	1.13
13:F:27:A:N3	36:O:181:TYR:CE2	2.16	1.13
1:A:1757:GLU:OE1	38:R:451:ILE:HG12	1.49	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:11:A:C2	14:G:12:G:C8	2.36	1.13
3:C:452:THR:CG2	3:C:577:PHE:CD2	2.31	1.13
3:C:679:PRO:HD2	3:C:807:GLN:HB3	1.16	1.13
1:A:705:LYS:HB2	38:R:251:ILE:HD12	1.28	1.13
2:B:42:U:N3	14:G:-3:A:C2	2.15	1.13
1:A:762:ARG:NH2	37:P:226:LYS:NZ	1.95	1.13
1:A:439:GLN:NE2	1:A:614:TYR:CZ	2.18	1.12
3:C:216:THR:HG22	3:C:245:HIS:HE1	0.97	1.12
23:3:440:HIS:ND1	23:3:733:PRO:HG3	1.63	1.12
3:C:81:VAL:HG13	40:T:201:SER:CB	1.77	1.12
3:C:140:HIS:CB	3:C:230:ASP:HB2	1.79	1.12
1:A:299:ILE:HD11	3:C:921:LEU:HB2	1.18	1.12
3:C:507:VAL:HG11	3:C:565:ILE:HG23	1.30	1.12
3:C:216:THR:HG22	3:C:245:HIS:CE1	1.85	1.12
13:F:68:C:C4	37:P:33:ARG:HB3	1.85	1.12
1:A:696:MET:CB	40:T:415:ILE:HD11	1.80	1.11
1:A:758:ARG:HB3	37:P:227:TYR:HE2	0.96	1.11
1:A:1548:TYR:CD2	1:A:1549:VAL:HG22	1.83	1.11
3:C:77:VAL:HG11	40:T:196:LEU:CB	1.79	1.11
14:G:-9:C:C4	41:U:18:TYR:CZ	2.38	1.11
1:A:762:ARG:NH2	37:P:226:LYS:CE	2.14	1.11
1:A:1548:TYR:HD2	1:A:1549:VAL:HG22	1.14	1.11
38:R:420:LYS:HE3	38:R:420:LYS:HA	1.18	1.11
29:L:216:PHE:HE1	36:O:112:VAL:C	1.53	1.11
46:Z:566:TYR:CE2	46:Z:584:TRP:CZ3	2.39	1.11
1:A:151:MET:HE3	1:A:628:GLY:O	1.49	1.10
1:A:692:ASP:HA	40:T:376:ARG:NH2	1.65	1.10
23:3:440:HIS:HE1	23:3:720:TRP:CZ3	1.67	1.10
1:A:1505:LYS:CE	46:Z:615:SER:OG	1.99	1.10
1:A:73:HIS:NE2	1:A:81:PHE:CE1	2.20	1.10
1:A:1900:GLU:HG2	46:Z:521:PRO:HG2	1.33	1.10
1:A:2287:ARG:NH2	4:D:1147:ASN:CB	2.14	1.10
28:J:225:LEU:HD21	29:L:211:ASN:HB2	1.29	1.10
32:I:296:PHE:HA	32:I:305:SER:CB	1.80	1.10
1:A:299:ILE:HG12	3:C:920:PRO:O	1.52	1.10
1:A:402:ILE:HG21	3:C:268:LYS:CE	1.81	1.10
1:A:1962:THR:HG22	46:Z:524:ARG:HB2	1.18	1.10
3:C:470:PRO:HB3	3:C:500:THR:HG23	1.34	1.10
36:O:149:LYS:HD2	36:O:290:LYS:HE2	1.12	1.10
38:R:92:SER:C	39:S:19:SER:HB2	1.71	1.10
1:A:529:THR:CG2	34:M:199:PRO:CD	2.28	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:ARG:NH2	37:P:226:LYS:HE2	1.66	1.09
1:A:73:HIS:HD2	1:A:81:PHE:CD2	1.69	1.09
3:C:66:TYR:CD2	40:T:457:GLY:HA2	1.87	1.09
14:G:-9:C:N4	41:U:18:TYR:OH	1.86	1.08
45:Y:85:GLU:O	46:Z:502:ALA:N	1.85	1.08
1:A:76:MET:CE	1:A:88:TYR:CD2	2.36	1.08
1:A:1342:TRP:CE2	3:C:921:LEU:HD13	1.86	1.08
3:C:465:MET:CE	3:C:475:MET:HG3	1.82	1.08
36:O:149:LYS:CD	36:O:290:LYS:NZ	2.16	1.08
46:Z:566:TYR:CE2	46:Z:584:TRP:HZ3	1.71	1.08
1:A:299:ILE:HD11	3:C:921:LEU:CA	1.84	1.08
1:A:783:TYR:CE1	37:P:228:ILE:HG21	1.88	1.08
39:S:39:PHE:HB3	39:S:129:PHE:CZ	1.85	1.08
28:J:259:GLN:HE22	29:L:220:PRO:CD	1.66	1.08
3:C:497:LEU:CD1	3:C:577:PHE:CZ	2.36	1.07
32:I:280:GLU:CA	32:I:288:THR:CB	2.32	1.07
1:A:546:LEU:HD11	1:A:595:LYS:HD2	1.12	1.07
24:4:17:VAL:HA	24:4:85:ARG:O	1.53	1.07
29:L:216:PHE:CE1	36:O:113:ASN:N	2.21	1.07
1:A:264:PHE:HE1	1:A:455:VAL:HG13	1.15	1.07
3:C:670:SER:CB	3:C:823:ALA:HB3	1.85	1.07
1:A:744:LYS:CE	37:P:213:ASP:HA	1.84	1.06
13:F:68:C:C4	37:P:33:ARG:CB	2.38	1.06
28:J:406:PHE:CD2	28:J:411:MET:HE3	1.90	1.06
1:A:86:ARG:HH22	38:R:211:ARG:HG2	1.15	1.05
1:A:264:PHE:CE1	1:A:455:VAL:HG13	1.90	1.05
36:O:132:ARG:HH11	39:S:149:SER:HB3	1.15	1.05
39:S:39:PHE:CB	39:S:129:PHE:CE2	2.40	1.05
1:A:305:ARG:HB3	3:C:879:ASP:OD1	1.55	1.05
1:A:532:THR:HG23	14:G:2:U:P	1.97	1.05
2:B:39:C:H4'	2:B:40:U:OP1	1.23	1.05
1:A:705:LYS:CG	38:R:251:ILE:HD12	1.86	1.05
1:A:1364:LEU:HD13	42:V:461:LEU:CB	1.86	1.05
3:C:452:THR:HG22	3:C:577:PHE:HD2	1.21	1.05
1:A:1342:TRP:CZ3	3:C:921:LEU:HD13	1.92	1.05
1:A:168:PRO:HG3	1:A:559:ASP:HB3	1.39	1.04
1:A:301:LYS:HE3	3:C:940:ARG:HA	1.38	1.04
1:A:844:GLU:CB	38:R:422:MET:HE1	1.83	1.04
40:T:399:LYS:CG	40:T:406:ILE:HD11	1.87	1.04
1:A:369:GLU:O	1:A:371:LEU:N	1.88	1.04
1:A:692:ASP:HA	40:T:376:ARG:HH22	1.18	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:228:PHE:HA	3:C:256:CYS:O	1.57	1.04
38:R:178:ARG:HD3	38:R:194:GLN:HE22	1.17	1.04
1:A:1449:LYS:HE3	38:R:428:GLY:HA3	1.37	1.04
3:C:78:GLU:HG2	3:C:80:ILE:HD11	1.06	1.04
1:A:755:HIS:ND1	37:P:223:PHE:CD1	2.26	1.04
2:B:43:U:H4'	13:F:67:G:H1	0.93	1.04
3:C:488:VAL:HG13	3:C:609:LYS:HE2	1.39	1.04
13:F:25:C:H4'	13:F:26:U:OP2	1.22	1.04
38:R:436:VAL:HG23	38:R:437:TYR:CD1	1.93	1.04
1:A:402:ILE:CG2	3:C:268:LYS:NZ	2.19	1.04
1:A:168:PRO:CG	1:A:559:ASP:HB3	1.87	1.03
1:A:1342:TRP:CE3	3:C:921:LEU:HD22	1.93	1.03
24:4:70:ALA:O	24:4:74:MET:CB	2.04	1.03
1:A:755:HIS:CE1	37:P:223:PHE:CD2	2.46	1.03
29:L:224:PHE:CD1	38:R:86:LEU:HD12	1.93	1.03
1:A:254:TYR:CZ	1:A:434:HIS:HB3	1.93	1.03
1:A:384:VAL:HG12	3:C:331:PHE:CD2	1.94	1.03
1:A:388:LEU:HB2	3:C:379:LYS:HD3	1.33	1.03
38:R:92:SER:HA	39:S:19:SER:HB3	1.35	1.03
1:A:76:MET:HE1	1:A:88:TYR:CD2	1.93	1.03
1:A:1306:LYS:NZ	2:B:38:C:O2'	1.90	1.03
28:J:273:TYR:CZ	38:R:228:PRO:HB3	1.94	1.03
1:A:299:ILE:CD1	1:A:1342:TRP:CZ3	2.42	1.03
4:D:754:GLU:CB	23:3:662:PHE:CZ	2.41	1.03
15:H:105:G:H2'	15:H:106:G:H5"	1.37	1.03
1:A:254:TYR:CE2	1:A:434:HIS:HB2	1.94	1.02
1:A:642:ARG:HD3	2:B:28:A:H1'	1.37	1.02
2:B:43:U:H5'	13:F:67:G:H22	1.19	1.02
3:C:452:THR:HG22	3:C:577:PHE:CD2	1.94	1.02
28:J:331:GLN:HG2	38:R:98:TYR:OH	1.59	1.02
46:Z:564:PRO:CB	46:Z:582:TYR:CG	2.41	1.02
3:C:387:ASP:O	3:C:388:VAL:CG1	2.07	1.02
38:R:420:LYS:HG3	38:R:421:GLY:H	1.20	1.02
1:A:384:VAL:CG1	3:C:331:PHE:CE2	2.42	1.02
2:B:42:U:O2'	13:F:69:A:N3	1.93	1.02
13:F:68:C:C5	37:P:33:ARG:CB	2.42	1.02
38:R:434:TYR:O	38:R:435:ASN:ND2	1.90	1.02
45:Y:37:TRP:CD1	45:Y:83:CYS:HB2	1.92	1.02
1:A:339:PHE:CE1	1:A:406:TRP:CE3	2.46	1.02
13:F:36:A:H3'	13:F:37:C:H5"	1.39	1.02
35:N:40:LYS:O	35:N:41:ARG:HG3	1.59	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:O:132:ARG:NH1	39:S:149:SER:HB3	1.73	1.02
38:R:442:ARG:HD2	38:R:444:GLY:H	0.97	1.02
23:3:440:HIS:CE1	23:3:720:TRP:CZ3	2.47	1.01
46:Z:525:TYR:CD1	46:Z:526:ILE:HG23	1.95	1.01
1:A:529:THR:HG22	34:M:199:PRO:HD3	1.04	1.01
3:C:511:GLY:O	3:C:576:ILE:CD1	2.07	1.01
1:A:532:THR:HG21	14:G:2:U:C5'	1.89	1.01
1:A:1457:HIS:HE1	1:A:1459:ARG:CG	1.74	1.01
1:A:1900:GLU:HG2	46:Z:521:PRO:CG	1.91	1.01
3:C:132:VAL:HG12	3:C:226:VAL:HG23	1.43	1.01
3:C:349:PHE:CD1	3:C:356:PHE:CE1	2.49	1.01
1:A:1900:GLU:OE2	46:Z:521:PRO:HB2	1.59	1.00
23:3:440:HIS:O	23:3:733:PRO:HG2	1.61	1.00
36:O:149:LYS:CG	36:O:290:LYS:NZ	2.25	1.00
43:W:420:ALA:O	43:W:438:ASP:N	1.93	1.00
3:C:261:ASP:OD2	51:C:1500:GTP:N1	1.92	1.00
3:C:703:GLU:OE2	3:C:740:THR:HG21	1.61	1.00
15:H:179:C:H2'	15:H:180:G:H8	1.25	1.00
3:C:705:VAL:CG2	3:C:717:PHE:CD2	2.39	1.00
14:G:17:U:O2	36:O:198:ILE:HD11	1.62	1.00
37:P:193:VAL:HG21	37:P:194:PHE:HD2	1.26	1.00
3:C:81:VAL:CG1	40:T:201:SER:HB3	1.90	1.00
23:3:303:ALA:O	23:3:310:ILE:HA	1.61	1.00
1:A:623:LYS:O	50:A:3000:IHP:P4	2.20	1.00
29:L:209:ASP:OD1	36:O:111:ASP:N	1.95	1.00
2:B:43:U:H4'	13:F:67:G:N1	1.75	1.00
3:C:85:ASP:HB3	40:T:238:LEU:HG	1.43	1.00
3:C:129:ILE:HG22	3:C:199:LEU:HB3	1.44	1.00
1:A:1162:PRO:HG2	37:P:194:PHE:CE2	1.97	1.00
46:Z:525:TYR:CE1	46:Z:526:ILE:HG23	1.96	1.00
1:A:779:LEU:HD21	37:P:223:PHE:CE2	1.97	0.99
23:3:440:HIS:CE1	23:3:733:PRO:CG	2.45	0.99
38:R:414:ARG:NE	46:Z:598:PHE:HZ	1.38	0.99
39:S:11:PRO:HB3	39:S:166:GLY:HA3	1.40	0.99
1:A:783:TYR:HB2	37:P:228:ILE:HG12	1.43	0.99
1:A:86:ARG:NH2	38:R:211:ARG:CG	2.24	0.99
1:A:529:THR:CG2	34:M:199:PRO:HD3	1.87	0.99
1:A:1505:LYS:HE3	46:Z:615:SER:OG	1.62	0.99
39:S:11:PRO:HB3	39:S:165:SER:O	1.62	0.99
1:A:264:PHE:CE1	1:A:459:LEU:HD13	1.96	0.99
13:F:28:A:HO2'	35:N:39:GLY:HA2	1.25	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:MET:CB	40:T:415:ILE:HD13	1.89	0.99
40:T:434:GLY:HA2	40:T:464:GLY:HA2	1.41	0.99
1:A:715:GLU:OE2	38:R:258:TRP:HZ3	1.43	0.99
46:Z:600:ARG:HB3	46:Z:600:ARG:HH11	1.24	0.99
3:C:64:LYS:HE3	37:P:206:LYS:HE2	1.45	0.99
3:C:137:HIS:CD2	3:C:236:MET:CB	2.45	0.99
13:F:68:C:C5	37:P:33:ARG:HB2	1.97	0.99
1:A:1457:HIS:NE2	38:R:425:GLY:N	2.09	0.99
1:A:2287:ARG:HH21	4:D:1147:ASN:CB	1.72	0.99
36:O:149:LYS:CG	36:O:290:LYS:HZ3	1.75	0.99
38:R:92:SER:CA	39:S:19:SER:CB	2.29	0.99
29:L:216:PHE:CE1	36:O:113:ASN:CA	2.46	0.99
1:A:1900:GLU:OE1	46:Z:522:LEU:CB	2.10	0.98
36:O:149:LYS:HZ3	36:O:290:LYS:HG2	1.23	0.98
3:C:78:GLU:O	40:T:198:ARG:CA	2.11	0.98
43:W:242:HIS:CB	43:W:325:LEU:O	2.10	0.98
1:A:1084:PRO:HG2	37:P:188:TRP:HZ2	1.26	0.98
13:F:27:A:C4	36:O:181:TYR:CE2	2.50	0.98
23:3:440:HIS:CE1	23:3:733:PRO:HG3	1.99	0.98
37:P:210:PHE:CD2	40:T:455:GLN:OE1	2.16	0.98
38:R:420:LYS:HB2	46:Z:610:LEU:HD11	1.44	0.98
1:A:1211:ASP:OD1	42:V:505:LYS:CB	2.12	0.98
3:C:306:ASN:OD1	3:C:437:HIS:CE1	2.16	0.98
36:O:149:LYS:CD	36:O:290:LYS:HE2	1.94	0.98
37:P:30:TYR:OH	38:R:162:ALA:HA	1.63	0.98
1:A:2074:ARG:NH2	4:D:1044:VAL:O	1.96	0.98
15:H:83:A:H2'	15:H:84:C:O4'	1.64	0.98
39:S:11:PRO:CB	39:S:165:SER:O	2.11	0.98
1:A:461:HIS:NE2	2:B:26:A:N6	2.12	0.97
3:C:84:GLU:O	40:T:238:LEU:CD2	2.12	0.97
3:C:670:SER:CA	3:C:823:ALA:HB3	1.94	0.97
39:S:100:MET:HG2	39:S:108:ASN:OD1	1.64	0.97
42:V:548:ALA:CB	42:V:585:ILE:CB	2.42	0.97
3:C:66:TYR:HB3	40:T:456:PRO:O	1.64	0.97
3:C:81:VAL:HG13	40:T:201:SER:HB3	0.99	0.97
45:Y:37:TRP:CZ3	46:Z:498:GLY:HA3	2.00	0.97
46:Z:566:TYR:HE2	46:Z:584:TRP:HZ3	1.05	0.97
3:C:711:ARG:HD3	3:C:730:ARG:HH11	1.29	0.97
1:A:1348:VAL:HG12	3:C:921:LEU:HD23	1.43	0.97
1:A:1364:LEU:HD12	42:V:461:LEU:CB	1.89	0.97
36:O:149:LYS:CD	36:O:290:LYS:HZ3	1.74	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:500:THR:HG22	3:C:545:PRO:HA	1.47	0.97
29:L:216:PHE:HD1	36:O:113:ASN:CA	1.59	0.97
3:C:670:SER:HA	3:C:823:ALA:HB3	1.43	0.97
1:A:1320:LYS:HE2	38:R:434:TYR:HE1	1.15	0.97
1:A:2328:ALA:HB2	4:D:788:GLY:HA2	1.43	0.97
3:C:670:SER:CA	3:C:823:ALA:CB	2.43	0.96
28:J:300:ASP:OD2	38:R:101:ILE:HG13	1.65	0.96
35:N:28:LYS:HZ3	43:W:190:ASP:HA	1.28	0.96
1:A:380:LEU:CD2	3:C:354:ARG:O	2.12	0.96
1:A:1293:ASN:HD22	41:U:14:GLY:HA2	1.28	0.96
23:3:440:HIS:NE2	23:3:733:PRO:HD3	1.70	0.96
1:A:296:PHE:CE1	3:C:591:ALA:HB1	2.01	0.96
1:A:546:LEU:HD11	1:A:595:LYS:CD	1.94	0.96
3:C:855:GLY:O	3:C:856:HIS:HB3	1.63	0.96
5:E:321:TYR:CE1	43:W:84:THR:HA	1.99	0.96
32:I:358:HIS:CB	32:I:376:ASN:CB	2.44	0.96
14:G:18:A:H5'	36:O:69:GLU:OE1	1.66	0.96
1:A:380:LEU:CB	3:C:354:ARG:NH1	2.27	0.96
40:T:352:THR:HG22	40:T:373:LYS:O	1.65	0.96
45:Y:37:TRP:HH2	46:Z:498:GLY:CA	1.70	0.96
1:A:303:ILE:HG21	3:C:933:PHE:CE1	2.01	0.96
1:A:47:GLU:O	1:A:50:LYS:HB2	1.64	0.96
3:C:135:CYS:SG	3:C:227:LEU:HD12	2.06	0.96
15:H:78:C:H2'	15:H:79:G:H8	1.27	0.96
1:A:121:HIS:NE2	1:A:481:PHE:CB	2.29	0.96
1:A:748:ASP:OD1	37:P:214:THR:HG22	1.64	0.96
1:A:1900:GLU:CD	46:Z:522:LEU:HB2	1.85	0.96
1:A:369:GLU:OE2	1:A:369:GLU:N	1.97	0.96
3:C:115:GLU:O	3:C:118:PHE:N	1.98	0.95
1:A:783:TYR:CD1	37:P:228:ILE:HG21	2.01	0.95
1:A:2298:LEU:CB	4:D:1283:PRO:CB	2.44	0.95
5:E:146:ARG:HH11	5:E:148:LYS:HE2	1.27	0.95
14:G:11:A:N3	14:G:12:G:H8	1.64	0.95
36:O:225:PRO:HB3	36:O:302:TRP:NE1	1.80	0.95
45:Y:37:TRP:CH2	46:Z:498:GLY:HA3	1.96	0.95
23:3:440:HIS:NE2	23:3:733:PRO:HD2	1.77	0.95
38:R:442:ARG:HD3	38:R:443:GLY:CA	1.96	0.95
1:A:171:ASP:O	1:A:520:TYR:CD2	2.20	0.95
15:H:156:U:H5"	15:H:156:U:C6	2.02	0.95
1:A:299:ILE:HD12	1:A:1342:TRP:CZ3	1.99	0.95
1:A:299:ILE:CB	1:A:1342:TRP:HZ3	1.79	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2335:ALA:O	4:D:570:THR:HA	1.65	0.95
3:C:145:PHE:CB	3:C:312:SER:HB3	1.97	0.95
13:F:22:A:H5"	35:N:116:ASN:O	1.66	0.95
36:O:149:LYS:CD	36:O:290:LYS:CE	2.44	0.95
38:R:442:ARG:HH11	38:R:444:GLY:N	1.64	0.95
1:A:388:LEU:O	3:C:379:LYS:NZ	2.00	0.95
3:C:700:ILE:HG23	3:C:735:PHE:CD2	2.01	0.95
1:A:264:PHE:CZ	1:A:459:LEU:CD1	2.50	0.95
1:A:705:LYS:HG2	38:R:251:ILE:HB	1.49	0.95
1:A:253:ASN:HB3	3:C:893:GLY:O	1.67	0.95
1:A:1505:LYS:HE2	46:Z:615:SER:OG	1.65	0.95
14:G:-9:C:N4	41:U:18:TYR:CZ	2.34	0.95
1:A:785:LYS:CE	37:P:215:LEU:HD11	1.97	0.94
14:G:11:A:C2	14:G:12:G:N7	2.34	0.94
1:A:384:VAL:CG1	3:C:331:PHE:CD2	2.50	0.94
1:A:1162:PRO:HG3	37:P:194:PHE:CD2	2.02	0.94
1:A:1457:HIS:CE1	38:R:424:SER:HA	2.01	0.94
28:J:339:TRP:CA	38:R:116:TYR:CE2	2.48	0.94
3:C:711:ARG:NH2	3:C:730:ARG:O	2.00	0.94
1:A:299:ILE:HG13	1:A:1342:TRP:CH2	2.02	0.94
13:F:49:G:N7	29:L:33:ARG:NH1	2.15	0.94
5:E:119:THR:CG2	5:E:161:ARG:HB3	1.97	0.94
15:H:180:G:H2'	15:H:181:G:H8	1.30	0.94
40:T:352:THR:HG22	40:T:373:LYS:C	1.86	0.94
13:F:27:A:P	35:N:41:ARG:HH21	1.90	0.94
1:A:1405:LEU:CB	38:R:415:LEU:CD2	2.45	0.94
1:A:1459:ARG:HE	38:R:423:ASP:HB2	1.31	0.94
1:A:1962:THR:CG2	46:Z:524:ARG:CB	2.45	0.94
3:C:145:PHE:HA	3:C:312:SER:HB2	0.95	0.94
3:C:445:ALA:HB3	3:C:466:SER:HA	1.50	0.94
14:G:-9:C:C5	41:U:18:TYR:HE1	1.79	0.94
15:H:79:G:H2'	15:H:80:A:H8	1.33	0.94
24:4:69:TYR:CZ	24:4:73:ILE:HG13	2.03	0.94
3:C:349:PHE:HD1	3:C:356:PHE:CD1	1.85	0.94
2:B:39:C:C4'	2:B:40:U:OP1	2.16	0.94
1:A:158:ARG:NH2	1:A:570:ASP:OD2	2.01	0.93
1:A:2113:LYS:CE	4:D:1229:ASP:O	2.16	0.93
13:F:8:C:H6	13:F:8:C:H5"	1.31	0.93
1:A:2268:LEU:CD2	4:D:1261:PRO:CB	2.46	0.93
1:A:461:HIS:CD2	2:B:27:U:O4	2.20	0.93
13:F:25:C:C4'	13:F:26:U:OP2	2.16	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:L:216:PHE:CE1	36:O:112:VAL:C	2.40	0.93
38:R:171:LEU:HD12	38:R:201:GLU:OE1	1.67	0.93
3:C:76:GLU:OE1	3:C:76:GLU:N	2.01	0.93
5:E:146:ARG:NH1	5:E:148:LYS:HE2	1.82	0.93
3:C:149:LEU:CD1	3:C:427:PHE:HD2	1.80	0.93
29:L:209:ASP:HA	36:O:110:SER:HB2	1.49	0.93
1:A:73:HIS:CD2	1:A:81:PHE:CE1	2.56	0.93
1:A:151:MET:CE	1:A:628:GLY:O	2.15	0.93
1:A:695:ASP:CB	40:T:374:SER:OG	2.15	0.93
3:C:449:ILE:HG21	3:C:457:VAL:CG1	1.99	0.93
28:J:259:GLN:NE2	29:L:220:PRO:CD	2.30	0.93
1:A:67:ARG:HD3	1:A:179:ALA:HB2	1.51	0.93
28:J:294:HIS:CE1	29:L:227:THR:HB	2.04	0.93
1:A:417:ARG:NH2	2:B:58:U:H5”	1.82	0.93
1:A:1900:GLU:OE2	46:Z:521:PRO:C	2.06	0.93
1:A:2314:PHE:CB	4:D:1125:SER:CA	2.47	0.93
3:C:497:LEU:HD13	3:C:577:PHE:HZ	1.17	0.93
13:F:68:C:C4	37:P:33:ARG:CG	2.52	0.93
1:A:548:ARG:NH2	1:A:549:GLU:OE2	2.01	0.92
2:B:43:U:C4’	13:F:67:G:H1	1.80	0.92
36:O:225:PRO:HG3	36:O:302:TRP:HE1	1.29	0.92
38:R:101:ILE:O	38:R:104:GLN:CG	2.16	0.92
1:A:299:ILE:HD12	1:A:1342:TRP:CE3	2.03	0.92
3:C:69:ALA:HA	40:T:456:PRO:HG3	1.49	0.92
3:C:449:ILE:CG2	3:C:457:VAL:CG1	2.46	0.92
3:C:678:THR:HG21	3:C:683:ASN:HD22	1.35	0.92
13:F:28:A:O2’	35:N:39:GLY:CA	2.17	0.92
43:W:258:PRO:O	43:W:260:ASP:N	2.02	0.92
1:A:2113:LYS:HE2	4:D:1229:ASP:CB	1.98	0.92
38:R:412:ASP:CG	38:R:413:GLN:H	1.69	0.92
36:O:223:LEU:HD13	36:O:224:ASP:N	1.84	0.92
3:C:77:VAL:CG1	40:T:196:LEU:CB	2.45	0.92
3:C:140:HIS:CG	3:C:230:ASP:HB3	2.03	0.92
38:R:414:ARG:NH1	46:Z:598:PHE:HE2	1.58	0.92
1:A:523:ASN:OD1	1:A:552:ARG:NH2	2.02	0.92
1:A:532:THR:CG2	14:G:2:U:O5’	2.17	0.92
3:C:445:ALA:O	3:C:449:ILE:N	2.03	0.92
3:C:476:CYS:HB3	3:C:565:ILE:HB	1.51	0.92
28:J:339:TRP:CA	38:R:116:TYR:CD2	2.51	0.92
1:A:228:TRP:O	1:A:415:SER:HA	1.70	0.92
23:3:440:HIS:HE1	23:3:720:TRP:HZ3	1.06	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:PHE:CE1	1:A:406:TRP:CZ3	2.58	0.92
3:C:670:SER:HB3	3:C:823:ALA:HB3	1.48	0.92
13:F:27:A:P	35:N:41:ARG:NH2	2.43	0.92
28:J:259:GLN:HE22	29:L:220:PRO:HD2	1.32	0.92
35:N:128:VAL:HG13	35:N:130:ARG:H	1.35	0.92
1:A:762:ARG:HH22	37:P:226:LYS:HZ1	1.08	0.92
1:A:651:TRP:NE1	13:F:66:C:C2	2.38	0.92
1:A:779:LEU:HD21	37:P:223:PHE:CZ	2.05	0.92
3:C:244:LYS:HA	3:C:292:TYR:HD2	1.34	0.91
38:R:106:GLN:HG2	38:R:110:LYS:HE2	1.51	0.91
3:C:483:SER:HA	3:C:490:PHE:HB3	1.52	0.91
3:C:674:CYS:SG	3:C:822:MET:SD	2.67	0.91
1:A:86:ARG:NH2	38:R:211:ARG:HG3	1.84	0.91
1:A:235:MET:CE	1:A:411:PHE:HA	1.99	0.91
3:C:86:THR:O	40:T:239:LYS:O	1.88	0.91
3:C:132:VAL:CG1	3:C:226:VAL:HG23	2.00	0.91
39:S:131:ARG:NH1	39:S:133:CYS:HA	1.86	0.91
1:A:171:ASP:HB3	1:A:519:ASP:HB2	1.53	0.91
1:A:305:ARG:HA	1:A:305:ARG:HH11	1.33	0.91
1:A:296:PHE:CE1	3:C:591:ALA:CB	2.54	0.91
1:A:1761:PRO:HB2	1:A:1930:TYR:OH	1.71	0.91
1:A:1962:THR:HG22	46:Z:524:ARG:CB	2.00	0.91
36:O:234:LEU:O	36:O:271:PHE:HA	1.70	0.91
1:A:1320:LYS:CE	38:R:434:TYR:CE1	2.54	0.91
23:3:699:VAL:HG22	23:3:716:SER:HB2	1.53	0.91
1:A:372:PRO:CG	3:C:342:ARG:HE	1.83	0.91
1:A:2328:ALA:CB	4:D:788:GLY:HA2	1.99	0.91
3:C:452:THR:HG22	3:C:577:PHE:HB3	1.52	0.91
29:L:224:PHE:CD1	38:R:86:LEU:CD1	2.53	0.91
3:C:145:PHE:N	3:C:312:SER:HB2	1.85	0.90
13:F:35:A:C8	14:G:12:G:C6	2.59	0.90
23:3:34:ARG:HB2	23:3:37:ILE:HB	1.51	0.90
1:A:232:LEU:HD22	1:A:404:LEU:HD13	1.53	0.90
3:C:230:ASP:OD2	3:C:233:GLU:HG2	1.70	0.90
1:A:1457:HIS:CE1	38:R:425:GLY:H	1.88	0.90
3:C:678:THR:OG1	3:C:680:ASN:O	1.89	0.90
1:A:76:MET:HE1	1:A:88:TYR:CG	2.06	0.90
1:A:1320:LYS:CE	38:R:434:TYR:HE1	1.85	0.90
45:Y:37:TRP:NE1	45:Y:83:CYS:HB2	1.87	0.90
1:A:623:LYS:HB3	50:A:3000:IHP:O34	1.72	0.90
1:A:1426:ASP:CG	38:R:421:GLY:HA3	1.91	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:221:ILE:CD1	3:C:479:THR:OG1	2.19	0.90
13:F:94:C:P	28:J:351:ASN:HD22	1.95	0.90
1:A:782:LEU:HD13	37:P:220:HIS:HE1	1.34	0.90
1:A:1290:LYS:HG2	41:U:13:SER:O	1.71	0.90
3:C:711:ARG:HD3	3:C:730:ARG:NH1	1.86	0.90
13:F:27:A:H1'	36:O:181:TYR:HE2	1.36	0.90
3:C:228:PHE:CA	3:C:256:CYS:O	2.20	0.90
1:A:705:LYS:HG2	38:R:251:ILE:CB	2.01	0.89
38:R:225:GLU:HB2	38:R:226:PRO:HD3	0.90	0.89
40:T:399:LYS:HG3	40:T:406:ILE:HD11	1.54	0.89
39:S:34:LYS:HE3	39:S:78:TYR:CE2	2.07	0.89
35:N:124:SER:O	35:N:127:GLU:HG2	1.71	0.89
45:Y:36:ALA:HB2	46:Z:499:LYS:O	1.72	0.89
1:A:227:ARG:CA	1:A:416:GLY:O	2.20	0.89
1:A:744:LYS:HE2	37:P:213:ASP:HA	1.52	0.89
1:A:525:LYS:HE2	34:M:194:ARG:CG	2.03	0.89
1:A:296:PHE:CB	3:C:656:ALA:HB2	2.02	0.89
37:P:192:VAL:HG12	37:P:194:PHE:H	1.35	0.89
1:A:387:PHE:CE2	3:C:399:LEU:HD23	2.07	0.89
1:A:748:ASP:HA	37:P:214:THR:HG21	1.54	0.89
1:A:254:TYR:CZ	1:A:434:HIS:CB	2.54	0.89
15:H:80:A:H2'	15:H:81:G:H8	1.36	0.89
38:R:81:LYS:HA	38:R:81:LYS:CE	2.02	0.89
1:A:1342:TRP:CE2	3:C:921:LEU:HD11	2.08	0.89
28:J:220:LEU:HD11	28:J:224:LYS:HE3	1.53	0.89
1:A:532:THR:OG1	14:G:2:U:O5'	1.89	0.89
15:H:81:G:H2'	15:H:82:G:H8	1.35	0.89
15:H:82:G:H2'	15:H:83:A:H8	1.38	0.89
38:R:92:SER:O	39:S:19:SER:HB2	1.73	0.89
38:R:442:ARG:CD	38:R:444:GLY:H	1.85	0.89
3:C:64:LYS:HZ1	37:P:206:LYS:HG2	1.38	0.88
37:P:193:VAL:HG21	37:P:194:PHE:CD2	2.02	0.88
1:A:529:THR:HG21	34:M:199:PRO:HG3	1.55	0.88
14:G:11:A:N3	14:G:12:G:C8	2.38	0.88
38:R:81:LYS:HA	38:R:81:LYS:NZ	1.88	0.88
1:A:586:GLY:C	1:A:1549:VAL:HG12	1.93	0.88
1:A:785:LYS:HE2	37:P:215:LEU:HD11	1.54	0.88
3:C:78:GLU:O	40:T:199:VAL:N	2.06	0.88
3:C:140:HIS:CE1	3:C:233:GLU:HB2	2.07	0.88
1:A:175:PRO:HG2	1:A:498:ARG:NH2	1.88	0.88
3:C:679:PRO:CG	3:C:807:GLN:OE1	2.21	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:ARG:NH2	1:A:423:ASP:O	2.06	0.88
3:C:678:THR:CG2	3:C:683:ASN:HB2	2.04	0.88
13:F:68:C:C4	37:P:33:ARG:HG2	2.07	0.88
1:A:384:VAL:HG12	3:C:331:PHE:HE2	1.08	0.88
1:A:1342:TRP:CD2	3:C:921:LEU:HD11	2.08	0.88
38:R:442:ARG:CD	38:R:444:GLY:N	2.34	0.88
1:A:715:GLU:OE2	38:R:258:TRP:CZ3	2.25	0.88
1:A:2314:PHE:HB2	4:D:1125:SER:CA	2.02	0.88
22:2:614:ARG:HH11	22:2:614:ARG:HG3	1.38	0.88
3:C:261:ASP:OD1	51:C:1500:GTP:O6	1.92	0.88
39:S:111:GLN:HE22	43:W:93:PHE:CB	1.86	0.88
1:A:1457:HIS:CE1	38:R:425:GLY:N	2.41	0.88
1:A:1459:ARG:HG3	38:R:422:MET:O	1.74	0.88
23:3:440:HIS:O	23:3:733:PRO:CG	2.22	0.88
37:P:224:MET:CE	37:P:228:ILE:HD13	2.04	0.88
1:A:278:LYS:NZ	14:G:-9:C:OP1	2.06	0.87
1:A:372:PRO:HG3	3:C:342:ARG:HE	1.38	0.87
3:C:97:VAL:CG2	37:P:45:GLN:HG3	2.03	0.87
15:H:179:C:O2'	15:H:180:G:H5'	1.74	0.87
3:C:149:LEU:HD12	3:C:427:PHE:HD2	1.39	0.87
3:C:700:ILE:HG23	3:C:735:PHE:CE2	2.09	0.87
23:3:812:LYS:O	23:3:816:LYS:HB2	1.74	0.87
14:G:137:C:H42	15:H:40:C:H42	1.22	0.87
23:3:545:VAL:HG12	23:3:546:LYS:HG2	1.57	0.87
24:4:75:ASN:OD1	24:4:86:VAL:HB	1.74	0.87
1:A:329:LEU:HD13	3:C:177:ARG:HE	1.40	0.87
3:C:523:GLN:OE1	3:C:524:ILE:N	2.07	0.87
1:A:433:GLU:OE1	1:A:436:PRO:HB3	1.74	0.87
3:C:705:VAL:HG21	3:C:717:PHE:CE2	2.07	0.87
5:E:243:LEU:CD1	5:E:247:GLY:HA2	2.04	0.87
15:H:68:G:O2'	15:H:69:U:H5'	1.74	0.87
15:H:78:C:H2'	15:H:79:G:C8	2.10	0.87
1:A:1162:PRO:CG	37:P:194:PHE:CE2	2.57	0.87
1:A:1370:ARG:HG2	42:V:464:GLN:HA	1.54	0.87
3:C:488:VAL:HG13	3:C:609:LYS:CE	2.05	0.87
15:H:154:C:O2	15:H:176:G:N2	2.07	0.87
28:J:339:TRP:CD2	38:R:116:TYR:HD2	1.93	0.87
38:R:423:ASP:O	38:R:424:SER:OG	1.92	0.87
15:H:180:G:H2'	15:H:181:G:C8	2.10	0.87
3:C:701:GLU:HA	3:C:740:THR:OG1	1.75	0.87
28:J:255:LEU:HD22	29:L:235:LEU:HD13	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:LEU:HD22	1:A:404:LEU:CD1	2.04	0.86
3:C:216:THR:CG2	3:C:245:HIS:HE1	1.84	0.86
38:R:442:ARG:NH1	38:R:443:GLY:O	2.07	0.86
13:F:27:A:OP2	35:N:41:ARG:NH2	2.09	0.86
1:A:318:TYR:CA	3:C:638:ASP:OD1	2.22	0.86
15:H:179:C:H2'	15:H:180:G:C8	2.09	0.86
1:A:86:ARG:NH2	38:R:211:ARG:HG2	1.85	0.86
33:Q:500:GLY:N	38:R:51:ILE:HD11	1.89	0.86
35:N:28:LYS:HZ1	43:W:190:ASP:H	1.18	0.86
36:O:20:PHE:CD1	38:R:177:ILE:HD11	2.11	0.86
38:R:225:GLU:CB	38:R:226:PRO:CD	2.43	0.86
1:A:1342:TRP:HB3	3:C:921:LEU:HD21	1.54	0.86
1:A:1757:GLU:CD	38:R:451:ILE:HG12	1.96	0.86
5:E:267:PHE:CE1	31:K:194:GLU:CB	2.59	0.86
15:H:148:C:O2'	15:H:149:A:H5'	1.75	0.86
21:1:1179:ASP:OD2	21:1:1185:ARG:NH1	2.08	0.86
40:T:399:LYS:HG2	40:T:406:ILE:HD11	1.53	0.86
5:E:269:PRO:O	5:E:270:LYS:HB3	1.76	0.86
13:F:26:U:H3'	13:F:27:A:H5"	1.56	0.86
28:J:256:LYS:O	29:L:232:TYR:CE2	2.29	0.86
37:P:210:PHE:HD2	40:T:455:GLN:OE1	1.53	0.86
38:R:147:THR:HG23	40:T:360:VAL:HG12	1.57	0.86
39:S:57:ILE:HD11	43:W:97:ASN:CB	2.03	0.86
23:3:442:LEU:HD12	23:3:733:PRO:O	1.76	0.86
40:T:417:ASN:OD1	40:T:432:ASP:OD1	1.94	0.86
1:A:299:ILE:CD1	1:A:1342:TRP:HZ3	1.85	0.86
1:A:402:ILE:CG2	3:C:268:LYS:HZ2	1.84	0.86
39:S:35:THR:O	39:S:129:PHE:CE1	2.29	0.86
1:A:296:PHE:HB3	3:C:656:ALA:CB	2.05	0.85
1:A:338:VAL:HG21	3:C:867:PRO:HG3	1.57	0.85
1:A:532:THR:CG2	14:G:2:U:C5'	2.52	0.85
38:R:135:PRO:O	38:R:136:ASP:OD1	1.94	0.85
1:A:299:ILE:CG1	3:C:920:PRO:O	2.24	0.85
38:R:420:LYS:HE3	38:R:420:LYS:CA	1.98	0.85
39:S:39:PHE:HB2	39:S:129:PHE:CE2	2.09	0.85
39:S:9:TRP:O	39:S:11:PRO:HD3	1.76	0.85
3:C:72:VAL:HG22	40:T:453:ALA:HB1	1.58	0.85
3:C:149:LEU:HD12	3:C:427:PHE:CD2	2.07	0.85
15:H:79:G:O2'	15:H:80:A:H5'	1.76	0.85
36:O:225:PRO:CG	36:O:302:TRP:HE1	1.88	0.85
39:S:35:THR:O	39:S:129:PHE:HE1	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:145:PHE:HB2	3:C:312:SER:HB3	1.57	0.85
21:1:672:ALA:HA	21:1:679:ILE:HD11	1.58	0.85
2:B:95:G:H4'	2:B:96:A:O4'	1.76	0.85
38:R:414:ARG:NH1	46:Z:598:PHE:HZ	1.44	0.85
5:E:162:ARG:NH2	5:E:203:ASP:O	2.10	0.85
5:E:267:PHE:CE1	31:K:194:GLU:HB3	2.10	0.85
1:A:152:ARG:HB3	1:A:152:ARG:HH11	1.40	0.85
38:R:414:ARG:HB2	38:R:414:ARG:NH2	1.92	0.85
39:S:35:THR:C	39:S:129:PHE:HE1	1.80	0.85
3:C:133:THR:O	3:C:226:VAL:N	2.10	0.85
43:W:137:TYR:HA	43:W:154:GLY:HA3	1.59	0.85
1:A:121:HIS:CG	1:A:481:PHE:O	2.30	0.85
1:A:338:VAL:HG23	3:C:867:PRO:HG3	1.58	0.85
14:G:1:G:N2	34:M:202:CYS:SG	2.50	0.85
1:A:452:LYS:NZ	2:B:48:A:OP1	2.10	0.84
1:A:1900:GLU:CG	46:Z:521:PRO:CG	2.55	0.84
3:C:94:ILE:HD13	37:P:44:ARG:NH1	1.92	0.84
15:H:156:U:H6	15:H:156:U:C5'	1.88	0.84
46:Z:600:ARG:HH11	46:Z:600:ARG:CB	1.90	0.84
2:B:40:U:H3	14:G:-1:G:H1	1.25	0.84
1:A:1900:GLU:OE2	46:Z:522:LEU:N	2.11	0.84
3:C:444:GLY:O	3:C:447:PRO:HD2	1.77	0.84
3:C:516:LEU:HD12	3:C:517:GLU:HG3	1.59	0.84
1:A:595:LYS:HE3	1:A:644:ILE:HD11	1.58	0.84
13:F:36:A:H2'	13:F:38:G:OP2	1.78	0.84
15:H:80:A:O2'	15:H:81:G:H5'	1.78	0.84
15:H:181:G:O2'	15:H:182:U:H5'	1.77	0.84
15:H:182:U:O2'	15:H:183:G:H5'	1.75	0.84
23:3:356:HIS:HB2	23:3:401:LEU:HB2	1.60	0.84
1:A:1348:VAL:CG1	3:C:921:LEU:HD23	2.06	0.84
3:C:80:ILE:O	40:T:200:ILE:HA	1.78	0.84
38:R:415:LEU:O	38:R:417:ASN:N	2.09	0.84
1:A:755:HIS:CE1	37:P:223:PHE:CB	2.60	0.84
3:C:711:ARG:HD3	3:C:730:ARG:HE	1.42	0.84
1:A:167:PRO:HD2	34:M:192:THR:HB	1.57	0.84
1:A:1505:LYS:HE2	46:Z:615:SER:CB	2.07	0.84
3:C:244:LYS:HA	3:C:292:TYR:CD2	2.13	0.84
3:C:365:SER:OG	3:C:371:GLU:OE2	1.95	0.84
3:C:725:ASP:OD1	3:C:727:LEU:N	2.10	0.84
15:H:78:C:O2'	15:H:79:G:H5'	1.77	0.84
38:R:178:ARG:HD3	38:R:194:GLN:NE2	1.91	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1426:ASP:CB	38:R:421:GLY:HA3	2.08	0.84
1:A:1457:HIS:CE1	1:A:1459:ARG:CG	2.61	0.84
1:A:1457:HIS:NE2	38:R:424:SER:HA	1.93	0.83
3:C:705:VAL:HG21	3:C:717:PHE:HE2	1.40	0.83
1:A:254:TYR:CE2	1:A:434:HIS:CB	2.61	0.83
1:A:1342:TRP:CZ2	3:C:921:LEU:HD13	2.13	0.83
3:C:79:THR:C	3:C:80:ILE:HD12	1.98	0.83
3:C:348:TYR:CD1	3:C:359:LYS:HB3	2.13	0.83
15:H:71:C:O2'	15:H:72:U:H5'	1.78	0.83
46:Z:566:TYR:CE2	46:Z:584:TRP:CE3	2.66	0.83
3:C:488:VAL:CG1	3:C:609:LYS:HE2	2.08	0.83
14:G:22:C:O2'	14:G:23:U:OP1	1.95	0.83
15:H:152:G:N2	15:H:153:A:N7	2.27	0.83
1:A:168:PRO:HG3	1:A:559:ASP:CB	2.07	0.83
5:E:74:PHE:CE1	5:E:81:LEU:CD2	2.62	0.83
45:Y:37:TRP:CZ2	46:Z:498:GLY:HA2	2.08	0.83
1:A:1757:GLU:CD	38:R:451:ILE:CG1	2.47	0.83
3:C:151:GLU:OE1	3:C:417:ARG:NH2	2.11	0.83
15:H:70:C:O2'	15:H:71:C:H5'	1.78	0.83
23:3:442:LEU:O	23:3:735:SER:N	2.10	0.83
38:R:117:THR:O	38:R:120:VAL:HG12	1.78	0.83
1:A:365:VAL:HG12	1:A:366:LYS:H	1.44	0.83
3:C:77:VAL:CG1	40:T:196:LEU:CG	2.35	0.83
1:A:1342:TRP:CH2	3:C:921:LEU:HD13	2.12	0.83
3:C:80:ILE:N	40:T:199:VAL:O	2.12	0.83
1:A:303:ILE:CG2	3:C:933:PHE:CE1	2.62	0.83
1:A:587:GLN:HB2	1:A:1549:VAL:HA	1.59	0.83
3:C:824:THR:HG23	3:C:824:THR:O	1.77	0.83
38:R:134:ARG:O	38:R:136:ASP:N	2.12	0.83
1:A:1457:HIS:HE1	1:A:1459:ARG:HG2	1.43	0.83
1:A:1900:GLU:OE2	46:Z:521:PRO:CB	2.26	0.83
3:C:145:PHE:CA	3:C:312:SER:HB3	2.04	0.83
15:H:72:U:O2'	15:H:73:C:H5'	1.77	0.83
3:C:470:PRO:HB3	3:C:500:THR:CG2	2.08	0.82
21:1:1108:ASN:ND2	21:1:1111:CYS:SG	2.52	0.82
15:H:73:C:O2'	15:H:74:U:H5'	1.79	0.82
1:A:1084:PRO:HG2	37:P:188:TRP:CZ2	2.12	0.82
1:A:1293:ASN:ND2	41:U:14:GLY:HA2	1.94	0.82
3:C:220:ARG:NH1	3:C:578:ARG:O	2.12	0.82
3:C:228:PHE:CB	3:C:256:CYS:O	2.27	0.82
3:C:482:TYR:HE2	3:C:493:PHE:CG	1.97	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:165:GLN:O	5:E:166:LEU:HD23	1.79	0.82
28:J:259:GLN:NE2	29:L:220:PRO:HD2	1.94	0.82
3:C:705:VAL:CB	3:C:717:PHE:CE2	2.61	0.82
14:G:11:A:C4	14:G:12:G:C8	2.67	0.82
15:H:69:U:O2'	15:H:70:C:H5'	1.80	0.82
38:R:103:ARG:HB3	38:R:103:ARG:HH11	1.44	0.82
1:A:532:THR:HG21	14:G:2:U:H5"	1.62	0.82
15:H:81:G:O2'	15:H:82:G:H5'	1.78	0.82
3:C:140:HIS:ND1	3:C:230:ASP:HB3	1.94	0.82
23:3:304:GLN:HE21	23:3:308:GLY:HA2	1.44	0.82
43:W:209:SER:O	43:W:213:GLN:N	2.12	0.82
1:A:132:ILE:CD1	2:B:57:G:OP1	2.27	0.82
3:C:489:GLN:O	3:C:489:GLN:NE2	2.13	0.82
15:H:105:G:C2'	15:H:106:G:H5"	2.10	0.82
37:P:30:TYR:OH	38:R:162:ALA:CA	2.27	0.82
1:A:615:ARG:O	1:A:618:THR:OG1	1.96	0.82
1:A:1342:TRP:CE3	3:C:921:LEU:CD2	2.62	0.82
1:A:1457:HIS:CE1	1:A:1459:ARG:HG2	2.15	0.82
3:C:259:LYS:HG2	3:C:262:ARG:CD	2.09	0.82
37:P:212:ASN:HB3	40:T:458:SER:HB2	1.61	0.82
1:A:1370:ARG:NH1	42:V:466:SER:O	2.10	0.82
1:A:303:ILE:CG2	3:C:933:PHE:HE1	1.93	0.81
1:A:2113:LYS:HE3	4:D:1229:ASP:C	2.01	0.81
5:E:74:PHE:CE2	5:E:343:ILE:HG12	2.14	0.81
45:Y:37:TRP:HA	45:Y:82:LEU:O	1.80	0.81
1:A:1900:GLU:CG	46:Z:521:PRO:HG2	2.09	0.81
3:C:64:LYS:HE3	37:P:206:LYS:CE	2.10	0.81
3:C:244:LYS:HB2	3:C:292:TYR:CE2	2.15	0.81
3:C:306:ASN:OD1	3:C:437:HIS:ND1	2.14	0.81
3:C:507:VAL:CG1	3:C:565:ILE:HG23	2.10	0.81
22:2:643:PRO:HD2	24:4:69:TYR:CD2	2.16	0.81
23:3:42:ARG:HE	23:3:53:LEU:HD11	1.45	0.81
23:3:210:PHE:HB2	23:3:224:TYR:HB2	1.60	0.81
26:6:49:CYS:HB3	26:6:87:LYS:HD3	1.61	0.81
35:N:111:THR:HG21	35:N:115:THR:O	1.79	0.81
37:P:193:VAL:HG23	37:P:194:PHE:CG	2.15	0.81
23:3:772:ALA:HB1	23:3:775:ASN:HD21	1.44	0.81
40:T:213:GLU:HG3	40:T:218:TRP:CE2	2.16	0.81
1:A:121:HIS:HA	1:A:482:PHE:HA	1.62	0.81
1:A:651:TRP:NE1	13:F:66:C:O2	2.14	0.81
3:C:511:GLY:O	3:C:576:ILE:HD13	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:R:443:GLY:HA2	38:R:446:ASP:HB3	1.62	0.81
39:S:39:PHE:CD2	39:S:129:PHE:CE2	2.68	0.81
1:A:247:THR:OG1	1:A:429:ASN:HB3	1.80	0.81
1:A:402:ILE:HG21	3:C:268:LYS:HE3	1.62	0.81
1:A:623:LYS:O	50:A:3000:IHP:O44	1.99	0.81
1:A:1184:ASN:OD1	1:A:1195:ARG:NH1	2.14	0.81
1:A:1426:ASP:HB2	38:R:421:GLY:CA	2.11	0.81
3:C:452:THR:HG21	3:C:577:PHE:HD2	1.43	0.81
5:E:74:PHE:CZ	5:E:81:LEU:HD21	2.16	0.81
5:E:281:VAL:CG2	43:W:148:VAL:HA	2.10	0.81
36:O:229:LYS:HG3	36:O:277:ARG:HH12	1.45	0.81
1:A:235:MET:HE1	1:A:411:PHE:HA	1.61	0.81
1:A:705:LYS:HB2	38:R:251:ILE:CD1	2.07	0.81
1:A:228:TRP:N	1:A:416:GLY:O	2.14	0.81
1:A:907:PRO:HD3	37:P:229:LYS:HB2	1.63	0.81
3:C:96:PRO:HA	37:P:48:GLN:HE21	1.44	0.81
3:C:140:HIS:NE2	3:C:233:GLU:HG3	1.95	0.81
39:S:39:PHE:CD1	39:S:129:PHE:HE2	1.97	0.81
1:A:296:PHE:CD1	3:C:656:ALA:HB2	2.16	0.81
3:C:140:HIS:ND1	3:C:230:ASP:N	2.28	0.81
3:C:452:THR:CB	3:C:577:PHE:HD2	1.93	0.81
3:C:507:VAL:HG11	3:C:565:ILE:CG2	2.09	0.81
3:C:711:ARG:HD3	3:C:730:ARG:NE	1.96	0.81
14:G:26:U:C1'	36:O:269:CYS:SG	2.68	0.81
15:H:183:G:H2'	15:H:184:C:H6	1.44	0.80
36:O:220:MET:SD	36:O:222:ARG:CB	2.70	0.80
1:A:461:HIS:CE1	2:B:23:C:C6	2.69	0.80
15:H:83:A:H2'	15:H:84:C:C1'	2.10	0.80
23:3:440:HIS:CG	23:3:733:PRO:HG3	2.15	0.80
2:B:18:C:O2'	2:B:19:A:O5'	1.98	0.80
13:F:68:C:H41	37:P:33:ARG:HB3	1.45	0.80
28:J:273:TYR:CE1	38:R:228:PRO:HB3	2.17	0.80
1:A:318:TYR:HB2	3:C:638:ASP:OD1	1.80	0.80
14:G:134:U:H3	15:H:42:G:H1	1.24	0.80
23:3:979:ARG:HD2	23:3:982:GLU:HB2	1.63	0.80
36:O:235:TYR:HD2	36:O:301:LYS:HB2	1.45	0.80
38:R:65:PRO:HG2	38:R:66:GLU:OE2	1.79	0.80
15:H:149:A:H2'	15:H:150:U:H6	1.44	0.80
22:2:682:LEU:HD13	22:2:687:PHE:HA	1.63	0.80
33:Q:500:GLY:N	38:R:51:ILE:CD1	2.44	0.80
1:A:748:ASP:CA	37:P:214:THR:HG21	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:705:VAL:CG2	3:C:717:PHE:HE2	1.84	0.80
15:H:82:G:O2'	15:H:83:A:H5'	1.81	0.80
1:A:596:TYR:CD2	14:G:-5:G:C6	2.70	0.80
3:C:87:GLN:OE1	3:C:91:GLU:HG2	1.82	0.80
3:C:140:HIS:CE1	3:C:230:ASP:HB3	2.16	0.80
3:C:776:GLU:O	3:C:781:ASP:OD1	2.00	0.80
5:E:265:ARG:H	5:E:272:ARG:NH2	1.80	0.80
13:F:68:C:N3	37:P:33:ARG:HG2	1.97	0.80
15:H:152:G:H5"	15:H:153:A:OP2	1.80	0.80
21:1:732:TRP:HE1	21:1:768:GLU:HG2	1.47	0.80
1:A:439:GLN:O	1:A:444:ARG:NH1	2.14	0.80
1:A:1764:SER:HB3	1:A:1766:GLN:HG2	1.64	0.80
2:B:31:U:H5"	37:P:32:SER:OG	1.81	0.80
1:A:245:LEU:HA	1:A:430:TRP:HZ2	1.46	0.80
1:A:264:PHE:HE1	1:A:455:VAL:CG1	1.94	0.80
1:A:293:TRP:CZ3	1:A:295:GLU:OE1	2.35	0.80
1:A:301:LYS:CE	3:C:940:ARG:HA	2.12	0.80
1:A:481:PHE:CE2	38:R:205:ASP:HA	2.17	0.80
3:C:445:ALA:HB1	3:C:449:ILE:HD11	1.63	0.80
3:C:738:ASP:HB2	3:C:740:THR:O	1.82	0.80
36:O:20:PHE:CE1	38:R:177:ILE:HD11	2.17	0.80
1:A:2314:PHE:HB3	4:D:1125:SER:CA	2.11	0.80
5:E:248:SER:HB2	5:E:249:TYR:CD1	2.17	0.80
13:F:22:A:C5'	35:N:116:ASN:O	2.30	0.80
23:3:637:PRO:HA	23:3:669:LEU:HA	1.63	0.80
24:4:28:LEU:O	24:4:32:LEU:CB	2.27	0.80
36:O:225:PRO:HB3	36:O:302:TRP:CE2	2.17	0.80
1:A:374:ASP:HB2	3:C:355:LYS:HD3	1.64	0.79
1:A:387:PHE:CD2	3:C:399:LEU:HD23	2.17	0.79
2:B:90:U:H5"	2:B:91:U:H5'	1.65	0.79
5:E:209:ILE:HG21	5:E:250:LEU:CD1	2.12	0.79
23:3:442:LEU:HD12	23:3:734:LEU:HD23	1.64	0.79
23:3:477:SER:HA	23:3:482:THR:HG22	1.65	0.79
29:L:222:LEU:H	29:L:222:LEU:HD22	1.45	0.79
1:A:825:ILE:HB	1:A:1001:VAL:HG12	1.65	0.79
3:C:145:PHE:N	3:C:312:SER:CB	2.41	0.79
14:G:-8:U:C6	41:U:16:ASN:HA	2.17	0.79
14:G:21:A:OP2	36:O:156:TYR:OH	1.99	0.79
39:S:11:PRO:CB	39:S:166:GLY:HA3	2.12	0.79
1:A:283:VAL:O	1:A:284:ARG:NE	2.15	0.79
29:L:216:PHE:HE1	36:O:112:VAL:O	1.66	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:T:292:TYR:CZ	40:T:308:ARG:HG3	2.18	0.79
1:A:546:LEU:CD1	1:A:595:LYS:HD2	2.06	0.79
3:C:77:VAL:HG11	40:T:196:LEU:HG	0.79	0.79
5:E:310:TYR:CE1	5:E:322:LYS:HD2	2.18	0.79
40:T:306:CYS:SG	40:T:336:VAL:HB	2.22	0.79
1:A:596:TYR:CZ	14:G:-5:G:C8	2.71	0.79
23:3:772:ALA:CB	23:3:775:ASN:HD21	1.95	0.79
43:W:212:GLU:O	43:W:214:LYS:N	2.14	0.79
1:A:1876:LEU:HD12	1:A:1884:ILE:HD11	1.65	0.79
3:C:244:LYS:HB2	3:C:292:TYR:HE2	1.47	0.79
15:H:153:A:H2'	15:H:154:C:H5'	1.65	0.79
38:R:67:ILE:HG22	38:R:69:VAL:HG23	1.65	0.79
39:S:34:LYS:HE3	39:S:78:TYR:HE2	1.47	0.79
37:P:212:ASN:O	40:T:458:SER:CA	2.23	0.79
38:R:420:LYS:HG3	38:R:421:GLY:N	1.97	0.79
40:T:351:ASP:O	40:T:352:THR:OG1	1.98	0.79
3:C:515:THR:O	3:C:517:GLU:N	2.16	0.79
3:C:705:VAL:HB	3:C:717:PHE:CE2	2.18	0.79
1:A:73:HIS:CD2	1:A:81:PHE:CD2	2.57	0.79
3:C:140:HIS:ND1	3:C:230:ASP:CB	2.46	0.79
3:C:259:LYS:HE2	3:C:262:ARG:CD	2.13	0.79
15:H:68:G:H1	15:H:84:C:H42	1.29	0.79
15:H:79:G:H2'	15:H:80:A:C8	2.17	0.79
1:A:596:TYR:CE2	14:G:-5:G:C5	2.71	0.78
1:A:602:ILE:CG2	1:A:1548:TYR:OH	2.32	0.78
13:F:34:G:N7	14:G:12:G:O6	2.16	0.78
15:H:101:U:H5"	15:H:102:U:H5'	1.64	0.78
46:Z:593:PHE:O	46:Z:597:ARG:HB2	1.83	0.78
1:A:1342:TRP:CE3	3:C:921:LEU:CD1	2.53	0.78
1:A:1767:ASN:O	1:A:1771:LEU:HB2	1.82	0.78
13:F:27:A:C4	36:O:181:TYR:CZ	2.71	0.78
39:S:111:GLN:NE2	43:W:93:PHE:CB	2.46	0.78
1:A:718:ARG:NH2	38:R:259:LYS:HE3	1.98	0.78
15:H:82:G:H2'	15:H:83:A:C8	2.17	0.78
23:3:1109:LEU:HD11	23:3:1128:ILE:HG21	1.65	0.78
1:A:695:ASP:OD2	40:T:350:HIS:HB3	1.83	0.78
23:3:641:CYS:HB2	23:3:701:LEU:HB3	1.64	0.78
39:S:39:PHE:HB3	39:S:129:PHE:HZ	1.26	0.78
41:U:1:MET:SD	41:U:1:MET:N	2.54	0.78
1:A:664:HIS:NE2	1:A:666:LYS:HD3	1.98	0.78
23:3:435:LEU:HD22	23:3:799:ILE:HD11	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:440:HIS:HE1	23:3:733:PRO:HD3	1.46	0.78
1:A:312:TYR:OH	3:C:853:ARG:NH2	2.17	0.78
38:R:132:LEU:HB3	40:T:399:LYS:NZ	1.99	0.78
1:A:299:ILE:HD12	3:C:921:LEU:HB2	1.66	0.78
1:A:705:LYS:HG2	38:R:251:ILE:HD12	1.65	0.78
1:A:758:ARG:CB	37:P:227:TYR:CE2	2.64	0.78
40:T:387:PHE:CE1	40:T:398:TRP:CD1	2.72	0.78
43:W:277:PRO:CB	43:W:578:TRP:C	2.51	0.78
24:4:17:VAL:HG22	24:4:86:VAL:HG22	1.66	0.78
40:T:434:GLY:HA2	40:T:464:GLY:CA	2.14	0.78
1:A:468:LYS:HD3	1:A:469:LYS:N	1.99	0.78
1:A:1505:LYS:HD2	46:Z:615:SER:HB3	1.66	0.78
3:C:133:THR:HB	3:C:225:VAL:HG23	1.65	0.78
23:3:295:THR:HG22	23:3:297:SER:H	1.48	0.78
36:O:149:LYS:HZ3	36:O:290:LYS:CG	1.97	0.78
3:C:452:THR:HG21	3:C:577:PHE:CD2	2.16	0.78
22:2:649:LYS:HB3	22:2:655:SER:HB2	1.65	0.78
24:4:17:VAL:O	24:4:56:TYR:HA	1.83	0.78
36:O:131:THR:HG23	43:W:111:LEU:H	1.48	0.78
37:P:224:MET:HE2	37:P:228:ILE:HD13	1.63	0.78
40:T:267:ASP:HB3	40:T:269:GLN:HG2	1.64	0.78
1:A:692:ASP:CA	40:T:376:ARG:HH22	1.97	0.77
1:A:919:ASP:OD2	1:A:1012:LYS:NZ	2.17	0.77
1:A:1838:LYS:HG2	1:A:1871:PRO:HG2	1.66	0.77
21:1:1053:ARG:NH1	22:2:559:PRO:O	2.17	0.77
23:3:590:MET:HG2	23:3:607:VAL:HA	1.63	0.77
23:3:805:ASN:ND2	23:3:858:GLY:O	2.14	0.77
1:A:168:PRO:HG2	1:A:559:ASP:HB3	1.64	0.77
3:C:449:ILE:HG21	3:C:457:VAL:HG12	1.66	0.77
3:C:677:GLU:OE2	3:C:684:LYS:HG2	1.83	0.77
21:1:941:ASN:HA	21:1:948:ARG:HH22	1.48	0.77
1:A:666:LYS:HB3	1:A:668:VAL:HG23	1.66	0.77
1:A:1405:LEU:CA	38:R:415:LEU:CD2	2.62	0.77
2:B:43:U:H5'	13:F:67:G:N2	1.98	0.77
3:C:449:ILE:CD1	3:C:466:SER:OG	2.33	0.77
15:H:80:A:H2'	15:H:81:G:C8	2.19	0.77
24:4:69:TYR:CE1	24:4:73:ILE:HG13	2.19	0.77
39:S:11:PRO:HB2	39:S:165:SER:O	1.83	0.77
46:Z:595:GLN:O	46:Z:599:ALA:N	2.14	0.77
1:A:456:LEU:O	1:A:460:LYS:HG2	1.84	0.77
1:A:1352:HIS:ND1	41:U:21:ARG:HA	1.98	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:140:HIS:HA	3:C:259:LYS:HZ3	1.47	0.77
3:C:349:PHE:CD1	3:C:356:PHE:CD1	2.68	0.77
5:E:277:PHE:HE2	5:E:300:ILE:CD1	1.98	0.77
13:F:8:C:H5"	13:F:8:C:C6	2.19	0.77
23:3:474:ILE:O	23:3:485:LEU:HB2	1.83	0.77
23:3:772:ALA:HB1	23:3:775:ASN:ND2	1.99	0.77
36:O:292:ILE:HG12	36:O:297:ARG:HA	1.66	0.77
1:A:651:TRP:CE2	13:F:66:C:C2	2.72	0.77
3:C:85:ASP:CB	40:T:238:LEU:HG	2.14	0.77
3:C:151:GLU:OE1	3:C:417:ARG:CZ	2.33	0.77
14:G:11:A:H2'	14:G:12:G:O4'	1.84	0.77
36:O:45:CYS:SG	53:O:502:ZN:ZN	1.71	0.77
45:Y:86:ASP:HA	46:Z:502:ALA:HB3	1.65	0.77
1:A:152:ARG:HH11	1:A:152:ARG:CB	1.97	0.77
1:A:362:ARG:O	1:A:362:ARG:NE	2.18	0.77
1:A:1505:LYS:CE	46:Z:615:SER:CB	2.62	0.77
28:J:291:GLN:NE2	29:L:230:GLU:OE2	2.17	0.77
40:T:318:ARG:HG3	40:T:319:THR:HG23	1.67	0.77
1:A:1757:GLU:OE2	38:R:451:ILE:HD11	1.85	0.77
3:C:482:TYR:HE2	3:C:493:PHE:CB	1.98	0.77
46:Z:603:SER:O	46:Z:607:VAL:HG23	1.84	0.77
1:A:43:LYS:HD2	43:W:168:PHE:CB	2.14	0.77
1:A:203:VAL:HG21	1:A:237:THR:CG2	2.14	0.77
1:A:1426:ASP:HB2	38:R:421:GLY:HA3	1.64	0.77
3:C:145:PHE:CZ	3:C:427:PHE:CE1	2.73	0.77
3:C:471:ASP:H	3:C:499:GLY:HA2	1.47	0.77
5:E:74:PHE:CD1	5:E:81:LEU:CD2	2.67	0.77
23:3:785:PRO:HA	23:3:800:ILE:O	1.84	0.77
1:A:623:LYS:CB	50:A:3000:IHP:O34	2.33	0.77
1:A:1342:TRP:HE3	3:C:921:LEU:HD22	1.49	0.77
3:C:567:GLU:HG2	3:C:572:GLU:OE2	1.85	0.77
15:H:177:A:H5"	15:H:178:A:OP1	1.84	0.77
23:3:981:CYS:SG	23:3:982:GLU:N	2.57	0.77
39:S:11:PRO:HB3	39:S:166:GLY:CA	2.14	0.77
1:A:782:LEU:HD13	37:P:220:HIS:CE1	2.18	0.76
3:C:82:GLN:CB	40:T:231:TRP:HZ3	1.98	0.76
3:C:711:ARG:HD3	3:C:730:ARG:CZ	2.16	0.76
5:E:146:ARG:HH12	5:E:148:LYS:HE3	1.49	0.76
36:O:132:ARG:NH1	39:S:149:SER:CB	2.46	0.76
36:O:149:LYS:NZ	36:O:290:LYS:HG2	1.99	0.76
36:O:177:GLU:OE1	36:O:177:GLU:N	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LEU:HD12	1:A:484:SER:HB2	1.67	0.76
1:A:630:TRP:O	1:A:632:ALA:N	2.18	0.76
21:1:473:GLN:HE22	25:5:93:ASN:H	1.33	0.76
38:R:420:LYS:HG2	38:R:423:ASP:OD2	1.84	0.76
1:A:43:LYS:CD	43:W:168:PHE:CB	2.63	0.76
1:A:230:PHE:N	1:A:414:ARG:O	2.18	0.76
1:A:705:LYS:CB	38:R:251:ILE:CD1	2.59	0.76
3:C:449:ILE:HD11	3:C:466:SER:N	1.99	0.76
15:H:143:A:H3'	15:H:143:A:N3	2.01	0.76
39:S:9:TRP:CZ2	39:S:44:ARG:HD3	2.20	0.76
39:S:13:ASN:HA	39:S:25:LEU:O	1.85	0.76
3:C:261:ASP:CG	51:C:1500:GTP:HN1	1.88	0.76
5:E:162:ARG:NH2	5:E:204:THR:HA	1.99	0.76
15:H:148:C:H2'	15:H:149:A:H8	1.48	0.76
39:S:9:TRP:HE3	39:S:11:PRO:HD3	1.49	0.76
1:A:1342:TRP:CB	3:C:921:LEU:HD21	2.13	0.76
3:C:471:ASP:OD1	3:C:472:GLY:N	2.19	0.76
22:2:611:ASP:O	22:2:614:ARG:HB3	1.86	0.76
38:R:412:ASP:CG	38:R:413:GLN:N	2.39	0.76
39:S:10:GLN:HA	39:S:29:TRP:CZ2	2.20	0.76
1:A:755:HIS:HA	37:P:223:PHE:CE1	2.20	0.76
23:3:423:LEU:HB2	23:3:438:LEU:HB2	1.66	0.76
1:A:529:THR:HG21	34:M:199:PRO:CG	2.16	0.76
15:H:168:A:H5'	15:H:169:C:OP2	1.86	0.76
46:Z:566:TYR:HD2	46:Z:580:PRO:HG2	1.50	0.76
3:C:750:LEU:O	3:C:754:VAL:HG23	1.84	0.76
13:F:40:U:H2'	13:F:41:A:C8	2.20	0.76
23:3:328:LYS:HB2	23:3:372:GLU:HG3	1.68	0.76
42:V:548:ALA:HB1	42:V:586:PHE:N	2.00	0.76
1:A:779:LEU:CD2	37:P:223:PHE:CE2	2.69	0.76
1:A:1301:ILE:HD11	1:A:1306:LYS:HE2	1.68	0.76
5:E:231:MET:HB3	5:E:262:TRP:CZ3	2.21	0.76
1:A:1162:PRO:CG	37:P:194:PHE:CD2	2.69	0.75
23:3:11:ALA:O	23:3:34:ARG:NH1	2.17	0.75
36:O:149:LYS:HG2	36:O:290:LYS:HZ3	1.49	0.75
46:Z:594:GLU:O	46:Z:598:PHE:HB2	1.86	0.75
1:A:318:TYR:N	3:C:638:ASP:OD1	2.19	0.75
32:I:720:ILE:O	32:I:721:LYS:CB	2.34	0.75
1:A:229:GLN:HG2	1:A:415:SER:HB2	1.68	0.75
1:A:532:THR:OG1	14:G:2:U:C5'	2.34	0.75
3:C:149:LEU:CD1	3:C:427:PHE:CG	2.53	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:593:GLU:HG3	3:C:594:PRO:HD2	1.67	0.75
14:G:132:G:H1	15:H:44:U:H3	1.34	0.75
23:3:784:THR:O	23:3:786:ARG:NH1	2.18	0.75
35:N:28:LYS:NZ	43:W:190:ASP:HA	2.01	0.75
38:R:66:GLU:OE2	38:R:66:GLU:N	2.19	0.75
38:R:181:PRO:O	38:R:182:SER:HB2	1.84	0.75
39:S:119:THR:OG1	39:S:122:LEU:HD12	1.87	0.75
1:A:318:TYR:CB	3:C:638:ASP:OD1	2.35	0.75
14:G:11:A:C4	14:G:12:G:H8	2.04	0.75
15:H:81:G:H2'	15:H:82:G:C8	2.19	0.75
23:3:905:VAL:HB	23:3:928:TYR:HB2	1.68	0.75
1:A:402:ILE:CG2	3:C:268:LYS:HZ1	1.97	0.75
1:A:1951:LYS:HD3	46:Z:521:PRO:O	1.85	0.75
23:3:720:TRP:HB3	23:3:731:LEU:HD11	1.69	0.75
36:O:20:PHE:CD1	38:R:177:ILE:CD1	2.70	0.75
3:C:470:PRO:HA	3:C:499:GLY:HA2	1.67	0.75
3:C:711:ARG:CD	3:C:730:ARG:HE	1.99	0.75
15:H:10:C:H2'	15:H:11:G:H8	1.52	0.75
23:3:441:GLY:HA3	23:3:734:LEU:O	1.85	0.75
23:3:1105:GLN:O	23:3:1118:VAL:HB	1.87	0.75
1:A:1762:TYR:O	1:A:1768:TYR:OH	2.05	0.75
13:F:36:A:C3'	13:F:37:C:H5"	2.16	0.75
28:J:339:TRP:CE3	38:R:116:TYR:HD2	2.04	0.75
42:V:515:CYS:HA	42:V:521:TYR:CB	2.17	0.75
3:C:82:GLN:HB2	40:T:231:TRP:HZ3	1.50	0.75
3:C:465:MET:HE1	3:C:475:MET:CG	2.13	0.75
15:H:71:C:H2'	15:H:72:U:C6	2.21	0.75
15:H:153:A:C2'	15:H:154:C:H5'	2.17	0.75
3:C:348:TYR:CE1	3:C:359:LYS:HB3	2.22	0.74
3:C:510:LEU:HD22	3:C:514:TYR:CE2	2.22	0.74
28:J:256:LYS:O	29:L:232:TYR:HD2	1.66	0.74
28:J:273:TYR:CG	38:R:228:PRO:HG2	2.21	0.74
1:A:1405:LEU:CA	38:R:415:LEU:HD21	2.15	0.74
1:A:1784:ASN:HD22	1:A:1897:LEU:HD12	1.50	0.74
1:A:2073:TRP:CD1	1:A:2074:ARG:HD2	2.22	0.74
3:C:449:ILE:CG2	3:C:457:VAL:HG12	2.17	0.74
36:O:225:PRO:CB	36:O:302:TRP:HE1	2.00	0.74
1:A:339:PHE:HE1	1:A:406:TRP:CZ3	2.01	0.74
1:A:532:THR:CG2	14:G:2:U:P	2.75	0.74
1:A:783:TYR:CB	37:P:228:ILE:HG12	2.17	0.74
46:Z:525:TYR:HD1	46:Z:526:ILE:HG23	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:LYS:CB	1:A:668:VAL:HG23	2.17	0.74
23:3:437:VAL:O	23:3:776:GLN:HA	1.87	0.74
43:W:198:LYS:O	43:W:199:TYR:O	2.04	0.74
1:A:318:TYR:C	3:C:638:ASP:OD1	2.25	0.74
1:A:380:LEU:O	3:C:354:ARG:CG	2.30	0.74
1:A:1457:HIS:CD2	38:R:425:GLY:H	2.04	0.74
3:C:137:HIS:CG	3:C:236:MET:HB2	2.22	0.74
15:H:180:G:O2'	15:H:181:G:H5'	1.88	0.74
38:R:70:ALA:O	38:R:71:GLN:O	2.05	0.74
1:A:73:HIS:NE2	1:A:81:PHE:CZ	2.51	0.74
1:A:203:VAL:CG2	1:A:237:THR:CG2	2.66	0.74
1:A:305:ARG:HB2	3:C:879:ASP:OD1	1.88	0.74
1:A:1405:LEU:HA	38:R:415:LEU:CD2	2.17	0.74
23:3:294:LYS:O	23:3:343:LYS:NZ	2.21	0.74
23:3:931:VAL:HG12	23:3:932:ASN:H	1.53	0.74
39:S:131:ARG:NH1	39:S:132:VAL:O	2.20	0.74
1:A:132:ILE:HD11	2:B:57:G:OP1	1.88	0.74
5:E:258:THR:HG22	5:E:260:ARG:HG2	1.68	0.74
1:A:744:LYS:HE3	37:P:213:ASP:HA	1.70	0.74
3:C:140:HIS:CA	3:C:230:ASP:HB2	2.17	0.74
13:F:34:G:H5"	13:F:34:G:N3	2.03	0.74
36:O:225:PRO:CB	36:O:302:TRP:NE1	2.50	0.74
38:R:422:MET:O	38:R:424:SER:N	2.17	0.74
40:T:385:TYR:O	40:T:400:PHE:HB2	1.88	0.74
1:A:260:LEU:HD23	1:A:455:VAL:HG22	1.70	0.74
3:C:445:ALA:HB1	3:C:449:ILE:CD1	2.17	0.74
13:F:1:G:O2'	35:N:99:ASN:ND2	2.20	0.74
1:A:380:LEU:CA	3:C:354:ARG:HG3	2.16	0.73
1:A:748:ASP:OD1	37:P:214:THR:CG2	2.36	0.73
5:E:243:LEU:HD11	5:E:247:GLY:HA2	1.68	0.73
1:A:176:LEU:HD13	1:A:181:ASN:HD22	1.52	0.73
23:3:555:VAL:HG23	23:3:592:LEU:HD22	1.70	0.73
28:J:406:PHE:CD2	28:J:411:MET:CE	2.70	0.73
1:A:312:TYR:CE2	3:C:882:GLY:HA3	2.23	0.73
1:A:593:ARG:HD3	14:G:-4:A:H4'	1.70	0.73
5:E:119:THR:HG21	5:E:161:ARG:CB	2.17	0.73
1:A:380:LEU:CB	3:C:354:ARG:CG	2.45	0.73
3:C:97:VAL:HG21	37:P:45:GLN:HG3	1.69	0.73
21:1:563:LEU:HD22	21:1:566:LEU:HD22	1.70	0.73
43:W:137:TYR:CB	43:W:159:ALA:HB2	2.17	0.73
1:A:1900:GLU:CD	46:Z:522:LEU:CB	2.55	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:42:U:C4'	13:F:70:A:H4'	2.18	0.73
3:C:94:ILE:HD11	37:P:44:ARG:NH2	2.03	0.73
23:3:772:ALA:O	23:3:775:ASN:ND2	2.21	0.73
1:A:294:ASN:OD1	3:C:654:LYS:HD3	1.89	0.73
1:A:530:LEU:HG	34:M:198:GLN:HE22	1.53	0.73
3:C:516:LEU:CD1	3:C:517:GLU:HG3	2.18	0.73
3:C:671:SER:O	3:C:672:LEU:HD13	1.89	0.73
15:H:69:U:H2'	15:H:70:C:C6	2.23	0.73
15:H:165:A:O2'	15:H:166:G:H5'	1.88	0.73
36:O:149:LYS:HG3	36:O:290:LYS:HZ1	1.54	0.73
36:O:247:ASP:OD2	36:O:294:ASN:ND2	2.21	0.73
39:S:131:ARG:NH1	39:S:133:CYS:CA	2.51	0.73
5:E:287:ASN:O	5:E:289:LEU:HD23	1.88	0.73
26:6:51:TYR:H	26:6:54:TYR:HB2	1.53	0.73
36:O:149:LYS:CG	36:O:290:LYS:HZ1	2.02	0.73
38:R:67:ILE:HG22	38:R:69:VAL:CG2	2.18	0.73
39:S:9:TRP:HZ2	39:S:44:ARG:HD3	1.52	0.73
39:S:100:MET:CG	39:S:108:ASN:OD1	2.36	0.73
1:A:1301:ILE:O	1:A:1303:LEU:O	2.06	0.73
1:A:2325:VAL:HG13	4:D:788:GLY:C	2.07	0.73
39:S:81:GLN:HA	39:S:108:ASN:O	1.88	0.73
1:A:2078:ILE:CG2	4:D:1047:PRO:CB	2.66	0.73
2:B:42:U:C2	14:G:-3:A:H2	2.07	0.73
15:H:106:G:H4'	15:H:107:A:O4'	1.89	0.73
23:3:1145:GLU:OE2	23:3:1149:ARG:NH2	2.21	0.73
28:J:339:TRP:CE3	38:R:116:TYR:CD2	2.76	0.73
43:W:101:THR:O	43:W:104:MET:N	2.22	0.73
3:C:711:ARG:CD	3:C:730:ARG:HH11	2.01	0.73
28:J:259:GLN:NE2	29:L:220:PRO:HD3	2.02	0.73
1:A:1290:LYS:HG2	41:U:13:SER:C	2.08	0.72
3:C:449:ILE:HG22	3:C:457:VAL:CG1	2.18	0.72
5:E:146:ARG:HH12	5:E:148:LYS:CE	1.99	0.72
5:E:250:LEU:HD23	5:E:250:LEU:O	1.88	0.72
15:H:70:C:H2'	15:H:71:C:C6	2.24	0.72
42:V:548:ALA:HB3	42:V:585:ILE:CB	2.19	0.72
1:A:1342:TRP:CZ2	3:C:921:LEU:CD1	2.71	0.72
3:C:508:LYS:HE3	3:C:566:THR:HG21	1.70	0.72
23:3:547:CYS:HA	23:3:555:VAL:O	1.89	0.72
40:T:434:GLY:CA	40:T:464:GLY:HA2	2.19	0.72
2:B:40:U:H4'	2:B:41:U:OP2	1.89	0.72
3:C:93:ILE:HD13	40:T:230:ILE:HD13	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:106:G:H21	15:H:107:A:N6	1.87	0.72
15:H:182:U:H2'	15:H:183:G:H8	1.53	0.72
21:1:428:ALA:O	21:1:432:THR:N	2.21	0.72
1:A:675:GLN:OE1	13:F:70:A:OP1	2.08	0.72
3:C:519:GLU:N	3:C:519:GLU:OE2	2.21	0.72
13:F:34:G:N3	13:F:34:G:H3'	2.05	0.72
1:A:549:GLU:OE1	1:A:552:ARG:NH1	2.23	0.72
1:A:1457:HIS:HE2	38:R:424:SER:CA	2.02	0.72
1:A:2324:GLU:HG2	1:A:2330:ARG:HH12	1.54	0.72
3:C:125:ASN:O	3:C:126:SER:OG	2.04	0.72
3:C:726:LEU:HD12	3:C:726:LEU:O	1.89	0.72
14:G:20:A:H1'	36:O:193:LEU:CD2	2.19	0.72
36:O:45:CYS:HG	53:O:502:ZN:ZN	1.01	0.72
40:T:352:THR:CG2	40:T:373:LYS:C	2.58	0.72
1:A:150:MET:SD	1:A:153:ARG:NH2	2.62	0.72
1:A:303:ILE:HD13	3:C:933:PHE:CD1	2.25	0.72
1:A:712:HIS:CE1	38:R:254:CYS:HB2	2.24	0.72
3:C:77:VAL:CG1	40:T:196:LEU:CA	2.68	0.72
3:C:449:ILE:HG21	3:C:457:VAL:HG11	1.70	0.72
13:F:5:U:H3'	13:F:7:G:H5"	1.71	0.72
1:A:1413:ASP:O	1:A:1418:ARG:NH1	2.21	0.72
1:A:2325:VAL:CG1	4:D:789:MET:HA	2.20	0.72
3:C:250:ARG:HE	3:C:451:HIS:CD2	2.07	0.72
23:3:442:LEU:CD1	23:3:734:LEU:HD23	2.19	0.72
1:A:107:PRO:O	1:A:111:GLU:OE1	2.08	0.72
1:A:193:LEU:HD12	1:A:194:GLU:H	1.55	0.72
1:A:1338:SER:OG	1:A:1351:THR:N	2.16	0.72
13:F:39:A:H61	14:G:8:C:H42	1.36	0.72
22:2:614:ARG:HG3	22:2:614:ARG:NH1	1.98	0.72
36:O:240:GLY:HA3	36:O:296:ARG:HH12	1.55	0.72
1:A:718:ARG:CZ	38:R:259:LYS:HE3	2.20	0.72
1:A:2078:ILE:HG21	4:D:1047:PRO:CB	2.20	0.72
5:E:264:VAL:HA	5:E:272:ARG:HH21	1.55	0.72
13:F:28:A:O4'	35:N:41:ARG:HA	1.90	0.72
23:3:783:TYR:HB2	23:3:801:GLU:HB3	1.72	0.72
43:W:491:GLN:O	43:W:493:ARG:N	2.23	0.72
1:A:785:LYS:HE3	37:P:215:LEU:HD11	1.71	0.72
2:B:42:U:O4'	13:F:70:A:H4'	1.89	0.72
15:H:165:A:C2'	15:H:166:G:H5'	2.20	0.72
23:3:440:HIS:CE1	23:3:720:TRP:HZ3	1.96	0.72
1:A:228:TRP:O	1:A:415:SER:CA	2.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:64:LYS:NZ	37:P:206:LYS:HG2	2.05	0.71
3:C:129:ILE:HA	3:C:199:LEU:O	1.90	0.71
1:A:203:VAL:HG23	1:A:237:THR:HG21	1.72	0.71
2:B:31:U:C5'	37:P:32:SER:OG	2.38	0.71
28:J:273:TYR:CE1	38:R:228:PRO:CB	2.72	0.71
29:L:224:PHE:CE1	38:R:86:LEU:CD1	2.73	0.71
37:P:66:ARG:HB2	37:P:66:ARG:HH11	1.55	0.71
1:A:168:PRO:CG	1:A:559:ASP:CB	2.64	0.71
1:A:529:THR:HG22	34:M:199:PRO:HD2	1.71	0.71
1:A:730:GLY:O	38:R:252:PRO:HG2	1.90	0.71
1:A:1402:ARG:HH22	46:Z:572:PRO:HA	1.53	0.71
21:1:1206:ASP:OD1	21:1:1207:SER:N	2.21	0.71
23:3:446:GLU:OE1	23:3:763:ARG:NH1	2.24	0.71
1:A:434:HIS:ND1	1:A:435:CYS:SG	2.62	0.71
1:A:462:ARG:HD2	1:A:462:ARG:N	2.05	0.71
15:H:153:A:H2'	15:H:154:C:C5'	2.19	0.71
21:1:405:ASP:HA	25:5:49:ARG:HH22	1.55	0.71
1:A:299:ILE:HD13	1:A:1346:THR:HG21	1.73	0.71
1:A:461:HIS:HD2	2:B:27:U:O4	1.71	0.71
3:C:706:GLN:HE21	3:C:708:THR:H	1.38	0.71
5:E:74:PHE:CE2	5:E:343:ILE:CG1	2.73	0.71
37:P:224:MET:CE	37:P:224:MET:HA	2.21	0.71
38:R:414:ARG:CZ	38:R:414:ARG:HB2	2.18	0.71
1:A:81:PHE:O	1:A:83:HIS:N	2.24	0.71
1:A:1962:THR:HG23	46:Z:524:ARG:HB2	1.68	0.71
3:C:700:ILE:HA	3:C:705:VAL:CG1	2.21	0.71
3:C:705:VAL:HG23	3:C:717:PHE:HD2	1.48	0.71
15:H:72:U:H2'	15:H:73:C:C6	2.26	0.71
1:A:76:MET:CE	1:A:506:LEU:HD11	2.21	0.71
1:A:264:PHE:CE2	1:A:459:LEU:CD1	2.73	0.71
1:A:1529:ILE:O	1:A:1532:ARG:N	2.24	0.71
3:C:80:ILE:HD12	3:C:80:ILE:N	2.05	0.71
3:C:94:ILE:HD13	37:P:44:ARG:CZ	2.20	0.71
3:C:441:PRO:O	3:C:444:GLY:HA3	1.90	0.71
3:C:490:PHE:CZ	3:C:612:LYS:HD2	2.26	0.71
36:O:235:TYR:HD1	36:O:271:PHE:HE1	1.37	0.71
37:P:191:ASP:N	37:P:191:ASP:OD1	2.23	0.71
43:W:277:PRO:CB	43:W:578:TRP:O	2.39	0.71
46:Z:612:TYR:O	46:Z:614:TRP:N	2.23	0.71
1:A:76:MET:HE3	1:A:506:LEU:HD11	1.72	0.71
1:A:1290:LYS:CG	41:U:13:SER:O	2.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:U:C4'	2:B:41:U:OP2	2.39	0.71
29:L:209:ASP:CG	36:O:111:ASP:HB2	2.11	0.71
42:V:549:LYS:O	42:V:552:ALA:HB3	1.91	0.71
1:A:365:VAL:HG12	1:A:366:LYS:N	2.06	0.71
1:A:402:ILE:HG21	3:C:268:LYS:HZ1	1.51	0.71
1:A:1459:ARG:CG	38:R:422:MET:O	2.39	0.71
1:A:2156:THR:OG1	1:A:2157:VAL:N	2.21	0.71
3:C:679:PRO:HG2	3:C:807:GLN:OE1	1.91	0.71
29:L:209:ASP:OD2	36:O:111:ASP:CB	2.30	0.71
38:R:422:MET:HG2	38:R:423:ASP:N	2.05	0.71
39:S:71:GLY:O	43:W:93:PHE:CB	2.39	0.71
1:A:705:LYS:HG2	38:R:251:ILE:CD1	2.21	0.71
1:A:1085:ILE:HG12	1:A:1099:PHE:HE1	1.56	0.71
21:1:1221:GLU:HG3	21:1:1223:SER:H	1.56	0.71
28:J:353:GLU:OE1	28:J:358:GLU:HB3	1.91	0.71
37:P:189:ASP:OD2	37:P:192:VAL:HG21	1.91	0.71
40:T:366:VAL:HG21	40:T:402:ASP:HA	1.72	0.71
1:A:719:CYS:SG	38:R:258:TRP:CH2	2.84	0.70
3:C:259:LYS:HG3	51:C:1500:GTP:C6	2.26	0.70
14:G:20:A:H1'	36:O:193:LEU:HD21	1.72	0.70
1:A:1342:TRP:CG	3:C:921:LEU:HD21	2.25	0.70
1:A:2328:ALA:HB3	4:D:788:GLY:N	2.05	0.70
15:H:160:A:O2'	15:H:161:U:H5'	1.90	0.70
29:L:209:ASP:CG	36:O:111:ASP:H	1.91	0.70
36:O:197:ASN:OD1	36:O:198:ILE:N	2.24	0.70
36:O:262:THR:HB	36:O:271:PHE:HB2	1.73	0.70
14:G:11:A:N3	14:G:11:A:H5"	2.05	0.70
15:H:168:A:N3	15:H:168:A:H2'	2.06	0.70
39:S:88:PRO:O	39:S:91:LYS:HE3	1.90	0.70
1:A:593:ARG:O	14:G:-4:A:H1'	1.91	0.70
13:F:24:A:H2	13:F:26:U:C2	2.09	0.70
36:O:144:SER:HA	36:O:148:LEU:HD13	1.73	0.70
38:R:189:ASN:HD21	38:R:195:ARG:NH2	1.90	0.70
40:T:267:ASP:O	40:T:268:LYS:HG3	1.91	0.70
1:A:171:ASP:O	1:A:520:TYR:CG	2.44	0.70
1:A:181:ASN:O	1:A:185:VAL:HG22	1.90	0.70
3:C:449:ILE:HD13	3:C:466:SER:OG	1.92	0.70
13:F:94:C:OP1	28:J:351:ASN:ND2	2.25	0.70
15:H:181:G:H2'	15:H:182:U:C6	2.26	0.70
21:1:901:GLN:HA	21:1:939:ARG:NH2	2.07	0.70
1:A:587:GLN:N	1:A:1549:VAL:HG12	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:L:216:PHE:CE1	36:O:112:VAL:HG12	2.25	0.70
38:R:103:ARG:HH11	38:R:103:ARG:CB	2.04	0.70
1:A:338:VAL:HG21	3:C:867:PRO:CG	2.22	0.70
3:C:457:VAL:CB	3:C:462:GLY:HA3	2.22	0.70
13:F:38:G:P	13:F:38:G:H8	2.14	0.70
13:F:68:C:C2	37:P:33:ARG:HG2	2.27	0.70
14:G:12:G:N3	14:G:12:G:H2'	2.07	0.70
21:1:1108:ASN:OD1	21:1:1110:VAL:N	2.25	0.70
42:V:536:ILE:O	42:V:578:SER:CB	2.39	0.70
43:W:101:THR:O	43:W:102:GLN:C	2.30	0.70
1:A:296:PHE:HE1	3:C:591:ALA:HB1	1.52	0.70
1:A:305:ARG:CG	3:C:879:ASP:OD1	2.39	0.70
1:A:1860:GLN:HG2	1:A:1883:VAL:HB	1.74	0.70
3:C:132:VAL:CG1	3:C:226:VAL:CG2	2.70	0.70
3:C:135:CYS:SG	3:C:227:LEU:CD1	2.80	0.70
13:F:27:A:H1'	36:O:181:TYR:CE2	2.23	0.70
14:G:-9:C:C6	41:U:18:TYR:CD1	2.80	0.70
38:R:220:ARG:NH1	38:R:220:ARG:HB2	2.06	0.70
39:S:10:GLN:HB3	39:S:29:TRP:CE3	2.27	0.70
39:S:39:PHE:HB2	39:S:129:PHE:HZ	1.10	0.70
1:A:76:MET:SD	1:A:88:TYR:CG	2.85	0.70
1:A:377:GLU:O	1:A:378:PHE:HB3	1.91	0.70
1:A:596:TYR:CD2	14:G:-5:G:C5	2.79	0.70
1:A:675:GLN:O	13:F:55:C:O2'	2.10	0.70
1:A:1318:THR:HB	1:A:1324:GLY:HA3	1.73	0.70
15:H:154:C:H2'	15:H:155:C:C6	2.27	0.70
21:1:1155:PHE:HA	21:1:1158:ILE:HG12	1.73	0.70
38:R:80:LYS:O	38:R:81:LYS:NZ	2.25	0.70
1:A:132:ILE:HD13	2:B:57:G:OP1	1.92	0.70
1:A:586:GLY:C	1:A:1549:VAL:CG1	2.59	0.70
1:A:719:CYS:SG	38:R:258:TRP:HH2	2.13	0.70
2:B:42:U:H4'	13:F:70:A:H5'	1.73	0.70
3:C:137:HIS:CE1	3:C:236:MET:SD	2.85	0.70
34:M:220:LEU:O	34:M:221:HIS:HB2	1.89	0.70
36:O:149:LYS:NZ	36:O:290:LYS:CG	2.55	0.70
1:A:481:PHE:CD2	38:R:205:ASP:HA	2.27	0.69
1:A:718:ARG:NE	38:R:259:LYS:HE3	2.06	0.69
3:C:452:THR:HB	3:C:577:PHE:CD2	2.26	0.69
23:3:722:SER:HA	23:3:730:HIS:O	1.92	0.69
1:A:461:HIS:CD2	2:B:26:A:N6	2.60	0.69
1:A:673:THR:O	1:A:677:VAL:HG23	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:64:LYS:NZ	37:P:206:LYS:CG	2.55	0.69
3:C:452:THR:O	3:C:577:PHE:HA	1.92	0.69
5:E:74:PHE:HE2	5:E:343:ILE:HG12	1.54	0.69
5:E:264:VAL:HA	5:E:272:ARG:NH2	2.07	0.69
36:O:48:CYS:SG	36:O:71:CYS:SG	2.91	0.69
1:A:529:THR:CG2	34:M:199:PRO:HD2	2.19	0.69
1:A:974:ASN:HB2	1:A:1178:TYR:HB3	1.73	0.69
1:A:71:ARG:HD2	1:A:177:ASP:OD2	1.92	0.69
1:A:338:VAL:CB	3:C:867:PRO:HG3	2.21	0.69
1:A:805:GLU:CB	37:P:194:PHE:HZ	2.04	0.69
1:A:2314:PHE:HD2	4:D:1123:TRP:CB	2.05	0.69
3:C:709:TRP:HB3	3:C:713:LYS:HD2	1.73	0.69
23:3:280:ASP:H	23:3:857:ALA:HB3	1.58	0.69
37:P:30:TYR:OH	38:R:161:ALA:O	2.10	0.69
38:R:436:VAL:HG23	38:R:437:TYR:CE1	2.26	0.69
1:A:76:MET:HE1	1:A:88:TYR:CB	2.22	0.69
1:A:755:HIS:HE1	37:P:223:PHE:CD2	2.06	0.69
14:G:19:G:H5"	36:O:159:ARG:HD2	1.74	0.69
15:H:149:A:H2'	15:H:150:U:C6	2.27	0.69
15:H:153:A:N6	15:H:177:A:C2	2.60	0.69
15:H:183:G:H2'	15:H:184:C:C6	2.26	0.69
29:L:209:ASP:OD1	36:O:111:ASP:CG	2.31	0.69
38:R:408:GLU:CG	38:R:409:VAL:H	2.04	0.69
1:A:1180:LYS:HA	1:A:1201:ARG:HH12	1.58	0.69
23:3:428:GLY:HA3	23:3:433:SER:HA	1.73	0.69
35:N:51:ARG:NH2	43:W:192:PHE:O	2.26	0.69
1:A:76:MET:CE	1:A:88:TYR:CG	2.70	0.69
1:A:229:GLN:CG	1:A:415:SER:HB2	2.21	0.69
1:A:296:PHE:HB3	3:C:656:ALA:HB2	1.66	0.69
1:A:762:ARG:NH2	37:P:226:LYS:HZ3	1.87	0.69
1:A:1342:TRP:HB3	3:C:921:LEU:CD2	2.22	0.69
1:A:1505:LYS:CD	46:Z:615:SER:HB3	2.22	0.69
3:C:89:LEU:HD23	3:C:89:LEU:C	2.14	0.69
3:C:482:TYR:CE2	3:C:493:PHE:HB2	2.28	0.69
5:E:178:LEU:CD1	5:E:222:LEU:CD2	2.71	0.69
15:H:83:A:C2'	15:H:84:C:O4'	2.39	0.69
23:3:452:LEU:HD11	23:3:762:LEU:HB2	1.74	0.69
25:5:18:ASN:OD1	25:5:19:ARG:N	2.25	0.69
44:X:185:ARG:O	44:X:189:HIS:HB2	1.93	0.69
1:A:529:THR:CG2	34:M:199:PRO:CG	2.71	0.69
1:A:1348:VAL:CG1	3:C:921:LEU:CD2	2.71	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1459:ARG:HG3	38:R:424:SER:H	1.57	0.69
1:A:2267:PHE:HA	4:D:1261:PRO:CB	2.23	0.69
3:C:93:ILE:CG2	40:T:218:TRP:CE2	2.76	0.69
3:C:736:GLY:CA	3:C:770:PHE:CE2	2.75	0.69
15:H:152:G:O3'	15:H:153:A:O4'	2.11	0.69
23:3:236:ILE:HB	23:3:249:LEU:HB2	1.75	0.69
28:J:353:GLU:OE1	28:J:358:GLU:CB	2.41	0.69
37:P:30:TYR:CZ	38:R:162:ALA:HA	2.28	0.69
37:P:224:MET:CE	37:P:228:ILE:CD1	2.71	0.69
43:W:474:LYS:HA	43:W:490:ALA:HB3	1.75	0.69
3:C:72:VAL:HG22	40:T:453:ALA:CB	2.23	0.69
3:C:256:CYS:SG	3:C:308:CYS:HB2	2.33	0.69
5:E:74:PHE:CD1	5:E:81:LEU:HD23	2.28	0.69
36:O:26:THR:OG1	36:O:159:ARG:NH2	2.26	0.69
1:A:338:VAL:CG2	3:C:867:PRO:CG	2.64	0.68
1:A:755:HIS:CE1	37:P:223:PHE:HB3	2.28	0.68
1:A:1076:ASP:O	1:A:1079:THR:OG1	2.11	0.68
13:F:37:C:H4'	13:F:38:G:OP2	1.91	0.68
22:2:487:LEU:O	22:2:490:HIS:N	2.26	0.68
23:3:718:ARG:NH2	23:3:734:LEU:O	2.25	0.68
1:A:299:ILE:CD1	3:C:921:LEU:CB	2.50	0.68
3:C:140:HIS:CD2	3:C:230:ASP:HB3	2.28	0.68
3:C:445:ALA:CB	3:C:466:SER:HA	2.20	0.68
3:C:725:ASP:OD1	3:C:728:ALA:N	2.25	0.68
38:R:434:TYR:HE2	38:R:436:VAL:HG22	1.57	0.68
1:A:73:HIS:NE2	1:A:81:PHE:CD1	2.59	0.68
1:A:203:VAL:CG2	1:A:237:THR:HG21	2.23	0.68
22:2:643:PRO:HD2	24:4:69:TYR:CG	2.27	0.68
37:P:72:ARG:NH1	37:P:72:ARG:HB2	2.08	0.68
38:R:106:GLN:CG	38:R:110:LYS:HE2	2.22	0.68
38:R:420:LYS:HG2	38:R:423:ASP:CG	2.13	0.68
45:Y:33:LYS:HA	45:Y:87:GLN:HE22	1.59	0.68
1:A:32:GLU:HG3	1:A:36:LYS:HE3	1.74	0.68
1:A:245:LEU:HA	1:A:430:TRP:CZ2	2.28	0.68
3:C:453:TYR:CZ	3:C:575:GLN:HB2	2.28	0.68
39:S:102:ASN:ND2	39:S:104:GLY:O	2.25	0.68
45:Y:86:ASP:HB2	46:Z:502:ALA:CB	2.23	0.68
1:A:44:ARG:HD2	1:A:45:TYR:CE2	2.28	0.68
1:A:121:HIS:HE2	1:A:481:PHE:HB3	1.51	0.68
1:A:171:ASP:OD2	1:A:519:ASP:OD2	2.12	0.68
1:A:1900:GLU:OE2	46:Z:522:LEU:HB2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2146:VAL:HG22	1:A:2272:MET:HB2	1.74	0.68
3:C:482:TYR:CE2	3:C:493:PHE:CB	2.77	0.68
3:C:678:THR:HG21	3:C:683:ASN:ND2	2.06	0.68
14:G:-2:C:H2'	14:G:-1:G:C8	2.28	0.68
23:3:441:GLY:O	23:3:775:ASN:CG	2.31	0.68
23:3:868:VAL:O	23:3:877:LEU:N	2.27	0.68
43:W:466:ALA:CB	43:W:512:CYS:O	2.41	0.68
1:A:296:PHE:CE1	3:C:591:ALA:HB3	2.27	0.68
1:A:384:VAL:HG11	3:C:331:PHE:CD2	2.28	0.68
5:E:108:HIS:CE1	5:E:128:SER:CB	2.77	0.68
15:H:147:G:O2'	15:H:148:C:H5'	1.94	0.68
23:3:524:ILE:HD11	23:3:556:ILE:HG21	1.74	0.68
29:L:216:PHE:CZ	36:O:112:VAL:HG12	2.29	0.68
36:O:137:LEU:HD12	36:O:140:ALA:HB3	1.76	0.68
37:P:63:LEU:O	37:P:63:LEU:HD23	1.94	0.68
38:R:414:ARG:NE	46:Z:598:PHE:CE1	2.47	0.68
43:W:212:GLU:C	43:W:214:LYS:H	1.97	0.68
1:A:91:ALA:O	1:A:93:LYS:N	2.27	0.68
1:A:380:LEU:C	3:C:354:ARG:HG2	2.14	0.68
1:A:779:LEU:CD2	37:P:223:PHE:HE2	2.06	0.68
1:A:1457:HIS:HE2	38:R:424:SER:HA	1.55	0.68
13:F:68:C:C5	37:P:33:ARG:HB3	2.20	0.68
38:R:88:ILE:CG2	38:R:96:ILE:CG2	2.71	0.68
1:A:299:ILE:HD11	3:C:921:LEU:HA	1.73	0.68
2:B:32:C:OP1	37:P:33:ARG:CZ	2.41	0.68
3:C:79:THR:HG23	40:T:199:VAL:CG2	2.24	0.68
3:C:452:THR:HG22	3:C:577:PHE:CB	2.23	0.68
5:E:74:PHE:CD1	5:E:81:LEU:HD21	2.29	0.68
38:R:92:SER:O	39:S:19:SER:O	2.11	0.68
46:Z:597:ARG:NH1	46:Z:601:LEU:CD1	2.57	0.68
1:A:228:TRP:O	1:A:416:GLY:N	2.26	0.68
1:A:758:ARG:HG3	1:A:779:LEU:HD11	1.75	0.68
1:A:1210:LYS:NZ	1:A:1369:TYR:OH	2.27	0.68
2:B:21:A:O3'	2:B:22:U:H4'	1.94	0.68
3:C:141:GLY:O	3:C:258:ASN:ND2	2.27	0.68
22:2:614:ARG:NH2	22:2:685:ASP:OD1	2.26	0.68
23:3:301:PHE:HB2	23:3:313:ILE:HB	1.76	0.68
27:7:48:ASP:O	27:7:51:ASN:N	2.27	0.68
28:J:360:ASP:O	28:J:363:ARG:HG3	1.93	0.68
45:Y:86:ASP:CA	46:Z:502:ALA:HB3	2.23	0.68
1:A:645:THR:HB	1:A:646:PRO:HD3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:94:ILE:CD1	37:P:44:ARG:NH1	2.57	0.68
13:F:35:A:H5”	13:F:35:A:N3	2.09	0.68
15:H:159:U:O2’	15:H:160:A:H5’	1.94	0.68
23:3:374:SER:HB3	23:3:377:MET:HG3	1.76	0.68
28:J:353:GLU:OE2	28:J:361:ARG:NH2	2.27	0.68
39:S:11:PRO:HB3	39:S:165:SER:C	2.15	0.68
3:C:94:ILE:CD1	37:P:44:ARG:CZ	2.72	0.67
3:C:360:ALA:H	3:C:361:PRO:HD3	1.59	0.67
3:C:534:VAL:HG12	3:C:535:ALA:H	1.59	0.67
38:R:420:LYS:HB2	46:Z:610:LEU:CD1	2.22	0.67
42:V:547:VAL:O	42:V:550:MET:N	2.27	0.67
1:A:75:ASP:OD1	1:A:75:ASP:N	2.26	0.67
1:A:2270:PHE:HD1	4:D:1264:PRO:CB	1.96	0.67
3:C:140:HIS:HB3	3:C:230:ASP:HB2	1.71	0.67
23:3:18:ILE:HD12	23:3:67:ALA:HB2	1.77	0.67
38:R:147:THR:CG2	40:T:360:VAL:HG12	2.23	0.67
1:A:122:ILE:CD1	1:A:483:GLN:HG3	2.24	0.67
3:C:140:HIS:CD2	3:C:230:ASP:CB	2.77	0.67
3:C:737:PRO:HG3	3:C:774:THR:OG1	1.93	0.67
21:1:437:PRO:O	44:X:262:TYR:HA	1.94	0.67
23:3:753:GLY:HA3	23:3:765:LEU:O	1.94	0.67
1:A:89:LEU:HD22	1:A:656:LEU:HD22	1.76	0.67
1:A:255:PHE:HE1	1:A:432:ARG:O	1.75	0.67
1:A:1072:LEU:HD22	1:A:1087:LEU:HD22	1.76	0.67
1:A:1962:THR:HG23	46:Z:524:ARG:HG3	1.74	0.67
3:C:259:LYS:HE2	3:C:262:ARG:HD2	1.74	0.67
21:1:1097:LEU:O	21:1:1100:ASN:ND2	2.24	0.67
23:3:412:ILE:HG12	23:3:423:LEU:HG	1.76	0.67
35:N:40:LYS:C	35:N:41:ARG:HG3	2.13	0.67
36:O:131:THR:HG23	43:W:111:LEU:N	2.10	0.67
1:A:76:MET:HE2	1:A:88:TYR:CD2	2.26	0.67
1:A:380:LEU:CA	3:C:354:ARG:CG	2.72	0.67
1:A:1422:LEU:HD22	21:1:88:VAL:CB	2.25	0.67
1:A:2113:LYS:CE	4:D:1229:ASP:CB	2.71	0.67
3:C:389:ASP:OD1	3:C:389:ASP:N	2.26	0.67
5:E:66:GLU:HB2	5:E:87:ASP:OD2	1.94	0.67
21:1:474:TYR:OH	25:5:93:ASN:ND2	2.27	0.67
21:1:798:THR:HG22	21:1:800:GLY:H	1.60	0.67
38:R:119:LEU:CB	38:R:232:MET:HG3	2.24	0.67
38:R:285:ASN:OD1	38:R:286:GLU:N	2.27	0.67
40:T:185:MET:CB	40:T:186:PRO:HD3	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:MET:SD	1:A:88:TYR:CD1	2.88	0.67
1:A:298:ASP:O	1:A:302:ILE:HG12	1.95	0.67
1:A:1281:THR:HG22	1:A:1284:LEU:H	1.59	0.67
3:C:94:ILE:HD11	37:P:44:ARG:HH22	1.60	0.67
3:C:132:VAL:HG12	3:C:226:VAL:CG2	2.23	0.67
5:E:246:GLU:HB2	5:E:248:SER:OG	1.94	0.67
40:T:455:GLN:HG3	40:T:485:THR:HG21	1.76	0.67
1:A:229:GLN:HA	1:A:414:ARG:O	1.94	0.67
1:A:299:ILE:CB	1:A:1342:TRP:CZ3	2.66	0.67
1:A:1258:LYS:HE2	38:R:432:GLU:HA	1.77	0.67
1:A:1661:TRP:CE2	1:A:1700:GLY:HA3	2.30	0.67
1:A:2300:ASN:OD1	4:D:1228:VAL:O	2.12	0.67
3:C:736:GLY:CA	3:C:770:PHE:HE2	2.07	0.67
36:O:131:THR:HG23	43:W:111:LEU:HA	1.77	0.67
45:Y:62:ILE:HA	45:Y:84:TYR:HA	1.75	0.67
45:Y:100:ILE:O	45:Y:106:THR:HA	1.94	0.67
46:Z:597:ARG:NH1	46:Z:601:LEU:HD12	2.08	0.67
1:A:296:PHE:CG	3:C:656:ALA:CB	2.62	0.67
1:A:696:MET:C	1:A:698:PRO:HD3	2.15	0.67
3:C:572:GLU:HG3	3:C:573:GLU:H	1.60	0.67
15:H:151:C:C2	15:H:152:G:C8	2.83	0.67
38:R:81:LYS:HA	38:R:81:LYS:HZ1	1.59	0.67
38:R:119:LEU:HA	38:R:232:MET:SD	2.34	0.67
40:T:272:CYS:HB3	40:T:282:ARG:HG3	1.76	0.67
1:A:134:TRP:HB3	1:A:418:THR:CG2	2.25	0.67
1:A:380:LEU:N	3:C:354:ARG:HB3	2.09	0.67
2:B:40:U:C5'	2:B:41:U:OP2	2.43	0.67
3:C:452:THR:CB	3:C:577:PHE:CD2	2.73	0.67
5:E:243:LEU:HD12	5:E:247:GLY:HA2	1.76	0.67
14:G:10:U:O5'	14:G:10:U:H6	1.78	0.67
15:H:169:C:O2'	15:H:170:C:H5'	1.95	0.67
23:3:63:ARG:NH2	23:3:119:GLN:OE1	2.22	0.67
23:3:470:PHE:HB3	23:3:747:SER:HA	1.75	0.67
23:3:802:THR:HA	23:3:863:ALA:O	1.95	0.67
3:C:149:LEU:HD13	3:C:427:PHE:CE2	2.22	0.67
3:C:510:LEU:HD22	3:C:514:TYR:CD2	2.30	0.67
13:F:27:A:N3	36:O:181:TYR:CD2	2.62	0.67
15:H:153:A:C3'	15:H:154:C:H5'	2.25	0.67
21:1:1126:PHE:HA	21:1:1165:TYR:OH	1.94	0.67
38:R:92:SER:C	39:S:19:SER:CB	2.56	0.67
38:R:135:PRO:O	38:R:136:ASP:CG	2.33	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:W:420:ALA:N	43:W:438:ASP:CB	2.57	0.67
1:A:225:TYR:O	1:A:418:THR:OG1	2.11	0.66
1:A:1984:LYS:HG3	1:A:2011:ILE:HD11	1.76	0.66
1:A:2306:HIS:CD2	1:A:2308:VAL:H	2.13	0.66
3:C:77:VAL:CG1	40:T:196:LEU:HB3	2.24	0.66
3:C:129:ILE:HG22	3:C:199:LEU:CB	2.23	0.66
23:3:1035:THR:HG21	23:3:1103:SER:HA	1.75	0.66
24:4:17:VAL:HG13	24:4:84:ILE:HG23	1.77	0.66
3:C:230:ASP:OD1	3:C:259:LYS:CB	2.43	0.66
15:H:143:A:H2'	15:H:144:C:H6	1.59	0.66
15:H:151:C:O2	15:H:152:G:C8	2.48	0.66
39:S:34:LYS:CE	39:S:78:TYR:CE2	2.77	0.66
39:S:77:ILE:HG13	39:S:78:TYR:HD1	1.58	0.66
1:A:439:GLN:NE2	1:A:614:TYR:OH	2.27	0.66
1:A:529:THR:CB	34:M:199:PRO:HD2	2.26	0.66
1:A:676:ARG:NE	13:F:56:A:OP1	2.28	0.66
1:A:1768:TYR:HA	1:A:1771:LEU:HB3	1.75	0.66
3:C:62:ASP:OD1	3:C:62:ASP:N	2.28	0.66
3:C:244:LYS:CB	3:C:292:TYR:CE2	2.79	0.66
15:H:151:C:H2'	15:H:152:G:H8	1.59	0.66
23:3:147:ASP:OD1	23:3:151:ARG:N	2.25	0.66
23:3:546:LYS:O	23:3:556:ILE:HA	1.94	0.66
23:3:947:GLU:HB3	23:3:963:VAL:HG22	1.75	0.66
1:A:532:THR:HG23	14:G:2:U:O5'	1.89	0.66
1:A:748:ASP:OD2	40:T:204:LEU:O	2.13	0.66
1:A:1386:TRP:HE1	1:A:1417:PRO:HD2	1.61	0.66
1:A:1457:HIS:CE1	1:A:1459:ARG:HB2	2.30	0.66
2:B:19:A:O2'	2:B:20:G:OP1	2.12	0.66
5:E:146:ARG:HH11	5:E:148:LYS:CE	1.83	0.66
15:H:73:C:H2'	15:H:74:U:C6	2.30	0.66
15:H:114:A:H61	15:H:142:C:H42	1.44	0.66
21:1:397:ARG:HD3	21:1:398:PRO:HD2	1.78	0.66
26:6:25:LYS:NZ	26:6:26:CYS:SG	2.68	0.66
1:A:254:TYR:OH	1:A:434:HIS:HB3	1.95	0.66
1:A:420:ARG:NH1	2:B:56:C:O2'	2.28	0.66
36:O:28:LEU:HD23	38:R:195:ARG:HE	1.61	0.66
1:A:532:THR:CB	14:G:2:U:O5'	2.42	0.66
3:C:473:PRO:O	3:C:474:LEU:HB3	1.96	0.66
3:C:474:LEU:HD23	3:C:474:LEU:C	2.16	0.66
15:H:47:U:H1'	15:H:48:A:H8	1.61	0.66
23:3:1017:ASN:OD1	23:3:1018:GLU:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:O:147:LEU:O	36:O:151:ALA:N	2.29	0.66
36:O:243:ILE:HG12	36:O:294:ASN:HD22	1.61	0.66
37:P:212:ASN:OD1	40:T:483:ASP:HA	1.96	0.66
40:T:314:ILE:HD12	40:T:324:HIS:HB2	1.75	0.66
45:Y:39:PHE:O	45:Y:109:VAL:HA	1.95	0.66
45:Y:98:ASN:OD1	45:Y:99:GLY:N	2.25	0.66
46:Z:525:TYR:HE1	46:Z:526:ILE:HG23	1.57	0.66
1:A:375:ASP:H	3:C:355:LYS:HZ2	1.44	0.66
1:A:377:GLU:O	1:A:378:PHE:CB	2.44	0.66
3:C:145:PHE:CE1	3:C:427:PHE:HE1	2.14	0.66
3:C:221:ILE:CG1	3:C:479:THR:OG1	2.43	0.66
40:T:342:GLU:HB3	40:T:343:PRO:CD	2.26	0.66
1:A:380:LEU:HB2	3:C:354:ARG:HG3	0.72	0.66
1:A:718:ARG:HH21	38:R:259:LYS:HE3	1.58	0.66
1:A:785:LYS:HE3	37:P:215:LEU:CD1	2.26	0.66
3:C:140:HIS:HA	3:C:259:LYS:NZ	2.10	0.66
5:E:116:HIS:O	5:E:124:LEU:HD12	1.95	0.66
5:E:281:VAL:HG22	43:W:148:VAL:HA	1.76	0.66
23:3:355:ASN:OD1	23:3:436:ARG:NH2	2.26	0.66
36:O:196:GLN:HE21	36:O:208:PRO:HG2	1.61	0.66
39:S:10:GLN:HB3	39:S:29:TRP:CD2	2.30	0.66
1:A:304:ILE:HD11	1:A:1342:TRP:CZ2	2.30	0.66
14:G:146:C:H41	21:1:1107:GLN:HG3	1.60	0.66
23:3:952:ILE:HG12	23:3:961:ILE:HG12	1.78	0.66
27:7:63:ARG:O	27:7:67:ASN:ND2	2.29	0.66
28:J:300:ASP:OD2	38:R:101:ILE:CG1	2.44	0.66
42:V:548:ALA:HB1	42:V:585:ILE:CB	2.25	0.66
1:A:406:TRP:HH2	3:C:265:LEU:O	1.79	0.66
1:A:755:HIS:HE1	37:P:223:PHE:HB3	1.61	0.66
1:A:829:PRO:O	1:A:882:LYS:NZ	2.27	0.66
1:A:1457:HIS:NE2	38:R:424:SER:CA	2.59	0.66
3:C:87:GLN:HE21	40:T:239:LYS:HD3	1.61	0.66
5:E:320:LEU:O	43:W:85:TYR:CB	2.44	0.66
23:3:330:PHE:O	23:3:394:ASN:ND2	2.29	0.66
35:N:28:LYS:HZ1	43:W:190:ASP:N	1.91	0.66
2:B:42:U:O4	14:G:-3:A:N1	2.29	0.65
3:C:77:VAL:HG12	40:T:197:TYR:CA	2.25	0.65
3:C:136:GLY:HA2	3:C:239:THR:HG22	1.77	0.65
5:E:178:LEU:HD11	5:E:222:LEU:CD2	2.26	0.65
38:R:124:VAL:HG13	38:R:125:MET:H	1.60	0.65
1:A:293:TRP:HZ3	1:A:295:GLU:OE1	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:TRP:CD1	13:F:66:C:H1'	2.31	0.65
1:A:1459:ARG:HE	38:R:423:ASP:CB	2.06	0.65
14:G:-12:G:H2'	14:G:-11:G:C8	2.30	0.65
23:3:440:HIS:CG	23:3:733:PRO:CG	2.79	0.65
40:T:439:TRP:CZ3	40:T:446:ASN:HB2	2.32	0.65
1:A:339:PHE:CD1	1:A:406:TRP:CE3	2.84	0.65
2:B:43:U:H3	14:G:-4:A:H2	1.37	0.65
2:B:43:U:O4	14:G:-4:A:N1	2.30	0.65
21:1:1171:PRO:O	21:1:1174:GLU:HB2	1.96	0.65
37:P:210:PHE:HB3	40:T:455:GLN:HE22	1.61	0.65
1:A:97:HIS:HD2	1:A:473:PHE:CZ	2.15	0.65
1:A:344:ASP:N	1:A:344:ASP:OD1	2.28	0.65
1:A:468:LYS:HD3	1:A:469:LYS:H	1.61	0.65
1:A:639:PHE:O	2:B:28:A:O2'	2.12	0.65
1:A:1356:GLY:O	41:U:15:THR:HG22	1.96	0.65
1:A:1459:ARG:CD	38:R:422:MET:O	2.45	0.65
1:A:1962:THR:O	46:Z:524:ARG:CG	2.45	0.65
2:B:63:A:H4'	5:E:106:LYS:NZ	2.12	0.65
21:1:713:ALA:HA	21:1:716:ALA:HB3	1.77	0.65
37:P:66:ARG:HH11	37:P:66:ARG:CB	2.09	0.65
1:A:301:LYS:HG2	3:C:940:ARG:N	2.12	0.65
3:C:457:VAL:HB	3:C:462:GLY:HA3	1.78	0.65
40:T:327:SER:O	40:T:357:TRP:HH2	1.79	0.65
3:C:700:ILE:HG21	3:C:741:GLY:O	1.97	0.65
14:G:137:C:H42	15:H:40:C:N4	1.95	0.65
21:1:584:ASP:OD1	21:1:585:GLU:N	2.29	0.65
22:2:487:LEU:HD12	27:7:28:LYS:HE3	1.78	0.65
22:2:511:LEU:HD23	22:2:593:GLU:HG3	1.79	0.65
23:3:458:ALA:HA	23:3:741:PHE:HB3	1.78	0.65
36:O:31:ASN:OD1	36:O:33:TYR:N	2.27	0.65
40:T:459:LEU:HD12	40:T:460:ASP:H	1.61	0.65
1:A:529:THR:HB	34:M:199:PRO:HD2	1.78	0.65
5:E:108:HIS:CE1	5:E:128:SER:HB3	2.31	0.65
13:F:24:A:H2	13:F:26:U:N3	1.94	0.65
1:A:155:LYS:NZ	1:A:624:GLY:O	2.29	0.65
1:A:318:TYR:HB2	3:C:638:ASP:CG	2.16	0.65
1:A:338:VAL:HG11	3:C:267:LEU:CD2	2.27	0.65
1:A:378:PHE:CD1	1:A:379:GLU:N	2.65	0.65
3:C:572:GLU:HG3	3:C:573:GLU:N	2.12	0.65
23:3:866:ILE:HB	23:3:880:VAL:HB	1.79	0.65
32:I:296:PHE:CA	32:I:305:SER:CB	2.66	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:O:68:THR:HA	36:O:83:THR:HG22	1.77	0.65
38:R:451:ILE:HD13	38:R:451:ILE:N	2.12	0.65
39:S:9:TRP:HE3	39:S:11:PRO:CD	2.10	0.65
40:T:458:SER:OG	40:T:459:LEU:N	2.30	0.65
23:3:791:HIS:HE1	23:3:934:GLY:HA3	1.62	0.65
24:4:75:ASN:OD1	24:4:86:VAL:CB	2.45	0.65
35:N:28:LYS:NZ	43:W:190:ASP:H	1.95	0.65
1:A:2314:PHE:CD2	4:D:1123:TRP:CB	2.80	0.65
2:B:44:A:C2	14:G:-5:G:N1	2.62	0.65
3:C:749:THR:O	3:C:753:GLU:N	2.27	0.65
13:F:33:G:OP2	13:F:33:G:H8	1.80	0.65
15:H:153:A:H3'	15:H:154:C:H5'	1.79	0.65
15:H:156:U:C6	15:H:156:U:C5'	2.72	0.65
21:1:1026:ASN:HD22	21:1:1031:VAL:HG11	1.60	0.65
36:O:253:TYR:OH	39:S:120:GLN:HG2	1.97	0.65
37:P:210:PHE:CE2	40:T:455:GLN:OE1	2.50	0.65
3:C:97:VAL:CG1	37:P:47:THR:OG1	2.45	0.64
3:C:463:GLU:OE1	3:C:463:GLU:N	2.29	0.64
3:C:488:VAL:HG13	3:C:609:LYS:NZ	2.12	0.64
5:E:277:PHE:HE2	5:E:300:ILE:HD13	1.61	0.64
21:1:912:ASN:OD1	21:1:957:ARG:NH1	2.30	0.64
38:R:171:LEU:CD1	38:R:201:GLU:OE1	2.44	0.64
2:B:19:A:H2'	2:B:20:G:H5"	1.78	0.64
3:C:72:VAL:CG2	40:T:453:ALA:HB1	2.26	0.64
14:G:11:A:N3	14:G:11:A:H3'	2.12	0.64
15:H:148:C:H2'	15:H:149:A:C8	2.30	0.64
3:C:141:GLY:C	3:C:258:ASN:HD22	2.01	0.64
5:E:153:PHE:O	5:E:171:SER:HB2	1.97	0.64
23:3:429:ARG:HH12	27:7:58:ASN:HA	1.62	0.64
23:3:635:ALA:HB3	23:3:669:LEU:HD23	1.79	0.64
1:A:779:LEU:HD21	37:P:223:PHE:HE2	1.59	0.64
1:A:1051:LEU:CD2	37:P:193:VAL:HG11	2.27	0.64
3:C:256:CYS:SG	3:C:308:CYS:CB	2.86	0.64
23:3:206:GLN:HG3	23:3:228:LEU:HD12	1.78	0.64
23:3:670:GLN:HA	23:3:698:PRO:HA	1.78	0.64
38:R:88:ILE:H	38:R:88:ILE:HD12	1.61	0.64
45:Y:24:ASP:O	45:Y:27:SER:N	2.30	0.64
46:Z:594:GLU:O	46:Z:598:PHE:N	2.25	0.64
1:A:299:ILE:HB	1:A:1342:TRP:CZ3	2.33	0.64
1:A:976:MET:HG2	1:A:1187:PHE:HB3	1.78	0.64
1:A:1069:ASN:OD1	1:A:1075:GLN:NE2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2328:ALA:CB	4:D:788:GLY:CA	2.74	0.64
2:B:40:U:H5'	2:B:41:U:OP2	1.97	0.64
3:C:97:VAL:HG22	37:P:45:GLN:HG3	1.77	0.64
3:C:482:TYR:HE2	3:C:493:PHE:CD2	2.14	0.64
1:A:176:LEU:HD13	1:A:181:ASN:ND2	2.12	0.64
15:H:68:G:H1	15:H:84:C:N4	1.95	0.64
23:3:714:ALA:O	23:3:720:TRP:HB2	1.97	0.64
36:O:223:LEU:O	36:O:223:LEU:HD22	1.98	0.64
36:O:225:PRO:HB2	36:O:226:PRO:HD2	1.80	0.64
38:R:419:SER:O	38:R:420:LYS:O	2.16	0.64
3:C:350:ASN:ND2	3:C:353:THR:HG23	2.13	0.64
3:C:705:VAL:HB	3:C:717:PHE:CZ	2.33	0.64
14:G:149:G:C2	14:G:150:U:H2'	2.32	0.64
21:1:847:ALA:O	21:1:851:SER:CB	2.46	0.64
38:R:433:ILE:HD12	38:R:435:ASN:ND2	2.12	0.64
39:S:10:GLN:OE1	39:S:10:GLN:N	2.31	0.64
1:A:380:LEU:CB	3:C:354:ARG:HH11	2.08	0.64
1:A:1342:TRP:CD2	3:C:921:LEU:CD2	2.80	0.64
3:C:824:THR:O	3:C:824:THR:CG2	2.45	0.64
13:F:38:G:H8	13:F:38:G:O5'	1.79	0.64
21:1:599:ASN:O	21:1:603:ALA:HB2	1.98	0.64
21:1:702:ARG:O	21:1:705:SER:OG	2.13	0.64
23:3:525:ARG:HG3	23:3:533:VAL:HG13	1.78	0.64
24:4:15:VAL:O	24:4:58:PHE:HA	1.97	0.64
29:L:224:PHE:HD1	38:R:86:LEU:HD12	1.54	0.64
1:A:175:PRO:HG2	1:A:498:ARG:CZ	2.27	0.64
1:A:481:PHE:CE2	38:R:205:ASP:CA	2.81	0.64
1:A:1134:TRP:O	1:A:1139:ARG:NH1	2.31	0.64
1:A:1252:GLY:HA2	1:A:1298:ARG:NH2	2.13	0.64
3:C:363:SER:O	3:C:364:SER:OG	2.11	0.64
14:G:-9:C:C6	41:U:18:TYR:CE1	2.84	0.64
15:H:25:G:H2'	15:H:26:A:H8	1.62	0.64
28:J:294:HIS:CE1	29:L:227:THR:CB	2.80	0.64
43:W:264:ASN:O	43:W:267:SER:CB	2.46	0.64
1:A:1215:ASN:HB3	1:A:1224:ARG:HD2	1.79	0.64
1:A:1457:HIS:CE1	38:R:424:SER:CA	2.79	0.64
2:B:12:U:O2'	2:B:13:C:O5'	2.14	0.64
3:C:678:THR:HG21	3:C:683:ASN:HB2	1.76	0.64
14:G:155:U:H4'	14:G:156:U:H5'	1.79	0.64
36:O:223:LEU:HD13	36:O:223:LEU:C	2.15	0.64
36:O:276:THR:HG23	36:O:279:ALA:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:S:13:ASN:HD22	39:S:24:VAL:HG11	1.62	0.64
1:A:134:TRP:HB3	1:A:418:THR:HG21	1.79	0.63
1:A:1337:GLN:O	1:A:1352:HIS:HB2	1.98	0.63
1:A:1962:THR:HG23	46:Z:524:ARG:CG	2.27	0.63
1:A:2319:LEU:HG	1:A:2320:LEU:N	2.11	0.63
3:C:482:TYR:CE2	3:C:493:PHE:CD2	2.86	0.63
4:D:1992:GLU:HA	4:D:1995:ALA:HB3	1.80	0.63
23:3:673:VAL:HA	23:3:691:THR:H	1.63	0.63
1:A:461:HIS:CE1	2:B:23:C:C5	2.86	0.63
1:A:643:GLY:HA3	2:B:29:A:O4'	1.99	0.63
3:C:481:MET:SD	3:C:492:ALA:HB2	2.37	0.63
3:C:596:ASN:HD22	3:C:596:ASN:N	1.96	0.63
13:F:94:C:OP1	28:J:351:ASN:HB2	1.98	0.63
14:G:-9:C:C5	41:U:18:TYR:CD1	2.84	0.63
14:G:26:U:C1'	36:O:269:CYS:HB3	2.28	0.63
15:H:152:G:C2	15:H:153:A:C5	2.87	0.63
23:3:524:ILE:HD11	23:3:556:ILE:HD13	1.80	0.63
24:4:75:ASN:OD1	24:4:86:VAL:N	2.31	0.63
3:C:77:VAL:HG12	40:T:196:LEU:O	1.70	0.63
5:E:119:THR:HG23	5:E:161:ARG:HB3	1.80	0.63
13:F:35:A:H2'	13:F:36:A:C5'	2.28	0.63
23:3:187:MET:HE2	23:3:206:GLN:HB3	1.80	0.63
23:3:931:VAL:N	23:3:936:LYS:O	2.29	0.63
25:5:20:ILE:HG12	25:5:63:VAL:HG22	1.78	0.63
1:A:755:HIS:CD2	37:P:219:PHE:HE2	2.15	0.63
13:F:27:A:OP1	35:N:41:ARG:NH2	2.30	0.63
13:F:58:G:H2'	13:F:59:G:C8	2.32	0.63
23:3:86:ARG:HA	23:3:105:GLU:O	1.98	0.63
23:3:174:ASP:OD2	23:3:240:GLY:N	2.31	0.63
23:3:489:GLU:HG2	23:3:748:GLU:HB3	1.80	0.63
36:O:78:LYS:O	36:O:97:ARG:NH2	2.32	0.63
43:W:463:SER:O	43:W:480:SER:HA	1.98	0.63
44:X:241:GLY:N	44:X:262:TYR:O	2.31	0.63
1:A:44:ARG:HD2	1:A:45:TYR:CZ	2.34	0.63
1:A:380:LEU:HB3	3:C:354:ARG:HH11	1.60	0.63
1:A:596:TYR:CE2	14:G:-5:G:N7	2.66	0.63
3:C:129:ILE:CG2	3:C:199:LEU:HB3	2.27	0.63
3:C:295:ASP:OD1	3:C:297:ASN:N	2.32	0.63
3:C:350:ASN:CG	3:C:353:THR:HG23	2.19	0.63
3:C:456:GLY:O	3:C:457:VAL:HG22	1.99	0.63
13:F:36:A:C5'	13:F:36:A:H8	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:R:132:LEU:HD23	38:R:132:LEU:H	1.63	0.63
1:A:1852:LEU:HD12	1:A:1853:PRO:HD2	1.80	0.63
13:F:28:A:H1'	35:N:39:GLY:O	1.98	0.63
23:3:794:SER:OG	23:3:796:ASN:OD1	2.15	0.63
38:R:123:GLU:OE1	38:R:124:VAL:N	2.30	0.63
1:A:43:LYS:NZ	43:W:168:PHE:O	2.30	0.63
1:A:460:LYS:NZ	2:B:49:A:OP2	2.29	0.63
1:A:1260:VAL:HG21	1:A:1325:LEU:HB3	1.80	0.63
1:A:1787:ARG:NH2	1:A:1804:ASN:O	2.31	0.63
1:A:1820:LYS:HD3	1:A:1914:MET:HE2	1.78	0.63
5:E:178:LEU:HD21	5:E:208:ILE:CD1	2.28	0.63
15:H:47:U:H1'	15:H:48:A:C8	2.34	0.63
21:1:812:PRO:HB2	21:1:813:PRO:HD3	1.81	0.63
25:5:23:ILE:HD12	25:5:89:VAL:HG12	1.81	0.63
36:O:115:GLU:HB3	38:R:218:ILE:HG21	1.80	0.63
1:A:319:LEU:N	3:C:638:ASP:OD1	2.31	0.63
1:A:693:ILE:HG13	1:A:738:MET:SD	2.38	0.63
1:A:1000:ILE:HG22	1:A:1001:VAL:HG13	1.81	0.63
3:C:93:ILE:CD1	40:T:230:ILE:HD13	2.29	0.63
3:C:476:CYS:CB	3:C:565:ILE:HB	2.27	0.63
21:1:698:GLN:O	21:1:702:ARG:NH1	2.32	0.63
23:3:399:ASP:OD1	23:3:400:GLU:N	2.32	0.63
23:3:521:PRO:HA	23:3:544:ILE:HG22	1.81	0.63
38:R:67:ILE:HD13	38:R:67:ILE:N	2.13	0.63
1:A:109:PRO:HD3	1:A:630:TRP:CZ2	2.33	0.63
3:C:259:LYS:HE2	3:C:262:ARG:HD3	1.79	0.63
13:F:26:U:C3'	13:F:27:A:H5"	2.29	0.63
13:F:40:U:H2'	13:F:41:A:H8	1.61	0.63
38:R:418:GLN:O	46:Z:606:ALA:HB2	1.97	0.63
1:A:595:LYS:HA	2:B:44:A:O3'	1.98	0.62
1:A:768:ASP:HB2	1:A:771:VAL:HG12	1.79	0.62
3:C:250:ARG:NE	3:C:451:HIS:NE2	2.47	0.62
5:E:265:ARG:H	5:E:272:ARG:HH21	1.47	0.62
15:H:179:C:C2	15:H:180:G:N7	2.67	0.62
38:R:250:LYS:HD3	38:R:251:ILE:N	2.13	0.62
42:V:549:LYS:O	42:V:552:ALA:N	2.32	0.62
46:Z:566:TYR:HB2	46:Z:581:GLY:O	1.98	0.62
1:A:630:TRP:O	1:A:631:ALA:C	2.37	0.62
1:A:1085:ILE:HG12	1:A:1099:PHE:CE1	2.34	0.62
5:E:251:LEU:HG	5:E:291:CYS:SG	2.39	0.62
35:N:116:ASN:OD1	35:N:116:ASN:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:O:219:THR:O	36:O:221:PRO:HD3	1.99	0.62
1:A:365:VAL:CG1	1:A:366:LYS:H	2.13	0.62
1:A:375:ASP:N	3:C:355:LYS:HZ2	1.97	0.62
3:C:79:THR:HG23	40:T:199:VAL:HB	0.68	0.62
21:1:1010:THR:OG1	21:1:1011:PRO:HD3	1.98	0.62
1:A:141:ILE:HG12	1:A:426:LEU:CD2	2.30	0.62
1:A:283:VAL:HG13	1:A:284:ARG:H	1.64	0.62
1:A:755:HIS:ND1	37:P:223:PHE:CD2	2.60	0.62
3:C:360:ALA:N	3:C:361:PRO:HD3	2.14	0.62
21:1:1257:PRO:HG3	22:2:482:ALA:HB2	1.81	0.62
23:3:553:GLN:NE2	23:3:565:TYR:OH	2.31	0.62
46:Z:566:TYR:CD2	46:Z:584:TRP:CE3	2.88	0.62
1:A:121:HIS:CE1	1:A:481:PHE:CB	2.68	0.62
1:A:203:VAL:HG21	1:A:237:THR:HG22	1.81	0.62
1:A:1306:LYS:NZ	2:B:38:C:C2'	2.62	0.62
2:B:43:U:N3	14:G:-4:A:C2	2.60	0.62
3:C:132:VAL:HG11	3:C:434:CYS:SG	2.39	0.62
23:3:27:GLN:OE1	23:3:42:ARG:NH1	2.32	0.62
23:3:380:GLU:O	23:3:383:ASP:N	2.32	0.62
36:O:19:ASP:OD1	36:O:20:PHE:N	2.33	0.62
38:R:250:LYS:HA	38:R:250:LYS:HE3	1.81	0.62
40:T:185:MET:HB3	40:T:186:PRO:HD3	1.81	0.62
43:W:280:GLN:HA	43:W:577:LEU:O	2.00	0.62
1:A:97:HIS:CD2	1:A:473:PHE:CZ	2.87	0.62
1:A:305:ARG:HA	1:A:305:ARG:NH1	2.09	0.62
1:A:312:TYR:CD2	3:C:882:GLY:HA3	2.34	0.62
1:A:402:ILE:HG22	3:C:268:LYS:NZ	2.10	0.62
1:A:755:HIS:HE1	37:P:223:PHE:CG	2.11	0.62
3:C:259:LYS:HG2	3:C:262:ARG:HD2	1.81	0.62
15:H:182:U:H2'	15:H:183:G:C8	2.34	0.62
23:3:273:ARG:O	23:3:386:PHE:HA	2.00	0.62
1:A:253:ASN:CB	3:C:893:GLY:O	2.46	0.62
1:A:800:TYR:CG	3:C:59:LEU:HD13	2.34	0.62
1:A:2105:ILE:HD13	1:A:2266:ARG:HH22	1.64	0.62
5:E:119:THR:HG21	5:E:161:ARG:HB3	1.72	0.62
23:3:440:HIS:CD2	23:3:733:PRO:CD	2.82	0.62
23:3:567:GLU:OE2	23:3:601:ARG:NE	2.29	0.62
37:P:211:VAL:HG13	40:T:457:GLY:HA3	0.75	0.62
40:T:356:LEU:N	40:T:356:LEU:HD12	2.15	0.62
1:A:282:LEU:C	1:A:282:LEU:HD23	2.20	0.62
5:E:146:ARG:CZ	5:E:148:LYS:HE3	2.27	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:847:ALA:O	21:1:851:SER:HB3	1.99	0.62
23:3:440:HIS:CE1	23:3:720:TRP:CH2	2.87	0.62
33:Q:500:GLY:N	38:R:51:ILE:HG13	2.14	0.62
46:Z:600:ARG:HH11	46:Z:600:ARG:CG	2.13	0.62
1:A:155:LYS:HD2	1:A:626:GLY:O	2.00	0.62
1:A:762:ARG:NH2	37:P:226:LYS:HZ1	1.79	0.62
1:A:2328:ALA:HB3	4:D:788:GLY:CA	2.30	0.62
15:H:154:C:H2'	15:H:155:C:H6	1.63	0.62
15:H:161:U:H6	15:H:161:U:O5'	1.83	0.62
21:1:664:GLY:HA2	21:1:667:ILE:HD12	1.80	0.62
21:1:696:ASP:OD1	21:1:697:GLU:N	2.33	0.62
21:1:1052:ALA:HA	21:1:1055:TRP:HD1	1.64	0.62
22:2:612:GLU:O	22:2:615:ILE:N	2.33	0.62
23:3:642:ILE:O	23:3:703:ARG:NH2	2.32	0.62
28:J:406:PHE:CE2	28:J:411:MET:CE	2.83	0.62
36:O:81:CYS:SG	53:O:501:ZN:ZN	1.88	0.62
39:S:9:TRP:CE3	39:S:11:PRO:CG	2.83	0.62
46:Z:573:PRO:HD2	46:Z:573:PRO:O	1.99	0.62
1:A:1217:GLN:NE2	42:V:592:GLU:O	2.32	0.62
3:C:230:ASP:OD1	3:C:259:LYS:HB3	2.00	0.62
4:D:754:GLU:CB	23:3:662:PHE:CE1	2.83	0.62
1:A:338:VAL:HG11	3:C:267:LEU:HD21	1.81	0.61
1:A:835:ASP:OD1	1:A:836:THR:N	2.32	0.61
5:E:277:PHE:HE2	5:E:300:ILE:HD12	1.63	0.61
23:3:811:THR:OG1	23:3:884:GLN:OE1	2.14	0.61
23:3:1004:ASP:OD1	23:3:1005:VAL:N	2.33	0.61
37:P:194:PHE:O	37:P:196:ASN:N	4.26	0.61
1:A:2068:SER:HB2	1:A:2072:GLU:HB2	1.81	0.61
3:C:141:GLY:C	3:C:258:ASN:ND2	2.53	0.61
13:F:24:A:C2	13:F:26:U:C2	2.88	0.61
14:G:13:C:H2'	14:G:14:A:C8	2.36	0.61
23:3:786:ARG:NH1	23:3:802:THR:O	2.33	0.61
28:J:262:ARG:HD3	29:L:220:PRO:HG2	1.82	0.61
39:S:131:ARG:HD3	39:S:132:VAL:C	2.09	0.61
46:Z:597:ARG:HH12	46:Z:601:LEU:HD12	1.66	0.61
1:A:344:ASP:OD1	1:A:347:LEU:CD1	2.49	0.61
1:A:783:TYR:HB2	37:P:228:ILE:CG1	2.26	0.61
13:F:38:G:P	13:F:38:G:C8	2.94	0.61
14:G:26:U:H5"	36:O:235:TYR:OH	2.00	0.61
21:1:866:LYS:HG3	21:1:909:VAL:HG11	1.82	0.61
23:3:317:THR:HA	23:3:322:VAL:HA	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1900:GLU:HG2	46:Z:521:PRO:HG3	1.82	0.61
14:G:146:C:H1'	15:H:33:G:N2	2.15	0.61
15:H:165:A:H8	15:H:165:A:O5'	1.84	0.61
38:R:55:LEU:O	38:R:73:PRO:O	2.19	0.61
38:R:92:SER:N	39:S:19:SER:HB2	2.15	0.61
44:X:343:ARG:HB3	44:X:378:GLU:HG3	1.83	0.61
46:Z:566:TYR:CD1	46:Z:567:SER:N	2.69	0.61
1:A:203:VAL:CG2	1:A:237:THR:HB	2.30	0.61
1:A:305:ARG:HG3	3:C:879:ASP:OD1	1.99	0.61
1:A:344:ASP:OD1	1:A:347:LEU:HD12	2.00	0.61
1:A:2106:LEU:HD12	1:A:2107:PRO:HD2	1.83	0.61
3:C:679:PRO:HD3	3:C:811:THR:OG1	1.99	0.61
3:C:750:LEU:C	3:C:750:LEU:HD12	2.21	0.61
15:H:56:A:H61	22:2:505:CYS:HA	1.66	0.61
15:H:68:G:H2'	15:H:69:U:C6	2.35	0.61
21:1:648:LEU:O	21:1:651:VAL:N	2.33	0.61
23:3:288:VAL:HG23	23:3:289:CYS:H	1.65	0.61
23:3:994:GLN:NE2	23:3:1036:ALA:O	2.33	0.61
40:T:327:SER:O	40:T:357:TRP:CH2	2.53	0.61
1:A:299:ILE:CD1	3:C:920:PRO:O	2.48	0.61
3:C:64:LYS:HZ2	37:P:206:LYS:HG3	1.63	0.61
3:C:97:VAL:HG13	37:P:47:THR:OG1	2.00	0.61
3:C:140:HIS:CG	3:C:230:ASP:H	2.18	0.61
3:C:809:ILE:HB	3:C:810:PRO:HD3	1.82	0.61
23:3:1191:LYS:NZ	23:3:1195:GLU:OE2	2.33	0.61
35:N:28:LYS:NZ	43:W:190:ASP:CA	2.64	0.61
42:V:537:HIS:HA	42:V:578:SER:CB	2.31	0.61
1:A:299:ILE:HD11	3:C:921:LEU:N	2.16	0.61
1:A:623:LYS:HD3	50:A:3000:IHP:O43	2.01	0.61
3:C:471:ASP:N	3:C:499:GLY:HA2	2.15	0.61
3:C:495:ARG:HD2	3:C:497:LEU:HD23	1.81	0.61
21:1:720:GLY:N	23:3:216:GLY:O	2.29	0.61
32:I:361:HIS:O	32:I:372:ARG:CB	2.48	0.61
36:O:283:ALA:O	36:O:287:SER:OG	2.18	0.61
38:R:185:GLY:O	38:R:186:VAL:HG22	2.00	0.61
40:T:339:GLN:NE2	40:T:342:GLU:O	2.34	0.61
40:T:355:ARG:C	40:T:356:LEU:HD12	2.21	0.61
43:W:290:GLY:CA	43:W:571:TRP:O	2.49	0.61
1:A:260:LEU:CD2	1:A:455:VAL:HG22	2.30	0.61
1:A:461:HIS:NE2	2:B:23:C:C6	2.69	0.61
1:A:1286:ASP:OD1	1:A:1354:ARG:NH2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:151:GLU:OE1	3:C:417:ARG:NH1	2.34	0.61
3:C:470:PRO:HA	3:C:499:GLY:CA	2.29	0.61
3:C:675:PHE:HD1	3:C:675:PHE:H	1.47	0.61
14:G:8:C:H2'	14:G:9:C:C6	2.35	0.61
15:H:106:G:N2	15:H:107:A:C6	2.67	0.61
15:H:142:C:C2'	15:H:143:A:H5'	2.30	0.61
15:H:157:G:H5"	15:H:157:G:H8	1.65	0.61
28:J:408:ASP:OD1	28:J:442:ARG:HG2	2.01	0.61
3:C:478:THR:OG1	3:C:563:ALA:O	2.14	0.61
3:C:705:VAL:HG22	3:C:705:VAL:O	2.00	0.61
15:H:153:A:N6	15:H:177:A:H2	1.98	0.61
23:3:452:LEU:HB3	23:3:478:PHE:HE1	1.66	0.61
29:L:74:LEU:HD23	29:L:77:LEU:HD12	1.83	0.61
36:O:196:GLN:NE2	36:O:209:VAL:HG23	2.14	0.61
45:Y:87:GLN:O	45:Y:90:THR:N	2.33	0.61
1:A:73:HIS:CD2	1:A:81:PHE:CG	2.89	0.61
1:A:73:HIS:CD2	1:A:81:PHE:CD1	2.88	0.61
1:A:256:TYR:CE1	3:C:888:ARG:CZ	2.83	0.61
5:E:108:HIS:CE1	5:E:128:SER:HB2	2.35	0.61
13:F:6:C:OP2	13:F:6:C:H4'	1.99	0.61
21:1:1203:GLY:O	23:3:1171:LYS:NZ	2.34	0.61
23:3:226:GLU:HG3	23:3:261:PHE:HZ	1.65	0.61
24:4:71:ILE:HD11	24:4:88:LYS:HB3	1.83	0.61
38:R:92:SER:O	39:S:19:SER:CB	2.48	0.61
38:R:92:SER:O	39:S:19:SER:C	2.39	0.61
40:T:349:SER:OG	40:T:351:ASP:OD1	2.18	0.61
1:A:296:PHE:CD2	3:C:656:ALA:HB2	2.30	0.60
1:A:1405:LEU:HA	38:R:415:LEU:HD21	1.78	0.60
3:C:133:THR:O	3:C:226:VAL:HB	2.01	0.60
3:C:135:CYS:O	3:C:228:PHE:N	2.28	0.60
3:C:449:ILE:HD11	3:C:466:SER:CA	2.31	0.60
3:C:710:ASN:O	3:C:713:LYS:N	2.31	0.60
13:F:27:A:C1'	36:O:181:TYR:HE2	2.11	0.60
15:H:143:A:H2'	15:H:144:C:C6	2.35	0.60
21:1:1293:ASN:HB3	27:7:76:CYS:HB3	1.83	0.60
28:J:406:PHE:CG	28:J:411:MET:HE3	2.36	0.60
36:O:235:TYR:CD2	36:O:301:LYS:HB2	2.33	0.60
46:Z:524:ARG:NE	46:Z:524:ARG:O	2.34	0.60
1:A:800:TYR:CD2	3:C:59:LEU:HD13	2.36	0.60
1:A:1457:HIS:CE1	1:A:1459:ARG:CB	2.83	0.60
21:1:918:VAL:HG12	21:1:961:VAL:HG21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:505:THR:HG21	23:3:508:CYS:SG	2.40	0.60
28:J:338:GLU:O	38:R:116:TYR:CD1	2.54	0.60
46:Z:491:ASP:O	46:Z:495:ALA:CB	2.48	0.60
1:A:151:MET:SD	1:A:628:GLY:C	2.80	0.60
1:A:158:ARG:HH12	1:A:573:GLN:HE21	1.48	0.60
28:J:291:GLN:OE1	29:L:230:GLU:HG3	2.01	0.60
40:T:339:GLN:HG2	40:T:340:ALA:N	2.16	0.60
46:Z:491:ASP:O	46:Z:495:ALA:HB2	2.01	0.60
1:A:82:ARG:HB3	1:A:83:HIS:ND1	2.17	0.60
1:A:532:THR:CG2	14:G:2:U:H5"	2.27	0.60
14:G:13:C:H2'	14:G:14:A:H8	1.66	0.60
23:3:441:GLY:O	23:3:775:ASN:HB2	2.00	0.60
24:4:31:GLU:O	24:4:35:GLN:HG2	2.02	0.60
40:T:292:TYR:CE2	40:T:308:ARG:HG3	2.36	0.60
1:A:48:LYS:O	1:A:53:PHE:CG	2.54	0.60
1:A:339:PHE:CE1	1:A:406:TRP:HE3	2.12	0.60
1:A:1827:TRP:HH2	1:A:1837:ALA:HB2	1.67	0.60
1:A:2073:TRP:CZ3	1:A:2310:ARG:HG2	2.36	0.60
5:E:178:LEU:HD21	5:E:208:ILE:HD13	1.82	0.60
5:E:266:PRO:HG3	29:L:785:GLN:NE2	2.16	0.60
23:3:833:GLU:HA	23:3:834:LEU:HB2	1.84	0.60
29:L:233:GLN:OE1	29:L:233:GLN:HA	2.01	0.60
38:R:171:LEU:CD1	38:R:201:GLU:CD	2.70	0.60
43:W:531:LYS:CB	43:W:546:PHE:O	2.50	0.60
1:A:623:LYS:CD	50:A:3000:IHP:O43	2.49	0.60
1:A:1447:VAL:HG11	1:A:1449:LYS:HE2	1.82	0.60
3:C:86:THR:HG22	40:T:238:LEU:O	2.01	0.60
3:C:452:THR:HG22	3:C:577:PHE:CG	2.37	0.60
3:C:706:GLN:NE2	3:C:708:THR:OG1	2.35	0.60
5:E:267:PHE:HE1	31:K:194:GLU:HB3	1.63	0.60
1:A:924:GLN:HE22	1:A:1439:ARG:CZ	2.14	0.60
3:C:221:ILE:HD11	3:C:479:THR:HG1	1.65	0.60
23:3:898:ASN:OD1	23:3:899:THR:N	2.34	0.60
42:V:483:GLU:O	42:V:486:THR:CB	2.49	0.60
1:A:705:LYS:HE2	38:R:251:ILE:HB	1.82	0.60
1:A:960:ASN:ND2	1:A:1225:THR:OG1	2.32	0.60
1:A:2298:LEU:CD1	4:D:1265:GLN:CB	2.79	0.60
3:C:77:VAL:HG21	40:T:196:LEU:HD23	1.83	0.60
3:C:148:CYS:HA	3:C:417:ARG:NH2	2.16	0.60
23:3:325:ILE:O	23:3:375:SER:N	2.35	0.60
40:T:267:ASP:O	40:T:268:LYS:CB	2.47	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:T:455:GLN:HG2	40:T:456:PRO:HD3	1.83	0.60
2:B:42:U:C4'	13:F:70:A:C4'	2.80	0.60
3:C:140:HIS:HA	3:C:230:ASP:HB2	1.83	0.60
3:C:567:GLU:OE2	3:C:570:GLY:HA3	2.02	0.60
13:F:7:G:H5'	13:F:7:G:H8	1.66	0.60
13:F:37:C:H41	14:G:5:G:P	2.24	0.60
15:H:83:A:C2	15:H:84:C:C2	2.90	0.60
29:L:77:LEU:HD22	38:R:289:ALA:HA	1.84	0.60
36:O:132:ARG:HG3	36:O:137:LEU:HD23	1.84	0.60
40:T:342:GLU:HB3	40:T:343:PRO:HD3	1.83	0.60
46:Z:563:ARG:HH21	46:Z:563:ARG:CG	2.14	0.60
1:A:1384:ARG:HH21	1:A:1414:ARG:HH12	1.50	0.60
1:A:1426:ASP:OD2	38:R:421:GLY:HA3	2.01	0.60
3:C:79:THR:CG2	40:T:199:VAL:CB	2.37	0.60
3:C:82:GLN:HB2	40:T:231:TRP:CZ3	2.36	0.60
3:C:94:ILE:CD1	37:P:44:ARG:NH2	2.65	0.60
3:C:443:VAL:O	3:C:447:PRO:HD3	2.02	0.60
3:C:678:THR:CG2	3:C:683:ASN:CB	2.79	0.60
14:G:26:U:C5'	36:O:235:TYR:OH	2.50	0.60
21:1:862:GLU:OE1	21:1:904:THR:OG1	2.19	0.60
23:3:457:ASN:ND2	23:3:478:PHE:O	2.35	0.60
33:Q:500:GLY:N	38:R:51:ILE:CG1	2.65	0.60
33:Q:500:GLY:CA	38:R:51:ILE:HD11	2.32	0.60
38:R:106:GLN:HG2	38:R:110:LYS:CE	2.28	0.60
40:T:185:MET:SD	40:T:442:ARG:NH1	2.71	0.60
1:A:122:ILE:HD13	1:A:483:GLN:CG	2.32	0.59
1:A:306:GLN:HG3	3:C:853:ARG:HG2	1.83	0.59
1:A:372:PRO:CG	3:C:342:ARG:NE	2.62	0.59
23:3:968:ARG:HD3	23:3:979:ARG:HD3	1.84	0.59
3:C:73:TYR:CD2	40:T:199:VAL:HG21	2.36	0.59
3:C:73:TYR:CZ	40:T:487:LYS:HE3	2.37	0.59
3:C:669:THR:HG22	3:C:690:GLU:HB3	1.84	0.59
28:J:406:PHE:CE2	28:J:411:MET:HE3	2.36	0.59
29:L:216:PHE:CE1	36:O:112:VAL:O	2.52	0.59
37:P:72:ARG:HB2	37:P:72:ARG:HH11	1.66	0.59
40:T:455:GLN:HG2	40:T:456:PRO:CD	2.32	0.59
1:A:122:ILE:N	1:A:481:PHE:O	2.34	0.59
1:A:525:LYS:CE	34:M:194:ARG:CG	2.79	0.59
1:A:532:THR:HG23	14:G:2:U:OP1	2.01	0.59
1:A:718:ARG:HE	38:R:259:LYS:HE3	1.67	0.59
3:C:186:VAL:HG22	3:C:535:ALA:HA	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:883:GLU:HG3	23:3:884:GLN:H	1.66	0.59
36:O:133:PRO:HD2	36:O:137:LEU:HD22	1.84	0.59
38:R:104:GLN:NE2	38:R:105:GLY:N	2.50	0.59
46:Z:574:ASN:O	46:Z:575:ARG:C	2.40	0.59
1:A:181:ASN:N	1:A:181:ASN:OD1	2.35	0.59
2:B:43:U:C4	14:G:-4:A:N1	2.71	0.59
5:E:233:GLY:O	5:E:260:ARG:NH2	2.35	0.59
13:F:27:A:C1'	36:O:181:TYR:CE2	2.86	0.59
14:G:22:C:O2'	14:G:23:U:P	2.60	0.59
28:J:493:ALA:HB1	28:J:499:ARG:CB	2.32	0.59
35:N:117:CYS:SG	35:N:119:CYS:HB3	2.42	0.59
38:R:124:VAL:HG22	38:R:125:MET:N	2.16	0.59
38:R:420:LYS:HA	38:R:420:LYS:CE	2.12	0.59
1:A:86:ARG:HG3	1:A:87:VAL:N	2.17	0.59
1:A:944:ASP:OD2	1:A:1435:GLY:N	2.34	0.59
1:A:1262:LYS:CG	38:R:431:ASP:CB	2.69	0.59
1:A:1405:LEU:HA	38:R:415:LEU:HD22	1.84	0.59
1:A:1962:THR:O	46:Z:524:ARG:HG3	2.02	0.59
3:C:298:LEU:HD13	3:C:298:LEU:N	2.18	0.59
15:H:56:A:H2'	15:H:57:A:C8	2.38	0.59
23:3:895:ARG:NH2	23:3:901:GLU:OE1	2.34	0.59
23:3:1040:ASP:OD1	23:3:1043:THR:N	2.35	0.59
29:L:209:ASP:OD1	36:O:111:ASP:CB	2.51	0.59
1:A:661:GLU:CD	38:R:214:ILE:HD11	2.22	0.59
1:A:692:ASP:O	1:A:696:MET:CB	2.50	0.59
1:A:942:PRO:HB2	1:A:1438:VAL:HG12	1.84	0.59
1:A:1076:ASP:OD1	1:A:1077:ILE:N	2.35	0.59
1:A:1363:GLN:HG2	1:A:1364:LEU:H	1.66	0.59
3:C:66:TYR:HE2	37:P:211:VAL:HG11	1.67	0.59
3:C:91:GLU:OE1	3:C:91:GLU:HA	2.01	0.59
3:C:145:PHE:CB	3:C:312:SER:CB	2.65	0.59
13:F:36:A:C5'	13:F:36:A:C8	2.85	0.59
15:H:112:G:H2'	15:H:113:G:H8	1.65	0.59
21:1:936:VAL:O	21:1:940:LEU:HB2	2.03	0.59
21:1:1125:PRO:HA	21:1:1128:VAL:HG22	1.84	0.59
23:3:740:GLU:HB2	23:3:757:ILE:HD12	1.83	0.59
36:O:132:ARG:HH11	39:S:149:SER:CB	2.00	0.59
36:O:155:PRO:HD3	38:R:188:PHE:CD1	2.38	0.59
40:T:345:ILE:HB	40:T:357:TRP:HB2	1.85	0.59
42:V:514:PHE:O	42:V:521:TYR:CB	2.51	0.59
1:A:338:VAL:HG21	3:C:867:PRO:CD	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:PHE:HE2	3:C:399:LEU:HD23	1.63	0.59
1:A:569:VAL:O	1:A:570:ASP:CB	2.50	0.59
1:A:1405:LEU:CB	38:R:415:LEU:HD22	2.33	0.59
1:A:2095:ASP:OD2	1:A:2258:ARG:NE	2.36	0.59
3:C:149:LEU:CD1	3:C:427:PHE:CB	2.80	0.59
23:3:224:TYR:HB3	23:3:261:PHE:HE2	1.66	0.59
23:3:1015:LYS:HE2	23:3:1065:GLU:HG2	1.85	0.59
28:J:225:LEU:CD2	29:L:211:ASN:HB2	2.20	0.59
38:R:90:VAL:CG1	38:R:94:GLY:O	2.50	0.59
38:R:110:LYS:HD2	38:R:110:LYS:C	2.23	0.59
38:R:226:PRO:HD2	38:R:226:PRO:O	2.00	0.59
39:S:10:GLN:HA	39:S:29:TRP:CH2	2.38	0.59
43:W:290:GLY:HA3	43:W:571:TRP:HA	1.84	0.59
45:Y:88:ARG:HH11	46:Z:576:PHE:HB3	1.68	0.59
1:A:44:ARG:CG	1:A:45:TYR:CD2	2.85	0.59
1:A:305:ARG:HH21	3:C:854:ARG:HD3	1.68	0.59
1:A:602:ILE:HG21	1:A:1548:TYR:OH	2.02	0.59
1:A:888:GLN:NE2	1:A:890:ALA:O	2.19	0.59
3:C:227:LEU:O	3:C:255:VAL:HA	2.03	0.59
23:3:613:THR:HG22	23:3:632:ALA:HA	1.84	0.59
23:3:784:THR:HB	23:3:786:ARG:HH12	1.67	0.59
23:3:1027:ASP:OD1	23:3:1028:THR:N	2.35	0.59
26:6:56:GLY:O	26:6:65:GLY:N	2.21	0.59
36:O:233:THR:HA	36:O:272:ILE:O	2.03	0.59
38:R:420:LYS:HG2	38:R:423:ASP:OD1	2.02	0.59
38:R:421:GLY:O	38:R:423:ASP:N	2.35	0.59
39:S:71:GLY:O	43:W:93:PHE:N	2.31	0.59
1:A:43:LYS:HD3	43:W:168:PHE:CB	2.32	0.59
3:C:137:HIS:CD2	3:C:236:MET:HB3	2.35	0.59
3:C:497:LEU:HD11	3:C:577:PHE:CZ	2.32	0.59
5:E:321:TYR:CD1	43:W:84:THR:HA	2.38	0.59
21:1:1223:SER:HB2	21:1:1226:VAL:HG12	1.83	0.59
1:A:232:LEU:HD13	1:A:401:GLY:HA2	1.85	0.59
2:B:44:A:H2	14:G:-5:G:H1	1.48	0.59
3:C:145:PHE:CE1	3:C:427:PHE:CE1	2.91	0.59
3:C:465:MET:CE	3:C:475:MET:CG	2.70	0.59
3:C:736:GLY:HA2	3:C:770:PHE:CE2	2.38	0.59
13:F:45:A:H1'	13:F:73:A:C2	2.38	0.59
21:1:522:LYS:HD3	21:1:526:PHE:CZ	2.38	0.59
23:3:22:PHE:HD2	23:3:29:GLU:HB2	1.68	0.59
23:3:587:VAL:HG11	23:3:590:MET:HG3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:J:259:GLN:HE22	29:L:220:PRO:CG	2.15	0.59
35:N:28:LYS:HZ3	43:W:190:ASP:CA	2.08	0.59
38:R:125:MET:CE	38:R:131:ASP:OD1	2.51	0.59
38:R:148:ARG:HG3	38:R:148:ARG:HH11	1.68	0.59
39:S:77:ILE:HG13	39:S:78:TYR:CD1	2.38	0.59
1:A:44:ARG:HG3	1:A:45:TYR:CD2	2.37	0.58
1:A:723:ASN:HB2	1:A:785:LYS:HG2	1.83	0.58
3:C:69:ALA:CA	40:T:456:PRO:HG3	2.28	0.58
3:C:359:LYS:HE3	3:C:359:LYS:O	2.02	0.58
13:F:35:A:O2'	13:F:36:A:OP1	2.21	0.58
21:1:1278:ASP:OD2	23:3:112:CYS:N	2.36	0.58
22:2:648:LEU:HD11	22:2:650:ILE:HG13	1.85	0.58
23:3:336:ALA:HA	23:3:351:SER:HA	1.85	0.58
23:3:463:ARG:HB2	23:3:510:LEU:HD22	1.85	0.58
28:J:339:TRP:CG	38:R:116:TYR:HD2	2.21	0.58
40:T:185:MET:SD	40:T:442:ARG:NH2	2.75	0.58
45:Y:52:ILE:HA	45:Y:55:VAL:HG22	1.84	0.58
1:A:76:MET:SD	1:A:88:TYR:CD2	2.95	0.58
1:A:695:ASP:CG	40:T:374:SER:OG	2.41	0.58
1:A:1352:HIS:CD2	41:U:5:ILE:CD1	2.86	0.58
1:A:1354:ARG:HH11	41:U:7:LEU:HG	1.68	0.58
1:A:2073:TRP:CD1	1:A:2074:ARG:N	2.71	0.58
1:A:2073:TRP:HD1	1:A:2074:ARG:HD2	1.67	0.58
1:A:2268:LEU:HD22	4:D:1261:PRO:O	1.96	0.58
2:B:42:U:C4	14:G:-3:A:N1	2.71	0.58
3:C:78:GLU:CD	40:T:198:ARG:HE	2.07	0.58
3:C:474:LEU:HD11	3:C:501:ILE:HG12	1.85	0.58
21:1:982:LEU:HD11	21:1:997:LEU:HD11	1.83	0.58
21:1:1147:VAL:O	21:1:1150:SER:OG	2.17	0.58
23:3:417:ASN:OD1	23:3:418:GLU:N	2.36	0.58
23:3:673:VAL:HG12	23:3:690:ARG:HA	1.84	0.58
23:3:797:LEU:HG	23:3:871:PRO:HG3	1.85	0.58
23:3:903:TRP:HB3	23:3:930:LEU:HD23	1.84	0.58
36:O:84:CYS:O	36:O:85:LEU:HB2	2.03	0.58
38:R:225:GLU:CG	38:R:226:PRO:CD	2.80	0.58
38:R:433:ILE:CD1	38:R:435:ASN:ND2	2.67	0.58
45:Y:86:ASP:CB	46:Z:502:ALA:HB3	2.33	0.58
1:A:32:GLU:OE2	1:A:36:LYS:HE3	2.03	0.58
1:A:229:GLN:HA	1:A:415:SER:HA	1.85	0.58
3:C:133:THR:O	3:C:226:VAL:CA	2.51	0.58
5:E:87:ASP:O	5:E:88:ARG:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:773:LEU:HD21	21:1:792:VAL:HG22	1.84	0.58
23:3:304:GLN:NE2	23:3:335:VAL:HA	2.18	0.58
23:3:638:GLU:H	23:3:669:LEU:HA	1.68	0.58
37:P:210:PHE:HD2	40:T:455:GLN:CD	2.05	0.58
38:R:233:HIS:CD2	38:R:233:HIS:H	2.22	0.58
43:W:97:ASN:C	43:W:99:PHE:H	2.06	0.58
1:A:1180:LYS:HA	1:A:1201:ARG:NH1	2.18	0.58
3:C:679:PRO:HD2	3:C:807:GLN:CB	2.10	0.58
23:3:440:HIS:O	23:3:718:ARG:NH2	2.36	0.58
28:J:338:GLU:O	38:R:116:TYR:CG	2.57	0.58
36:O:245:GLU:O	36:O:248:LEU:N	2.37	0.58
1:A:299:ILE:CD1	1:A:1346:THR:HG21	2.32	0.58
1:A:1367:ASN:OD1	1:A:1368:LEU:N	2.37	0.58
1:A:1900:GLU:OE1	46:Z:522:LEU:HB3	2.00	0.58
3:C:750:LEU:O	3:C:750:LEU:HD12	2.03	0.58
5:E:263:ASP:HB3	5:E:274:VAL:HG21	1.84	0.58
46:Z:566:TYR:CD2	46:Z:584:TRP:HE3	2.20	0.58
1:A:1863:VAL:HG11	1:A:1868:MET:HB2	1.84	0.58
1:A:2310:ARG:NH1	1:A:2314:PHE:HE1	2.02	0.58
5:E:87:ASP:O	5:E:88:ARG:CB	2.51	0.58
23:3:224:TYR:HB3	23:3:261:PHE:CE2	2.39	0.58
24:4:18:GLY:H	24:4:85:ARG:HB2	1.67	0.58
37:P:35:LEU:HB3	37:P:36:PRO:HD2	1.86	0.58
42:V:497:CYS:CB	42:V:507:PHE:CB	2.81	0.58
1:A:388:LEU:HD13	3:C:379:LYS:HB3	1.85	0.58
1:A:798:GLY:HA2	38:R:288:PHE:CE2	2.39	0.58
1:A:1962:THR:O	46:Z:524:ARG:HG2	2.03	0.58
1:A:2325:VAL:O	4:D:788:GLY:HA2	2.03	0.58
3:C:509:VAL:O	3:C:510:LEU:HD23	2.04	0.58
15:H:147:G:H2'	15:H:148:C:C6	2.38	0.58
34:M:196:ASP:O	34:M:198:GLN:N	2.36	0.58
1:A:121:HIS:ND1	1:A:481:PHE:O	2.36	0.58
1:A:152:ARG:HH11	1:A:152:ARG:CG	2.16	0.58
1:A:264:PHE:CE1	1:A:455:VAL:CG1	2.75	0.58
1:A:535:ARG:CZ	1:A:535:ARG:HB3	2.33	0.58
1:A:1757:GLU:OE1	38:R:451:ILE:CG1	2.36	0.58
3:C:140:HIS:NE2	3:C:233:GLU:CG	2.66	0.58
15:H:80:A:C2	15:H:81:G:C5	2.92	0.58
23:3:461:THR:HA	23:3:473:TYR:O	2.03	0.58
25:5:24:ARG:HG2	25:5:59:THR:HG22	1.86	0.58
37:P:188:TRP:C	37:P:190:ASP:N	2.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:V:609:GLN:O	42:V:612:PHE:N	2.36	0.58
3:C:140:HIS:NE2	3:C:233:GLU:CB	2.67	0.58
14:G:141:C:H2'	14:G:142:U:H6	1.69	0.58
21:1:415:LEU:O	25:5:36:TYR:OH	2.21	0.58
21:1:1109:ARG:NH2	21:1:1142:ASN:HB2	2.19	0.58
21:1:1165:TYR:HE1	22:2:575:PHE:CD1	2.21	0.58
23:3:878:ASP:OD1	23:3:879:LEU:N	2.37	0.58
38:R:124:VAL:HG22	38:R:126:ASN:H	1.68	0.58
46:Z:566:TYR:HE2	46:Z:584:TRP:CZ3	1.92	0.58
1:A:249:LEU:HD22	1:A:254:TYR:HB2	1.86	0.58
1:A:280:GLU:OE2	1:A:281:PRO:HD2	2.03	0.58
3:C:573:GLU:N	3:C:573:GLU:OE1	2.37	0.58
14:G:18:A:C5'	36:O:69:GLU:OE1	2.46	0.58
23:3:8:LEU:HD23	23:3:774:PHE:HZ	1.68	0.58
23:3:753:GLY:CA	23:3:765:LEU:O	2.51	0.58
38:R:125:MET:HE3	38:R:131:ASP:OD1	2.03	0.58
38:R:171:LEU:HD23	38:R:171:LEU:O	2.03	0.58
1:A:232:LEU:HD22	1:A:404:LEU:HD12	1.86	0.57
2:B:44:A:H2	14:G:-5:G:N1	2.02	0.57
3:C:145:PHE:CD1	3:C:312:SER:HB3	2.39	0.57
5:E:165:GLN:HG3	5:E:181:ILE:HD11	1.85	0.57
38:R:189:ASN:HD21	38:R:195:ARG:HH22	1.50	0.57
38:R:415:LEU:C	38:R:417:ASN:H	2.05	0.57
40:T:399:LYS:HG2	40:T:406:ILE:CD1	2.31	0.57
1:A:48:LYS:O	1:A:53:PHE:CD2	2.57	0.57
5:E:277:PHE:CE2	5:E:300:ILE:CD1	2.85	0.57
13:F:39:A:N6	14:G:8:C:H42	2.02	0.57
14:G:12:G:N2	14:G:13:C:O4'	2.38	0.57
23:3:440:HIS:CD2	23:3:733:PRO:HD2	2.39	0.57
23:3:781:LEU:HB3	23:3:801:GLU:OE2	2.04	0.57
37:P:188:TRP:O	37:P:189:ASP:C	2.42	0.57
1:A:60:ASP:OD1	1:A:60:ASP:N	2.36	0.57
3:C:749:THR:OG1	3:C:752:SER:HB2	2.04	0.57
36:O:131:THR:HG23	43:W:111:LEU:CA	2.34	0.57
44:X:285:ARG:NH1	44:X:304:ALA:O	2.35	0.57
1:A:439:GLN:NE2	1:A:614:TYR:CE2	2.49	0.57
1:A:800:TYR:HB3	3:C:59:LEU:CD1	2.34	0.57
2:B:41:U:C4	14:G:-1:G:N1	2.73	0.57
2:B:42:U:H3	14:G:-3:A:H2	0.70	0.57
3:C:617:LEU:HD11	3:C:629:ILE:HG23	1.87	0.57
23:3:306:GLU:OE2	27:7:63:ARG:HG3	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:1050:PHE:HB3	23:3:1167:TYR:CE2	2.38	0.57
29:L:73:HIS:O	29:L:77:LEU:HG	2.04	0.57
38:R:171:LEU:HD12	38:R:201:GLU:CD	2.25	0.57
1:A:50:LYS:O	1:A:51:PHE:C	2.43	0.57
1:A:1771:LEU:HD11	1:A:1777:ILE:HG21	1.86	0.57
3:C:79:THR:HG23	40:T:199:VAL:CG1	2.27	0.57
21:1:850:ILE:O	21:1:854:VAL:HG23	2.04	0.57
23:3:791:HIS:CE1	23:3:934:GLY:HA3	2.39	0.57
38:R:55:LEU:CB	38:R:73:PRO:O	2.53	0.57
1:A:785:LYS:CE	37:P:215:LEU:CD1	2.78	0.57
2:B:20:G:O6	2:B:24:G:OP1	2.21	0.57
3:C:93:ILE:O	3:C:94:ILE:HB	2.04	0.57
3:C:572:GLU:O	3:C:573:GLU:HB2	2.04	0.57
3:C:669:THR:CG2	3:C:690:GLU:OE1	2.52	0.57
5:E:267:PHE:CE1	31:K:194:GLU:HB2	2.40	0.57
14:G:137:C:N4	15:H:40:C:H42	1.99	0.57
23:3:211:TYR:CE1	23:3:222:ARG:HG2	2.40	0.57
23:3:429:ARG:NH1	27:7:58:ASN:OD1	2.38	0.57
23:3:635:ALA:H	23:3:669:LEU:HD21	1.70	0.57
37:P:73:GLU:O	37:P:76:ARG:HG2	2.04	0.57
37:P:188:TRP:N	37:P:188:TRP:CE3	2.73	0.57
1:A:569:VAL:O	1:A:570:ASP:HB2	2.04	0.57
1:A:623:LYS:O	50:A:3000:IHP:O24	2.22	0.57
1:A:745:ALA:HB2	40:T:206:TRP:CZ2	2.40	0.57
1:A:783:TYR:CG	37:P:228:ILE:HG12	2.39	0.57
3:C:140:HIS:HE2	3:C:233:GLU:HG3	1.68	0.57
15:H:166:G:OP2	15:H:166:G:N2	2.27	0.57
29:L:33:ARG:O	29:L:36:SER:OG	2.20	0.57
29:L:215:PRO:O	36:O:113:ASN:CA	2.53	0.57
35:N:28:LYS:NZ	43:W:190:ASP:N	2.52	0.57
36:O:240:GLY:HA3	36:O:296:ARG:HH22	1.68	0.57
37:P:31:SER:N	37:P:34:ASP:OD2	2.37	0.57
1:A:293:TRP:HB2	1:A:1136:ARG:NH2	2.19	0.57
1:A:705:LYS:CG	38:R:251:ILE:HB	2.27	0.57
1:A:2153:THR:HG22	1:A:2154:HIS:H	1.70	0.57
3:C:140:HIS:CE1	3:C:233:GLU:CB	2.83	0.57
3:C:487:GLY:HA3	3:C:489:GLN:OE1	2.05	0.57
3:C:490:PHE:HZ	3:C:612:LYS:HD2	1.69	0.57
3:C:511:GLY:O	3:C:576:ILE:HD12	2.02	0.57
15:H:148:C:O5'	15:H:148:C:H6	1.87	0.57
21:1:1109:ARG:HH22	21:1:1142:ASN:HB2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:1258:ALA:HB3	21:1:1261:VAL:HG12	1.86	0.57
23:3:184:CYS:SG	23:3:209:THR:OG1	2.56	0.57
23:3:275:ARG:HE	23:3:386:PHE:HD2	1.51	0.57
38:R:434:TYR:CD2	38:R:435:ASN:N	2.73	0.57
1:A:387:PHE:CD2	3:C:399:LEU:CD2	2.87	0.57
1:A:692:ASP:CA	40:T:376:ARG:NH2	2.53	0.57
1:A:705:LYS:CG	38:R:251:ILE:CD1	2.70	0.57
1:A:1757:GLU:HG3	38:R:451:ILE:HG13	1.87	0.57
5:E:310:TYR:CE1	5:E:322:LYS:CD	2.86	0.57
15:H:152:G:N2	15:H:153:A:C5	2.73	0.57
21:1:1098:LEU:HD13	21:1:1135:GLU:HG3	1.85	0.57
21:1:1126:PHE:CE2	22:2:572:HIS:HA	2.39	0.57
28:J:224:LYS:HE2	28:J:255:LEU:HD13	1.85	0.57
39:S:131:ARG:NH1	39:S:133:CYS:CB	2.68	0.57
46:Z:525:TYR:CD1	46:Z:526:ILE:N	2.73	0.57
1:A:532:THR:CB	14:G:2:U:C5’	2.83	0.57
1:A:832:TYR:CE2	1:A:834:HIS:HB2	2.40	0.57
3:C:508:LYS:HE3	3:C:566:THR:CG2	2.34	0.57
21:1:807:LYS:HA	21:1:811:LEU:HD12	1.87	0.57
21:1:942:ASN:HD22	21:1:947:VAL:HG11	1.70	0.57
23:3:442:LEU:CD1	23:3:733:PRO:O	2.50	0.57
38:R:181:PRO:O	43:W:112:SER:O	2.21	0.57
40:T:347:THR:CG2	40:T:357:TRP:HE1	2.18	0.57
42:V:489:LEU:O	42:V:492:MET:CB	2.53	0.57
43:W:420:ALA:H	43:W:438:ASP:CB	2.17	0.57
46:Z:611:ALA:O	46:Z:614:TRP:HB3	2.05	0.57
1:A:32:GLU:CG	1:A:36:LYS:HE3	2.35	0.56
2:B:27:U:O2’	2:B:28:A:O5’	2.23	0.56
3:C:261:ASP:OD1	51:C:1500:GTP:C6	2.57	0.56
3:C:456:GLY:C	3:C:457:VAL:HG13	2.25	0.56
39:S:10:GLN:CB	39:S:29:TRP:CD2	2.88	0.56
40:T:306:CYS:SG	40:T:336:VAL:CG1	2.93	0.56
1:A:790:ARG:NE	1:A:986:GLU:OE2	2.38	0.56
1:A:1233:ASP:OD1	1:A:1234:ASP:N	2.37	0.56
1:A:1252:GLY:HA2	1:A:1298:ARG:HH21	1.69	0.56
13:F:57:U:H2’	13:F:58:G:H8	1.69	0.56
14:G:7:G:H2’	14:G:8:C:C6	2.40	0.56
15:H:78:C:HO2’	15:H:79:G:H5’	1.70	0.56
15:H:141:C:C2	15:H:142:C:C5	2.94	0.56
23:3:327:LEU:O	23:3:373:PHE:HB2	2.05	0.56
23:3:478:PHE:O	23:3:504:PRO:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:J:273:TYR:CG	38:R:228:PRO:CG	2.88	0.56
38:R:409:VAL:O	38:R:410:GLN:HG2	2.05	0.56
42:V:483:GLU:O	42:V:486:THR:N	2.33	0.56
46:Z:524:ARG:HB3	46:Z:524:ARG:CZ	2.35	0.56
1:A:36:LYS:NZ	43:W:163:GLN:CB	2.69	0.56
1:A:36:LYS:HZ1	43:W:163:GLN:CB	2.18	0.56
1:A:178:TYR:CD2	1:A:491:GLU:HB2	2.40	0.56
1:A:356:ILE:HG22	1:A:357:ASN:N	2.20	0.56
1:A:434:HIS:CE1	1:A:435:CYS:SG	2.98	0.56
1:A:532:THR:CB	14:G:2:U:H5"	2.35	0.56
1:A:587:GLN:O	1:A:587:GLN:HG2	2.04	0.56
1:A:1301:ILE:HD11	1:A:1306:LYS:CE	2.35	0.56
1:A:1386:TRP:HZ2	1:A:1417:PRO:HB2	1.69	0.56
1:A:1548:TYR:CD2	1:A:1549:VAL:CG2	2.75	0.56
3:C:426:GLU:O	3:C:427:PHE:HB2	2.05	0.56
3:C:449:ILE:CG2	3:C:457:VAL:HG11	2.30	0.56
5:E:250:LEU:CD2	5:E:262:TRP:HB2	2.35	0.56
15:H:152:G:N2	15:H:153:A:C8	2.73	0.56
21:1:847:ALA:O	21:1:851:SER:OG	2.24	0.56
22:2:643:PRO:CD	24:4:69:TYR:CG	2.88	0.56
23:3:438:LEU:HA	23:3:775:ASN:O	2.06	0.56
23:3:520:TYR:HB2	23:3:521:PRO:HD2	1.87	0.56
23:3:633:LEU:HD13	23:3:667:ILE:HG21	1.87	0.56
29:L:209:ASP:CG	36:O:111:ASP:CB	2.73	0.56
35:N:38:GLU:C	35:N:40:LYS:H	2.08	0.56
37:P:76:ARG:HG3	37:P:77:ASP:N	2.19	0.56
38:R:89:GLN:OE1	39:S:146:GLU:N	2.38	0.56
39:S:131:ARG:HH12	39:S:133:CYS:HA	1.68	0.56
1:A:120:TYR:N	1:A:483:GLN:O	2.33	0.56
1:A:226:GLN:HA	1:A:418:THR:OG1	2.06	0.56
1:A:570:ASP:OD1	1:A:571:ALA:N	2.38	0.56
3:C:223:ASP:OD1	3:C:495:ARG:NH2	2.38	0.56
3:C:457:VAL:HA	3:C:462:GLY:HA3	1.88	0.56
3:C:673:LYS:HG3	3:C:686:THR:CG2	2.36	0.56
3:C:701:GLU:HA	3:C:740:THR:HG1	1.70	0.56
14:G:22:C:O2	14:G:22:C:H2'	2.06	0.56
21:1:944:SER:O	21:1:948:ARG:HG3	2.04	0.56
21:1:1279:ALA:HA	23:3:1167:TYR:CE1	2.41	0.56
24:4:75:ASN:ND2	24:4:86:VAL:O	2.38	0.56
34:M:201:ILE:HA	34:M:220:LEU:HB3	1.85	0.56
1:A:226:GLN:OE1	1:A:417:ARG:NE	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:ASP:OD1	40:T:376:ARG:NH2	2.38	0.56
1:A:1163:ARG:NH2	3:C:61:GLU:OE2	2.35	0.56
5:E:267:PHE:CZ	31:K:194:GLU:CG	2.88	0.56
13:F:26:U:O2'	13:F:27:A:OP1	2.18	0.56
23:3:550:ASN:HD21	23:3:595:VAL:H	1.53	0.56
27:7:32:LEU:O	27:7:36:HIS:ND1	2.23	0.56
28:J:311:GLN:OE1	28:J:311:GLN:N	2.33	0.56
1:A:282:LEU:HD23	1:A:282:LEU:O	2.05	0.56
1:A:301:LYS:HG2	3:C:940:ARG:CA	2.35	0.56
3:C:301:SER:O	3:C:304:LEU:N	2.30	0.56
3:C:619:THR:C	3:C:620:LYS:HG3	2.25	0.56
13:F:50:A:O2'	13:F:51:U:OP1	2.23	0.56
43:W:101:THR:O	43:W:103:GLN:N	2.38	0.56
1:A:283:VAL:HG22	1:A:284:ARG:HG2	1.88	0.56
1:A:651:TRP:CZ2	13:F:66:C:N3	2.73	0.56
1:A:812:THR:HG23	1:A:1055:LEU:HD11	1.88	0.56
1:A:2320:LEU:HD23	1:A:2322:GLU:H	1.71	0.56
3:C:140:HIS:CB	3:C:230:ASP:CB	2.66	0.56
24:4:79:LEU:HB2	24:4:84:ILE:HD11	1.88	0.56
29:L:721:LEU:HA	29:L:724:TYR:CG	2.41	0.56
35:N:128:VAL:HG13	35:N:130:ARG:N	2.14	0.56
1:A:44:ARG:NH2	5:E:285:GLU:O	2.38	0.56
1:A:229:GLN:HG2	1:A:415:SER:CB	2.36	0.56
1:A:579:GLN:NE2	1:A:613:TYR:CE1	2.74	0.56
1:A:849:ALA:O	1:A:1449:LYS:NZ	2.36	0.56
3:C:85:ASP:HB3	40:T:238:LEU:CG	2.27	0.56
3:C:677:GLU:HA	3:C:683:ASN:O	2.05	0.56
5:E:277:PHE:CE2	5:E:300:ILE:HD13	2.40	0.56
14:G:20:A:C1'	36:O:193:LEU:HD21	2.35	0.56
21:1:1026:ASN:ND2	21:1:1031:VAL:HG11	2.21	0.56
23:3:745:PHE:HE2	23:3:750:CYS:HB3	1.71	0.56
1:A:378:PHE:C	1:A:379:GLU:HG2	2.25	0.56
2:B:40:U:H3'	2:B:40:U:O2	2.05	0.56
3:C:385:VAL:HG23	3:C:386:GLY:N	2.20	0.56
5:E:153:PHE:HD1	5:E:153:PHE:H	1.54	0.56
15:H:150:U:C2	15:H:151:C:C5	2.94	0.56
21:1:689:ILE:O	21:1:692:HIS:ND1	2.39	0.56
21:1:718:PRO:HA	21:1:756:LEU:HG	1.88	0.56
23:3:669:LEU:HB2	23:3:673:VAL:HG22	1.88	0.56
25:5:93:ASN:OD1	25:5:94:ALA:N	2.34	0.56
28:J:433:ARG:HH12	28:J:461:LYS:CB	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:O:236:VAL:O	36:O:269:CYS:HA	2.06	0.56
40:T:342:GLU:CB	40:T:343:PRO:CD	2.83	0.56
46:Z:612:TYR:O	46:Z:613:LYS:C	2.43	0.56
1:A:89:LEU:HD13	1:A:660:PHE:CZ	2.41	0.56
1:A:339:PHE:CD1	1:A:406:TRP:CZ3	2.93	0.56
1:A:1451:ASN:OD1	1:A:1453:PHE:N	2.39	0.56
3:C:631:GLY:HA3	3:C:637:LEU:HD21	1.88	0.56
15:H:83:A:N1	15:H:84:C:C4	2.74	0.56
21:1:1293:ASN:HA	27:7:76:CYS:O	2.05	0.56
21:1:1295:TYR:CE2	27:7:28:LYS:HE2	2.41	0.56
23:3:29:GLU:HB3	23:3:40:LEU:HD11	1.87	0.56
23:3:804:HIS:HD2	23:3:862:TRP:CZ2	2.24	0.56
23:3:1028:THR:HG22	23:3:1088:LYS:HD3	1.86	0.56
35:N:59:TYR:CE1	43:W:187:SER:HA	2.41	0.56
1:A:295:GLU:OE2	3:C:593:GLU:OE2	2.23	0.55
1:A:783:TYR:CD1	37:P:228:ILE:HG12	2.41	0.55
14:G:16:G:H4'	14:G:17:U:O5'	2.04	0.55
15:H:154:C:O2'	15:H:155:C:H5'	2.04	0.55
21:1:570:TYR:HD1	21:1:573:LYS:HD2	1.71	0.55
39:S:131:ARG:HH11	39:S:133:CYS:HA	1.69	0.55
1:A:417:ARG:HH12	2:B:58:U:H4'	1.70	0.55
1:A:2113:LYS:CE	4:D:1229:ASP:CA	2.84	0.55
15:H:141:C:H2'	15:H:142:C:H6	1.71	0.55
15:H:149:A:C4	15:H:150:U:C5	2.95	0.55
15:H:180:G:C2	15:H:181:G:C5	2.94	0.55
36:O:225:PRO:HG3	36:O:302:TRP:NE1	2.12	0.55
1:A:89:LEU:HD13	1:A:660:PHE:HZ	1.71	0.55
1:A:296:PHE:HB3	3:C:656:ALA:HB1	1.86	0.55
1:A:1321:GLU:O	1:A:1503:TRP:NE1	2.39	0.55
1:A:1418:ARG:HE	1:A:1464:LEU:HD23	1.72	0.55
1:A:2325:VAL:CG1	4:D:788:GLY:O	2.33	0.55
3:C:674:CYS:HG	3:C:822:MET:CE	2.16	0.55
5:E:250:LEU:HD22	5:E:262:TRP:HB2	1.88	0.55
21:1:1137:ARG:HH21	22:2:524:LEU:HD13	1.72	0.55
37:P:224:MET:HA	37:P:224:MET:HE3	1.88	0.55
3:C:77:VAL:HG13	40:T:196:LEU:C	1.90	0.55
3:C:706:GLN:NE2	3:C:708:THR:H	2.02	0.55
22:2:650:ILE:HG12	22:2:688:GLY:HA3	1.89	0.55
1:A:151:MET:CE	1:A:628:GLY:C	2.75	0.55
1:A:1035:GLN:HA	1:A:1446:GLN:NE2	2.21	0.55
1:A:1364:LEU:HD13	42:V:461:LEU:C	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1370:ARG:HH22	42:V:506:PHE:CB	2.19	0.55
1:A:1690:ASP:OD1	1:A:1691:ASN:N	2.39	0.55
2:B:47:A:O2'	2:B:48:A:H5"	2.06	0.55
2:B:94:U:H2'	2:B:95:G:H5"	1.89	0.55
3:C:185:PRO:HG3	3:C:482:TYR:CZ	2.41	0.55
3:C:439:PRO:HB2	3:C:443:VAL:HB	1.88	0.55
21:1:1166:ILE:O	21:1:1170:THR:HG23	2.07	0.55
23:3:526:HIS:HB3	23:3:534:ASN:HB2	1.88	0.55
24:4:29:LEU:HD22	24:4:33:PHE:HE2	1.72	0.55
39:S:13:ASN:HD22	39:S:24:VAL:CG1	2.19	0.55
46:Z:566:TYR:CD2	46:Z:580:PRO:HG2	2.36	0.55
1:A:89:LEU:O	1:A:89:LEU:HD23	2.05	0.55
1:A:1364:LEU:HD11	42:V:461:LEU:CB	2.29	0.55
1:A:1607:GLU:N	1:A:1632:PHE:O	2.38	0.55
1:A:1930:TYR:O	1:A:1933:PHE:HB3	2.06	0.55
1:A:2073:TRP:HD1	1:A:2074:ARG:N	2.04	0.55
3:C:516:LEU:HD13	3:C:516:LEU:C	2.26	0.55
3:C:702:ASN:O	3:C:703:GLU:HB2	2.07	0.55
5:E:162:ARG:CZ	5:E:203:ASP:O	2.55	0.55
15:H:165:A:H2'	15:H:166:G:H5'	1.88	0.55
23:3:996:ILE:HG23	23:3:999:ARG:H	1.72	0.55
1:A:1233:ASP:O	1:A:1236:SER:OG	2.23	0.55
1:A:1899:VAL:HB	1:A:1902:PHE:HD2	1.71	0.55
3:C:78:GLU:OE1	40:T:198:ARG:NE	2.36	0.55
3:C:79:THR:CG2	40:T:199:VAL:CG1	2.84	0.55
3:C:567:GLU:OE1	3:C:572:GLU:HB3	2.06	0.55
5:E:260:ARG:NH1	5:E:276:ILE:HD11	2.22	0.55
14:G:23:U:O2	14:G:23:U:H2'	2.07	0.55
21:1:1255:PHE:CD2	22:2:487:LEU:HD22	2.42	0.55
37:P:33:ARG:HG3	37:P:33:ARG:HH11	1.72	0.55
45:Y:22:VAL:HG22	45:Y:26:VAL:HG13	1.88	0.55
46:Z:600:ARG:HB3	46:Z:600:ARG:NH1	2.08	0.55
1:A:283:VAL:HG13	1:A:284:ARG:N	2.22	0.55
1:A:464:PRO:O	1:A:465:LYS:HB3	2.05	0.55
1:A:715:GLU:CD	38:R:258:TRP:CZ3	2.79	0.55
1:A:1099:PHE:HE2	1:A:1153:VAL:HG13	1.72	0.55
1:A:1457:HIS:HE1	1:A:1459:ARG:HG3	1.68	0.55
1:A:1971:LEU:HB2	1:A:1976:TRP:CE2	2.42	0.55
21:1:1017:LEU:HD13	21:1:1050:VAL:HG21	1.89	0.55
21:1:1076:ALA:O	21:1:1080:THR:HG23	2.07	0.55
23:3:441:GLY:O	23:3:775:ASN:CB	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:K:135:TRP:O	31:K:138:TYR:CG	2.60	0.55
38:R:74:LEU:HD23	38:R:75:ASP:OD1	2.06	0.55
38:R:436:VAL:CG2	38:R:437:TYR:CE1	2.89	0.55
42:V:641:ASP:O	42:V:644:ARG:N	2.39	0.55
45:Y:85:GLU:O	46:Z:502:ALA:CB	2.55	0.55
1:A:436:PRO:O	1:A:437:ALA:HB3	2.07	0.55
1:A:623:LYS:CG	50:A:3000:IHP:O34	2.55	0.55
3:C:149:LEU:HA	3:C:427:PHE:CD2	2.41	0.55
5:E:114:GLU:CD	5:E:116:HIS:HE2	2.09	0.55
14:G:142:U:H2'	14:G:143:U:C6	2.42	0.55
15:H:150:U:H2'	15:H:151:C:H6	1.71	0.55
25:5:17:VAL:HG23	25:5:67:ILE:HD11	1.89	0.55
45:Y:37:TRP:HZ3	46:Z:498:GLY:HA3	1.66	0.55
1:A:119:LEU:HD11	1:A:477:LYS:HG3	1.88	0.55
1:A:168:PRO:HG2	1:A:559:ASP:CB	2.36	0.55
1:A:1457:HIS:HE2	38:R:425:GLY:H	1.46	0.55
1:A:1505:LYS:HE3	46:Z:615:SER:HG	1.68	0.55
1:A:1645:LEU:HB2	1:A:1714:ALA:HB3	1.88	0.55
1:A:2306:HIS:HD2	1:A:2308:VAL:H	1.54	0.55
3:C:220:ARG:HG2	3:C:479:THR:HG21	1.89	0.55
21:1:1174:GLU:OE2	21:1:1210:HIS:NE2	2.35	0.55
23:3:452:LEU:HB3	23:3:478:PHE:CE1	2.42	0.55
29:L:224:PHE:CD1	38:R:86:LEU:O	2.59	0.55
35:N:139:CYS:SG	35:N:140:ARG:N	2.80	0.55
37:P:188:TRP:O	37:P:190:ASP:N	2.39	0.55
38:R:74:LEU:HD23	38:R:74:LEU:C	2.27	0.55
39:S:131:ARG:HH11	39:S:133:CYS:CA	2.17	0.55
46:Z:574:ASN:O	46:Z:577:ASN:N	2.33	0.55
1:A:148:TRP:CH2	1:A:616:PHE:HB2	2.42	0.54
1:A:356:ILE:HG22	1:A:357:ASN:H	1.72	0.54
4:D:1048:VAL:O	4:D:1050:GLU:N	2.40	0.54
23:3:309:ASP:HA	23:3:332:THR:HG22	1.88	0.54
23:3:848:PRO:HB2	23:3:851:ILE:HG22	1.89	0.54
24:4:14:THR:CA	24:4:59:VAL:O	2.28	0.54
26:6:39:PRO:HB3	26:6:70:TYR:HB2	1.88	0.54
28:J:294:HIS:HE1	29:L:227:THR:HB	1.70	0.54
36:O:166:SER:HA	36:O:169:VAL:HG12	1.89	0.54
36:O:232:THR:HG22	36:O:277:ARG:HA	1.89	0.54
37:P:228:ILE:O	37:P:229:LYS:C	2.45	0.54
38:R:86:LEU:HD12	38:R:86:LEU:O	2.06	0.54
43:W:185:ASP:O	43:W:186:ALA:HB3	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:C:H2'	41:U:11:ARG:HH12	1.71	0.54
5:E:119:THR:HG21	5:E:161:ARG:HB2	1.87	0.54
15:H:153:A:C3'	15:H:154:C:C5'	2.86	0.54
21:1:1179:ASP:HB3	22:2:511:LEU:CD1	2.37	0.54
21:1:1279:ALA:HA	23:3:1167:TYR:HE1	1.70	0.54
35:N:38:GLU:O	35:N:40:LYS:N	2.38	0.54
44:X:312:GLU:O	44:X:327:TYR:HB2	2.07	0.54
1:A:592:TYR:HA	1:A:595:LYS:O	2.08	0.54
1:A:1132:LYS:HA	1:A:1139:ARG:HD3	1.90	0.54
3:C:140:HIS:CD2	3:C:233:GLU:HG3	2.41	0.54
3:C:510:LEU:HB3	3:C:576:ILE:HD11	1.89	0.54
13:F:27:A:N9	36:O:181:TYR:OH	2.37	0.54
13:F:36:A:H2'	13:F:37:C:H4'	1.89	0.54
13:F:38:G:H2'	13:F:39:A:C8	2.42	0.54
13:F:56:A:C2	15:H:20:G:C2	2.96	0.54
23:3:553:GLN:HA	23:3:566:PHE:O	2.07	0.54
23:3:1014:TYR:OH	23:3:1019:ASN:OD1	2.24	0.54
28:J:218:GLU:HG3	28:J:219:GLU:OE2	2.07	0.54
36:O:196:GLN:HE22	36:O:209:VAL:HG23	1.71	0.54
43:W:198:LYS:O	43:W:199:TYR:C	2.45	0.54
1:A:151:MET:SD	1:A:628:GLY:O	2.65	0.54
1:A:596:TYR:CZ	14:G:-5:G:N7	2.75	0.54
1:A:676:ARG:HG3	13:F:56:A:P	2.48	0.54
3:C:749:THR:HG1	3:C:752:SER:HB2	1.72	0.54
36:O:102:SER:OG	36:O:139:LYS:NZ	2.25	0.54
38:R:402:ASN:HB3	44:X:191:GLN:HB2	1.90	0.54
45:Y:10:ILE:HD13	45:Y:98:ASN:HD21	1.73	0.54
1:A:173:GLU:O	1:A:520:TYR:CD2	2.61	0.54
1:A:329:LEU:HD13	3:C:177:ARG:NE	2.17	0.54
1:A:699:GLU:O	1:A:701:ILE:HD12	2.07	0.54
1:A:1459:ARG:HG3	38:R:424:SER:N	2.22	0.54
3:C:145:PHE:CZ	3:C:427:PHE:HE1	2.21	0.54
5:E:161:ARG:NH1	5:E:203:ASP:OD1	2.40	0.54
23:3:913:LEU:HD23	23:3:920:VAL:HG12	1.89	0.54
28:J:262:ARG:HD3	29:L:220:PRO:CG	2.38	0.54
29:L:224:PHE:HD1	38:R:86:LEU:O	1.91	0.54
37:P:63:LEU:HD23	37:P:63:LEU:C	2.28	0.54
40:T:455:GLN:NE2	40:T:456:PRO:HD2	2.22	0.54
1:A:705:LYS:HG2	38:R:251:ILE:CG1	2.38	0.54
1:A:1285:LEU:HB3	1:A:1335:ILE:HD12	1.90	0.54
1:A:1333:VAL:HG11	1:A:1367:ASN:HD22	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1351:THR:HG22	41:U:25:LEU:HD21	1.88	0.54
1:A:2095:ASP:OD1	1:A:2095:ASP:N	2.41	0.54
2:B:42:U:H4'	13:F:70:A:C4'	2.37	0.54
5:E:108:HIS:ND1	5:E:128:SER:CB	2.70	0.54
5:E:310:TYR:CZ	5:E:322:LYS:HD2	2.42	0.54
23:3:138:GLN:HG2	23:3:161:HIS:CE1	2.43	0.54
23:3:336:ALA:HB2	23:3:349:VAL:HG13	1.90	0.54
38:R:131:ASP:OD2	38:R:132:LEU:HD23	2.07	0.54
1:A:530:LEU:HG	34:M:198:GLN:NE2	2.20	0.54
1:A:978:GLU:OE2	1:A:1187:PHE:HB2	2.07	0.54
1:A:1328:LEU:HD22	1:A:1368:LEU:HD21	1.89	0.54
1:A:1342:TRP:CG	3:C:921:LEU:HD11	2.42	0.54
1:A:2325:VAL:O	4:D:788:GLY:CA	2.56	0.54
3:C:259:LYS:CE	3:C:262:ARG:HD2	2.36	0.54
3:C:482:TYR:CD2	3:C:493:PHE:HB2	2.42	0.54
3:C:700:ILE:CG2	3:C:735:PHE:CD2	2.83	0.54
21:1:470:ASP:OD1	21:1:471:ASP:N	2.41	0.54
21:1:624:VAL:O	21:1:628:THR:OG1	2.14	0.54
21:1:632:PHE:HA	21:1:635:VAL:HG22	1.90	0.54
23:3:144:LEU:HB3	23:3:152:LEU:HD11	1.89	0.54
23:3:253:GLU:OE2	23:3:254:ASN:ND2	2.41	0.54
23:3:440:HIS:C	23:3:733:PRO:HG2	2.28	0.54
28:J:408:ASP:OD1	28:J:443:ILE:HG22	2.07	0.54
3:C:230:ASP:CG	3:C:259:LYS:NZ	2.61	0.54
15:H:183:G:C4	15:H:184:C:C5	2.95	0.54
21:1:331:ALA:O	21:1:335:LYS:N	2.34	0.54
37:P:228:ILE:HD12	37:P:228:ILE:N	2.23	0.54
39:S:55:ARG:CZ	43:W:95:PRO:O	2.56	0.54
40:T:356:LEU:N	40:T:356:LEU:CD1	2.70	0.54
46:Z:612:TYR:O	46:Z:615:SER:N	2.29	0.54
1:A:375:ASP:N	3:C:355:LYS:NZ	2.56	0.54
1:A:628:GLY:O	1:A:629:PHE:HB2	2.08	0.54
1:A:1778:TRP:CE2	1:A:1858:PRO:HG3	2.42	0.54
1:A:2067:PHE:CE2	1:A:2069:SER:HA	2.43	0.54
3:C:135:CYS:SG	3:C:227:LEU:HB2	2.47	0.54
21:1:893:ILE:HG13	21:1:928:TYR:CD2	2.43	0.54
22:2:476:GLU:N	22:2:479:ASP:OD2	2.41	0.54
27:7:15:GLN:O	27:7:21:THR:OG1	2.22	0.54
28:J:255:LEU:HD22	29:L:235:LEU:CD1	2.35	0.54
38:R:232:MET:O	38:R:232:MET:HG2	2.07	0.54
1:A:339:PHE:HE1	1:A:406:TRP:HZ3	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:LYS:HG2	50:A:3000:IHP:O34	2.07	0.54
1:A:1838:LYS:HG3	1:A:1868:MET:SD	2.49	0.54
1:A:2113:LYS:HE3	4:D:1229:ASP:CA	2.38	0.54
1:A:2325:VAL:HG13	4:D:789:MET:HA	1.88	0.54
3:C:79:THR:HA	40:T:199:VAL:H	1.73	0.54
14:G:137:C:H2'	14:G:138:A:O4'	2.07	0.54
15:H:3:C:H2'	15:H:4:G:H8	1.73	0.54
21:1:826:ASP:OD1	21:1:827:ARG:N	2.39	0.54
21:1:1010:THR:O	21:1:1012:PRO:HD3	2.08	0.54
27:7:60:SER:HG	27:7:63:ARG:H	1.55	0.54
36:O:50:ARG:NH1	36:O:122:GLU:OE1	2.41	0.54
36:O:57:TRP:CD1	36:O:57:TRP:C	2.81	0.54
36:O:235:TYR:HD1	36:O:271:PHE:CE1	2.24	0.54
38:R:135:PRO:HD2	40:T:341:ALA:HB1	1.90	0.54
38:R:442:ARG:CD	38:R:443:GLY:CA	2.70	0.54
43:W:474:LYS:CA	43:W:490:ALA:HB3	2.37	0.54
1:A:148:TRP:CZ2	1:A:616:PHE:HA	2.43	0.53
1:A:2117:ILE:O	1:A:2304:PHE:HB2	2.07	0.53
3:C:700:ILE:HA	3:C:705:VAL:HG12	1.89	0.53
3:C:742:PRO:HB2	3:C:786:ASN:H	1.72	0.53
5:E:178:LEU:CD1	5:E:222:LEU:HD22	2.37	0.53
14:G:-8:U:C6	41:U:16:ASN:CA	2.90	0.53
38:R:442:ARG:NH1	38:R:444:GLY:N	2.41	0.53
40:T:287:HIS:CE1	40:T:313:ARG:HG3	2.43	0.53
43:W:481:MET:O	43:W:483:ASN:N	2.41	0.53
43:W:531:LYS:HA	43:W:546:PHE:O	2.07	0.53
46:Z:485:GLU:O	46:Z:489:GLU:CB	2.56	0.53
1:A:71:ARG:NH1	1:A:177:ASP:OD2	2.32	0.53
1:A:254:TYR:O	1:A:434:HIS:HD2	1.91	0.53
1:A:705:LYS:HG2	38:R:251:ILE:CG2	2.38	0.53
1:A:1403:LEU:O	38:R:412:ASP:HB2	2.08	0.53
1:A:1930:TYR:CD2	1:A:1931:THR:N	2.76	0.53
14:G:135:G:H1	15:H:41:U:H3	1.56	0.53
15:H:84:C:O2	15:H:84:C:H2'	2.09	0.53
23:3:166:LEU:O	23:3:186:GLU:HA	2.08	0.53
40:T:454:VAL:HG12	40:T:455:GLN:N	2.24	0.53
1:A:1605:GLU:OE2	1:A:2286:VAL:HG21	2.07	0.53
1:A:1962:THR:CG2	46:Z:524:ARG:CG	2.86	0.53
5:E:87:ASP:O	5:E:88:ARG:HB2	2.07	0.53
13:F:53:A:H2'	13:F:54:G:O4'	2.09	0.53
21:1:626:ASN:ND2	21:1:630:ARG:HH12	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:1299:GLU:HA	21:1:1302:TYR:CE2	2.44	0.53
35:N:27:GLN:NE2	35:N:31:GLU:OE2	2.41	0.53
36:O:165:CYS:HB2	36:O:181:TYR:HB2	1.90	0.53
40:T:384:HIS:O	40:T:385:TYR:CB	2.55	0.53
42:V:525:PHE:O	42:V:528:ILE:N	2.41	0.53
44:X:181:PHE:HA	45:Y:50:GLY:H	1.73	0.53
1:A:1352:HIS:CD2	41:U:5:ILE:HD13	2.44	0.53
3:C:449:ILE:CD1	3:C:466:SER:N	2.71	0.53
21:1:822:ARG:HH11	45:Y:31:GLU:HG2	1.74	0.53
21:1:1077:THR:O	21:1:1080:THR:OG1	2.22	0.53
21:1:1127:THR:HA	22:2:571:LEU:HB3	1.88	0.53
23:3:3:LEU:HD12	23:3:1093:MET:SD	2.48	0.53
28:J:218:GLU:HG3	28:J:219:GLU:N	2.23	0.53
38:R:103:ARG:HH11	38:R:103:ARG:CG	2.21	0.53
38:R:225:GLU:CG	38:R:226:PRO:HD3	2.36	0.53
1:A:122:ILE:HD13	1:A:483:GLN:HG3	1.90	0.53
1:A:348:PRO:HB3	1:A:394:TYR:CE2	2.43	0.53
1:A:2073:TRP:CH2	1:A:2310:ARG:HG2	2.44	0.53
1:A:2298:LEU:HD13	4:D:1265:GLN:CB	2.39	0.53
3:C:481:MET:SD	3:C:559:ILE:HD11	2.48	0.53
23:3:712:VAL:HG23	23:3:722:SER:HB3	1.91	0.53
1:A:881:ILE:HG23	1:A:918:THR:HG23	1.88	0.53
1:A:1457:HIS:HE2	38:R:425:GLY:N	2.04	0.53
1:A:2310:ARG:HH12	1:A:2314:PHE:HE1	1.56	0.53
3:C:115:GLU:O	3:C:116:MET:C	2.43	0.53
3:C:220:ARG:O	3:C:448:LYS:HE2	2.08	0.53
3:C:360:ALA:N	3:C:361:PRO:CD	2.71	0.53
15:H:147:G:C2	15:H:148:C:C2	2.97	0.53
15:H:153:A:H3'	15:H:154:C:C5'	2.38	0.53
21:1:1157:TYR:O	26:6:38:ARG:NH2	2.40	0.53
23:3:195:ASP:OD1	23:3:197:THR:OG1	2.23	0.53
23:3:250:ILE:HD13	23:3:259:LYS:HB3	1.91	0.53
23:3:547:CYS:HB3	23:3:556:ILE:HG22	1.90	0.53
23:3:667:ILE:HB	23:3:675:LEU:HB2	1.91	0.53
37:P:41:ILE:HD11	40:T:318:ARG:HB2	1.90	0.53
39:S:20:MET:HE1	39:S:141:ARG:HB3	1.91	0.53
1:A:465:LYS:HG3	1:A:465:LYS:O	2.08	0.53
3:C:449:ILE:HG22	3:C:457:VAL:HG13	1.88	0.53
5:E:108:HIS:ND1	5:E:128:SER:HB2	2.24	0.53
5:E:178:LEU:CD2	5:E:208:ILE:CD1	2.87	0.53
15:H:68:G:C2'	15:H:69:U:H5'	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:141:VAL:HG11	23:3:213:LEU:HD12	1.89	0.53
23:3:440:HIS:CD2	23:3:733:PRO:CG	2.92	0.53
1:A:525:LYS:HE2	34:M:194:ARG:CB	2.38	0.53
1:A:642:ARG:CD	2:B:28:A:H1'	2.24	0.53
2:B:18:C:C2'	2:B:19:A:O5'	2.56	0.53
2:B:32:C:H5"	37:P:33:ARG:NH1	2.24	0.53
3:C:82:GLN:CG	40:T:237:LYS:HA	2.38	0.53
15:H:79:G:C2	15:H:80:A:C5	2.97	0.53
21:1:944:SER:HA	21:1:948:ARG:NE	2.23	0.53
28:J:359:VAL:O	28:J:363:ARG:HG2	2.08	0.53
35:N:55:GLN:NE2	43:W:192:PHE:CB	2.71	0.53
35:N:128:VAL:CG1	35:N:130:ARG:HB3	2.38	0.53
38:R:132:LEU:HB3	40:T:399:LYS:HZ2	1.70	0.53
40:T:318:ARG:HH11	40:T:318:ARG:CG	2.22	0.53
41:U:23:LEU:O	41:U:23:LEU:HD13	2.08	0.53
46:Z:571:PRO:HD3	46:Z:579:TRP:CH2	2.43	0.53
1:A:372:PRO:CB	3:C:342:ARG:HH21	2.22	0.53
1:A:595:LYS:NZ	2:B:45:C:OP1	2.31	0.53
1:A:1199:LYS:NZ	1:A:1206:GLU:OE2	2.32	0.53
3:C:259:LYS:HG2	3:C:262:ARG:HG3	1.90	0.53
5:E:232:ARG:O	5:E:262:TRP:HH2	1.91	0.53
21:1:516:LEU:O	21:1:520:THR:HG23	2.08	0.53
24:4:47:ASP:HB3	24:4:52:GLN:O	2.08	0.53
32:I:362:LYS:HA	32:I:372:ARG:CB	2.39	0.53
1:A:204:LEU:HD23	1:A:205:ASP:OD1	2.09	0.53
1:A:602:ILE:HG22	1:A:1548:TYR:OH	2.06	0.53
1:A:723:ASN:ND2	1:A:788:GLN:OE1	2.41	0.53
1:A:748:ASP:HA	37:P:214:THR:CG2	2.34	0.53
1:A:1275:ARG:HD2	1:A:1375:TRP:CD1	2.44	0.53
1:A:1425:LYS:CG	38:R:417:ASN:OD1	2.56	0.53
1:A:1781:ASP:HB3	1:A:1808:PHE:HB3	1.90	0.53
2:B:42:U:H4'	13:F:70:A:C5'	2.37	0.53
3:C:250:ARG:NE	3:C:451:HIS:CD2	2.76	0.53
3:C:516:LEU:HB2	3:C:575:GLN:HE22	1.73	0.53
13:F:50:A:H2'	13:F:51:U:C6	2.44	0.53
13:F:56:A:C6	15:H:20:G:C6	2.96	0.53
22:2:614:ARG:HH11	22:2:614:ARG:CG	2.14	0.53
23:3:211:TYR:HE1	23:3:222:ARG:HG2	1.74	0.53
23:3:605:LEU:O	23:3:616:ILE:HA	2.08	0.53
23:3:719:SER:OG	23:3:739:LEU:HD11	2.09	0.53
39:S:34:LYS:CE	39:S:78:TYR:CD2	2.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:891:PHE:O	29:L:83:ARG:NH1	2.42	0.52
3:C:671:SER:C	3:C:672:LEU:HD22	2.30	0.52
21:1:599:ASN:O	21:1:603:ALA:CB	2.57	0.52
23:3:519:VAL:HG22	23:3:524:ILE:HG12	1.90	0.52
23:3:639:SER:OG	23:3:701:LEU:N	2.42	0.52
23:3:1148:LEU:O	23:3:1152:HIS:N	2.39	0.52
38:R:95:LYS:HD3	38:R:95:LYS:N	2.25	0.52
1:A:191:ILE:HG23	1:A:572:PHE:CZ	2.44	0.52
1:A:245:LEU:HD22	1:A:430:TRP:CH2	2.44	0.52
1:A:596:TYR:HB2	14:G:-5:G:C2	2.43	0.52
1:A:1701:VAL:HA	1:A:1716:GLY:HA3	1.90	0.52
3:C:943:LEU:HD23	3:C:943:LEU:N	2.24	0.52
13:F:48:A:N3	29:L:33:ARG:NH2	2.57	0.52
13:F:94:C:OP1	28:J:351:ASN:CB	2.57	0.52
14:G:153:C:H4’	14:G:154:U:OP1	2.10	0.52
15:H:81:G:C2	15:H:82:G:C5	2.97	0.52
23:3:550:ASN:HB3	23:3:553:GLN:HB2	1.90	0.52
42:V:530:LYS:O	42:V:532:GLN:N	2.42	0.52
43:W:212:GLU:C	43:W:214:LYS:N	2.61	0.52
3:C:97:VAL:HG12	37:P:47:THR:OG1	2.10	0.52
13:F:34:G:H2’	13:F:35:A:O5’	2.10	0.52
14:G:-4:A:H2’	14:G:-3:A:C8	2.44	0.52
15:H:148:C:C2’	15:H:149:A:H5’	2.39	0.52
21:1:516:LEU:HD11	21:1:558:ARG:HD3	1.91	0.52
21:1:1090:PRO:HG3	21:1:1123:CYS:HB2	1.91	0.52
23:3:128:ARG:HH21	23:3:180:PRO:HG3	1.73	0.52
23:3:159:GLU:OE2	26:6:14:GLN:HB2	2.09	0.52
23:3:755:VAL:HG22	23:3:764:ILE:HD12	1.89	0.52
36:O:229:LYS:HA	36:O:277:ARG:NH2	2.24	0.52
37:P:189:ASP:O	37:P:191:ASP:N	2.43	0.52
38:R:233:HIS:H	38:R:233:HIS:HD2	1.56	0.52
39:S:39:PHE:CD2	39:S:129:PHE:HE2	2.10	0.52
40:T:351:ASP:C	40:T:352:THR:HG1	2.11	0.52
41:U:9:THR:HG23	41:U:9:THR:O	2.09	0.52
43:W:531:LYS:CA	43:W:546:PHE:O	2.58	0.52
1:A:830:LEU:HA	1:A:882:LYS:HZ2	1.74	0.52
1:A:1214:TRP:CE2	1:A:1230:LEU:HD11	2.45	0.52
5:E:178:LEU:N	5:E:178:LEU:HD23	2.25	0.52
14:G:-12:G:H4’	14:G:-11:G:OP1	2.09	0.52
21:1:1108:ASN:OD1	21:1:1109:ARG:N	2.43	0.52
23:3:114:ARG:NE	23:3:136:GLU:OE1	2.32	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:O:75:SER:O	36:O:79:ASN:N	2.42	0.52
36:O:80:VAL:HG11	36:O:94:ILE:HD11	1.90	0.52
36:O:243:ILE:HG22	36:O:244:THR:O	2.08	0.52
38:R:52:PRO:O	38:R:53:ARG:HB2	2.09	0.52
38:R:81:LYS:HA	38:R:81:LYS:HE3	1.87	0.52
1:A:299:ILE:HD11	3:C:920:PRO:C	2.29	0.52
1:A:1275:ARG:NH1	1:A:1378:GLU:OE1	2.43	0.52
1:A:1306:LYS:HB2	14:G:-6:C:H4'	1.92	0.52
3:C:80:ILE:CD1	3:C:80:ILE:N	2.73	0.52
3:C:143:THR:HB	51:C:1500:GTP:O1A	2.09	0.52
3:C:700:ILE:CG2	3:C:741:GLY:O	2.57	0.52
13:F:36:A:C8	13:F:36:A:C4'	2.93	0.52
13:F:57:U:H2'	13:F:58:G:C8	2.45	0.52
21:1:717:THR:HG22	21:1:718:PRO:CD	2.39	0.52
21:1:762:ALA:O	21:1:766:THR:OG1	2.19	0.52
23:3:159:GLU:HB3	23:3:161:HIS:CD2	2.44	0.52
35:N:40:LYS:O	35:N:41:ARG:CG	2.47	0.52
46:Z:524:ARG:HD2	46:Z:525:TYR:HB3	1.92	0.52
1:A:91:ALA:O	1:A:92:LEU:C	2.45	0.52
1:A:107:PRO:O	1:A:111:GLU:CD	2.48	0.52
1:A:115:ASP:HB3	1:A:486:LYS:HE2	1.91	0.52
1:A:121:HIS:HE2	1:A:481:PHE:CB	2.14	0.52
1:A:121:HIS:CD2	1:A:481:PHE:HB3	2.36	0.52
1:A:1631:LEU:HD12	1:A:1660:TYR:HD2	1.74	0.52
1:A:2133:PRO:HD2	1:A:2139:VAL:HG13	1.92	0.52
2:B:42:U:O2'	13:F:69:A:C2	2.58	0.52
2:B:43:U:C5'	13:F:67:G:H22	2.08	0.52
3:C:78:GLU:O	40:T:198:ARG:C	2.47	0.52
3:C:78:GLU:CG	3:C:80:ILE:CD1	2.54	0.52
3:C:139:HIS:O	3:C:259:LYS:NZ	2.36	0.52
3:C:449:ILE:HD11	3:C:466:SER:HA	1.91	0.52
3:C:508:LYS:HB3	3:C:566:THR:CG2	2.39	0.52
3:C:710:ASN:O	3:C:712:LYS:N	2.42	0.52
21:1:1254:LEU:O	21:1:1262:ARG:HG2	2.09	0.52
23:3:1059:PRO:O	23:3:1062:THR:HG23	2.08	0.52
36:O:72:GLN:O	36:O:75:SER:OG	2.19	0.52
40:T:267:ASP:O	40:T:268:LYS:CG	2.56	0.52
40:T:351:ASP:C	40:T:352:THR:OG1	2.48	0.52
46:Z:597:ARG:NH1	46:Z:601:LEU:HD13	2.24	0.52
1:A:1131:LYS:HE3	1:A:1174:PHE:CD1	2.44	0.52
1:A:1162:PRO:HG3	37:P:194:PHE:CG	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1459:ARG:HD2	38:R:422:MET:O	2.09	0.52
14:G:11:A:N1	14:G:12:G:C8	2.77	0.52
23:3:285:MET:SD	23:3:305:THR:HB	2.49	0.52
23:3:304:GLN:HE22	23:3:335:VAL:HA	1.73	0.52
24:4:41:ASN:HB2	24:4:60:GLU:HB3	1.92	0.52
40:T:318:ARG:HH11	40:T:319:THR:HG23	1.74	0.52
1:A:47:GLU:OE1	1:A:47:GLU:N	2.35	0.52
1:A:206:TRP:CD1	1:A:213:LEU:HD21	2.45	0.52
1:A:651:TRP:CZ2	13:F:66:C:C4	2.97	0.52
3:C:711:ARG:CZ	3:C:730:ARG:O	2.57	0.52
3:C:902:HIS:ND1	3:C:903:HIS:HB2	2.25	0.52
21:1:1289:ASN:HB3	21:1:1295:TYR:H	1.75	0.52
23:3:108:GLY:O	26:6:82:ARG:HD3	2.09	0.52
23:3:232:GLY:HA2	23:3:252:SER:HA	1.90	0.52
24:4:34:LEU:HA	24:4:37:GLY:O	2.10	0.52
36:O:24:CYS:HB2	36:O:27:CYS:SG	2.49	0.52
38:R:135:PRO:O	38:R:136:ASP:CB	2.58	0.52
1:A:380:LEU:HB2	3:C:354:ARG:NH1	2.18	0.52
1:A:1136:ARG:H	1:A:1345:GLN:HA	1.75	0.52
3:C:259:LYS:HG2	3:C:262:ARG:CG	2.39	0.52
3:C:510:LEU:HD22	3:C:514:TYR:HE2	1.75	0.52
21:1:901:GLN:HA	21:1:939:ARG:HH22	1.72	0.52
37:P:193:VAL:HG23	37:P:194:PHE:N	2.25	0.52
39:S:9:TRP:CE3	39:S:11:PRO:HG2	2.45	0.52
40:T:347:THR:O	40:T:354:ILE:HG23	2.10	0.52
43:W:518:PRO:O	43:W:519:ASP:CB	2.57	0.52
1:A:666:LYS:HB2	1:A:668:VAL:HG23	1.92	0.52
1:A:676:ARG:HG3	13:F:55:C:O3'	2.09	0.52
3:C:449:ILE:CD1	3:C:466:SER:CA	2.88	0.52
3:C:600:LEU:N	3:C:601:PRO:HD2	2.25	0.52
13:F:27:A:N9	36:O:181:TYR:CZ	2.77	0.52
21:1:661:ARG:NH1	21:1:696:ASP:OD2	2.39	0.52
21:1:1070:LYS:HB3	21:1:1073:ILE:HD12	1.91	0.52
21:1:1096:THR:HA	21:1:1099:ASN:ND2	2.25	0.52
23:3:259:LYS:HG3	23:3:266:ASP:OD1	2.09	0.52
23:3:1048:ASP:HB3	23:3:1052:ASN:H	1.75	0.52
36:O:113:ASN:O	36:O:116:TYR:N	2.43	0.52
37:P:189:ASP:OD2	37:P:192:VAL:CG2	2.59	0.52
38:R:70:ALA:O	38:R:71:GLN:C	2.48	0.52
38:R:442:ARG:CD	38:R:443:GLY:C	2.77	0.52
45:Y:69:ARG:NH2	45:Y:74:GLY:O	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:PHE:CD1	1:A:473:PHE:CZ	2.98	0.51
1:A:941:LYS:HG3	1:A:1071:PHE:CE1	2.46	0.51
1:A:1275:ARG:HD2	1:A:1375:TRP:NE1	2.25	0.51
1:A:1425:LYS:C	1:A:1425:LYS:HD3	2.31	0.51
3:C:64:LYS:NZ	37:P:206:LYS:HG3	2.22	0.51
3:C:89:LEU:O	3:C:91:GLU:N	2.43	0.51
21:1:1256:HIS:ND1	21:1:1261:VAL:HG11	2.24	0.51
23:3:460:TRP:CZ2	23:3:507:SER:HA	2.46	0.51
23:3:476:VAL:HG22	23:3:762:LEU:HD22	1.91	0.51
23:3:1134:SER:HB2	23:3:1136:GLU:OE1	2.09	0.51
35:N:43:VAL:O	35:N:47:TRP:NE1	2.44	0.51
37:P:32:SER:O	37:P:35:LEU:HD12	2.09	0.51
1:A:203:VAL:CG2	1:A:237:THR:CB	2.88	0.51
1:A:672:VAL:HG21	40:T:267:ASP:OD1	2.10	0.51
1:A:805:GLU:CB	37:P:194:PHE:CZ	2.89	0.51
3:C:77:VAL:HG13	40:T:196:LEU:HB3	1.91	0.51
13:F:36:A:H3'	13:F:37:C:C5'	2.26	0.51
21:1:1253:GLY:HA3	21:1:1265:TYR:CG	2.45	0.51
26:6:54:TYR:HA	26:6:57:ARG:HB2	1.92	0.51
29:L:224:PHE:CE1	38:R:86:LEU:HD13	2.44	0.51
40:T:392:PRO:HA	40:T:414:ALA:O	2.09	0.51
43:W:425:VAL:O	43:W:433:PHE:CB	2.59	0.51
1:A:339:PHE:C	1:A:340:ILE:HD13	2.31	0.51
1:A:461:HIS:HD2	2:B:27:U:C4	2.28	0.51
1:A:750:TRP:CZ2	1:A:778:ARG:HG2	2.45	0.51
1:A:1179:SER:O	1:A:1182:ASN:N	2.44	0.51
1:A:1784:ASN:ND2	1:A:1897:LEU:HD12	2.22	0.51
3:C:674:CYS:SG	3:C:822:MET:CE	2.99	0.51
13:F:45:A:N1	22:2:554:ARG:NH2	2.53	0.51
21:1:1179:ASP:HB2	21:1:1185:ARG:HD3	1.93	0.51
23:3:331:ASP:OD2	23:3:394:ASN:HB2	2.11	0.51
32:I:729:SER:O	32:I:732:ALA:HB3	2.09	0.51
38:R:125:MET:O	38:R:126:ASN:HB3	2.11	0.51
40:T:267:ASP:O	40:T:268:LYS:HB2	2.09	0.51
40:T:454:VAL:CG2	40:T:463:SER:OG	2.58	0.51
1:A:308:ILE:HG22	1:A:308:ILE:O	2.09	0.51
1:A:384:VAL:CG1	3:C:331:PHE:HD2	2.16	0.51
1:A:782:LEU:HB3	37:P:224:MET:SD	2.50	0.51
3:C:300:LEU:HD13	3:C:300:LEU:N	2.25	0.51
3:C:388:VAL:O	3:C:388:VAL:HG22	2.10	0.51
15:H:55:U:H1'	15:H:58:U:H5	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:107:A:C6	15:H:108:G:C5	2.99	0.51
46:Z:593:PHE:O	46:Z:597:ARG:CB	2.57	0.51
1:A:122:ILE:CD1	1:A:483:GLN:CG	2.89	0.51
1:A:593:ARG:NE	14:G:-4:A:O5'	2.43	0.51
1:A:1667:ARG:HD2	1:A:1679:TYR:CE2	2.46	0.51
1:A:2147:MET:O	1:A:2274:PRO:HD3	2.10	0.51
3:C:678:THR:HG23	3:C:683:ASN:H	1.75	0.51
5:E:231:MET:SD	5:E:262:TRP:CE3	3.04	0.51
13:F:68:C:N4	37:P:33:ARG:CB	2.45	0.51
14:G:20:A:P	36:O:159:ARG:HD3	2.50	0.51
21:1:1054:GLU:OE1	21:1:1057:ARG:NH1	2.36	0.51
23:3:854:ALA:HB1	23:3:856:LYS:HD2	1.93	0.51
23:3:1002:VAL:HB	23:3:1010:ILE:HB	1.93	0.51
1:A:1447:VAL:HG12	1:A:1449:LYS:HG2	1.92	0.51
13:F:43:A:O2'	13:F:44:G:H5'	2.11	0.51
14:G:26:U:C1'	36:O:269:CYS:CB	2.88	0.51
21:1:231:ARG:HA	21:1:607:ALA:HB2	1.92	0.51
23:3:264:GLN:HE22	23:3:322:VAL:H	1.58	0.51
23:3:745:PHE:CZ	23:3:747:SER:HB3	2.46	0.51
39:S:36:CYS:HA	39:S:129:PHE:CE1	2.45	0.51
40:T:318:ARG:HG3	40:T:318:ARG:HH11	1.76	0.51
1:A:203:VAL:HG23	1:A:237:THR:CG2	2.35	0.51
1:A:589:THR:OG1	1:A:590:GLY:N	2.44	0.51
1:A:978:GLU:CD	1:A:1188:ASN:H	2.14	0.51
1:A:1320:LYS:NZ	38:R:434:TYR:CD1	2.77	0.51
1:A:1962:THR:HG23	46:Z:524:ARG:CB	2.28	0.51
1:A:2090:ILE:HA	1:A:2223:CYS:O	2.10	0.51
3:C:220:ARG:O	3:C:448:LYS:CE	2.58	0.51
13:F:34:G:N3	13:F:34:G:C3'	2.72	0.51
13:F:94:C:H5"	28:J:347:HIS:HB3	1.92	0.51
22:2:469:VAL:HG12	22:2:471:ARG:H	1.76	0.51
23:3:113:ARG:HB2	23:3:116:VAL:HB	1.91	0.51
23:3:971:ASP:OD1	23:3:972:LEU:N	2.43	0.51
36:O:20:PHE:CE1	38:R:197:ILE:HD13	2.46	0.51
36:O:75:SER:OG	36:O:76:LYS:N	2.44	0.51
39:S:35:THR:O	39:S:129:PHE:CZ	2.63	0.51
40:T:459:LEU:HD12	40:T:460:ASP:N	2.25	0.51
45:Y:37:TRP:CH2	46:Z:498:GLY:N	2.74	0.51
1:A:95:MET:N	1:A:96:PRO:HD2	2.26	0.51
1:A:586:GLY:HA3	1:A:1549:VAL:HG11	1.92	0.51
1:A:595:LYS:HB3	2:B:45:C:OP1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1629:ILE:HB	1:A:1662:ILE:HB	1.92	0.51
1:A:1923:TRP:HB3	1:A:1927:ILE:HD11	1.93	0.51
1:A:2081:ALA:HB1	4:D:1010:SER:CB	2.40	0.51
3:C:133:THR:O	3:C:226:VAL:O	2.29	0.51
13:F:34:G:N3	13:F:34:G:C5'	2.73	0.51
13:F:35:A:N3	13:F:35:A:C5'	2.73	0.51
23:3:354:GLY:HA3	23:3:432:ARG:HH12	1.76	0.51
24:4:16:TYR:HA	24:4:57:GLY:O	2.10	0.51
24:4:16:TYR:HD1	24:4:58:PHE:CE2	2.28	0.51
28:J:257:GLU:HA	29:L:232:TYR:CE2	2.46	0.51
28:J:273:TYR:CD2	38:R:228:PRO:CG	2.94	0.51
39:S:11:PRO:CA	39:S:166:GLY:HA3	2.41	0.51
1:A:184:ASP:OD1	35:N:1:MET:N	2.35	0.51
1:A:744:LYS:HZ1	37:P:212:ASN:C	2.14	0.51
1:A:975:VAL:HB	1:A:1099:PHE:HB2	1.93	0.51
1:A:1373:GLN:HB3	1:A:1378:GLU:OE2	2.11	0.51
1:A:1502:PHE:CZ	1:A:1505:LYS:HB3	2.45	0.51
3:C:131:ASN:ND2	3:C:223:ASP:OD2	2.44	0.51
14:G:11:A:N3	14:G:11:A:C5'	2.73	0.51
14:G:11:A:N1	14:G:12:G:N7	2.59	0.51
14:G:20:A:OP2	36:O:159:ARG:CD	2.58	0.51
21:1:669:GLN:O	21:1:672:ALA:N	2.44	0.51
23:3:246:SER:O	23:3:260:ASN:ND2	2.44	0.51
23:3:404:LEU:HD23	23:3:407:ILE:HD11	1.92	0.51
23:3:520:TYR:CE1	23:3:522:ASP:HB2	2.46	0.51
23:3:896:PHE:HB2	23:3:899:THR:HG22	1.93	0.51
28:J:273:TYR:CD1	38:R:228:PRO:HG2	2.46	0.51
39:S:131:ARG:HH11	39:S:132:VAL:C	2.12	0.51
40:T:300:ILE:O	40:T:301:ASP:HB2	2.11	0.51
1:A:331:TRP:C	1:A:331:TRP:HE3	2.14	0.51
1:A:338:VAL:CG1	3:C:267:LEU:HD23	2.41	0.51
1:A:748:ASP:OD2	40:T:484:LYS:NZ	2.43	0.51
1:A:823:SER:OG	1:A:933:ARG:NH1	2.44	0.51
1:A:1276:GLU:O	1:A:1279:VAL:HG12	2.11	0.51
3:C:93:ILE:CD1	40:T:230:ILE:CD1	2.89	0.51
15:H:111:G:O3'	15:H:112:G:O4'	2.29	0.51
21:1:475:PHE:CE1	21:1:502:LEU:HB2	2.46	0.51
21:1:582:LEU:HD23	21:1:630:ARG:HB3	1.93	0.51
23:3:556:ILE:HD11	23:3:564:VAL:HB	1.93	0.51
23:3:1144:VAL:O	23:3:1148:LEU:HB2	2.11	0.51
36:O:283:ALA:O	36:O:287:SER:CB	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:T:385:TYR:CE2	40:T:400:PHE:HB3	2.46	0.51
1:A:86:ARG:HH21	38:R:211:ARG:HG3	1.74	0.50
1:A:227:ARG:C	1:A:416:GLY:O	2.48	0.50
1:A:1435:GLY:O	1:A:1438:VAL:HG22	2.10	0.50
3:C:215:VAL:HG11	3:C:242:LEU:HD22	1.93	0.50
3:C:559:ILE:C	3:C:559:ILE:HD12	2.31	0.50
23:3:28:GLN:HE22	23:3:343:LYS:HG2	1.77	0.50
23:3:80:VAL:HB	23:3:88:VAL:HG23	1.93	0.50
23:3:110:SER:HB3	26:6:82:ARG:HH12	1.75	0.50
28:J:252:GLU:OE1	28:J:260:ARG:HB3	2.12	0.50
28:J:360:ASP:HA	28:J:363:ARG:HD2	1.91	0.50
38:R:220:ARG:CB	38:R:220:ARG:HH11	2.24	0.50
40:T:233:LEU:HD23	40:T:233:LEU:C	2.32	0.50
43:W:474:LYS:C	43:W:490:ALA:CB	2.80	0.50
1:A:863:GLU:OE2	1:A:916:LYS:NZ	2.36	0.50
1:A:1757:GLU:CD	38:R:451:ILE:HD11	2.30	0.50
1:A:1930:TYR:HD2	1:A:1931:THR:N	2.09	0.50
1:A:2298:LEU:CD1	4:D:1285:SER:CA	2.89	0.50
2:B:20:G:H1'	2:B:21:A:OP1	2.12	0.50
2:B:44:A:P	13:F:66:C:H42	2.33	0.50
3:C:452:THR:O	3:C:578:ARG:N	2.43	0.50
3:C:457:VAL:HG12	3:C:462:GLY:CA	2.41	0.50
3:C:619:THR:O	3:C:620:LYS:HG3	2.11	0.50
5:E:229:TYR:CE2	5:E:272:ARG:NH1	2.77	0.50
15:H:51:A:N6	15:H:63:G:O6	2.44	0.50
23:3:506:LEU:HB3	23:3:547:CYS:SG	2.52	0.50
23:3:669:LEU:HD22	23:3:673:VAL:HG21	1.93	0.50
36:O:149:LYS:NZ	36:O:290:LYS:HG3	2.26	0.50
39:S:10:GLN:HA	39:S:29:TRP:CE2	2.46	0.50
46:Z:574:ASN:O	46:Z:576:PHE:N	2.44	0.50
1:A:227:ARG:H	1:A:417:ARG:HA	1.75	0.50
1:A:264:PHE:CE1	1:A:459:LEU:CD1	2.81	0.50
1:A:844:GLU:CB	38:R:422:MET:HE2	2.23	0.50
3:C:94:ILE:HG21	40:T:259:PRO:HB3	1.92	0.50
3:C:387:ASP:O	3:C:389:ASP:OD1	2.30	0.50
3:C:659:VAL:HG12	3:C:660:VAL:N	2.26	0.50
14:G:-12:G:O2'	14:G:-11:G:O5'	2.30	0.50
15:H:153:A:C2'	15:H:154:C:C5'	2.86	0.50
15:H:182:U:C2'	15:H:183:G:H5'	2.41	0.50
21:1:1156:GLU:O	26:6:38:ARG:NH1	2.45	0.50
27:7:32:LEU:HA	27:7:35:GLN:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:O:44:GLU:HA	36:O:50:ARG:O	2.10	0.50
38:R:178:ARG:CD	38:R:194:GLN:HE22	2.07	0.50
38:R:422:MET:C	38:R:424:SER:H	2.12	0.50
38:R:434:TYR:CD1	46:Z:616:VAL:CB	2.95	0.50
40:T:329:HIS:CE1	40:T:355:ARG:HG3	2.46	0.50
42:V:576:THR:O	42:V:580:ARG:N	2.36	0.50
1:A:305:ARG:HE	3:C:854:ARG:NH1	2.10	0.50
1:A:338:VAL:HB	3:C:867:PRO:HG3	1.93	0.50
1:A:1379:PHE:O	1:A:1382:SER:OG	2.17	0.50
1:A:2073:TRP:HH2	1:A:2310:ARG:NH1	2.09	0.50
2:B:63:A:H4'	5:E:106:LYS:HZ2	1.75	0.50
3:C:134:LEU:HD23	3:C:226:VAL:HB	1.94	0.50
3:C:140:HIS:HB3	3:C:230:ASP:N	2.26	0.50
3:C:456:GLY:O	3:C:457:VAL:HG13	2.11	0.50
5:E:277:PHE:CE2	5:E:300:ILE:HD12	2.46	0.50
13:F:35:A:C8	14:G:12:G:N1	2.80	0.50
13:F:37:C:N4	14:G:5:G:OP1	2.44	0.50
14:G:-4:A:H2'	14:G:-3:A:H8	1.76	0.50
21:1:897:LEU:HD11	21:1:932:ILE:HD13	1.93	0.50
23:3:757:ILE:HG23	23:3:762:LEU:HD13	1.94	0.50
23:3:996:ILE:HD13	23:3:1041:TYR:HD1	1.75	0.50
36:O:253:TYR:OH	39:S:120:GLN:HA	2.12	0.50
38:R:434:TYR:CE2	38:R:436:VAL:HG22	2.43	0.50
40:T:306:CYS:SG	40:T:336:VAL:CB	2.97	0.50
45:Y:86:ASP:HB2	46:Z:502:ALA:HB3	1.93	0.50
1:A:693:ILE:O	1:A:697:MET:N	2.42	0.50
3:C:93:ILE:HG21	40:T:218:TRP:CE2	2.46	0.50
3:C:846:VAL:HG22	3:C:887:LEU:HD11	1.94	0.50
14:G:-11:G:OP1	41:U:21:ARG:NE	2.40	0.50
14:G:132:G:H2'	14:G:133:A:C8	2.46	0.50
21:1:822:ARG:HD3	45:Y:32:TYR:OH	2.12	0.50
23:3:550:ASN:OD1	23:3:551:GLN:N	2.41	0.50
23:3:685:ASP:OD1	23:3:686:LEU:N	2.44	0.50
23:3:807:TYR:HE1	23:3:861:GLN:HG3	1.76	0.50
29:L:216:PHE:CZ	36:O:112:VAL:CG1	2.95	0.50
31:K:196:GLU:O	31:K:199:ILE:CG1	2.59	0.50
36:O:106:ASP:CG	36:O:107:MET:H	2.15	0.50
38:R:101:ILE:O	38:R:104:GLN:HG2	2.08	0.50
38:R:442:ARG:HH11	38:R:443:GLY:CA	2.15	0.50
40:T:297:HIS:HD2	40:T:338:CYS:SG	2.34	0.50
1:A:117:PRO:HG2	1:A:131:GLU:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:848:GLU:CD	38:R:424:SER:OG	2.50	0.50
1:A:2073:TRP:CH2	1:A:2310:ARG:NH1	2.80	0.50
2:B:100:C:H2'	2:B:101:U:C6	2.47	0.50
13:F:36:A:C3'	13:F:37:C:C5'	2.85	0.50
15:H:25:G:H2'	15:H:26:A:C8	2.45	0.50
15:H:46:U:O2'	15:H:47:U:OP2	2.25	0.50
15:H:70:C:O5'	15:H:70:C:H6	1.94	0.50
15:H:147:G:N2	15:H:148:C:C2	2.80	0.50
21:1:1003:VAL:HG23	21:1:1004:ILE:H	1.77	0.50
21:1:1132:LEU:O	21:1:1135:GLU:N	2.45	0.50
23:3:300:PHE:CG	23:3:312:LYS:HE2	2.46	0.50
35:N:105:CYS:SG	35:N:119:CYS:SG	3.10	0.50
37:P:41:ILE:HD11	40:T:318:ARG:HA	1.92	0.50
37:P:210:PHE:CG	40:T:201:SER:OG	2.64	0.50
42:V:484:SER:C	42:V:486:THR:H	2.15	0.50
1:A:121:HIS:HA	1:A:481:PHE:O	2.12	0.50
1:A:402:ILE:HD13	3:C:268:LYS:HE3	1.94	0.50
1:A:525:LYS:CD	34:M:194:ARG:CG	2.90	0.50
1:A:1209:HIS:CG	1:A:1210:LYS:H	2.30	0.50
36:O:222:ARG:HA	36:O:288:PHE:HD2	1.76	0.50
1:A:89:LEU:CD2	1:A:656:LEU:HD22	2.42	0.50
1:A:948:PRO:O	1:A:951:LEU:HB2	2.12	0.50
1:A:1505:LYS:HE2	46:Z:615:SER:CA	2.40	0.50
1:A:1757:GLU:CD	38:R:451:ILE:CD1	2.80	0.50
3:C:66:TYR:CD2	40:T:457:GLY:CA	2.79	0.50
3:C:244:LYS:CA	3:C:292:TYR:CD2	2.92	0.50
15:H:148:C:HO2'	15:H:149:A:H5'	1.77	0.50
23:3:1050:PHE:HB3	23:3:1167:TYR:HE2	1.75	0.50
23:3:1147:HIS:O	23:3:1151:GLU:HB2	2.10	0.50
40:T:281:ILE:HD12	40:T:282:ARG:HG2	1.92	0.50
43:W:290:GLY:HA2	43:W:573:GLY:HA2	1.94	0.50
1:A:1402:ARG:HH21	46:Z:573:PRO:HG3	1.77	0.50
3:C:259:LYS:HE2	3:C:262:ARG:HH11	1.77	0.50
5:E:228:THR:HG22	5:E:229:TYR:HD1	1.77	0.50
13:F:41:A:H2'	13:F:42:C:C6	2.47	0.50
15:H:74:U:O5'	15:H:74:U:H6	1.95	0.50
21:1:595:GLU:O	21:1:599:ASN:ND2	2.45	0.50
23:3:12:THR:HA	23:3:34:ARG:NH1	2.27	0.50
23:3:819:MET:O	23:3:823:MET:HG3	2.12	0.50
44:X:282:LEU:HD23	44:X:295:ASP:HA	1.94	0.50
1:A:55:ASP:OD1	1:A:55:ASP:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:ARG:HH11	1:A:710:LEU:HD13	1.77	0.49
3:C:144:CYS:C	3:C:312:SER:HB2	2.33	0.49
3:C:499:GLY:O	3:C:500:THR:CG2	2.60	0.49
21:1:1040:GLY:HA2	21:1:1080:THR:HG22	1.94	0.49
23:3:4:TYR:HB2	23:3:1132:PHE:CZ	2.47	0.49
23:3:458:ALA:HB3	23:3:477:SER:HB3	1.94	0.49
23:3:550:ASN:HD21	23:3:595:VAL:N	2.10	0.49
23:3:1188:ASN:O	23:3:1192:ASN:ND2	2.31	0.49
37:P:66:ARG:HH11	37:P:66:ARG:CG	2.24	0.49
46:Z:612:TYR:C	46:Z:614:TRP:N	2.63	0.49
46:Z:614:TRP:CD1	46:Z:614:TRP:C	2.85	0.49
1:A:348:PRO:O	1:A:350:PHE:N	2.45	0.49
1:A:965:VAL:HG13	1:A:966:TRP:CD1	2.47	0.49
1:A:1403:LEU:O	38:R:412:ASP:CB	2.60	0.49
1:A:1700:GLY:H	1:A:1717:ASN:HD22	1.60	0.49
2:B:40:U:H3	14:G:-1:G:H22	1.59	0.49
3:C:116:MET:O	3:C:119:LEU:HB3	2.12	0.49
3:C:854:ARG:NH1	3:C:879:ASP:OD2	2.45	0.49
5:E:265:ARG:N	5:E:272:ARG:HH21	2.10	0.49
13:F:27:A:N9	36:O:181:TYR:CE2	2.80	0.49
15:H:181:G:N2	15:H:182:U:C2	2.80	0.49
21:1:717:THR:HG22	21:1:718:PRO:HD3	1.93	0.49
23:3:274:ARG:HG2	23:3:387:PHE:CE1	2.47	0.49
23:3:755:VAL:HG13	23:3:762:LEU:HD11	1.93	0.49
38:R:132:LEU:HB3	40:T:399:LYS:HZ1	1.77	0.49
39:S:34:LYS:HE3	39:S:78:TYR:CD2	2.47	0.49
43:W:430:ASN:O	43:W:447:TRP:CB	2.59	0.49
45:Y:48:THR:OG1	45:Y:49:GLU:OE1	2.30	0.49
1:A:152:ARG:CG	1:A:152:ARG:NH1	2.73	0.49
1:A:296:PHE:CD1	3:C:591:ALA:HB3	2.47	0.49
1:A:380:LEU:CB	3:C:354:ARG:CZ	2.88	0.49
1:A:409:ARG:N	1:A:410:PRO:HD2	2.26	0.49
1:A:596:TYR:CD1	14:G:-5:G:C4	3.01	0.49
1:A:2298:LEU:C	4:D:1283:PRO:CB	2.78	0.49
3:C:65:TYR:C	3:C:66:TYR:CG	2.86	0.49
3:C:78:GLU:OE1	40:T:198:ARG:NH2	2.45	0.49
3:C:297:ASN:HB3	3:C:298:LEU:HD13	1.95	0.49
3:C:493:PHE:HD2	3:C:551:LEU:HD21	1.76	0.49
3:C:715:GLY:HA2	3:C:729:ALA:HB1	1.93	0.49
5:E:164:PRO:O	5:E:166:LEU:HG	2.13	0.49
21:1:499:LYS:HD3	21:1:534:GLN:NE2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:652:CYS:HB3	21:1:692:HIS:CE1	2.46	0.49
21:1:827:ARG:O	21:1:830:TYR:HB3	2.12	0.49
23:3:235:LEU:HG	23:3:250:ILE:HG13	1.93	0.49
23:3:1008:SER:OG	23:3:1009:PHE:N	2.45	0.49
35:N:59:TYR:CD1	43:W:187:SER:HA	2.48	0.49
36:O:225:PRO:CB	36:O:226:PRO:HD2	2.42	0.49
39:S:110:SER:O	39:S:111:GLN:C	2.50	0.49
43:W:474:LYS:C	43:W:490:ALA:HB3	2.33	0.49
1:A:76:MET:SD	1:A:88:TYR:CE1	3.05	0.49
1:A:800:TYR:CB	3:C:59:LEU:HD13	2.43	0.49
1:A:1056:HIS:NE2	1:A:1060:GLU:OE2	2.44	0.49
1:A:1310:ARG:NH2	1:A:1563:HIS:O	2.45	0.49
1:A:1760:GLU:HB2	1:A:1761:PRO:HD2	1.93	0.49
1:A:1807:ILE:HB	1:A:1820:LYS:HB3	1.92	0.49
1:A:2325:VAL:HG11	4:D:789:MET:HA	1.94	0.49
3:C:62:ASP:HB3	37:P:206:LYS:NZ	2.27	0.49
3:C:66:TYR:CE2	37:P:211:VAL:HG11	2.45	0.49
3:C:349:PHE:CD1	3:C:356:PHE:HE1	2.22	0.49
15:H:37:U:H2'	15:H:38:A:H8	1.77	0.49
23:3:253:GLU:OE2	23:3:284:GLY:HA3	2.12	0.49
23:3:483:LEU:HD11	23:3:493:GLU:HG3	1.94	0.49
28:J:220:LEU:HD13	28:J:220:LEU:C	2.32	0.49
35:N:1:MET:HB3	35:N:2:PRO:HD3	1.94	0.49
36:O:147:LEU:HA	36:O:150:LEU:HG	1.94	0.49
38:R:433:ILE:HG13	38:R:434:TYR:O	2.12	0.49
1:A:115:ASP:CB	1:A:486:LYS:HE2	2.43	0.49
1:A:1405:LEU:N	38:R:415:LEU:HD21	2.27	0.49
1:A:1818:PHE:CD2	1:A:1848:LEU:HD21	2.47	0.49
1:A:1930:TYR:CD2	1:A:1930:TYR:C	2.85	0.49
3:C:133:THR:O	3:C:226:VAL:CB	2.60	0.49
3:C:335:ASN:OD1	3:C:336:TYR:N	2.45	0.49
3:C:709:TRP:N	3:C:709:TRP:CD1	2.79	0.49
23:3:994:GLN:HE22	23:3:1037:SER:HA	1.78	0.49
32:I:511:LEU:CB	32:I:547:LEU:CA	2.91	0.49
36:O:106:ASP:OD1	36:O:107:MET:N	2.42	0.49
36:O:161:ARG:NH2	36:O:182:ARG:HD2	2.27	0.49
38:R:231:VAL:HG23	38:R:232:MET:N	2.26	0.49
38:R:241:MET:SD	38:R:245:GLU:CD	2.91	0.49
38:R:450:SER:OG	38:R:452:TYR:O	2.30	0.49
46:Z:563:ARG:CG	46:Z:563:ARG:NH2	2.73	0.49
1:A:529:THR:CB	34:M:199:PRO:CD	2.88	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:690:MET:HG3	1:A:694:LEU:HD12	1.95	0.49
1:A:1723:LYS:HB3	1:A:1724:PRO:HD3	1.95	0.49
1:A:1809:ILE:HD11	1:A:1845:VAL:HG22	1.93	0.49
2:B:42:U:O4'	13:F:70:A:C4'	2.58	0.49
5:E:266:PRO:HB3	29:L:785:GLN:HB2	1.95	0.49
13:F:36:A:C8	13:F:36:A:H5'	2.48	0.49
21:1:805:TYR:CE1	21:1:809:GLU:HG3	2.46	0.49
23:3:23:SER:HA	23:3:94:PRO:HG3	1.95	0.49
23:3:794:SER:HB2	23:3:933:ASN:O	2.12	0.49
23:3:1048:ASP:OD1	23:3:1049:LYS:N	2.45	0.49
28:J:331:GLN:CG	38:R:98:TYR:OH	2.47	0.49
35:N:40:LYS:C	35:N:41:ARG:CG	2.81	0.49
36:O:240:GLY:HA3	36:O:296:ARG:NH1	2.24	0.49
46:Z:526:ILE:N	46:Z:526:ILE:HD12	2.27	0.49
1:A:365:VAL:CG1	1:A:366:LYS:N	2.73	0.49
1:A:461:HIS:NE2	2:B:23:C:C5	2.80	0.49
1:A:800:TYR:HB3	3:C:59:LEU:HD13	1.95	0.49
1:A:2097:ILE:HD12	1:A:2099:GLU:HB2	1.93	0.49
3:C:140:HIS:O	3:C:258:ASN:HB3	2.13	0.49
3:C:363:SER:O	3:C:364:SER:CB	2.60	0.49
14:G:-9:C:N3	41:U:18:TYR:CZ	2.77	0.49
21:1:498:MET:HE1	21:1:531:LEU:HD12	1.93	0.49
21:1:1017:LEU:HD21	21:1:1058:ILE:HD11	1.93	0.49
21:1:1273:TYR:OH	21:1:1277:GLN:NE2	2.46	0.49
23:3:31:VAL:HG21	23:3:78:ILE:HD11	1.95	0.49
23:3:440:HIS:ND1	23:3:720:TRP:CH2	2.80	0.49
23:3:527:ILE:HA	23:3:532:ARG:O	2.12	0.49
37:P:30:TYR:OH	38:R:162:ALA:C	2.50	0.49
43:W:210:GLU:HA	43:W:213:GLN:CB	2.42	0.49
46:Z:597:ARG:HH12	46:Z:601:LEU:CD1	2.22	0.49
1:A:380:LEU:HB3	3:C:354:ARG:HH12	1.64	0.49
1:A:532:THR:HG21	14:G:2:U:H5'	1.88	0.49
1:A:1618:LYS:HD2	1:A:1626:CYS:H	1.78	0.49
1:A:1718:TRP:HZ3	1:A:1726:ILE:HD12	1.77	0.49
1:A:2287:ARG:HH22	4:D:1147:ASN:CB	2.15	0.49
2:B:20:G:OP1	2:B:20:G:H4'	2.12	0.49
2:B:63:A:H5"	5:E:106:LYS:HZ3	1.76	0.49
3:C:73:TYR:CZ	40:T:487:LYS:CE	2.95	0.49
3:C:137:HIS:NE2	3:C:236:MET:CE	2.75	0.49
3:C:705:VAL:HG21	3:C:718:PHE:CZ	2.47	0.49
5:E:74:PHE:HE1	5:E:95:VAL:CG2	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:F:53:A:C6	13:F:54:G:C5	3.00	0.49
14:G:5:G:H2'	14:G:5:G:N3	2.28	0.49
14:G:155:U:H4'	14:G:156:U:OP2	2.13	0.49
15:H:107:A:C2	15:H:108:G:C4	3.01	0.49
15:H:143:A:N3	15:H:143:A:C3'	2.73	0.49
21:1:175:LYS:O	21:1:179:GLY:HA3	2.11	0.49
21:1:1134:ASN:ND2	22:2:534:GLN:HA	2.28	0.49
23:3:47:THR:HG23	23:3:49:LYS:H	1.77	0.49
23:3:785:PRO:HA	23:3:801:GLU:HA	1.95	0.49
24:4:32:LEU:HD21	24:4:79:LEU:HD21	1.94	0.49
38:R:55:LEU:CA	38:R:73:PRO:O	2.61	0.49
1:A:258:PHE:HZ	1:A:275:GLY:O	1.96	0.49
1:A:331:TRP:CZ2	3:C:896:PHE:CE1	3.01	0.49
1:A:347:LEU:HD13	1:A:351:TYR:OH	2.12	0.49
1:A:1393:ARG:O	1:A:1397:ILE:HG13	2.12	0.49
3:C:301:SER:O	3:C:303:LEU:N	2.44	0.49
3:C:499:GLY:O	3:C:500:THR:HG23	2.13	0.49
5:E:219:VAL:HB	5:E:229:TYR:HB2	1.95	0.49
26:6:43:VAL:HG21	26:6:69:ALA:HB3	1.94	0.49
28:J:560:ALA:H	32:I:766:MET:CB	2.26	0.49
36:O:235:TYR:CD1	36:O:271:PHE:HE1	2.24	0.49
38:R:131:ASP:OD2	38:R:132:LEU:CD2	2.60	0.49
38:R:171:LEU:HD11	38:R:201:GLU:CD	2.32	0.49
40:T:442:ARG:HB3	40:T:443:THR:HG23	1.95	0.49
45:Y:38:ILE:HG22	45:Y:90:THR:HG23	1.95	0.49
1:A:304:ILE:HD11	1:A:1342:TRP:HZ2	1.77	0.49
1:A:494:LEU:HD21	1:A:562:VAL:HG21	1.95	0.49
1:A:623:LYS:HG2	50:A:3000:IHP:O43	2.13	0.49
1:A:2113:LYS:HE2	4:D:1229:ASP:CA	2.41	0.49
3:C:381:LEU:CD2	3:C:416:LEU:HD22	2.42	0.49
5:E:74:PHE:HE1	5:E:95:VAL:HG22	1.77	0.49
15:H:71:C:H2'	15:H:72:U:H6	1.75	0.49
35:N:55:GLN:CD	43:W:192:PHE:CB	2.81	0.49
36:O:155:PRO:HG3	38:R:188:PHE:HA	1.94	0.49
38:R:433:ILE:O	38:R:434:TYR:HB3	2.13	0.49
43:W:536:ASP:O	43:W:540:THR:N	2.42	0.49
45:Y:24:ASP:CG	45:Y:25:LYS:H	2.14	0.49
1:A:44:ARG:CG	1:A:45:TYR:CE2	2.95	0.48
1:A:322:ASN:OD1	3:C:655:VAL:HB	2.12	0.48
1:A:380:LEU:N	3:C:354:ARG:CB	2.75	0.48
1:A:433:GLU:OE1	1:A:436:PRO:CB	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1870:ASP:HB2	1:A:1871:PRO:HD3	1.95	0.48
1:A:1998:ASN:O	1:A:2001:SER:OG	2.23	0.48
3:C:82:GLN:HG3	40:T:237:LYS:HA	1.94	0.48
3:C:334:ILE:HD12	3:C:334:ILE:O	2.13	0.48
5:E:153:PHE:N	5:E:153:PHE:CD1	2.78	0.48
13:F:26:U:H3'	13:F:27:A:C5'	2.37	0.48
15:H:182:U:HO2'	15:H:183:G:H5'	1.76	0.48
21:1:408:PHE:HB2	25:5:49:ARG:NH1	2.28	0.48
23:3:734:LEU:HD13	23:3:767:LEU:HD21	1.94	0.48
38:R:82:MET:HE2	38:R:82:MET:O	2.13	0.48
45:Y:32:TYR:C	45:Y:34:ASP:H	2.15	0.48
1:A:595:LYS:CE	1:A:644:ILE:HD11	2.38	0.48
1:A:794:TYR:CD2	1:A:1028:TYR:HB2	2.47	0.48
2:B:40:U:H3	14:G:-1:G:N2	2.11	0.48
3:C:78:GLU:C	40:T:198:ARG:HA	2.25	0.48
3:C:508:LYS:HB3	3:C:566:THR:HG23	1.95	0.48
3:C:855:GLY:O	3:C:856:HIS:CB	2.44	0.48
5:E:162:ARG:HH22	5:E:204:THR:HA	1.74	0.48
13:F:54:G:N2	15:H:22:U:C2	2.81	0.48
14:G:11:A:N3	14:G:11:A:C3'	2.76	0.48
15:H:5:C:H2'	15:H:6:U:H6	1.78	0.48
21:1:483:ASP:OD1	21:1:484:GLU:N	2.46	0.48
28:J:360:ASP:HA	28:J:363:ARG:CG	2.44	0.48
39:S:131:ARG:HH12	39:S:133:CYS:CB	2.26	0.48
1:A:122:ILE:HD12	1:A:483:GLN:HG3	1.94	0.48
1:A:828:PRO:HG3	1:A:925:TYR:CZ	2.48	0.48
1:A:1214:TRP:CZ2	1:A:1230:LEU:HD11	2.48	0.48
1:A:2298:LEU:HD11	4:D:1285:SER:CA	2.43	0.48
3:C:73:TYR:CE1	40:T:453:ALA:O	2.67	0.48
3:C:297:ASN:HD22	3:C:298:LEU:CD1	2.26	0.48
3:C:333:ASP:OD1	3:C:333:ASP:N	2.42	0.48
3:C:401:ILE:HD11	3:C:423:PHE:HB2	1.96	0.48
13:F:49:G:H2'	13:F:50:A:H8	1.78	0.48
14:G:-8:U:C5	41:U:16:ASN:HB3	2.48	0.48
14:G:138:A:H5"	29:L:12:ARG:NE	2.28	0.48
15:H:10:C:H2'	15:H:11:G:C8	2.40	0.48
23:3:157:PRO:HD2	26:6:16:GLY:HA2	1.95	0.48
23:3:870:ASN:ND2	23:3:873:GLN:H	2.10	0.48
35:N:65:TYR:OH	35:N:93:LYS:HE2	2.13	0.48
38:R:433:ILE:HG13	38:R:434:TYR:N	2.27	0.48
40:T:302:VAL:HG23	40:T:315:TRP:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:W:97:ASN:C	43:W:99:PHE:N	2.66	0.48
46:Z:604:LYS:HA	46:Z:607:VAL:HG23	1.94	0.48
1:A:273:ILE:CG2	1:A:274:PRO:HD2	2.43	0.48
1:A:296:PHE:CD2	3:C:656:ALA:N	2.81	0.48
1:A:2149:PRO:O	1:A:2160:PRO:HD3	2.13	0.48
3:C:291:MET:CG	3:C:292:TYR:CE1	2.96	0.48
3:C:443:VAL:O	3:C:447:PRO:CD	2.62	0.48
3:C:452:THR:O	3:C:577:PHE:CA	2.60	0.48
13:F:8:C:H6	13:F:8:C:C5'	2.15	0.48
13:F:66:C:H2'	13:F:67:G:O4'	2.12	0.48
14:G:-8:U:H2'	14:G:-7:C:O4'	2.13	0.48
14:G:9:C:H2'	14:G:10:U:C6	2.48	0.48
14:G:19:G:C5'	36:O:159:ARG:HD2	2.40	0.48
15:H:25:G:N3	15:H:26:A:C8	2.82	0.48
23:3:886:GLU:OE1	23:3:926:TYR:OH	2.24	0.48
23:3:1149:ARG:HH12	23:3:1161:LEU:HD13	1.79	0.48
28:J:406:PHE:HB3	28:J:411:MET:HG2	1.96	0.48
44:X:212:ASN:H	44:X:307:GLN:HE22	1.60	0.48
1:A:774:LYS:HG2	15:H:23:A:C8	2.48	0.48
1:A:1214:TRP:NE1	1:A:1276:GLU:OE1	2.23	0.48
13:F:45:A:H4'	13:F:46:G:OP2	2.14	0.48
13:F:53:A:C6	15:H:25:G:C4	3.02	0.48
23:3:457:ASN:HD21	23:3:504:PRO:HB3	1.79	0.48
23:3:624:CYS:SG	23:3:625:LEU:HD13	2.54	0.48
23:3:930:LEU:HA	23:3:937:LEU:HD23	1.95	0.48
27:7:40:TYR:HA	27:7:43:TYR:CD2	2.49	0.48
29:L:733:LYS:O	29:L:736:ASN:CG	2.52	0.48
36:O:229:LYS:HA	36:O:277:ARG:HH22	1.78	0.48
38:R:103:ARG:CG	38:R:103:ARG:NH1	2.75	0.48
40:T:185:MET:CB	40:T:186:PRO:CD	2.90	0.48
40:T:213:GLU:HB2	40:T:218:TRP:O	2.14	0.48
1:A:279:PHE:CZ	1:A:452:LYS:HG3	2.49	0.48
1:A:593:ARG:HE	14:G:-4:A:P	2.37	0.48
1:A:718:ARG:HH21	38:R:259:LYS:CE	2.25	0.48
3:C:350:ASN:HB3	3:C:353:THR:HG23	1.94	0.48
3:C:445:ALA:O	3:C:449:ILE:HG13	2.12	0.48
3:C:678:THR:HG23	3:C:683:ASN:CA	2.43	0.48
3:C:736:GLY:N	3:C:770:PHE:HE2	2.10	0.48
21:1:1212:LEU:HD13	21:1:1237:LEU:HD13	1.96	0.48
23:3:142:TYR:CE1	23:3:157:PRO:HB3	2.48	0.48
23:3:565:TYR:CG	23:3:619:LEU:HD13	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:R:215:ASN:HD22	38:R:216:LYS:N	2.11	0.48
42:V:549:LYS:O	42:V:552:ALA:CB	2.60	0.48
1:A:247:THR:HG1	1:A:429:ASN:HB3	1.76	0.48
1:A:279:PHE:CE1	1:A:452:LYS:HE3	2.48	0.48
1:A:330:THR:O	1:A:331:TRP:CB	2.62	0.48
1:A:409:ARG:HD2	1:A:409:ARG:O	2.14	0.48
1:A:1295:ILE:HG13	1:A:1296:GLN:N	2.29	0.48
3:C:135:CYS:SG	3:C:227:LEU:HA	2.54	0.48
3:C:149:LEU:CA	3:C:427:PHE:CE2	2.97	0.48
3:C:349:PHE:HB2	3:C:356:PHE:CE1	2.48	0.48
3:C:514:TYR:CD1	3:C:515:THR:N	2.82	0.48
15:H:83:A:C2	15:H:84:C:N3	2.82	0.48
23:3:842:PHE:HD2	23:3:843:LEU:HD12	1.78	0.48
23:3:926:TYR:HE1	23:3:942:LYS:HG3	1.77	0.48
28:J:273:TYR:CZ	38:R:228:PRO:CB	2.82	0.48
36:O:223:LEU:HD22	36:O:223:LEU:C	2.34	0.48
40:T:387:PHE:CD1	40:T:387:PHE:C	2.87	0.48
1:A:121:HIS:O	1:A:123:THR:N	2.47	0.48
1:A:299:ILE:CD1	3:C:920:PRO:C	2.82	0.48
1:A:596:TYR:O	1:A:597:LYS:C	2.50	0.48
1:A:1119:ASP:OD2	1:A:1124:ASN:N	2.44	0.48
1:A:1332:HIS:HB3	1:A:1359:HIS:HE1	1.78	0.48
1:A:2298:LEU:HD11	4:D:1265:GLN:CB	2.44	0.48
3:C:82:GLN:O	40:T:202:GLY:HA3	2.13	0.48
3:C:457:VAL:HG12	3:C:462:GLY:HA3	1.96	0.48
3:C:477:HIS:HD1	3:C:478:THR:N	2.12	0.48
5:E:243:LEU:HD11	5:E:247:GLY:CA	2.41	0.48
14:G:17:U:H2'	14:G:18:A:C8	2.49	0.48
15:H:83:A:C2	15:H:84:C:C4	3.01	0.48
21:1:1297:ARG:NH1	27:7:39:SER:OG	2.46	0.48
22:2:504:TRP:C	22:2:506:PHE:H	2.17	0.48
40:T:384:HIS:O	40:T:385:TYR:HB3	2.13	0.48
42:V:576:THR:O	42:V:579:SER:N	2.47	0.48
43:W:528:GLY:O	43:W:552:VAL:CB	2.62	0.48
1:A:592:TYR:O	1:A:595:LYS:O	2.32	0.48
1:A:1892:PRO:HD3	1:A:1941:ARG:HH21	1.79	0.48
3:C:128:LEU:O	3:C:199:LEU:N	2.37	0.48
3:C:690:GLU:HB2	3:C:691:PRO:HD2	1.95	0.48
13:F:44:G:H2'	22:2:554:ARG:HG2	1.96	0.48
14:G:20:A:OP2	36:O:159:ARG:HD3	2.14	0.48
15:H:37:U:H2'	15:H:38:A:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:2:652:GLY:N	22:2:655:SER:O	2.45	0.48
23:3:21:ASN:HD21	23:3:28:GLN:HG2	1.77	0.48
23:3:58:VAL:HG12	23:3:1155:LEU:HB3	1.95	0.48
23:3:539:PRO:HD2	23:3:558:LEU:HD21	1.95	0.48
23:3:891:VAL:HA	23:3:906:LEU:O	2.13	0.48
23:3:1057:ARG:HG2	23:3:1058:LEU:O	2.13	0.48
38:R:184:GLN:O	38:R:188:PHE:HB2	2.13	0.48
45:Y:110:ASP:OD1	45:Y:111:HIS:N	2.43	0.48
1:A:232:LEU:HD13	1:A:404:LEU:HD12	1.95	0.48
1:A:238:LEU:HB3	1:A:411:PHE:HE2	1.79	0.48
1:A:380:LEU:HB2	3:C:354:ARG:CZ	2.44	0.48
1:A:380:LEU:N	3:C:354:ARG:CG	2.77	0.48
1:A:412:ASN:OD1	1:A:413:LEU:HD23	2.13	0.48
1:A:731:LEU:HD23	1:A:736:GLU:HB2	1.94	0.48
1:A:2310:ARG:HH11	1:A:2310:ARG:CG	2.27	0.48
3:C:93:ILE:O	3:C:94:ILE:CB	2.62	0.48
3:C:145:PHE:HB2	3:C:312:SER:CB	2.32	0.48
13:F:27:A:N3	36:O:181:TYR:HE2	1.98	0.48
21:1:208:PRO:N	21:1:656:LYS:HE3	2.29	0.48
23:3:476:VAL:O	23:3:482:THR:HA	2.14	0.48
23:3:981:CYS:SG	23:3:1021:LEU:HG	2.54	0.48
38:R:402:ASN:HB2	44:X:192:ARG:CG	2.43	0.48
1:A:203:VAL:HG12	1:A:207:PHE:CD1	2.49	0.47
1:A:296:PHE:CZ	3:C:591:ALA:C	2.88	0.47
1:A:735:ILE:O	1:A:738:MET:HE2	2.14	0.47
1:A:758:ARG:HD2	1:A:775:ASN:ND2	2.28	0.47
1:A:1183:PRO:HA	1:A:1201:ARG:HE	1.78	0.47
1:A:1754:TYR:CD1	21:1:948:ARG:NH1	2.82	0.47
1:A:1768:TYR:HA	1:A:1771:LEU:CB	2.40	0.47
3:C:557:GLN:N	3:C:558:PRO:HD2	2.29	0.47
5:E:263:ASP:OD1	5:E:272:ARG:HB3	2.13	0.47
13:F:44:G:N2	14:G:3:A:C8	2.82	0.47
21:1:209:GLY:HA3	21:1:614:ARG:NH1	2.29	0.47
23:3:353:PHE:HB3	23:3:406:PRO:HD3	1.96	0.47
23:3:814:GLN:O	23:3:818:GLN:HB2	2.13	0.47
26:6:19:ILE:HD12	26:6:42:LEU:HD21	1.96	0.47
28:J:273:TYR:CD2	38:R:228:PRO:HG3	2.49	0.47
38:R:120:VAL:CG2	38:R:121:PRO:HD2	2.44	0.47
44:X:246:TYR:H	44:X:386:ASP:HA	1.79	0.47
1:A:312:TYR:N	1:A:312:TYR:CD1	2.78	0.47
1:A:1045:GLY:HA3	1:A:1090:ARG:NH2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1270:LEU:HD12	1:A:1274:PHE:CD2	2.49	0.47
1:A:1551:PHE:O	1:A:1553:VAL:HG23	2.14	0.47
3:C:753:GLU:O	3:C:755:ASP:N	2.45	0.47
5:E:269:PRO:O	5:E:270:LYS:CB	2.54	0.47
13:F:12:G:H2'	13:F:13:G:O4'	2.14	0.47
15:H:151:C:C2	15:H:152:G:N7	2.82	0.47
23:3:675:LEU:HD23	23:3:686:LEU:HD11	1.96	0.47
23:3:1095:TYR:CZ	23:3:1164:ARG:HD2	2.49	0.47
26:6:23:CYS:HB3	26:6:58:CYS:HB2	1.97	0.47
27:7:69:MET:HA	27:7:72:MET:HG2	1.96	0.47
28:J:436:TYR:OH	28:J:458:PHE:HA	2.14	0.47
36:O:253:TYR:OH	39:S:120:GLN:CG	2.62	0.47
40:T:416:ILE:O	40:T:416:ILE:HD13	2.14	0.47
42:V:484:SER:C	42:V:486:THR:N	2.67	0.47
42:V:527:GLY:O	42:V:530:LYS:N	2.47	0.47
42:V:625:ARG:O	42:V:629:ASN:CB	2.62	0.47
1:A:385:GLU:OE1	1:A:386:PRO:HD2	2.14	0.47
1:A:388:LEU:CD1	3:C:379:LYS:HB3	2.45	0.47
1:A:1211:ASP:CG	42:V:505:LYS:CB	2.82	0.47
1:A:1258:LYS:HE2	38:R:432:GLU:CA	2.44	0.47
1:A:2148:VAL:O	1:A:2150:GLN:HG2	2.14	0.47
3:C:66:TYR:OH	37:P:216:ARG:HD2	2.13	0.47
3:C:73:TYR:HE1	40:T:453:ALA:O	1.97	0.47
3:C:441:PRO:O	3:C:444:GLY:CA	2.61	0.47
3:C:449:ILE:HD12	3:C:466:SER:OG	2.13	0.47
3:C:673:LYS:HB3	3:C:688:ILE:HG22	1.96	0.47
5:E:178:LEU:CD2	5:E:208:ILE:HD13	2.44	0.47
14:G:138:A:H2'	14:G:139:U:C6	2.49	0.47
21:1:1252:GLN:HG2	22:2:492:LYS:HA	1.96	0.47
23:3:240:GLY:HA3	23:3:246:SER:HB2	1.95	0.47
27:7:33:VAL:HG23	27:7:75:PRO:HG2	1.96	0.47
38:R:73:PRO:HG2	38:R:74:LEU:H	1.79	0.47
38:R:189:ASN:HD21	38:R:195:ARG:CZ	2.26	0.47
39:S:9:TRP:CE3	39:S:11:PRO:CD	2.95	0.47
45:Y:63:VAL:HG23	45:Y:64:ASN:H	1.78	0.47
1:A:1192:PHE:HE1	1:A:1274:PHE:CD1	2.32	0.47
1:A:1439:ARG:O	1:A:1443:LYS:HG2	2.15	0.47
3:C:240:GLU:OE2	3:C:292:TYR:OH	2.18	0.47
3:C:438:ILE:CD1	3:C:438:ILE:N	2.76	0.47
14:G:17:U:H2'	14:G:18:A:H8	1.79	0.47
14:G:149:G:N2	14:G:150:U:H2'	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:464:LEU:HD23	21:1:478:LEU:HD21	1.95	0.47
21:1:781:ASP:HB3	21:1:784:MET:HB2	1.95	0.47
23:3:54:LEU:HD22	23:3:98:MET:HA	1.97	0.47
23:3:120:PHE:HB2	23:3:133:SER:OG	2.15	0.47
26:6:21:ARG:HG3	26:6:56:GLY:HA2	1.96	0.47
37:P:224:MET:HE2	37:P:228:ILE:CD1	2.39	0.47
37:P:228:ILE:CD1	37:P:228:ILE:N	2.78	0.47
1:A:171:ASP:CG	1:A:519:ASP:OD2	2.53	0.47
1:A:277:PRO:HA	1:A:448:GLN:HG3	1.96	0.47
1:A:340:ILE:HD13	1:A:340:ILE:N	2.29	0.47
1:A:546:LEU:HD11	1:A:595:LYS:CG	2.43	0.47
1:A:2252:LEU:HD23	1:A:2253:PRO:HD2	1.96	0.47
3:C:73:TYR:OH	40:T:487:LYS:CE	2.62	0.47
3:C:185:PRO:HD3	3:C:482:TYR:CE1	2.50	0.47
5:E:161:ARG:HH11	5:E:161:ARG:CG	2.26	0.47
13:F:22:A:H3'	35:N:115:THR:HG21	1.96	0.47
21:1:1172:LEU:HA	22:2:522:PHE:HE1	1.79	0.47
23:3:354:GLY:HA3	23:3:432:ARG:NH1	2.30	0.47
37:P:192:VAL:HG12	37:P:193:VAL:N	2.29	0.47
38:R:103:ARG:NH2	38:R:110:LYS:O	2.40	0.47
38:R:178:ARG:CD	38:R:194:GLN:NE2	2.72	0.47
1:A:323:LEU:N	1:A:324:PRO:CD	2.77	0.47
1:A:338:VAL:HB	3:C:867:PRO:CG	2.45	0.47
1:A:380:LEU:H	3:C:354:ARG:HB3	1.79	0.47
2:B:42:U:H2'	2:B:43:U:O4'	2.13	0.47
3:C:507:VAL:HG12	3:C:508:LYS:N	2.29	0.47
3:C:710:ASN:O	3:C:711:ARG:C	2.53	0.47
14:G:-5:G:O2'	14:G:-4:A:H8	1.98	0.47
15:H:57:A:H2'	15:H:58:U:O4'	2.14	0.47
21:1:1140:GLU:O	21:1:1144:GLN:HG3	2.15	0.47
23:3:459:VAL:HB	23:3:757:ILE:HG23	1.97	0.47
23:3:554:VAL:HB	23:3:566:PHE:HB2	1.97	0.47
28:J:216:ASP:O	28:J:219:GLU:N	2.47	0.47
38:R:51:ILE:N	38:R:52:PRO:CD	2.77	0.47
38:R:90:VAL:HB	39:S:20:MET:SD	2.55	0.47
39:S:34:LYS:HE2	39:S:78:TYR:CD2	2.48	0.47
40:T:318:ARG:HH11	40:T:319:THR:CG2	2.28	0.47
1:A:735:ILE:O	1:A:738:MET:HB3	2.15	0.47
1:A:1241:HIS:ND1	1:A:1287:LEU:HD11	2.29	0.47
3:C:78:GLU:CD	3:C:80:ILE:HD11	2.30	0.47
3:C:749:THR:O	3:C:753:GLU:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:903:GLN:HE22	21:1:910:MET:HG3	1.80	0.47
23:3:18:ILE:HD13	23:3:65:LEU:HG	1.96	0.47
23:3:931:VAL:O	23:3:936:LYS:N	2.40	0.47
23:3:1032:TRP:O	23:3:1048:ASP:HA	2.15	0.47
28:J:273:TYR:CE2	38:R:228:PRO:HB3	2.46	0.47
34:M:205:TYR:CD2	34:M:221:HIS:O	2.68	0.47
35:N:27:GLN:HE21	35:N:31:GLU:HG2	1.79	0.47
36:O:236:VAL:HB	36:O:270:ALA:O	2.15	0.47
37:P:227:TYR:N	37:P:227:TYR:CD1	2.81	0.47
39:S:125:LYS:HE3	39:S:125:LYS:N	2.30	0.47
40:T:257:ARG:HD3	40:T:301:ASP:OD1	2.14	0.47
42:V:467:LEU:O	42:V:468:ASP:CB	2.62	0.47
45:Y:40:LEU:HB2	45:Y:43:LEU:HD11	1.96	0.47
1:A:195:LEU:H	1:A:195:LEU:HD12	1.80	0.47
1:A:229:GLN:CB	1:A:415:SER:HB2	2.45	0.47
1:A:1455:TRP:CE3	1:A:1456:THR:HB	2.50	0.47
3:C:115:GLU:O	3:C:118:PHE:CA	2.61	0.47
3:C:457:VAL:CA	3:C:462:GLY:HA3	2.44	0.47
21:1:207:THR:HA	21:1:656:LYS:NZ	2.28	0.47
21:1:699:GLN:HA	21:1:702:ARG:CZ	2.45	0.47
23:3:164:ASN:ND2	23:3:189:TYR:OH	2.34	0.47
23:3:304:GLN:HA	23:3:309:ASP:O	2.15	0.47
23:3:931:VAL:HG12	23:3:932:ASN:N	2.26	0.47
25:5:14:PRO:HB2	25:5:16:GLU:OE1	2.15	0.47
40:T:246:ILE:HB	40:T:267:ASP:OD1	2.15	0.47
1:A:134:TRP:HB3	1:A:418:THR:HG22	1.95	0.47
1:A:596:TYR:CZ	14:G:-5:G:C5	3.03	0.47
1:A:695:ASP:HB3	40:T:374:SER:CB	2.38	0.47
1:A:1608:THR:HG22	1:A:1632:PHE:HB2	1.97	0.47
2:B:42:U:O5'	2:B:42:U:H6	1.97	0.47
21:1:535:ILE:O	21:1:538:LEU:N	2.47	0.47
21:1:760:GLU:N	21:1:760:GLU:OE1	2.47	0.47
21:1:1132:LEU:HD11	21:1:1150:SER:OG	2.14	0.47
23:3:5:ASN:OD1	23:3:6:LEU:N	2.47	0.47
23:3:212:GLU:OE1	23:3:223:LYS:HD2	2.15	0.47
23:3:498:GLY:HA3	23:3:531:LYS:NZ	2.30	0.47
38:R:67:ILE:HG22	38:R:69:VAL:HG21	1.97	0.47
38:R:82:MET:HE3	38:R:82:MET:C	2.36	0.47
1:A:91:ALA:O	1:A:94:TYR:N	2.43	0.47
1:A:331:TRP:CZ2	3:C:896:PHE:HE1	2.33	0.47
1:A:596:TYR:CE1	14:G:-5:G:C4	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:A:O2'	2:B:30:A:H5'	2.15	0.47
3:C:470:PRO:CA	3:C:499:GLY:HA2	2.42	0.47
3:C:490:PHE:CE1	3:C:612:LYS:HD2	2.49	0.47
13:F:49:G:H2'	13:F:50:A:C8	2.50	0.47
14:G:156:U:P	14:G:156:U:H3'	2.54	0.47
15:H:6:U:H2'	15:H:7:U:H6	1.80	0.47
15:H:47:U:H4'	15:H:48:A:OP1	2.15	0.47
15:H:153:A:C8	15:H:154:C:H5'	2.50	0.47
21:1:1185:ARG:HD2	21:1:1218:ASN:CG	2.35	0.47
22:2:642:PRO:HG3	22:2:648:LEU:HD22	1.97	0.47
23:3:182:PHE:O	23:3:210:PHE:HA	2.15	0.47
23:3:458:ALA:HA	23:3:741:PHE:CB	2.45	0.47
28:J:255:LEU:CD2	29:L:235:LEU:HD13	2.38	0.47
1:A:755:HIS:HE1	37:P:223:PHE:CB	2.14	0.46
1:A:1256:PHE:CZ	1:A:1302:GLY:HA3	2.51	0.46
1:A:1718:TRP:CZ3	1:A:1723:LYS:HA	2.50	0.46
3:C:82:GLN:HG3	40:T:238:LEU:N	2.30	0.46
3:C:244:LYS:HG3	3:C:292:TYR:CD2	2.50	0.46
3:C:449:ILE:HD11	3:C:465:MET:C	2.35	0.46
3:C:571:ASN:O	3:C:572:GLU:HB3	2.16	0.46
21:1:815:PHE:HA	21:1:819:TRP:HD1	1.81	0.46
21:1:1058:ILE:O	21:1:1062:LEU:HG	2.16	0.46
23:3:248:VAL:HG23	23:3:250:ILE:HD11	1.96	0.46
37:P:64:GLU:OE2	37:P:68:ARG:NE	2.48	0.46
43:W:481:MET:C	43:W:483:ASN:H	2.18	0.46
1:A:299:ILE:HD12	3:C:921:LEU:HD22	1.97	0.46
1:A:519:ASP:C	1:A:519:ASP:OD1	2.54	0.46
1:A:1209:HIS:CG	1:A:1210:LYS:N	2.83	0.46
1:A:1212:GLY:HA3	1:A:1280:ASN:ND2	2.31	0.46
1:A:1824:THR:HA	1:A:1827:TRP:HD1	1.80	0.46
1:A:1892:PRO:HG3	1:A:1941:ARG:HE	1.81	0.46
2:B:41:U:H2'	2:B:42:U:C6	2.49	0.46
3:C:262:ARG:HG2	51:C:1500:GTP:N2	2.30	0.46
3:C:350:ASN:CB	3:C:353:THR:HG23	2.45	0.46
13:F:78:A:H8	13:F:78:A:OP2	1.98	0.46
15:H:150:U:H2'	15:H:151:C:C6	2.50	0.46
21:1:732:TRP:HB2	21:1:765:TYR:HE1	1.79	0.46
21:1:738:HIS:CE1	21:1:746:PHE:HE2	2.32	0.46
21:1:1169:VAL:HG12	21:1:1173:LEU:HG	1.97	0.46
23:3:28:GLN:NE2	23:3:343:LYS:HG2	2.31	0.46
23:3:1005:VAL:O	23:3:1032:TRP:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:N:128:VAL:HG11	35:N:130:ARG:HB3	1.96	0.46
39:S:13:ASN:ND2	39:S:24:VAL:CG1	2.79	0.46
39:S:101:ALA:HB1	43:W:94:GLY:HA3	1.96	0.46
45:Y:48:THR:HG1	45:Y:49:GLU:H	1.63	0.46
1:A:232:LEU:O	1:A:404:LEU:HD11	2.16	0.46
1:A:298:ASP:OD1	1:A:300:ASN:N	2.48	0.46
1:A:437:ALA:O	1:A:439:GLN:HG2	2.15	0.46
1:A:532:THR:CG2	14:G:2:U:OP1	2.63	0.46
1:A:844:GLU:O	1:A:848:GLU:HG2	2.15	0.46
1:A:982:GLU:HG3	1:A:1169:GLN:HG3	1.97	0.46
1:A:1761:PRO:CB	1:A:1930:TYR:OH	2.55	0.46
1:A:1821:ILE:O	1:A:1912:PRO:HA	2.15	0.46
3:C:221:ILE:HG23	3:C:495:ARG:HB3	1.96	0.46
5:E:87:ASP:O	5:E:88:ARG:CG	2.63	0.46
13:F:28:A:O2'	35:N:39:GLY:C	2.53	0.46
21:1:728:LEU:O	21:1:731:LEU:N	2.48	0.46
23:3:274:ARG:NH2	23:3:307:GLN:OE1	2.48	0.46
38:R:195:ARG:HB3	38:R:195:ARG:HH11	1.80	0.46
45:Y:37:TRP:CZ3	46:Z:498:GLY:C	2.86	0.46
1:A:97:HIS:HD2	1:A:473:PHE:HZ	1.59	0.46
1:A:338:VAL:HG21	3:C:867:PRO:HD3	1.97	0.46
1:A:468:LYS:HD3	1:A:468:LYS:C	2.35	0.46
1:A:1370:ARG:NH2	42:V:506:PHE:CB	2.78	0.46
1:A:1607:GLU:HB2	1:A:1634:SER:HA	1.96	0.46
1:A:1733:ILE:HG23	1:A:1737:ASN:HB2	1.98	0.46
1:A:2070:LYS:HA	1:A:2070:LYS:HD3	1.67	0.46
1:A:2121:ARG:O	1:A:2154:HIS:HA	2.15	0.46
1:A:2314:PHE:HB3	4:D:1125:SER:N	2.29	0.46
3:C:66:TYR:CG	40:T:457:GLY:HA2	2.46	0.46
3:C:80:ILE:HD13	40:T:198:ARG:HG3	1.98	0.46
3:C:678:THR:HG21	3:C:683:ASN:CB	2.43	0.46
5:E:260:ARG:CZ	5:E:276:ILE:HD11	2.46	0.46
13:F:27:A:C2	36:O:181:TYR:CD2	3.03	0.46
13:F:37:C:O2	13:F:37:C:H2'	2.15	0.46
14:G:149:G:H2'	14:G:150:U:C6	2.50	0.46
15:H:71:C:O5'	15:H:71:C:H6	1.98	0.46
15:H:79:G:N3	15:H:80:A:C8	2.83	0.46
15:H:142:C:H2'	15:H:143:A:H5'	1.98	0.46
21:1:572:HIS:HB2	21:1:612:THR:HG23	1.96	0.46
21:1:722:GLU:O	21:1:725:ASP:HB2	2.14	0.46
21:1:842:ASN:HA	21:1:879:LEU:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:1210:HIS:CD2	22:2:584:LEU:HD22	2.51	0.46
23:3:30:ILE:HG22	23:3:32:VAL:HG13	1.98	0.46
23:3:228:LEU:HD23	23:3:259:LYS:NZ	2.30	0.46
23:3:238:VAL:HB	23:3:247:GLY:O	2.16	0.46
23:3:718:ARG:HG2	23:3:719:SER:N	2.30	0.46
23:3:801:GLU:O	23:3:864:SER:HA	2.16	0.46
36:O:146:MET:O	36:O:149:LYS:N	2.40	0.46
39:S:81:GLN:HB3	39:S:108:ASN:N	2.31	0.46
40:T:213:GLU:HG3	40:T:218:TRP:NE1	2.29	0.46
1:A:67:ARG:HD3	1:A:179:ALA:CB	2.34	0.46
1:A:1354:ARG:NH1	41:U:7:LEU:CD2	2.79	0.46
1:A:1700:GLY:O	1:A:1717:ASN:N	2.41	0.46
1:A:1782:ASP:OD1	1:A:1865:ARG:HD3	2.15	0.46
3:C:385:VAL:CG2	3:C:386:GLY:N	2.78	0.46
15:H:80:A:N3	15:H:81:G:C8	2.84	0.46
21:1:478:LEU:HA	21:1:496:LYS:HE3	1.97	0.46
21:1:579:GLU:HB3	21:1:627:THR:OG1	2.16	0.46
21:1:903:GLN:HG3	21:1:950:GLN:HE22	1.81	0.46
21:1:1186:GLN:HE22	21:1:1225:HIS:HB3	1.79	0.46
21:1:1253:GLY:HA3	21:1:1265:TYR:CD1	2.51	0.46
23:3:195:ASP:OD2	23:3:200:ALA:N	2.43	0.46
23:3:787:LYS:HB3	23:3:800:ILE:HD11	1.96	0.46
23:3:828:GLY:O	23:3:834:LEU:N	2.49	0.46
23:3:851:ILE:HG23	23:3:852:PHE:CD2	2.50	0.46
25:5:78:SER:HA	25:5:89:VAL:HG21	1.97	0.46
36:O:193:LEU:HD23	36:O:193:LEU:O	2.15	0.46
38:R:134:ARG:O	38:R:135:PRO:C	2.54	0.46
1:A:270:ASN:HD21	41:U:8:PRO:HA	1.81	0.46
1:A:596:TYR:OH	14:G:-5:G:C8	2.68	0.46
1:A:748:ASP:CB	37:P:214:THR:HG21	2.46	0.46
1:A:1397:ILE:HG12	38:R:408:GLU:CG	2.45	0.46
3:C:145:PHE:CG	3:C:312:SER:HB3	2.49	0.46
3:C:149:LEU:N	3:C:427:PHE:HE2	2.14	0.46
5:E:281:VAL:HG21	43:W:148:VAL:HA	1.95	0.46
21:1:862:GLU:O	21:1:865:ARG:N	2.48	0.46
21:1:972:GLY:O	21:1:976:VAL:HG22	2.15	0.46
23:3:253:GLU:HG3	23:3:254:ASN:HD22	1.81	0.46
23:3:488:GLY:C	23:3:490:THR:H	2.19	0.46
25:5:81:ASN:OD1	25:5:82:VAL:N	2.48	0.46
34:M:220:LEU:O	34:M:221:HIS:CB	2.61	0.46
36:O:78:LYS:HG3	36:O:202:TYR:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:O:123:ARG:O	36:O:126:SER:OG	2.16	0.46
40:T:185:MET:HB2	40:T:186:PRO:HD3	1.98	0.46
1:A:75:ASP:HB2	1:A:77:THR:OG1	2.16	0.46
1:A:201:ALA:HA	1:A:204:LEU:HB3	1.98	0.46
1:A:388:LEU:HB3	1:A:391:THR:OG1	2.16	0.46
2:B:12:U:H3	2:B:65:G:H1	1.62	0.46
3:C:66:TYR:N	3:C:66:TYR:CD1	2.81	0.46
3:C:507:VAL:HG13	3:C:566:THR:O	2.16	0.46
3:C:559:ILE:HD12	3:C:559:ILE:O	2.15	0.46
3:C:569:ARG:O	3:C:569:ARG:HG2	2.16	0.46
3:C:671:SER:OG	3:C:672:LEU:HD22	2.15	0.46
3:C:853:ARG:O	3:C:854:ARG:CB	2.62	0.46
3:C:934:MET:HE2	3:C:934:MET:HB2	1.77	0.46
5:E:276:ILE:C	5:E:277:PHE:HD1	2.19	0.46
14:G:135:G:O6	14:G:137:C:N4	2.48	0.46
15:H:30:A:C8	29:L:7:LYS:HD3	2.51	0.46
15:H:107:A:C6	15:H:108:G:C6	3.04	0.46
21:1:859:ASP:OD1	21:1:860:GLU:N	2.47	0.46
23:3:448:ALA:HB3	23:3:764:ILE:HB	1.97	0.46
29:L:78:MET:HB3	29:L:81:GLN:OE1	2.16	0.46
36:O:20:PHE:CG	36:O:21:PRO:HD2	2.51	0.46
46:Z:604:LYS:HA	46:Z:607:VAL:CG2	2.46	0.46
1:A:780:THR:HG22	1:A:898:PHE:CD2	2.50	0.46
1:A:802:THR:HG22	1:A:803:ALA:H	1.80	0.46
1:A:1237:MET:HG2	1:A:1284:LEU:HD21	1.98	0.46
1:A:1312:PRO:O	1:A:1315:VAL:HG22	2.14	0.46
1:A:1399:GLN:HB3	1:A:1401:ARG:HG2	1.98	0.46
1:A:2112:LYS:HE2	1:A:2112:LYS:HB3	1.67	0.46
13:F:56:A:N1	15:H:20:G:C6	2.84	0.46
15:H:78:C:O5'	15:H:78:C:H6	1.98	0.46
21:1:588:TYR:HA	21:1:591:VAL:HG12	1.98	0.46
21:1:608:THR:O	21:1:612:THR:OG1	2.15	0.46
21:1:759:ALA:O	21:1:763:ASN:HB2	2.16	0.46
23:3:69:ARG:HG2	23:3:70:LEU:O	2.16	0.46
23:3:509:SER:CB	23:3:549:VAL:HG21	2.45	0.46
35:N:5:LYS:HD2	35:N:77:TYR:OH	2.16	0.46
35:N:17:LEU:HD12	35:N:18:ILE:HG23	1.98	0.46
38:R:88:ILE:HG22	38:R:96:ILE:HG23	1.98	0.46
38:R:92:SER:O	39:S:19:SER:CA	2.64	0.46
38:R:220:ARG:NH1	38:R:220:ARG:CB	2.76	0.46
1:A:532:THR:OG1	14:G:2:U:H5"	2.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:841:LEU:HD13	1:A:1433:ASP:HB2	1.98	0.46
1:A:1306:LYS:NZ	2:B:38:C:H2'	2.30	0.46
1:A:1388:GLU:O	1:A:1392:LYS:HG2	2.16	0.46
1:A:1718:TRP:CZ3	1:A:1726:ILE:HD12	2.50	0.46
3:C:725:ASP:OD1	3:C:727:LEU:CA	2.64	0.46
5:E:266:PRO:HB3	29:L:785:GLN:CB	2.46	0.46
5:E:276:ILE:C	5:E:277:PHE:CD1	2.89	0.46
13:F:43:A:H2	14:G:4:A:H61	1.64	0.46
15:H:114:A:H2'	15:H:115:G:H8	1.81	0.46
21:1:647:PHE:O	21:1:651:VAL:HG23	2.16	0.46
21:1:1125:PRO:O	21:1:1128:VAL:N	2.49	0.46
21:1:1181:ASP:H	21:1:1184:HIS:HD2	1.64	0.46
23:3:71:THR:HG23	23:3:126:LYS:HD2	1.98	0.46
23:3:482:THR:HG23	23:3:503:THR:O	2.15	0.46
23:3:616:ILE:O	23:3:628:LEU:HB2	2.16	0.46
24:4:29:LEU:HD22	24:4:33:PHE:CE2	2.49	0.46
24:4:32:LEU:CD2	24:4:79:LEU:HD21	2.46	0.46
25:5:46:ARG:HB3	25:5:63:VAL:HG12	1.97	0.46
28:J:406:PHE:CG	28:J:411:MET:CE	2.97	0.46
36:O:63:MET:SD	36:O:160:ASN:HB2	2.56	0.46
37:P:54:VAL:HG13	37:P:59:PHE:HZ	1.80	0.46
38:R:185:GLY:C	38:R:186:VAL:HG13	2.35	0.46
1:A:34:ALA:HA	5:E:213:ILE:CD1	2.46	0.46
1:A:296:PHE:CB	3:C:656:ALA:CB	2.71	0.46
1:A:331:TRP:NE1	3:C:884:GLU:OE2	2.49	0.46
1:A:586:GLY:O	1:A:592:TYR:CE2	2.69	0.46
1:A:738:MET:HE3	1:A:739:ILE:HG13	1.97	0.46
1:A:1328:LEU:HD23	1:A:1470:TYR:CE2	2.51	0.46
1:A:1505:LYS:CD	46:Z:615:SER:CB	2.91	0.46
1:A:2272:MET:HB3	1:A:2272:MET:HE3	1.68	0.46
3:C:678:THR:HG23	3:C:683:ASN:N	2.31	0.46
5:E:248:SER:HB2	5:E:249:TYR:HD1	1.75	0.46
21:1:888:LEU:O	21:1:892:LEU:HG	2.15	0.46
23:3:287:PHE:CD1	23:3:303:ALA:HB1	2.50	0.46
36:O:84:CYS:HB3	36:O:86:LEU:HG	1.98	0.46
37:P:48:GLN:O	37:P:49:ASP:CB	2.64	0.46
38:R:148:ARG:HG3	38:R:148:ARG:NH1	2.31	0.46
38:R:226:PRO:CD	38:R:226:PRO:O	2.64	0.46
1:A:121:HIS:HD2	1:A:482:PHE:CE1	2.35	0.45
1:A:892:LYS:HD2	1:A:912:GLU:OE1	2.16	0.45
1:A:903:SER:OG	1:A:904:HIS:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1026:ASN:ND2	1:A:1029:GLY:O	2.45	0.45
1:A:1348:VAL:HG11	3:C:921:LEU:HD21	1.98	0.45
5:E:232:ARG:O	5:E:262:TRP:CH2	2.69	0.45
21:1:744:ALA:O	21:1:787:ILE:HG21	2.16	0.45
21:1:1165:TYR:HE1	22:2:575:PHE:CG	2.33	0.45
23:3:58:VAL:HG12	23:3:1155:LEU:HD23	1.98	0.45
23:3:233:ASN:ND2	23:3:286:ILE:HD12	2.31	0.45
23:3:462:VAL:HG21	23:3:508:CYS:HB3	1.98	0.45
23:3:1012:VAL:HA	23:3:1022:ILE:O	2.17	0.45
38:R:65:PRO:HA	39:S:93:THR:O	2.16	0.45
1:A:303:ILE:HG23	3:C:933:PHE:CE1	2.50	0.45
1:A:671:THR:OG1	13:F:69:A:OP1	2.34	0.45
1:A:1084:PRO:HB3	1:A:1101:PHE:CE1	2.51	0.45
3:C:136:GLY:HA3	3:C:228:PHE:O	2.16	0.45
3:C:301:SER:C	3:C:303:LEU:N	2.68	0.45
3:C:499:GLY:C	3:C:500:THR:HG23	2.36	0.45
3:C:753:GLU:C	3:C:755:ASP:H	2.19	0.45
13:F:57:U:C2	13:F:58:G:N7	2.84	0.45
14:G:10:U:O2'	14:G:11:A:OP1	2.28	0.45
21:1:701:VAL:O	21:1:705:SER:HB3	2.16	0.45
23:3:536:TRP:CG	23:3:566:PHE:HZ	2.33	0.45
23:3:700:LYS:NZ	23:3:740:GLU:O	2.41	0.45
23:3:701:LEU:HA	23:3:713:LEU:O	2.16	0.45
39:S:39:PHE:CD1	39:S:129:PHE:CE2	2.88	0.45
39:S:82:PHE:H	39:S:108:ASN:H	1.64	0.45
41:U:1:MET:O	41:U:3:ASN:N	2.48	0.45
1:A:359:ILE:O	1:A:360:SER:HB3	2.16	0.45
1:A:907:PRO:CD	37:P:229:LYS:HB2	2.39	0.45
1:A:1301:ILE:CD1	1:A:1306:LYS:HE2	2.41	0.45
1:A:1957:ASP:HB3	1:A:1960:THR:HG23	1.98	0.45
3:C:336:TYR:CD1	3:C:336:TYR:C	2.89	0.45
5:E:146:ARG:NH1	5:E:148:LYS:NZ	2.62	0.45
15:H:60:U:H2'	15:H:61:C:H6	1.81	0.45
21:1:1074:ARG:HD2	21:1:1111:CYS:SG	2.55	0.45
23:3:169:HIS:CD2	23:3:170:VAL:H	2.34	0.45
23:3:526:HIS:HB3	23:3:534:ASN:O	2.17	0.45
23:3:544:ILE:HD11	23:3:556:ILE:HG21	1.98	0.45
23:3:805:ASN:O	23:3:856:LYS:HB3	2.16	0.45
31:K:188:LEU:C	31:K:188:LEU:HD13	2.36	0.45
37:P:227:TYR:N	37:P:227:TYR:HD1	2.14	0.45
40:T:306:CYS:SG	40:T:336:VAL:HG12	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:W:426:PHE:HA	43:W:433:PHE:HA	1.99	0.45
1:A:331:TRP:C	1:A:331:TRP:CE3	2.90	0.45
1:A:374:ASP:O	1:A:375:ASP:HB3	2.16	0.45
1:A:434:HIS:C	1:A:434:HIS:HD1	2.19	0.45
1:A:592:TYR:CE1	14:G:-5:G:H4'	2.51	0.45
1:A:651:TRP:CD1	13:F:66:C:C1'	2.98	0.45
1:A:1434:LYS:O	1:A:1439:ARG:NH1	2.45	0.45
3:C:193:THR:HG22	3:C:428:THR:HG21	1.97	0.45
3:C:482:TYR:CE2	3:C:493:PHE:CG	2.89	0.45
5:E:119:THR:CG2	5:E:161:ARG:CB	2.73	0.45
5:E:157:CYS:HA	5:E:168:CYS:O	2.16	0.45
15:H:181:G:C2	15:H:182:U:N3	2.84	0.45
21:1:427:PRO:O	21:1:431:LEU:N	2.45	0.45
21:1:834:VAL:O	21:1:838:VAL:HG23	2.16	0.45
21:1:1181:ASP:OD1	21:1:1182:LEU:N	2.46	0.45
23:3:257:THR:OG1	23:3:268:ARG:HG2	2.16	0.45
23:3:482:THR:HG21	23:3:505:THR:OG1	2.17	0.45
23:3:897:SER:HB2	23:3:957:GLY:HA3	1.97	0.45
23:3:905:VAL:HG23	23:3:930:LEU:HB2	1.98	0.45
27:7:73:LEU:HD12	27:7:74:GLN:N	2.32	0.45
32:I:712:VAL:O	32:I:715:GLY:N	2.49	0.45
35:N:47:TRP:HB2	35:N:48:PRO:HD3	1.99	0.45
35:N:125:LYS:HD2	43:W:167:VAL:O	2.17	0.45
36:O:234:LEU:HB2	36:O:272:ILE:HB	1.98	0.45
37:P:193:VAL:CG2	37:P:194:PHE:N	2.79	0.45
38:R:88:ILE:HD12	38:R:88:ILE:N	2.29	0.45
38:R:181:PRO:O	38:R:182:SER:CB	2.58	0.45
1:A:259:ASP:C	1:A:259:ASP:OD1	2.55	0.45
1:A:535:ARG:NH1	14:G:2:U:OP2	2.50	0.45
1:A:658:ARG:N	37:P:29:GLN:OE1	2.49	0.45
1:A:966:TRP:HE3	1:A:1178:TYR:CZ	2.35	0.45
1:A:1426:ASP:OD2	38:R:421:GLY:CA	2.64	0.45
1:A:1809:ILE:HB	1:A:1818:PHE:HB2	1.97	0.45
1:A:1900:GLU:OE2	46:Z:521:PRO:CA	2.64	0.45
3:C:183:SER:OG	3:C:480:LYS:NZ	2.50	0.45
3:C:230:ASP:CG	3:C:259:LYS:HZ1	2.19	0.45
5:E:243:LEU:CD1	5:E:247:GLY:CA	2.84	0.45
14:G:26:U:C2'	36:O:269:CYS:SG	3.04	0.45
15:H:25:G:C2	15:H:26:A:C5	3.04	0.45
15:H:150:U:H3	15:H:181:G:H1	1.62	0.45
15:H:152:G:O2'	15:H:153:A:H1'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:796:ASN:HA	23:3:871:PRO:HD3	1.98	0.45
28:J:360:ASP:HA	28:J:363:ARG:CD	2.46	0.45
29:L:789:ALA:O	29:L:792:LEU:CG	2.64	0.45
39:S:34:LYS:HG3	39:S:78:TYR:CE2	2.52	0.45
40:T:409:LEU:HD12	40:T:409:LEU:N	2.31	0.45
43:W:266:ARG:O	43:W:267:SER:O	2.35	0.45
1:A:61:MET:HB3	1:A:62:PRO:HD2	1.98	0.45
1:A:730:GLY:O	1:A:731:LEU:HB2	2.16	0.45
1:A:1413:ASP:OD1	1:A:1414:ARG:HG3	2.17	0.45
1:A:1604:LEU:HD11	1:A:1725:LEU:HD22	1.98	0.45
1:A:2169:LEU:HD21	1:A:2272:MET:HG3	1.99	0.45
1:A:2303:GLU:CD	1:A:2303:GLU:H	2.19	0.45
3:C:66:TYR:CB	40:T:456:PRO:O	2.51	0.45
3:C:495:ARG:HG3	3:C:495:ARG:O	2.16	0.45
3:C:497:LEU:CD1	3:C:577:PHE:CE1	2.94	0.45
3:C:852:ARG:NH2	14:G:-12:G:OP1	2.50	0.45
4:D:1349:GLY:HA2	4:D:1491:SER:O	2.16	0.45
5:E:260:ARG:CD	5:E:276:ILE:HG12	2.47	0.45
13:F:94:C:H2'	13:F:95:G:H8	1.82	0.45
14:G:-12:G:HO2'	14:G:-11:G:C5'	2.29	0.45
23:3:115:ILE:HD11	27:7:18:TYR:CE1	2.51	0.45
38:R:179:TYR:CE2	38:R:181:PRO:HG3	2.52	0.45
40:T:297:HIS:CD2	40:T:338:CYS:SG	3.09	0.45
43:W:516:PHE:HA	43:W:522:TYR:O	2.16	0.45
46:Z:525:TYR:CE1	46:Z:526:ILE:CG2	2.86	0.45
1:A:317:PRO:HB2	1:A:327:VAL:HG11	1.98	0.45
1:A:536:LYS:HD3	13:F:72:G:O2'	2.16	0.45
1:A:1768:TYR:HE1	1:A:1930:TYR:CE1	2.34	0.45
2:B:57:G:H2'	2:B:58:U:H5'	1.99	0.45
3:C:926:ALA:N	3:C:927:PRO:HD2	2.32	0.45
5:E:178:LEU:HG	5:E:188:GLN:HB2	1.98	0.45
5:E:277:PHE:CD1	5:E:277:PHE:N	2.83	0.45
13:F:22:A:P	35:N:115:THR:OG1	2.74	0.45
21:1:86:ALA:O	21:1:89:ALA:HB3	2.17	0.45
21:1:476:ASP:OD1	21:1:477:LYS:N	2.49	0.45
21:1:1110:VAL:O	21:1:1113:THR:HB	2.17	0.45
21:1:1251:LEU:HD12	22:2:497:SER:OG	2.16	0.45
23:3:223:LYS:HE2	23:3:224:TYR:CZ	2.52	0.45
23:3:429:ARG:HH12	27:7:59:GLU:H	1.65	0.45
23:3:1114:SER:HB2	23:3:1215:TYR:CE1	2.51	0.45
28:J:338:GLU:O	38:R:116:TYR:CE1	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:O:225:PRO:HB3	36:O:302:TRP:CZ2	2.51	0.45
38:R:128:ASP:OD2	38:R:133:GLN:OE1	2.34	0.45
40:T:393:ASP:O	40:T:413:ASN:ND2	2.49	0.45
46:Z:564:PRO:O	46:Z:582:TYR:CG	2.69	0.45
46:Z:600:ARG:CG	46:Z:600:ARG:NH1	2.73	0.45
1:A:76:MET:SD	1:A:88:TYR:CE2	3.10	0.45
1:A:402:ILE:HG22	3:C:268:LYS:HZ1	1.77	0.45
1:A:755:HIS:CG	37:P:219:PHE:HE2	2.35	0.45
1:A:833:LYS:HG3	1:A:834:HIS:CD2	2.52	0.45
1:A:975:VAL:HG11	1:A:1153:VAL:HG21	1.98	0.45
1:A:1342:TRP:CE3	3:C:921:LEU:CG	3.00	0.45
1:A:1963:GLU:HB2	1:A:1966:HIS:HD2	1.81	0.45
2:B:22:U:O2	2:B:22:U:H2'	2.15	0.45
3:C:144:CYS:SG	3:C:148:CYS:SG	3.15	0.45
13:F:38:G:OP2	13:F:38:G:C8	2.70	0.45
14:G:6:A:H2'	14:G:7:G:H8	1.82	0.45
21:1:501:LEU:O	21:1:504:ILE:N	2.48	0.45
21:1:592:GLU:O	21:1:596:ILE:HG23	2.16	0.45
21:1:629:ALA:HA	21:1:667:ILE:HG12	1.99	0.45
23:3:383:ASP:OD1	23:3:384:THR:N	2.50	0.45
23:3:1057:ARG:HB2	23:3:1092:ILE:HD13	1.98	0.45
38:R:82:MET:C	38:R:82:MET:CE	2.86	0.45
43:W:466:ALA:HB2	43:W:512:CYS:O	2.17	0.45
45:Y:41:GLY:HA2	45:Y:79:PHE:HB3	1.99	0.45
1:A:733:THR:OG1	1:A:734:PRO:HD3	2.16	0.45
1:A:1013:ASN:OD1	1:A:1030:ILE:HG13	2.16	0.45
1:A:1125:ILE:HG22	1:A:1147:VAL:HG21	1.99	0.45
1:A:1904:ASP:O	1:A:1908:LYS:HG2	2.16	0.45
1:A:1949:ARG:HA	1:A:1952:VAL:HG23	1.98	0.45
1:A:2074:ARG:O	1:A:2078:ILE:HD13	2.17	0.45
2:B:40:U:OP2	2:B:40:U:C6	2.70	0.45
3:C:137:HIS:HD2	3:C:236:MET:HB2	1.61	0.45
3:C:191:PRO:HG2	3:C:426:GLU:OE1	2.17	0.45
3:C:445:ALA:HB1	3:C:449:ILE:CG1	2.45	0.45
5:E:162:ARG:HH21	5:E:204:THR:HA	1.78	0.45
13:F:51:U:H2'	13:F:52:U:O4'	2.17	0.45
14:G:20:A:OP2	36:O:159:ARG:HG3	2.16	0.45
21:1:552:LEU:HA	21:1:555:VAL:HG12	1.98	0.45
21:1:822:ARG:NH1	45:Y:31:GLU:HG2	2.32	0.45
21:1:897:LEU:O	21:1:901:GLN:HG3	2.17	0.45
21:1:1186:GLN:NE2	21:1:1225:HIS:HB3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:643:VAL:HG12	23:3:664:TYR:O	2.17	0.45
25:5:48:ILE:HG12	25:5:62:VAL:HG23	1.99	0.45
28:J:406:PHE:CB	28:J:411:MET:HG2	2.47	0.45
36:O:205:ILE:O	36:O:207:ASP:N	2.50	0.45
36:O:259:ARG:HD2	36:O:273:GLN:HG2	1.99	0.45
40:T:342:GLU:CB	40:T:343:PRO:HD2	2.47	0.45
40:T:454:VAL:HG22	40:T:463:SER:OG	2.16	0.45
40:T:455:GLN:CG	40:T:456:PRO:CD	2.94	0.45
1:A:44:ARG:CD	1:A:45:TYR:CE2	2.99	0.45
1:A:845:ARG:NH2	1:A:1439:ARG:HE	2.15	0.45
1:A:1258:LYS:HE2	38:R:432:GLU:CB	2.47	0.45
1:A:1780:VAL:HG22	1:A:1809:ILE:HG12	1.99	0.45
3:C:65:TYR:O	3:C:66:TYR:CB	2.65	0.45
3:C:230:ASP:OD2	3:C:233:GLU:CG	2.55	0.45
3:C:502:HIS:ND1	3:C:543:ARG:HB3	2.32	0.45
3:C:926:ALA:HA	3:C:929:LEU:HG	1.98	0.45
13:F:50:A:H2'	13:F:51:U:H6	1.82	0.45
14:G:6:A:H2'	14:G:7:G:C8	2.52	0.45
14:G:12:G:N3	14:G:12:G:C2'	2.79	0.45
14:G:157:U:H5'	21:1:622:GLU:OE1	2.17	0.45
15:H:113:G:H2'	15:H:114:A:H8	1.82	0.45
21:1:1002:ASN:OD1	21:1:1041:ARG:NH2	2.50	0.45
22:2:611:ASP:O	22:2:614:ARG:CB	2.60	0.45
23:3:462:VAL:O	23:3:472:ALA:N	2.46	0.45
23:3:509:SER:OG	23:3:517:VAL:O	2.20	0.45
23:3:883:GLU:HG3	23:3:884:GLN:N	2.32	0.45
23:3:1051:GLY:HA2	23:3:1100:THR:HA	1.99	0.45
25:5:26:LEU:HD12	25:5:87:LEU:HD22	1.98	0.45
27:7:31:TRP:HE3	27:7:32:LEU:HD12	1.82	0.45
29:L:226:ASP:OD1	38:R:83:SER:HB2	2.16	0.45
32:I:433:ALA:O	32:I:437:CYS:N	2.50	0.45
35:N:91:LYS:HD3	35:N:91:LYS:HA	1.81	0.45
36:O:197:ASN:O	36:O:201:ARG:HG3	2.17	0.45
38:R:88:ILE:HG21	38:R:96:ILE:CG2	2.46	0.45
38:R:89:GLN:OE1	39:S:145:VAL:HG13	2.17	0.45
38:R:408:GLU:CG	38:R:409:VAL:N	2.78	0.45
44:X:336:GLY:HA3	44:X:378:GLU:HB2	1.99	0.45
46:Z:524:ARG:HD2	46:Z:525:TYR:CB	2.46	0.45
1:A:1348:VAL:HG11	3:C:921:LEU:CD2	2.47	0.44
3:C:93:ILE:CG2	40:T:218:TRP:NE1	2.80	0.44
5:E:276:ILE:O	5:E:277:PHE:HD1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:F:68:C:C5	37:P:33:ARG:HG2	2.52	0.44
13:F:94:C:H2'	13:F:95:G:C8	2.52	0.44
15:H:7:U:H2'	15:H:8:C:C6	2.52	0.44
15:H:81:G:N3	15:H:82:G:C8	2.85	0.44
15:H:141:C:H2'	15:H:142:C:C6	2.50	0.44
21:1:810:ILE:O	21:1:813:PRO:HD2	2.17	0.44
23:3:460:TRP:CE2	23:3:507:SER:HA	2.52	0.44
23:3:723:TYR:CD1	23:3:725:TYR:HB2	2.53	0.44
23:3:1140:PHE:O	23:3:1144:VAL:HG23	2.17	0.44
36:O:56:ARG:HG2	36:O:67:LYS:HB3	1.99	0.44
36:O:131:THR:O	36:O:132:ARG:HB2	2.17	0.44
36:O:294:ASN:O	36:O:296:ARG:HG3	2.17	0.44
38:R:147:THR:HG23	40:T:360:VAL:CG1	2.40	0.44
38:R:416:PHE:O	38:R:416:PHE:CG	2.70	0.44
42:V:548:ALA:HB2	42:V:585:ILE:CB	2.42	0.44
1:A:280:GLU:OE1	41:U:9:THR:HG21	2.17	0.44
1:A:1088:PHE:HD1	1:A:1097:ILE:HG12	1.82	0.44
1:A:1430:LEU:HD11	38:R:422:MET:HA	1.98	0.44
1:A:1591:MET:SD	1:A:1611:LYS:NZ	2.75	0.44
1:A:1788:VAL:HA	1:A:1802:PRO:HA	1.98	0.44
1:A:2196:HIS:HB3	1:A:2230:LEU:HD11	1.98	0.44
1:A:2222:SER:OG	1:A:2223:CYS:N	2.50	0.44
1:A:2334:TYR:CE1	4:D:591:GLU:CB	3.00	0.44
2:B:44:A:OP1	13:F:66:C:N4	2.30	0.44
3:C:93:ILE:CG2	40:T:218:TRP:CZ2	3.00	0.44
3:C:388:VAL:HA	3:C:392:LEU:HB2	1.99	0.44
5:E:132:THR:HG21	5:E:146:ARG:HG2	1.98	0.44
13:F:58:G:O2'	13:F:59:G:OP1	2.31	0.44
15:H:143:A:OP2	15:H:143:A:C2	2.71	0.44
15:H:157:G:H5"	15:H:157:G:C8	2.50	0.44
21:1:762:ALA:O	21:1:766:THR:CB	2.64	0.44
21:1:1252:GLN:NE2	22:2:492:LYS:O	2.51	0.44
22:2:613:LEU:HD21	24:4:32:LEU:HD13	1.99	0.44
23:3:404:LEU:HB3	23:3:407:ILE:HD11	1.99	0.44
23:3:536:TRP:CD1	23:3:566:PHE:HZ	2.35	0.44
23:3:607:VAL:HB	23:3:615:ARG:O	2.17	0.44
23:3:1159:ASP:OD1	23:3:1160:HIS:N	2.49	0.44
28:J:297:ASN:OD1	29:L:223:GLY:O	2.34	0.44
29:L:213:GLU:CB	36:O:110:SER:HB3	2.47	0.44
36:O:230:THR:H	36:O:277:ARG:NH1	2.15	0.44
39:S:38:ASN:HD22	39:S:100:MET:CE	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:LEU:HD12	1:A:194:GLU:N	2.29	0.44
1:A:380:LEU:HD22	3:C:354:ARG:C	2.21	0.44
1:A:380:LEU:CD2	3:C:354:ARG:C	2.84	0.44
1:A:1136:ARG:CZ	1:A:1139:ARG:HH21	2.30	0.44
1:A:1136:ARG:NE	1:A:1139:ARG:HH21	2.16	0.44
1:A:1459:ARG:HD3	1:A:1459:ARG:HA	1.75	0.44
1:A:1785:VAL:O	1:A:1805:GLY:HA3	2.17	0.44
1:A:2328:ALA:CB	4:D:788:GLY:N	2.79	0.44
2:B:63:A:H5"	5:E:106:LYS:NZ	2.32	0.44
3:C:140:HIS:HB3	3:C:230:ASP:CB	2.43	0.44
3:C:671:SER:CB	3:C:672:LEU:HD22	2.46	0.44
4:D:721:VAL:HA	4:D:825:THR:O	2.17	0.44
5:E:209:ILE:HG21	5:E:250:LEU:HD11	1.94	0.44
13:F:39:A:H2'	13:F:40:U:C6	2.52	0.44
14:G:20:A:OP2	36:O:159:ARG:CG	2.64	0.44
21:1:529:GLY:HA2	21:1:570:TYR:CZ	2.51	0.44
23:3:205:GLN:HB2	23:3:228:LEU:O	2.17	0.44
23:3:747:SER:N	23:3:750:CYS:O	2.51	0.44
25:5:98:PHE:O	25:5:100:LYS:N	2.50	0.44
36:O:33:TYR:OH	43:W:139:LEU:O	2.30	0.44
37:P:188:TRP:N	37:P:188:TRP:CD2	2.86	0.44
38:R:416:PHE:O	38:R:416:PHE:CD1	2.70	0.44
40:T:387:PHE:CZ	40:T:398:TRP:CD1	3.04	0.44
46:Z:500:GLY:O	46:Z:503:GLN:N	2.50	0.44
46:Z:573:PRO:O	46:Z:573:PRO:CD	2.65	0.44
46:Z:597:ARG:CZ	46:Z:601:LEU:HD13	2.47	0.44
1:A:121:HIS:CA	1:A:481:PHE:O	2.66	0.44
1:A:394:TYR:CD1	1:A:394:TYR:N	2.86	0.44
1:A:532:THR:OG1	14:G:2:U:H3'	2.17	0.44
1:A:661:GLU:HA	38:R:213:LYS:HA	2.00	0.44
1:A:777:GLY:O	1:A:780:THR:OG1	2.25	0.44
1:A:1074:PHE:HB3	1:A:1079:THR:OG1	2.17	0.44
1:A:1354:ARG:NH1	41:U:7:LEU:HD21	2.32	0.44
1:A:1631:LEU:HD12	1:A:1660:TYR:CD2	2.51	0.44
13:F:5:U:H5'	13:F:6:C:OP2	2.17	0.44
15:H:159:U:H2'	15:H:160:A:C8	2.52	0.44
15:H:165:A:C6	15:H:166:G:O6	2.71	0.44
21:1:937:LEU:O	21:1:940:LEU:HB3	2.18	0.44
22:2:611:ASP:O	22:2:614:ARG:N	2.50	0.44
23:3:1063:ASN:H	23:3:1087:GLN:HE22	1.65	0.44
23:3:1096:HIS:NE2	23:3:1098:GLY:HA2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:P:189:ASP:C	37:P:191:ASP:N	2.68	0.44
40:T:439:TRP:CE3	40:T:446:ASN:HB2	2.52	0.44
45:Y:36:ALA:CB	46:Z:499:LYS:O	2.54	0.44
1:A:141:ILE:HG12	1:A:426:LEU:HD23	1.99	0.44
1:A:507:LEU:HD12	1:A:507:LEU:HA	1.79	0.44
1:A:1402:ARG:HD2	38:R:412:ASP:HA	1.98	0.44
1:A:1533:ARG:HD2	1:A:1751:LEU:O	2.18	0.44
1:A:1553:VAL:O	1:A:1561:PHE:HA	2.18	0.44
1:A:1957:ASP:O	1:A:1960:THR:OG1	2.19	0.44
1:A:2073:TRP:CZ3	1:A:2313:HIS:CE1	3.05	0.44
3:C:135:CYS:SG	3:C:227:LEU:CB	3.06	0.44
3:C:259:LYS:HD2	51:C:1500:GTP:C5	2.52	0.44
3:C:673:LYS:HG3	3:C:686:THR:HG23	2.00	0.44
14:G:21:A:O3'	14:G:22:C:C6	2.71	0.44
15:H:60:U:H2'	15:H:61:C:C6	2.52	0.44
21:1:1211:LEU:O	21:1:1215:VAL:HG23	2.17	0.44
23:3:442:LEU:HD11	23:3:732:THR:OG1	2.17	0.44
23:3:636:GLN:O	23:3:670:GLN:HG2	2.17	0.44
26:6:58:CYS:N	26:6:63:GLY:O	2.46	0.44
36:O:258:ILE:HG22	36:O:260:THR:N	2.32	0.44
45:Y:58:GLN:HB2	46:Z:584:TRP:NE1	2.33	0.44
1:A:79:ARG:HD2	1:A:79:ARG:O	2.18	0.44
1:A:305:ARG:NH2	3:C:854:ARG:HD3	2.32	0.44
1:A:611:LEU:HA	1:A:611:LEU:HD12	1.85	0.44
1:A:707:ARG:O	1:A:711:GLN:HG3	2.17	0.44
1:A:978:GLU:OE2	1:A:1188:ASN:N	2.36	0.44
1:A:1134:TRP:CZ2	1:A:1195:ARG:HB2	2.53	0.44
1:A:1407:ASP:OD1	1:A:1407:ASP:N	2.51	0.44
1:A:1667:ARG:HD2	1:A:1679:TYR:CD2	2.52	0.44
1:A:2125:ALA:O	1:A:2150:GLN:NE2	2.50	0.44
1:A:2237:TRP:HZ2	1:A:2248:PRO:HB2	1.81	0.44
3:C:457:VAL:CG1	3:C:462:GLY:HA3	2.46	0.44
15:H:34:U:C4	15:H:35:A:N7	2.85	0.44
15:H:73:C:O5'	15:H:73:C:H6	2.01	0.44
15:H:142:C:O2'	15:H:143:A:H5'	2.18	0.44
15:H:147:G:C6	15:H:148:C:N4	2.86	0.44
21:1:1108:ASN:OD1	21:1:1110:VAL:HG12	2.17	0.44
22:2:569:GLN:CB	43:W:460:SER:CB	2.95	0.44
23:3:812:LYS:O	23:3:816:LYS:CB	2.57	0.44
36:O:68:THR:HA	36:O:83:THR:CG2	2.45	0.44
37:P:193:VAL:HG23	37:P:194:PHE:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:S:9:TRP:HE3	39:S:11:PRO:CG	2.29	0.44
45:Y:63:VAL:HG23	45:Y:64:ASN:N	2.33	0.44
1:A:67:ARG:HE	1:A:67:ARG:HB2	1.58	0.44
1:A:193:LEU:HB3	1:A:208:TYR:OH	2.17	0.44
1:A:373:ASP:OD1	1:A:374:ASP:N	2.51	0.44
1:A:460:LYS:NZ	2:B:49:A:P	2.91	0.44
1:A:1362:ASP:OD1	1:A:1362:ASP:N	2.51	0.44
1:A:1674:HIS:HB3	1:A:1709:TYR:CE2	2.53	0.44
1:A:2121:ARG:HA	1:A:2121:ARG:HD2	1.55	0.44
3:C:145:PHE:HD1	3:C:312:SER:HB3	1.83	0.44
5:E:266:PRO:CG	29:L:785:GLN:HB3	2.48	0.44
13:F:9:U:H2'	13:F:10:U:C6	2.52	0.44
13:F:68:C:C5	37:P:33:ARG:CG	2.95	0.44
15:H:26:A:C6	15:H:27:U:C4	3.05	0.44
21:1:1072:ALA:O	21:1:1075:ARG:HB3	2.18	0.44
23:3:929:LYS:HD3	23:3:938:GLU:OE2	2.17	0.44
29:L:224:PHE:CE1	38:R:86:LEU:HD12	2.43	0.44
40:T:342:GLU:O	40:T:343:PRO:C	2.56	0.44
42:V:525:PHE:O	42:V:526:GLU:C	2.55	0.44
43:W:476:LEU:O	43:W:487:ILE:HA	2.16	0.44
46:Z:584:TRP:CZ3	46:Z:586:GLY:HA2	2.53	0.44
1:A:148:TRP:HE3	1:A:629:PHE:CD1	2.35	0.44
1:A:402:ILE:HG21	3:C:268:LYS:HZ2	1.47	0.44
1:A:1034:LEU:HB2	1:A:1037:ALA:HB2	1.98	0.44
1:A:1457:HIS:CE1	38:R:424:SER:C	2.90	0.44
1:A:1555:LEU:HD12	1:A:1560:ILE:HB	2.00	0.44
1:A:1557:LEU:HD13	1:A:1580:HIS:CE1	2.53	0.44
1:A:2280:ASN:HB3	1:A:2309:HIS:CD2	2.53	0.44
14:G:21:A:P	36:O:156:TYR:HH	2.35	0.44
14:G:26:U:H5'	36:O:235:TYR:OH	2.18	0.44
21:1:601:ALA:HB2	21:1:635:VAL:HG12	2.00	0.44
21:1:969:LYS:O	21:1:973:HIS:ND1	2.36	0.44
23:3:353:PHE:CD1	23:3:406:PRO:HD3	2.53	0.44
23:3:607:VAL:HG21	23:3:617:ILE:HD12	1.99	0.44
23:3:930:LEU:HG	23:3:934:GLY:HA2	1.98	0.44
24:4:79:LEU:HG	24:4:84:ILE:HG13	2.00	0.44
37:P:66:ARG:HB2	37:P:66:ARG:NH1	2.30	0.44
38:R:124:VAL:HG22	38:R:125:MET:H	1.83	0.44
38:R:132:LEU:HD23	38:R:132:LEU:N	2.31	0.44
38:R:208:GLU:OE2	38:R:211:ARG:NH1	2.51	0.44
38:R:415:LEU:H	38:R:415:LEU:HG	1.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:T:358:ASP:HB2	40:T:365:ARG:HD2	2.00	0.44
46:Z:524:ARG:CD	46:Z:524:ARG:C	2.85	0.44
1:A:82:ARG:NH1	14:G:16:G:O6	2.49	0.44
1:A:106:MET:HG2	1:A:489:TRP:CZ2	2.53	0.44
1:A:300:ASN:O	3:C:936:LYS:CB	2.66	0.44
1:A:382:GLU:O	1:A:383:PHE:CD2	2.70	0.44
1:A:941:LYS:HE3	1:A:951:LEU:HD21	2.00	0.44
1:A:1038:SER:HA	1:A:1442:PHE:HE2	1.83	0.44
1:A:1900:GLU:CG	46:Z:521:PRO:HG3	2.39	0.44
3:C:439:PRO:O	3:C:440:SER:CB	2.66	0.44
3:C:465:MET:HE1	3:C:475:MET:CE	2.47	0.44
3:C:779:LEU:HD11	3:C:825:PRO:HB2	1.99	0.44
14:G:-8:U:C2	41:U:15:THR:O	2.71	0.44
14:G:11:A:C5	14:G:12:G:C8	3.06	0.44
14:G:21:A:O3'	14:G:22:C:H6	2.00	0.44
15:H:6:U:H2'	15:H:7:U:C6	2.53	0.44
21:1:503:LYS:HD2	21:1:515:ALA:HB2	2.00	0.44
21:1:779:SER:HB3	21:1:784:MET:HG2	2.00	0.44
21:1:1131:ALA:O	21:1:1135:GLU:HG2	2.17	0.44
23:3:411:GLN:HA	23:3:1105:GLN:OE1	2.18	0.44
23:3:798:ILE:HA	23:3:867:ARG:O	2.18	0.44
25:5:46:ARG:N	25:5:63:VAL:O	2.50	0.44
35:N:125:LYS:HA	35:N:125:LYS:HD3	1.74	0.44
36:O:28:LEU:CD2	38:R:195:ARG:HE	2.29	0.44
39:S:81:GLN:HB3	39:S:108:ASN:H	1.82	0.44
43:W:420:ALA:HB3	43:W:438:ASP:CB	2.48	0.44
1:A:44:ARG:HG2	1:A:45:TYR:CD2	2.53	0.43
1:A:330:THR:O	1:A:331:TRP:HB2	2.17	0.43
1:A:402:ILE:HD13	3:C:268:LYS:CE	2.47	0.43
1:A:1306:LYS:HZ1	2:B:38:C:H2'	1.83	0.43
1:A:2073:TRP:CH2	1:A:2313:HIS:CG	3.06	0.43
3:C:229:ILE:CG2	3:C:234:GLY:O	2.66	0.43
5:E:248:SER:HB2	5:E:249:TYR:CE1	2.53	0.43
13:F:35:A:C8	14:G:12:G:O6	2.71	0.43
13:F:68:C:H42	40:T:283:HIS:CE1	2.35	0.43
21:1:903:GLN:HG3	21:1:950:GLN:NE2	2.33	0.43
23:3:176:GLY:O	23:3:178:GLU:HG2	2.17	0.43
23:3:446:GLU:CD	23:3:763:ARG:HD3	2.38	0.43
23:3:745:PHE:HB2	23:3:755:VAL:HG23	2.00	0.43
23:3:998:HIS:HE1	23:3:1064:ASP:OD2	2.00	0.43
23:3:1207:LYS:HA	23:3:1210:ASP:OD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:5:53:THR:O	25:5:57:ARG:HG3	2.18	0.43
28:J:339:TRP:C	38:R:116:TYR:CE2	2.92	0.43
38:R:109:ASP:OD1	38:R:110:LYS:N	2.51	0.43
40:T:454:VAL:CG1	40:T:455:GLN:N	2.81	0.43
1:A:73:HIS:HA	1:A:81:PHE:CE2	2.53	0.43
1:A:89:LEU:CD2	1:A:656:LEU:CD2	2.95	0.43
1:A:331:TRP:HE3	1:A:332:TYR:CA	2.30	0.43
1:A:664:HIS:CE1	1:A:666:LYS:HD3	2.53	0.43
1:A:694:LEU:O	1:A:698:PRO:HG3	2.18	0.43
1:A:970:GLU:HB2	1:A:972:GLU:OE2	2.17	0.43
1:A:1532:ARG:HG2	1:A:1572:SER:OG	2.18	0.43
1:A:2310:ARG:HH11	1:A:2310:ARG:HB3	1.83	0.43
3:C:135:CYS:N	3:C:226:VAL:O	2.50	0.43
3:C:392:LEU:HD12	3:C:392:LEU:O	2.18	0.43
3:C:508:LYS:O	3:C:566:THR:HG22	2.18	0.43
3:C:674:CYS:HB2	3:C:818:SER:HB3	2.00	0.43
3:C:703:GLU:OE2	3:C:740:THR:CG2	2.50	0.43
5:E:251:LEU:CG	5:E:291:CYS:SG	3.05	0.43
15:H:159:U:H2'	15:H:160:A:H8	1.83	0.43
15:H:182:U:H6	15:H:182:U:O5'	2.01	0.43
21:1:528:ALA:HB2	21:1:563:LEU:HD13	2.00	0.43
21:1:732:TRP:O	21:1:735:ILE:HB	2.19	0.43
22:2:556:LYS:O	22:2:559:PRO:HD3	2.18	0.43
23:3:409:PHE:HD2	23:3:788:PHE:CE2	2.36	0.43
23:3:484:VAL:HG21	23:3:499:PHE:HB2	1.99	0.43
23:3:791:HIS:ND1	23:3:794:SER:HB3	2.33	0.43
23:3:837:GLU:O	23:3:837:GLU:HG2	2.17	0.43
38:R:419:SER:C	38:R:420:LYS:O	2.55	0.43
1:A:908:VAL:HA	1:A:1445:TYR:O	2.18	0.43
1:A:1071:PHE:CD2	1:A:1072:LEU:HG	2.53	0.43
1:A:1544:ARG:HB3	1:A:1672:ASP:OD2	2.19	0.43
1:A:2067:PHE:HB2	1:A:2072:GLU:HG2	2.00	0.43
3:C:131:ASN:HB3	3:C:549:TRP:CZ2	2.52	0.43
3:C:524:ILE:O	3:C:525:CYS:SG	2.74	0.43
15:H:64:A:H2'	15:H:65:U:C6	2.53	0.43
15:H:153:A:H2'	15:H:154:C:H5"	1.99	0.43
21:1:840:LEU:O	21:1:844:VAL:HG12	2.19	0.43
22:2:482:ALA:O	22:2:485:PRO:HD3	2.18	0.43
23:3:88:VAL:HA	23:3:103:HIS:O	2.18	0.43
23:3:458:ALA:C	23:3:757:ILE:HG12	2.39	0.43
23:3:511:LEU:HB2	23:3:517:VAL:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:1056:VAL:HG22	23:3:1091:VAL:HG22	2.01	0.43
24:4:67:ALA:HA	24:4:70:ALA:HB3	2.00	0.43
31:K:134:ALA:O	31:K:137:VAL:HG12	2.17	0.43
36:O:27:CYS:O	36:O:28:LEU:C	2.56	0.43
38:R:88:ILE:HG22	38:R:96:ILE:CG2	2.49	0.43
40:T:406:ILE:HG22	40:T:407:GLN:N	2.33	0.43
43:W:309:MET:HA	43:W:334:ALA:HB1	2.00	0.43
1:A:167:PRO:CD	34:M:192:THR:HB	2.38	0.43
1:A:338:VAL:CB	3:C:867:PRO:CG	2.96	0.43
1:A:406:TRP:CH2	3:C:265:LEU:O	2.64	0.43
1:A:741:ARG:NH2	40:T:432:ASP:O	2.41	0.43
1:A:1263:TRP:CE3	1:A:1295:ILE:HD13	2.53	0.43
2:B:99:C:H2'	2:B:100:C:C6	2.53	0.43
3:C:133:THR:CB	3:C:225:VAL:HG23	2.43	0.43
3:C:297:ASN:HD22	3:C:298:LEU:HD12	1.83	0.43
3:C:350:ASN:HB3	3:C:353:THR:CG2	2.49	0.43
3:C:505:GLN:HG2	3:C:506:PRO:HD2	2.00	0.43
3:C:776:GLU:O	3:C:781:ASP:HA	2.18	0.43
13:F:42:C:H2'	13:F:43:A:C8	2.53	0.43
21:1:885:ASP:OD1	21:1:888:LEU:HB3	2.18	0.43
21:1:1119:VAL:O	21:1:1122:THR:HG22	2.17	0.43
21:1:1120:ALA:HB1	21:1:1125:PRO:HB3	2.01	0.43
21:1:1179:ASP:HB3	22:2:511:LEU:HD12	2.00	0.43
22:2:630:PRO:HA	22:2:631:PRO:HD3	1.77	0.43
23:3:136:GLU:OE2	23:3:189:TYR:OH	2.10	0.43
29:L:63:TRP:CH2	29:L:99:HIS:HB2	2.54	0.43
29:L:101:GLU:O	29:L:105:ASP:HB2	2.18	0.43
36:O:90:TYR:HB3	36:O:92:LEU:HD12	1.98	0.43
38:R:54:LEU:HD12	38:R:54:LEU:HA	1.86	0.43
38:R:55:LEU:C	38:R:73:PRO:O	2.56	0.43
40:T:399:LYS:HG3	40:T:406:ILE:CD1	2.37	0.43
45:Y:36:ALA:HB3	46:Z:498:GLY:O	2.18	0.43
1:A:459:LEU:HD12	1:A:459:LEU:HA	1.75	0.43
3:C:145:PHE:N	3:C:312:SER:OG	2.50	0.43
3:C:736:GLY:HA3	3:C:770:PHE:CE2	2.53	0.43
5:E:67:GLY:N	5:E:87:ASP:OD1	2.42	0.43
14:G:-5:G:O2'	14:G:-4:A:H5"	2.18	0.43
15:H:83:A:C4	15:H:84:C:C6	3.07	0.43
15:H:98:G:H5'	15:H:104:U:OP2	2.18	0.43
15:H:154:C:O2'	15:H:155:C:C5'	2.66	0.43
15:H:181:G:C2	15:H:182:U:C4	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:897:LEU:HD21	21:1:932:ILE:HD13	2.00	0.43
21:1:1235:GLU:O	21:1:1238:ARG:HB3	2.18	0.43
23:3:139:LYS:HB2	23:3:160:ALA:HB3	2.00	0.43
23:3:868:VAL:HG12	23:3:877:LEU:HB2	1.99	0.43
36:O:58:CYS:HB2	36:O:65:PHE:CE1	2.52	0.43
36:O:230:THR:H	36:O:277:ARG:CZ	2.32	0.43
38:R:126:ASN:HD22	38:R:128:ASP:H	1.66	0.43
45:Y:29:HIS:CG	45:Y:91:ILE:HG23	2.53	0.43
1:A:648:LEU:HA	1:A:648:LEU:HD23	1.79	0.43
1:A:1382:SER:HB3	1:A:1416:ILE:HG12	2.00	0.43
1:A:1771:LEU:HD12	1:A:1777:ILE:HD13	2.00	0.43
1:A:2284:MET:HE1	1:A:2311:PRO:HG3	2.01	0.43
2:B:27:U:HO2'	2:B:28:A:P	2.41	0.43
3:C:60:HIS:ND1	3:C:60:HIS:O	2.51	0.43
13:F:36:A:C3'	13:F:36:A:C8	3.01	0.43
15:H:157:G:H2'	15:H:158:G:O4'	2.19	0.43
21:1:889:GLU:HA	21:1:892:LEU:HD12	2.00	0.43
22:2:613:LEU:HD11	24:4:32:LEU:HD13	1.99	0.43
23:3:32:VAL:HG23	23:3:39:GLU:HB3	1.99	0.43
25:5:114:LYS:HA	25:5:119:ILE:O	2.19	0.43
29:L:73:HIS:CD2	29:L:77:LEU:HD11	2.53	0.43
36:O:45:CYS:SG	36:O:48:CYS:N	2.92	0.43
36:O:45:CYS:O	36:O:49:ALA:HA	2.18	0.43
36:O:147:LEU:HD12	36:O:148:LEU:N	2.34	0.43
38:R:52:PRO:HB3	38:R:57:ASP:OD2	2.17	0.43
38:R:119:LEU:HA	38:R:232:MET:CE	2.49	0.43
38:R:120:VAL:HG23	38:R:121:PRO:HD2	2.01	0.43
39:S:10:GLN:CA	39:S:29:TRP:CE2	3.01	0.43
40:T:459:LEU:HG	40:T:461:SER:OG	2.18	0.43
1:A:345:PRO:O	1:A:346:ASP:O	2.35	0.43
1:A:372:PRO:HB2	3:C:342:ARG:HH21	1.84	0.43
1:A:790:ARG:HG3	3:C:60:HIS:HD2	1.82	0.43
1:A:1921:ASP:OD2	1:A:1966:HIS:HB3	2.19	0.43
1:A:2073:TRP:CD1	1:A:2073:TRP:C	2.91	0.43
1:A:2328:ALA:HB3	4:D:787:ALA:C	2.38	0.43
2:B:87:A:H5'	2:B:93:U:OP2	2.19	0.43
3:C:61:GLU:OE1	3:C:62:ASP:N	2.51	0.43
3:C:295:ASP:OD1	3:C:297:ASN:HB2	2.19	0.43
3:C:461:LEU:HD23	3:C:461:LEU:HA	1.78	0.43
4:D:441:GLY:O	4:D:693:THR:N	2.36	0.43
21:1:471:ASP:OD2	21:1:505:LYS:NZ	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:L:216:PHE:HZ	36:O:112:VAL:CG1	2.31	0.43
35:N:59:TYR:CZ	35:N:63:LEU:HD11	2.53	0.43
38:R:242:THR:HG22	38:R:244:LYS:H	1.84	0.43
38:R:443:GLY:O	38:R:447:MET:CB	2.67	0.43
39:S:56:ILE:HD12	39:S:153:PRO:HG3	2.00	0.43
39:S:131:ARG:HH12	39:S:133:CYS:HB2	1.83	0.43
1:A:293:TRP:HB2	1:A:1136:ARG:HH22	1.83	0.43
1:A:470:ARG:CZ	1:A:470:ARG:HB2	2.49	0.43
1:A:643:GLY:O	1:A:646:PRO:HD2	2.19	0.43
1:A:781:ARG:NH2	15:H:24:A:H5'	2.34	0.43
1:A:1433:ASP:O	1:A:1434:LYS:HD3	2.19	0.43
1:A:1437:ARG:O	1:A:1440:THR:OG1	2.36	0.43
3:C:73:TYR:CE1	40:T:487:LYS:HE2	2.52	0.43
3:C:137:HIS:HD2	3:C:236:MET:CB	2.22	0.43
3:C:275:TYR:OH	3:C:345:GLY:HA2	2.19	0.43
3:C:349:PHE:CG	3:C:356:PHE:HE1	2.36	0.43
3:C:941:LYS:HG2	3:C:942:GLY:N	2.34	0.43
13:F:28:A:C4'	35:N:41:ARG:HA	2.48	0.43
13:F:46:G:H2'	13:F:47:A:C8	2.54	0.43
15:H:166:G:N3	15:H:166:G:H2'	2.33	0.43
15:H:180:G:N3	15:H:181:G:C8	2.87	0.43
21:1:892:LEU:HD23	21:1:892:LEU:HA	1.91	0.43
27:7:51:ASN:OD1	27:7:61:LYS:HE2	2.18	0.43
35:N:46:LEU:HD23	35:N:46:LEU:HA	1.92	0.43
35:N:128:VAL:HG13	35:N:130:ARG:CB	2.48	0.43
37:P:191:ASP:O	37:P:192:VAL:HG23	2.18	0.43
39:S:55:ARG:NH2	43:W:95:PRO:O	2.52	0.43
40:T:225:ASP:O	40:T:226:ARG:HB2	2.18	0.43
1:A:235:MET:CE	1:A:411:PHE:CA	2.85	0.43
1:A:283:VAL:O	1:A:284:ARG:CZ	2.67	0.43
1:A:284:ARG:HE	1:A:284:ARG:HB3	1.70	0.43
1:A:371:LEU:HD12	1:A:372:PRO:HD2	2.00	0.43
1:A:380:LEU:HD22	1:A:380:LEU:H	1.84	0.43
1:A:843:LEU:HD22	1:A:867:ILE:HG23	2.01	0.43
3:C:289:ILE:CD1	3:C:300:LEU:HD21	2.49	0.43
3:C:381:LEU:HD23	3:C:416:LEU:HD22	1.99	0.43
5:E:255:MET:C	5:E:257:ASN:H	2.22	0.43
13:F:39:A:H61	14:G:8:C:N4	2.11	0.43
14:G:12:G:C2	14:G:13:C:O4'	2.71	0.43
21:1:184:VAL:O	21:1:188:ALA:CB	2.66	0.43
23:3:633:LEU:HD12	23:3:637:PRO:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:J:339:TRP:CG	38:R:116:TYR:CD2	3.06	0.43
38:R:250:LYS:HD3	38:R:250:LYS:C	2.39	0.43
40:T:347:THR:HG21	40:T:357:TRP:HE1	1.82	0.43
44:X:307:GLN:HB3	44:X:331:LEU:HD13	2.01	0.43
1:A:30:LEU:HB3	5:E:194:TYR:CZ	2.53	0.43
1:A:61:MET:HE1	35:N:104:ARG:HD2	2.01	0.43
1:A:151:MET:SD	1:A:628:GLY:HA3	2.59	0.43
1:A:210:HIS:CD2	1:A:210:HIS:C	2.92	0.43
1:A:344:ASP:OD1	1:A:347:LEU:HD11	2.19	0.43
1:A:1735:LYS:NZ	1:A:1765:SER:O	2.50	0.43
2:B:12:U:O2'	2:B:13:C:P	2.77	0.43
3:C:669:THR:HG22	3:C:690:GLU:CB	2.48	0.43
5:E:178:LEU:CD1	5:E:222:LEU:HD21	2.46	0.43
5:E:321:TYR:OH	5:E:356:ILE:HG23	2.19	0.43
15:H:68:G:C6	15:H:84:C:N4	2.85	0.43
21:1:900:PHE:HA	21:1:903:GLN:HE21	1.83	0.43
21:1:968:GLU:OE1	21:1:968:GLU:N	2.51	0.43
23:3:253:GLU:HA	23:3:286:ILE:HG22	2.01	0.43
23:3:820:ALA:HB2	23:3:843:LEU:HD11	2.00	0.43
23:3:1055:VAL:HB	23:3:1093:MET:HB3	2.00	0.43
26:6:14:GLN:O	26:6:46:CYS:HB3	2.18	0.43
29:L:209:ASP:HA	36:O:110:SER:CB	2.34	0.43
38:R:113:TYR:CG	38:R:118:ASP:OD2	2.72	0.43
40:T:399:LYS:CG	40:T:406:ILE:CD1	2.78	0.43
45:Y:37:TRP:CE2	45:Y:83:CYS:SG	3.11	0.43
45:Y:85:GLU:O	46:Z:502:ALA:CA	2.65	0.43
1:A:76:MET:CE	1:A:88:TYR:CE2	2.99	0.42
1:A:369:GLU:HB2	1:A:370:PRO:HD2	2.00	0.42
1:A:1373:GLN:NE2	1:A:1381:ASP:OD2	2.52	0.42
1:A:1539:SER:OG	1:A:1540:PRO:HD3	2.19	0.42
1:A:1630:LEU:HA	1:A:1630:LEU:HD23	1.80	0.42
1:A:1900:GLU:CD	46:Z:521:PRO:HB2	2.34	0.42
1:A:2302:LYS:HD2	1:A:2306:HIS:CE1	2.54	0.42
1:A:2328:ALA:CB	4:D:787:ALA:C	2.87	0.42
3:C:77:VAL:CB	40:T:196:LEU:HG	2.41	0.42
3:C:457:VAL:O	3:C:458:ASP:CB	2.67	0.42
13:F:55:C:OP2	13:F:74:U:O2'	2.36	0.42
23:3:169:HIS:H	23:3:185:LEU:HB2	1.83	0.42
23:3:226:GLU:HG3	23:3:261:PHE:CZ	2.51	0.42
23:3:498:GLY:HA3	23:3:531:LYS:HZ3	1.83	0.42
23:3:520:TYR:HE1	23:3:522:ASP:HB2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:640:LEU:HD22	23:3:667:ILE:HG12	2.01	0.42
23:3:1188:ASN:OD1	23:3:1189:LYS:N	2.51	0.42
26:6:57:ARG:HD2	26:6:62:GLY:C	2.40	0.42
35:N:2:PRO:HG2	35:N:4:VAL:H	1.84	0.42
35:N:60:ILE:HD13	35:N:78:CYS:HB3	2.00	0.42
36:O:77:LEU:HD12	36:O:77:LEU:HA	1.89	0.42
36:O:278:GLN:O	36:O:282:VAL:HG23	2.19	0.42
38:R:124:VAL:HG22	38:R:126:ASN:N	2.34	0.42
40:T:284:TYR:N	40:T:284:TYR:CD1	2.87	0.42
42:V:585:ILE:O	42:V:586:PHE:C	2.58	0.42
43:W:491:GLN:O	43:W:492:ASN:C	2.57	0.42
45:Y:92:LEU:O	45:Y:96:ASN:CB	2.67	0.42
1:A:39:GLN:OE1	43:W:169:GLU:CB	2.67	0.42
1:A:332:TYR:C	1:A:332:TYR:CD1	2.92	0.42
1:A:1425:LYS:HG2	38:R:417:ASN:OD1	2.18	0.42
1:A:2072:GLU:O	1:A:2076:ARG:HG3	2.18	0.42
1:A:2310:ARG:HG2	1:A:2310:ARG:HH11	1.84	0.42
3:C:93:ILE:HG21	40:T:218:TRP:CZ2	2.54	0.42
3:C:481:MET:SD	3:C:492:ALA:CB	3.06	0.42
15:H:168:A:N3	15:H:168:A:C2'	2.77	0.42
21:1:404:LEU:HD23	25:5:47:GLN:CD	2.39	0.42
21:1:744:ALA:HB2	21:1:784:MET:SD	2.59	0.42
21:1:1289:ASN:HB2	21:1:1294:THR:HA	2.00	0.42
23:3:274:ARG:NH2	23:3:309:ASP:OD2	2.50	0.42
33:Q:500:GLY:HA2	38:R:51:ILE:HD11	2.00	0.42
38:R:118:ASP:OD1	38:R:232:MET:HE1	2.19	0.42
38:R:220:ARG:HB2	38:R:220:ARG:CZ	2.49	0.42
45:Y:37:TRP:NE1	45:Y:83:CYS:CB	2.70	0.42
1:A:32:GLU:OE2	1:A:36:LYS:CE	2.68	0.42
1:A:407:ALA:HA	1:A:408:PRO:HD3	1.87	0.42
1:A:962:LEU:HB2	1:A:965:VAL:HB	1.99	0.42
1:A:1052:VAL:HG22	1:A:1161:LEU:HD21	2.01	0.42
1:A:1099:PHE:HZ	1:A:1157:ILE:HD11	1.85	0.42
1:A:1353:PHE:HE2	41:U:22:ASN:CG	2.23	0.42
1:A:1457:HIS:HE2	38:R:424:SER:CB	2.32	0.42
1:A:1772:PHE:CD1	1:A:1773:SER:N	2.87	0.42
1:A:1810:PHE:CE1	1:A:1919:LEU:HD12	2.55	0.42
3:C:242:LEU:HD23	3:C:242:LEU:HA	1.84	0.42
3:C:413:ARG:HB2	3:C:414:PRO:HD3	1.99	0.42
15:H:3:C:H2'	15:H:4:G:C8	2.53	0.42
15:H:178:A:N3	15:H:178:A:H2'	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:707:LEU:O	21:1:710:ALA:HB3	2.20	0.42
21:1:811:LEU:HB2	21:1:812:PRO:HD3	2.00	0.42
21:1:1040:GLY:CA	21:1:1080:THR:HG22	2.48	0.42
22:2:613:LEU:HA	22:2:616:SER:OG	2.20	0.42
23:3:310:ILE:O	23:3:330:PHE:HB3	2.19	0.42
23:3:961:ILE:HB	23:3:970:TYR:CD2	2.54	0.42
28:J:375:ASP:O	28:J:376:VAL:C	2.58	0.42
35:N:15:TRP:HE3	35:N:74:LEU:HD11	1.83	0.42
36:O:185:LYS:HG2	36:O:186:PRO:HD2	2.00	0.42
43:W:155:SER:O	43:W:156:VAL:CB	2.67	0.42
1:A:32:GLU:CD	1:A:36:LYS:HE3	2.39	0.42
1:A:173:GLU:O	1:A:520:TYR:HD2	2.02	0.42
1:A:232:LEU:N	1:A:233:PRO:CD	2.83	0.42
1:A:1354:ARG:NH1	41:U:7:LEU:HG	2.34	0.42
2:B:94:U:O2'	2:B:95:G:H3'	2.18	0.42
3:C:323:PHE:CE1	3:C:424:PHE:HE1	2.37	0.42
3:C:706:GLN:HE21	3:C:708:THR:N	2.12	0.42
3:C:863:ILE:HA	3:C:864:PRO:HD3	1.88	0.42
5:E:67:GLY:H	5:E:87:ASP:CG	2.20	0.42
15:H:5:C:H2'	15:H:6:U:C6	2.54	0.42
21:1:413:LYS:HG3	21:1:415:LEU:HD11	2.01	0.42
21:1:619:ASN:ND2	21:1:624:VAL:HG21	2.34	0.42
21:1:619:ASN:OD1	21:1:620:MET:N	2.52	0.42
21:1:722:GLU:O	21:1:725:ASP:CB	2.67	0.42
23:3:185:LEU:HD11	23:3:235:LEU:HD13	2.01	0.42
23:3:287:PHE:HA	23:3:304:GLN:O	2.19	0.42
23:3:1014:TYR:CE2	23:3:1016:ARG:HA	2.55	0.42
23:3:1052:ASN:OD1	23:3:1096:HIS:ND1	2.39	0.42
23:3:1201:PRO:HB2	23:3:1202:PRO:HD3	2.02	0.42
26:6:47:ASP:HA	26:6:50:ASN:O	2.20	0.42
28:J:331:GLN:HG2	38:R:98:TYR:HH	1.76	0.42
28:J:339:TRP:CD2	38:R:116:TYR:CD2	2.85	0.42
29:L:63:TRP:CZ2	29:L:99:HIS:HB2	2.54	0.42
35:N:12:PRO:HG2	35:N:74:LEU:HA	2.02	0.42
36:O:240:GLY:HA3	36:O:296:ARG:NH2	2.34	0.42
37:P:188:TRP:C	37:P:190:ASP:H	2.21	0.42
38:R:183:GLN:HB3	38:R:188:PHE:CD2	2.54	0.42
39:S:125:LYS:HB3	39:S:126:HIS:CE1	2.54	0.42
43:W:528:GLY:HA2	43:W:552:VAL:CB	2.49	0.42
45:Y:69:ARG:HA	45:Y:76:SER:HA	2.02	0.42
1:A:61:MET:CE	35:N:104:ARG:HD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:TYR:HE1	1:A:485:THR:HB	1.84	0.42
1:A:378:PHE:CD1	1:A:378:PHE:C	2.93	0.42
1:A:549:GLU:CD	1:A:552:ARG:NH1	2.72	0.42
1:A:596:TYR:CE1	14:G:-5:G:N9	2.88	0.42
1:A:718:ARG:NH2	38:R:259:LYS:CE	2.78	0.42
1:A:1263:TRP:CD2	1:A:1295:ILE:HD13	2.54	0.42
1:A:1363:GLN:O	1:A:1364:LEU:HG	2.18	0.42
3:C:669:THR:HG22	3:C:690:GLU:OE1	2.19	0.42
3:C:712:LYS:O	3:C:716:GLU:HG3	2.18	0.42
5:E:277:PHE:CE1	5:E:317:ARG:HG2	2.53	0.42
14:G:5:G:C2	14:G:6:A:C5	3.08	0.42
14:G:136:U:O4	21:1:515:ALA:HA	2.19	0.42
21:1:494:GLU:HA	21:1:497:ILE:HG22	2.01	0.42
21:1:940:LEU:O	21:1:948:ARG:NH2	2.51	0.42
21:1:1255:PHE:HD2	22:2:487:LEU:HD22	1.81	0.42
23:3:456:PRO:HB2	23:3:757:ILE:HD13	2.02	0.42
23:3:508:CYS:SG	23:3:518:GLN:NE2	2.92	0.42
23:3:784:THR:HB	23:3:786:ARG:NH1	2.32	0.42
36:O:104:LYS:HG3	36:O:139:LYS:HZ1	1.84	0.42
36:O:133:PRO:HG2	36:O:137:LEU:HB2	2.01	0.42
36:O:248:LEU:O	36:O:252:PHE:HD2	2.03	0.42
38:R:129:ASP:HB3	38:R:131:ASP:CG	2.40	0.42
40:T:318:ARG:CG	40:T:318:ARG:NH1	2.82	0.42
1:A:385:GLU:HB3	1:A:386:PRO:HD2	2.00	0.42
1:A:494:LEU:HD23	1:A:494:LEU:HA	1.84	0.42
1:A:715:GLU:OE1	38:R:258:TRP:CE3	2.73	0.42
1:A:791:GLN:NE2	1:A:1026:ASN:OD1	2.52	0.42
1:A:1759:THR:N	21:1:938:TRP:CD1	2.88	0.42
1:A:1948:ASP:O	1:A:1951:LYS:HB2	2.20	0.42
1:A:1953:ILE:HD11	1:A:1986:LEU:HD13	2.01	0.42
1:A:2216:CYS:HA	1:A:2225:LEU:HB3	2.01	0.42
3:C:85:ASP:OD2	40:T:240:LEU:HA	2.20	0.42
3:C:90:THR:O	3:C:92:PRO:HD3	2.19	0.42
15:H:107:A:N1	15:H:108:G:C5	2.88	0.42
21:1:1075:ARG:HE	21:1:1075:ARG:HB2	1.64	0.42
23:3:146:ARG:HB2	23:3:150:ALA:HA	2.02	0.42
23:3:353:PHE:O	23:3:432:ARG:NH1	2.44	0.42
23:3:774:PHE:N	23:3:774:PHE:CD2	2.86	0.42
27:7:30:GLU:HA	27:7:33:VAL:HG12	2.02	0.42
29:L:209:ASP:CG	36:O:111:ASP:N	2.63	0.42
29:L:219:LYS:NZ	36:O:105:ASP:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:I:712:VAL:O	32:I:713:ARG:C	2.57	0.42
34:M:202:CYS:HB2	34:M:219:PHE:HB2	2.02	0.42
36:O:224:ASP:N	36:O:225:PRO:HD2	2.34	0.42
38:R:71:GLN:HE21	38:R:71:GLN:HB2	1.61	0.42
39:S:98:LEU:HD21	39:S:129:PHE:HD2	1.84	0.42
39:S:102:ASN:OD1	39:S:107:THR:O	2.37	0.42
40:T:188:PRO:HG3	40:T:443:THR:HG21	2.01	0.42
45:Y:38:ILE:HG12	45:Y:82:LEU:HB3	2.02	0.42
1:A:48:LYS:HG2	1:A:49:ARG:N	2.35	0.42
1:A:384:VAL:O	1:A:385:GLU:HG2	2.20	0.42
1:A:651:TRP:CD1	13:F:66:C:C2	3.07	0.42
1:A:1560:ILE:HG12	1:A:1668:TRP:CB	2.49	0.42
1:A:1889:LEU:HD11	1:A:2012:LEU:HG	2.02	0.42
2:B:19:A:H2'	2:B:20:G:C5'	2.49	0.42
2:B:32:C:OP1	37:P:33:ARG:NE	2.53	0.42
3:C:77:VAL:HG13	40:T:196:LEU:CB	2.41	0.42
3:C:140:HIS:CB	3:C:230:ASP:H	2.33	0.42
3:C:259:LYS:HD2	51:C:1500:GTP:C4	2.55	0.42
3:C:452:THR:HB	3:C:577:PHE:CE2	2.55	0.42
5:E:152:SER:OG	5:E:153:PHE:HD1	2.03	0.42
13:F:58:G:O2'	13:F:59:G:P	2.78	0.42
14:G:141:C:H2'	14:G:142:U:C6	2.52	0.42
15:H:179:C:C2	15:H:180:G:C8	3.07	0.42
21:1:401:ASP:HA	21:1:404:LEU:HB2	2.00	0.42
21:1:848:GLU:O	21:1:851:SER:OG	2.32	0.42
21:1:1179:ASP:OD1	21:1:1181:ASP:N	2.52	0.42
23:3:3:LEU:HA	23:3:1130:VAL:O	2.20	0.42
23:3:228:LEU:HD23	23:3:259:LYS:HZ2	1.84	0.42
23:3:482:THR:OG1	23:3:501:GLY:HA3	2.19	0.42
23:3:691:THR:HG22	23:3:716:SER:HB3	2.02	0.42
23:3:718:ARG:HG2	23:3:719:SER:H	1.84	0.42
25:5:25:ASN:HB3	25:5:87:LEU:HA	2.02	0.42
28:J:294:HIS:HE1	29:L:227:THR:CB	2.26	0.42
29:L:703:MET:O	29:L:707:ALA:HB3	2.18	0.42
31:K:157:ARG:O	31:K:160:ILE:CG1	2.68	0.42
36:O:219:THR:O	36:O:220:MET:C	2.58	0.42
37:P:226:LYS:HD3	37:P:227:TYR:HE1	1.83	0.42
38:R:67:ILE:CG1	38:R:71:GLN:OE1	2.68	0.42
42:V:484:SER:O	42:V:486:THR:N	2.53	0.42
42:V:547:VAL:O	42:V:548:ALA:C	2.58	0.42
43:W:571:TRP:O	43:W:573:GLY:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:TYR:CE1	1:A:485:THR:HG22	2.54	0.42
1:A:372:PRO:HB2	3:C:342:ARG:NH2	2.34	0.42
1:A:382:GLU:O	1:A:383:PHE:CG	2.73	0.42
1:A:651:TRP:CE2	13:F:66:C:N3	2.88	0.42
1:A:816:TRP:CE2	1:A:820:ARG:HG3	2.55	0.42
1:A:1436:TRP:HA	1:A:1439:ARG:CZ	2.50	0.42
2:B:19:A:HO2'	2:B:20:G:P	2.37	0.42
3:C:149:LEU:HA	3:C:427:PHE:HD2	1.82	0.42
13:F:28:A:O4'	35:N:41:ARG:CA	2.64	0.42
14:G:-3:A:H2'	14:G:-2:C:C6	2.55	0.42
15:H:82:G:C2	15:H:83:A:C5	3.08	0.42
21:1:527:GLY:O	21:1:531:LEU:HD13	2.20	0.42
22:2:525:PRO:HD2	22:2:528:ILE:HD12	2.00	0.42
23:3:412:ILE:HD12	23:3:1118:VAL:HG11	2.01	0.42
36:O:24:CYS:HB3	36:O:26:THR:H	1.85	0.42
40:T:187:LYS:N	40:T:188:PRO:CD	2.83	0.42
40:T:233:LEU:HD23	40:T:233:LEU:O	2.20	0.42
43:W:431:ARG:O	43:W:446:GLU:HA	2.19	0.42
45:Y:37:TRP:HH2	46:Z:498:GLY:N	2.15	0.42
45:Y:59:TYR:HB3	45:Y:92:LEU:HD23	2.01	0.42
1:A:137:GLU:N	1:A:138:PRO:HD2	2.35	0.42
1:A:303:ILE:CG2	3:C:933:PHE:CD1	3.03	0.42
1:A:434:HIS:ND1	1:A:434:HIS:C	2.73	0.42
1:A:629:PHE:CD2	1:A:629:PHE:O	2.73	0.42
1:A:697:MET:N	1:A:698:PRO:HD3	2.34	0.42
1:A:833:LYS:HE3	1:A:834:HIS:NE2	2.35	0.42
1:A:1416:ILE:HB	1:A:1417:PRO:HD3	2.01	0.42
1:A:1457:HIS:HE1	38:R:424:SER:HA	1.74	0.42
1:A:1529:ILE:O	1:A:1530:PRO:C	2.59	0.42
2:B:92:U:C3'	2:B:93:U:H5'	2.50	0.42
3:C:140:HIS:HB3	3:C:230:ASP:H	1.85	0.42
3:C:149:LEU:HA	3:C:427:PHE:CE2	2.54	0.42
14:G:139:U:H2'	14:G:140:A:C8	2.55	0.42
15:H:26:A:C5	15:H:27:U:C5	3.08	0.42
21:1:687:VAL:HA	21:1:690:ILE:HG22	2.01	0.42
21:1:727:VAL:HG12	21:1:731:LEU:HD11	2.02	0.42
21:1:790:LYS:O	21:1:793:LYS:HB3	2.19	0.42
23:3:1039:LEU:HB2	23:3:1043:THR:OG1	2.20	0.42
28:J:240:THR:O	28:J:241:VAL:HB	2.19	0.42
28:J:259:GLN:HE21	29:L:220:PRO:HD3	1.82	0.42
36:O:253:TYR:CZ	39:S:120:GLN:CG	3.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:P:58:ASP:OD2	37:P:61:ARG:HB2	2.19	0.42
37:P:192:VAL:CG1	37:P:193:VAL:N	2.83	0.42
1:A:86:ARG:HH22	38:R:211:ARG:HA	1.85	0.42
1:A:1188:ASN:ND2	1:A:1233:ASP:OD2	2.47	0.42
1:A:1371:TYR:OH	42:V:464:GLN:CB	2.67	0.42
1:A:1399:GLN:C	1:A:1401:ARG:H	2.24	0.42
1:A:1489:LEU:O	1:A:1492:GLY:N	2.45	0.42
1:A:1503:TRP:CZ2	1:A:1753:LEU:HD21	2.55	0.42
1:A:1555:LEU:HB2	1:A:1558:THR:OG1	2.19	0.42
1:A:1763:LEU:HD23	1:A:1764:SER:O	2.20	0.42
1:A:2117:ILE:H	1:A:2117:ILE:HG12	1.64	0.42
3:C:220:ARG:HD3	3:C:477:HIS:NE2	2.34	0.42
3:C:474:LEU:HD12	3:C:500:THR:O	2.20	0.42
5:E:274:VAL:C	5:E:275:LYS:HG3	2.40	0.42
15:H:147:G:C2	15:H:148:C:N3	2.87	0.42
15:H:155:C:H2'	15:H:156:U:H5"	2.02	0.42
15:H:179:C:O2	15:H:180:G:C8	2.72	0.42
21:1:555:VAL:O	21:1:559:ILE:HG12	2.19	0.42
22:2:643:PRO:HG2	24:4:66:ASP:HA	2.01	0.42
23:3:259:LYS:HE3	23:3:266:ASP:OD2	2.20	0.42
23:3:261:PHE:HD1	23:3:261:PHE:HA	1.72	0.42
23:3:288:VAL:HG23	23:3:289:CYS:N	2.33	0.42
23:3:519:VAL:HG22	23:3:524:ILE:HG23	2.02	0.42
23:3:673:VAL:HA	23:3:690:ARG:HA	2.02	0.42
23:3:968:ARG:CZ	23:3:979:ARG:HH11	2.33	0.42
23:3:1011:TRP:HB3	23:3:1024:PHE:CZ	2.55	0.42
28:J:216:ASP:O	28:J:218:GLU:N	2.53	0.42
35:N:56:LYS:HE2	35:N:83:TYR:O	2.20	0.42
36:O:292:ILE:HG23	36:O:296:ARG:C	2.40	0.42
40:T:281:ILE:CD1	40:T:282:ARG:HG2	2.50	0.42
1:A:1320:LYS:NZ	38:R:434:TYR:CE1	2.88	0.41
1:A:1402:ARG:CD	38:R:412:ASP:HA	2.50	0.41
1:A:1942:ALA:CB	1:A:1983:LEU:HD22	2.50	0.41
3:C:291:MET:HG2	3:C:292:TYR:CE1	2.54	0.41
3:C:445:ALA:HB1	3:C:449:ILE:HG13	2.02	0.41
3:C:829:GLU:HG3	3:C:830:PRO:HD2	2.01	0.41
13:F:8:C:C6	13:F:8:C:C5'	2.98	0.41
13:F:31:U:H2'	13:F:32:U:C6	2.55	0.41
15:H:68:G:H2'	15:H:69:U:H6	1.82	0.41
21:1:783:GLU:O	21:1:787:ILE:HG12	2.20	0.41
21:1:1025:LYS:HE2	34:M:210:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:443:GLU:HA	23:3:735:SER:OG	2.20	0.41
23:3:812:LYS:NZ	23:3:855:PRO:HG2	2.35	0.41
27:7:23:HIS:H	27:7:26:THR:HG1	1.68	0.41
28:J:239:ARG:C	28:J:239:ARG:HD3	2.40	0.41
28:J:262:ARG:HB3	29:L:220:PRO:HG3	2.02	0.41
28:J:368:ARG:O	28:J:372:VAL:HG23	2.20	0.41
38:R:131:ASP:OD2	38:R:132:LEU:N	2.53	0.41
39:S:15:TYR:HB2	39:S:163:TYR:HB2	2.02	0.41
1:A:61:MET:HB3	1:A:62:PRO:CD	2.51	0.41
1:A:121:HIS:CD2	1:A:481:PHE:O	2.70	0.41
1:A:151:MET:SD	1:A:628:GLY:CA	3.08	0.41
1:A:151:MET:HE1	1:A:629:PHE:HA	2.02	0.41
1:A:155:LYS:CE	1:A:624:GLY:O	2.68	0.41
1:A:372:PRO:HG2	3:C:342:ARG:HE	1.80	0.41
1:A:1051:LEU:HD22	37:P:193:VAL:HG11	2.00	0.41
1:A:1428:HIS:O	1:A:1429:THR:C	2.59	0.41
1:A:1823:HIS:O	1:A:1826:VAL:HG22	2.20	0.41
3:C:73:TYR:HB3	3:C:77:VAL:HG21	2.02	0.41
3:C:89:LEU:C	3:C:89:LEU:CD2	2.82	0.41
3:C:259:LYS:HG2	3:C:262:ARG:HD3	1.99	0.41
3:C:449:ILE:CD1	3:C:466:SER:HA	2.50	0.41
14:G:-8:U:H5	41:U:16:ASN:HB3	1.85	0.41
15:H:80:A:C2	15:H:81:G:N7	2.88	0.41
15:H:153:A:H62	15:H:177:A:H2	1.67	0.41
21:1:1185:ARG:HD2	21:1:1218:ASN:OD1	2.20	0.41
23:3:425:VAL:O	23:3:435:LEU:HD12	2.20	0.41
23:3:436:ARG:HG2	23:3:778:ALA:HA	2.01	0.41
29:L:31:TRP:CH2	29:L:47:LYS:HA	2.55	0.41
35:N:37:HIS:CD2	35:N:37:HIS:O	2.74	0.41
35:N:75:TYR:CZ	35:N:79:ILE:HD11	2.55	0.41
36:O:132:ARG:HG3	36:O:137:LEU:CD2	2.50	0.41
36:O:164:ILE:HD12	36:O:164:ILE:HA	1.91	0.41
36:O:219:THR:O	36:O:221:PRO:CD	2.66	0.41
38:R:88:ILE:CG2	38:R:96:ILE:HG23	2.48	0.41
38:R:418:GLN:HE21	38:R:418:GLN:HB2	1.64	0.41
38:R:442:ARG:NH1	38:R:443:GLY:CA	2.78	0.41
43:W:371:THR:O	43:W:372:ASN:CB	2.68	0.41
43:W:458:GLU:O	43:W:459:PRO:C	2.58	0.41
45:Y:64:ASN:O	45:Y:83:CYS:HB3	2.19	0.41
46:Z:572:PRO:CG	46:Z:588:ASP:OD2	2.67	0.41
1:A:206:TRP:CE3	1:A:212:PRO:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:GLN:HA	1:A:212:PRO:HD3	1.82	0.41
1:A:428:LYS:HE3	1:A:454:TYR:CE1	2.55	0.41
1:A:434:HIS:CG	3:C:892:GLN:OE1	2.74	0.41
1:A:638:LEU:HA	1:A:638:LEU:HD23	1.70	0.41
1:A:1883:VAL:HG12	1:A:1885:LYS:HG3	2.01	0.41
1:A:2111:LEU:HD21	1:A:2225:LEU:HD21	2.03	0.41
3:C:148:CYS:SG	3:C:312:SER:O	2.78	0.41
3:C:512:GLU:HG3	3:C:562:THR:O	2.19	0.41
5:E:263:ASP:O	5:E:272:ARG:NE	2.32	0.41
21:1:520:THR:HG21	21:1:558:ARG:HE	1.85	0.41
21:1:1124:SER:O	21:1:1127:THR:OG1	2.28	0.41
23:3:8:LEU:HD23	23:3:774:PHE:CZ	2.52	0.41
29:L:219:LYS:NZ	36:O:104:LYS:O	2.51	0.41
29:L:741:GLN:O	29:L:744:GLN:CG	2.69	0.41
36:O:214:LEU:HD23	36:O:214:LEU:HA	1.82	0.41
40:T:225:ASP:O	40:T:226:ARG:CB	2.67	0.41
1:A:54:VAL:O	1:A:54:VAL:HG23	2.20	0.41
1:A:258:PHE:CD2	1:A:434:HIS:HA	2.55	0.41
1:A:800:TYR:HB3	3:C:59:LEU:HD11	2.02	0.41
1:A:1554:GLN:NE2	1:A:1620:TYR:O	2.49	0.41
1:A:1730:MET:O	1:A:1734:MET:HG2	2.19	0.41
1:A:2172:MET:HB2	1:A:2172:MET:HE3	1.79	0.41
3:C:261:ASP:CG	51:C:1500:GTP:N1	2.61	0.41
3:C:445:ALA:CB	3:C:449:ILE:HD11	2.43	0.41
3:C:853:ARG:O	3:C:854:ARG:HB3	2.20	0.41
15:H:152:G:H2'	15:H:152:G:N3	2.36	0.41
15:H:154:C:N3	15:H:176:G:N1	2.61	0.41
21:1:642:PRO:HB3	21:1:682:HIS:NE2	2.36	0.41
21:1:1136:TYR:CE1	21:1:1144:GLN:HB3	2.55	0.41
23:3:199:GLU:HB3	23:3:203:ASN:HD21	1.85	0.41
28:J:220:LEU:O	28:J:223:TYR:HB3	2.21	0.41
38:R:155:VAL:O	38:R:159:VAL:HG23	2.20	0.41
43:W:97:ASN:O	43:W:99:PHE:N	2.53	0.41
1:A:331:TRP:HE3	1:A:332:TYR:N	2.18	0.41
3:C:589:LYS:HB3	3:C:659:VAL:O	2.20	0.41
3:C:704:VAL:O	3:C:709:TRP:CZ2	2.74	0.41
3:C:707:ILE:HD11	3:C:735:PHE:HB2	2.01	0.41
13:F:40:U:O4	13:F:41:A:N6	2.54	0.41
15:H:103:U:C3'	15:H:104:U:H5'	2.51	0.41
21:1:621:ASP:OD2	21:1:623:TYR:HB3	2.19	0.41
21:1:719:TYR:CD1	23:3:218:ASN:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:116:VAL:HA	23:3:117:PRO:HD3	1.95	0.41
23:3:896:PHE:CZ	23:3:972:LEU:HB2	2.55	0.41
24:4:69:TYR:OH	24:4:73:ILE:HG13	2.20	0.41
28:J:340:GLN:N	28:J:341:PRO:HD3	2.35	0.41
29:L:717:MET:O	29:L:721:LEU:N	2.48	0.41
37:P:189:ASP:O	37:P:190:ASP:C	2.58	0.41
40:T:223:SER:OG	40:T:224:ALA:N	2.53	0.41
44:X:173:GLN:NE2	44:X:176:GLU:HA	2.36	0.41
1:A:107:PRO:O	1:A:108:MET:HB2	2.21	0.41
1:A:118:VAL:HG12	1:A:119:LEU:N	2.36	0.41
1:A:1325:LEU:HD23	1:A:1325:LEU:HA	1.86	0.41
1:A:1948:ASP:HA	1:A:1951:LYS:HD2	2.01	0.41
1:A:2073:TRP:CZ3	1:A:2313:HIS:CG	3.09	0.41
1:A:2117:ILE:HG21	1:A:2301:PRO:HB2	2.02	0.41
1:A:2120:LEU:HD12	1:A:2120:LEU:N	2.35	0.41
3:C:97:VAL:HG21	37:P:45:GLN:CG	2.46	0.41
3:C:137:HIS:NE2	3:C:236:MET:SD	2.93	0.41
13:F:39:A:H2'	13:F:40:U:O4'	2.21	0.41
14:G:-2:C:H2'	14:G:-1:G:H8	1.82	0.41
15:H:72:U:H6	15:H:72:U:O5'	2.03	0.41
15:H:171:U:H2'	15:H:172:C:O4'	2.21	0.41
21:1:815:PHE:HA	21:1:819:TRP:CD1	2.56	0.41
23:3:168:TYR:CE1	27:7:69:MET:HB3	2.55	0.41
23:3:442:LEU:HD13	23:3:734:LEU:HD23	1.99	0.41
23:3:587:VAL:CG1	23:3:590:MET:HG3	2.49	0.41
32:I:296:PHE:CB	32:I:305:SER:O	2.68	0.41
39:S:9:TRP:C	39:S:11:PRO:HD3	2.39	0.41
40:T:297:HIS:CE1	40:T:300:ILE:HD12	2.56	0.41
40:T:455:GLN:CG	40:T:456:PRO:HD2	2.51	0.41
45:Y:24:ASP:O	45:Y:26:VAL:N	2.54	0.41
1:A:148:TRP:CZ2	1:A:616:PHE:CA	3.02	0.41
1:A:175:PRO:CG	1:A:498:ARG:NH2	2.73	0.41
1:A:294:ASN:OD1	3:C:654:LYS:CD	2.66	0.41
1:A:596:TYR:O	1:A:598:LEU:N	2.54	0.41
1:A:866:LEU:O	1:A:869:GLN:HB3	2.21	0.41
1:A:1035:GLN:HA	1:A:1446:GLN:HE22	1.84	0.41
1:A:1099:PHE:CE2	1:A:1153:VAL:HG13	2.53	0.41
1:A:1221:THR:O	1:A:1223:GLU:HG3	2.20	0.41
1:A:1342:TRP:CG	3:C:921:LEU:CD2	2.99	0.41
1:A:1430:LEU:HD21	38:R:422:MET:HA	2.03	0.41
1:A:1458:GLN:HE21	1:A:1463:LYS:HG3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:C:H6	2:B:26:A:H62	1.67	0.41
2:B:40:U:O2	2:B:40:U:C2'	2.69	0.41
2:B:63:A:C4'	5:E:106:LYS:NZ	2.81	0.41
3:C:230:ASP:OD1	3:C:259:LYS:HB2	2.17	0.41
3:C:270:PRO:HA	3:C:271:PRO:HD3	1.87	0.41
4:D:577:LYS:O	4:D:581:SER:N	2.54	0.41
14:G:26:U:H2'	36:O:269:CYS:SG	2.61	0.41
14:G:155:U:C4'	14:G:156:U:H5'	2.49	0.41
15:H:4:G:H2'	15:H:5:C:C6	2.55	0.41
15:H:83:A:H2'	15:H:84:C:H1'	2.00	0.41
21:1:1127:THR:O	22:2:571:LEU:HD13	2.21	0.41
23:3:314:THR:HG22	23:3:315:LEU:N	2.36	0.41
23:3:521:PRO:HA	23:3:544:ILE:CG2	2.49	0.41
23:3:524:ILE:CD1	23:3:556:ILE:HD13	2.49	0.41
24:4:67:ALA:O	24:4:70:ALA:HB3	2.21	0.41
28:J:273:TYR:CD1	38:R:228:PRO:CB	3.04	0.41
36:O:149:LYS:CE	36:O:290:LYS:HE2	2.48	0.41
39:S:11:PRO:HB3	39:S:166:GLY:N	2.34	0.41
1:A:143:GLN:O	1:A:146:SER:HB3	2.20	0.41
1:A:362:ARG:C	1:A:362:ARG:CD	2.88	0.41
1:A:642:ARG:CZ	2:B:28:A:C4	3.04	0.41
1:A:1342:TRP:CD1	3:C:921:LEU:HD11	2.55	0.41
1:A:1891:LEU:HB2	1:A:1893:PHE:CE2	2.55	0.41
1:A:2090:ILE:H	1:A:2090:ILE:HD13	1.86	0.41
1:A:2259:VAL:HG22	1:A:2260:GLN:H	1.86	0.41
2:B:41:U:C4	2:B:42:U:O4	2.73	0.41
3:C:300:LEU:N	3:C:300:LEU:CD1	2.84	0.41
13:F:60:C:H5"	38:R:219:PRO:HB3	2.01	0.41
14:G:21:A:OP1	36:O:156:TYR:CE2	2.73	0.41
15:H:160:A:H2'	15:H:161:U:C6	2.55	0.41
21:1:719:TYR:HB3	23:3:216:GLY:O	2.20	0.41
21:1:1016:LEU:O	21:1:1019:ARG:HB3	2.20	0.41
21:1:1055:TRP:O	21:1:1058:ILE:HB	2.20	0.41
21:1:1092:ASP:OD1	21:1:1092:ASP:N	2.53	0.41
23:3:86:ARG:CD	23:3:104:GLN:HE21	2.33	0.41
23:3:205:GLN:HE21	23:3:227:PRO:HB3	1.85	0.41
23:3:554:VAL:HG12	23:3:556:ILE:HG23	2.01	0.41
26:6:90:ASN:OD1	26:6:91:LEU:N	2.54	0.41
31:K:134:ALA:C	31:K:137:VAL:HG12	2.40	0.41
34:M:208:THR:HG22	34:M:210:PHE:HD2	1.85	0.41
35:N:68:LYS:HD3	35:N:68:LYS:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:N:117:CYS:C	35:N:119:CYS:N	2.73	0.41
36:O:104:LYS:H	36:O:104:LYS:HG2	1.71	0.41
38:R:129:ASP:C	38:R:131:ASP:N	2.73	0.41
39:S:66:ASP:C	39:S:66:ASP:OD1	2.59	0.41
40:T:309:ASP:C	40:T:309:ASP:OD1	2.59	0.41
43:W:290:GLY:HA2	43:W:571:TRP:O	2.19	0.41
46:Z:522:LEU:HD13	46:Z:522:LEU:C	2.41	0.41
46:Z:525:TYR:HD1	46:Z:526:ILE:CG2	2.29	0.41
1:A:128:PHE:CD1	1:A:473:PHE:CE1	3.09	0.41
1:A:225:TYR:O	1:A:418:THR:CB	2.68	0.41
1:A:293:TRP:HD1	1:A:1136:ARG:NH2	2.19	0.41
1:A:965:VAL:O	1:A:1100:ARG:NH1	2.54	0.41
1:A:1052:VAL:CG2	1:A:1161:LEU:HD21	2.51	0.41
1:A:1661:TRP:NE1	1:A:1697:SER:O	2.53	0.41
1:A:1757:GLU:CG	38:R:451:ILE:HG13	2.51	0.41
1:A:1776:ILE:O	1:A:1859:LYS:N	2.48	0.41
1:A:1788:VAL:HG21	1:A:1800:THR:HB	2.03	0.41
1:A:2117:ILE:HG22	1:A:2303:GLU:HA	2.03	0.41
1:A:2320:LEU:HD21	1:A:2322:GLU:CD	2.41	0.41
3:C:64:LYS:HE2	3:C:64:LYS:HA	2.02	0.41
3:C:65:TYR:O	3:C:66:TYR:CG	2.73	0.41
3:C:79:THR:HA	40:T:199:VAL:O	2.20	0.41
3:C:132:VAL:HG11	3:C:226:VAL:CG2	2.49	0.41
3:C:133:THR:HB	3:C:225:VAL:HA	2.02	0.41
3:C:513:ASN:O	3:C:513:ASN:ND2	2.54	0.41
3:C:518:ASP:N	3:C:519:GLU:OE2	2.54	0.41
5:E:115:LEU:O	5:E:116:HIS:CD2	2.74	0.41
5:E:177:LYS:C	5:E:178:LEU:HD23	2.41	0.41
5:E:243:LEU:HD22	5:E:243:LEU:HA	1.80	0.41
5:E:266:PRO:CB	29:L:785:GLN:HB3	2.51	0.41
15:H:152:G:H2'	15:H:153:A:C1'	2.51	0.41
21:1:184:VAL:O	21:1:188:ALA:HB2	2.21	0.41
21:1:517:ARG:O	21:1:520:THR:OG1	2.20	0.41
21:1:664:GLY:O	21:1:667:ILE:HB	2.21	0.41
21:1:770:MET:O	21:1:774:ILE:HG12	2.21	0.41
21:1:963:LYS:HG2	21:1:1003:VAL:HB	2.02	0.41
21:1:1080:THR:HA	21:1:1083:TYR:CD2	2.56	0.41
21:1:1092:ASP:OD1	21:1:1093:VAL:N	2.54	0.41
21:1:1227:ILE:O	21:1:1231:MET:HG2	2.20	0.41
21:1:1252:GLN:OE1	22:2:499:PRO:HA	2.20	0.41
23:3:65:LEU:HD12	23:3:79:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:631:GLN:HG2	23:3:632:ALA:O	2.21	0.41
23:3:910:ALA:HB2	23:3:948:VAL:HG23	2.02	0.41
32:I:606:TRP:O	32:I:609:ALA:HB3	2.21	0.41
32:I:616:TYR:O	32:I:618:ARG:N	2.54	0.41
38:R:69:VAL:HG12	38:R:70:ALA:N	2.36	0.41
38:R:132:LEU:HD13	40:T:399:LYS:HE3	2.02	0.41
38:R:414:ARG:NH2	38:R:414:ARG:CB	2.73	0.41
40:T:209:CYS:O	40:T:221:THR:HA	2.21	0.41
40:T:210:ILE:HG12	40:T:221:THR:HG22	2.03	0.41
40:T:294:LEU:N	40:T:294:LEU:HD23	2.36	0.41
40:T:400:PHE:HD1	40:T:401:PRO:HA	1.86	0.41
42:V:530:LYS:C	42:V:532:GLN:N	2.74	0.41
43:W:298:PRO:O	43:W:299:LEU:CB	2.68	0.41
44:X:303:HIS:CB	44:X:383:ASP:HB3	2.51	0.41
45:Y:10:ILE:O	45:Y:13:LEU:N	2.53	0.41
45:Y:67:LEU:HA	45:Y:80:CYS:HA	2.02	0.41
46:Z:566:TYR:CE2	46:Z:584:TRP:HE3	2.29	0.41
1:A:293:TRP:CE3	1:A:293:TRP:C	2.94	0.41
1:A:842:ALA:HB1	1:A:920:ALA:HB1	2.03	0.41
1:A:1425:LYS:CB	38:R:417:ASN:OD1	2.69	0.41
1:A:1771:LEU:O	1:A:1777:ILE:HD12	2.20	0.41
1:A:1776:ILE:HD13	1:A:1813:ARG:HD3	2.03	0.41
3:C:149:LEU:HD11	3:C:427:PHE:CB	2.51	0.41
3:C:354:ARG:CG	3:C:354:ARG:HH11	2.34	0.41
13:F:42:C:C2	13:F:43:A:C8	3.09	0.41
21:1:1286:ARG:N	23:3:1006:GLN:HE22	2.19	0.41
23:3:274:ARG:HD2	23:3:389:PRO:HD3	2.02	0.41
25:5:14:PRO:O	25:5:17:VAL:HG22	2.21	0.41
28:J:423:GLU:OE1	28:J:423:GLU:HA	2.21	0.41
29:L:49:ARG:NH1	29:L:53:TRP:HB3	2.36	0.41
35:N:40:LYS:O	35:N:44:GLU:HB3	2.21	0.41
35:N:113:PHE:HD1	38:R:200:VAL:HG21	1.86	0.41
39:S:11:PRO:O	39:S:29:TRP:NE1	2.41	0.41
39:S:20:MET:CE	39:S:141:ARG:HD2	2.51	0.41
40:T:399:LYS:HB2	40:T:404:SER:HB3	2.03	0.41
40:T:434:GLY:HA2	40:T:464:GLY:N	2.36	0.41
42:V:585:ILE:O	42:V:588:GLN:N	2.54	0.41
1:A:121:HIS:C	1:A:123:THR:H	2.23	0.40
1:A:329:LEU:HD12	3:C:177:ARG:HG2	2.03	0.40
1:A:460:LYS:HZ1	2:B:49:A:P	2.41	0.40
1:A:593:ARG:CD	14:G:-4:A:H4'	2.43	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1528:GLN:HG3	1:A:1530:PRO:CD	2.51	0.40
1:A:1957:ASP:OD2	1:A:1959:THR:OG1	2.37	0.40
3:C:221:ILE:HG13	3:C:479:THR:OG1	2.21	0.40
3:C:235:VAL:HG13	3:C:239:THR:OG1	2.22	0.40
3:C:392:LEU:N	3:C:393:PRO:CD	2.84	0.40
4:D:419:GLY:C	4:D:421:HIS:H	2.25	0.40
5:E:178:LEU:CD2	5:E:208:ILE:HD11	2.51	0.40
5:E:257:ASN:ND2	43:W:149:SER:O	2.53	0.40
14:G:146:C:C4	14:G:147:C:N4	2.89	0.40
15:H:112:G:O5'	15:H:112:G:H8	2.04	0.40
21:1:498:MET:HE1	21:1:530:PRO:HB2	2.02	0.40
21:1:765:TYR:O	21:1:769:VAL:HG23	2.20	0.40
21:1:806:ILE:HG12	21:1:810:ILE:HD12	2.03	0.40
21:1:997:LEU:O	21:1:1001:VAL:HG23	2.21	0.40
21:1:1126:PHE:HA	21:1:1165:TYR:CZ	2.56	0.40
23:3:6:LEU:HD12	23:3:1128:ILE:HD11	2.03	0.40
23:3:194:ASN:O	23:3:196:PRO:HD3	2.21	0.40
23:3:259:LYS:HG3	23:3:266:ASP:CG	2.42	0.40
25:5:27:PRO:HG3	25:5:85:ARG:NH1	2.36	0.40
35:N:70:ILE:HG23	35:N:74:LEU:HD23	2.01	0.40
36:O:155:PRO:HD3	38:R:188:PHE:CE1	2.56	0.40
44:X:263:PRO:CG	44:X:265:LYS:H	2.34	0.40
46:Z:563:ARG:HH21	46:Z:563:ARG:HG3	1.83	0.40
1:A:1251:SER:O	1:A:1298:ARG:NH2	2.55	0.40
1:A:1263:TRP:CZ2	1:A:1292:GLU:HG2	2.56	0.40
1:A:1451:ASN:HB2	38:R:428:GLY:O	2.21	0.40
1:A:1529:ILE:HG13	1:A:1530:PRO:HD3	2.03	0.40
3:C:64:LYS:NZ	37:P:209:ARG:NH1	2.70	0.40
3:C:85:ASP:HA	40:T:238:LEU:HB3	2.03	0.40
3:C:534:VAL:HG12	3:C:535:ALA:N	2.31	0.40
13:F:42:C:H2'	13:F:43:A:O4'	2.21	0.40
15:H:2:U:H2'	15:H:3:C:C6	2.55	0.40
15:H:149:A:N3	15:H:150:U:C6	2.89	0.40
21:1:658:TRP:CZ3	21:1:700:LYS:HD2	2.55	0.40
21:1:935:THR:O	21:1:939:ARG:HG2	2.21	0.40
21:1:1126:PHE:HA	21:1:1165:TYR:CE2	2.56	0.40
22:2:614:ARG:O	22:2:618:GLY:N	2.51	0.40
22:2:648:LEU:O	22:2:649:LYS:HD3	2.21	0.40
23:3:983:ASN:HB2	23:3:1021:LEU:HB2	2.03	0.40
24:4:17:VAL:HG13	24:4:84:ILE:CG2	2.48	0.40
28:J:338:GLU:O	38:R:116:TYR:CD2	2.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:J:376:VAL:HG13	28:J:377:LYS:N	2.36	0.40
37:P:44:ARG:HG3	40:T:258:SER:CA	2.51	0.40
39:S:12:PRO:CD	39:S:166:GLY:HA2	2.51	0.40
39:S:25:LEU:HD12	39:S:25:LEU:N	2.36	0.40
39:S:55:ARG:HH12	43:W:96:GLU:HA	1.86	0.40
42:V:512:GLY:O	42:V:513:ARG:C	2.60	0.40
43:W:528:GLY:O	43:W:552:VAL:HA	2.21	0.40
44:X:238:THR:O	44:X:393:VAL:HG23	2.21	0.40
1:A:164:MET:CE	1:A:560:SER:HA	2.51	0.40
1:A:212:PRO:HD2	1:A:225:TYR:OH	2.21	0.40
1:A:652:LEU:HD23	1:A:652:LEU:HA	1.84	0.40
1:A:1057:ARG:O	1:A:1060:GLU:HB2	2.22	0.40
1:A:1273:TYR:HD2	1:A:1274:PHE:CD2	2.39	0.40
1:A:1342:TRP:CD2	3:C:921:LEU:HD21	2.50	0.40
1:A:1581:LEU:HD22	1:A:1746:ARG:NH1	2.36	0.40
1:A:2144:CYS:HB2	1:A:2270:PHE:CE1	2.57	0.40
3:C:375:GLU:N	3:C:376:PRO:HD2	2.37	0.40
5:E:255:MET:O	5:E:257:ASN:N	2.54	0.40
21:1:922:GLY:O	21:1:925:VAL:HG12	2.22	0.40
21:1:933:CYS:HA	21:1:936:VAL:HB	2.02	0.40
21:1:1130:PRO:HB3	22:2:528:ILE:HG23	2.04	0.40
23:3:63:ARG:HD2	23:3:83:ASP:HA	2.03	0.40
23:3:379:LEU:HB2	23:3:383:ASP:HB3	2.04	0.40
23:3:388:GLN:NE2	23:3:389:PRO:HD2	2.36	0.40
23:3:606:ALA:HA	23:3:616:ILE:HD13	2.04	0.40
39:S:15:TYR:CE2	39:S:22:ILE:HG21	2.57	0.40
39:S:65:GLY:O	39:S:110:SER:OG	2.40	0.40
40:T:339:GLN:CG	40:T:340:ALA:N	2.84	0.40
45:Y:37:TRP:HH2	46:Z:498:GLY:HA3	1.59	0.40
46:Z:491:ASP:O	46:Z:495:ALA:HB3	2.21	0.40
1:A:121:HIS:C	1:A:123:THR:N	2.74	0.40
1:A:372:PRO:CG	3:C:342:ARG:HG2	2.51	0.40
1:A:460:LYS:HA	1:A:460:LYS:HD2	1.94	0.40
1:A:938:PRO:O	1:A:941:LYS:HD3	2.22	0.40
1:A:2120:LEU:HD12	1:A:2120:LEU:H	1.86	0.40
3:C:229:ILE:HG12	3:C:239:THR:HG21	2.04	0.40
3:C:567:GLU:O	3:C:567:GLU:HG3	2.20	0.40
13:F:96:U:H2'	13:F:97:U:C6	2.56	0.40
21:1:1052:ALA:HA	21:1:1055:TRP:CD1	2.51	0.40
21:1:1248:GLN:NE2	23:3:1030:PRO:HD3	2.36	0.40
23:3:179:ASN:HB3	23:3:213:LEU:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:192:ALA:HA	23:3:200:ALA:HB3	2.02	0.40
23:3:464:ARG:NH1	23:3:473:TYR:OH	2.53	0.40
23:3:535:GLU:HG2	23:3:536:TRP:N	2.36	0.40
25:5:42:TYR:CZ	25:5:73:ALA:HA	2.56	0.40
38:R:89:GLN:HG2	39:S:155:ASP:OD2	2.21	0.40
39:S:100:MET:HE3	39:S:109:GLY:O	2.22	0.40
40:T:220:VAL:HG12	40:T:221:THR:N	2.37	0.40
1:A:109:PRO:HD3	1:A:630:TRP:HZ2	1.83	0.40
1:A:120:TYR:CE1	1:A:485:THR:CG2	3.04	0.40
1:A:460:LYS:O	1:A:462:ARG:HD2	2.22	0.40
1:A:692:ASP:HA	40:T:376:ARG:HH21	1.72	0.40
1:A:718:ARG:NH2	38:R:259:LYS:HG3	2.36	0.40
1:A:787:GLU:OE1	1:A:790:ARG:NH2	2.53	0.40
1:A:923:ASP:OD2	1:A:1439:ARG:HD3	2.22	0.40
1:A:1161:LEU:HD23	1:A:1161:LEU:HA	1.85	0.40
1:A:2195:THR:O	1:A:2199:ILE:HG12	2.21	0.40
1:A:2332:ASP:O	1:A:2334:TYR:N	2.54	0.40
2:B:20:G:C1'	2:B:21:A:OP1	2.69	0.40
2:B:57:G:C2'	2:B:58:U:H5'	2.51	0.40
3:C:259:LYS:HG3	51:C:1500:GTP:C5	2.57	0.40
3:C:592:VAL:HG12	3:C:603:MET:SD	2.62	0.40
3:C:673:LYS:HD3	3:C:673:LYS:H	1.86	0.40
3:C:738:ASP:N	3:C:738:ASP:OD1	2.54	0.40
3:C:926:ALA:N	3:C:927:PRO:CD	2.84	0.40
13:F:58:G:HO2'	13:F:59:G:P	2.44	0.40
21:1:570:TYR:O	21:1:574:ILE:HG12	2.22	0.40
21:1:839:GLU:O	21:1:842:ASN:HB2	2.22	0.40
21:1:1023:ILE:O	21:1:1026:ASN:HB2	2.21	0.40
23:3:561:GLY:O	23:3:582:GLU:HA	2.22	0.40
23:3:999:ARG:NE	23:3:1041:TYR:OH	2.54	0.40
32:I:365:ALA:CA	32:I:369:GLY:N	2.85	0.40
38:R:123:GLU:C	38:R:124:VAL:HG12	2.41	0.40
39:S:12:PRO:HB2	39:S:13:ASN:H	1.75	0.40
40:T:218:TRP:HZ3	40:T:220:VAL:CG2	2.35	0.40
44:X:231:ALA:O	44:X:236:THR:OG1	2.39	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	2224/2335 (95%)	2081 (94%)	115 (5%)	28 (1%)	10 42
3	C	854/972 (88%)	777 (91%)	57 (7%)	20 (2%)	5 28
4	D	1720/2136 (80%)	1632 (95%)	85 (5%)	3 (0%)	44 78
5	E	297/357 (83%)	272 (92%)	16 (5%)	9 (3%)	3 22
6	a	77/126 (61%)	76 (99%)	1 (1%)	0	100 100
6	h	76/126 (60%)	75 (99%)	1 (1%)	0	100 100
7	b	80/231 (35%)	78 (98%)	2 (2%)	0	100 100
7	i	84/231 (36%)	82 (98%)	2 (2%)	0	100 100
8	c	80/119 (67%)	77 (96%)	3 (4%)	0	100 100
8	j	80/119 (67%)	77 (96%)	3 (4%)	0	100 100
9	d	95/118 (80%)	91 (96%)	4 (4%)	0	100 100
9	k	81/118 (69%)	78 (96%)	3 (4%)	0	100 100
10	f	72/86 (84%)	69 (96%)	3 (4%)	0	100 100
10	m	72/86 (84%)	68 (94%)	4 (6%)	0	100 100
11	e	77/92 (84%)	76 (99%)	1 (1%)	0	100 100
11	l	77/92 (84%)	76 (99%)	1 (1%)	0	100 100
12	g	72/76 (95%)	70 (97%)	2 (3%)	0	100 100
12	n	64/76 (84%)	62 (97%)	2 (3%)	0	100 100
16	o	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	10 42
17	p	159/225 (71%)	138 (87%)	9 (6%)	12 (8%)	1 10
18	w	419/501 (84%)	378 (90%)	38 (9%)	3 (1%)	19 56
19	u	94/793 (12%)	87 (93%)	5 (5%)	2 (2%)	5 29
20	v	155/464 (33%)	125 (81%)	22 (14%)	8 (5%)	1 15
21	1	1022/1304 (78%)	897 (88%)	119 (12%)	6 (1%)	22 59
22	2	171/895 (19%)	154 (90%)	17 (10%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
23	3	1165/1217 (96%)	1086 (93%)	78 (7%)	1 (0%)	48 83
24	4	76/424 (18%)	69 (91%)	6 (8%)	1 (1%)	10 42
25	5	106/125 (85%)	90 (85%)	16 (15%)	0	100 100
26	6	83/110 (76%)	76 (92%)	7 (8%)	0	100 100
27	7	64/86 (74%)	55 (86%)	9 (14%)	0	100 100
28	J	483/848 (57%)	452 (94%)	24 (5%)	7 (1%)	9 40
29	L	324/802 (40%)	304 (94%)	18 (6%)	2 (1%)	22 59
30	q	130/504 (26%)	119 (92%)	7 (5%)	4 (3%)	3 22
30	r	129/504 (26%)	118 (92%)	9 (7%)	2 (2%)	8 37
30	s	65/504 (13%)	62 (95%)	2 (3%)	1 (2%)	8 39
30	t	65/504 (13%)	64 (98%)	0	1 (2%)	8 39
31	K	144/225 (64%)	134 (93%)	6 (4%)	4 (3%)	4 24
32	I	498/855 (58%)	479 (96%)	11 (2%)	8 (2%)	8 37
33	Q	1297/1485 (87%)	1271 (98%)	26 (2%)	0	100 100
34	M	34/343 (10%)	30 (88%)	3 (9%)	1 (3%)	3 23
35	N	141/144 (98%)	126 (89%)	12 (8%)	3 (2%)	5 29
36	O	283/420 (67%)	247 (87%)	26 (9%)	10 (4%)	3 20
37	P	92/229 (40%)	82 (89%)	8 (9%)	2 (2%)	5 29
38	R	295/540 (55%)	249 (84%)	31 (10%)	15 (5%)	1 15
39	S	157/166 (95%)	144 (92%)	10 (6%)	3 (2%)	6 32
40	T	311/514 (60%)	282 (91%)	17 (6%)	12 (4%)	2 18
41	U	24/2752 (1%)	20 (83%)	3 (12%)	1 (4%)	2 17
42	V	444/908 (49%)	412 (93%)	27 (6%)	5 (1%)	12 46
43	W	475/579 (82%)	419 (88%)	32 (7%)	24 (5%)	1 15
44	X	143/396 (36%)	133 (93%)	10 (7%)	0	100 100
45	Y	103/322 (32%)	92 (89%)	11 (11%)	0	100 100
46	Z	109/619 (18%)	93 (85%)	10 (9%)	6 (6%)	1 15
47	z	176/472 (37%)	170 (97%)	6 (3%)	0	100 100
48	x	562/1041 (54%)	537 (96%)	20 (4%)	5 (1%)	14 50
49	y	224/301 (74%)	217 (97%)	7 (3%)	0	100 100
All	All	16564/29872 (55%)	15374 (93%)	979 (6%)	211 (1%)	13 42

All (211) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	ARG
1	A	92	LEU
1	A	167	PRO
1	A	188	LEU
1	A	331	TRP
1	A	346	ASP
1	A	383	PHE
1	A	570	ASP
1	A	629	PHE
1	A	701	ILE
3	C	388	VAL
3	C	427	PHE
3	C	444	GLY
3	C	457	VAL
3	C	458	ASP
3	C	516	LEU
3	C	824	THR
4	D	957	VAL
4	D	1584	ILE
5	E	193	THR
17	p	157	ASN
17	p	183	VAL
17	p	195	GLU
18	w	284	ARG
20	v	139	PRO
20	v	162	PRO
20	v	165	ARG
20	v	218	PRO
28	J	413	GLU
30	q	59	HIS
30	q	60	PRO
30	s	71	ILE
30	t	69	THR
31	K	78	PRO
31	K	90	PRO
32	I	463	PRO
32	I	721	LYS
32	I	797	PHE
35	N	36	PRO
36	O	20	PHE
36	O	107	MET
36	O	225	PRO

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Mol	Chain	Res	Type
36	O	226	PRO
37	P	49	ASP
38	R	71	GLN
38	R	135	PRO
38	R	136	ASP
38	R	186	VAL
38	R	412	ASP
38	R	416	PHE
38	R	420	LYS
38	R	425	GLY
39	S	164	PRO
40	T	186	PRO
40	T	268	LYS
40	T	341	ALA
40	T	343	PRO
40	T	495	ALA
42	V	596	LEU
42	V	597	PRO
43	W	156	VAL
43	W	199	TYR
43	W	213	GLN
43	W	243	VAL
43	W	258	PRO
43	W	259	GLN
43	W	263	VAL
43	W	267	SER
43	W	279	LYS
43	W	299	LEU
43	W	325	LEU
43	W	372	ASN
43	W	492	ASN
46	Z	499	LYS
46	Z	531	LEU
46	Z	536	ARG
46	Z	569	PRO
48	x	937	ILE
1	A	122	ILE
1	A	308	ILE
1	A	349	ALA
1	A	370	PRO
1	A	374	ASP
1	A	631	ALA

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Mol	Chain	Res	Type
3	C	90	THR
3	C	364	SER
3	C	572	GLU
3	C	711	ARG
16	o	160	LYS
17	p	159	PRO
17	p	160	GLU
17	p	177	PHE
17	p	186	ARG
19	u	280	VAL
20	v	115	PRO
21	1	112	ILE
28	J	217	GLU
28	J	341	PRO
28	J	376	VAL
28	J	709	VAL
30	q	9	ASN
32	I	618	ARG
32	I	634	ILE
35	N	39	GLY
36	O	132	ARG
36	O	206	ASN
37	P	190	ASP
38	R	191	GLY
38	R	422	MET
39	S	12	PRO
40	T	301	ASP
41	U	2	TYR
42	V	485	GLN
43	W	191	GLY
43	W	318	VAL
43	W	482	ASP
46	Z	613	LYS
1	A	51	PHE
1	A	212	PRO
1	A	378	PHE
1	A	699	GLU
5	E	60	MET
5	E	88	ARG
5	E	256	ASP
17	p	222	TYR
18	w	177	ARG

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Mol	Chain	Res	Type
30	q	19	PRO
30	r	9	ASN
32	I	601	GLN
32	I	752	ALA
34	M	197	TYR
36	O	222	ARG
38	R	104	GLN
38	R	173	PRO
40	T	406	ILE
42	V	578	SER
43	W	102	GLN
48	x	1005	SER
1	A	363	HIS
1	A	480	LYS
1	A	698	PRO
1	A	1092	ILE
1	A	1828	ALA
3	C	63	LYS
3	C	754	VAL
3	C	856	HIS
5	E	162	ARG
16	o	32	PRO
17	p	208	GLN
17	p	209	GLY
21	1	417	PRO
21	1	456	VAL
28	J	604	PRO
29	L	585	TYR
31	K	65	ILE
32	I	617	GLU
36	O	134	VAL
36	O	230	THR
38	R	124	VAL
39	S	10	GLN
40	T	401	PRO
43	W	272	GLU
43	W	554	ILE
48	x	935	ASP
1	A	359	ILE
3	C	361	PRO
3	C	615	PRO
5	E	159	PRO

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Mol	Chain	Res	Type
20	v	217	PRO
36	O	239	LEU
38	R	126	ASN
38	R	423	ASP
40	T	185	MET
40	T	189	GLN
40	T	226	ARG
43	W	301	GLY
43	W	330	GLY
48	x	980	GLN
48	x	981	PRO
3	C	94	ILE
3	C	360	ALA
3	C	623	GLU
5	E	270	LYS
17	p	173	GLN
20	v	141	ILE
20	v	220	PRO
21	1	944	SER
29	L	215	PRO
42	V	609	GLN
43	W	376	PRO
43	W	549	HIS
3	C	66	TYR
5	E	149	GLY
46	Z	571	PRO
1	A	186	GLU
19	u	221	PRO
31	K	17	PRO
1	A	384	VAL
18	w	229	TRP
21	1	418	PRO
24	4	27	PRO
28	J	241	VAL
40	T	411	GLY
43	W	270	PRO
4	D	585	ILE
5	E	324	PRO
17	p	184	PRO
30	r	60	PRO
35	N	4	VAL
21	1	932	ILE

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Mol	Chain	Res	Type
23	3	491	VAL

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	2001/2108 (95%)	1902 (95%)	99 (5%)	21 42
3	C	745/866 (86%)	677 (91%)	68 (9%)	7 24
5	E	256/300 (85%)	244 (95%)	12 (5%)	22 44
18	w	49/446 (11%)	47 (96%)	2 (4%)	26 47
20	v	30/382 (8%)	28 (93%)	2 (7%)	13 34
21	1	735/1104 (67%)	735 (100%)	0	100 100
22	2	94/776 (12%)	90 (96%)	4 (4%)	25 46
23	3	1018/1051 (97%)	1017 (100%)	1 (0%)	92 95
24	4	39/336 (12%)	37 (95%)	2 (5%)	20 41
25	5	74/109 (68%)	74 (100%)	0	100 100
26	6	73/95 (77%)	73 (100%)	0	100 100
27	7	57/77 (74%)	57 (100%)	0	100 100
28	J	205/751 (27%)	194 (95%)	11 (5%)	18 40
29	L	131/709 (18%)	122 (93%)	9 (7%)	13 33
31	K	54/196 (28%)	49 (91%)	5 (9%)	7 23
34	M	25/294 (8%)	24 (96%)	1 (4%)	27 48
35	N	130/130 (100%)	125 (96%)	5 (4%)	28 49
36	O	250/361 (69%)	239 (96%)	11 (4%)	24 46
37	P	90/203 (44%)	77 (86%)	13 (14%)	2 13
38	R	220/463 (48%)	170 (77%)	50 (23%)	0 5
39	S	129/134 (96%)	119 (92%)	10 (8%)	10 29
40	T	268/441 (61%)	251 (94%)	17 (6%)	15 36
41	U	21/2432 (1%)	16 (76%)	5 (24%)	0 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
44	X	52/349 (15%)	46 (88%)	6 (12%)	4 17
45	Y	57/291 (20%)	56 (98%)	1 (2%)	54 71
46	Z	47/545 (9%)	39 (83%)	8 (17%)	1 9
47	z	146/416 (35%)	146 (100%)	0	100 100
48	x	1/897 (0%)	1 (100%)	0	100 100
All	All	6997/16262 (43%)	6655 (95%)	342 (5%)	23 42

All (342) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	48	LYS
1	A	49	ARG
1	A	50	LYS
1	A	55	ASP
1	A	59	GLU
1	A	60	ASP
1	A	75	ASP
1	A	77	THR
1	A	78	ASN
1	A	82	ARG
1	A	86	ARG
1	A	88	TYR
1	A	89	LEU
1	A	152	ARG
1	A	163	ARG
1	A	177	ASP
1	A	181	ASN
1	A	185	VAL
1	A	204	LEU
1	A	233	PRO
1	A	250	VAL
1	A	258	PHE
1	A	284	ARG
1	A	294	ASN
1	A	295	GLU
1	A	325	HIS
1	A	330	THR
1	A	331	TRP
1	A	336	ASN

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Mol	Chain	Res	Type
1	A	344	ASP
1	A	352	PHE
1	A	359	ILE
1	A	362	ARG
1	A	363	HIS
1	A	364	SER
1	A	366	LYS
1	A	371	LEU
1	A	377	GLU
1	A	382	GLU
1	A	383	PHE
1	A	389	LYS
1	A	391	THR
1	A	394	TYR
1	A	409	ARG
1	A	413	LEU
1	A	433	GLU
1	A	459	LEU
1	A	462	ARG
1	A	467	GLN
1	A	468	LYS
1	A	535	ARG
1	A	546	LEU
1	A	579	GLN
1	A	606	LYS
1	A	627	CYS
1	A	630	TRP
1	A	671	THR
1	A	673	THR
1	A	674	LYS
1	A	675	GLN
1	A	679	SER
1	A	1163	ARG
1	A	1425	LYS
1	A	1549	VAL
1	A	1930	TYR
1	A	2067	PHE
1	A	2073	TRP
1	A	2074	ARG
1	A	2078	ILE
1	A	2085	LEU
1	A	2087	THR

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Mol	Chain	Res	Type
1	A	2090	ILE
1	A	2103	THR
1	A	2108	LYS
1	A	2117	ILE
1	A	2143	ARG
1	A	2156	THR
1	A	2157	VAL
1	A	2159	LEU
1	A	2171	GLU
1	A	2193	VAL
1	A	2194	THR
1	A	2219	THR
1	A	2223	CYS
1	A	2233	SER
1	A	2239	ARG
1	A	2242	THR
1	A	2254	SER
1	A	2259	VAL
1	A	2261	MET
1	A	2273	VAL
1	A	2284	MET
1	A	2293	LYS
1	A	2298	LEU
1	A	2310	ARG
1	A	2312	SER
1	A	2319	LEU
1	A	2329	ASP
3	C	61	GLU
3	C	62	ASP
3	C	63	LYS
3	C	64	LYS
3	C	66	TYR
3	C	68	THR
3	C	71	GLU
3	C	79	THR
3	C	97	VAL
3	C	131	ASN
3	C	227	LEU
3	C	256	CYS
3	C	259	LYS
3	C	295	ASP
3	C	296	GLU

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Mol	Chain	Res	Type
3	C	297	ASN
3	C	298	LEU
3	C	300	LEU
3	C	333	ASP
3	C	336	TYR
3	C	354	ARG
3	C	359	LYS
3	C	362	THR
3	C	366	GLN
3	C	387	ASP
3	C	389	ASP
3	C	427	PHE
3	C	428	THR
3	C	438	ILE
3	C	446	LYS
3	C	452	THR
3	C	454	THR
3	C	457	VAL
3	C	458	ASP
3	C	459	SER
3	C	463	GLU
3	C	468	CYS
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	512	GLU
3	C	517	GLU
3	C	519	GLU
3	C	571	ASN
3	C	572	GLU
3	C	573	GLU
3	C	596	ASN
3	C	673	LYS
3	C	675	PHE
3	C	677	GLU
3	C	704	VAL
3	C	706	GLN
3	C	709	TRP
3	C	712	LYS

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Mol	Chain	Res	Type
3	C	724	TRP
3	C	725	ASP
3	C	730	ARG
3	C	738	ASP
3	C	749	THR
3	C	750	LEU
3	C	763	LYS
3	C	826	ARG
3	C	856	HIS
3	C	941	LYS
3	C	943	LEU
5	E	74	PHE
5	E	153	PHE
5	E	161	ARG
5	E	229	TYR
5	E	243	LEU
5	E	248	SER
5	E	250	LEU
5	E	265	ARG
5	E	270	LYS
5	E	271	GLU
5	E	289	LEU
5	E	290	ARG
18	w	419	PRO
18	w	441	PRO
20	v	18	SER
20	v	56	CYS
22	2	498	VAL
22	2	520	PRO
22	2	614	ARG
22	2	616	SER
23	3	442	LEU
24	4	27	PRO
24	4	83	PRO
28	J	217	GLU
28	J	218	GLU
28	J	219	GLU
28	J	221	ASN
28	J	229	LYS
28	J	239	ARG
28	J	281	LYS
28	J	308	ARG

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Mol	Chain	Res	Type
28	J	363	ARG
28	J	410	HIS
28	J	411	MET
29	L	219	LYS
29	L	222	LEU
29	L	227	THR
29	L	228	SER
29	L	235	LEU
29	L	731	LEU
29	L	761	SER
29	L	766	ARG
29	L	781	GLU
31	K	38	GLU
31	K	90	PRO
31	K	117	GLN
31	K	126	LEU
31	K	171	GLN
34	M	221	HIS
35	N	24	GLU
35	N	41	ARG
35	N	42	LYS
35	N	116	ASN
35	N	125	LYS
36	O	45	CYS
36	O	69	GLU
36	O	74	CYS
36	O	115	GLU
36	O	150	LEU
36	O	220	MET
36	O	223	LEU
36	O	225	PRO
36	O	226	PRO
36	O	228	ASP
36	O	229	LYS
37	P	28	LYS
37	P	29	GLN
37	P	30	TYR
37	P	33	ARG
37	P	66	ARG
37	P	67	GLU
37	P	76	ARG
37	P	78	ARG

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Mol	Chain	Res	Type
37	P	188	TRP
37	P	190	ASP
37	P	191	ASP
37	P	212	ASN
37	P	224	MET
38	R	56	GLU
38	R	66	GLU
38	R	71	GLN
38	R	72	TYR
38	R	75	ASP
38	R	80	LYS
38	R	81	LYS
38	R	82	MET
38	R	86	LEU
38	R	89	GLN
38	R	92	SER
38	R	95	LYS
38	R	103	ARG
38	R	104	GLN
38	R	106	GLN
38	R	118	ASP
38	R	122	LYS
38	R	125	MET
38	R	128	ASP
38	R	129	ASP
38	R	137	GLU
38	R	158	LYS
38	R	170	LYS
38	R	171	LEU
38	R	175	GLN
38	R	181	PRO
38	R	183	GLN
38	R	186	VAL
38	R	188	PHE
38	R	189	ASN
38	R	195	ARG
38	R	211	ARG
38	R	212	PHE
38	R	213	LYS
38	R	214	ILE
38	R	215	ASN
38	R	220	ARG

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Mol	Chain	Res	Type
38	R	233	HIS
38	R	245	GLU
38	R	250	LYS
38	R	403	PRO
38	R	409	VAL
38	R	411	TYR
38	R	415	LEU
38	R	418	GLN
38	R	420	LYS
38	R	422	MET
38	R	426	PHE
38	R	434	TYR
38	R	435	ASN
39	S	10	GLN
39	S	15	TYR
39	S	91	LYS
39	S	100	MET
39	S	102	ASN
39	S	108	ASN
39	S	125	LYS
39	S	129	PHE
39	S	131	ARG
39	S	133	CYS
40	T	257	ARG
40	T	282	ARG
40	T	308	ARG
40	T	318	ARG
40	T	387	PHE
40	T	399	LYS
40	T	400	PHE
40	T	401	PRO
40	T	402	ASP
40	T	412	HIS
40	T	416	ILE
40	T	418	THR
40	T	455	GLN
40	T	460	ASP
40	T	461	SER
40	T	463	SER
40	T	478	LEU
41	U	1	MET
41	U	11	ARG

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Mol	Chain	Res	Type
41	U	20	GLN
41	U	23	LEU
41	U	25	LEU
44	X	209	PRO
44	X	224	PRO
44	X	249	PRO
44	X	263	PRO
44	X	293	PRO
44	X	297	PRO
45	Y	44	PRO
46	Z	524	ARG
46	Z	526	ILE
46	Z	563	ARG
46	Z	569	PRO
46	Z	597	ARG
46	Z	598	PHE
46	Z	600	ARG
46	Z	613	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (111) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	73	HIS
1	A	78	ASN
1	A	97	HIS
1	A	210	HIS
1	A	270	ASN
1	A	297	ASN
1	A	325	HIS
1	A	448	GLN
1	A	573	GLN
1	A	584	HIS
1	A	601	GLN
1	A	675	GLN
1	A	775	ASN
1	A	924	GLN
1	A	1024	HIS
1	A	1069	ASN
1	A	1075	GLN
1	A	1096	HIS
1	A	1217	GLN

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Mol	Chain	Res	Type
1	A	1293	ASN
1	A	1296	GLN
1	A	1337	GLN
1	A	1359	HIS
1	A	1458	GLN
1	A	1460	HIS
1	A	1527	ASN
1	A	1580	HIS
1	A	1717	ASN
1	A	1784	ASN
1	A	1966	HIS
1	A	2123	GLN
1	A	2300	ASN
1	A	2306	HIS
3	C	87	GLN
3	C	245	HIS
3	C	297	ASN
3	C	437	HIS
3	C	513	ASN
3	C	575	GLN
3	C	583	ASN
3	C	596	ASN
3	C	706	GLN
3	C	924	GLN
5	E	165	GLN
18	w	425	HIS
18	w	485	ASN
20	v	23	ASN
20	v	78	HIS
21	1	473	GLN
21	1	599	ASN
21	1	903	GLN
21	1	942	ASN
21	1	1026	ASN
21	1	1186	GLN
21	1	1209	ASN
21	1	1248	GLN
21	1	1277	GLN
22	2	490	HIS
23	3	21	ASN
23	3	104	GLN
23	3	254	ASN

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Mol	Chain	Res	Type
23	3	264	GLN
23	3	293	HIS
23	3	304	GLN
23	3	388	GLN
23	3	440	HIS
23	3	518	GLN
23	3	775	ASN
23	3	870	ASN
23	3	1087	GLN
28	J	221	ASN
28	J	259	GLN
28	J	294	HIS
28	J	351	ASN
29	L	39	HIS
29	L	73	HIS
31	K	117	GLN
31	K	171	GLN
35	N	27	GLN
35	N	37	HIS
35	N	99	ASN
35	N	107	GLN
36	O	163	HIS
36	O	196	GLN
36	O	254	GLN
36	O	268	GLN
36	O	294	ASN
37	P	212	ASN
37	P	220	HIS
38	R	104	GLN
38	R	106	GLN
38	R	126	ASN
38	R	189	ASN
38	R	194	GLN
38	R	215	ASN
38	R	233	HIS
38	R	283	HIS
38	R	418	GLN
40	T	217	GLN
40	T	278	ASN
40	T	297	HIS
40	T	413	ASN
40	T	417	ASN

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Mol	Chain	Res	Type
40	T	446	ASN
40	T	451	HIS
40	T	455	GLN
44	X	307	GLN
45	Y	87	GLN
47	z	112	GLN
47	z	127	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	F	91/107 (85%)	37 (40%)	12 (13%)
14	G	76/274 (27%)	48 (63%)	9 (11%)
15	H	130/188 (69%)	33 (25%)	4 (3%)
2	B	82/117 (70%)	19 (23%)	10 (12%)
All	All	379/686 (55%)	137 (36%)	35 (9%)

All (137) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	12	U
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	24	G
2	B	25	C
2	B	26	A
2	B	28	A
2	B	36	C
2	B	38	C
2	B	40	U
2	B	41	U
2	B	45	C
2	B	57	G
2	B	70	A
2	B	71	C
13	F	6	C
13	F	7	G

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Mol	Chain	Res	Type
13	F	8	C
13	F	10	U
13	F	12	G
13	F	25	C
13	F	26	U
13	F	27	A
13	F	28	A
13	F	29	A
13	F	33	G
13	F	34	G
13	F	36	A
13	F	37	C
13	F	38	G
13	F	44	G
13	F	45	A
13	F	46	G
13	F	47	A
13	F	48	A
13	F	49	G
13	F	51	U
13	F	54	G
13	F	55	C
13	F	56	A
13	F	58	G
13	F	59	G
13	F	60	C
13	F	61	C
13	F	62	C
13	F	68	C
13	F	74	U
13	F	78	A
13	F	79	C
13	F	85	U
13	F	86	U
13	F	87	C
14	G	-11	G
14	G	-6	C
14	G	-4	A
14	G	-3	A
14	G	1	G
14	G	2	U
14	G	3	A

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Mol	Chain	Res	Type
14	G	4	A
14	G	5	G
14	G	7	G
14	G	8	C
14	G	10	U
14	G	11	A
14	G	12	G
14	G	13	C
14	G	17	U
14	G	21	A
14	G	22	C
14	G	23	U
14	G	24	G
14	G	25	G
14	G	26	U
14	G	27	U
14	G	28	A
14	G	29	C
14	G	30	C
14	G	31	U
14	G	131	U
14	G	132	G
14	G	135	G
14	G	136	U
14	G	137	C
14	G	143	U
14	G	144	A
14	G	145	U
14	G	146	C
14	G	147	C
14	G	148	U
14	G	149	G
14	G	150	U
14	G	151	C
14	G	152	C
14	G	154	U
14	G	156	U
14	G	159	U
14	G	161	U
14	G	162	C
14	G	163	C
15	H	14	C

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Mol	Chain	Res	Type
15	H	20	G
15	H	23	A
15	H	24	A
15	H	25	G
15	H	29	A
15	H	30	A
15	H	31	G
15	H	44	U
15	H	45	C
15	H	46	U
15	H	47	U
15	H	48	A
15	H	65	U
15	H	112	G
15	H	143	A
15	H	147	G
15	H	149	A
15	H	152	G
15	H	153	A
15	H	154	C
15	H	156	U
15	H	157	G
15	H	160	A
15	H	163	G
15	H	164	C
15	H	166	G
15	H	167	U
15	H	169	C
15	H	177	A
15	H	178	A
15	H	179	C
15	H	183	G

All (35) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	12	U
2	B	18	C
2	B	19	A
2	B	20	G
2	B	23	C
2	B	24	G

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Mol	Chain	Res	Type
2	B	25	C
2	B	27	U
2	B	39	C
2	B	40	U
13	F	5	U
13	F	7	G
13	F	25	C
13	F	33	G
13	F	35	A
13	F	36	A
13	F	37	C
13	F	47	A
13	F	48	A
13	F	50	A
13	F	58	G
13	F	59	G
14	G	-12	G
14	G	16	G
14	G	21	A
14	G	22	C
14	G	136	U
14	G	148	U
14	G	151	C
14	G	153	C
14	G	155	U
15	H	29	A
15	H	46	U
15	H	47	U
15	H	156	U

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 21 ligands modelled in this entry, 19 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	$\#\|Z\| > 2$
51	GTP	C	1500	52	26,34,34	1.18	1 (3%)	32,54,54	1.81	8 (25%)
50	IHP	A	3000	-	36,36,36	1.01	2 (5%)	54,60,60	1.62	12 (22%)

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
51	GTP	C	1500	52	-	7/18/38/38	0/3/3/3
50	IHP	A	3000	-	-	6/30/54/54	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	C	1500	GTP	C6-N1	-3.52	1.32	1.37
50	A	3000	IHP	P5-O45	-2.86	1.43	1.54
50	A	3000	IHP	P2-O12	2.65	1.64	1.59

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	A	3000	IHP	O45-P5-O35	4.10	123.30	107.64
50	A	3000	IHP	O35-P5-O15	-3.97	88.19	105.99
51	C	1500	GTP	C5-C6-N1	3.79	120.64	113.95
51	C	1500	GTP	PA-O3A-PB	-3.79	119.84	132.83
51	C	1500	GTP	O6-C6-C5	-3.73	117.08	124.37
50	A	3000	IHP	O16-C6-C1	3.32	116.50	108.69
50	A	3000	IHP	C6-C1-C2	-3.22	103.37	110.41
51	C	1500	GTP	PB-O3B-PG	-3.16	121.97	132.83
51	C	1500	GTP	C2-N1-C6	-3.02	119.53	125.10
51	C	1500	GTP	O2G-PG-O3B	2.89	114.34	104.64
50	A	3000	IHP	O44-P4-O34	2.73	118.06	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	A	3000	IHP	C5-C6-C1	-2.65	104.62	110.41
51	C	1500	GTP	C3'-C2'-C1'	2.32	104.47	100.98
51	C	1500	GTP	O4'-C4'-C3'	2.30	109.66	105.11
50	A	3000	IHP	O35-P5-O25	2.25	119.48	110.68
50	A	3000	IHP	O12-C2-C3	2.14	113.74	108.69
50	A	3000	IHP	O15-C5-C4	-2.13	103.66	108.69
50	A	3000	IHP	O42-P2-O22	2.10	118.91	110.68
50	A	3000	IHP	O31-P1-O11	-2.09	96.62	105.99
50	A	3000	IHP	C4-C3-C2	2.08	114.96	110.41

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
50	A	3000	IHP	C4-C5-O15-P5
50	A	3000	IHP	C6-C5-O15-P5
51	C	1500	GTP	PB-O3B-PG-O3G
51	C	1500	GTP	C5'-O5'-PA-O3A
51	C	1500	GTP	C5'-O5'-PA-O1A
51	C	1500	GTP	C5'-O5'-PA-O2A
51	C	1500	GTP	O4'-C4'-C5'-O5'
51	C	1500	GTP	C3'-C4'-C5'-O5'
50	A	3000	IHP	C2-O12-P2-O22
50	A	3000	IHP	C1-O11-P1-O21
50	A	3000	IHP	C1-O11-P1-O31
50	A	3000	IHP	C5-O15-P5-O35
51	C	1500	GTP	PG-O3B-PB-O2B

There are no ring outliers.

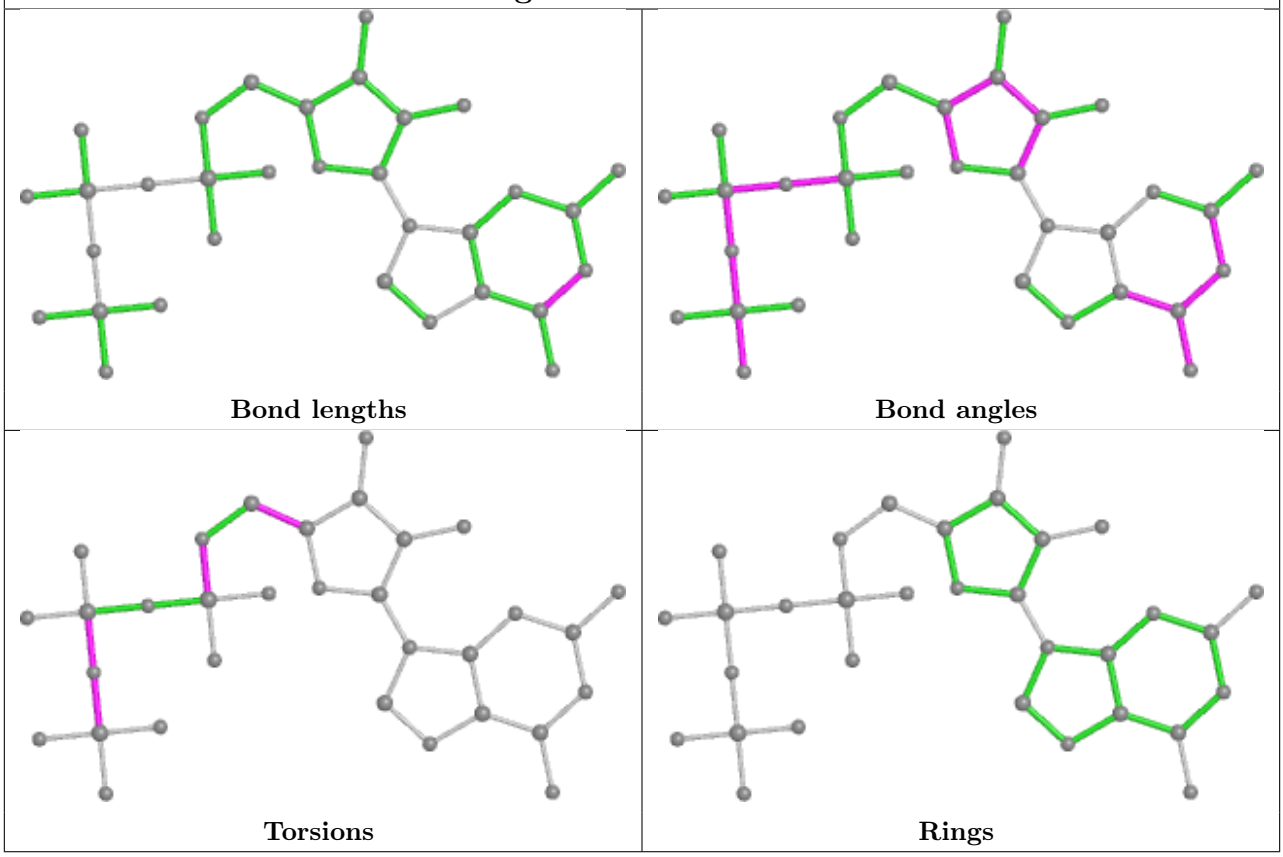
2 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	C	1500	GTP	11	0
50	A	3000	IHP	10	0

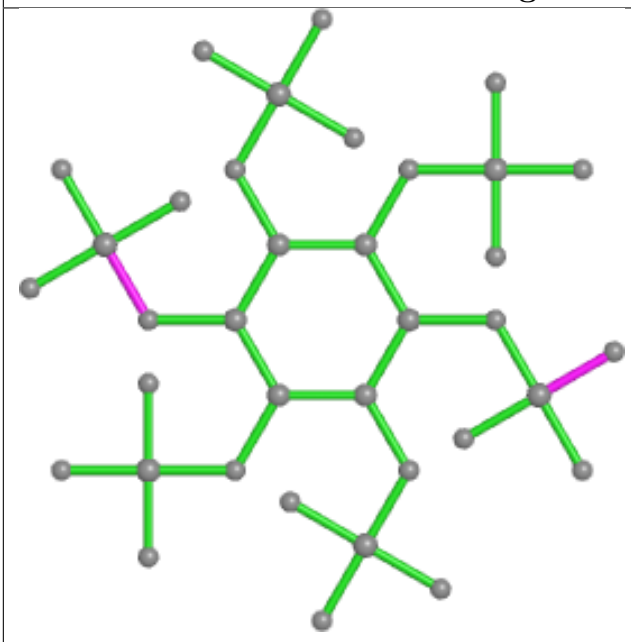
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

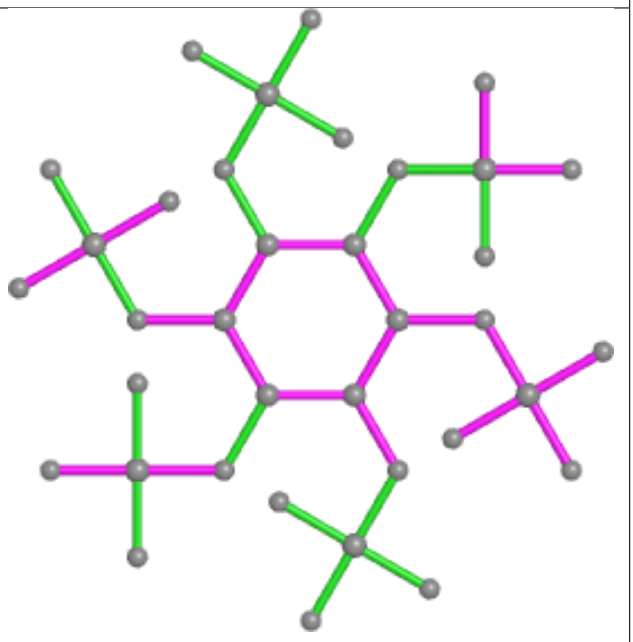
Ligand GTP C 1500



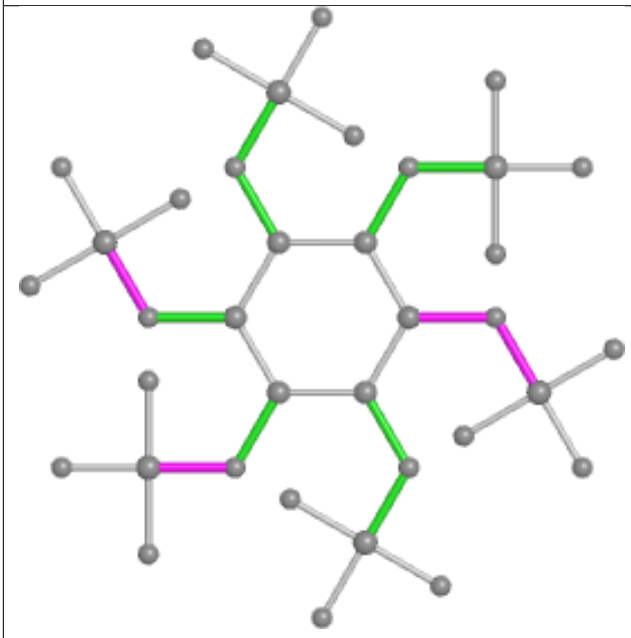
Ligand IHP A 3000



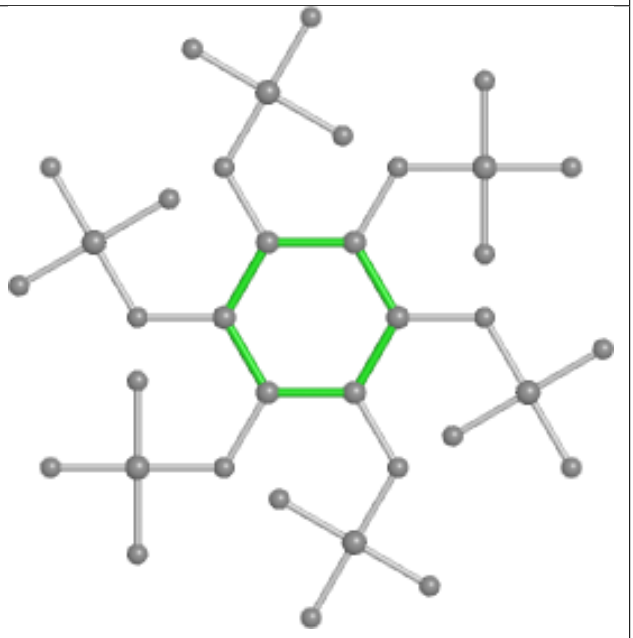
Bond lengths



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.

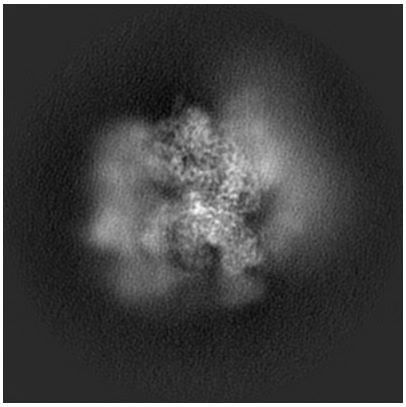
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6889. These allow visual inspection of the internal detail of the map and identification of artifacts.

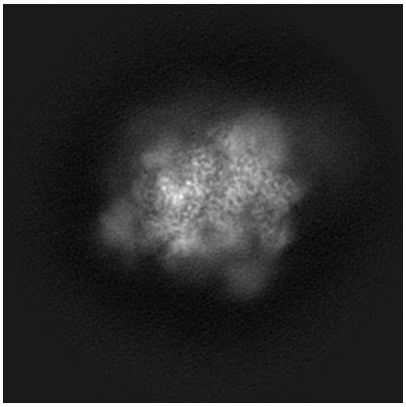
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

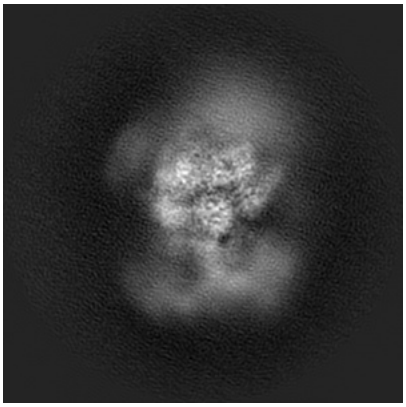
6.1.1 Primary map



X



Y

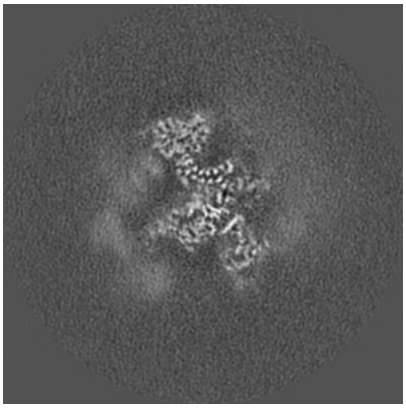


Z

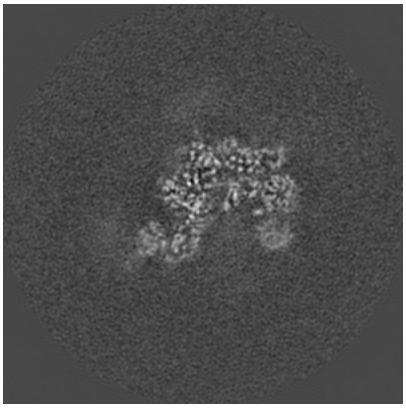
The images above show the map projected in three orthogonal directions.

6.2 Central slices

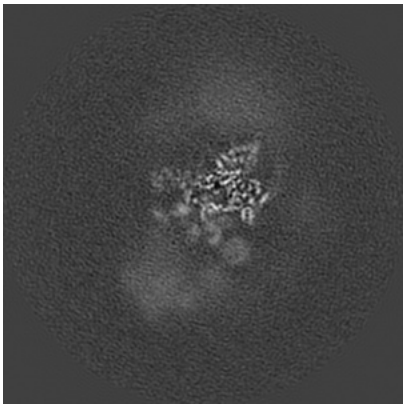
6.2.1 Primary map



X Index: 200



Y Index: 200

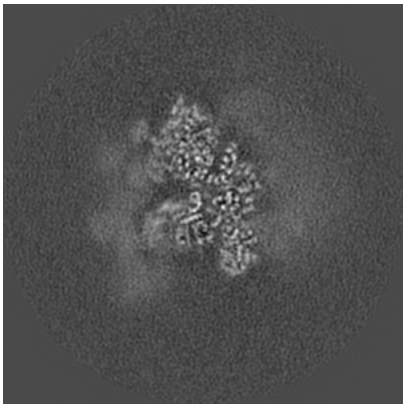


Z Index: 200

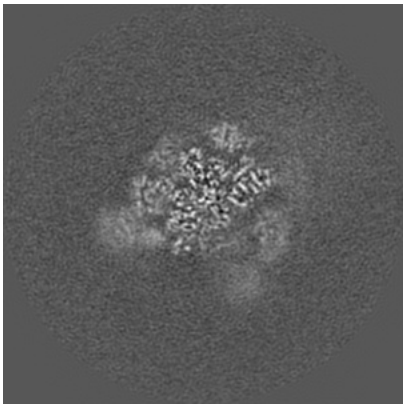
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

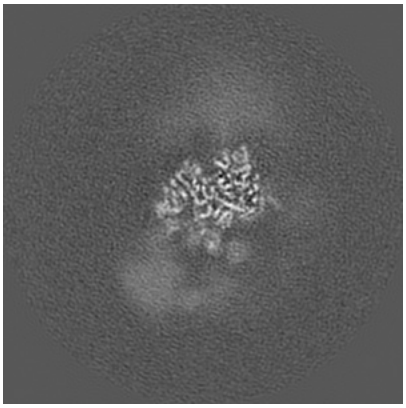
6.3.1 Primary map



X Index: 212



Y Index: 225

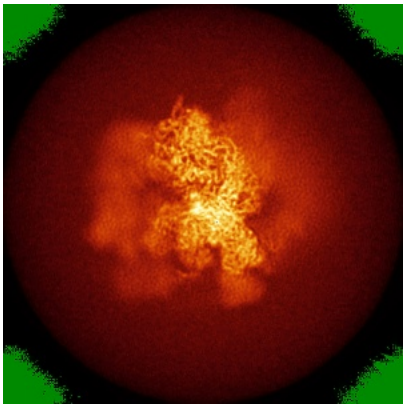


Z Index: 192

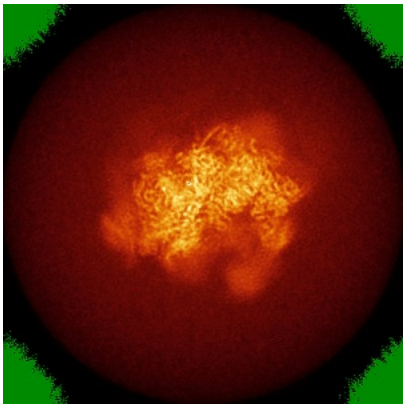
The images above show the largest variance slices of the map in three orthogonal directions.

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

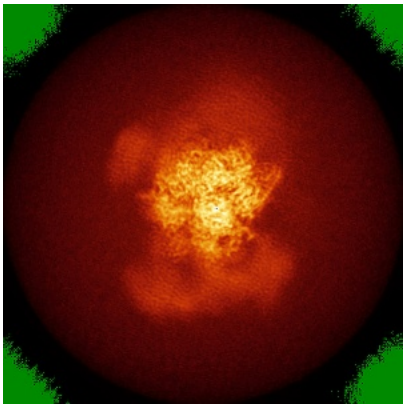
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0374. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

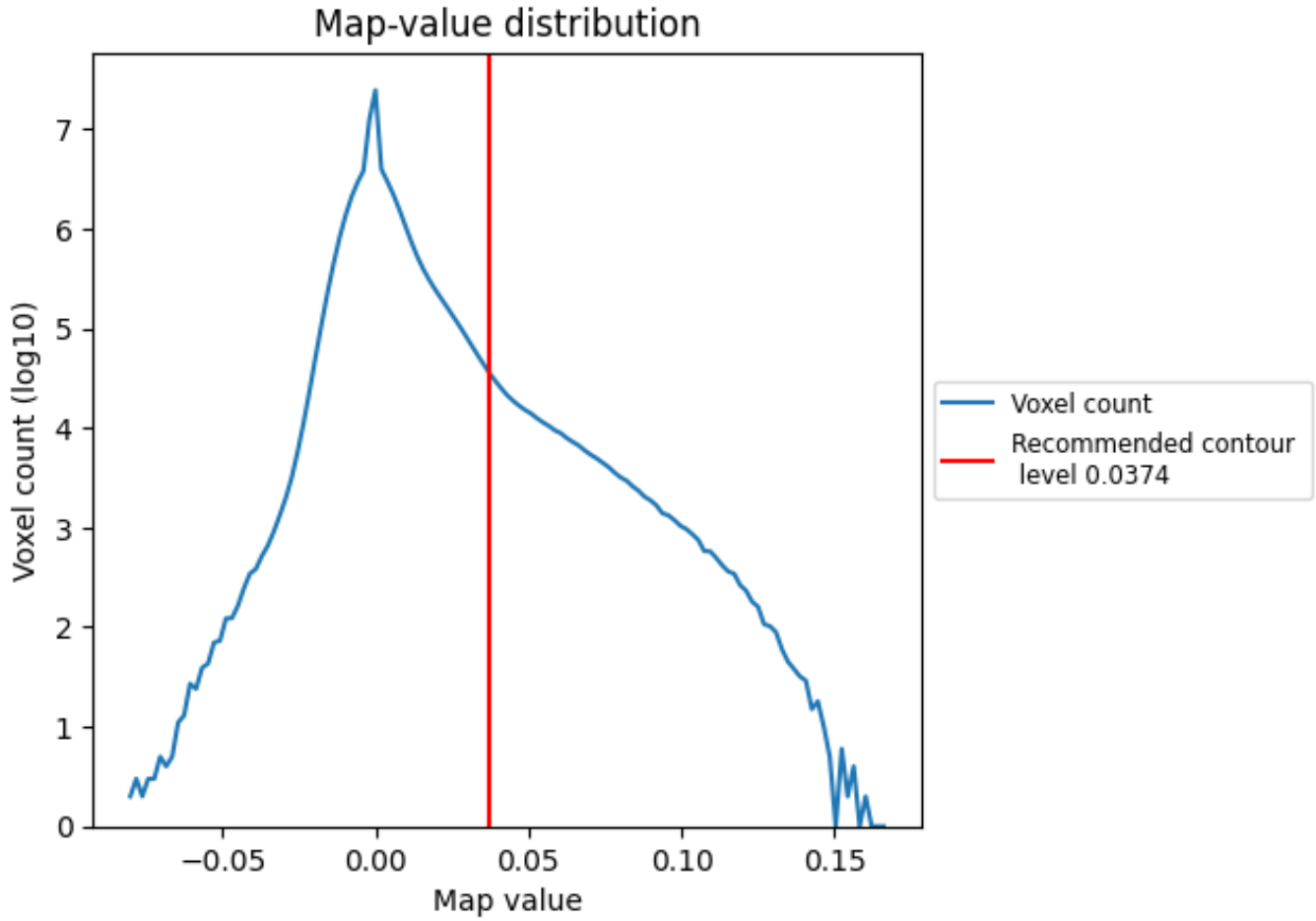
6.6 Mask visualisation (i)

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

7 Map analysis

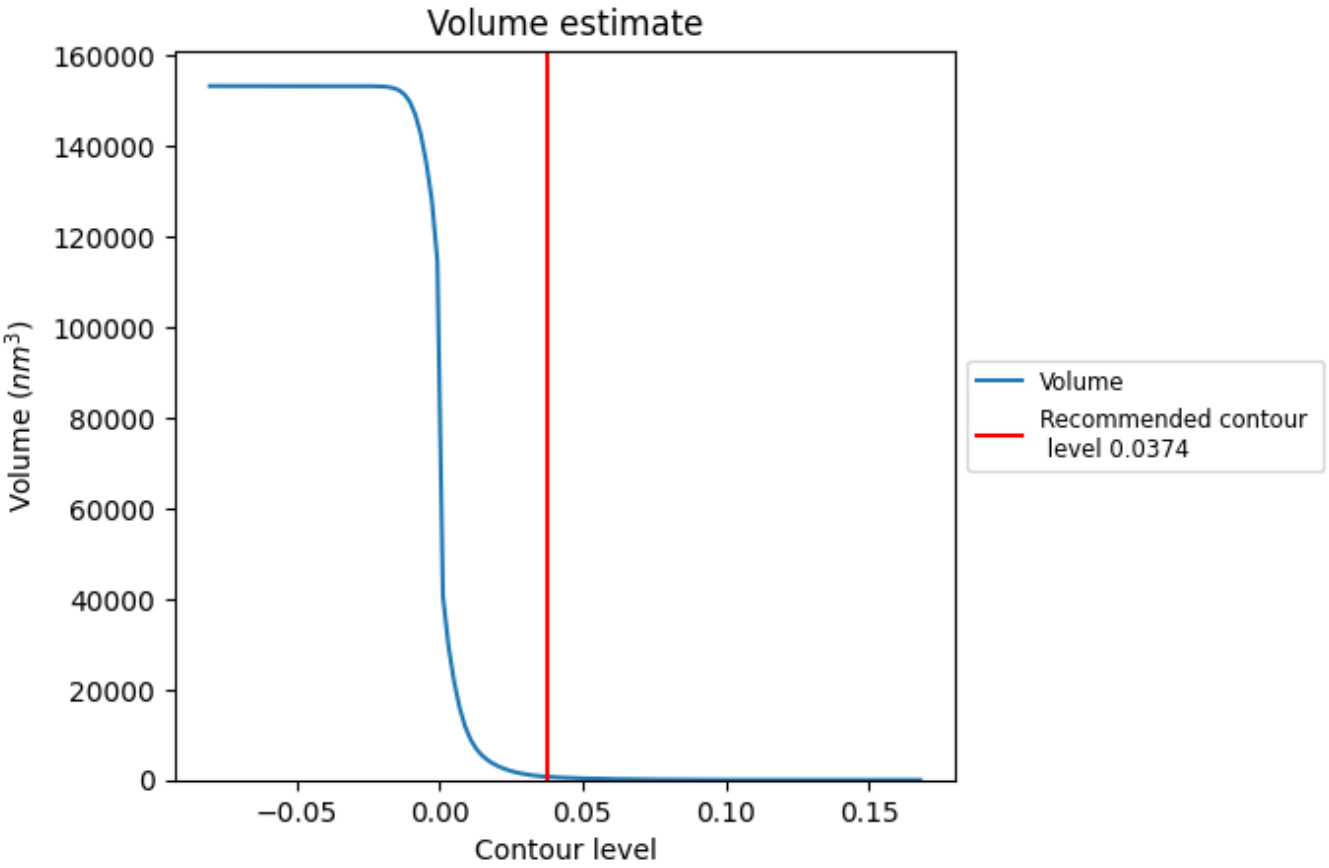
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

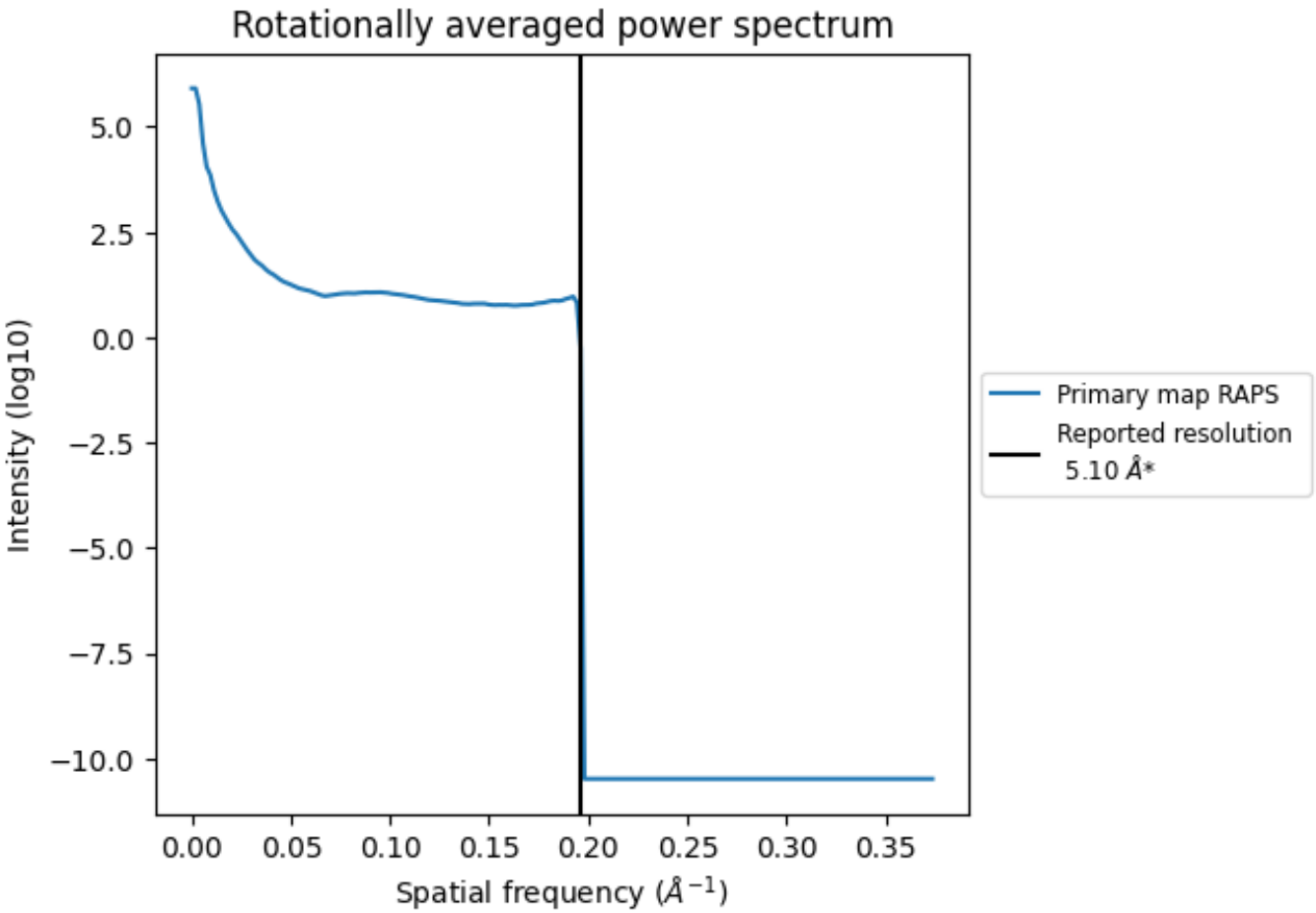
7.2 Volume estimate



The volume at the recommended contour level is 725 nm^3; this corresponds to an approximate mass of 654 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 0.196 $Å^{-1}$

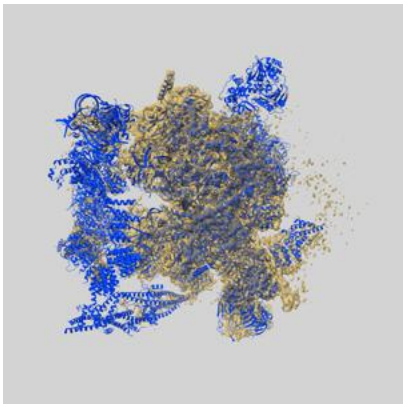
8 Fourier-Shell correlation

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

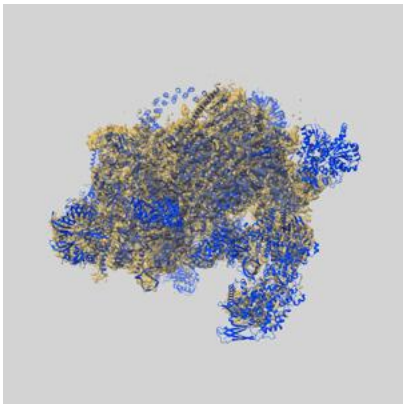
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6889 and PDB model 5Z56. Per-residue inclusion information can be found in section 3 on page 16.

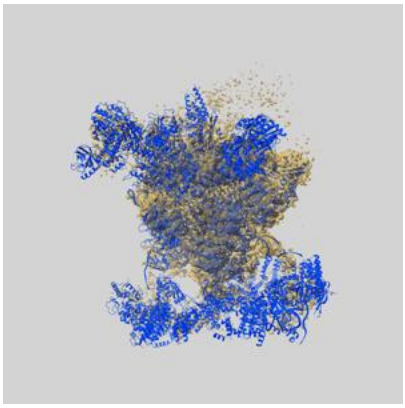
9.1 Map-model overlay



X



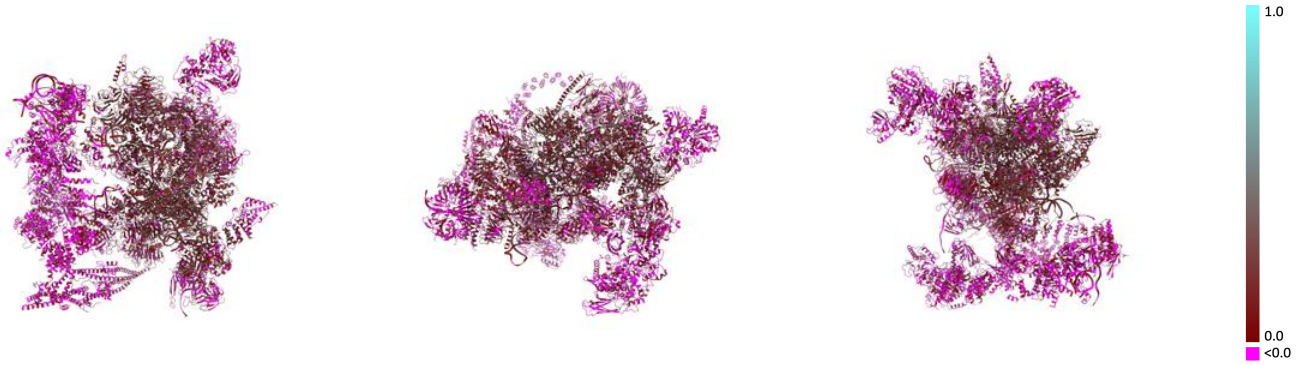
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0374 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

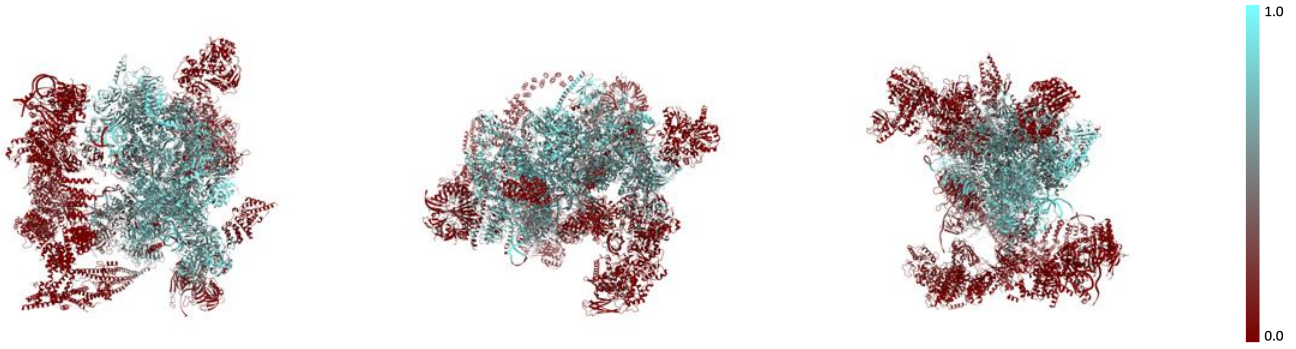
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

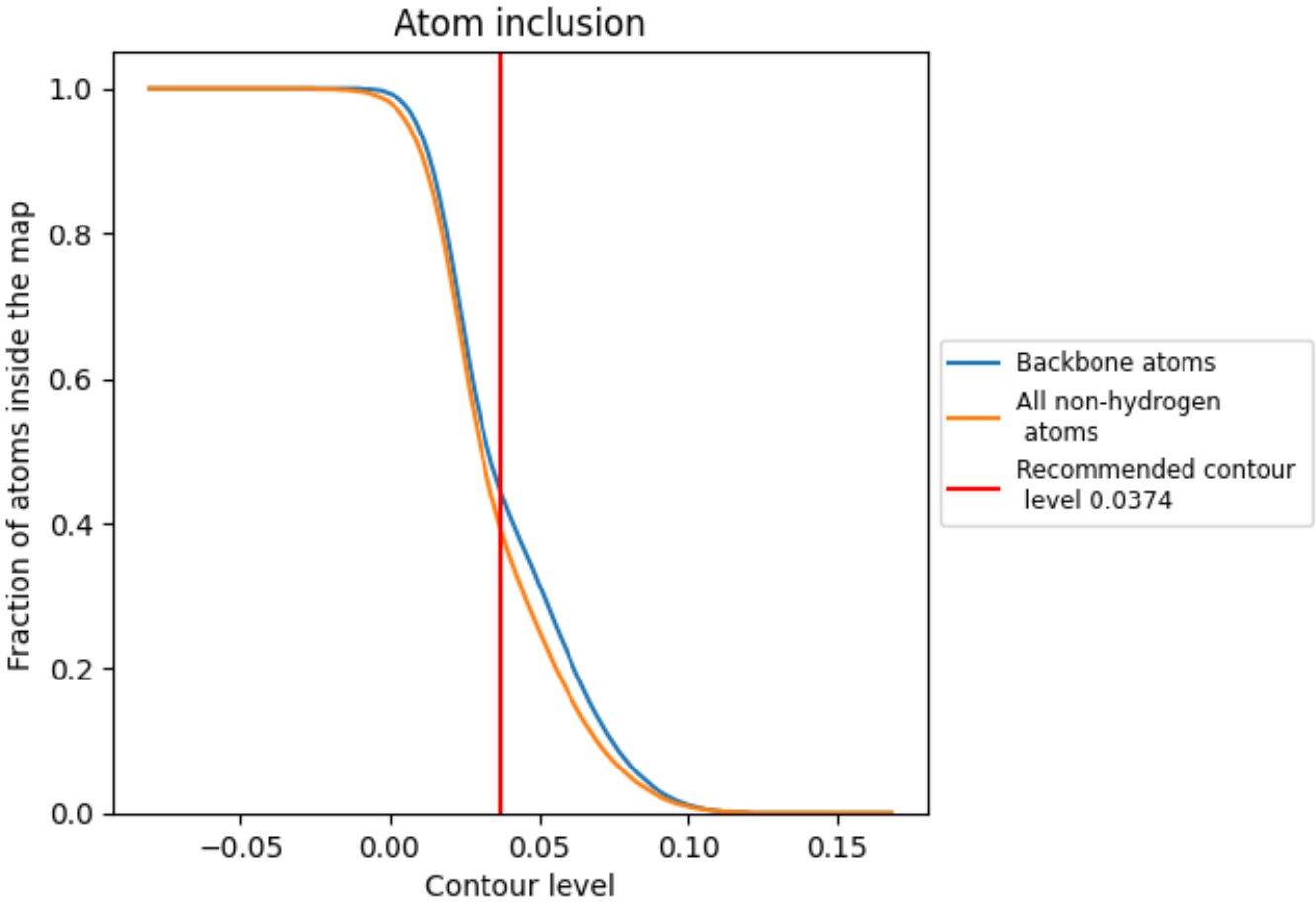
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0374).

9.4 Atom inclusion (i)



At the recommended contour level, 44% of all backbone atoms, 39% 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 (0.0374) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3900	0.1310
1	0.6320	0.2170
2	0.5230	0.1780
3	0.6060	0.1710
4	0.2310	0.0610
5	0.6450	0.2070
6	0.6670	0.2070
7	0.6700	0.2160
A	0.5630	0.2060
B	0.7040	0.1870
C	0.6430	0.1910
D	0.1000	0.0630
E	0.5400	0.1430
F	0.7610	0.2100
G	0.7270	0.2080
H	0.3810	0.1180
I	0.0210	0.0120
J	0.2700	0.0700
K	0.0710	0.0420
L	0.2920	0.1050
M	0.2260	0.1790
N	0.6190	0.1720
O	0.4390	0.1590
P	0.2840	0.1630
Q	0.0090	-0.0050
R	0.4890	0.2030
S	0.3280	0.0920
T	0.6900	0.1960
U	0.4870	0.2470
V	0.3750	0.1280
W	0.1590	0.0700
X	0.6110	0.1900
Y	0.7010	0.2550
Z	0.6410	0.2540
a	0.0550	0.0050

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Chain	Atom inclusion	Q-score
b	0.0960	0.0920
c	0.1870	-0.0010
d	0.1830	0.0510
e	0.1690	0.0540
f	0.1690	-0.0090
g	0.1180	0.0210
h	0.0280	0.0350
i	0.0090	0.0050
j	0.0370	-0.0030
k	0.0240	0.0350
l	0.0050	-0.0000
m	0.0220	0.0220
n	0.0270	0.0070
o	0.0110	0.0180
p	0.0320	0.0150
q	0.0020	-0.0120
r	0.0120	0.0120
s	0.0480	0.0470
t	0.0030	-0.0040
u	0.0020	0.0250
v	0.3360	0.1070
w	0.1970	0.0420
x	0.0010	-0.0010
y	0.0470	0.0010
z	0.1700	0.1660