Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 05:13 AM JST

PDB ID	:	7DVQ
EMDB ID	:	EMD-30875
Title	:	Cryo-EM Structure of the Activated Human Minor Spliceosome (minor Bact Complex)
Authors	:	Bai, R.; Wan, R.; Wang, L.; Xu, K.; Zhang, Q.; Lei, J.; Shi, Y.
Deposited on	:	2021-01-14
Resolution	:	2.89 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:

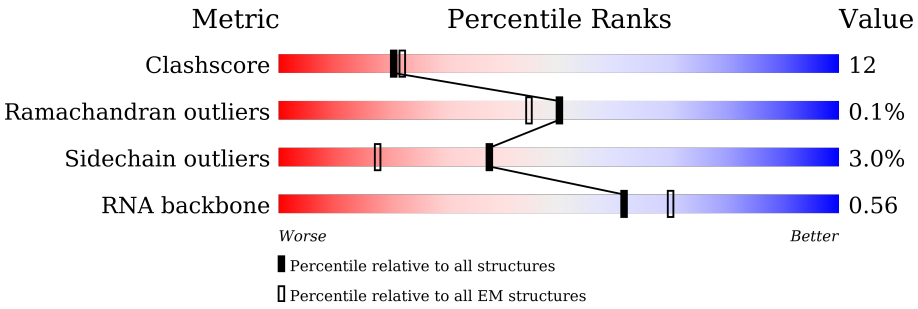
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.89 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	11% 79% 15% • 5%
2	B	117	24% 40% 31% 6% 23%
3	C	972	• 75% 17% • 7%
4	D	2136	55% 78% 6% • 16%
5	E	357	83% 53% 29% • 16%
6	a	126	62% 64% 36%
6	h	126	63% 63% 37%

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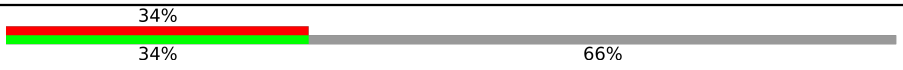
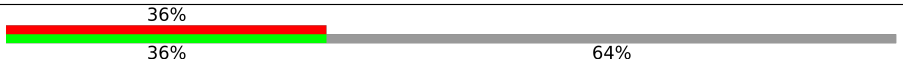
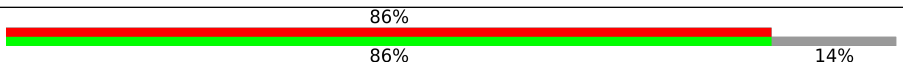
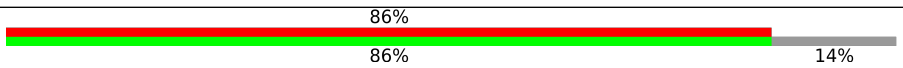
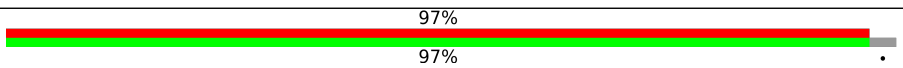
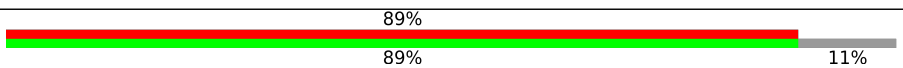
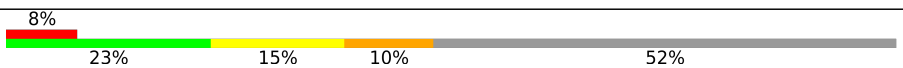
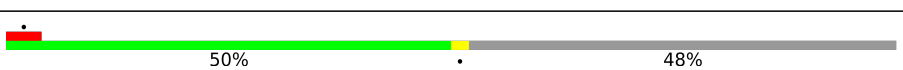
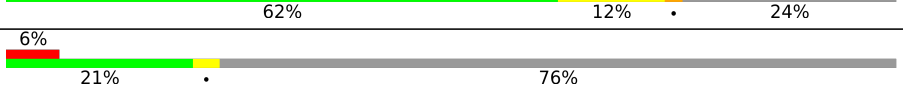
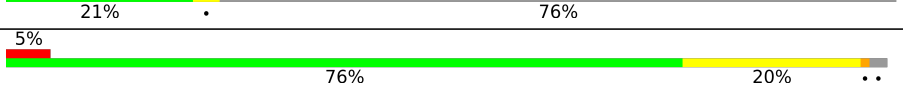
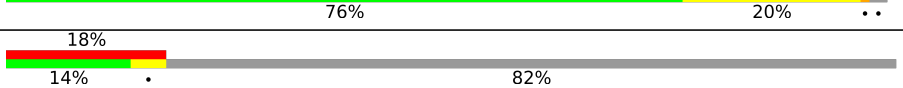
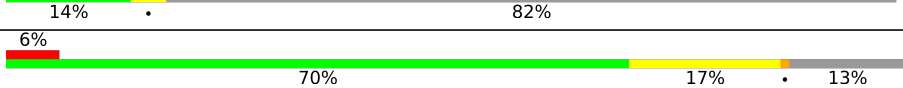
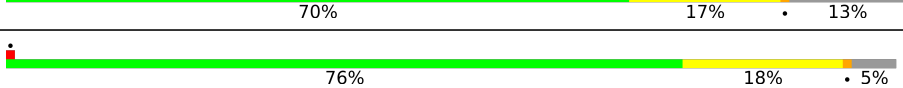
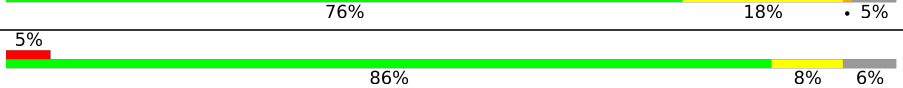
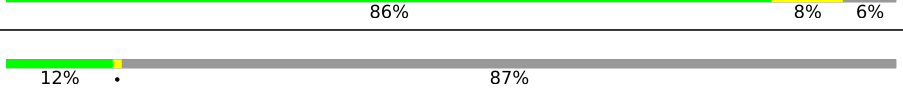
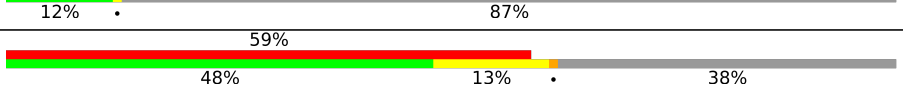
Mol	Chain	Length	Quality of chain
7	b	240	
7	i	240	
8	c	119	
8	j	119	
9	d	118	
9	k	118	
10	f	86	
10	m	86	
11	e	92	
11	l	92	
12	g	76	
12	n	76	
13	F	124	
14	G	142	
15	H	150	
16	v	230	
17	1	1304	
18	2	895	
19	3	1217	
20	4	424	
21	5	125	
22	6	110	
23	7	86	
24	L	802	
25	J	848	

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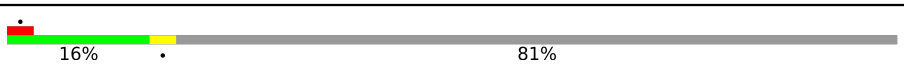
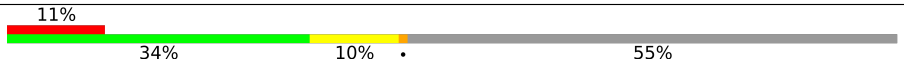
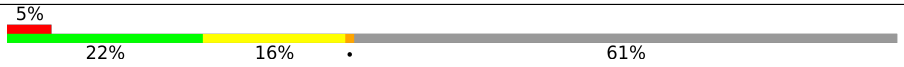
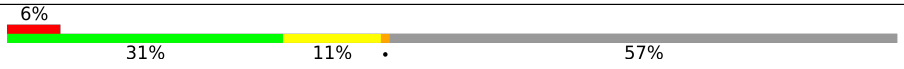
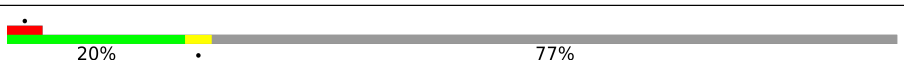
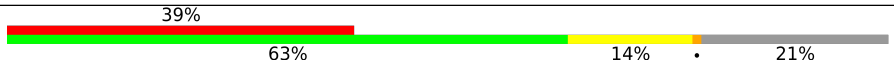
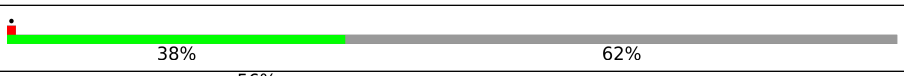
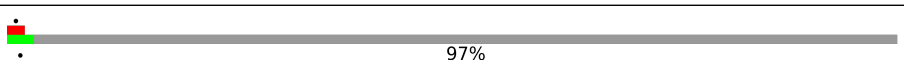
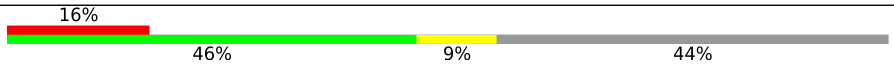
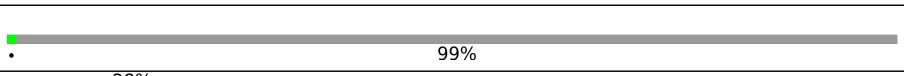
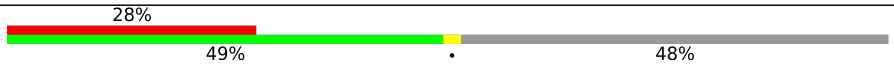
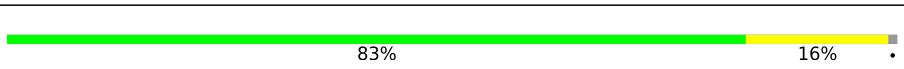
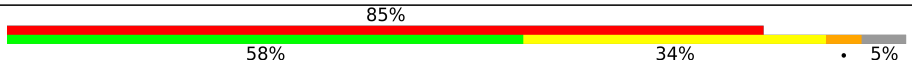
Mol	Chain	Length	Quality of chain
26	P	229	
27	R	536	
28	T	514	
29	X	396	
30	Y	322	
31	Z	619	
32	9	520	
33	z	472	
34	x	1041	
35	y	476	
36	M	343	
37	U	2752	
38	V	908	
39	8	904	
40	0	101	
41	I	367	
42	K	198	

2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 99906 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	2223	18354	11832	3206	3236	80	0	0

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	90	1898	850	320	638	90	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	902	7125	4560	1185	1345	35	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	1803	9215	5522	1841	1851	1	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	2337	1470	409	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 392	C 233	N 79	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	C	N	O	0	0
			363	215	74	74		
12	n	68	Total	C	N	O	0	0
			334	198	68	68		

- Molecule 13 is a RNA chain called U6atac snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	60	Total	C	N	O	P	0	0
			1294	577	242	415	60		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	63	Total	C	N	O	P	0	0
			1303	585	197	458	63		

- Molecule 15 is a RNA chain called U12 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	63	Total	C	N	O	P	0	0
			1350	604	247	436	63		

- Molecule 16 is a protein called Sodium channel modifier 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	v	119	Total	C	N	O	S	0	0
			963	601	179	178	5		

- Molecule 17 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	1	986	Total	C	N	O	P	S	0	0
			7879	5035	1361	1435	1	47		

- Molecule 18 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	2	216	Total	C	N	O	S	0	0
			1674	1067	296	305	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
19	3	1193	Total	C	N	O	P	S	0	0
			9352	5932	1590	1784	1	45		

- Molecule 20 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	4	78	Total	C	N	O	0	0
			383	227	78	78		

- Molecule 21 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	5	109	Total	C	N	O	S	0	0
			906	582	157	163	4		

- Molecule 22 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	6	105	Total	C	N	O	S	0	0
			811	502	145	151	13		

- Molecule 23 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	7	81	Total	C	N	O	S	0	0
			669	422	117	124	6		

- Molecule 24 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	L	101	Total	C	N	O	S	0	0
			843	540	152	147	4		

- Molecule 25 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	J	522	Total	C	N	O	S	0	0
			3457	2153	654	645	5		

- Molecule 26 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	P	44	Total	C	N	O	S	0	0
			384	243	71	68	2		

- Molecule 27 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	R	241	Total	C	N	O	S	0	0
			1923	1191	347	374	11		

- Molecule 28 is a protein called Pleiotropic regulator 1.

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

- Molecule 29 is a protein called Smad nuclear-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	X	156	Total	C	N	O	S	0	0
			1271	815	227	227	2		

- Molecule 30 is a protein called RNA-binding motif protein, X-linked 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	140	Total	C	N	O	S	0	0
			1095	692	192	206	5		

- Molecule 31 is a protein called BUD13 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Z	140	Total	C	N	O	S	0	0
			1129	703	214	207	5		

- Molecule 32 is a protein called RING-type E3 ubiquitin-protein ligase PPIL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	9	409	Total	C	N	O	S	0	0
			2691	1672	487	525	7		

- Molecule 33 is a protein called Peptidyl-prolyl cis-trans isomerase CWC27 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	z	177	Total	C	N	O	S	0	0
			1400	883	245	267	5		

- Molecule 34 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase DHX16.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	x	599	Total	C	N	O	S	0	0
			3007	1794	607	605	1		

- Molecule 35 is a protein called G-patch domain and KOW motifs-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	y	13	Total	C	N	O	0	0
			105	66	22	17		

- Molecule 36 is a protein called RING finger protein 113A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	M	191	Total	C	N	O	S	0	0
			1572	983	282	295	12		

- Molecule 37 is a protein called Serine/arginine repetitive matrix protein 2.

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

- Molecule 38 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	V	468	Total	C	N	O	S	0	0
			3008	1873	548	574	13		

- Molecule 39 is a protein called Serine/arginine repetitive matrix protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	8	126	Total	C	N	O	S	0	0
			1011	652	168	185	6		

- Molecule 40 is a protein called Cysteine-rich PDZ-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	0	100	Total	C	N	O	S	0	0
			770	475	142	144	9		

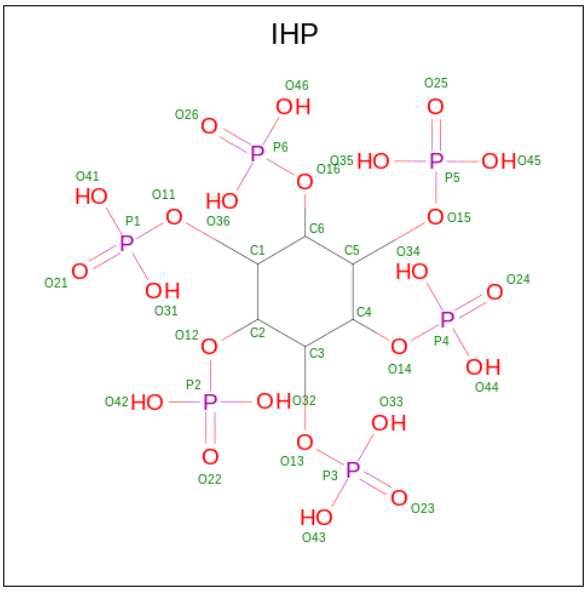
- Molecule 41 is a protein called RNA-binding protein 48.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	I	128	Total	C	N	O	S	0	0
			1062	683	184	190	5		

- Molecule 42 is a protein called Armadillo repeat-containing protein 7.

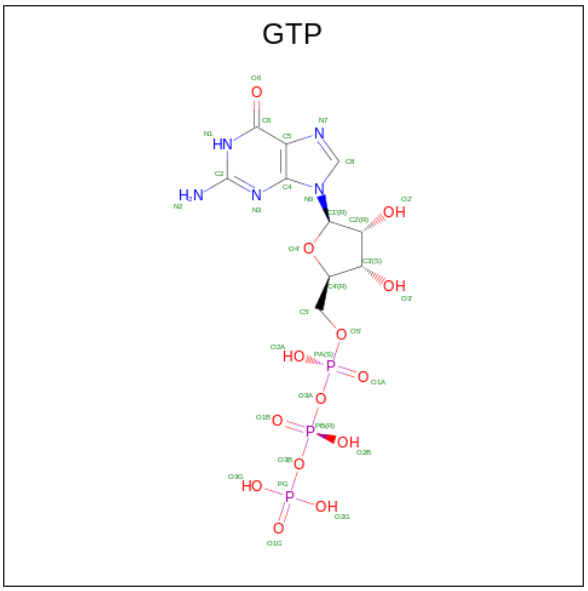
Mol	Chain	Residues	Atoms					AltConf	Trace
42	K	188	Total	C	N	O	S	0	0
			1314	824	229	256	5		

- Molecule 43 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 44 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



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

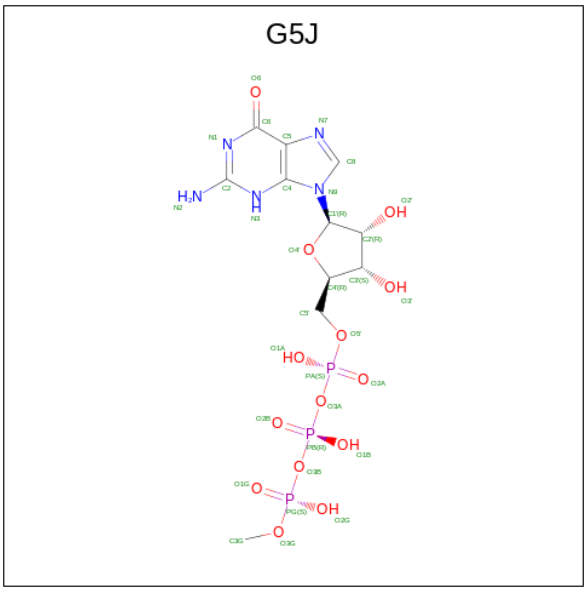
- Molecule 45 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 46 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
46	F	2	Total	K	0
			2	2	

- Molecule 47 is 5'-O-[(S)-hydroxy{[(R)-hydroxy{[(S)-hydroxy(methoxy)phosphoryl]oxy}phosphoryl]oxy}phosphoryl]guanosine (three-letter code: G5J) (formula: $C_{11}H_{18}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
47	F	1	Total	C	N	O	P	0
			33	11	5	14	3	

- Molecule 48 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
48	v	1	Total	Zn	0
			1	1	
48	6	3	Total	Zn	0
			3	3	
48	M	1	Total	Zn	0
			1	1	
48	0	2	Total	Zn	0
			2	2	

- Molecule 49 is water.

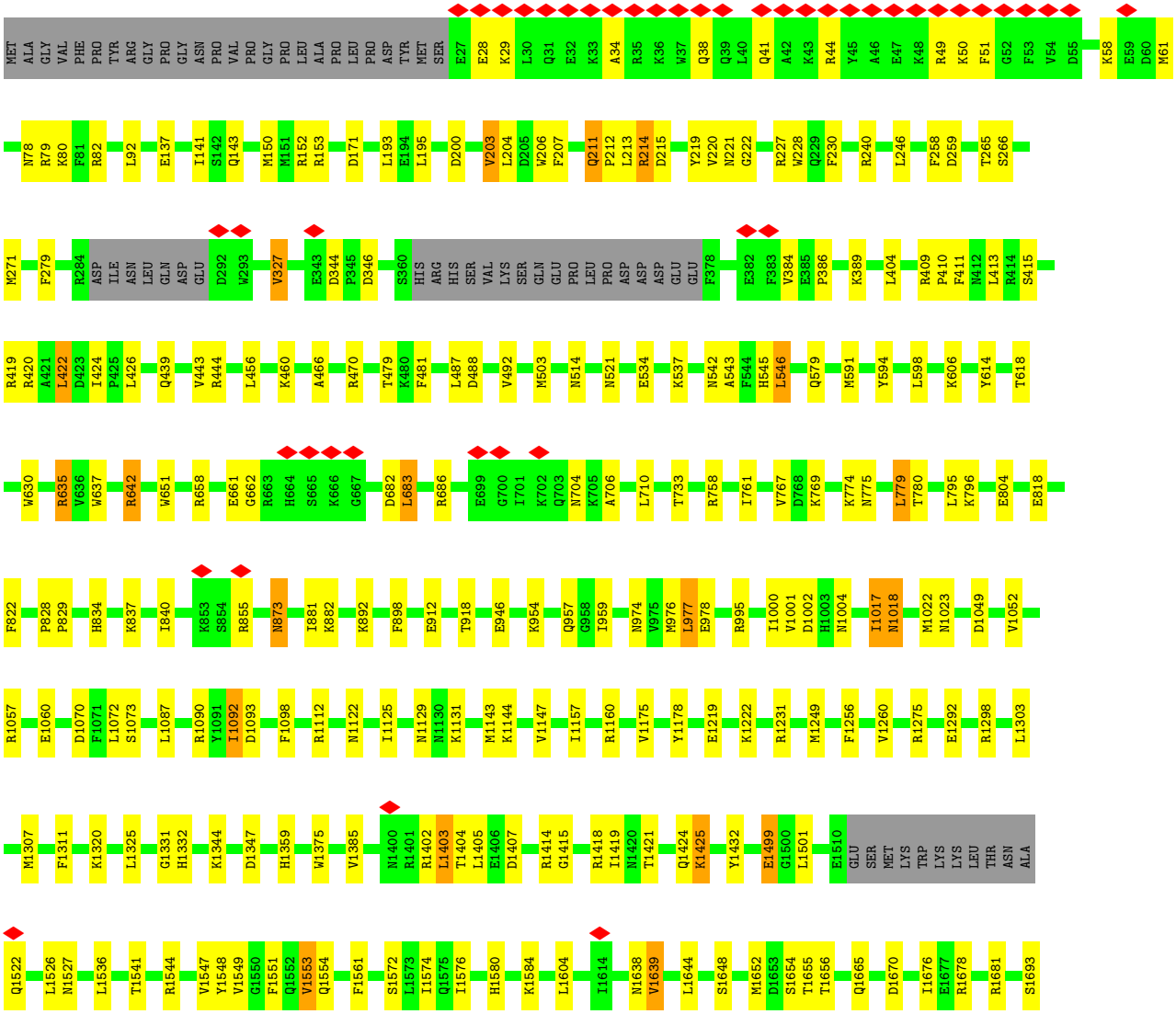
Mol	Chain	Residues	Atoms		AltConf
49	C	3	Total	O	0
			3	3	

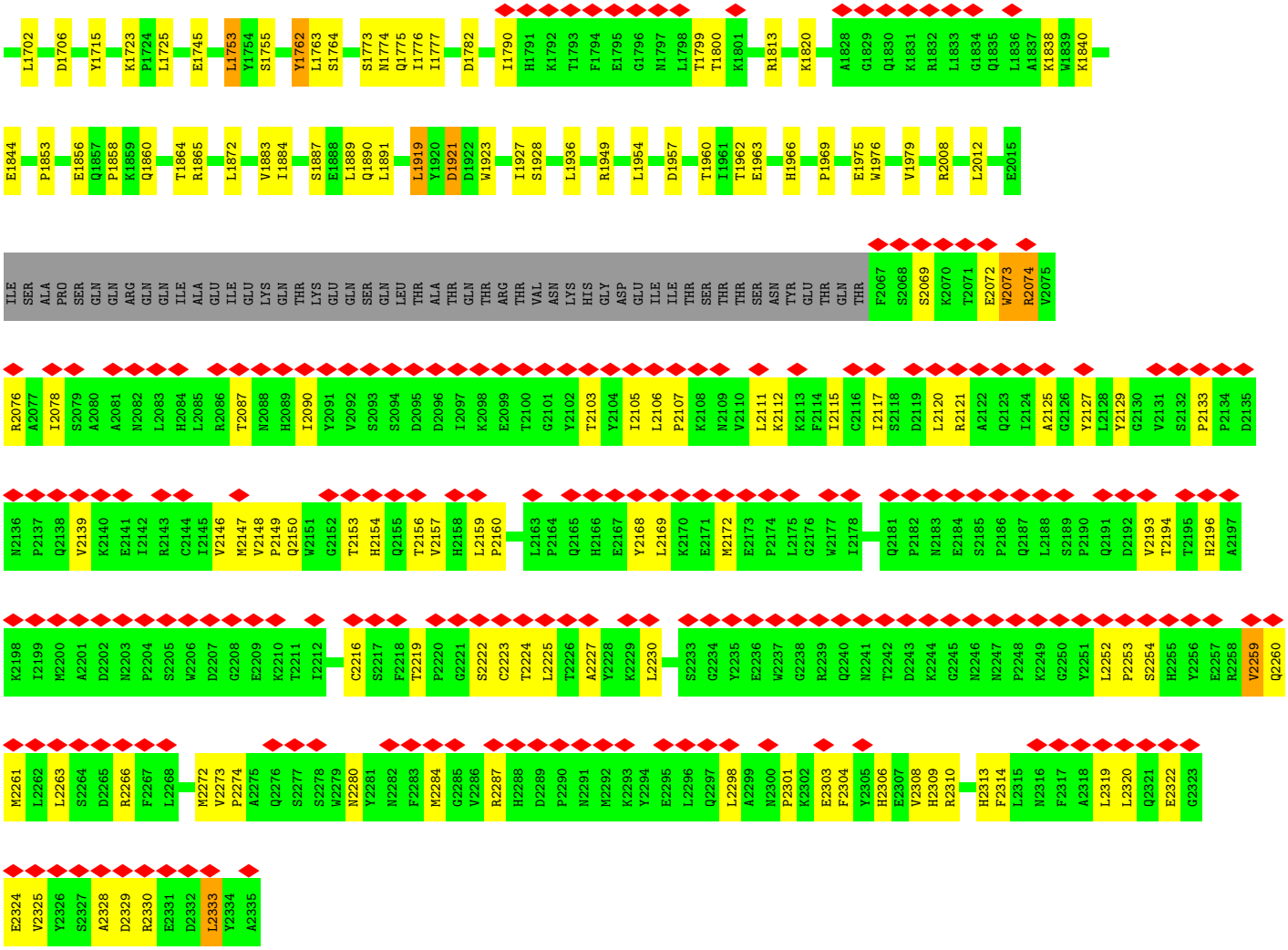
3 Residue-property plots (i)

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

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

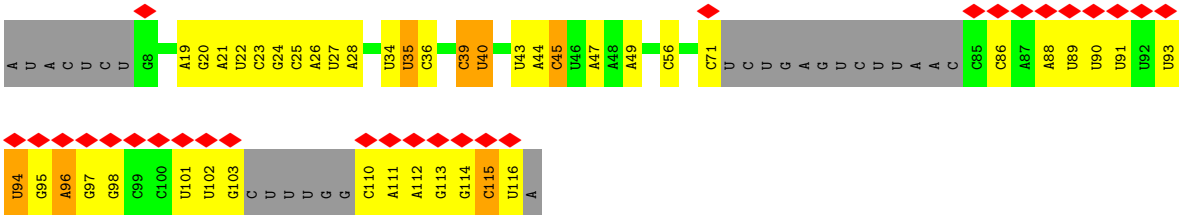
Chain A:





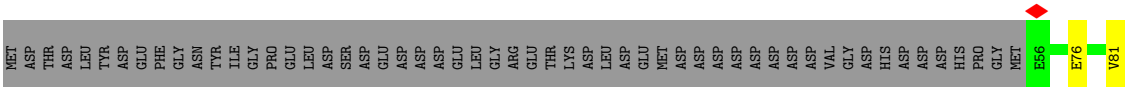
• Molecule 2: U5 snRNA

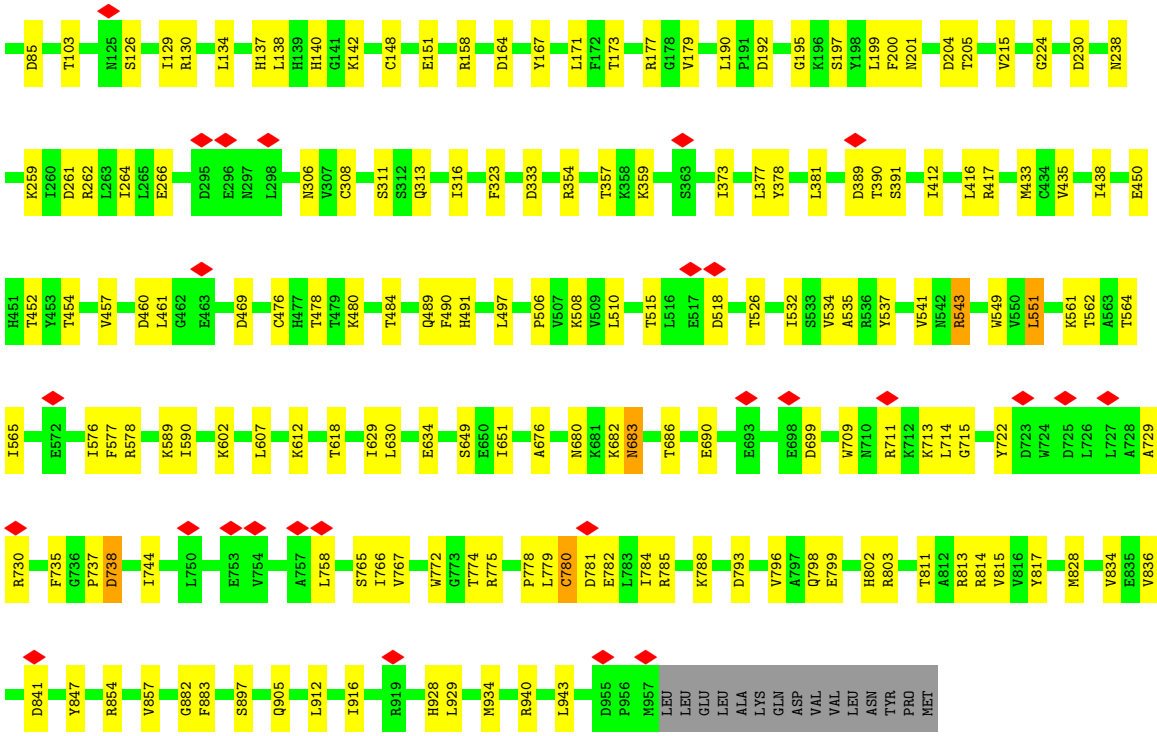
Chain B:



• Molecule 3: 116 kDa U5 small nuclear ribonucleoprotein component

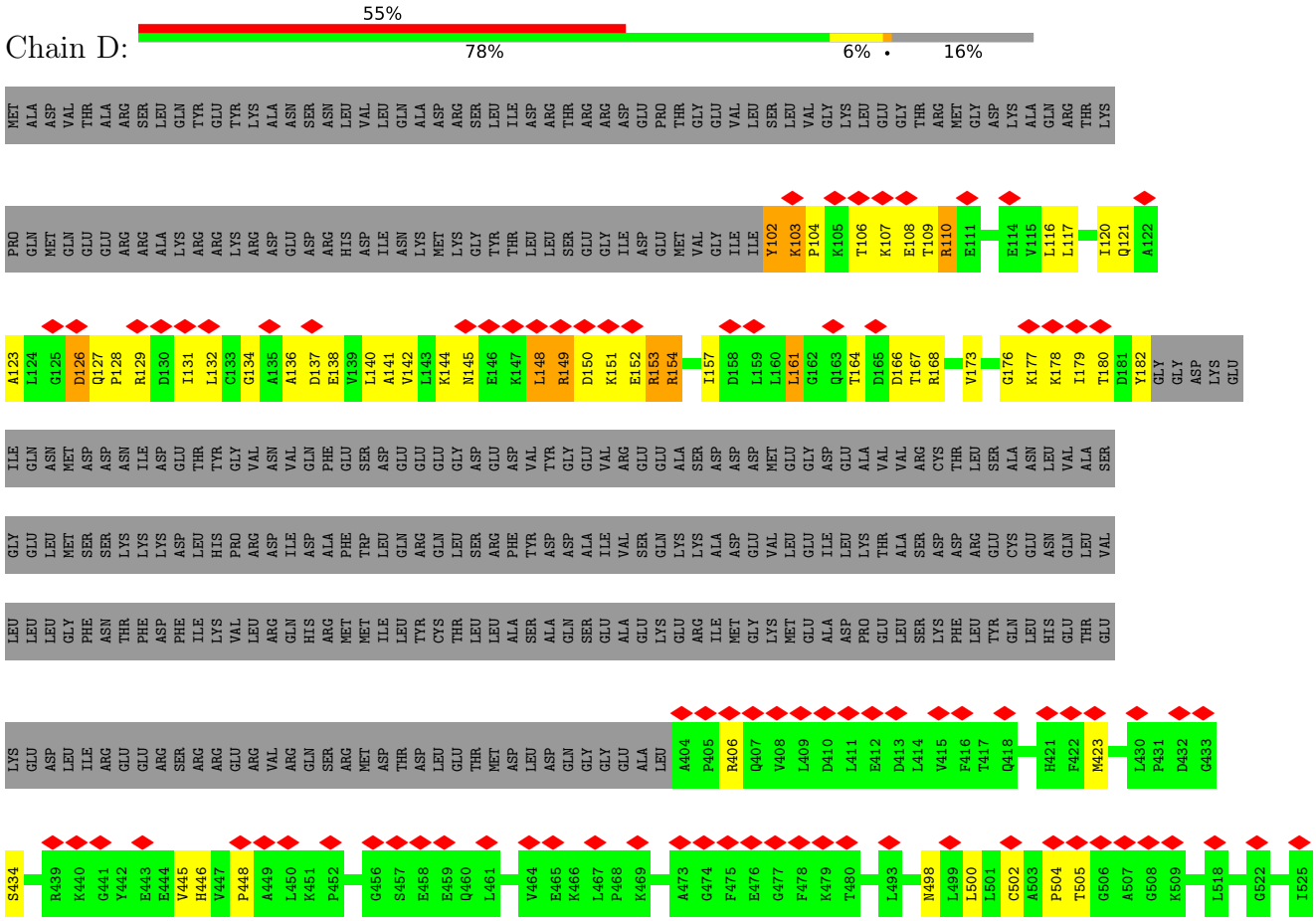
Chain C:

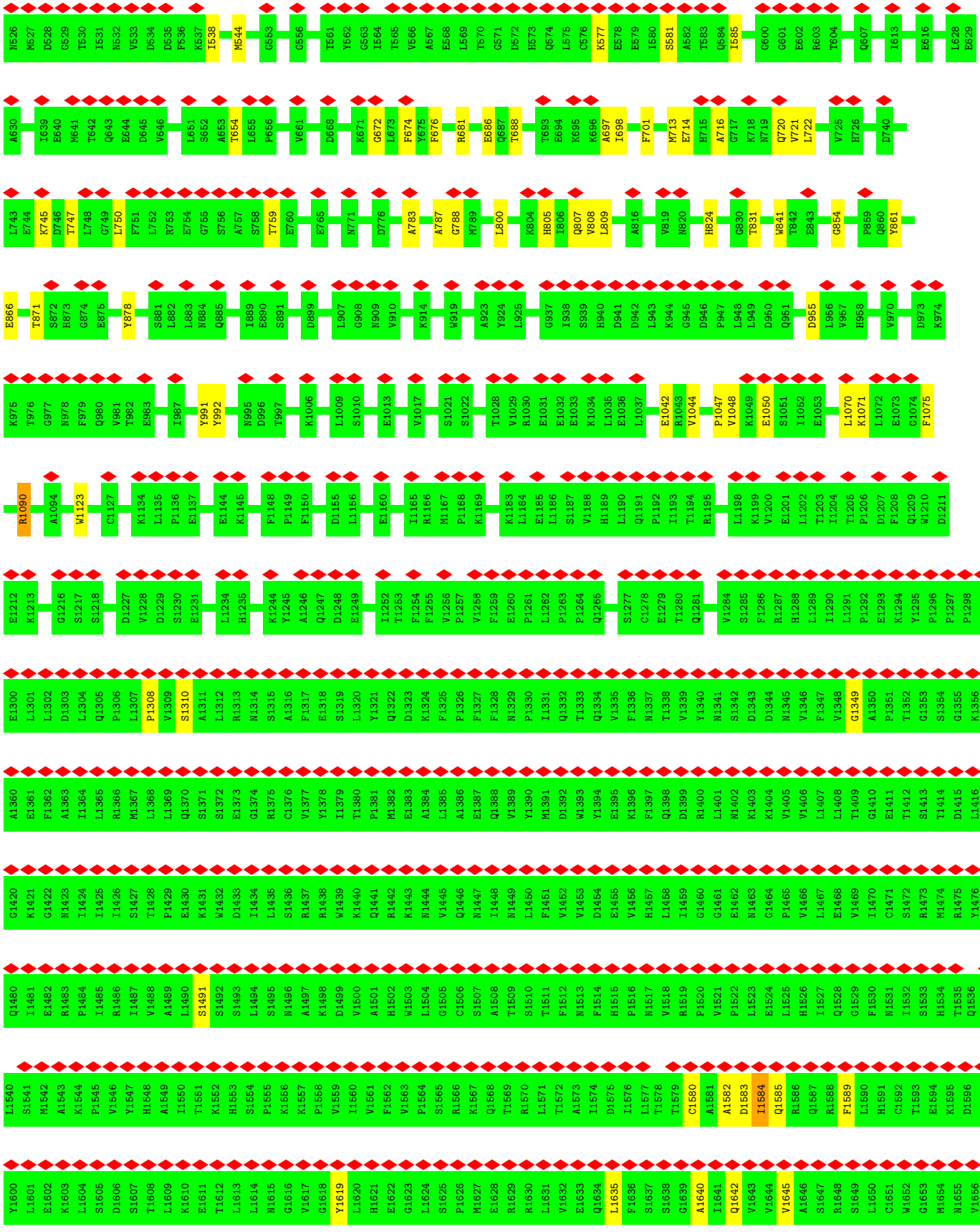




• Molecule 4: U5 small nuclear ribonucleoprotein 200 kDa helicase

Chain D:

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A630 I639 E640 M641 T642 Q643 E644 D645 V646 L651 S652 A653 T654 L655 F656 V661 D668 K671 G672 L673 F674 Y675 F676 R681 E686 Q687 T688 T693 E694 K695 K696 A697 I698 F701 M713 E714 H715 A716 G717 K718 N719 Q720 V721 L722 V725 H726 D740
L743 E744 K745 D746 T747 L748 G749 L750 F751 L752 R753 E754 G755 S756 A757 S758 T759 E760 E765 N771 D776 A783 A787 G788 M789 L800 K804 H805 I806 Q807 V808 L809 A816 V819 N820 H824 G830 T831 W841 T842 E843 G854 P859 Q860 Y861
E866 T871 S872 H873 G874 E875 Y878 S881 L882 L883 N884 Q885 I889 E890 S891 D899 L907 G908 N909 V910 K914 W919 A923 Y924 L925 G937 I938 S939 H940 D941 D942 L943 K944 G945 D946 P947 L948 L949 D950 Q951 D955 L956 V957 H958 V970 D973 K974
K975 T976 G977 N978 F979 Q980 V981 T982 E983 I987 Y991 Y992 N995 D996 T997 K1006 L1009 S1010 E1013 V1017 S1021 S1022 T1028 V1029 R1030 E1031 E1032 E1033 K1034 L1035 E1036 L1037 E1042 R1043 V1044 P1047 V1048 K1049 E1050 S1051 I1052 E1053 L1070 K1071 L1072 E1073 G1074 F1075
R1090 A1094 W1123 C1127 K1134 L1135 P1136 E1137 E1144 K1145 F1148 P1149 F1150 D1155 L1156 E1160 I1165 R1166 M1167 P1168 K1169 K1183 L1184 E1185 L1186 S1187 V1188 H1189 L1190 Q1191 P1192 I1193 T1194 R1195 L1198 K1199 V1200 E1201 L1202 T1203 I1204 T1205 P1206 D1207 F1208 Q1209 W1210 D1211
E1212 K1213 G1216 S1217 S1218 D1227 V1228 D1229 S1230 E1231 L1234 H1235 K1244 Y1245 A1246 Q1247 D1248 E1249 I1252 T1253 F1254 F1255 V1256 P1257 V1258 F1259 E1260 P1261 L1262 P1263 P1264 Q1265 S1277 C1278 E1279 T1280 Q1281 V1284 S1285 F1286 R1287 H1288 L1289 I1290 L1291 P1292 E1293 K1294 Y1295 P1296 P1297 P1298 T1299
E1300 L1301 L1302 D1303 L1304 Q1305 P1306 L1307 P1308 V1309 S1310 A1311 L1312 R1313 N1314 S1315 A1316 F1317 E1318 S1319 L1320 Y1321 Q1322 D1323 K1324 F1325 P1326 F1327 F1328 N1329 P1330 I1331 Q1332 T1333 Q1334 V1335 F1336 N1337 T1338 V1339 Y1340 N1341 S1342 D1343 D1344 N1345 V1346 F1347 V1348 G1349 A1350 P1351 T1352 G1353 S1354 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 R1414 D1415 L1416 K1417 L1418 L1419
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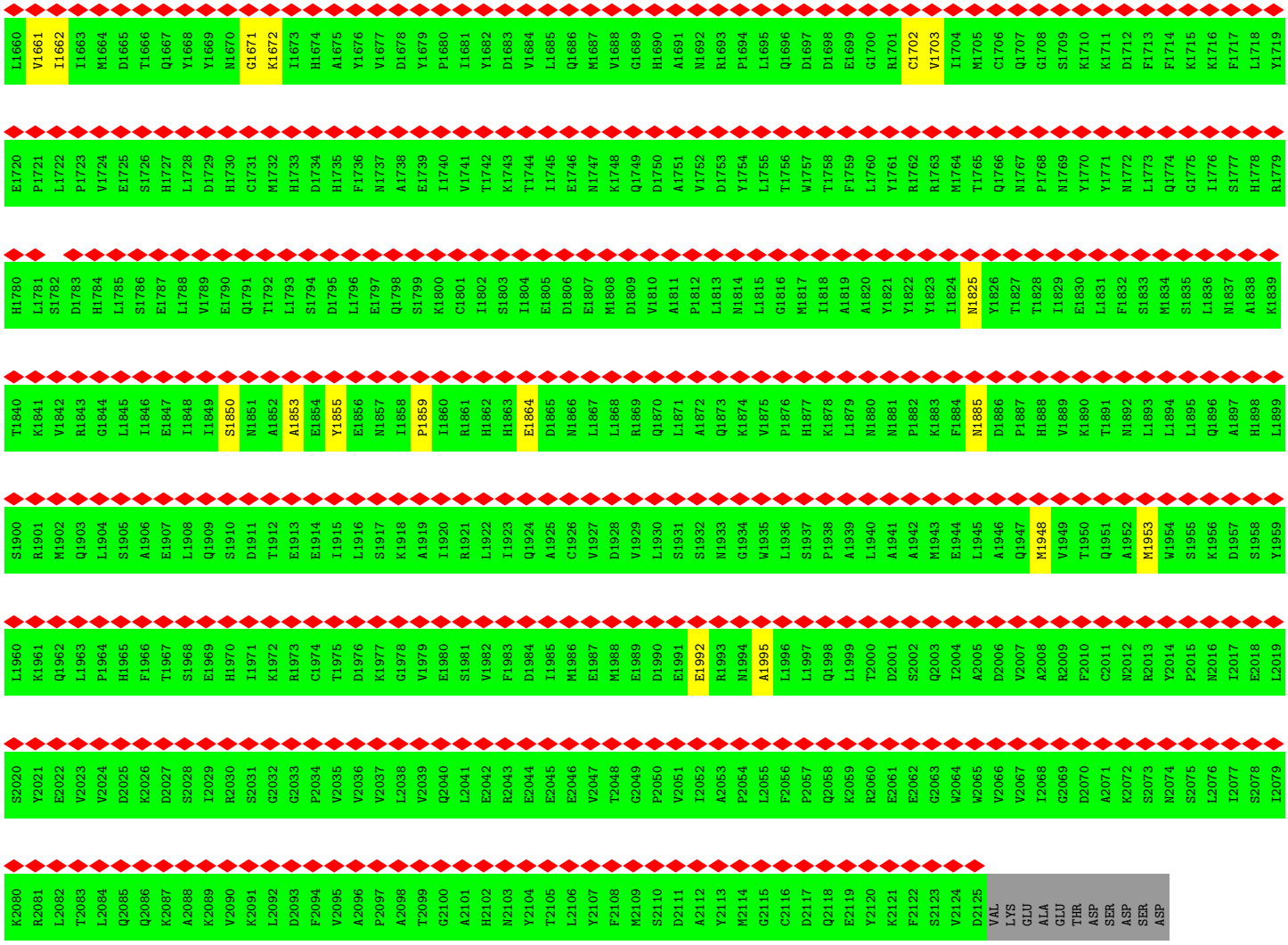
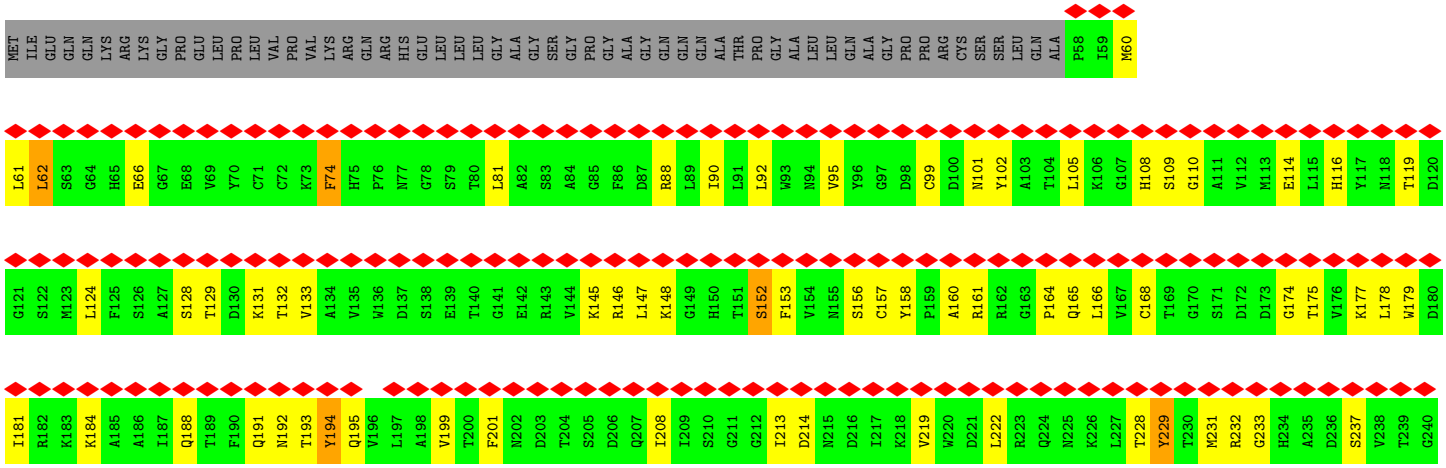
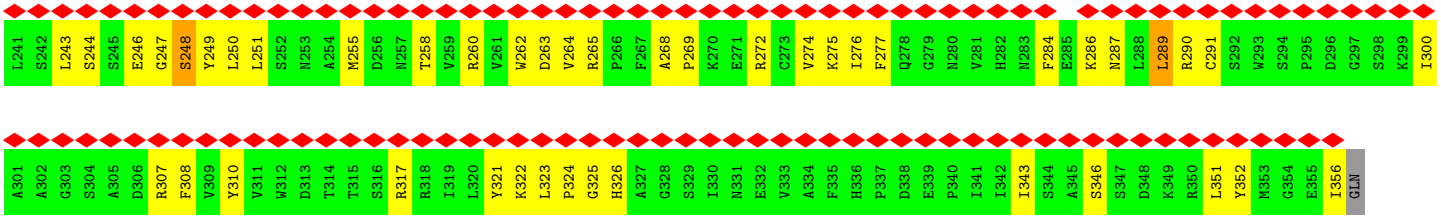
L1540 S1541 M1542 A1543 K1544 P1545 Y1546 Y1547 H1548 A1549 I1550 T1551 K1552 H1553 S1554 P1555 K1556 K1557 P1558 V1559 I1560 V1561 F1562 V1563 P1564 S1565 R1566 K1567 Q1568 T1569 R1570 L1571 T1572 A1573 I1574 D1575 I1576 L1577 T1578 T1579 C1580 A1581 A1582 D1583 I1584 Q1585 R1586 Q1587 R1588 F1589 L1590 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 C1651 W1652 G1653 M1654 N1655 V1656 A1657 A1658 H1659



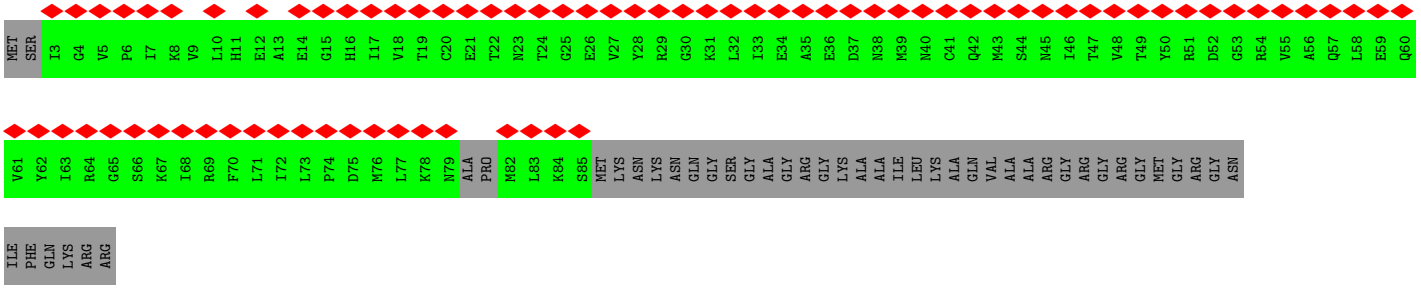
• Molecule 5: U5 small nuclear ribonucleoprotein 40 kDa protein

Chain E:

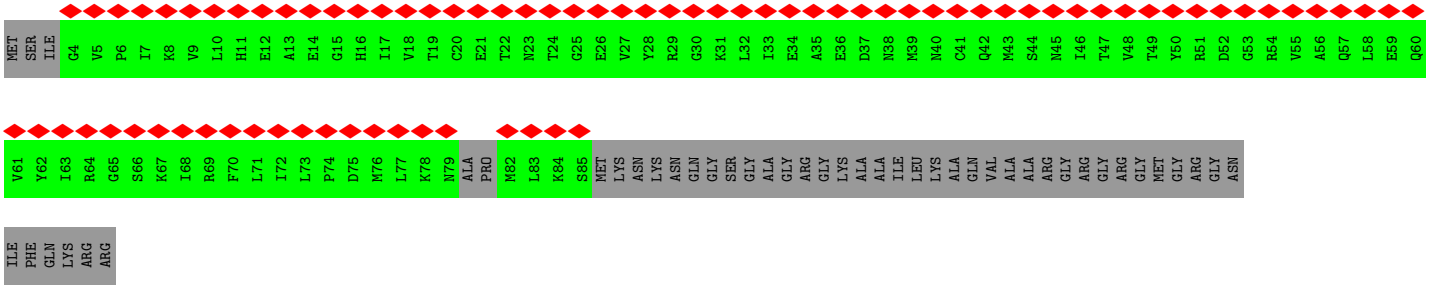




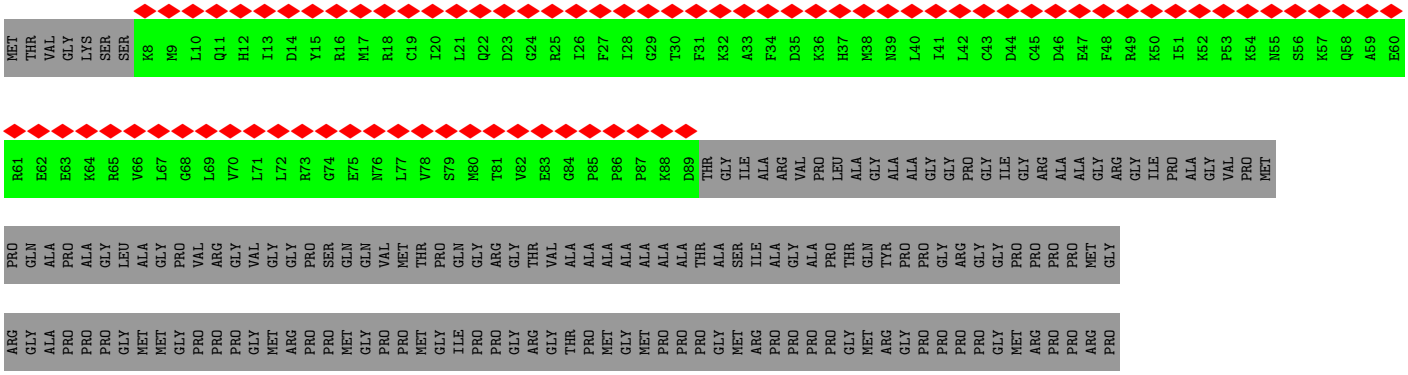
• Molecule 6: Small nuclear ribonucleoprotein Sm D3



• Molecule 6: Small nuclear ribonucleoprotein Sm D3

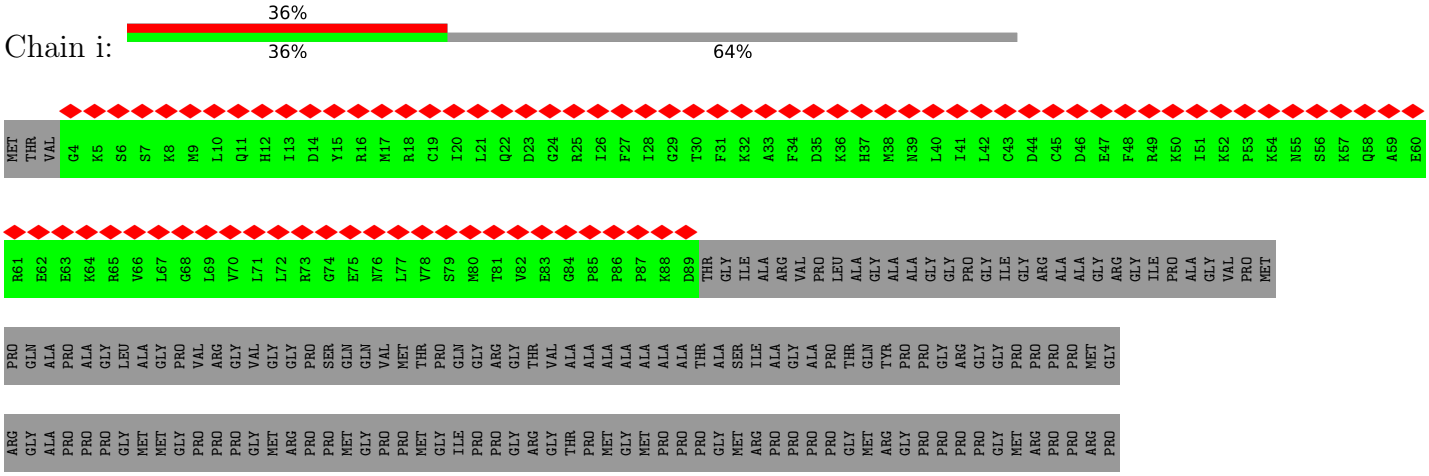


• Molecule 7: Small nuclear ribonucleoprotein-associated proteins B and B'



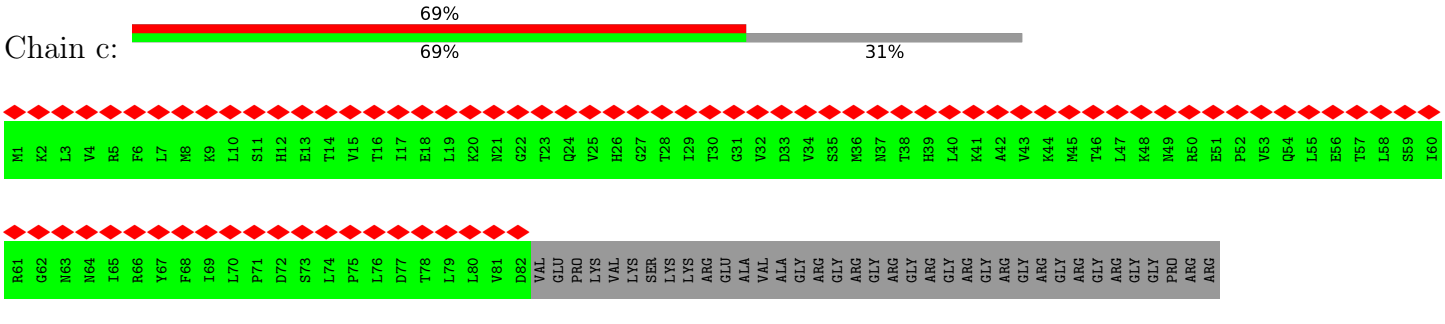
• Molecule 7: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain i:



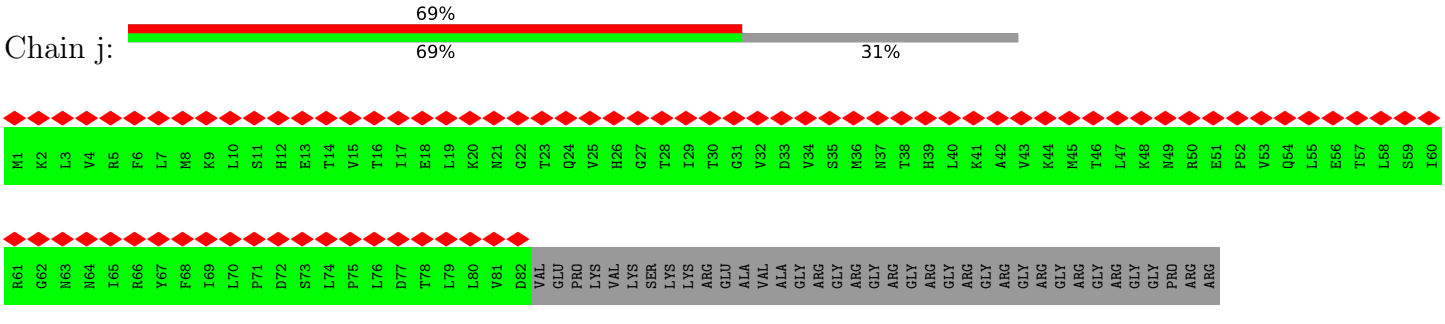
• Molecule 8: Small nuclear ribonucleoprotein Sm D1

Chain c:



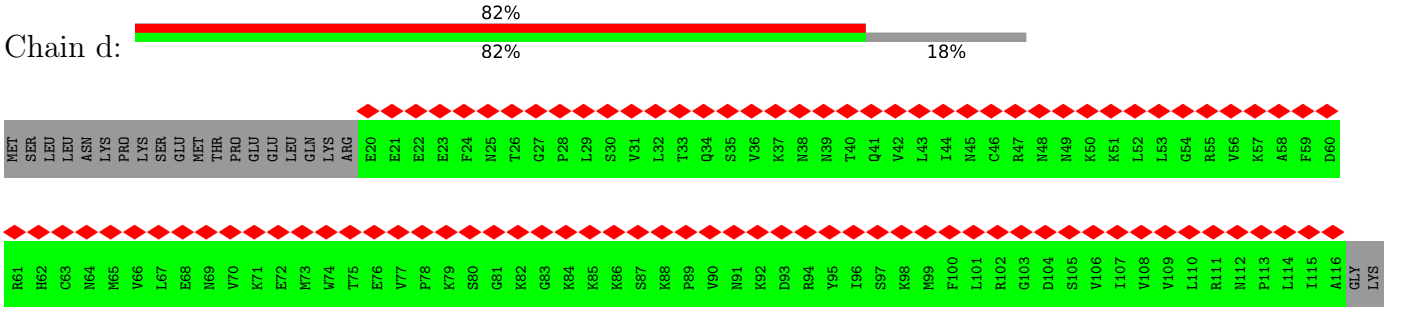
• Molecule 8: Small nuclear ribonucleoprotein Sm D1

Chain j:



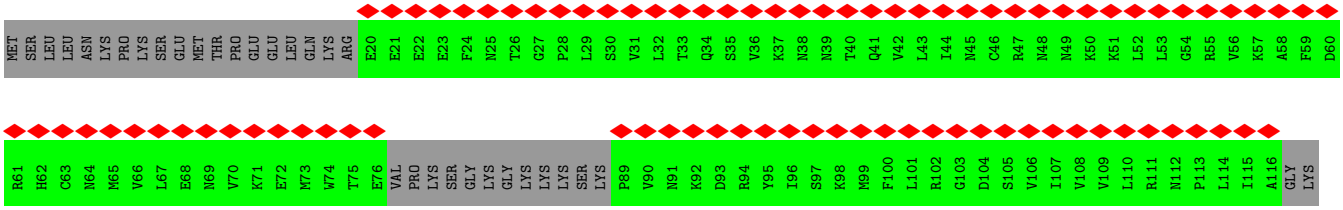
• Molecule 9: Small nuclear ribonucleoprotein Sm D2

Chain d:

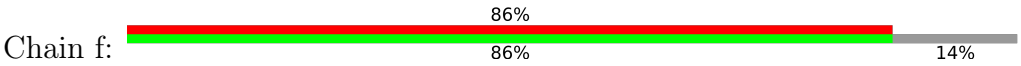


• Molecule 9: Small nuclear ribonucleoprotein Sm D2

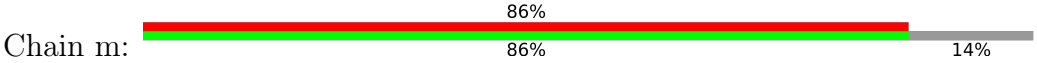
Chain k:



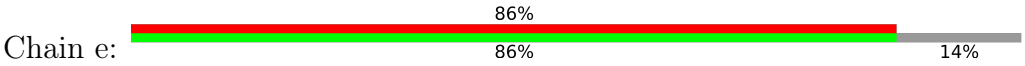
• Molecule 10: Small nuclear ribonucleoprotein F

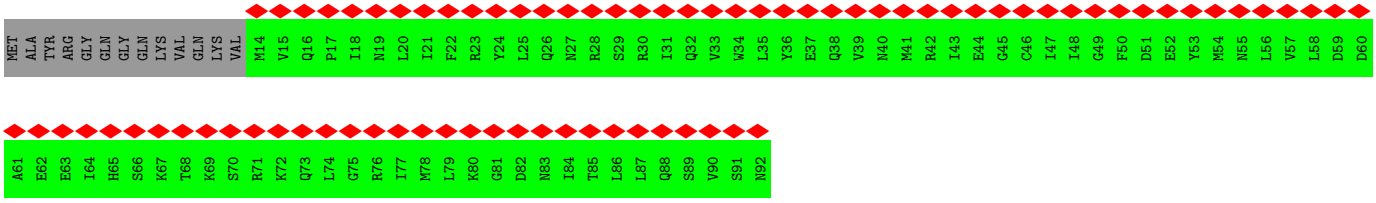


• Molecule 10: Small nuclear ribonucleoprotein F

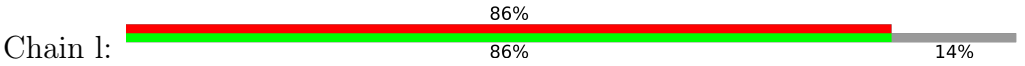


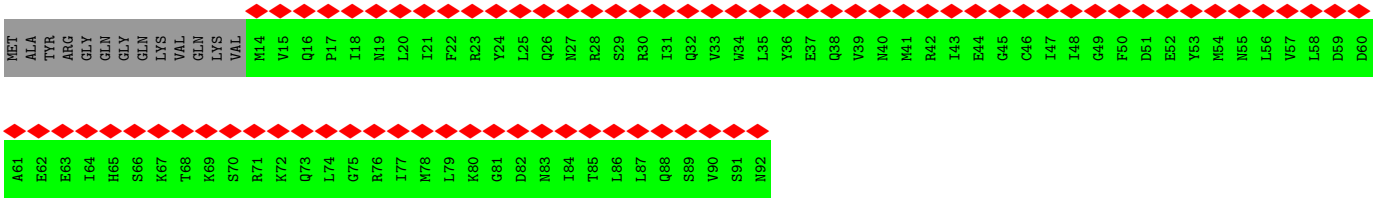
• Molecule 11: Small nuclear ribonucleoprotein E





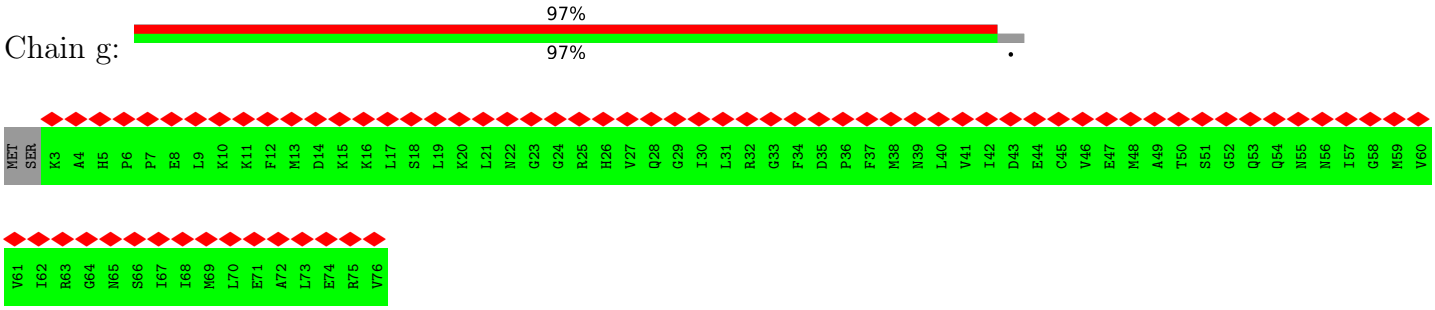
• Molecule 11: Small nuclear ribonucleoprotein E





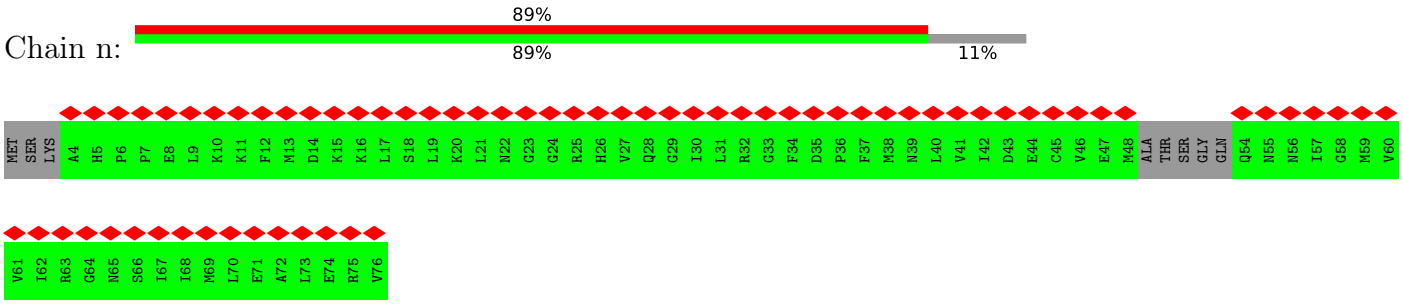
• Molecule 12: Small nuclear ribonucleoprotein G

Chain g:



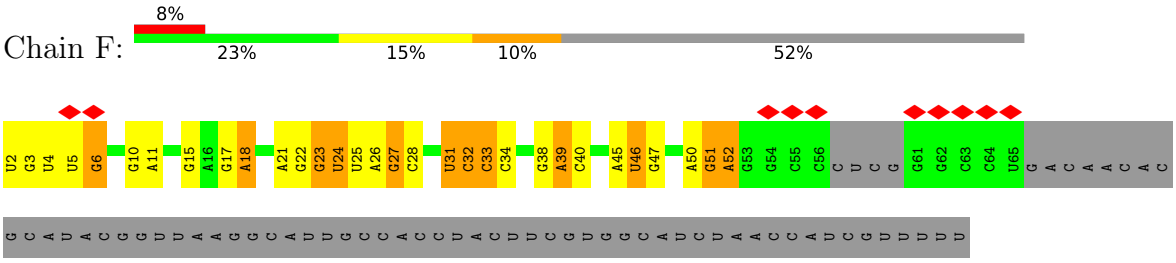
• Molecule 12: Small nuclear ribonucleoprotein G

Chain n:



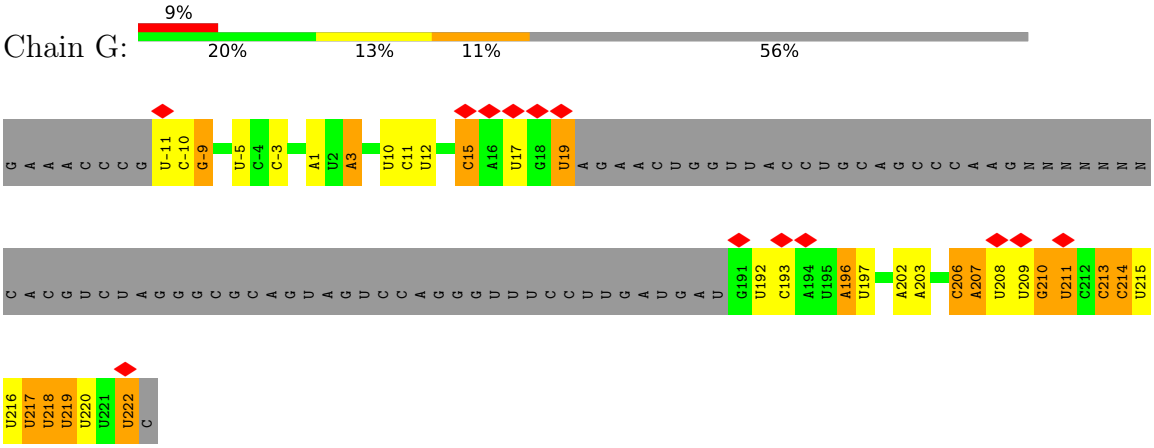
• Molecule 13: U6atac snRNA

Chain F:



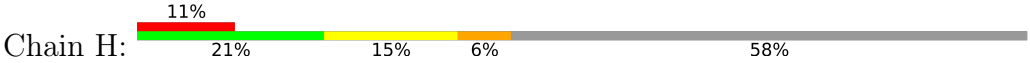
• Molecule 14: pre-mRNA

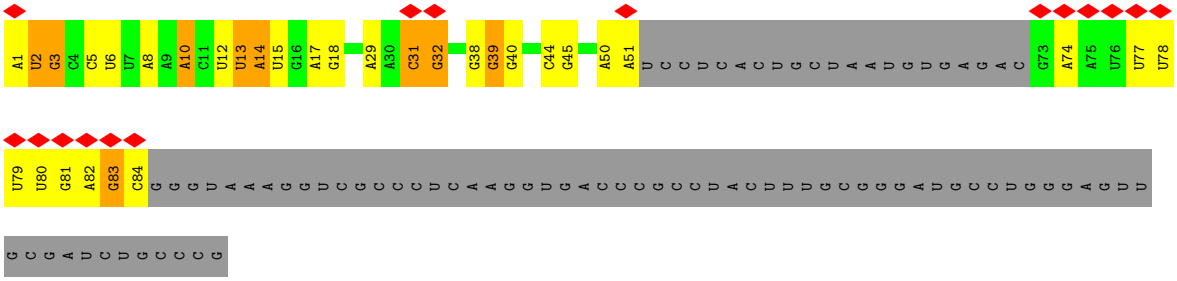
Chain G:



• Molecule 15: U12 snRNA

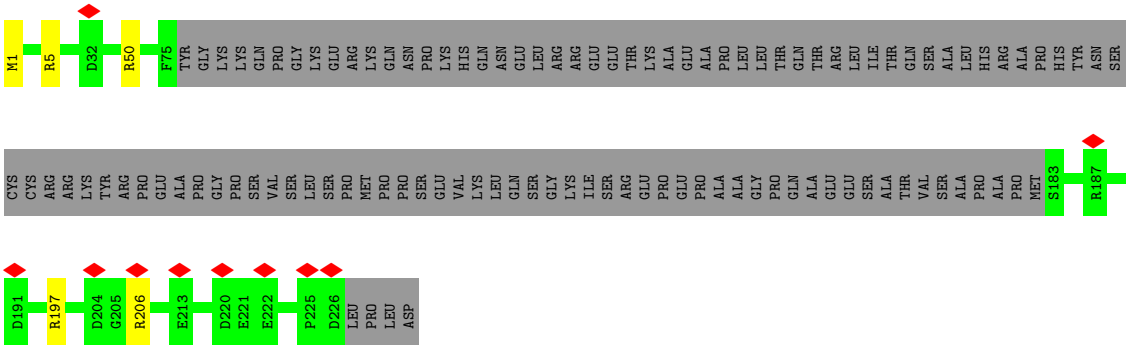
Chain H:





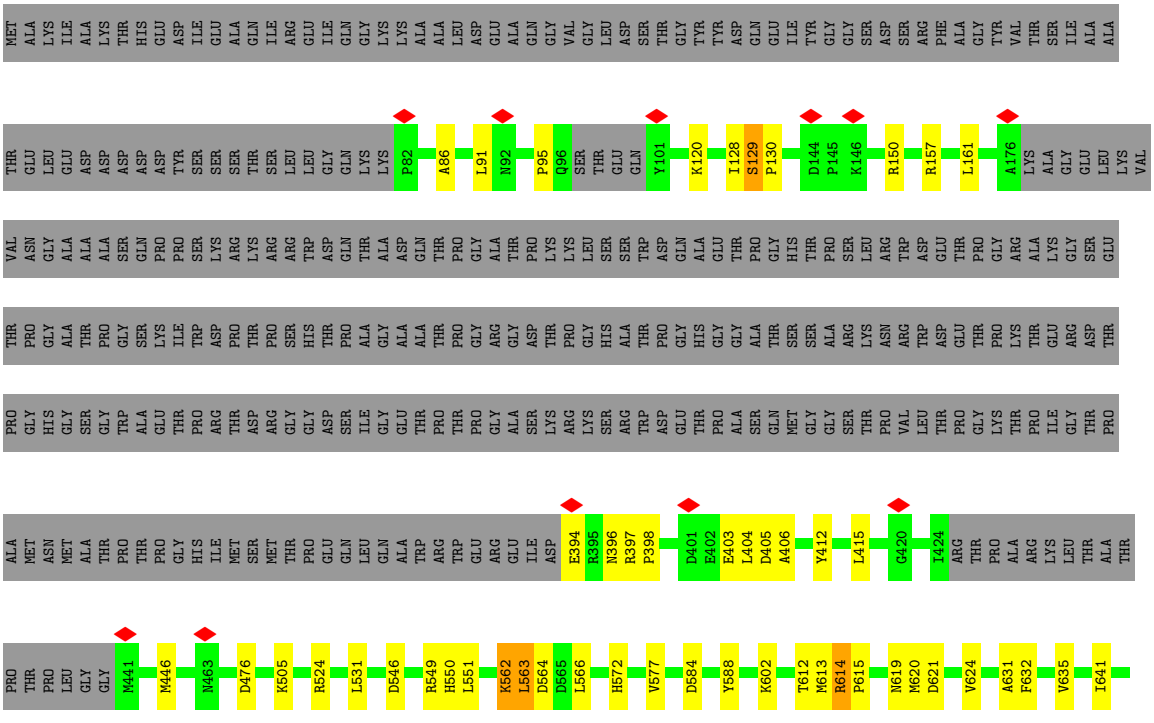
• Molecule 16: Sodium channel modifier 1

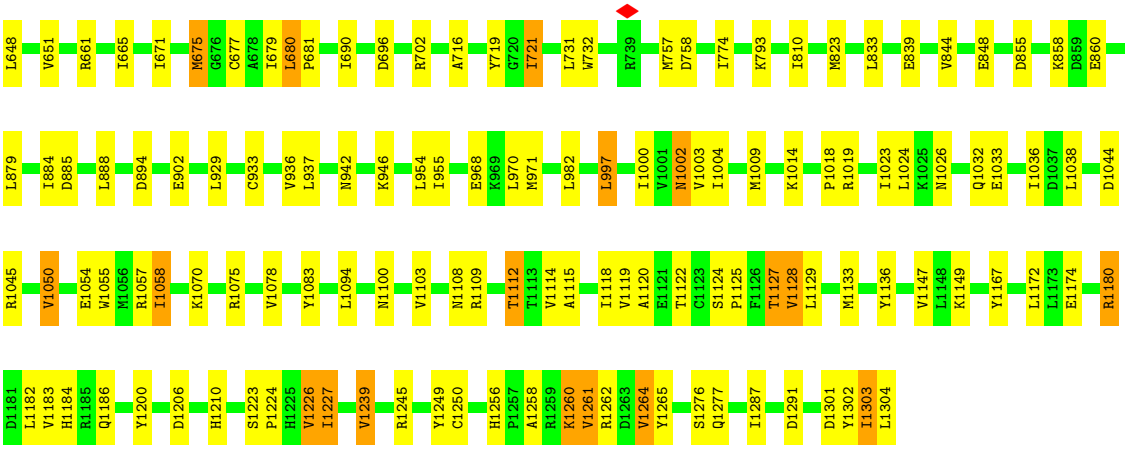
Chain v:



• Molecule 17: Splicing factor 3B subunit 1

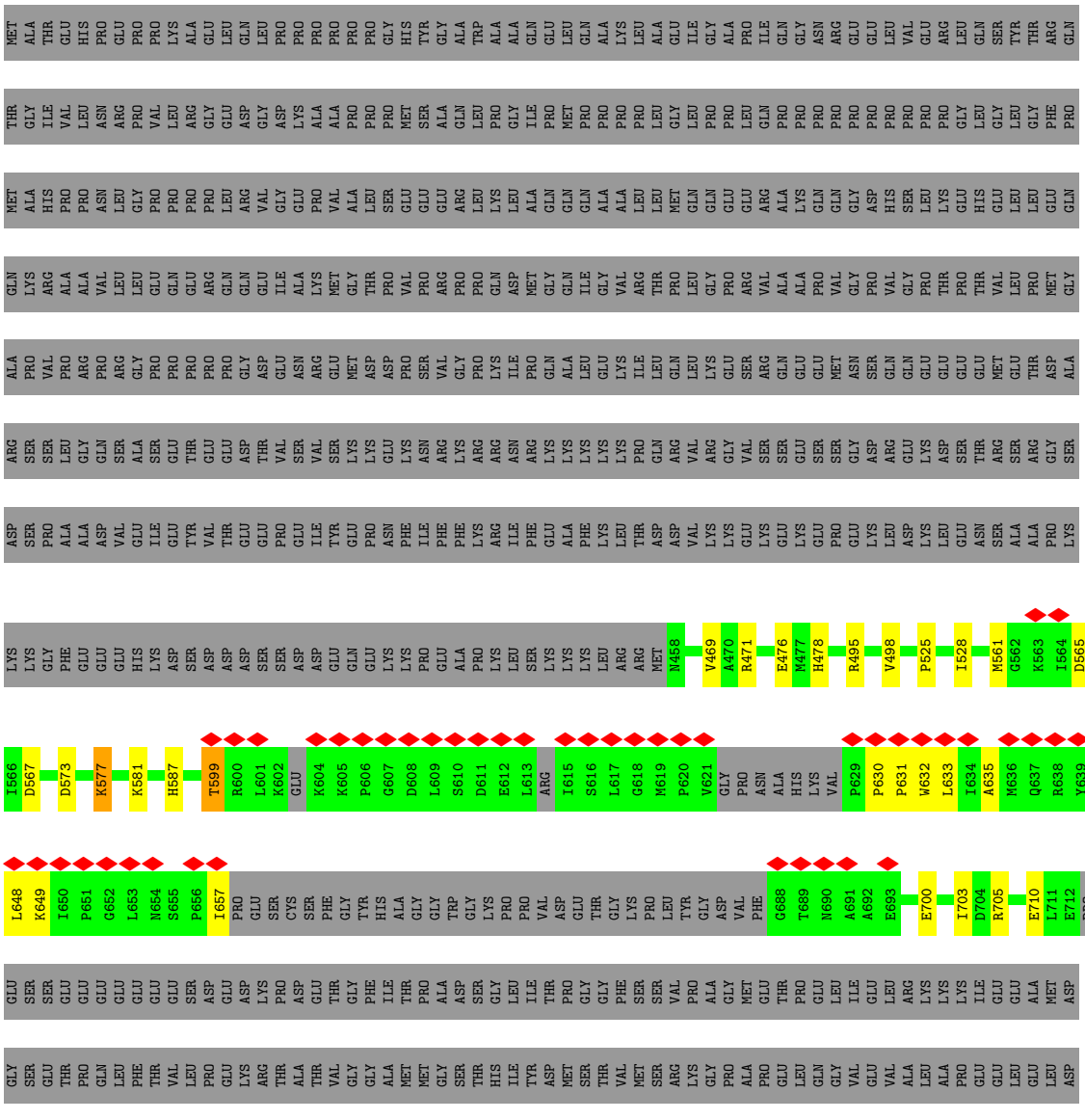
Chain 1:





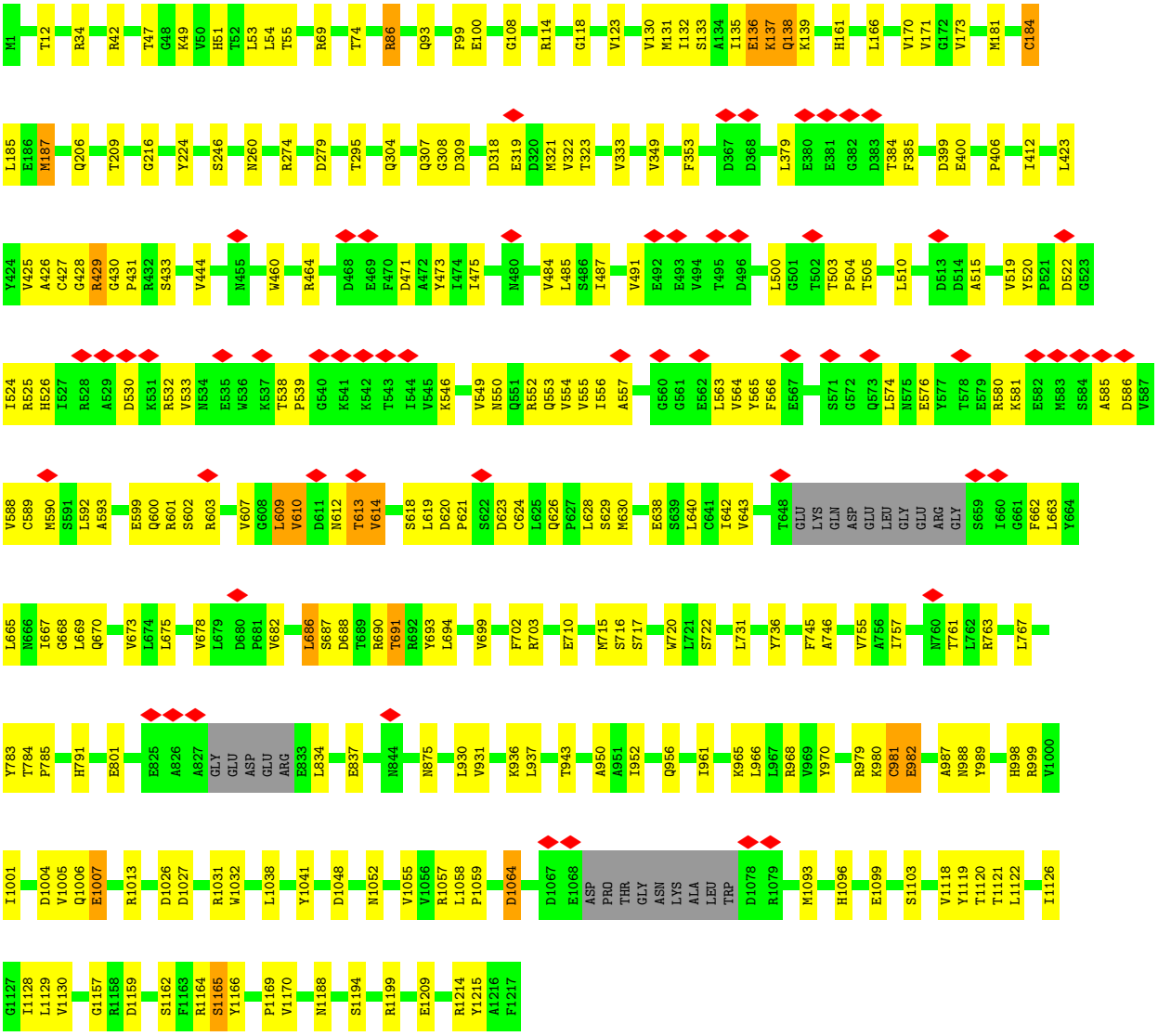
• Molecule 18: Splicing factor 3B subunit 2

Chain 2:



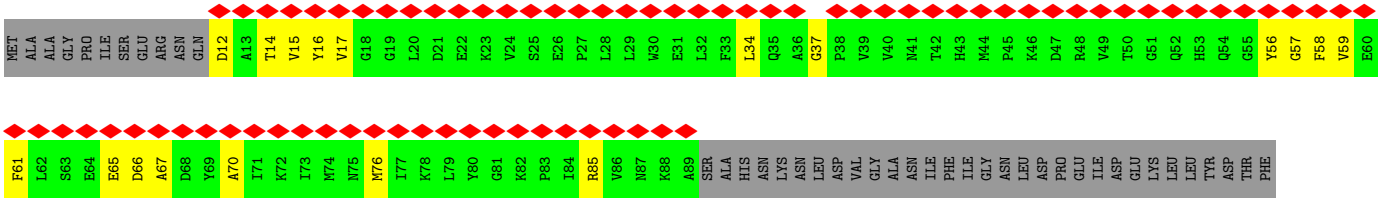
• Molecule 19: Splicing factor 3B subunit 3

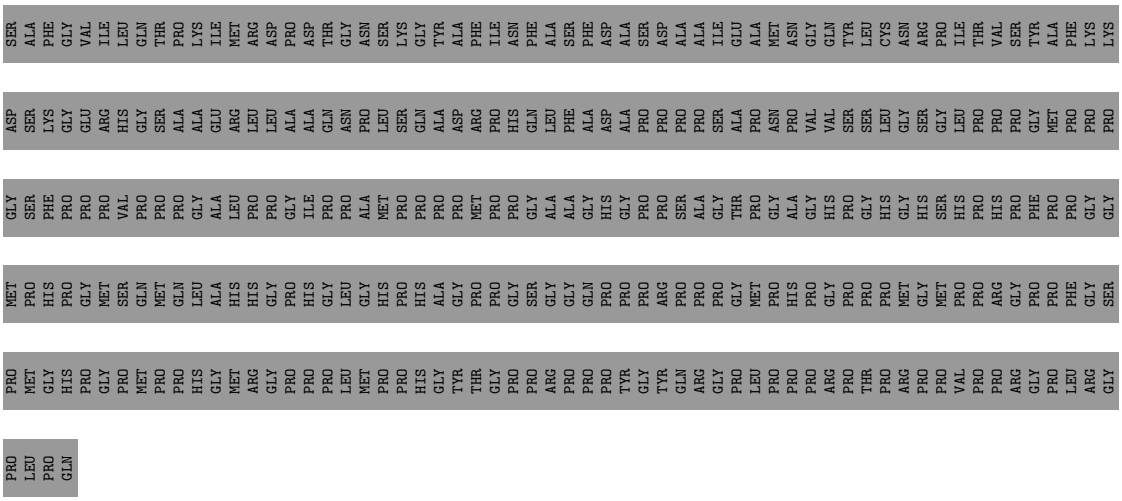
Chain 3:



• Molecule 20: Splicing factor 3B subunit 4

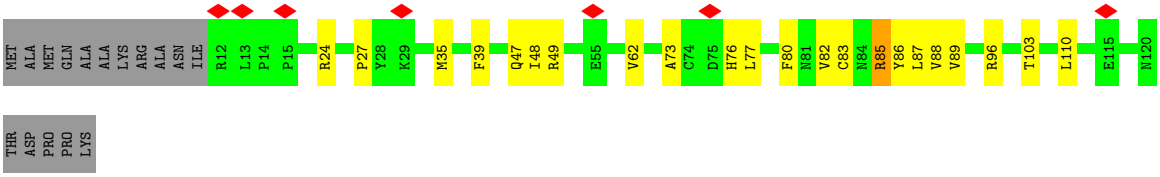
Chain 4:





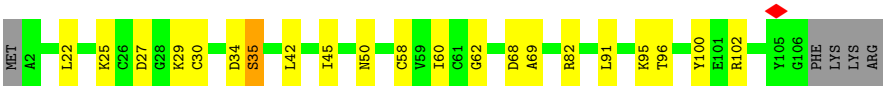
• Molecule 21: Splicing factor 3B subunit 6

Chain 5:



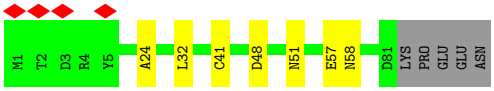
• Molecule 22: PHD finger-like domain-containing protein 5A

Chain 6:



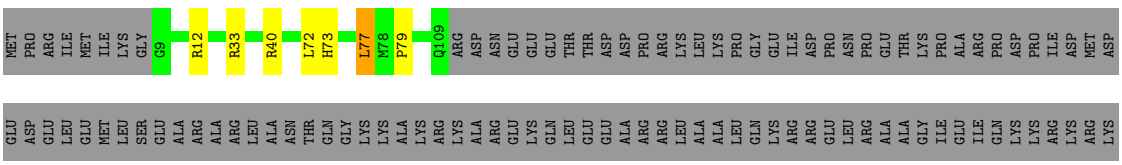
• Molecule 23: Splicing factor 3B subunit 5

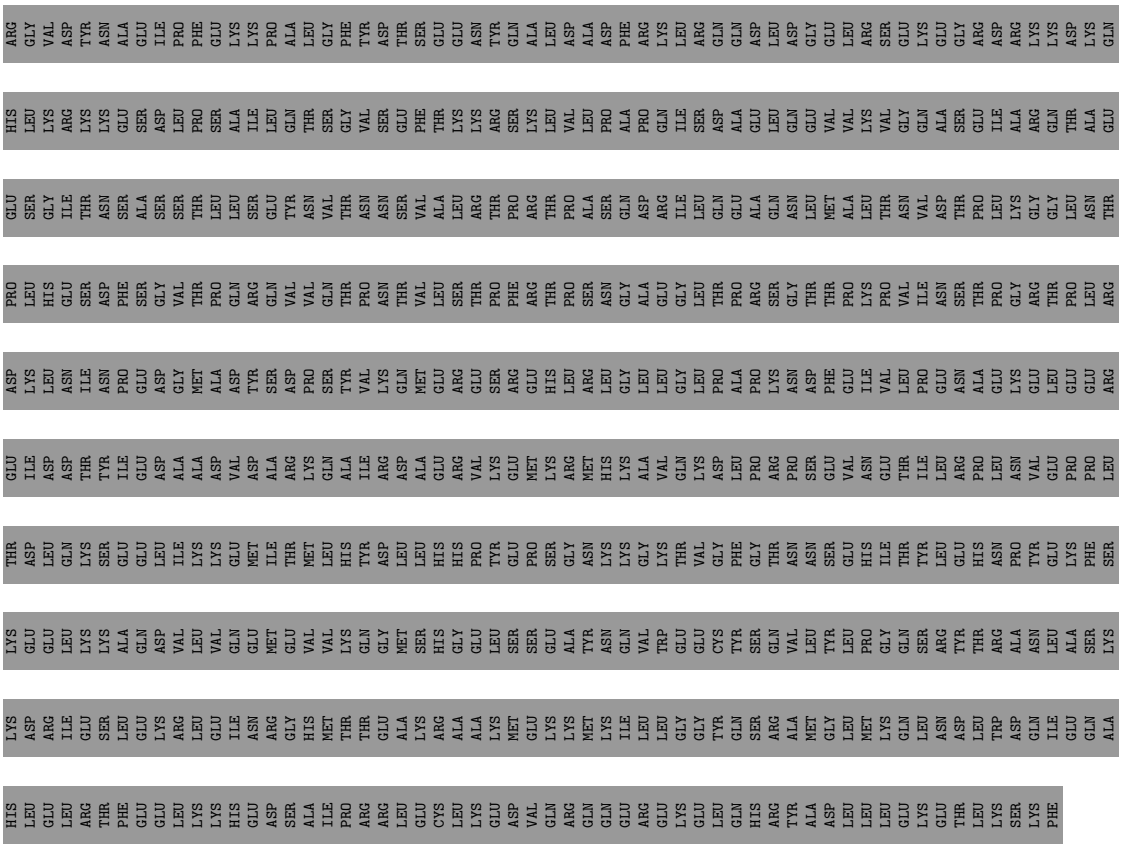
Chain 7:



• Molecule 24: Cell division cycle 5-like protein

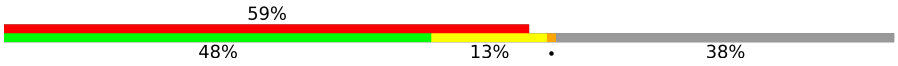
Chain L:

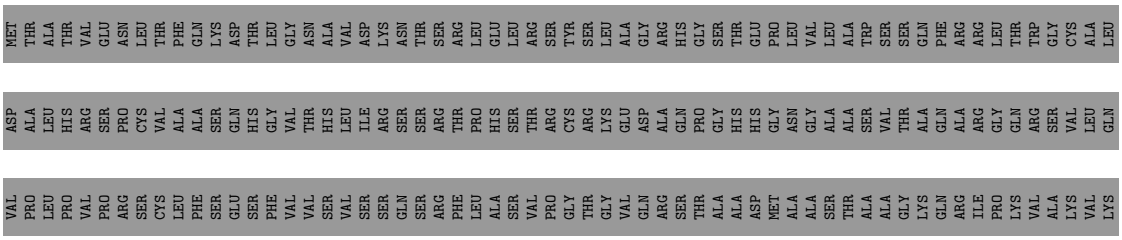


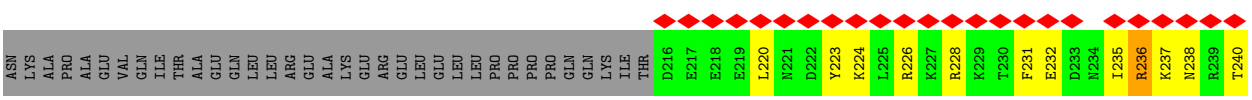


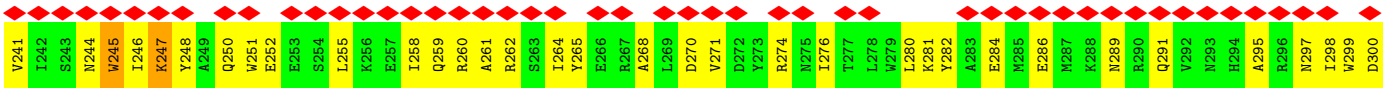
• Molecule 25: Crooked neck-like protein 1

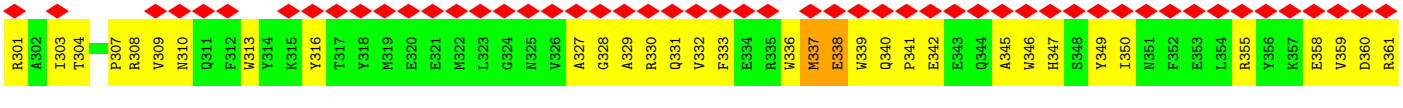
Chain J:

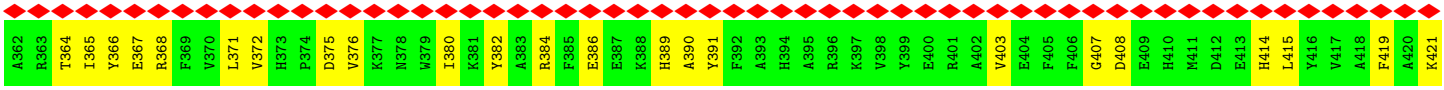


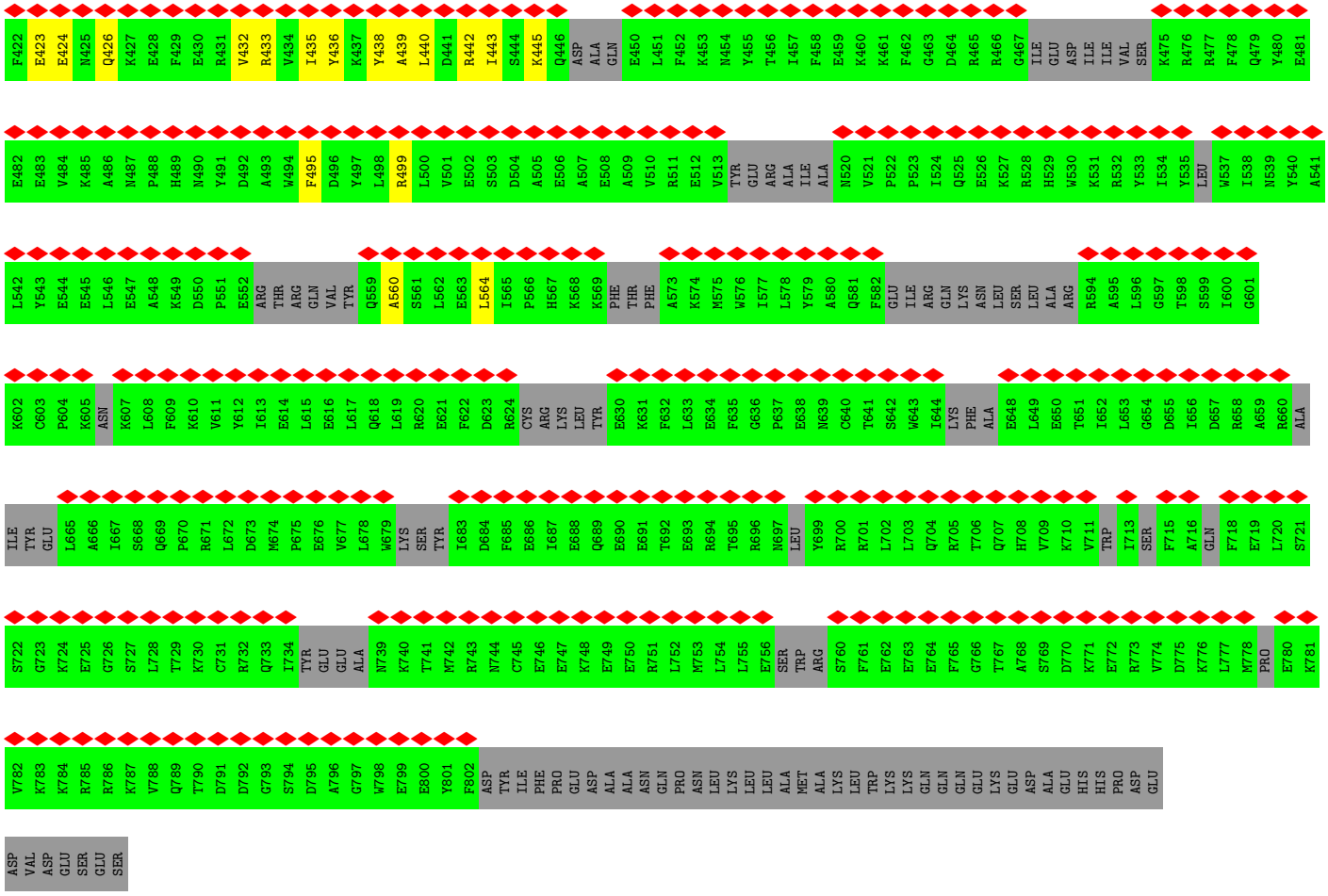






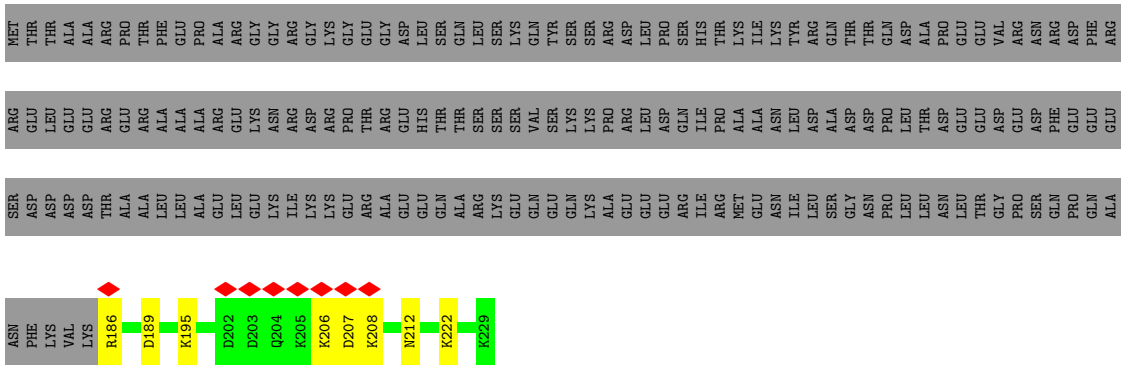






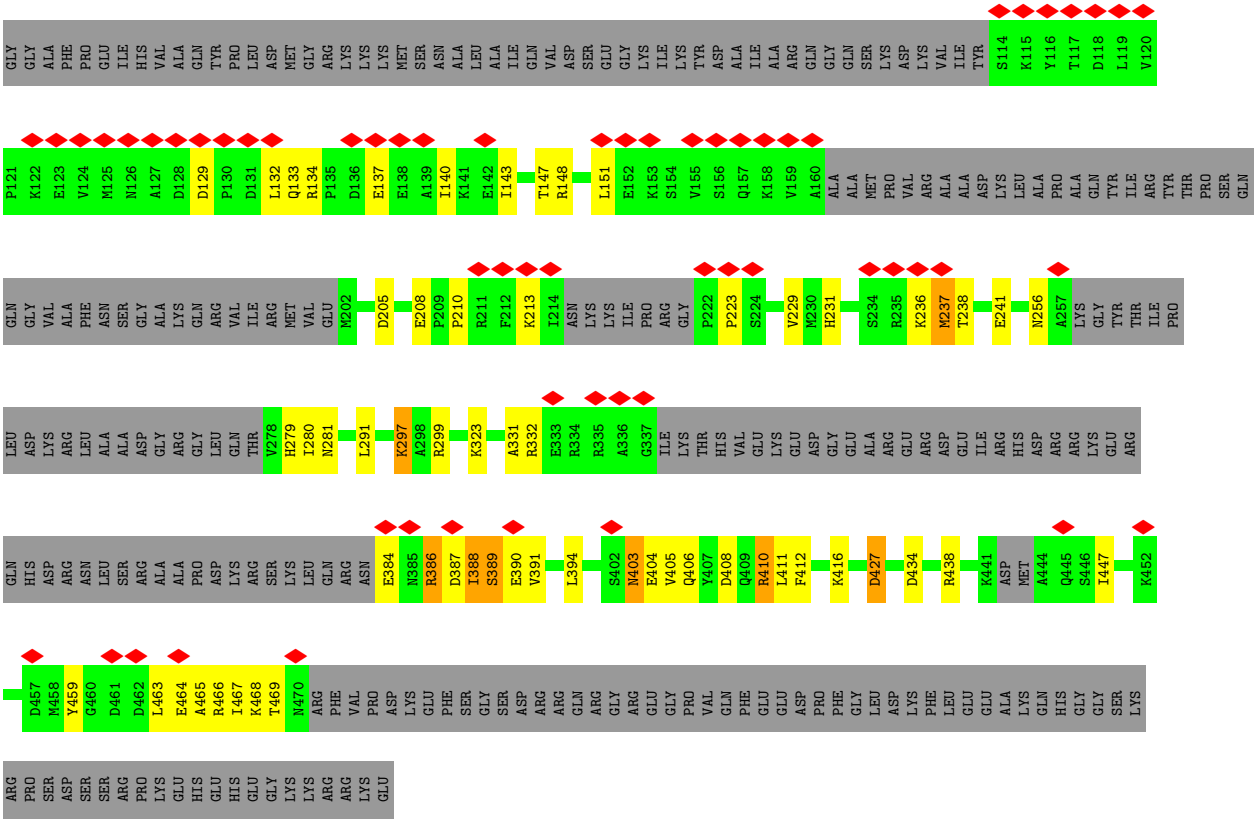
• Molecule 26: Spliceosome-associated protein CWC15 homolog

Chain P:



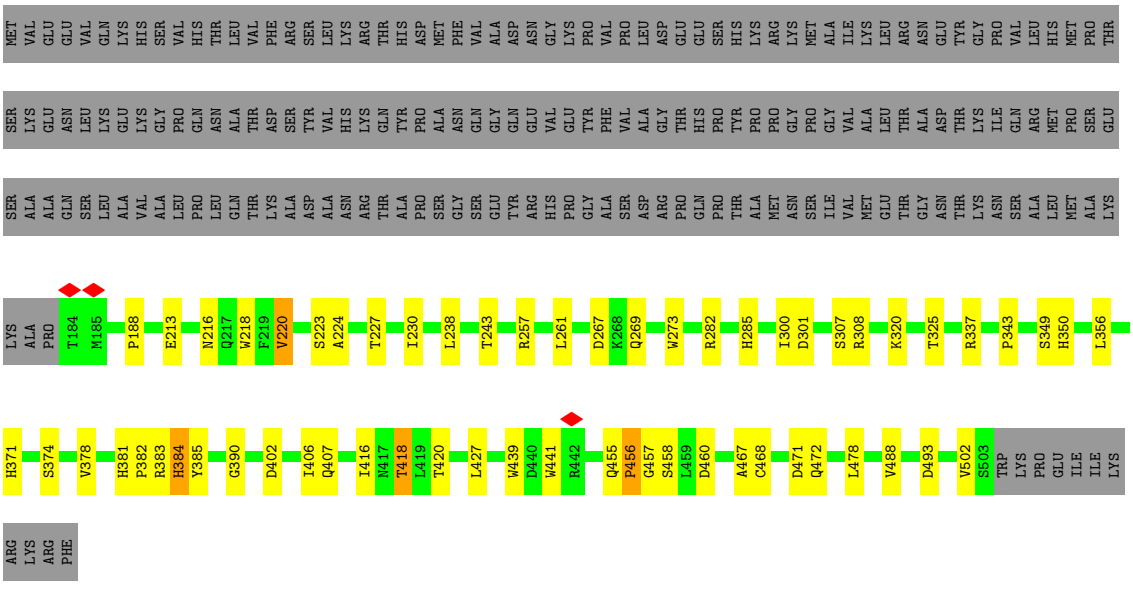
• Molecule 27: SNW domain-containing protein 1

Chain R:



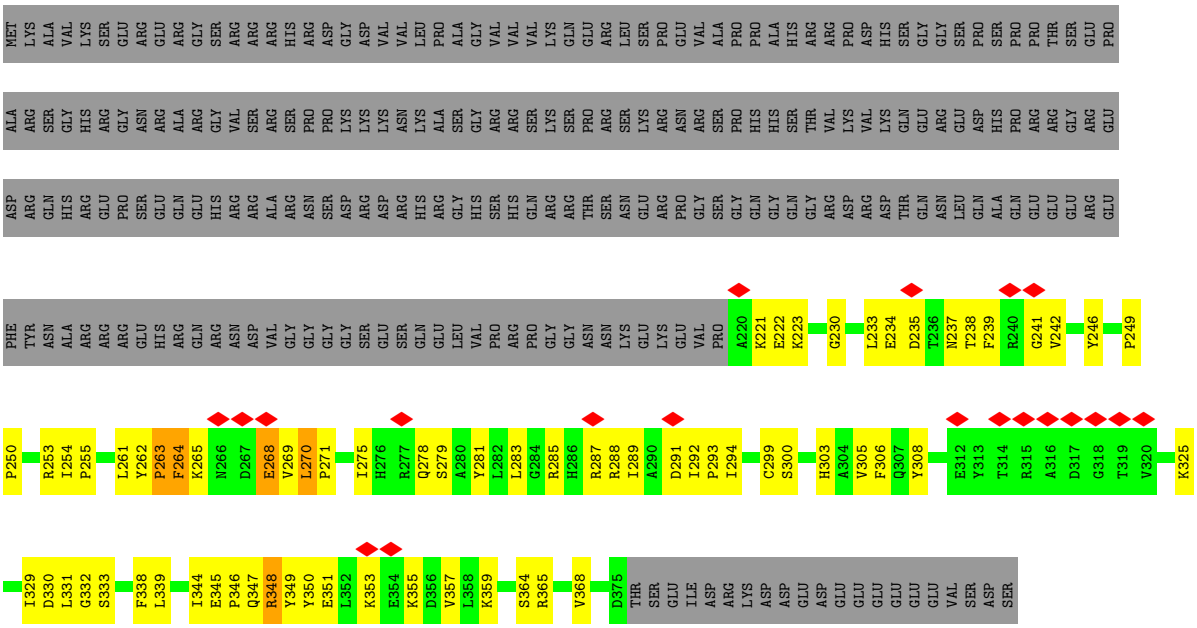
• Molecule 28: Pleiotropic regulator 1

Chain T:

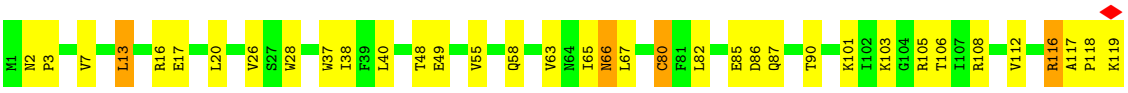


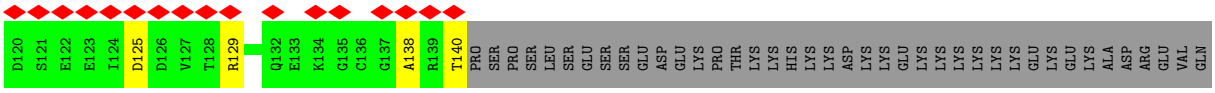
• Molecule 29: Smad nuclear-interacting protein 1

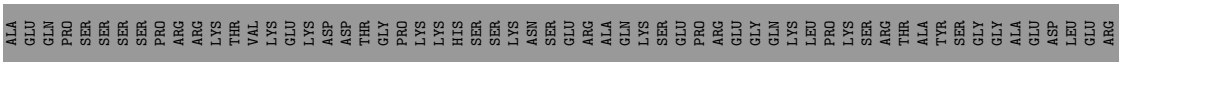
Chain X:



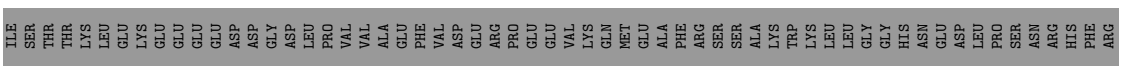
• Molecule 30: RNA-binding motif protein, X-linked 2

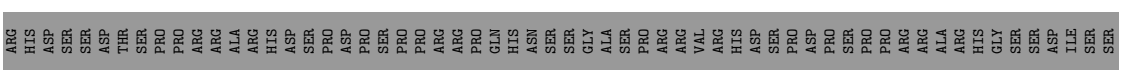


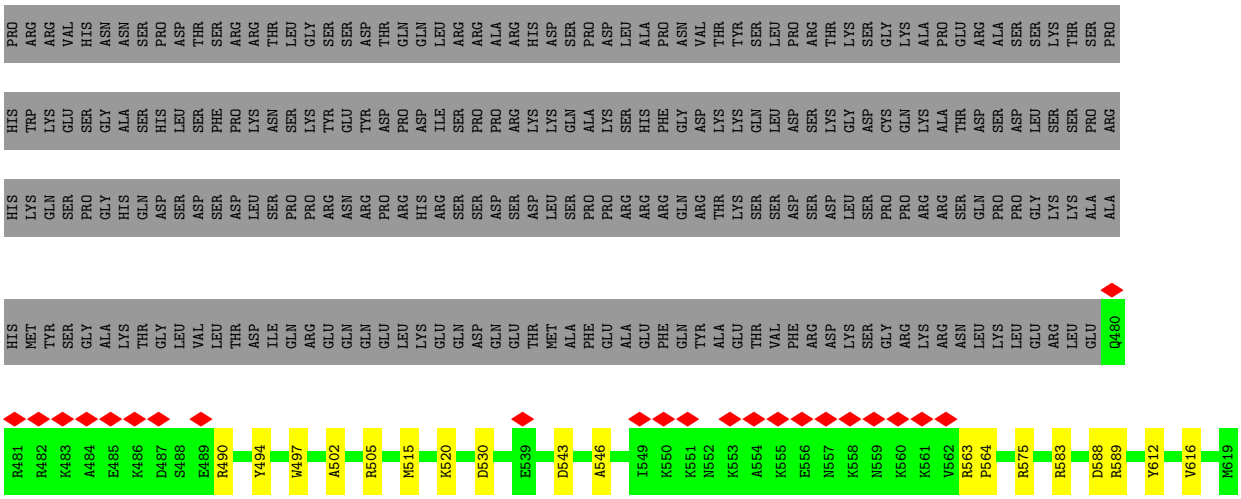




• Molecule 31: BUD13 homolog

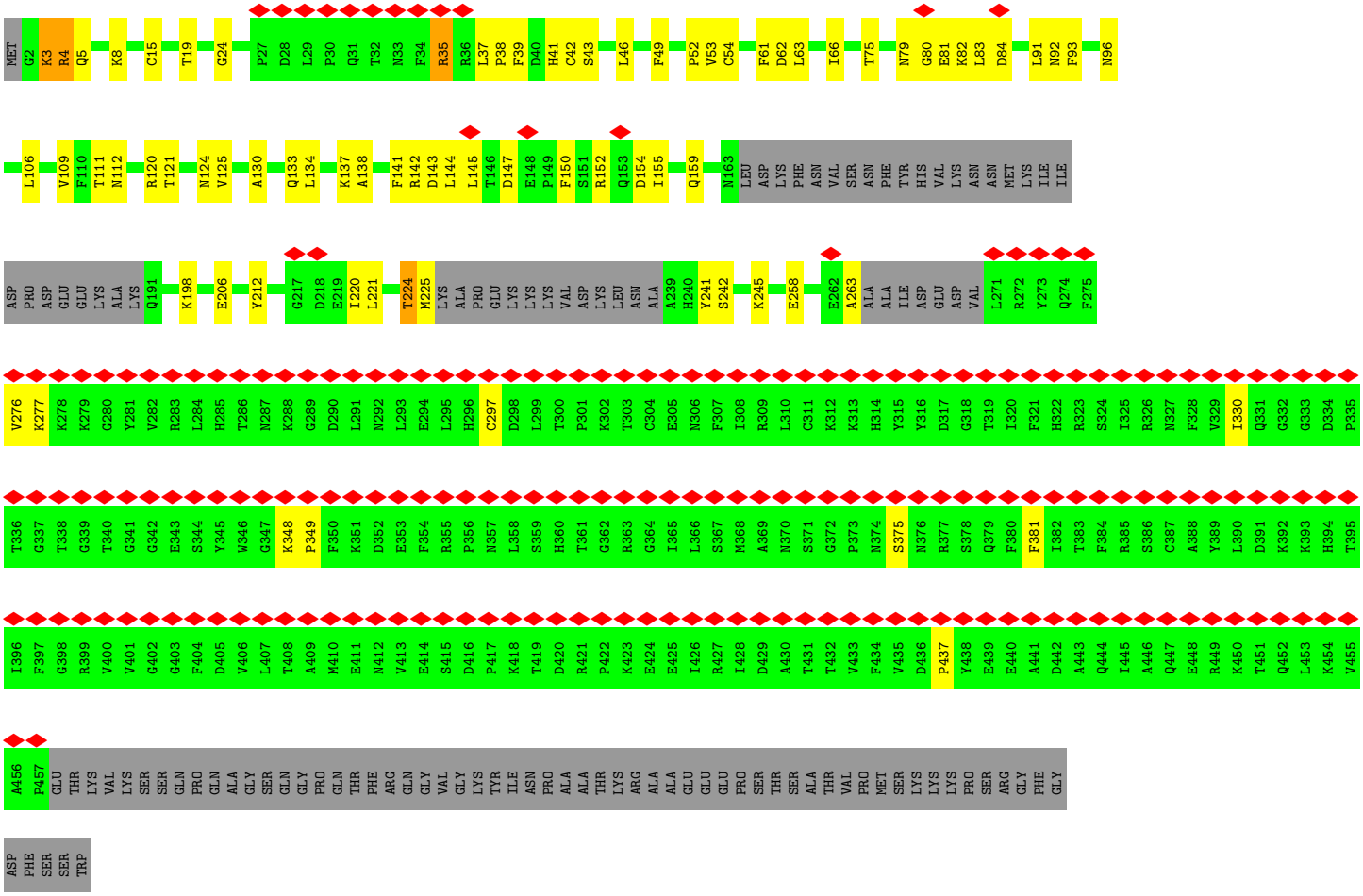






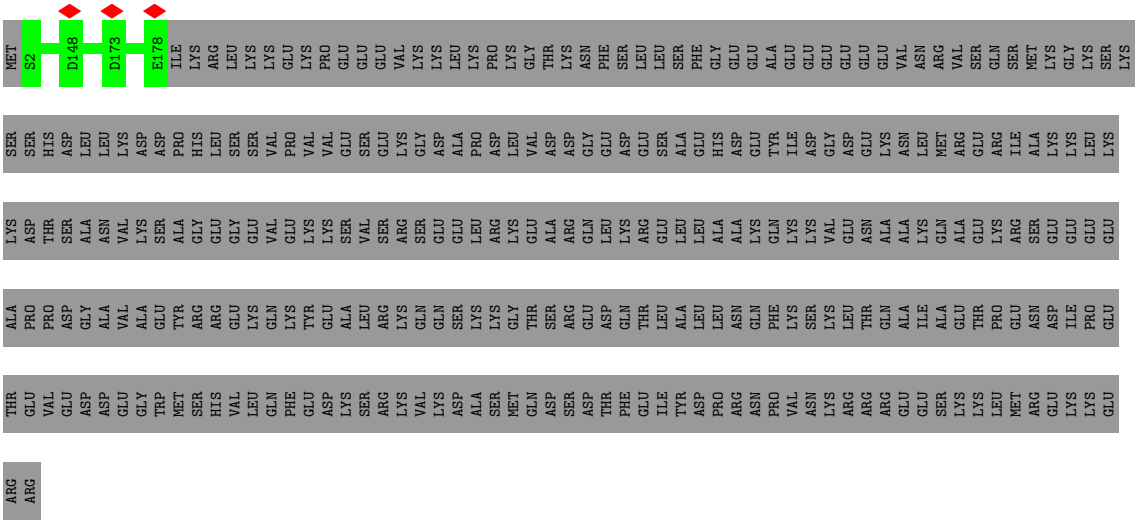
• Molecule 32: RING-type E3 ubiquitin-protein ligase PPIL2

Chain 9:



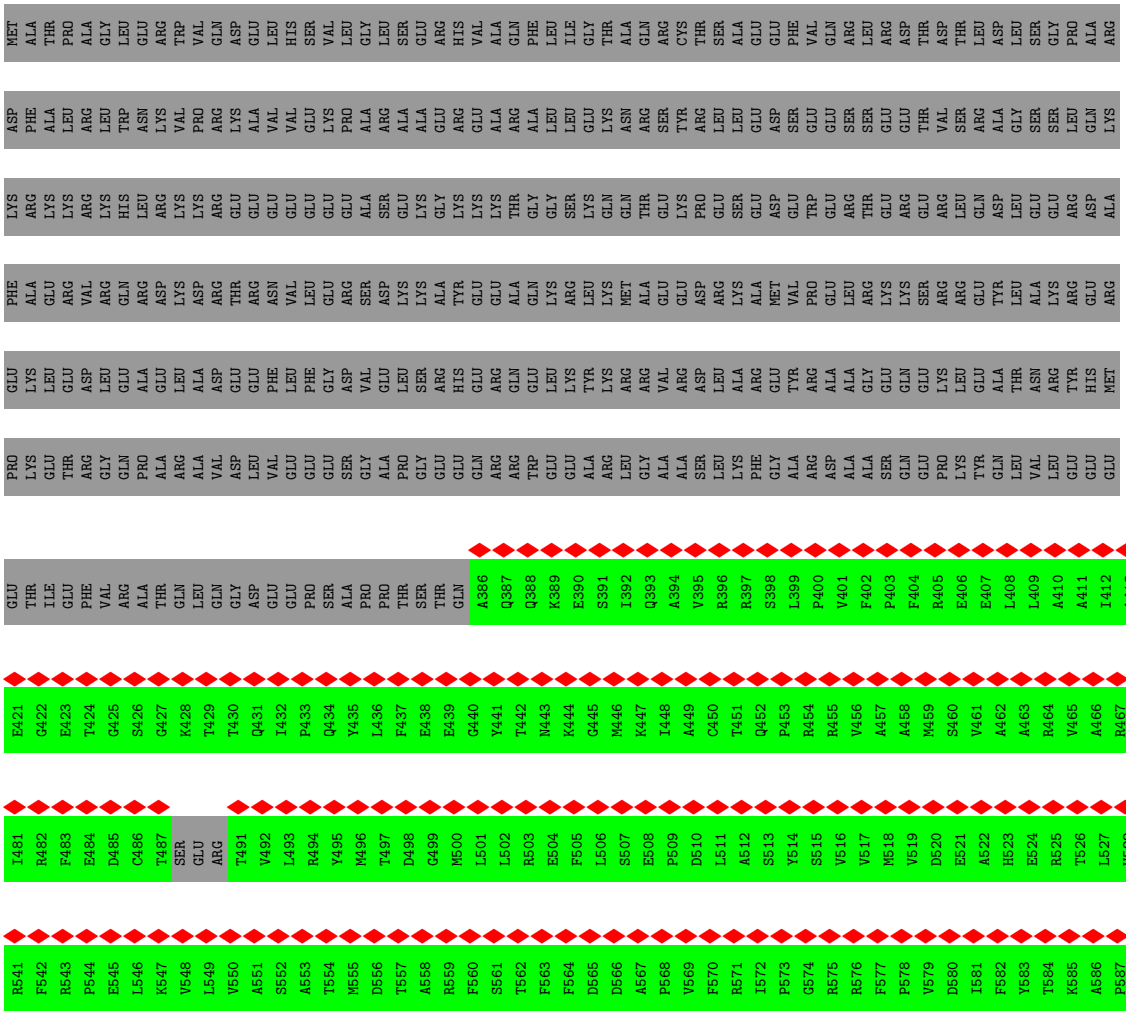
• Molecule 33: Peptidyl-prolyl cis-trans isomerase CWC27 homolog

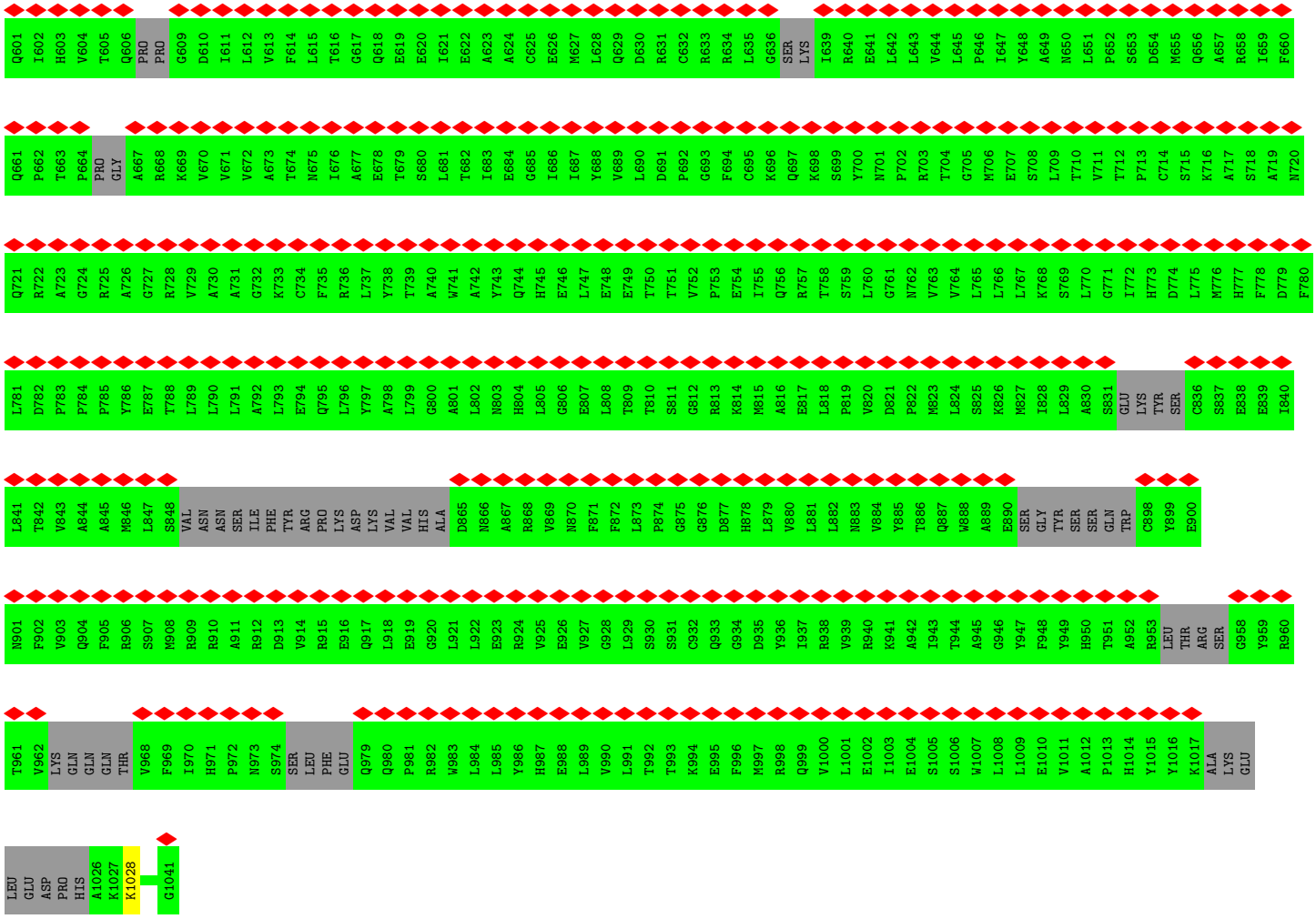
Chain z:



• Molecule 34: Pre-mRNA-splicing factor ATP-dependent RNA helicase DHX16

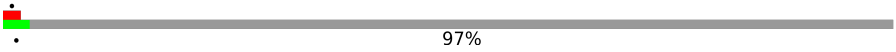
Chain x:

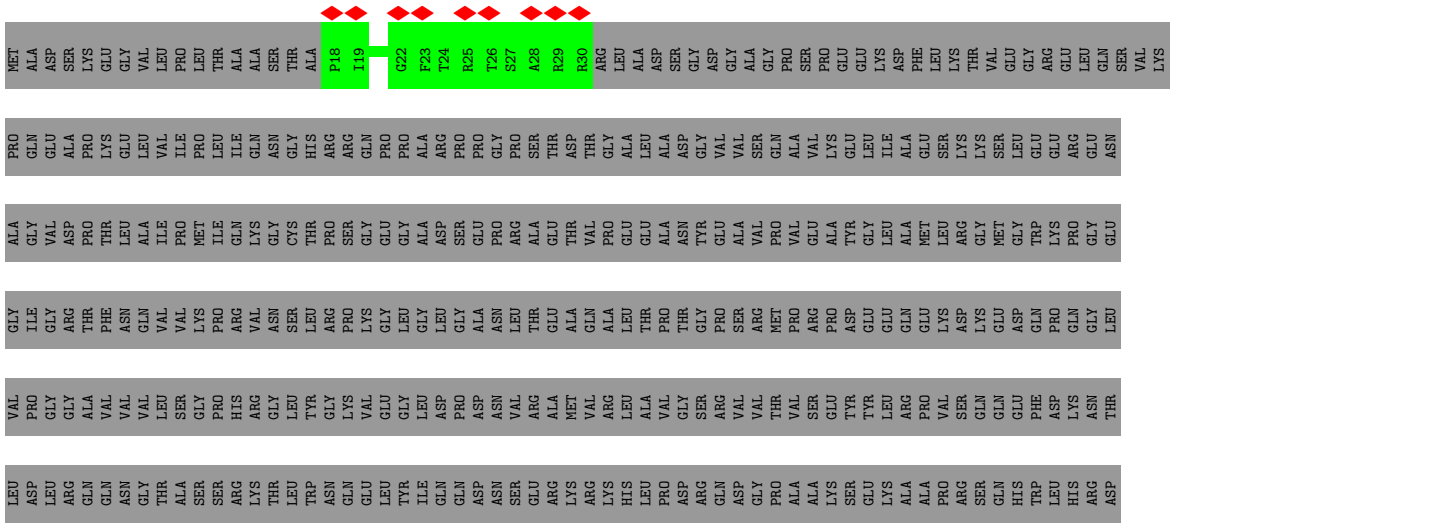


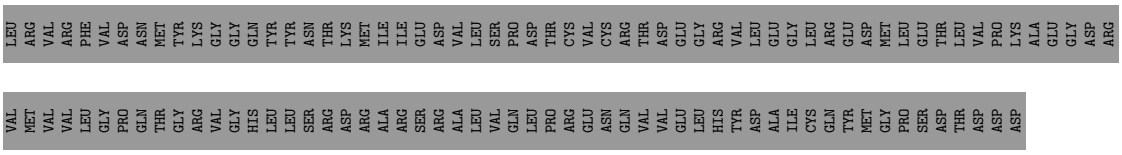


• Molecule 35: G-patch domain and KOW motifs-containing protein

Chain y:

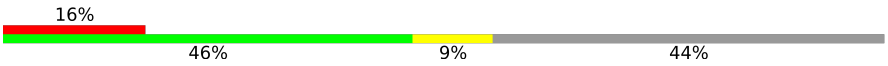


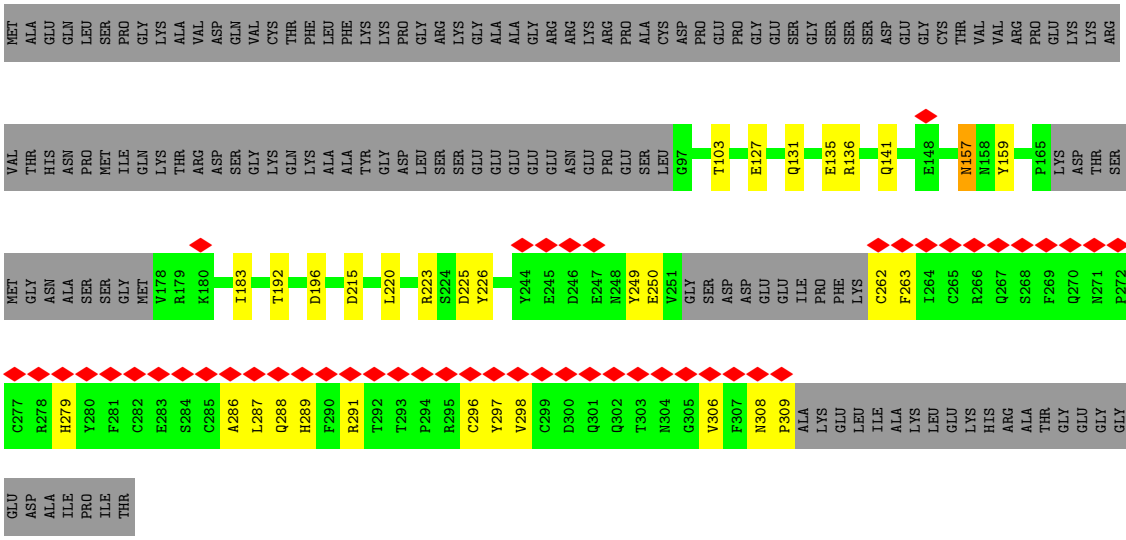




• Molecule 36: RING finger protein 113A

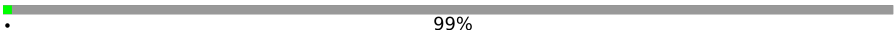
Chain M:

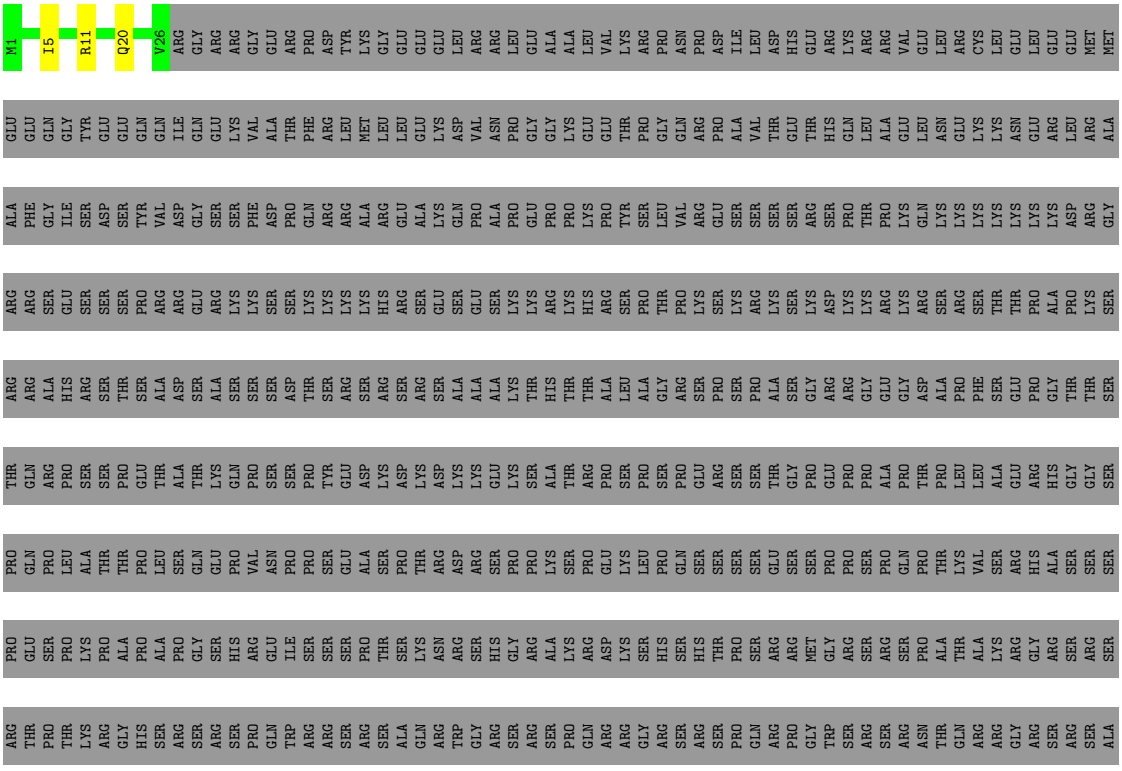


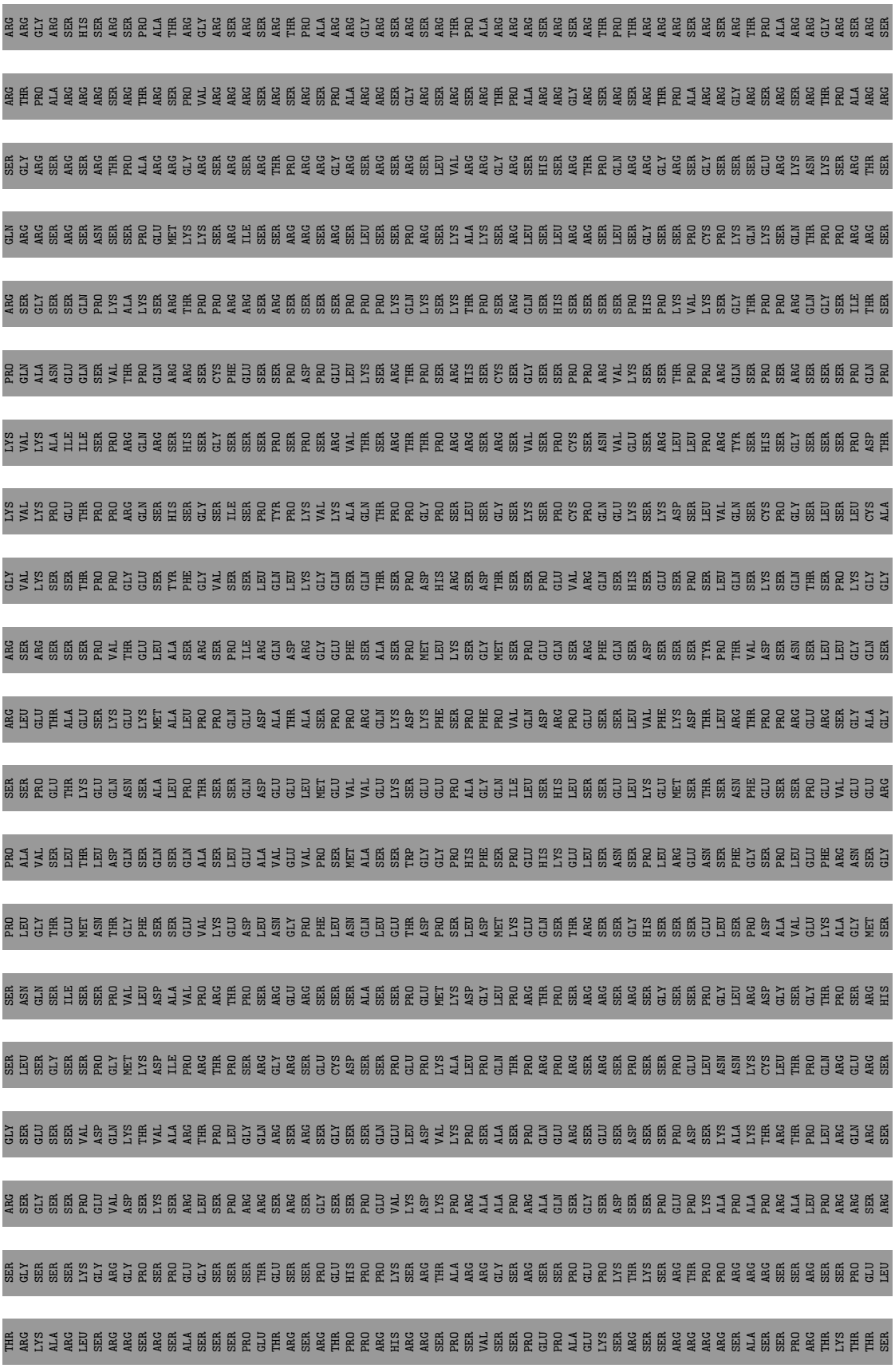


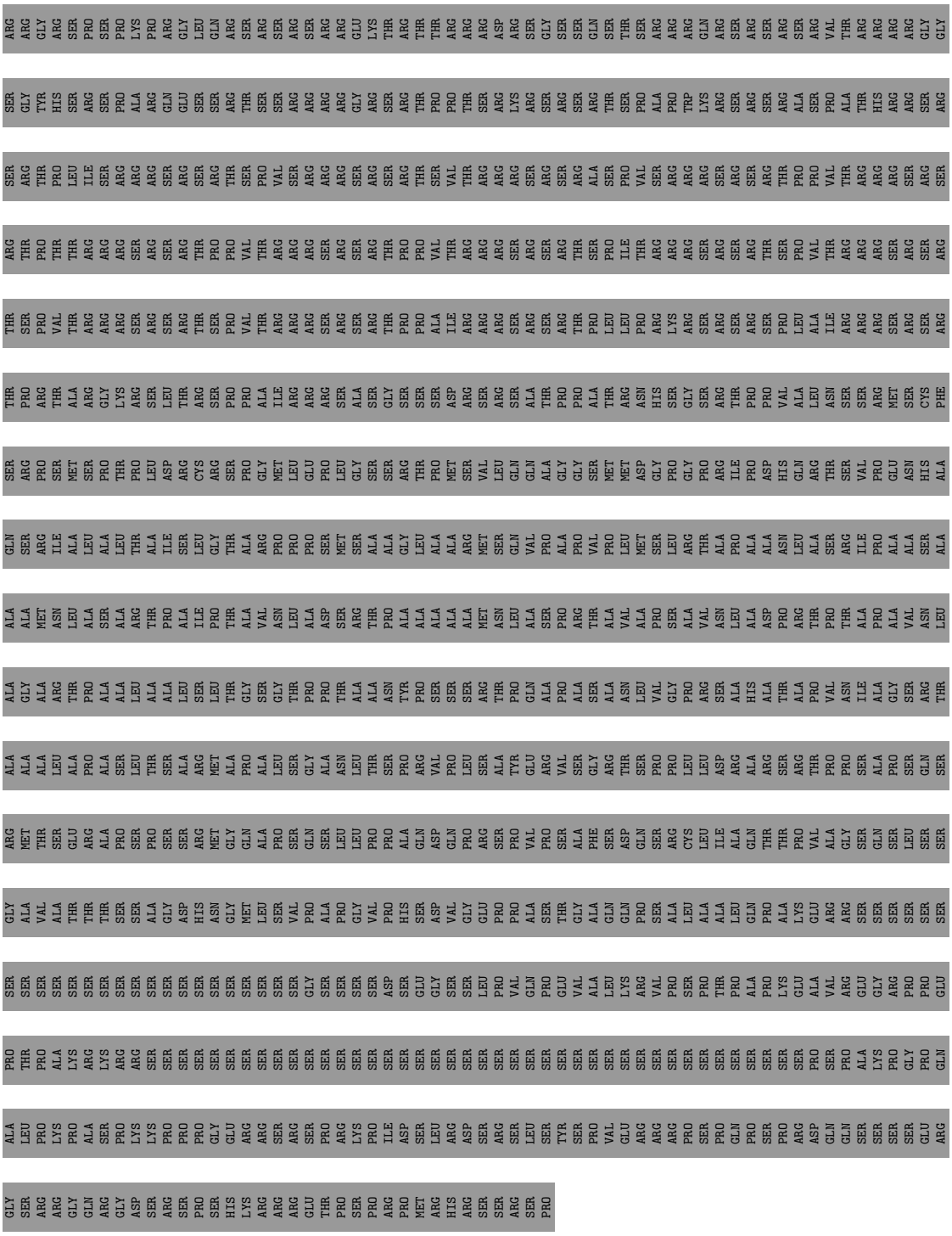
• Molecule 37: Serine/arginine repetitive matrix protein 2

Chain U:



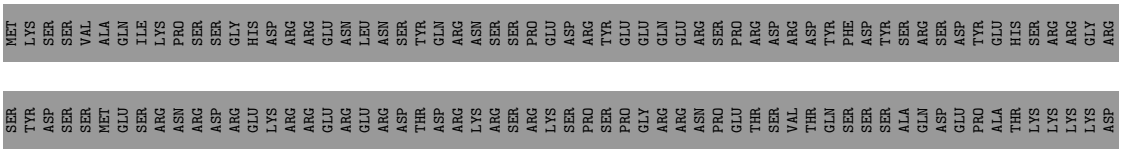


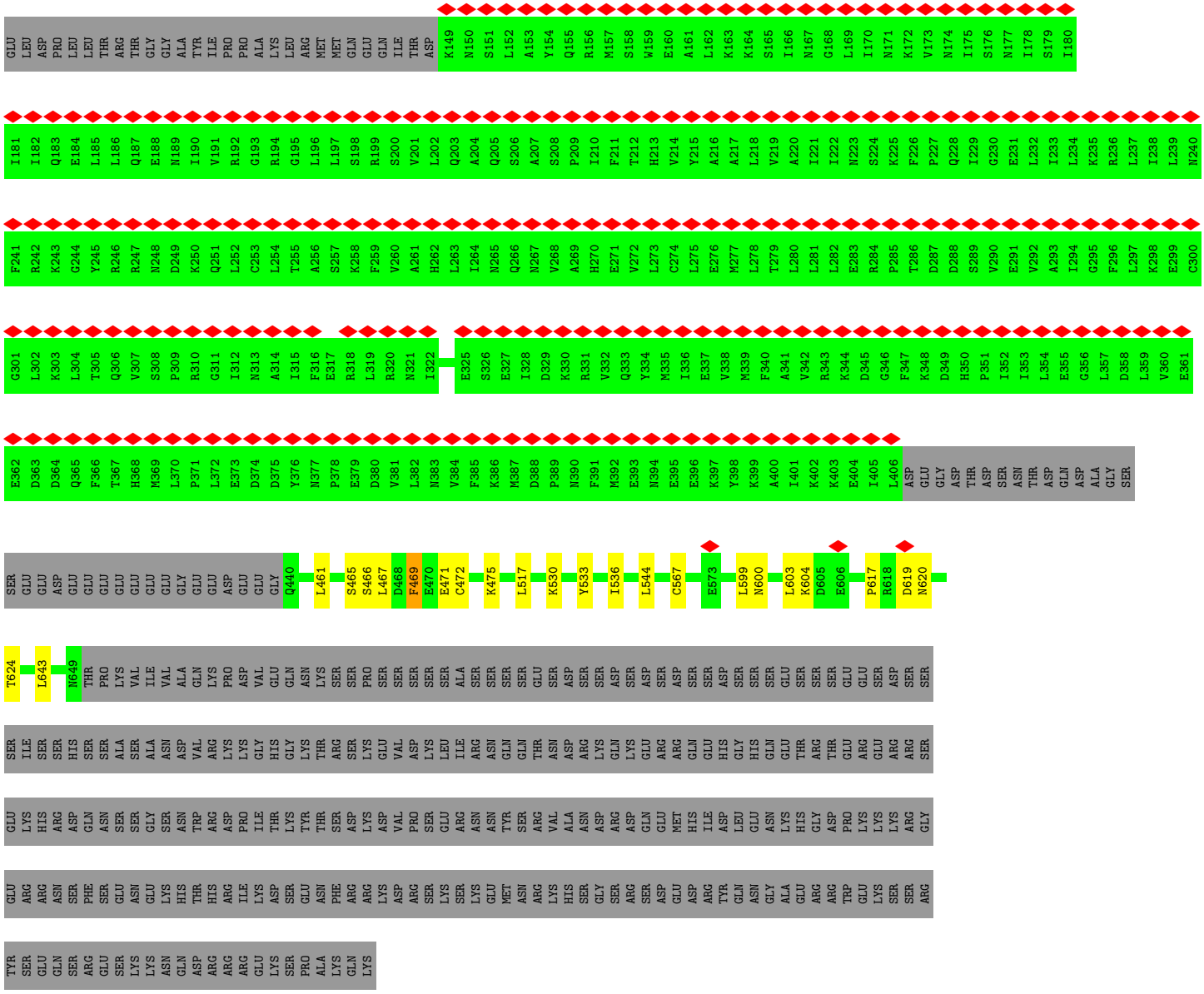




• Molecule 38: Pre-mRNA-splicing factor CWC22 homolog

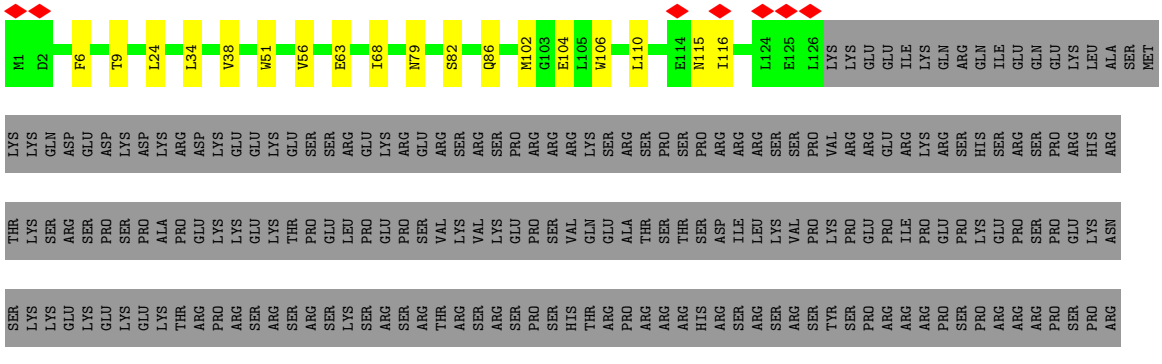
Chain V:

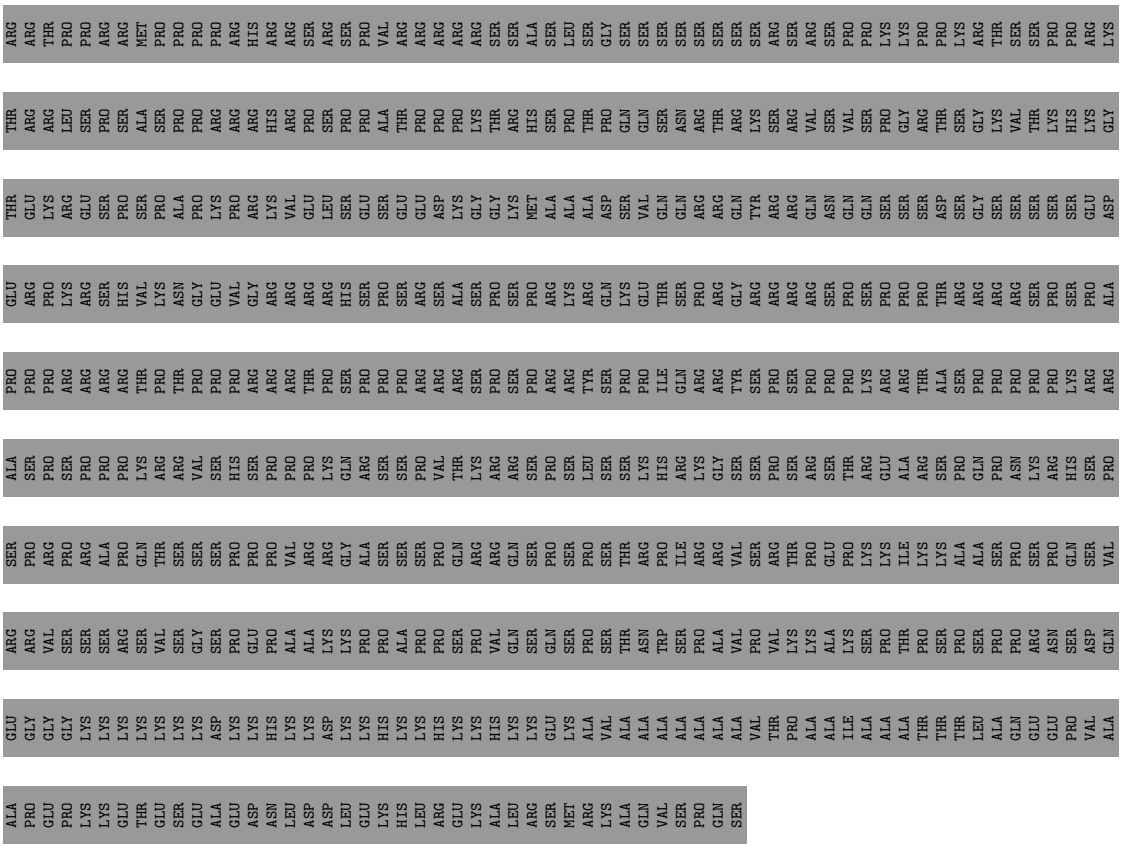




• Molecule 39: Serine/arginine repetitive matrix protein 1

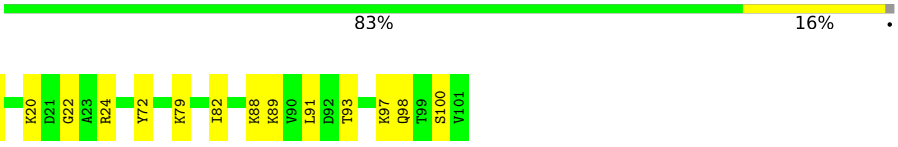
Chain 8:





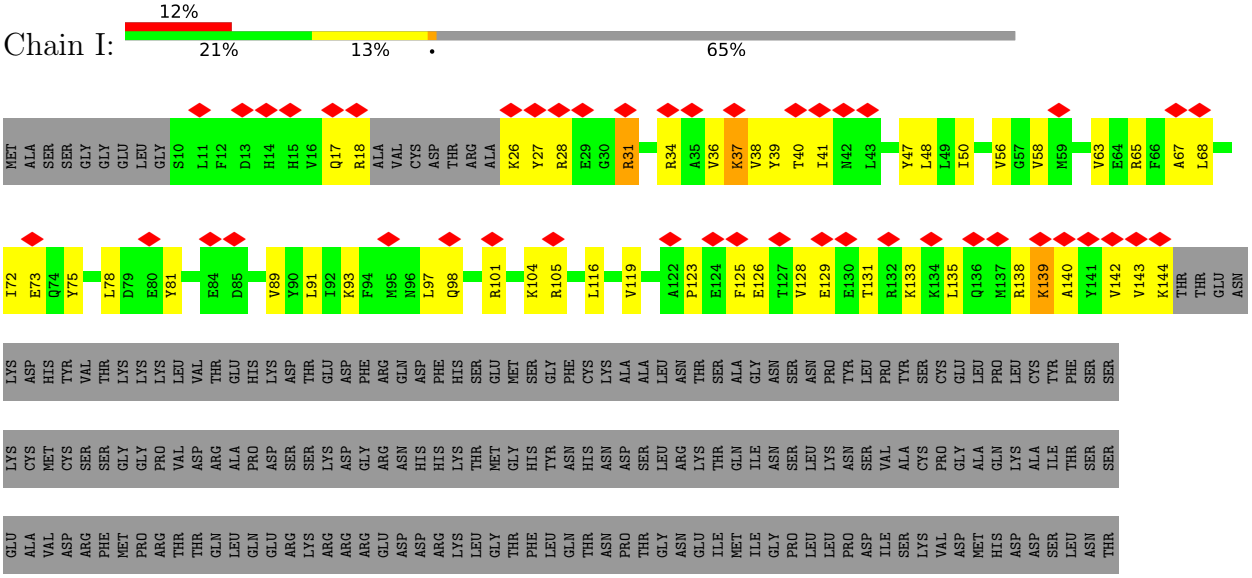
• Molecule 40: Cysteine-rich PDZ-binding protein

Chain 0:



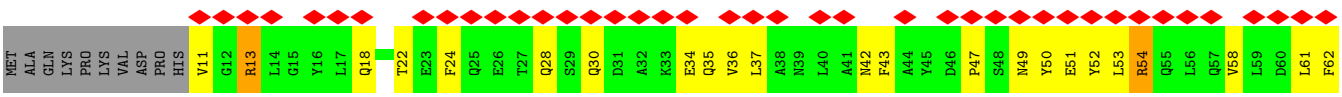
• Molecule 41: RNA-binding protein 48

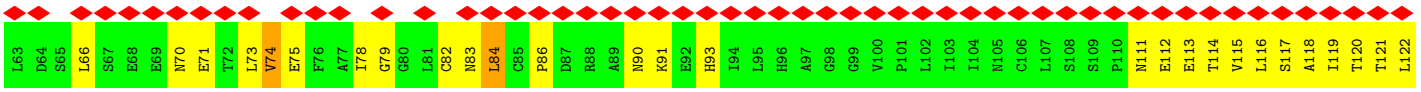
Chain I:

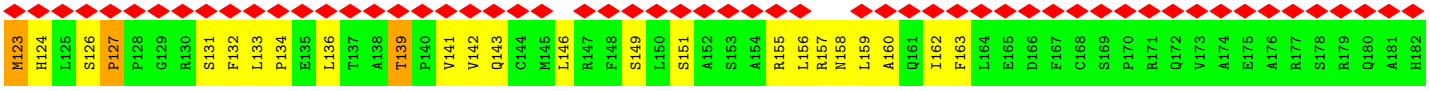


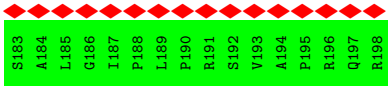
• Molecule 42: Armadillo repeat-containing protein 7

Chain K:









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	101443	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.134	Depositor
Minimum map value	-0.056	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	644.52, 644.52, 644.52	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, K, TPO, SEP, IHP, GTP, G5J

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	1.19	1/18863 (0.0%)	0.77	0/25599
2	B	0.51	0/2115	0.92	0/3284
3	C	1.03	1/7287 (0.0%)	0.79	0/9902
4	D	0.32	0/9225	0.58	0/12826
5	E	0.60	0/2390	0.75	0/3238
6	a	0.43	0/397	0.58	0/549
6	h	0.47	0/390	0.62	0/539
7	b	0.50	0/404	0.72	0/561
7	i	0.50	0/421	0.73	0/583
8	c	0.58	0/405	0.73	0/563
8	j	0.57	0/405	0.73	0/563
9	d	0.66	0/479	0.82	0/666
9	k	0.67	0/420	0.81	0/583
10	f	0.75	0/360	0.82	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	0.81	0/542
12	g	0.54	0/362	0.71	0/501
12	n	0.54	0/332	0.73	0/458
13	F	0.43	0/1449	0.77	0/2257
14	G	0.31	0/1445	0.71	0/2238
15	H	0.45	0/1511	0.72	0/2351
16	v	0.94	0/984	0.66	0/1326
17	1	1.13	0/8025	0.79	0/10859
18	2	1.01	0/1710	0.70	0/2306
19	3	1.03	0/9531	0.74	0/12931
20	4	0.60	0/382	0.70	0/529
21	5	0.88	0/925	0.71	0/1247
22	6	1.15	0/825	0.77	0/1106
23	7	1.29	0/688	0.85	0/930
24	L	1.26	0/864	0.78	0/1165
25	J	0.35	0/3494	0.52	0/4743

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
26	P	1.18	0/391	0.72	0/517
27	R	0.78	0/1954	0.58	0/2622
28	T	1.28	0/2574	0.84	0/3511
29	X	0.31	0/1304	0.52	0/1760
30	Y	1.05	0/1113	0.72	0/1501
31	Z	1.08	0/1153	0.70	0/1548
32	9	0.57	0/2732	0.60	0/3733
33	z	1.09	0/1434	0.76	0/1941
34	x	0.37	0/2996	0.49	0/4142
35	y	0.25	0/107	0.47	0/141
36	M	1.03	0/1609	0.70	0/2164
37	U	0.91	0/196	0.66	0/265
38	V	0.88	0/3042	0.70	0/4152
39	8	0.95	0/1028	0.75	0/1379
40	0	1.01	0/782	0.68	0/1043
41	I	0.42	0/1083	0.53	0/1454
42	K	0.29	0/1333	0.50	0/1826
All	All	0.91	2/102059 (0.0%)	0.72	0/140180

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	204	ASP	C-N	-5.74	1.20	1.34
1	A	279	PHE	C-N	-5.65	1.21	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	18354	0	18178	381	0
2	B	1898	0	963	36	0
3	C	7125	0	7130	122	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	9215	0	4458	170	0
5	E	2337	0	2272	194	0
6	a	399	0	173	0	0
6	h	392	0	168	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	1294	0	650	41	0
14	G	1303	0	667	46	0
15	H	1350	0	679	30	0
16	v	963	0	945	0	0
17	1	7879	0	8044	165	0
18	2	1674	0	1580	23	0
19	3	9352	0	9273	220	0
20	4	383	0	173	24	0
21	5	906	0	913	31	0
22	6	811	0	788	20	0
23	7	669	0	631	6	0
24	L	843	0	852	15	0
25	J	3457	0	2537	157	0
26	P	384	0	382	10	0
27	R	1923	0	1889	117	0
28	T	2507	0	2451	41	0
29	X	1271	0	1252	92	0
30	Y	1095	0	1083	59	0
31	Z	1129	0	1077	20	0
32	9	2691	0	2121	91	0
33	z	1400	0	1344	0	0
34	x	3007	0	1453	0	0
35	y	105	0	107	0	0
36	M	1572	0	1483	36	0
37	U	193	0	196	3	0
38	V	3008	0	2291	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	8	1011	0	1035	17	0
40	0	770	0	778	28	0
41	I	1062	0	1067	67	0
42	K	1314	0	1177	100	0
43	A	36	0	6	0	0
44	C	32	0	12	3	0
45	C	1	0	0	0	0
45	F	4	0	0	0	0
46	F	2	0	0	0	0
47	F	33	0	0	3	0
48	0	2	0	0	0	0
48	6	3	0	0	0	0
48	M	1	0	0	0	0
48	v	1	0	0	0	0
49	C	3	0	0	0	0
All	All	99906	0	84285	2086	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 12.

All (2086) 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)
17:1:641:ILE:HD11	17:1:675:MET:CE	1.58	1.34
20:4:14:THR:HA	20:4:59:VAL:O	1.32	1.30
25:J:337:MET:HE2	25:J:346:TRP:CH2	1.69	1.26
5:E:62:LEU:HD12	5:E:351:LEU:CD1	1.66	1.26
5:E:62:LEU:CD1	5:E:351:LEU:HD12	1.68	1.23
5:E:326:HIS:CE1	5:E:346:SER:HB3	1.73	1.22
32:9:3:LYS:HD3	32:9:5:GLN:HB2	1.20	1.18
29:X:345:GLU:OE2	29:X:348:ARG:HD2	1.44	1.17
25:J:337:MET:CE	25:J:346:TRP:CZ3	2.29	1.15
25:J:337:MET:HE2	25:J:346:TRP:CZ3	1.81	1.14
5:E:74:PHE:CE1	5:E:81:LEU:HD21	1.81	1.13
24:L:77:LEU:HD21	32:9:221:LEU:HD11	1.30	1.13
1:A:2168:TYR:CZ	1:A:2298:LEU:HD11	1.83	1.12
25:J:316:TYR:HE1	25:J:332:VAL:HG21	1.15	1.12
4:D:176:GLY:O	4:D:179:ILE:HG22	1.47	1.11
17:1:641:ILE:CD1	17:1:675:MET:CE	2.27	1.11
20:4:12:ASP:CB	20:4:67:ALA:HB1	1.80	1.10
5:E:60:MET:SD	5:E:99:CYS:SG	2.50	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:950:ALA:HB2	19:3:989:TYR:OH	1.53	1.08
42:K:119:ILE:HG23	42:K:163:PHE:HD2	1.19	1.08
17:1:641:ILE:HD11	17:1:675:MET:HE2	1.09	1.07
41:I:31:ARG:HB3	41:I:31:ARG:HH11	1.16	1.07
19:3:630:MET:CE	36:M:287:LEU:HD21	1.83	1.07
1:A:1838:LYS:HE3	1:A:1865:ARG:CZ	1.83	1.07
5:E:119:THR:HG21	5:E:161:ARG:HB2	1.37	1.06
20:4:17:VAL:HA	20:4:85:ARG:O	1.53	1.06
39:8:56:VAL:HG21	39:8:68:ILE:HD13	1.39	1.05
5:E:132:THR:CG2	5:E:146:ARG:HB2	1.86	1.04
5:E:258:THR:HG21	5:E:260:ARG:HH11	1.11	1.04
27:R:279:HIS:HA	32:9:224:THR:CG2	1.87	1.04
14:G:222:U:C6	30:Y:119:LYS:HE2	1.91	1.04
19:3:687:SER:O	36:M:306:VAL:HG21	1.55	1.04
29:X:265:LYS:HG3	29:X:364:SER:OG	1.58	1.03
4:D:406:ARG:CB	4:D:955:ASP:HA	1.87	1.03
5:E:326:HIS:CE1	5:E:346:SER:CB	2.40	1.03
27:R:386:ARG:HH12	29:X:353:LYS:HG3	1.20	1.03
5:E:88:ARG:HG2	5:E:110:GLY:O	1.57	1.03
5:E:260:ARG:HD2	5:E:276:ILE:HG12	1.34	1.03
4:D:164:THR:HA	4:D:168:ARG:NH1	1.73	1.03
17:1:971:MET:HE1	17:1:1003:VAL:HG11	1.40	1.03
1:A:2325:VAL:HG13	4:D:788:GLY:O	1.59	1.03
27:R:279:HIS:HA	32:9:224:THR:HG23	1.37	1.02
5:E:193:THR:HG23	5:E:194:TYR:CD1	1.94	1.02
27:R:387:ASP:HB2	29:X:351:GLU:HB2	1.36	1.02
29:X:241:GLY:HA2	29:X:288:ARG:NH2	1.74	1.01
27:R:280:ILE:H	32:9:224:THR:CG2	1.72	1.01
25:J:359:VAL:HG21	25:J:389:HIS:NE2	1.77	1.00
1:A:1122:ASN:HB2	32:9:35:ARG:HH21	1.27	0.99
19:3:1130:VAL:CG1	19:3:1215:TYR:CE1	2.46	0.98
25:J:337:MET:CE	25:J:346:TRP:CH2	2.45	0.97
4:D:120:ILE:HD12	4:D:161:LEU:CD2	1.93	0.97
1:A:1122:ASN:HB2	32:9:35:ARG:NH2	1.79	0.97
1:A:2325:VAL:HG13	4:D:788:GLY:C	1.83	0.97
4:D:148:LEU:CD2	4:D:152:GLU:HB3	1.93	0.96
19:3:47:THR:CG2	19:3:49:LYS:HG2	1.96	0.96
19:3:630:MET:SD	36:M:287:LEU:HD21	2.04	0.96
19:3:630:MET:HE1	36:M:287:LEU:HD21	1.44	0.96
1:A:265:THR:HG23	1:A:327:VAL:HG22	1.48	0.96
17:1:641:ILE:CG1	17:1:675:MET:CE	2.45	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:5:39:PHE:HE1	21:5:77:LEU:HD21	1.28	0.95
19:3:54:LEU:HD23	19:3:99:PHE:CE2	2.00	0.95
42:K:149:SER:O	42:K:157:ARG:HG2	1.65	0.95
5:E:147:LEU:HD13	5:E:179:TRP:CG	1.99	0.95
17:1:641:ILE:CG1	17:1:675:MET:HE1	1.96	0.95
41:I:37:LYS:HD3	41:I:39:TYR:CZ	2.01	0.94
1:A:2103:THR:HG21	1:A:2260:GLN:OE1	1.66	0.94
5:E:260:ARG:CD	5:E:276:ILE:HG12	1.96	0.94
27:R:386:ARG:NH1	29:X:353:LYS:HG3	1.83	0.94
1:A:1307:MET:SD	1:A:1547:VAL:HG11	2.07	0.94
1:A:2219:THR:HG23	1:A:2224:THR:HG22	1.47	0.94
25:J:316:TYR:CE1	25:J:332:VAL:HG21	2.03	0.94
1:A:1092:ILE:HG22	1:A:1093:ASP:H	1.31	0.93
20:4:12:ASP:CB	20:4:67:ALA:CB	2.47	0.92
25:J:232:GLU:HA	25:J:235:ILE:CG2	2.00	0.92
25:J:313:TRP:CZ3	25:J:336:TRP:NE1	2.37	0.92
39:8:56:VAL:HG21	39:8:68:ILE:CD1	1.98	0.92
1:A:1976:TRP:HA	1:A:1979:VAL:HG22	1.52	0.92
42:K:119:ILE:HG23	42:K:163:PHE:CD2	2.05	0.91
19:3:170:VAL:HG22	19:3:184:CYS:SG	2.10	0.91
25:J:333:PHE:CD1	25:J:349:TYR:CD1	2.58	0.91
19:3:1130:VAL:CG1	19:3:1215:TYR:CZ	2.53	0.91
5:E:62:LEU:HD12	5:E:351:LEU:HD12	0.91	0.91
19:3:586:ASP:OD1	19:3:610:VAL:HG11	1.71	0.91
1:A:1921:ASP:HB3	1:A:1966:HIS:ND1	1.86	0.91
19:3:1004:ASP:OD2	19:3:1007:GLU:HB2	1.70	0.91
19:3:429:ARG:HG2	19:3:429:ARG:HH21	1.35	0.91
5:E:258:THR:HG21	5:E:260:ARG:NH1	1.86	0.90
1:A:2284:MET:SD	1:A:2287:ARG:HD2	2.10	0.90
17:1:1004:ILE:HD11	17:1:1009:MET:SD	2.12	0.90
42:K:78:ILE:HG21	42:K:114:THR:HG23	1.54	0.90
29:X:253:ARG:HH21	29:X:253:ARG:HG3	1.36	0.90
4:D:131:ILE:CG1	4:D:697:ALA:HB1	2.02	0.90
5:E:258:THR:HG22	5:E:260:ARG:HG2	1.53	0.90
27:R:280:ILE:H	32:9:224:THR:HG22	1.35	0.89
4:D:126:ASP:OD2	4:D:1075:PHE:CB	2.20	0.89
42:K:24:PHE:HB2	42:K:36:VAL:HG11	1.53	0.89
5:E:193:THR:CG2	5:E:194:TYR:CD1	2.55	0.89
19:3:1057:ARG:HG3	19:3:1057:ARG:HH11	1.38	0.89
1:A:591:MET:HB3	1:A:598:LEU:CD2	2.02	0.88
27:R:391:VAL:HA	29:X:347:GLN:O	1.72	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1:614:ARG:O	17:1:614:ARG:HD2	1.74	0.88
42:K:78:ILE:HG12	42:K:117:SER:HB2	1.54	0.88
30:Y:67:LEU:HA	30:Y:80:CYS:HB2	1.56	0.88
29:X:241:GLY:HA2	29:X:288:ARG:CZ	2.04	0.88
29:X:345:GLU:OE2	29:X:348:ARG:CD	2.22	0.88
32:9:3:LYS:CD	32:9:5:GLN:HB2	2.04	0.88
3:C:779:LEU:HD21	3:C:912:LEU:HD11	1.56	0.88
32:9:220:ILE:H	32:9:220:ILE:HD12	1.37	0.87
27:R:438:ARG:HG3	27:R:438:ARG:HH21	1.35	0.87
5:E:145:LYS:HE2	5:E:184:LYS:HE2	1.56	0.87
19:3:630:MET:HE2	36:M:287:LEU:HD11	1.54	0.87
29:X:241:GLY:HA3	29:X:289:ILE:HD11	1.56	0.87
19:3:49:LYS:HG3	19:3:51:HIS:CE1	2.10	0.86
4:D:1589:PHE:O	4:D:1642:GLN:CB	2.23	0.86
5:E:193:THR:CG2	5:E:194:TYR:CE1	2.58	0.86
5:E:326:HIS:ND1	5:E:346:SER:CB	2.38	0.86
4:D:123:ALA:HB3	4:D:161:LEU:HD11	1.56	0.86
5:E:193:THR:HG23	5:E:194:TYR:HD1	1.37	0.86
1:A:1976:TRP:HA	1:A:1979:VAL:CG2	2.05	0.86
4:D:148:LEU:HD21	4:D:152:GLU:HB3	1.55	0.86
18:2:657:ILE:O	18:2:657:ILE:HG22	1.73	0.86
19:3:1130:VAL:HG11	19:3:1215:TYR:CE2	2.09	0.86
1:A:1639:VAL:HG12	1:A:1655:THR:CG2	2.05	0.86
32:9:3:LYS:HD3	32:9:5:GLN:CB	2.04	0.85
1:A:2219:THR:HG23	1:A:2224:THR:CG2	2.05	0.85
4:D:800:LEU:O	4:D:805:HIS:CB	2.24	0.85
25:J:247:LYS:NZ	25:J:247:LYS:HB3	1.92	0.85
19:3:1130:VAL:HG11	19:3:1215:TYR:CD2	2.11	0.85
1:A:1092:ILE:HG22	1:A:1093:ASP:N	1.91	0.85
19:3:1130:VAL:HG13	19:3:1215:TYR:CE1	2.10	0.85
4:D:142:VAL:HA	4:D:145:ASN:ND2	1.90	0.85
1:A:1762:TYR:O	1:A:2008:ARG:HD3	1.77	0.84
4:D:120:ILE:HD12	4:D:161:LEU:HD21	1.55	0.84
20:4:61:PHE:CB	20:4:66:ASP:CB	2.54	0.84
21:5:39:PHE:HE1	21:5:77:LEU:CD2	1.90	0.84
42:K:133:LEU:N	42:K:134:PRO:HD2	1.92	0.84
1:A:2090:ILE:HD12	1:A:2263:LEU:HD11	1.59	0.84
4:D:120:ILE:CD1	4:D:161:LEU:HD22	2.06	0.84
1:A:1122:ASN:HB3	32:9:35:ARG:HD3	1.59	0.84
1:A:2090:ILE:CD1	1:A:2263:LEU:CD1	2.54	0.84
17:1:641:ILE:HG13	17:1:675:MET:HE1	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:5:27:PRO:HG2	21:5:83:CYS:HB3	1.60	0.84
41:I:31:ARG:HH11	41:I:31:ARG:CB	1.90	0.84
25:J:245:TRP:CZ3	25:J:264:ILE:HG23	2.11	0.84
1:A:2168:TYR:CE2	1:A:2298:LEU:HD11	2.13	0.84
1:A:2310:ARG:HG2	1:A:2313:HIS:ND1	1.93	0.84
30:Y:67:LEU:HA	30:Y:80:CYS:CB	2.08	0.83
25:J:246:ILE:HD12	25:J:281:LYS:HG3	1.60	0.83
19:3:968:ARG:HG2	19:3:982:GLU:HB2	1.60	0.83
42:K:37:LEU:HD12	42:K:73:LEU:HG	1.60	0.83
1:A:1385:VAL:CG1	1:A:1419:ILE:HD11	2.09	0.83
1:A:1402:ARG:HD3	27:R:408:ASP:HB3	1.61	0.83
19:3:47:THR:HG22	19:3:49:LYS:HG2	1.58	0.82
1:A:1018:ASN:HB2	1:A:1023:ASN:HB3	1.59	0.82
17:1:641:ILE:CD1	17:1:675:MET:HE3	2.10	0.82
21:5:73:ALA:O	21:5:77:LEU:HB3	1.77	0.82
3:C:262:ARG:HD2	3:C:266:GLU:OE2	1.80	0.82
4:D:131:ILE:HG13	4:D:697:ALA:HB1	1.59	0.82
42:K:158:ASN:O	42:K:162:ILE:HG12	1.80	0.82
1:A:1122:ASN:CB	32:9:35:ARG:HD3	2.09	0.82
1:A:2306:HIS:HE1	1:A:2308:VAL:HG23	1.44	0.82
40:0:93:THR:CG2	40:0:98:GLN:HE22	1.93	0.82
17:1:971:MET:HE1	17:1:1003:VAL:CG1	2.09	0.82
5:E:74:PHE:CE2	5:E:343:ILE:HG12	2.15	0.81
5:E:193:THR:HG22	5:E:194:TYR:CE1	2.15	0.81
25:J:238:ASN:HB3	25:J:240:THR:HG22	1.62	0.81
1:A:2090:ILE:HD11	1:A:2263:LEU:CD1	2.10	0.81
1:A:2310:ARG:CG	1:A:2313:HIS:ND1	2.43	0.81
5:E:132:THR:HG21	5:E:146:ARG:HD2	1.60	0.81
5:E:165:GLN:O	5:E:166:LEU:HD23	1.79	0.81
5:E:326:HIS:ND1	5:E:346:SER:HB3	1.95	0.81
19:3:585:ALA:HB3	19:3:609:LEU:CD2	2.10	0.81
42:K:66:LEU:HA	42:K:74:VAL:HG23	1.60	0.81
25:J:236:ARG:NH1	25:J:236:ARG:O	2.14	0.81
4:D:148:LEU:CD2	4:D:152:GLU:CB	2.59	0.81
26:P:212:ASN:HD22	28:T:458:SER:HB3	1.46	0.81
19:3:699:VAL:HG12	19:3:716:SER:HB2	1.63	0.81
27:R:387:ASP:HB2	29:X:351:GLU:CB	2.12	0.80
5:E:74:PHE:CE1	5:E:81:LEU:CD2	2.62	0.80
17:1:641:ILE:HD11	17:1:675:MET:HE3	1.61	0.80
25:J:359:VAL:CG2	25:J:389:HIS:NE2	2.43	0.80
41:I:139:LYS:HZ3	41:I:139:LYS:HB3	1.45	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1:1058:ILE:HD13	17:1:1058:ILE:O	1.81	0.80
19:3:1130:VAL:HG11	19:3:1215:TYR:CZ	2.15	0.80
5:E:74:PHE:CZ	5:E:81:LEU:HD21	2.16	0.80
5:E:248:SER:HB2	5:E:249:TYR:CD1	2.17	0.80
5:E:265:ARG:H	5:E:272:ARG:NH2	1.80	0.80
27:R:237:MET:CE	27:R:237:MET:H	1.95	0.80
29:X:241:GLY:CA	29:X:288:ARG:NH2	2.44	0.80
39:8:56:VAL:CG2	39:8:68:ILE:CD1	2.60	0.80
5:E:174:GLY:HA3	5:E:192:ASN:O	1.82	0.80
17:1:1260:LYS:O	17:1:1264:VAL:HG12	1.82	0.79
1:A:2219:THR:CG2	1:A:2224:THR:CG2	2.60	0.79
4:D:150:ASP:OD1	17:1:879:LEU:HD22	1.81	0.79
27:R:280:ILE:N	32:9:224:THR:CG2	2.45	0.79
1:A:1385:VAL:CG1	1:A:1419:ILE:CD1	2.61	0.79
5:E:147:LEU:HD13	5:E:179:TRP:CD2	2.17	0.79
27:R:280:ILE:H	32:9:224:THR:HG21	1.47	0.79
4:D:129:ARG:HG2	4:D:841:TRP:HE1	1.45	0.79
5:E:310:TYR:CE1	5:E:322:LYS:HD2	2.18	0.78
15:H:77:U:H5”	15:H:78:U:H5’	1.64	0.78
20:4:17:VAL:O	20:4:56:TYR:HA	1.83	0.78
21:5:39:PHE:CE1	21:5:77:LEU:HD21	2.18	0.78
25:J:232:GLU:HA	25:J:235:ILE:HG22	1.64	0.78
1:A:2219:THR:HG21	1:A:2224:THR:HG21	1.66	0.78
3:C:76:GLU:OE1	3:C:76:GLU:N	2.16	0.78
27:R:403:ASN:HB2	29:X:250:PRO:O	1.82	0.78
41:I:128:VAL:HA	42:K:158:ASN:OD1	1.84	0.78
4:D:123:ALA:CB	4:D:161:LEU:HD11	2.13	0.78
19:3:429:ARG:HG2	19:3:429:ARG:NH2	1.97	0.77
36:M:249:TYR:HB3	40:0:72:TYR:OH	1.83	0.77
1:A:2306:HIS:CE1	1:A:2308:VAL:HG23	2.18	0.77
1:A:2090:ILE:HD11	1:A:2263:LEU:HD13	1.67	0.77
19:3:950:ALA:HB2	19:3:989:TYR:HH	1.50	0.77
28:T:282:ARG:HB2	28:T:320:LYS:HD3	1.67	0.77
1:A:2117:ILE:HD11	1:A:2147:MET:CE	2.15	0.77
5:E:119:THR:CG2	5:E:161:ARG:HB2	2.12	0.77
5:E:148:LYS:O	5:E:179:TRP:HH2	1.67	0.77
25:J:299:TRP:HB3	25:J:316:TYR:HD2	1.47	0.77
42:K:120:THR:HG22	42:K:124:HIS:CD2	2.19	0.77
1:A:598:LEU:HD11	1:A:637:TRP:HZ3	1.50	0.77
1:A:2219:THR:CG2	1:A:2224:THR:HG21	2.15	0.77
1:A:1639:VAL:CG1	1:A:1655:THR:HG23	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:1130:VAL:HG11	19:3:1215:TYR:CG	2.20	0.77
21:5:27:PRO:HG3	21:5:85:ARG:HD2	1.65	0.77
25:J:236:ARG:HH11	25:J:236:ARG:CA	1.98	0.77
5:E:74:PHE:CD1	5:E:81:LEU:CD2	2.67	0.76
19:3:539:PRO:HG2	19:3:580:ARG:HH22	1.48	0.76
30:Y:140:THR:HG22	31:Z:563:ARG:HG3	1.65	0.76
4:D:173:VAL:CG1	4:D:177:LYS:HE2	2.15	0.76
5:E:61:LEU:HD13	5:E:352:TYR:CE1	2.20	0.76
5:E:231:MET:HB3	5:E:262:TRP:CZ3	2.21	0.76
19:3:47:THR:HG21	19:3:49:LYS:HG2	1.67	0.76
1:A:2117:ILE:HD11	1:A:2147:MET:HE1	1.67	0.76
19:3:675:LEU:CD2	19:3:691:THR:HG22	2.15	0.76
4:D:120:ILE:HG21	4:D:136:ALA:HB2	1.65	0.76
5:E:277:PHE:HE2	5:E:300:ILE:CD1	1.98	0.76
17:1:641:ILE:HG13	17:1:675:MET:CE	2.12	0.76
4:D:151:LYS:HE2	4:D:151:LYS:HA	1.65	0.75
30:Y:138:ALA:HB1	31:Z:564:PRO:HD2	1.68	0.75
1:A:2325:VAL:CG1	4:D:788:GLY:O	2.34	0.75
27:R:387:ASP:H	29:X:351:GLU:HB3	1.51	0.75
29:X:238:THR:O	29:X:238:THR:HG23	1.85	0.75
4:D:120:ILE:HD12	4:D:161:LEU:HD22	1.65	0.75
32:9:277:LYS:O	32:9:437:PRO:CB	2.35	0.75
1:A:2090:ILE:HG22	1:A:2223:CYS:HB3	1.68	0.75
4:D:783:ALA:O	4:D:809:LEU:HA	1.85	0.75
25:J:337:MET:CE	25:J:346:TRP:CE3	2.70	0.75
41:I:26:LYS:HG3	41:I:28:ARG:H	1.52	0.75
1:A:1275:ARG:HD2	1:A:1375:TRP:NE1	2.02	0.75
5:E:287:ASN:O	5:E:289:LEU:HD23	1.87	0.74
19:3:1057:ARG:HG3	19:3:1057:ARG:NH1	1.97	0.74
5:E:250:LEU:HD12	5:E:250:LEU:O	1.87	0.74
5:E:326:HIS:CE1	5:E:346:SER:OG	2.39	0.74
25:J:270:ASP:OD1	27:R:223:PRO:CD	2.35	0.74
5:E:62:LEU:HB2	5:E:351:LEU:HB2	1.69	0.74
14:G:222:U:C6	30:Y:119:LYS:CE	2.71	0.74
1:A:1639:VAL:HG12	1:A:1655:THR:HG23	1.69	0.74
5:E:132:THR:HG23	5:E:146:ARG:HB2	1.67	0.74
32:9:220:ILE:HD12	32:9:220:ILE:N	2.02	0.74
41:I:37:LYS:CD	41:I:39:TYR:CZ	2.71	0.74
1:A:1838:LYS:HE3	1:A:1865:ARG:NE	2.03	0.74
19:3:662:PHE:CE2	19:3:678:VAL:HG13	2.23	0.74
20:4:12:ASP:C	20:4:67:ALA:CB	2.56	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:R:410:ARG:HH21	27:R:410:ARG:HG3	1.52	0.74
27:R:410:ARG:HG3	27:R:410:ARG:NH2	2.03	0.74
25:J:238:ASN:HB3	25:J:240:THR:CG2	2.17	0.74
25:J:333:PHE:CD1	25:J:349:TYR:HD1	2.03	0.73
39:8:56:VAL:CG2	39:8:68:ILE:HD11	2.17	0.73
1:A:228:TRP:CH2	1:A:413:LEU:HD11	2.23	0.73
1:A:1923:TRP:O	1:A:1927:ILE:HG12	1.87	0.73
27:R:237:MET:H	27:R:237:MET:HE3	1.53	0.73
14:G:213:C:C4'	14:G:214:C:OP2	2.37	0.73
27:R:387:ASP:CB	29:X:351:GLU:HB2	2.18	0.73
4:D:154:ARG:HH22	4:D:166:ASP:HA	1.53	0.73
19:3:1130:VAL:CG1	19:3:1215:TYR:CD1	2.71	0.73
1:A:51:PHE:CZ	5:E:66:GLU:OE1	2.42	0.73
3:C:81:VAL:HB	26:P:208:LYS:NZ	2.03	0.73
4:D:747:THR:CB	4:D:750:LEU:CB	2.67	0.73
5:E:133:VAL:O	5:E:146:ARG:HA	1.89	0.73
17:1:721:ILE:HD12	17:1:721:ILE:O	1.88	0.73
17:1:968:GLU:HA	17:1:971:MET:HG2	1.71	0.73
38:V:536:ILE:HG23	38:V:544:LEU:HD11	1.71	0.73
17:1:614:ARG:HD2	17:1:614:ARG:C	2.07	0.72
19:3:662:PHE:HE2	19:3:678:VAL:HG13	1.53	0.72
1:A:2069:SER:CB	1:A:2072:GLU:OE1	2.37	0.72
21:5:73:ALA:O	21:5:77:LEU:CB	2.37	0.72
25:J:340:GLN:HG3	25:J:372:VAL:HG21	1.69	0.72
27:R:394:LEU:CD1	29:X:331:LEU:HD22	2.20	0.72
27:R:438:ARG:HG3	27:R:438:ARG:NH2	2.00	0.72
30:Y:17:GLU:OE1	30:Y:28:TRP:HD1	1.71	0.72
1:A:829:PRO:HB3	21:5:86:TYR:CE2	2.25	0.72
3:C:683:ASN:ND2	3:C:683:ASN:H	1.85	0.72
5:E:148:LYS:O	5:E:179:TRP:CH2	2.43	0.72
5:E:260:ARG:CD	5:E:276:ILE:CG1	2.68	0.72
25:J:337:MET:HE1	25:J:346:TRP:CZ3	2.24	0.72
4:D:109:THR:HG22	4:D:180:THR:OG1	1.90	0.72
19:3:1165:SER:OG	19:3:1170:VAL:HG23	1.90	0.72
25:J:231:PHE:O	25:J:235:ILE:HG22	1.89	0.72
1:A:1774:ASN:OD1	1:A:1775:GLN:N	2.23	0.72
1:A:1298:ARG:NH2	2:B:39:C:H3'	2.05	0.71
1:A:2168:TYR:CE1	1:A:2298:LEU:HD11	2.24	0.71
38:V:536:ILE:HD12	38:V:544:LEU:CD1	2.19	0.71
1:A:1122:ASN:CB	32:9:35:ARG:HH21	2.01	0.71
14:G:206:C:O2'	14:G:207:A:OP2	2.07	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:47:THR:CG2	19:3:49:LYS:HE3	2.20	0.71
41:I:37:LYS:HD3	41:I:39:TYR:CE1	2.25	0.71
1:A:2324:GLU:HG2	1:A:2330:ARG:HH12	1.54	0.71
5:E:74:PHE:HE2	5:E:343:ILE:HG12	1.54	0.71
5:E:133:VAL:HB	5:E:147:LEU:HG	1.72	0.71
1:A:2074:ARG:NH2	4:D:1044:VAL:O	2.22	0.71
1:A:2090:ILE:HD12	1:A:2263:LEU:CD1	2.18	0.71
4:D:161:LEU:HD12	4:D:161:LEU:O	1.91	0.71
1:A:481:PHE:CZ	27:R:205:ASP:HB3	2.26	0.71
5:E:264:VAL:HA	5:E:272:ARG:HH21	1.55	0.71
17:1:641:ILE:CD1	17:1:675:MET:HE2	2.01	0.71
25:J:313:TRP:CE3	25:J:336:TRP:CE2	2.78	0.71
41:I:28:ARG:HH12	42:K:11:VAL:CG2	2.03	0.71
5:E:268:ALA:HB1	5:E:269:PRO:HD2	1.70	0.71
14:G:213:C:H4'	14:G:214:C:H5'	1.72	0.71
17:1:1075:ARG:HA	17:1:1078:VAL:HG22	1.72	0.71
27:R:386:ARG:HH11	27:R:386:ARG:HG3	1.53	0.71
1:A:1536:LEU:HG	1:A:1572:SER:HB3	1.72	0.71
4:D:121:GLN:HG2	4:D:132:LEU:HD21	1.73	0.71
19:3:550:ASN:HB2	19:3:592:LEU:HD23	1.71	0.71
5:E:74:PHE:CE2	5:E:343:ILE:CG1	2.73	0.70
30:Y:65:ILE:HD13	30:Y:82:LEU:HD21	1.73	0.70
41:I:37:LYS:CD	41:I:39:TYR:CE1	2.74	0.70
18:2:644:SER:CB	20:4:65:GLU:CB	2.69	0.70
29:X:265:LYS:HG3	29:X:364:SER:HG	1.54	0.70
1:A:1921:ASP:HB3	1:A:1966:HIS:CG	2.26	0.70
17:1:1109:ARG:HA	17:1:1112:THR:CG2	2.21	0.70
42:K:51:GLU:HA	42:K:54:ARG:NH2	2.06	0.70
19:3:630:MET:HE1	36:M:287:LEU:CD2	2.21	0.70
22:6:27:ASP:OD2	40:0:20:LYS:CE	2.38	0.70
25:J:386:GLU:O	25:J:390:ALA:N	2.24	0.70
27:R:386:ARG:NH1	27:R:386:ARG:HG3	2.03	0.70
42:K:78:ILE:HD11	42:K:118:ALA:CA	2.21	0.70
19:3:1130:VAL:HG11	19:3:1215:TYR:CD1	2.27	0.70
19:3:585:ALA:HB3	19:3:609:LEU:HD23	1.73	0.70
29:X:345:GLU:OE2	29:X:348:ARG:NH1	2.25	0.70
1:A:2319:LEU:HD22	4:D:1070:LEU:HA	1.72	0.70
4:D:1671:GLY:O	4:D:1885:ASN:CB	2.40	0.70
5:E:326:HIS:ND1	5:E:346:SER:OG	2.25	0.70
19:3:1130:VAL:HG11	19:3:1215:TYR:CE1	2.25	0.70
20:4:12:ASP:C	20:4:67:ALA:HB2	2.12	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:J:261:ALA:HA	25:J:264:ILE:HD12	1.73	0.70
24:L:73:HIS:CD2	32:9:220:ILE:HD13	2.26	0.70
25:J:358:GLU:HG2	25:J:361:ARG:HD3	1.73	0.70
41:I:128:VAL:CA	42:K:158:ASN:OD1	2.40	0.70
1:A:409:ARG:HG2	1:A:410:PRO:HA	1.74	0.70
5:E:264:VAL:HA	5:E:272:ARG:NH2	2.07	0.69
32:9:349:PRO:CB	32:9:375:SER:HA	2.22	0.69
40:0:93:THR:CG2	40:0:98:GLN:NE2	2.55	0.69
1:A:1385:VAL:HG21	1:A:1414:ARG:HB3	1.74	0.69
4:D:1850:SER:O	4:D:1855:TYR:CB	2.40	0.69
17:1:1100:ASN:O	17:1:1103:VAL:HG23	1.92	0.69
1:A:2072:GLU:O	1:A:2076:ARG:HG3	1.92	0.69
1:A:2146:VAL:HG22	1:A:2272:MET:HB2	1.74	0.69
29:X:253:ARG:HG3	29:X:253:ARG:NH2	2.08	0.69
1:A:2127:TYR:OH	1:A:2159:LEU:CD1	2.40	0.69
14:G:215:U:H2'	30:Y:2:ASN:ND2	2.07	0.69
15:H:1:A:H3'	15:H:1:A:N3	2.08	0.69
19:3:138:GLN:HG3	19:3:161:HIS:CE1	2.27	0.69
4:D:131:ILE:HG12	4:D:697:ALA:HB1	1.74	0.69
3:C:454:THR:HG22	3:C:578:ARG:HG3	1.75	0.69
5:E:132:THR:HG22	5:E:146:ARG:HB2	1.72	0.69
42:K:78:ILE:HD11	42:K:118:ALA:N	2.08	0.69
3:C:534:VAL:HB	3:C:537:TYR:O	1.92	0.69
1:A:1275:ARG:HD2	1:A:1375:TRP:CD1	2.28	0.69
5:E:119:THR:HG21	5:E:161:ARG:CB	2.19	0.69
17:1:394:GLU:HG3	17:1:396:ASN:H	1.58	0.69
19:3:54:LEU:HD23	19:3:99:PHE:CD2	2.28	0.69
27:R:280:ILE:N	32:9:224:THR:HG21	2.07	0.69
2:B:23:C:O2	2:B:23:C:H3'	1.93	0.69
5:E:74:PHE:CD1	5:E:81:LEU:HD23	2.28	0.69
25:J:329:ALA:O	25:J:333:PHE:HD2	1.76	0.69
1:A:1385:VAL:HG12	1:A:1419:ILE:HD11	1.73	0.69
4:D:142:VAL:HA	4:D:145:ASN:HD21	1.55	0.69
4:D:423:MET:CB	4:D:878:TYR:CB	2.71	0.69
5:E:243:LEU:HG	5:E:244:SER:O	1.92	0.69
13:F:21:A:C2	24:L:33:ARG:CZ	2.76	0.69
41:I:139:LYS:HB3	41:I:139:LYS:NZ	2.07	0.69
14:G:218:U:C5	30:Y:105:ARG:CZ	2.76	0.68
19:3:586:ASP:OD1	19:3:610:VAL:CG1	2.41	0.68
27:R:134:ARG:HE	28:T:383:ARG:HA	1.55	0.68
1:A:598:LEU:HD11	1:A:637:TRP:CZ3	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1639:VAL:CG1	1:A:1655:THR:CG2	2.72	0.68
3:C:690:GLU:OE2	3:C:788:LYS:NZ	2.25	0.68
41:I:50:ILE:HG12	41:I:119:VAL:HG12	1.73	0.68
1:A:1307:MET:SD	1:A:1547:VAL:CG1	2.80	0.68
13:F:21:A:H3'	13:F:21:A:N3	2.08	0.68
4:D:106:THR:HG22	4:D:107:LYS:N	2.09	0.68
4:D:141:ALA:HA	4:D:182:TYR:OH	1.94	0.68
5:E:178:LEU:CD1	5:E:222:LEU:CD2	2.70	0.68
1:A:1219:GLU:O	1:A:1222:LYS:NZ	2.26	0.68
1:A:1639:VAL:HG12	1:A:1655:THR:HG22	1.74	0.68
1:A:2168:TYR:CZ	1:A:2298:LEU:CD1	2.71	0.68
27:R:390:GLU:OE1	27:R:390:GLU:N	2.20	0.68
1:A:2219:THR:OG1	1:A:2222:SER:HB3	1.93	0.68
41:I:28:ARG:HH12	42:K:11:VAL:HG21	1.58	0.68
4:D:128:PRO:HD2	4:D:131:ILE:HD12	1.75	0.68
31:Z:612:TYR:O	31:Z:616:VAL:HG22	1.94	0.68
1:A:2219:THR:CG2	1:A:2224:THR:HG22	2.23	0.68
4:D:504:PRO:CB	4:D:681:ARG:CB	2.71	0.68
25:J:307:PRO:HB2	25:J:339:TRP:CZ2	2.29	0.68
19:3:970:TYR:HE1	19:3:979:ARG:HB2	1.57	0.67
27:R:386:ARG:HH21	29:X:339:LEU:HD11	1.59	0.67
32:9:120:ARG:HG2	32:9:120:ARG:HH21	1.59	0.67
19:3:114:ARG:HG3	23:7:41:CYS:SG	2.34	0.67
19:3:761:THR:HG21	19:3:763:ARG:HH21	1.59	0.67
27:R:331:ALA:HB2	29:X:355:LYS:HD2	1.76	0.67
3:C:224:GLY:HA3	3:C:438:ILE:HD12	1.75	0.67
5:E:108:HIS:CE1	5:E:128:SER:CB	2.77	0.67
19:3:487:ILE:HA	19:3:491:VAL:HG22	1.76	0.67
5:E:246:GLU:HB2	5:E:248:SER:OG	1.94	0.67
5:E:119:THR:CG2	5:E:161:ARG:CB	2.72	0.67
17:1:632:PHE:HA	17:1:635:VAL:HG13	1.77	0.67
3:C:452:THR:HG22	3:C:577:PHE:HD2	1.58	0.67
30:Y:86:ASP:OD1	31:Z:502:ALA:CB	2.43	0.67
19:3:783:TYR:HB2	19:3:801:GLU:HB3	1.77	0.67
1:A:439:GLN:HB3	1:A:443:VAL:CG2	2.25	0.67
27:R:394:LEU:HD13	29:X:331:LEU:HD22	1.76	0.67
27:R:394:LEU:HD11	29:X:331:LEU:CD2	2.25	0.67
1:A:1773:SER:O	1:A:1813:ARG:NH1	2.28	0.67
30:Y:67:LEU:CA	30:Y:80:CYS:HB2	2.25	0.67
2:B:35:U:OP1	32:9:15:CYS:HB2	1.95	0.66
5:E:116:HIS:O	5:E:124:LEU:HD12	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:R:467:ILE:HG23	31:Z:515:MET:HE2	1.77	0.66
22:6:29:LYS:HD3	22:6:34:ASP:OD1	1.94	0.66
3:C:129:ILE:HG22	3:C:199:LEU:HB3	1.78	0.66
42:K:82:CYS:SG	42:K:120:THR:HB	2.36	0.66
15:H:84:C:O5'	15:H:84:C:H6	1.78	0.66
25:J:232:GLU:O	25:J:235:ILE:HG23	1.95	0.66
27:R:388:ILE:HG23	29:X:350:TYR:CD1	2.30	0.66
1:A:1544:ARG:HH21	36:M:183:ILE:HG12	1.61	0.66
19:3:930:LEU:HD12	19:3:937:LEU:HD23	1.77	0.66
4:D:445:VAL:O	4:D:688:THR:CB	2.43	0.66
5:E:178:LEU:HD11	5:E:222:LEU:CD2	2.26	0.66
5:E:258:THR:HG22	5:E:260:ARG:CG	2.25	0.66
5:E:108:HIS:CE1	5:E:128:SER:HB3	2.31	0.66
1:A:228:TRP:CH2	1:A:413:LEU:CD1	2.78	0.66
4:D:1090:ARG:HG2	4:D:1090:ARG:HH21	1.61	0.66
14:G:210:G:H3'	14:G:210:G:N3	2.11	0.66
17:1:1044:ASP:OD1	17:1:1044:ASP:N	2.28	0.66
19:3:630:MET:CE	36:M:287:LEU:HD11	2.26	0.66
42:K:120:THR:HG22	42:K:124:HIS:HD2	1.60	0.66
5:E:175:THR:CG2	5:E:191:GLN:OE1	2.44	0.65
27:R:281:ASN:O	32:9:221:LEU:HD13	1.96	0.65
5:E:62:LEU:CB	5:E:351:LEU:HB2	2.26	0.65
5:E:268:ALA:HB1	5:E:269:PRO:CD	2.26	0.65
19:3:687:SER:O	36:M:306:VAL:CG2	2.41	0.65
19:3:736:TYR:OH	19:3:763:ARG:NH1	2.28	0.65
13:F:22:G:OP1	24:L:33:ARG:NH1	2.30	0.65
27:R:434:ASP:N	27:R:434:ASP:OD1	2.27	0.65
30:Y:55:VAL:HG13	31:Z:589:ARG:HD2	1.78	0.65
31:Z:530:ASP:OD1	31:Z:530:ASP:N	2.25	0.65
25:J:329:ALA:O	25:J:333:PHE:CD2	2.50	0.65
25:J:340:GLN:HB2	25:J:346:TRP:CZ2	2.31	0.65
1:A:1975:GLU:O	1:A:1979:VAL:HG22	1.97	0.65
14:G:217:U:H6	14:G:217:U:H5'	1.61	0.65
19:3:586:ASP:O	19:3:610:VAL:HG13	1.97	0.65
25:J:349:TYR:HE2	25:J:365:ILE:HG13	1.61	0.65
1:A:413:LEU:HD13	1:A:415:SER:O	1.97	0.65
32:9:37:LEU:HD12	32:9:38:PRO:HD2	1.78	0.65
1:A:213:LEU:HD12	1:A:230:PHE:CE1	2.31	0.65
1:A:977:LEU:C	1:A:977:LEU:HD12	2.17	0.65
5:E:277:PHE:HE2	5:E:300:ILE:HD13	1.61	0.65
47:F:207:G5J:O1G	41:I:37:LYS:HE2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:J:340:GLN:HB2	25:J:346:TRP:HZ2	1.61	0.65
1:A:977:LEU:HD12	1:A:977:LEU:O	1.97	0.65
25:J:313:TRP:CH2	25:J:336:TRP:CD1	2.85	0.65
27:R:388:ILE:HG23	29:X:350:TYR:CE1	2.30	0.65
30:Y:140:THR:HG22	31:Z:563:ARG:CG	2.25	0.65
14:G:219:U:H6	14:G:219:U:OP1	1.80	0.65
41:I:28:ARG:NH1	42:K:11:VAL:HG21	2.11	0.65
41:I:73:GLU:HB3	41:I:93:LYS:HG2	1.79	0.65
4:D:151:LYS:HE2	4:D:151:LYS:CA	2.27	0.64
17:1:1115:ALA:O	17:1:1119:VAL:HG12	1.97	0.64
19:3:1006:GLN:O	19:3:1006:GLN:HG2	1.96	0.64
1:A:228:TRP:CZ2	1:A:413:LEU:HD11	2.32	0.64
5:E:243:LEU:HD21	5:E:247:GLY:HA2	1.79	0.64
5:E:326:HIS:HD1	5:E:346:SER:CB	2.10	0.64
25:J:340:GLN:HG3	25:J:372:VAL:CG2	2.28	0.64
42:K:78:ILE:HG12	42:K:117:SER:CB	2.26	0.64
25:J:359:VAL:HG21	25:J:389:HIS:CE1	2.33	0.64
1:A:661:GLU:O	27:R:213:LYS:HG3	1.97	0.64
1:A:1385:VAL:HG21	1:A:1414:ARG:CB	2.28	0.64
17:1:95:PRO:HB2	27:R:412:PHE:HE2	1.61	0.64
19:3:47:THR:HG22	19:3:49:LYS:H	1.62	0.64
32:9:220:ILE:H	32:9:220:ILE:CD1	2.11	0.64
2:B:102:U:H6	2:B:102:U:O5'	1.81	0.64
5:E:74:PHE:CD1	5:E:81:LEU:HD21	2.29	0.64
18:2:657:ILE:O	18:2:657:ILE:CG2	2.45	0.64
30:Y:116:ARG:HG2	30:Y:116:ARG:HH11	1.63	0.64
1:A:246:LEU:HD11	1:A:411:PHE:CE2	2.32	0.64
17:1:1180:ARG:HH21	17:1:1180:ARG:HB2	1.62	0.64
22:6:27:ASP:OD2	40:0:20:LYS:NZ	2.31	0.64
1:A:2074:ARG:NH1	4:D:1042:GLU:HA	2.12	0.64
28:T:381:HIS:ND1	28:T:382:PRO:HD2	2.13	0.64
1:A:1544:ARG:NH2	36:M:183:ILE:HG12	2.14	0.63
17:1:1261:VAL:O	17:1:1264:VAL:HG13	1.98	0.63
4:D:1992:GLU:HA	4:D:1995:ALA:HB3	1.81	0.63
5:E:178:LEU:HD21	5:E:208:ILE:CD1	2.28	0.63
14:G:222:U:H6	30:Y:119:LYS:HE2	1.59	0.63
24:L:77:LEU:CD2	32:9:221:LEU:HD11	2.20	0.63
39:8:56:VAL:CG2	39:8:68:ILE:HD13	2.22	0.63
13:F:31:U:O2'	13:F:32:C:P	2.56	0.63
17:1:550:HIS:CE1	22:6:96:THR:HG22	2.33	0.63
17:1:1108:ASN:O	17:1:1112:THR:HG22	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:0:93:THR:HG22	40:0:98:GLN:HE22	1.62	0.63
42:K:151:SER:HB3	42:K:156:LEU:HD23	1.79	0.63
1:A:51:PHE:O	5:E:88:ARG:NH2	2.31	0.63
1:A:2325:VAL:HG13	4:D:788:GLY:CA	2.27	0.63
2:B:96:A:H3'	2:B:96:A:N3	2.13	0.63
1:A:1777:ILE:HG12	1:A:1860:GLN:HB2	1.80	0.63
4:D:148:LEU:HD22	4:D:153:ARG:N	2.13	0.63
17:1:661:ARG:NH1	17:1:696:ASP:OD2	2.30	0.63
1:A:481:PHE:CE1	27:R:205:ASP:HB3	2.34	0.63
1:A:591:MET:HB3	1:A:598:LEU:HD22	1.81	0.63
1:A:1144:LYS:HG3	32:9:46:LEU:HD22	1.80	0.63
17:1:404:LEU:HD23	21:5:47:GLN:OE1	1.98	0.63
1:A:211:GLN:HB3	1:A:214:ARG:HB2	1.81	0.63
3:C:779:LEU:HD21	3:C:912:LEU:CD1	2.27	0.63
19:3:791:HIS:CE1	19:3:930:LEU:HD23	2.34	0.63
21:5:77:LEU:CD2	21:5:89:VAL:HG11	2.29	0.63
1:A:1541:THR:O	1:A:1544:ARG:HG3	1.99	0.63
1:A:1838:LYS:HG3	1:A:1865:ARG:NH2	2.14	0.63
2:B:43:U:OP2	32:9:3:LYS:HE2	1.99	0.63
27:R:280:ILE:HB	32:9:221:LEU:HD22	1.80	0.63
4:D:164:THR:HA	4:D:168:ARG:HH11	1.64	0.62
5:E:251:LEU:HG	5:E:291:CYS:SG	2.39	0.62
17:1:696:ASP:O	17:1:702:ARG:NH1	2.29	0.62
19:3:1164:ARG:O	19:3:1170:VAL:HG22	1.98	0.62
27:R:427:ASP:OD1	27:R:427:ASP:N	2.30	0.62
1:A:2090:ILE:CD1	1:A:2263:LEU:HD13	2.26	0.62
4:D:713:MET:O	4:D:716:ALA:HB2	1.98	0.62
4:D:1948:MET:HA	4:D:1953:MET:O	1.98	0.62
5:E:308:PHE:CE1	5:E:324:PRO:HB3	2.34	0.62
20:4:15:VAL:O	20:4:58:PHE:HA	1.98	0.62
28:T:390:GLY:HA3	28:T:416:ILE:HD11	1.81	0.62
36:M:157:ASN:OD1	36:M:157:ASN:N	2.32	0.62
42:K:82:CYS:SG	42:K:120:THR:CG2	2.87	0.62
4:D:131:ILE:HG21	4:D:701:PHE:CB	2.29	0.62
27:R:404:GLU:N	29:X:253:ARG:HH11	1.97	0.62
32:9:75:THR:HA	32:9:82:LYS:HA	1.81	0.62
41:I:142:VAL:HG11	42:K:86:PRO:HB2	1.79	0.62
5:E:174:GLY:O	5:E:192:ASN:N	2.32	0.62
17:1:1055:TRP:HA	17:1:1058:ILE:HG22	1.81	0.62
25:J:245:TRP:HZ3	25:J:264:ILE:HG23	1.60	0.62
25:J:347:HIS:HA	25:J:350:ILE:HD12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:325:LYS:HD3	29:X:351:GLU:OE2	1.99	0.62
13:F:23:G:O2'	13:F:24:U:P	2.57	0.62
25:J:560:ALA:O	25:J:564:LEU:CB	2.48	0.62
32:9:112:ASN:O	32:9:159:GLN:NE2	2.32	0.62
1:A:1774:ASN:OD1	1:A:1775:GLN:CG	2.48	0.62
5:E:147:LEU:HD13	5:E:179:TRP:CD1	2.34	0.62
17:1:665:ILE:HG23	17:1:690:ILE:HD12	1.82	0.62
25:J:232:GLU:CA	25:J:235:ILE:HG22	2.30	0.62
29:X:270:LEU:HB3	29:X:271:PRO:HD2	1.81	0.62
1:A:2105:ILE:HD13	1:A:2266:ARG:HH22	1.64	0.62
4:D:406:ARG:CB	4:D:955:ASP:CA	2.71	0.62
13:F:4:U:H5'	41:I:31:ARG:NH2	2.14	0.62
17:1:1083:TYR:CE1	40:0:13:VAL:HG23	2.35	0.62
20:4:12:ASP:O	20:4:67:ALA:CB	2.48	0.62
29:X:233:LEU:HD11	29:X:237:ASN:HD21	1.64	0.62
1:A:2284:MET:HG3	1:A:2284:MET:O	1.99	0.62
18:2:644:SER:HA	20:4:65:GLU:CB	2.30	0.62
19:3:47:THR:HG21	19:3:49:LYS:HE3	1.81	0.62
30:Y:63:VAL:HG11	31:Z:497:TRP:CD1	2.34	0.62
32:9:49:PHE:CD1	32:9:52:PRO:HG3	2.34	0.62
1:A:1385:VAL:HG11	1:A:1419:ILE:CD1	2.29	0.62
3:C:151:GLU:HG2	3:C:158:ARG:HH11	1.64	0.62
30:Y:117:ALA:HB2	31:Z:494:TYR:CE2	2.35	0.62
36:M:127:GLU:O	36:M:136:ARG:NH2	2.30	0.62
42:K:78:ILE:HG21	42:K:114:THR:CG2	2.29	0.62
1:A:1774:ASN:OD1	1:A:1775:GLN:HG2	2.00	0.62
3:C:532:ILE:HD11	3:C:541:VAL:HG11	1.82	0.62
17:1:588:TYR:CZ	22:6:91:LEU:HD21	2.35	0.62
17:1:1109:ARG:O	17:1:1112:THR:HG23	2.00	0.62
19:3:669:LEU:HD12	19:3:673:VAL:HG23	1.82	0.62
27:R:387:ASP:O	29:X:351:GLU:N	2.29	0.62
36:M:279:HIS:ND1	36:M:296:CYS:SG	2.73	0.62
1:A:200:ASP:OD1	1:A:240:ARG:NH2	2.32	0.61
1:A:2328:ALA:CB	4:D:787:ALA:HB3	2.30	0.61
2:B:45:C:C5	32:9:3:LYS:HG3	2.34	0.61
5:E:108:HIS:CE1	5:E:128:SER:HB2	2.35	0.61
13:F:21:A:H2	24:L:33:ARG:CZ	2.13	0.61
4:D:1090:ARG:HH21	4:D:1090:ARG:CG	2.13	0.61
5:E:160:ALA:HB2	5:E:201:PHE:CD2	2.35	0.61
17:1:1224:PRO:HA	17:1:1227:ILE:HG22	1.81	0.61
1:A:213:LEU:HD12	1:A:230:PHE:HE1	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:502:CYS:CB	4:D:654:THR:HA	2.30	0.61
17:1:971:MET:CE	17:1:1003:VAL:HG11	2.23	0.61
29:X:222:GLU:OE1	29:X:222:GLU:N	2.26	0.61
4:D:759:THR:HA	19:3:682:VAL:HG21	1.81	0.61
5:E:178:LEU:HD21	5:E:208:ILE:HD13	1.82	0.61
17:1:719:TYR:HB3	19:3:216:GLY:O	2.00	0.61
1:A:171:ASP:OD1	1:A:521:ASN:ND2	2.29	0.61
4:D:149:ARG:HH11	4:D:149:ARG:CG	2.14	0.61
18:2:599:THR:HG23	18:2:599:THR:O	2.00	0.61
4:D:131:ILE:HG12	4:D:697:ALA:O	1.99	0.61
27:R:280:ILE:N	32:9:224:THR:HG22	2.09	0.61
32:9:49:PHE:CE1	32:9:52:PRO:HG3	2.34	0.61
30:Y:7:VAL:HG22	30:Y:108:ARG:HB3	1.83	0.61
1:A:1864:THR:HA	1:A:1890:GLN:HG2	1.83	0.61
5:E:62:LEU:CG	5:E:351:LEU:HB2	2.30	0.61
5:E:260:ARG:HD3	5:E:276:ILE:HD13	1.82	0.61
13:F:3:G:O6	42:K:13:ARG:HD3	2.00	0.61
19:3:93:GLN:NE2	19:3:100:GLU:OE1	2.34	0.61
19:3:1130:VAL:HG13	19:3:1215:TYR:CD1	2.33	0.61
1:A:466:ALA:HB1	2:B:19:A:C8	2.36	0.61
5:E:277:PHE:HE2	5:E:300:ILE:HD12	1.64	0.61
17:1:1018:PRO:HB2	36:M:223:ARG:HG2	1.82	0.61
19:3:406:PRO:HA	19:3:1122:LEU:O	2.00	0.61
38:V:624:THR:HG23	38:V:643:LEU:HD12	1.83	0.61
1:A:1755:SER:O	17:1:942:ASN:HB2	1.99	0.61
1:A:2227:ALA:HB2	1:A:2261:MET:SD	2.40	0.61
14:G:214:C:OP1	30:Y:2:ASN:HB2	2.01	0.61
17:1:602:LYS:NZ	39:8:9:THR:OG1	2.34	0.61
21:5:76:HIS:O	21:5:76:HIS:ND1	2.27	0.61
25:J:236:ARG:HH11	25:J:236:ARG:CG	2.13	0.61
27:R:410:ARG:HH21	27:R:410:ARG:CG	2.14	0.61
1:A:1923:TRP:HB3	1:A:1927:ILE:HD11	1.83	0.60
3:C:167:TYR:CE2	3:C:535:ALA:HB3	2.36	0.60
14:G:213:C:H4'	14:G:214:C:OP2	1.99	0.60
19:3:86:ARG:HD2	19:3:1157:GLY:O	2.01	0.60
25:J:438:TYR:O	25:J:442:ARG:N	2.32	0.60
27:R:391:VAL:HG23	29:X:347:GLN:HB3	1.82	0.60
29:X:357:VAL:HG22	29:X:368:VAL:HG22	1.83	0.60
4:D:1589:PHE:CA	4:D:1642:GLN:CB	2.79	0.60
25:J:231:PHE:HD2	25:J:248:TYR:HD1	1.49	0.60
25:J:265:TYR:CD2	25:J:282:TYR:HD1	2.20	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:J:333:PHE:CE1	25:J:349:TYR:HD1	2.19	0.60
1:A:2106:LEU:HD12	1:A:2107:PRO:HD2	1.83	0.60
1:A:2117:ILE:CD1	1:A:2147:MET:CE	2.79	0.60
5:E:258:THR:CG2	5:E:260:ARG:HH11	2.01	0.60
1:A:1919:LEU:HD12	1:A:1936:LEU:HD21	1.82	0.60
4:D:129:ARG:HG2	4:D:841:TRP:NE1	2.17	0.60
4:D:173:VAL:HG12	4:D:177:LYS:HE2	1.83	0.60
5:E:265:ARG:H	5:E:272:ARG:HH21	1.47	0.60
17:1:129:SEP:O2P	17:1:572:HIS:ND1	2.29	0.60
5:E:233:GLY:O	5:E:260:ARG:NH2	2.35	0.60
17:1:621:ASP:HB2	17:1:624:VAL:HG22	1.82	0.60
18:2:703:ILE:HG21	18:2:705:ARG:HE	1.66	0.60
1:A:1072:LEU:HD22	1:A:1087:LEU:HD22	1.83	0.60
5:E:260:ARG:CD	5:E:276:ILE:CD1	2.79	0.60
19:3:412:ILE:HG12	19:3:423:LEU:HG	1.82	0.60
1:A:481:PHE:CE2	27:R:205:ASP:HB3	2.36	0.60
5:E:145:LYS:HE2	5:E:184:LYS:CE	2.29	0.60
14:G:206:C:O2'	14:G:207:A:P	2.60	0.60
22:6:22:LEU:HD22	22:6:60:ILE:HD12	1.83	0.60
30:Y:117:ALA:HB2	31:Z:494:TYR:CD2	2.37	0.60
32:9:276:VAL:CB	32:9:297:CYS:CB	2.79	0.60
42:K:119:ILE:CG2	42:K:163:PHE:HD2	2.05	0.60
1:A:150:MET:SD	1:A:153:ARG:HD3	2.42	0.60
25:J:340:GLN:HG2	25:J:340:GLN:O	2.01	0.60
1:A:1762:TYR:O	1:A:2008:ARG:CD	2.50	0.60
3:C:772:TRP:CZ2	32:9:133:GLN:HG3	2.37	0.60
17:1:549:ARG:NH2	17:1:584:ASP:OD2	2.34	0.59
15:H:31:C:H2'	15:H:32:G:H5"	1.83	0.59
1:A:143:GLN:NE2	1:A:207:PHE:O	2.34	0.59
20:4:12:ASP:C	20:4:67:ALA:HB1	2.22	0.59
27:R:279:HIS:CA	32:9:224:THR:CG2	2.73	0.59
29:X:283:LEU:HD11	29:X:292:ILE:HD12	1.83	0.59
3:C:589:LYS:HE2	3:C:940:ARG:HH12	1.67	0.59
17:1:405:ASP:OD1	21:5:49:ARG:NH2	2.35	0.59
1:A:386:PRO:HD2	1:A:389:LYS:HD2	1.85	0.59
1:A:767:VAL:HG11	2:B:39:C:C6	2.37	0.59
1:A:1790:ILE:HG12	1:A:1800:THR:HG22	1.84	0.59
1:A:1976:TRP:CA	1:A:1979:VAL:HG22	2.31	0.59
1:A:2127:TYR:OH	1:A:2159:LEU:HD11	2.02	0.59
5:E:263:ASP:HB3	5:E:274:VAL:HG21	1.84	0.59
25:J:328:GLY:O	25:J:332:VAL:HG23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1092:ILE:CG2	1:A:1093:ASP:N	2.64	0.59
1:A:1921:ASP:HB3	1:A:1966:HIS:CE1	2.38	0.59
27:R:386:ARG:HH11	27:R:386:ARG:CG	2.14	0.59
3:C:699:ASP:OD2	3:C:722:TYR:OH	2.20	0.59
27:R:237:MET:H	27:R:237:MET:HE2	1.67	0.59
1:A:2090:ILE:HA	1:A:2223:CYS:O	2.03	0.59
41:I:56:VAL:HG23	41:I:58:VAL:HG13	1.84	0.59
3:C:778:PRO:HD3	3:C:817:TYR:CE1	2.38	0.59
17:1:1000:ILE:O	17:1:1004:ILE:HG12	2.03	0.59
17:1:1109:ARG:HA	17:1:1112:THR:HG22	1.83	0.59
5:E:165:GLN:HG3	5:E:181:ILE:HD11	1.85	0.59
3:C:532:ILE:CD1	3:C:541:VAL:HG11	2.33	0.58
4:D:176:GLY:O	4:D:179:ILE:CG2	2.38	0.58
17:1:631:ALA:O	17:1:635:VAL:HG13	2.03	0.58
21:5:24:ARG:HB2	21:5:88:VAL:HB	1.85	0.58
25:J:236:ARG:HH11	25:J:236:ARG:HA	1.68	0.58
29:X:241:GLY:CA	29:X:288:ARG:CZ	2.76	0.58
42:K:62:PHE:O	42:K:66:LEU:HD12	2.03	0.58
19:3:108:GLY:O	22:6:82:ARG:NH1	2.35	0.58
22:6:58:CYS:HB3	22:6:62:GLY:H	1.67	0.58
25:J:333:PHE:CG	25:J:349:TYR:CE1	2.91	0.58
1:A:2319:LEU:HD22	4:D:1070:LEU:CA	2.33	0.58
19:3:471:ASP:OD2	19:3:746:ALA:N	2.34	0.58
29:X:246:TYR:OH	29:X:249:PRO:HD3	2.04	0.58
36:M:296:CYS:SG	36:M:297:TYR:N	2.75	0.58
1:A:855:ARG:HH22	1:A:1522:GLN:HA	1.69	0.58
1:A:1838:LYS:HE3	1:A:1865:ARG:NH2	2.19	0.58
17:1:774:ILE:HD11	17:1:810:ILE:HD13	1.84	0.58
19:3:585:ALA:HB3	19:3:609:LEU:HD22	1.84	0.58
19:3:675:LEU:HD21	19:3:691:THR:HG22	1.85	0.58
21:5:77:LEU:HD23	21:5:89:VAL:HG11	1.84	0.58
1:A:439:GLN:HB3	1:A:443:VAL:HG21	1.84	0.58
3:C:81:VAL:HB	26:P:208:LYS:HZ2	1.68	0.58
17:1:546:ASP:N	17:1:546:ASP:OD1	2.32	0.58
41:I:128:VAL:CG1	42:K:158:ASN:OD1	2.51	0.58
1:A:1547:VAL:HG12	1:A:1548:TYR:HD1	1.69	0.58
1:A:206:TRP:O	1:A:212:PRO:HB3	2.02	0.58
1:A:1549:VAL:O	1:A:1549:VAL:HG12	2.04	0.58
4:D:1825:ASN:CB	4:D:1853:ALA:HB3	2.33	0.58
19:3:47:THR:HG23	19:3:49:LYS:HE3	1.85	0.58
41:I:129:GLU:HB2	41:I:133:LYS:NZ	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:243:LEU:HD11	5:E:247:GLY:HA2	1.83	0.58
5:E:277:PHE:CE2	5:E:300:ILE:CD1	2.85	0.58
5:E:310:TYR:CE1	5:E:322:LYS:CD	2.86	0.58
40:0:93:THR:HB	40:0:98:GLN:NE2	2.19	0.58
42:K:70:ASN:HD22	42:K:73:LEU:HD13	1.69	0.58
4:D:131:ILE:HG23	4:D:698:ILE:HA	1.86	0.58
4:D:1662:ILE:HA	4:D:1703:VAL:O	2.04	0.58
3:C:780:CYS:SG	3:C:782:GLU:CG	2.92	0.58
42:K:78:ILE:HD11	42:K:118:ALA:HB2	1.85	0.58
1:A:977:LEU:HB2	1:A:1175:VAL:HG22	1.85	0.57
3:C:450:GLU:HA	3:C:457:VAL:HG22	1.86	0.57
4:D:164:THR:HA	4:D:168:ARG:HH12	1.67	0.57
19:3:429:ARG:HD2	23:7:58:ASN:OD1	2.04	0.57
13:F:23:G:O2’	13:F:24:U:OP1	2.23	0.57
25:J:247:LYS:HB3	25:J:247:LYS:HZ1	1.69	0.57
27:R:236:LYS:HG2	27:R:237:MET:HE3	1.85	0.57
29:X:283:LEU:HG	29:X:292:ILE:HB	1.85	0.57
40:0:97:LYS:O	40:0:97:LYS:HG3	2.04	0.57
42:K:111:ASN:OD1	42:K:112:GLU:N	2.38	0.57
1:A:1052:VAL:O	1:A:1160:ARG:NH1	2.38	0.57
25:J:333:PHE:CG	25:J:349:TYR:CD1	2.92	0.57
41:I:37:LYS:HD2	41:I:39:TYR:CE1	2.37	0.57
1:A:137:GLU:HG3	1:A:424:ILE:HD13	1.87	0.57
3:C:460:ASP:N	3:C:460:ASP:OD1	2.36	0.57
3:C:711:ARG:NH2	3:C:730:ARG:O	2.37	0.57
4:D:120:ILE:CD1	4:D:161:LEU:CD2	2.67	0.57
14:G:217:U:H5’	14:G:217:U:C6	2.39	0.57
19:3:1130:VAL:HG12	19:3:1215:TYR:CZ	2.36	0.57
27:R:237:MET:O	27:R:237:MET:HG2	2.03	0.57
1:A:822:PHE:CE2	1:A:1000:ILE:HD12	2.40	0.57
1:A:1143:MET:O	1:A:1147:VAL:HG22	2.04	0.57
3:C:715:GLY:HA2	3:C:729:ALA:HB1	1.87	0.57
4:D:1619:TYR:HA	4:D:1645:VAL:O	2.05	0.57
32:9:143:ASP:OD1	32:9:144:LEU:N	2.37	0.57
36:M:141:GLN:NE2	36:M:159:TYR:O	2.38	0.57
41:I:128:VAL:HG12	42:K:158:ASN:OD1	2.03	0.57
42:K:116:LEU:HD23	42:K:159:LEU:HD12	1.85	0.57
17:1:1276:SER:O	17:1:1276:SER:OG	2.19	0.57
21:5:39:PHE:CE1	21:5:77:LEU:CD2	2.80	0.57
19:3:524:ILE:HD11	19:3:556:ILE:HG21	1.87	0.57
5:E:277:PHE:CE2	5:E:300:ILE:HD13	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:T:337:ARG:HG3	28:T:378:VAL:HG23	1.86	0.57
42:K:82:CYS:SG	42:K:120:THR:HG21	2.43	0.57
42:K:82:CYS:HA	42:K:121:THR:HG22	1.86	0.57
13:F:2:U:O2	42:K:42:ASN:HB3	2.05	0.57
25:J:359:VAL:HG11	25:J:389:HIS:CD2	2.40	0.57
25:J:380:ILE:HD13	25:J:414:HIS:ND1	2.19	0.57
1:A:460:LYS:HE2	2:B:49:A:OP2	2.04	0.57
5:E:147:LEU:CD1	5:E:179:TRP:CD1	2.88	0.57
28:T:349:SER:OG	28:T:350:HIS:N	2.37	0.57
28:T:418:THR:HG21	28:T:467:ALA:HA	1.87	0.57
30:Y:17:GLU:OE1	30:Y:28:TRP:CD1	2.55	0.57
1:A:774:LYS:NZ	15:H:5:C:O2'	2.28	0.56
3:C:618:THR:HB	3:C:630:LEU:HB2	1.87	0.56
4:D:140:LEU:HD23	4:D:144:LYS:HG2	1.87	0.56
5:E:194:TYR:CD1	5:E:194:TYR:N	2.73	0.56
17:1:1045:ARG:NH1	40:0:22:GLY:O	2.37	0.56
30:Y:37:TRP:O	30:Y:112:VAL:HG22	2.04	0.56
39:8:34:LEU:HD22	39:8:82:SER:HB2	1.86	0.56
42:K:127:PRO:HG2	42:K:131:SER:HB3	1.87	0.56
42:K:132:PHE:C	42:K:134:PRO:HD2	2.24	0.56
1:A:215:ASP:OD1	1:A:215:ASP:N	2.37	0.56
1:A:1144:LYS:CG	32:9:46:LEU:HD22	2.35	0.56
1:A:2117:ILE:CD1	1:A:2147:MET:HE2	2.36	0.56
1:A:2153:THR:HG22	1:A:2154:HIS:H	1.70	0.56
3:C:389:ASP:OD1	3:C:389:ASP:N	2.33	0.56
25:J:301:ARG:O	25:J:304:THR:HB	2.06	0.56
28:T:350:HIS:HA	28:T:374:SER:HB2	1.88	0.56
38:V:536:ILE:HD12	38:V:544:LEU:HD12	1.87	0.56
1:A:683:LEU:HD12	1:A:683:LEU:O	2.06	0.56
1:A:1125:ILE:HD12	32:9:35:ARG:HG3	1.87	0.56
1:A:1670:ASP:N	1:A:1670:ASP:OD1	2.35	0.56
15:H:38:G:H2'	15:H:39:G:H5'	1.86	0.56
19:3:549:VAL:HG13	19:3:554:VAL:HG22	1.87	0.56
1:A:780:THR:HG22	1:A:898:PHE:CD2	2.41	0.56
17:1:1258:ALA:HB3	17:1:1261:VAL:CG1	2.35	0.56
19:3:565:TYR:OH	19:3:624:CYS:SG	2.62	0.56
19:3:1027:ASP:OD2	19:3:1031:ARG:NH1	2.39	0.56
36:M:262:CYS:SG	36:M:263:PHE:N	2.78	0.56
42:K:53:LEU:HD22	42:K:58:VAL:HG11	1.87	0.56
4:D:448:PRO:C	4:D:686:GLU:CB	2.73	0.56
14:G:192:U:H2'	14:G:193:C:C6	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:R:237:MET:HE3	27:R:237:MET:N	2.20	0.56
1:A:50:LYS:HD2	5:E:88:ARG:HH12	1.71	0.56
1:A:1049:ASP:OD1	1:A:1090:ARG:HD3	2.05	0.56
3:C:381:LEU:HD22	3:C:416:LEU:HD21	1.88	0.56
5:E:88:ARG:HD3	5:E:109:SER:O	2.06	0.56
13:F:31:U:O2'	13:F:32:C:OP1	2.24	0.56
15:H:81:G:H2'	15:H:82:A:H5"	1.87	0.56
25:J:327:ALA:O	25:J:331:GLN:OE1	2.24	0.56
1:A:682:ASP:OD2	15:H:3:G:O2'	2.23	0.56
1:A:704:ASN:ND2	1:A:706:ALA:HB2	2.21	0.56
25:J:297:ASN:O	25:J:300:ASP:HB3	2.05	0.56
27:R:391:VAL:HG23	29:X:347:GLN:CB	2.35	0.56
28:T:216:ASN:HD21	28:T:472:GLN:HB2	1.70	0.56
42:K:78:ILE:HD13	42:K:114:THR:O	2.06	0.56
1:A:1782:ASP:OD2	1:A:1865:ARG:NH2	2.39	0.56
3:C:735:PHE:CE1	3:C:744:ILE:HG12	2.41	0.56
4:D:141:ALA:CA	4:D:182:TYR:OH	2.54	0.56
4:D:178:LYS:O	4:D:178:LYS:HG2	2.05	0.56
19:3:429:ARG:HH21	19:3:429:ARG:CG	2.13	0.56
19:3:1188:ASN:OD1	19:3:1188:ASN:N	2.38	0.56
1:A:774:LYS:HG2	15:H:6:U:C6	2.40	0.55
3:C:709:TRP:HB3	3:C:713:LYS:HE3	1.89	0.55
5:E:114:GLU:CD	5:E:116:HIS:HE2	2.09	0.55
15:H:38:G:H2'	15:H:39:G:C5'	2.36	0.55
42:K:70:ASN:HB3	42:K:73:LEU:HB2	1.88	0.55
1:A:662:GLY:CA	27:R:213:LYS:NZ	2.69	0.55
1:A:1385:VAL:HG21	1:A:1414:ARG:HG2	1.88	0.55
3:C:81:VAL:HB	26:P:208:LYS:HZ3	1.71	0.55
4:D:502:CYS:O	4:D:676:PHE:O	2.23	0.55
5:E:132:THR:CG2	5:E:146:ARG:HD2	2.33	0.55
17:1:855:ASP:N	17:1:855:ASP:OD1	2.34	0.55
19:3:638:GLU:OE2	19:3:670:GLN:HG3	2.06	0.55
1:A:804:GLU:OE2	32:9:212:TYR:OH	2.22	0.55
1:A:2284:MET:O	1:A:2284:MET:CG	2.55	0.55
4:D:142:VAL:O	4:D:145:ASN:OD1	2.24	0.55
19:3:613:TPO:HG21	19:3:613:TPO:O1P	2.04	0.55
25:J:403:VAL:HA	25:J:407:GLY:HA3	1.89	0.55
29:X:264:PHE:N	29:X:264:PHE:CD1	2.73	0.55
1:A:1763:LEU:HD22	1:A:2012:LEU:HD13	1.87	0.55
1:A:2310:ARG:HD2	1:A:2313:HIS:CG	2.41	0.55
4:D:505:THR:CB	4:D:854:GLY:HA3	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Y:86:ASP:OD1	31:Z:502:ALA:HB3	2.06	0.55
41:I:41:ILE:HD13	41:I:138:ARG:HD3	1.89	0.55
5:E:131:LYS:HG2	5:E:152:SER:O	2.06	0.55
5:E:174:GLY:O	5:E:192:ASN:CB	2.54	0.55
25:J:327:ALA:HA	25:J:330:ARG:HG3	1.87	0.55
27:R:390:GLU:H	27:R:390:GLU:CD	2.09	0.55
41:I:18:ARG:NH1	42:K:35:GLN:OE1	2.39	0.55
42:K:133:LEU:N	42:K:134:PRO:CD	2.67	0.55
1:A:1405:LEU:HD23	27:R:411:LEU:HD23	1.87	0.55
5:E:310:TYR:CZ	5:E:322:LYS:HD2	2.42	0.55
15:H:15:U:H3'	24:L:40:ARG:NH1	2.22	0.55
25:J:340:GLN:N	25:J:341:PRO:HD3	2.22	0.55
27:R:463:LEU:O	27:R:467:ILE:HG12	2.06	0.55
29:X:254:ILE:HD13	29:X:279:SER:HB3	1.88	0.55
2:B:47:A:O4'	37:U:11:ARG:NH1	2.40	0.55
4:D:1048:VAL:O	4:D:1050:GLU:N	2.40	0.55
5:E:108:HIS:ND1	5:E:128:SER:CB	2.70	0.55
19:3:525:ARG:HE	19:3:533:VAL:HG21	1.72	0.55
22:6:27:ASP:OD2	40:0:20:LYS:HE3	2.07	0.55
1:A:346:ASP:OD1	1:A:346:ASP:N	2.39	0.55
1:A:2306:HIS:HE1	1:A:2308:VAL:CG2	2.19	0.55
30:Y:85:GLU:OE2	31:Z:505:ARG:NH2	2.40	0.55
38:V:536:ILE:HD12	38:V:544:LEU:HD11	1.89	0.55
40:0:93:THR:HB	40:0:98:GLN:HE21	1.71	0.55
1:A:796:LYS:O	32:9:225:MET:HE1	2.07	0.55
4:D:1589:PHE:HA	4:D:1642:GLN:CB	2.37	0.55
5:E:269:PRO:HD2	5:E:272:ARG:HG2	1.89	0.55
25:J:310:ASN:ND2	25:J:342:GLU:OE1	2.40	0.55
26:P:195:LYS:HD3	32:9:198:LYS:HB3	1.88	0.55
1:A:2320:LEU:HD23	1:A:2322:GLU:H	1.71	0.55
3:C:737:PRO:HG3	3:C:774:THR:O	2.07	0.55
4:D:164:THR:HG22	4:D:168:ARG:HH11	1.72	0.55
4:D:991:TYR:O	4:D:1090:ARG:NH2	2.39	0.55
19:3:678:VAL:O	19:3:686:LEU:HA	2.07	0.55
19:3:1004:ASP:CG	19:3:1007:GLU:HB2	2.27	0.55
32:9:143:ASP:OD1	32:9:145:LEU:N	2.40	0.55
41:I:139:LYS:HD3	42:K:124:HIS:ND1	2.22	0.55
1:A:873:ASN:N	1:A:873:ASN:OD1	2.38	0.54
4:D:1825:ASN:CB	4:D:1853:ALA:CB	2.85	0.54
5:E:260:ARG:HD3	5:E:276:ILE:CD1	2.37	0.54
32:9:53:VAL:HG11	32:9:63:LEU:HD13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:M:279:HIS:HD1	36:M:296:CYS:HG	1.50	0.54
13:F:21:A:C2	24:L:33:ARG:NH2	2.75	0.54
19:3:618:SER:HB2	19:3:628:LEU:HD11	1.89	0.54
19:3:1103:SER:O	19:3:1119:TYR:HA	2.08	0.54
19:3:1130:VAL:CG1	19:3:1215:TYR:CE2	2.84	0.54
1:A:1820:LYS:NZ	1:A:1844:GLU:OE1	2.40	0.54
17:1:1223:SER:HB3	17:1:1226:VAL:CG1	2.37	0.54
19:3:279:ASP:OD2	19:3:307:GLN:NE2	2.40	0.54
26:P:207:ASP:OD1	26:P:208:LYS:N	2.40	0.54
29:X:238:THR:O	29:X:238:THR:CG2	2.54	0.54
31:Z:543:ASP:HB3	31:Z:546:ALA:HB2	1.90	0.54
1:A:50:LYS:HD2	5:E:88:ARG:NH1	2.22	0.54
1:A:51:PHE:HZ	5:E:66:GLU:OE1	1.91	0.54
5:E:174:GLY:CA	5:E:192:ASN:O	2.54	0.54
3:C:543:ARG:CG	3:C:543:ARG:HH11	2.19	0.54
5:E:326:HIS:HE1	5:E:346:SER:CB	2.13	0.54
13:F:28:C:OP2	13:F:46:U:O2'	2.21	0.54
14:G:213:C:O4'	14:G:214:C:OP2	2.26	0.54
19:3:1165:SER:HB3	19:3:1169:PRO:HA	1.90	0.54
29:X:300:SER:OG	29:X:303:HIS:ND1	2.28	0.54
41:I:47:TYR:HE1	41:I:93:LYS:HD2	1.72	0.54
42:K:78:ILE:CG2	42:K:114:THR:HG23	2.31	0.54
17:1:1128:VAL:HG23	17:1:1128:VAL:O	2.07	0.54
25:J:270:ASP:OD1	27:R:223:PRO:CG	2.56	0.54
30:Y:101:LYS:HG2	30:Y:106:THR:HG22	1.89	0.54
1:A:1604:LEU:HD11	1:A:1725:LEU:HD22	1.88	0.54
30:Y:66:ASN:O	30:Y:80:CYS:HB2	2.08	0.54
3:C:313:GLN:O	3:C:417:ARG:NH1	2.41	0.54
5:E:178:LEU:CD1	5:E:222:LEU:HD22	2.37	0.54
14:G:222:U:H4'	14:G:222:U:OP1	2.08	0.54
25:J:403:VAL:O	25:J:408:ASP:N	2.38	0.54
5:E:147:LEU:CD1	5:E:179:TRP:CG	2.83	0.54
17:1:1058:ILE:HD13	17:1:1058:ILE:C	2.28	0.54
19:3:304:GLN:HE21	19:3:308:GLY:HA2	1.73	0.54
25:J:259:GLN:OE1	25:J:262:ARG:NH1	2.41	0.54
27:R:394:LEU:CD1	29:X:331:LEU:CD2	2.84	0.54
25:J:236:ARG:NH1	25:J:236:ARG:HG3	2.22	0.54
25:J:274:ARG:NE	27:R:229:VAL:HG22	2.22	0.54
1:A:2117:ILE:O	1:A:2304:PHE:HB2	2.07	0.53
1:A:2319:LEU:HD11	4:D:1071:LYS:CB	2.38	0.53
15:H:10:A:C2'	15:H:10:A:N3	2.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2:525:PRO:HG2	18:2:528:ILE:HD12	1.89	0.53
19:3:185:LEU:HB3	19:3:206:GLN:HE21	1.73	0.53
19:3:555:VAL:HG22	19:3:565:TYR:HB3	1.90	0.53
19:3:950:ALA:HB2	19:3:989:TYR:CZ	2.42	0.53
25:J:313:TRP:CE3	25:J:336:TRP:NE1	2.76	0.53
28:T:471:ASP:OD1	28:T:471:ASP:N	2.41	0.53
1:A:651:TRP:CD1	13:F:38:G:H1'	2.42	0.53
13:F:31:U:O2'	13:F:32:C:O5'	2.25	0.53
18:2:567:ASP:OD1	18:2:567:ASP:N	2.40	0.53
27:R:279:HIS:HA	32:9:224:THR:HG22	1.86	0.53
41:I:31:ARG:HB3	41:I:31:ARG:NH1	2.01	0.53
41:I:140:ALA:O	41:I:144:LYS:HE2	2.09	0.53
1:A:44:ARG:HA	1:A:49:ARG:NH1	2.23	0.53
1:A:995:ARG:HG3	27:R:291:LEU:HD13	1.89	0.53
1:A:2103:THR:CG2	1:A:2260:GLN:OE1	2.48	0.53
4:D:141:ALA:CB	4:D:182:TYR:OH	2.56	0.53
5:E:229:TYR:CE2	5:E:272:ARG:NH1	2.77	0.53
17:1:550:HIS:CE1	22:6:96:THR:CG2	2.91	0.53
20:4:12:ASP:O	20:4:67:ALA:HB1	2.08	0.53
28:T:307:SER:OG	28:T:308:ARG:N	2.39	0.53
14:G:213:C:H4'	14:G:214:C:C5'	2.37	0.53
38:V:466:SER:OG	38:V:472:CYS:HB2	2.08	0.53
1:A:2328:ALA:HB3	4:D:787:ALA:HB3	1.89	0.53
15:H:10:A:N3	15:H:10:A:H3'	2.23	0.53
18:2:469:VAL:HG12	18:2:471:ARG:H	1.74	0.53
4:D:131:ILE:HG12	4:D:697:ALA:C	2.29	0.53
32:9:106:LEU:HG	32:9:130:ALA:HB2	1.90	0.53
1:A:661:GLU:O	27:R:213:LYS:HA	2.09	0.53
5:E:178:LEU:CD2	5:E:208:ILE:CD1	2.87	0.53
13:F:31:U:C2'	13:F:32:C:O5'	2.56	0.53
17:1:631:ALA:O	17:1:635:VAL:CG1	2.57	0.53
23:7:48:ASP:OD1	23:7:51:ASN:ND2	2.41	0.53
29:X:347:GLN:N	29:X:347:GLN:NE2	2.56	0.53
30:Y:58:GLN:NE2	31:Z:588:ASP:OD1	2.41	0.53
40:0:93:THR:HG21	40:0:98:GLN:NE2	2.23	0.53
1:A:1762:TYR:HD1	1:A:1762:TYR:H	1.56	0.53
1:A:1949:ARG:CD	27:R:463:LEU:HD13	2.39	0.53
2:B:23:C:O2	2:B:23:C:C3'	2.57	0.53
3:C:778:PRO:HD3	3:C:817:TYR:CD1	2.43	0.53
17:1:1174:GLU:OE1	17:1:1210:HIS:NE2	2.36	0.53
19:3:675:LEU:HD21	19:3:691:THR:CG2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:J:313:TRP:CZ3	25:J:336:TRP:CD1	2.97	0.53
28:T:216:ASN:ND2	28:T:472:GLN:HB2	2.24	0.53
42:K:54:ARG:CB	42:K:54:ARG:CZ	2.86	0.53
1:A:58:LYS:NZ	1:A:479:THR:O	2.42	0.53
1:A:1002:ASP:OD2	1:A:1004:ASN:HB2	2.09	0.53
3:C:484:THR:OG1	3:C:489:GLN:O	2.26	0.53
5:E:325:GLY:O	5:E:352:TYR:CE2	2.62	0.53
14:G:196:A:N3	14:G:196:A:H5"	2.23	0.53
15:H:2:U:OP1	15:H:2:U:H2'	2.09	0.53
19:3:460:TRP:CZ3	19:3:505:THR:HG23	2.44	0.53
5:E:260:ARG:NE	5:E:276:ILE:CD1	2.72	0.53
13:F:23:G:C2'	13:F:24:U:O5'	2.57	0.53
17:1:1054:GLU:OE1	17:1:1057:ARG:NH1	2.42	0.53
1:A:2333:LEU:HD21	4:D:544:MET:HA	1.91	0.52
5:E:263:ASP:O	5:E:272:ARG:NE	2.32	0.52
25:J:355:ARG:HB3	25:J:355:ARG:NH1	2.23	0.52
32:9:43:SER:H	32:9:61:PHE:HB3	1.74	0.52
4:D:148:LEU:HD23	4:D:152:GLU:CB	2.39	0.52
5:E:62:LEU:HB2	5:E:351:LEU:CB	2.39	0.52
17:1:680:LEU:HB3	17:1:681:PRO:HD3	1.92	0.52
19:3:970:TYR:CE1	19:3:979:ARG:HB2	2.42	0.52
19:3:1055:VAL:HB	19:3:1093:MET:HB3	1.91	0.52
25:J:337:MET:HE1	25:J:346:TRP:CE3	2.41	0.52
1:A:542:ASN:O	1:A:546:LEU:HB2	2.09	0.52
1:A:2074:ARG:HH12	4:D:1042:GLU:HA	1.72	0.52
3:C:828:MET:HA	3:C:905:GLN:O	2.08	0.52
4:D:1090:ARG:HB2	4:D:1090:ARG:CZ	2.38	0.52
4:D:1948:MET:CB	4:D:1953:MET:O	2.57	0.52
5:E:108:HIS:ND1	5:E:128:SER:HB2	2.24	0.52
5:E:232:ARG:O	5:E:262:TRP:HH2	1.91	0.52
15:H:10:A:N3	15:H:10:A:H2'	2.25	0.52
32:9:120:ARG:NH1	32:9:154:ASP:OD1	2.42	0.52
2:B:115:C:O2	2:B:115:C:H2'	2.09	0.52
14:G:19:U:O2	14:G:19:U:H2'	2.09	0.52
17:1:524:ARG:HH11	17:1:566:LEU:HD11	1.74	0.52
19:3:426:ALA:HB1	19:3:785:PRO:CG	2.39	0.52
31:Z:520:LYS:NZ	31:Z:530:ASP:OD2	2.43	0.52
1:A:422:LEU:O	1:A:635:ARG:NE	2.43	0.52
1:A:2133:PRO:HD2	1:A:2139:VAL:HG13	1.92	0.52
3:C:138:LEU:HD11	3:C:179:VAL:HG23	1.91	0.52
3:C:173:THR:O	3:C:177:ARG:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:178:LEU:N	5:E:178:LEU:HD23	2.25	0.52
5:E:260:ARG:HD3	5:E:276:ILE:CG1	2.38	0.52
19:3:722:SER:HB3	19:3:731:LEU:HD13	1.92	0.52
25:J:236:ARG:NH1	25:J:236:ARG:HA	2.24	0.52
25:J:368:ARG:HG2	25:J:368:ARG:HH11	1.74	0.52
28:T:381:HIS:CG	28:T:384:HIS:HB2	2.45	0.52
1:A:34:ALA:O	5:E:195:GLN:NE2	2.39	0.52
1:A:1838:LYS:CE	1:A:1865:ARG:NE	2.72	0.52
3:C:164:ASP:OD1	3:C:164:ASP:N	2.33	0.52
4:D:538:ILE:O	4:D:585:ILE:HA	2.09	0.52
5:E:250:LEU:HD11	5:E:262:TRP:HB2	1.91	0.52
17:1:613:MET:CE	17:1:635:VAL:HG11	2.40	0.52
19:3:1159:ASP:HB3	19:3:1162:SER:HB3	1.92	0.52
25:J:349:TYR:CE2	25:J:365:ILE:HG13	2.43	0.52
30:Y:37:TRP:HB3	30:Y:112:VAL:CG2	2.40	0.52
3:C:390:THR:OG1	3:C:391:SER:N	2.42	0.52
19:3:69:ARG:NH2	19:3:74:THR:O	2.43	0.52
21:5:27:PRO:CG	21:5:83:CYS:HB3	2.35	0.52
27:R:408:ASP:OD2	27:R:410:ARG:NH2	2.43	0.52
4:D:1948:MET:CA	4:D:1953:MET:O	2.57	0.52
19:3:209:THR:HA	19:3:224:TYR:O	2.10	0.52
29:X:303:HIS:CE1	29:X:333:SER:HB2	2.44	0.52
1:A:1957:ASP:HB2	1:A:1960:THR:HG23	1.92	0.52
4:D:128:PRO:CD	4:D:131:ILE:HD12	2.39	0.52
4:D:141:ALA:HA	4:D:182:TYR:CZ	2.44	0.52
20:4:16:TYR:HA	20:4:57:GLY:O	2.10	0.52
21:5:77:LEU:HG	21:5:89:VAL:HG11	1.92	0.52
25:J:268:ALA:O	25:J:271:VAL:HG12	2.10	0.52
32:9:92:ASN:OD1	32:9:124:ASN:HA	2.09	0.52
1:A:481:PHE:CD1	27:R:205:ASP:HB3	2.45	0.52
1:A:662:GLY:HA3	27:R:213:LYS:HG3	1.91	0.52
3:C:765:SER:OG	3:C:766:ILE:N	2.42	0.52
5:E:175:THR:HG22	5:E:191:GLN:OE1	2.10	0.52
14:G:210:G:N3	14:G:210:G:C2'	2.73	0.52
3:C:261:ASP:N	3:C:261:ASP:OD1	2.42	0.51
47:F:207:G5J:O1A	41:I:34:ARG:HG3	2.10	0.51
17:1:968:GLU:OE1	17:1:971:MET:SD	2.69	0.51
20:4:12:ASP:O	20:4:67:ALA:HB2	2.10	0.51
27:R:231:HIS:NE2	28:T:371:HIS:O	2.43	0.51
27:R:459:TYR:CE2	27:R:463:LEU:HD12	2.45	0.51
3:C:85:ASP:OD1	3:C:85:ASP:N	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1:1083:TYR:CZ	40:0:13:VAL:HG23	2.46	0.51
20:4:34:LEU:HA	20:4:37:GLY:O	2.09	0.51
42:K:78:ILE:HD11	42:K:118:ALA:CB	2.40	0.51
1:A:213:LEU:O	1:A:220:VAL:HG22	2.10	0.51
1:A:661:GLU:OE2	27:R:210:PRO:HG2	2.10	0.51
3:C:137:HIS:CE1	3:C:238:ASN:H	2.28	0.51
3:C:682:LYS:HD2	3:C:802:HIS:CD2	2.45	0.51
25:J:386:GLU:OE2	25:J:391:TYR:HB2	2.10	0.51
1:A:466:ALA:HB1	2:B:19:A:N7	2.25	0.51
1:A:976:MET:HE1	1:A:1098:PHE:HD1	1.75	0.51
1:A:2219:THR:HG21	1:A:2224:THR:CG2	2.34	0.51
5:E:231:MET:SD	5:E:262:TRP:CE3	3.04	0.51
14:G:218:U:C6	30:Y:105:ARG:NH1	2.78	0.51
17:1:823:MET:HG2	17:1:833:LEU:HD22	1.92	0.51
18:2:476:GLU:OE1	18:2:478:HIS:NE2	2.43	0.51
19:3:1032:TRP:O	19:3:1048:ASP:HA	2.10	0.51
22:6:22:LEU:HG	22:6:69:ALA:HB2	1.92	0.51
28:T:478:LEU:HD23	28:T:488:VAL:HG22	1.93	0.51
32:9:121:THR:HG23	32:9:154:ASP:OD2	2.11	0.51
41:I:31:ARG:HH11	41:I:31:ARG:CG	2.24	0.51
1:A:1963:GLU:HB2	1:A:1966:HIS:CD2	2.46	0.51
5:E:132:THR:CG2	5:E:146:ARG:CB	2.75	0.51
25:J:439:ALA:HA	25:J:442:ARG:HB3	1.93	0.51
4:D:179:ILE:HG23	4:D:179:ILE:O	2.11	0.51
19:3:464:ARG:NH2	19:3:473:TYR:OH	2.43	0.51
28:T:261:LEU:HB3	28:T:273:TRP:HB2	1.92	0.51
32:9:19:THR:HA	32:9:24:GLY:HA3	1.92	0.51
38:V:536:ILE:HG23	38:V:544:LEU:CD1	2.39	0.51
3:C:134:LEU:O	3:C:205:THR:OG1	2.28	0.51
3:C:735:PHE:HE1	3:C:744:ILE:HG12	1.74	0.51
4:D:106:THR:HG22	4:D:107:LYS:H	1.76	0.51
25:J:336:TRP:CH2	25:J:345:ALA:HB1	2.46	0.51
25:J:349:TYR:CD2	25:J:365:ILE:HG21	2.46	0.51
42:K:50:TYR:CE1	42:K:84:LEU:HD12	2.46	0.51
2:B:111:A:H2'	2:B:112:A:C8	2.46	0.51
4:D:106:THR:CG2	4:D:107:LYS:N	2.73	0.51
17:1:858:LYS:NZ	17:1:894:ASP:OD2	2.37	0.51
42:K:50:TYR:OH	42:K:83:ASN:O	2.29	0.51
1:A:2310:ARG:CD	1:A:2313:HIS:ND1	2.73	0.51
4:D:140:LEU:HD23	4:D:140:LEU:O	2.10	0.51
17:1:933:CYS:SG	17:1:970:LEU:HD21	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2147:MET:O	1:A:2274:PRO:HD3	2.10	0.51
15:H:12:U:O2'	15:H:13:U:P	2.69	0.51
19:3:522:ASP:O	19:3:538:THR:HG23	2.10	0.51
19:3:678:VAL:HG23	19:3:688:ASP:OD1	2.11	0.51
19:3:703:ARG:HD3	19:3:710:GLU:OE2	2.11	0.51
25:J:236:ARG:HH11	25:J:236:ARG:CB	2.24	0.51
30:Y:87:GLN:O	30:Y:90:THR:OG1	2.25	0.51
36:M:288:GLN:HA	36:M:291:ARG:HD3	1.93	0.51
41:I:128:VAL:N	42:K:158:ASN:OD1	2.44	0.51
1:A:837:LYS:HA	1:A:840:ILE:HG22	1.92	0.50
1:A:2115:ILE:HD11	1:A:2223:CYS:SG	2.51	0.50
2:B:113:G:H2'	2:B:114:G:C8	2.46	0.50
3:C:151:GLU:OE1	3:C:417:ARG:NH2	2.37	0.50
17:1:1256:HIS:ND1	17:1:1261:VAL:HG11	2.26	0.50
19:3:623:ASP:HB2	19:3:626:GLN:HG3	1.93	0.50
20:4:14:THR:CA	20:4:59:VAL:O	2.28	0.50
27:R:129:ASP:O	27:R:133:GLN:HG2	2.11	0.50
29:X:268:GLU:H	29:X:268:GLU:CD	2.13	0.50
29:X:278:GLN:HG2	29:X:281:TYR:CZ	2.46	0.50
1:A:266:SER:OG	1:A:271:MET:O	2.26	0.50
17:1:614:ARG:HB3	17:1:615:PRO:HD3	1.93	0.50
19:3:430:GLY:H	19:3:784:THR:HG22	1.77	0.50
1:A:591:MET:HB3	1:A:598:LEU:HD21	1.87	0.50
2:B:113:G:H2'	2:B:114:G:H8	1.77	0.50
3:C:686:THR:HB	3:C:793:ASP:HB3	1.94	0.50
4:D:1582:ALA:C	4:D:1584:ILE:H	2.15	0.50
4:D:1589:PHE:C	4:D:1642:GLN:CB	2.79	0.50
19:3:428:GLY:HA3	19:3:433:SER:HA	1.93	0.50
19:3:564:VAL:HG22	19:3:580:ARG:HG2	1.93	0.50
28:T:460:ASP:OD1	28:T:460:ASP:N	2.45	0.50
42:K:51:GLU:CA	42:K:54:ARG:NH2	2.74	0.50
42:K:83:ASN:OD1	42:K:84:LEU:N	2.44	0.50
1:A:488:ASP:O	1:A:492:VAL:HG23	2.11	0.50
1:A:2127:TYR:OH	1:A:2159:LEU:HD13	2.11	0.50
3:C:142:LYS:N	44:C:1500:GTP:O1B	2.40	0.50
5:E:175:THR:HG22	5:E:191:GLN:CD	2.31	0.50
13:F:32:C:H4'	25:J:236:ARG:O	2.12	0.50
18:2:700:GLU:HA	18:2:703:ILE:HD12	1.94	0.50
21:5:76:HIS:HD1	21:5:76:HIS:C	2.13	0.50
41:I:17:GLN:OE1	41:I:17:GLN:N	2.45	0.50
3:C:357:THR:OG1	3:C:359:LYS:O	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:158:TYR:HB2	5:E:199:VAL:O	2.12	0.50
13:F:32:C:O2'	13:F:33:C:OP2	2.27	0.50
19:3:589:CYS:SG	19:3:640:LEU:HD12	2.52	0.50
28:T:420:THR:HG1	28:T:468:CYS:HG	1.59	0.50
42:K:82:CYS:SG	42:K:120:THR:CB	2.99	0.50
1:A:344:ASP:OD1	1:A:344:ASP:N	2.35	0.50
2:B:110:C:H2'	2:B:111:A:H8	1.76	0.50
4:D:134:GLY:O	4:D:138:GLU:HG3	2.12	0.50
5:E:265:ARG:N	5:E:272:ARG:HH21	2.10	0.50
29:X:305:VAL:HB	29:X:329:ILE:CG2	2.42	0.50
30:Y:118:PRO:O	31:Z:490:ARG:NH1	2.45	0.50
32:9:61:PHE:HE1	32:9:66:ILE:HB	1.77	0.50
42:K:51:GLU:HA	42:K:54:ARG:CZ	2.41	0.50
3:C:841:ASP:N	3:C:841:ASP:OD1	2.43	0.50
13:F:21:A:N6	27:R:256:ASN:OD1	2.44	0.50
14:G:206:C:H4'	14:G:207:A:O5'	2.11	0.50
17:1:1075:ARG:HA	17:1:1078:VAL:CG2	2.39	0.50
19:3:716:SER:OG	19:3:717:SER:N	2.45	0.50
28:T:406:ILE:HG22	28:T:407:GLN:HB2	1.94	0.50
1:A:80:LYS:HB2	41:I:116:LEU:HD11	1.92	0.50
1:A:1070:ASP:OD1	1:A:1073:SER:OG	2.29	0.50
1:A:1762:TYR:N	1:A:1762:TYR:CD1	2.80	0.50
2:B:101:U:H2'	2:B:102:U:C6	2.47	0.50
4:D:721:VAL:N	4:D:807:GLN:O	2.42	0.50
5:E:194:TYR:CD2	5:E:214:ASP:HB3	2.47	0.50
5:E:194:TYR:CE2	5:E:214:ASP:OD2	2.64	0.50
25:J:380:ILE:O	25:J:384:ARG:HD3	2.12	0.50
32:9:93:PHE:CD1	32:9:125:VAL:HG11	2.46	0.50
1:A:213:LEU:CD1	1:A:230:PHE:CE1	2.94	0.50
1:A:780:THR:HG22	1:A:898:PHE:HD2	1.75	0.50
1:A:892:LYS:HD2	1:A:912:GLU:HG3	1.94	0.50
1:A:1790:ILE:HA	1:A:1799:THR:O	2.12	0.50
13:F:18:A:H4'	13:F:45:A:C2	2.47	0.50
3:C:564:THR:HG21	3:C:576:ILE:HA	1.94	0.49
5:E:164:PRO:O	5:E:166:LEU:HG	2.12	0.49
13:F:32:C:H5'	25:J:237:LYS:O	2.11	0.49
25:J:232:GLU:HA	25:J:235:ILE:HG21	1.88	0.49
25:J:232:GLU:CA	25:J:235:ILE:CG2	2.81	0.49
28:T:267:ASP:OD1	28:T:267:ASP:N	2.36	0.49
42:K:93:HIS:C	42:K:93:HIS:CD2	2.85	0.49
2:B:96:A:N3	2:B:96:A:C2'	2.74	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1:619:ASN:OD1	17:1:620:MET:N	2.45	0.49
19:3:118:GLY:HA2	19:3:132:ILE:HD11	1.94	0.49
28:T:223:SER:OG	28:T:224:ALA:N	2.45	0.49
28:T:343:PRO:HG3	28:T:356:LEU:HD23	1.94	0.49
42:K:78:ILE:CG1	42:K:117:SER:HB2	2.35	0.49
2:B:91:U:O5'	2:B:91:U:H6	1.95	0.49
4:D:106:THR:O	4:D:110:ARG:N	2.41	0.49
4:D:116:LEU:HD22	4:D:140:LEU:HD12	1.92	0.49
5:E:74:PHE:HE1	5:E:95:VAL:CG2	2.25	0.49
5:E:277:PHE:CE2	5:E:300:ILE:HD12	2.46	0.49
19:3:384:THR:OG1	19:3:385:PHE:N	2.45	0.49
19:3:546:LYS:HG3	19:3:588:VAL:O	2.13	0.49
19:3:968:ARG:CG	19:3:982:GLU:HB2	2.39	0.49
25:J:280:LEU:O	25:J:284:GLU:HG2	2.13	0.49
27:R:408:ASP:OD1	27:R:408:ASP:N	2.44	0.49
29:X:330:ASP:OD1	29:X:346:PRO:HA	2.12	0.49
32:9:142:ARG:HH11	32:9:147:ASP:HB3	1.76	0.49
42:K:111:ASN:O	42:K:115:VAL:HG23	2.12	0.49
1:A:635:ARG:HH22	2:B:27:U:P	2.34	0.49
1:A:758:ARG:HD3	1:A:779:LEU:HD11	1.94	0.49
14:G:218:U:C5	30:Y:105:ARG:NH2	2.81	0.49
18:2:644:SER:CA	20:4:65:GLU:CB	2.91	0.49
25:J:337:MET:CE	25:J:346:TRP:CZ2	2.95	0.49
42:K:18:GLN:HE21	42:K:22:THR:HG23	1.78	0.49
3:C:737:PRO:HG3	3:C:774:THR:C	2.33	0.49
4:D:1090:ARG:CG	4:D:1090:ARG:NH2	2.73	0.49
5:E:74:PHE:HE1	5:E:95:VAL:HG22	1.76	0.49
14:G:202:A:OP1	17:1:1149:LYS:HE3	2.11	0.49
27:R:388:ILE:CG2	29:X:350:TYR:CE1	2.95	0.49
29:X:235:ASP:OD1	30:Y:103:LYS:HD2	2.12	0.49
1:A:1275:ARG:HD2	1:A:1375:TRP:CE2	2.48	0.49
1:A:1403:LEU:HD12	1:A:1407:ASP:OD2	2.13	0.49
3:C:680:ASN:O	3:C:682:LYS:N	2.44	0.49
4:D:149:ARG:CG	4:D:149:ARG:NH1	2.73	0.49
19:3:630:MET:CE	36:M:287:LEU:CD2	2.73	0.49
27:R:205:ASP:OD1	27:R:208:GLU:HG3	2.12	0.49
29:X:241:GLY:CA	29:X:288:ARG:HH21	2.20	0.49
42:K:122:LEU:HB2	42:K:163:PHE:HE2	1.78	0.49
1:A:444:ARG:HG3	1:A:444:ARG:HH11	1.77	0.49
1:A:487:LEU:HD12	1:A:492:VAL:HG22	1.95	0.49
1:A:2225:LEU:HD13	1:A:2261:MET:CE	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:219:VAL:HB	5:E:229:TYR:HB2	1.95	0.49
14:G:210:G:N3	14:G:210:G:C3'	2.75	0.49
19:3:318:ASP:HB2	19:3:323:THR:HG21	1.94	0.49
19:3:333:VAL:HG11	19:3:349:VAL:HG21	1.94	0.49
29:X:268:GLU:OE1	29:X:268:GLU:N	2.39	0.49
36:M:274:VAL:N	36:M:308:ASN:O	2.41	0.49
40:0:93:THR:HG21	40:0:98:GLN:HE22	1.72	0.49
1:A:137:GLU:HG2	1:A:410:PRO:HG3	1.95	0.49
3:C:515:THR:HG23	3:C:518:ASP:H	1.77	0.49
19:3:552:ARG:HD3	19:3:600:GLN:O	2.12	0.49
25:J:236:ARG:NH1	25:J:236:ARG:CA	2.73	0.49
32:9:54:CYS:HB2	32:9:91:LEU:HD11	1.94	0.49
36:M:286:ALA:HA	36:M:289:HIS:HB3	1.95	0.49
1:A:481:PHE:CD2	27:R:205:ASP:HB3	2.47	0.49
2:B:111:A:H2'	2:B:112:A:H8	1.78	0.49
3:C:683:ASN:H	3:C:683:ASN:HD22	1.57	0.49
4:D:148:LEU:CD2	4:D:152:GLU:HB2	2.42	0.49
4:D:720:GLN:H	4:D:824:HIS:CB	2.25	0.49
19:3:530:ASP:OD1	19:3:532:ARG:HG2	2.13	0.49
30:Y:37:TRP:CB	30:Y:112:VAL:CG2	2.91	0.49
1:A:733:THR:HG23	32:9:241:TYR:HA	1.94	0.49
1:A:1644:LEU:O	1:A:1723:LYS:NZ	2.46	0.49
1:A:1776:ILE:HB	1:A:1858:PRO:HA	1.95	0.49
5:E:308:PHE:HE1	5:E:324:PRO:HB3	1.75	0.49
17:1:562:LYS:HA	17:1:562:LYS:HD2	1.60	0.49
17:1:1180:ARG:HH21	17:1:1180:ARG:CB	2.26	0.49
1:A:213:LEU:HD13	1:A:219:TYR:CB	2.42	0.48
1:A:2314:PHE:HD2	4:D:1123:TRP:CB	2.26	0.48
4:D:713:MET:O	4:D:716:ALA:CB	2.60	0.48
13:F:40:C:O4'	28:T:285:HIS:CE1	2.66	0.48
14:G:197:U:H4'	24:L:12:ARG:HD2	1.95	0.48
14:G:218:U:C5	30:Y:105:ARG:NH1	2.81	0.48
15:H:2:U:O2'	15:H:3:G:P	2.71	0.48
17:1:130:PRO:HG2	17:1:150:ARG:HD2	1.95	0.48
17:1:614:ARG:N	17:1:615:PRO:CD	2.76	0.48
19:3:757:ILE:HG13	19:3:757:ILE:O	2.12	0.48
42:K:122:LEU:HB2	42:K:163:PHE:CE2	2.47	0.48
1:A:2328:ALA:HB1	4:D:787:ALA:HB3	1.94	0.48
3:C:103:THR:HG22	3:C:171:LEU:HD23	1.96	0.48
5:E:263:ASP:OD1	5:E:272:ARG:HB3	2.13	0.48
14:G:211:U:H2'	14:G:213:C:OP2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1:671:ILE:HG23	17:1:675:MET:HG3	1.95	0.48
19:3:630:MET:SD	36:M:287:LEU:CD2	2.91	0.48
25:J:282:TYR:CE2	25:J:298:ILE:HG21	2.48	0.48
25:J:495:PHE:O	25:J:499:ARG:N	2.46	0.48
29:X:332:GLY:HA2	29:X:346:PRO:HB3	1.96	0.48
32:9:152:ARG:O	32:9:155:ILE:HG22	2.12	0.48
1:A:2149:PRO:O	1:A:2160:PRO:HD3	2.12	0.48
3:C:564:THR:CG2	3:C:576:ILE:HG22	2.43	0.48
3:C:796:VAL:HB	3:C:803:ARG:HH11	1.78	0.48
4:D:104:PRO:HB2	4:D:110:ARG:HG3	1.95	0.48
4:D:423:MET:CB	4:D:878:TYR:HA	2.43	0.48
25:J:299:TRP:HB3	25:J:316:TYR:CD2	2.39	0.48
25:J:349:TYR:HD2	25:J:365:ILE:HG21	1.77	0.48
1:A:828:PRO:HB2	1:A:882:LYS:HE3	1.95	0.48
1:A:1962:THR:HG22	1:A:1969:PRO:HA	1.94	0.48
1:A:2073:TRP:CD1	1:A:2073:TRP:C	2.85	0.48
4:D:1090:ARG:CZ	4:D:1090:ARG:CB	2.91	0.48
5:E:157:CYS:HA	5:E:168:CYS:O	2.13	0.48
19:3:970:TYR:HE1	19:3:979:ARG:CB	2.25	0.48
25:J:316:TYR:CE1	25:J:332:VAL:CG2	2.89	0.48
28:T:188:PRO:HG2	28:T:502:VAL:HG11	1.96	0.48
28:T:227:THR:HG22	28:T:243:THR:HG22	1.95	0.48
28:T:267:ASP:OD2	28:T:269:GLN:NE2	2.46	0.48
28:T:427:LEU:HB3	28:T:439:TRP:HB2	1.95	0.48
1:A:422:LEU:HD23	1:A:422:LEU:H	1.78	0.48
1:A:545:HIS:HB3	1:A:594:TYR:CZ	2.49	0.48
2:B:102:U:H2'	2:B:103:G:C8	2.48	0.48
5:E:129:THR:HB	5:E:153:PHE:CD1	2.48	0.48
5:E:284:PHE:O	5:E:286:LYS:HG2	2.14	0.48
19:3:54:LEU:CD2	19:3:99:PHE:CD2	2.96	0.48
19:3:138:GLN:HG3	19:3:161:HIS:HE1	1.75	0.48
19:3:720:TRP:CE3	19:3:731:LEU:HG	2.49	0.48
22:6:91:LEU:HD13	39:8:6:PHE:CE2	2.49	0.48
29:X:241:GLY:CA	29:X:289:ILE:HD11	2.36	0.48
41:I:78:LEU:HD23	41:I:78:LEU:H	1.78	0.48
2:B:110:C:H2'	2:B:111:A:C8	2.49	0.48
17:1:933:CYS:SG	17:1:970:LEU:HD11	2.54	0.48
19:3:49:LYS:CG	19:3:51:HIS:CE1	2.92	0.48
19:3:123:VAL:HG12	19:3:130:VAL:HG23	1.96	0.48
19:3:1118:VAL:HG22	19:3:1128:ILE:HG22	1.96	0.48
25:J:236:ARG:HH11	25:J:236:ARG:C	2.15	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:I:47:TYR:CE1	41:I:93:LYS:HD2	2.49	0.48
41:I:63:VAL:HG21	41:I:75:TYR:CD2	2.48	0.48
1:A:2252:LEU:HD23	1:A:2253:PRO:HD2	1.96	0.48
4:D:123:ALA:CB	4:D:161:LEU:CD1	2.88	0.48
5:E:175:THR:HG22	5:E:191:GLN:HA	1.95	0.48
5:E:228:THR:HG22	5:E:229:TYR:HD1	1.77	0.48
14:G:215:U:H2'	30:Y:2:ASN:HD21	1.75	0.48
28:T:402:ASP:OD1	28:T:402:ASP:N	2.40	0.48
1:A:2328:ALA:HB1	4:D:787:ALA:CB	2.44	0.48
4:D:721:VAL:O	4:D:808:VAL:HA	2.14	0.48
5:E:62:LEU:HB2	5:E:351:LEU:H	1.79	0.48
5:E:129:THR:HB	5:E:153:PHE:HD1	1.78	0.48
29:X:261:LEU:HG	29:X:275:ILE:HG13	1.95	0.48
30:Y:48:THR:OG1	30:Y:49:GLU:N	2.46	0.48
32:9:37:LEU:HD12	32:9:38:PRO:CD	2.43	0.48
42:K:54:ARG:HB3	42:K:54:ARG:NH1	2.29	0.48
5:E:178:LEU:CD2	5:E:208:ILE:HD13	2.44	0.48
42:K:78:ILE:CD1	42:K:118:ALA:HB2	2.43	0.48
1:A:439:GLN:O	1:A:444:ARG:NH1	2.47	0.48
1:A:1057:ARG:NH1	1:A:1060:GLU:OE1	2.41	0.48
13:F:21:A:H2	24:L:33:ARG:NH2	2.10	0.48
19:3:952:ILE:HG12	19:3:961:ILE:HG12	1.96	0.48
22:6:22:LEU:CD2	22:6:60:ILE:HD12	2.44	0.48
25:J:260:ARG:O	25:J:264:ILE:HG13	2.13	0.48
25:J:274:ARG:HE	27:R:229:VAL:HG22	1.78	0.48
29:X:345:GLU:OE2	29:X:348:ARG:CZ	2.62	0.48
32:9:79:ASN:OD1	32:9:80:GLY:N	2.47	0.48
41:I:91:LEU:HD11	41:I:125:PHE:CE2	2.49	0.48
13:F:31:U:HO2'	13:F:32:C:P	2.35	0.47
17:1:936:VAL:CG2	17:1:954:LEU:HD23	2.44	0.47
29:X:285:ARG:N	29:X:300:SER:O	2.45	0.47
32:9:38:PRO:HB2	32:9:41:HIS:ND1	2.29	0.47
41:I:139:LYS:NZ	41:I:139:LYS:CB	2.73	0.47
42:K:54:ARG:HD3	42:K:90:ASN:ND2	2.29	0.47
1:A:1553:VAL:HG13	36:M:196:ASP:HB2	1.95	0.47
1:A:2129:TYR:HB3	1:A:2172:MET:HE3	1.95	0.47
4:D:759:THR:HA	19:3:682:VAL:CG2	2.43	0.47
17:1:1094:LEU:HD22	17:1:1128:VAL:HB	1.96	0.47
25:J:308:ARG:HG3	27:R:231:HIS:O	2.14	0.47
29:X:253:ARG:NH2	29:X:253:ARG:CG	2.73	0.47
1:A:1407:ASP:OD1	1:A:1407:ASP:N	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2325:VAL:HG22	4:D:788:GLY:O	2.14	0.47
3:C:834:VAL:HG11	3:C:883:PHE:HE2	1.79	0.47
5:E:258:THR:CG2	5:E:260:ARG:CG	2.93	0.47
13:F:32:C:O2'	13:F:33:C:P	2.73	0.47
17:1:1033:GLU:OE1	17:1:1070:LYS:HE2	2.15	0.47
25:J:232:GLU:OE1	25:J:235:ILE:HG21	2.14	0.47
25:J:270:ASP:OD1	27:R:223:PRO:HD3	2.15	0.47
29:X:230:GLY:O	29:X:234:GLU:HG3	2.14	0.47
1:A:651:TRP:CG	13:F:38:G:H1'	2.49	0.47
1:A:1385:VAL:HG11	1:A:1419:ILE:HD12	1.94	0.47
3:C:264:ILE:HG12	3:C:378:TYR:CE1	2.49	0.47
3:C:811:THR:O	3:C:815:VAL:HG23	2.14	0.47
4:D:714:GLU:C	4:D:716:ALA:H	2.17	0.47
5:E:258:THR:CG2	5:E:260:ARG:HG2	2.37	0.47
29:X:364:SER:O	29:X:365:ARG:HG2	2.14	0.47
30:Y:37:TRP:HB3	30:Y:112:VAL:HG21	1.96	0.47
3:C:780:CYS:SG	3:C:782:GLU:HG3	2.54	0.47
4:D:423:MET:CB	4:D:878:TYR:CA	2.92	0.47
5:E:160:ALA:HB2	5:E:201:PHE:CE2	2.50	0.47
14:G:211:U:O2'	14:G:213:C:OP2	2.25	0.47
25:J:313:TRP:CH2	25:J:339:TRP:CD1	3.03	0.47
29:X:329:ILE:O	29:X:329:ILE:HG23	2.13	0.47
32:9:141:PHE:HB3	32:9:150:PHE:O	2.14	0.47
1:A:976:MET:HE1	1:A:1098:PHE:CD1	2.50	0.47
1:A:1762:TYR:HD1	1:A:1762:TYR:N	2.12	0.47
1:A:1872:LEU:HD22	1:A:1884:ILE:HG12	1.96	0.47
3:C:478:THR:O	3:C:562:THR:OG1	2.26	0.47
5:E:88:ARG:CG	5:E:110:GLY:O	2.46	0.47
5:E:248:SER:HB2	5:E:249:TYR:HD1	1.75	0.47
17:1:758:ASP:N	17:1:758:ASP:OD1	2.48	0.47
17:1:1124:SER:O	17:1:1127:THR:OG1	2.30	0.47
18:2:633:LEU:C	18:2:635:ALA:H	2.16	0.47
20:4:67:ALA:O	20:4:70:ALA:HB3	2.15	0.47
27:R:388:ILE:HD13	29:X:350:TYR:HD1	1.79	0.47
29:X:246:TYR:HH	29:X:249:PRO:HD3	1.79	0.47
41:I:81:TYR:HD2	41:I:89:VAL:HG21	1.79	0.47
1:A:152:ARG:NH2	1:A:618:THR:O	2.47	0.47
1:A:206:TRP:HB2	1:A:212:PRO:HB2	1.95	0.47
1:A:974:ASN:HB2	1:A:1178:TYR:HB3	1.95	0.47
14:G:218:U:C4	30:Y:105:ARG:CZ	2.98	0.47
15:H:15:U:H3'	24:L:40:ARG:HH12	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:399:ASP:OD1	19:3:400:GLU:N	2.48	0.47
19:3:720:TRP:HE3	19:3:731:LEU:HG	1.80	0.47
21:5:80:PHE:CD2	21:5:82:VAL:HG23	2.50	0.47
22:6:30:CYS:O	22:6:34:ASP:HA	2.15	0.47
28:T:493:ASP:OD1	28:T:493:ASP:N	2.37	0.47
1:A:761:ILE:HD12	1:A:775:ASN:HD22	1.80	0.47
3:C:649:SER:HB3	3:C:651:ILE:HG12	1.95	0.47
3:C:774:THR:HA	3:C:784:ILE:HD12	1.96	0.47
17:1:128:ILE:HB	21:5:96:ARG:HB3	1.97	0.47
17:1:415:LEU:HD23	17:1:415:LEU:HA	1.79	0.47
19:3:629:SER:OG	19:3:686:LEU:HD12	2.15	0.47
19:3:987:ALA:HB3	19:3:1007:GLU:HG2	1.96	0.47
25:J:276:ILE:HD11	25:J:309:VAL:HG11	1.96	0.47
25:J:303:ILE:HD13	25:J:313:TRP:CD1	2.50	0.47
42:K:120:THR:CG2	42:K:124:HIS:CD2	2.96	0.47
1:A:2148:VAL:O	1:A:2150:GLN:HG2	2.14	0.47
2:B:96:A:N3	2:B:96:A:C3'	2.77	0.47
3:C:543:ARG:CG	3:C:543:ARG:NH1	2.77	0.47
4:D:141:ALA:HB2	4:D:182:TYR:OH	2.15	0.47
5:E:277:PHE:N	5:E:277:PHE:CD1	2.82	0.47
15:H:2:U:O2'	15:H:3:G:OP2	2.26	0.47
19:3:353:PHE:HE2	19:3:429:ARG:NH1	2.13	0.47
19:3:1004:ASP:OD2	19:3:1007:GLU:CB	2.55	0.47
29:X:338:PHE:HD2	29:X:359:LYS:HB3	1.79	0.47
30:Y:65:ILE:CD1	30:Y:82:LEU:HD21	2.44	0.47
1:A:662:GLY:HA3	27:R:213:LYS:NZ	2.30	0.47
1:A:1122:ASN:HB2	32:9:35:ARG:HD3	1.94	0.47
1:A:2121:ARG:O	1:A:2154:HIS:HA	2.15	0.47
4:D:1672:LYS:HA	4:D:1885:ASN:O	2.15	0.47
27:R:389:SER:HB3	29:X:349:TYR:HB2	1.97	0.47
32:9:79:ASN:ND2	32:9:81:GLU:HG2	2.30	0.47
3:C:813:ARG:NH1	32:9:106:LEU:HD22	2.30	0.46
17:1:1032:GLN:O	17:1:1036:ILE:HG22	2.15	0.46
18:2:565:ASP:OD1	18:2:565:ASP:N	2.47	0.46
21:5:77:LEU:CG	21:5:89:VAL:HG11	2.45	0.46
27:R:403:ASN:ND2	27:R:403:ASN:O	2.47	0.46
28:T:381:HIS:HD2	28:T:441:TRP:CE2	2.33	0.46
40:0:82:ILE:HA	40:0:89:LYS:HA	1.98	0.46
42:K:113:GLU:HA	42:K:116:LEU:HD12	1.97	0.46
1:A:28:GLU:HG2	1:A:29:LYS:N	2.31	0.46
1:A:642:ARG:HG3	2:B:56:C:H1'	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:881:ILE:HG23	1:A:918:THR:HG23	1.97	0.46
1:A:1093:ASP:N	1:A:1093:ASP:OD2	2.49	0.46
13:F:17:G:O2'	13:F:18:A:N7	2.46	0.46
14:G:-9:G:N2	37:U:5:ILE:O	2.44	0.46
15:H:13:U:H5'	15:H:14:A:C5'	2.45	0.46
15:H:39:G:H2'	15:H:40:G:O4'	2.15	0.46
25:J:232:GLU:O	25:J:235:ILE:CG2	2.63	0.46
25:J:236:ARG:HH11	25:J:236:ARG:HG3	1.79	0.46
27:R:140:ILE:HA	27:R:143:ILE:HG22	1.97	0.46
36:M:249:TYR:HB3	40:0:72:TYR:CZ	2.51	0.46
36:M:287:LEU:O	36:M:291:ARG:HG3	2.14	0.46
39:8:51:TRP:HH2	39:8:104:GLU:HG3	1.79	0.46
39:8:56:VAL:HG23	39:8:68:ILE:HD11	1.96	0.46
40:0:93:THR:CB	40:0:98:GLN:NE2	2.78	0.46
42:K:146:LEU:C	42:K:146:LEU:HD23	2.36	0.46
1:A:1129:ASN:OD1	1:A:1129:ASN:N	2.46	0.46
1:A:1347:ASP:OD1	1:A:1347:ASP:N	2.35	0.46
4:D:498:ASN:O	4:D:672:GLY:O	2.33	0.46
5:E:243:LEU:HD11	5:E:247:GLY:CA	2.44	0.46
17:1:675:MET:HB2	17:1:679:ILE:HG23	1.97	0.46
20:4:12:ASP:CB	20:4:67:ALA:HB3	2.43	0.46
21:5:48:ILE:HG12	21:5:62:VAL:HG22	1.98	0.46
32:9:52:PRO:HB2	32:9:91:LEU:HB2	1.96	0.46
41:I:104:LYS:HG3	41:I:119:VAL:HG23	1.98	0.46
1:A:1415:GLY:O	1:A:1418:ARG:NH1	2.47	0.46
1:A:1853:PRO:HD2	1:A:1856:GLU:HG3	1.98	0.46
19:3:1064:ASP:OD1	19:3:1064:ASP:N	2.28	0.46
1:A:443:VAL:HG11	1:A:614:TYR:CD1	2.51	0.46
5:E:119:THR:CG2	5:E:161:ARG:HB3	2.46	0.46
5:E:178:LEU:HG	5:E:188:GLN:HB2	1.98	0.46
19:3:643:VAL:O	19:3:663:LEU:HD12	2.16	0.46
25:J:236:ARG:NH1	25:J:236:ARG:CG	2.73	0.46
25:J:376:VAL:HG23	25:J:415:LEU:HD12	1.97	0.46
27:R:237:MET:HB2	27:R:241:GLU:OE2	2.16	0.46
29:X:344:ILE:HB	29:X:350:TYR:CE2	2.50	0.46
32:9:75:THR:HG22	32:9:82:LYS:HB3	1.97	0.46
41:I:97:LEU:O	41:I:101:ARG:HG3	2.15	0.46
42:K:139:THR:HB	42:K:141:VAL:HG22	1.96	0.46
3:C:506:PRO:HB3	3:C:526:THR:HG22	1.98	0.46
17:1:129:SEP:O3P	17:1:150:ARG:NH2	2.30	0.46
17:1:933:CYS:O	17:1:937:LEU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2:633:LEU:C	18:2:635:ALA:N	2.69	0.46
41:I:123:PRO:O	41:I:126:GLU:HG2	2.16	0.46
1:A:514:ASN:N	1:A:514:ASN:OD1	2.44	0.46
1:A:1260:VAL:HG21	1:A:1325:LEU:HB3	1.97	0.46
1:A:1527:ASN:HB2	36:M:215:ASP:HB3	1.98	0.46
4:D:783:ALA:O	4:D:809:LEU:CA	2.60	0.46
13:F:6:G:H2'	13:F:6:G:N3	2.30	0.46
17:1:937:LEU:HD23	17:1:937:LEU:HA	1.78	0.46
19:3:55:THR:O	19:3:55:THR:HG23	2.16	0.46
19:3:515:ALA:HB1	19:3:526:HIS:NE2	2.31	0.46
19:3:557:ALA:HB2	19:3:590:MET:HE1	1.98	0.46
25:J:308:ARG:HH21	25:J:341:PRO:HB3	1.80	0.46
29:X:332:GLY:CA	29:X:346:PRO:HB3	2.46	0.46
41:I:78:LEU:HD21	41:I:89:VAL:HG12	1.96	0.46
1:A:1292:GLU:OE2	1:A:1331:GLY:N	2.41	0.46
1:A:1648:SER:HB3	1:A:1883:VAL:HG12	1.97	0.46
4:D:1349:GLY:HA2	4:D:1491:SER:O	2.16	0.46
5:E:250:LEU:CD1	5:E:262:TRP:HB2	2.45	0.46
15:H:38:G:C2'	15:H:39:G:H5"	2.46	0.46
22:6:45:ILE:HD11	22:6:50:ASN:HB3	1.97	0.46
1:A:774:LYS:HZ1	15:H:5:C:HO2'	1.58	0.46
1:A:1000:ILE:HG22	1:A:1001:VAL:HG13	1.96	0.46
17:1:1250:CYS:HA	17:1:1265:TYR:CE2	2.51	0.46
19:3:519:VAL:HG23	19:3:524:ILE:HG12	1.98	0.46
19:3:950:ALA:CB	19:3:989:TYR:OH	2.44	0.46
25:J:270:ASP:OD1	27:R:223:PRO:HG3	2.16	0.46
25:J:366:TYR:CE2	25:J:382:TYR:HA	2.51	0.46
30:Y:67:LEU:HA	30:Y:80:CYS:HB3	1.92	0.46
42:K:123:MET:HE2	42:K:123:MET:HB2	1.73	0.46
1:A:1536:LEU:HD11	1:A:1576:ILE:HD11	1.98	0.46
1:A:2225:LEU:HD13	1:A:2261:MET:HE1	1.98	0.46
3:C:683:ASN:ND2	3:C:683:ASN:N	2.60	0.46
5:E:260:ARG:NE	5:E:276:ILE:HD11	2.31	0.46
18:2:648:LEU:HD12	18:2:649:LYS:H	1.81	0.46
28:T:455:GLN:HG2	28:T:456:PRO:HD2	1.97	0.46
30:Y:67:LEU:CD1	30:Y:80:CYS:HB3	2.45	0.46
38:V:619:ASP:OD1	38:V:620:ASN:N	2.49	0.46
39:8:38:VAL:O	39:8:79:ASN:ND2	2.49	0.46
41:I:28:ARG:HA	41:I:28:ARG:HD2	1.57	0.46
41:I:139:LYS:O	41:I:143:VAL:HG23	2.16	0.46
3:C:126:SER:O	3:C:126:SER:OG	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:151:LYS:HE2	4:D:151:LYS:N	2.31	0.45
5:E:232:ARG:O	5:E:262:TRP:CH2	2.69	0.45
19:3:614:VAL:HG11	19:3:667:ILE:HD13	1.98	0.45
25:J:286:GLU:HB3	25:J:295:ALA:HB2	1.97	0.45
25:J:436:TYR:CZ	25:J:440:LEU:HD22	2.50	0.45
25:J:439:ALA:O	25:J:443:ILE:HG12	2.15	0.45
29:X:345:GLU:CD	29:X:348:ARG:HH11	2.18	0.45
42:K:143:GLN:H	42:K:143:GLN:HG3	1.53	0.45
1:A:1385:VAL:HG21	1:A:1414:ARG:CG	2.45	0.45
4:D:500:LEU:O	4:D:674:PHE:O	2.34	0.45
5:E:260:ARG:CD	5:E:276:ILE:HD13	2.45	0.45
14:G:11:C:H2'	14:G:12:U:O4'	2.16	0.45
17:1:577:VAL:O	17:1:577:VAL:HG12	2.17	0.45
17:1:716:ALA:O	17:1:719:TYR:N	2.40	0.45
17:1:902:GLU:OE1	27:R:447:ILE:HD12	2.16	0.45
19:3:137:LYS:O	19:3:137:LYS:HD3	2.15	0.45
29:X:287:ARG:HA	29:X:293:PRO:HB3	1.98	0.45
30:Y:140:THR:CG2	31:Z:563:ARG:CG	2.93	0.45
36:M:225:ASP:N	36:M:225:ASP:OD1	2.49	0.45
1:A:34:ALA:HA	5:E:213:ILE:CD1	2.46	0.45
1:A:1404:THR:O	1:A:1407:ASP:OD1	2.35	0.45
1:A:1774:ASN:OD1	1:A:1775:GLN:HG3	2.15	0.45
1:A:1860:GLN:HG2	1:A:1883:VAL:HG22	1.98	0.45
1:A:2196:HIS:HB3	1:A:2230:LEU:HD11	1.98	0.45
3:C:490:PHE:HE2	3:C:612:LYS:HB2	1.80	0.45
5:E:276:ILE:C	5:E:277:PHE:CD1	2.89	0.45
17:1:613:MET:HE3	17:1:635:VAL:HG11	1.98	0.45
19:3:173:VAL:HB	19:3:181:MET:HB2	1.98	0.45
19:3:1004:ASP:OD1	19:3:1005:VAL:N	2.49	0.45
27:R:465:ALA:O	27:R:469:THR:HG23	2.16	0.45
28:T:381:HIS:ND1	28:T:384:HIS:HB2	2.32	0.45
32:9:42:CYS:SG	32:9:61:PHE:HB2	2.56	0.45
1:A:635:ARG:NH2	2:B:26:A:O3'	2.49	0.45
1:A:2169:LEU:HD21	1:A:2272:MET:HG3	1.98	0.45
5:E:178:LEU:CD1	5:E:222:LEU:HD21	2.46	0.45
5:E:276:ILE:C	5:E:277:PHE:HD1	2.19	0.45
19:3:593:ALA:HB3	19:3:602:SER:OG	2.16	0.45
25:J:223:TYR:HA	25:J:226:ARG:NE	2.32	0.45
27:R:391:VAL:O	27:R:391:VAL:HG13	2.17	0.45
1:A:44:ARG:HA	1:A:49:ARG:HH12	1.81	0.45
1:A:79:ARG:O	1:A:82:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:A:N3	2:B:96:A:H2'	2.32	0.45
4:D:131:ILE:HG12	4:D:697:ALA:CB	2.46	0.45
17:1:982:LEU:HD12	17:1:1019:ARG:HG2	1.97	0.45
1:A:2303:GLU:CD	1:A:2303:GLU:H	2.19	0.45
3:C:676:ALA:HB3	3:C:815:VAL:HG22	1.99	0.45
4:D:831:THR:CB	4:D:871:THR:HA	2.47	0.45
5:E:250:LEU:HD12	5:E:250:LEU:C	2.37	0.45
19:3:136:GLU:HB3	19:3:166:LEU:HD23	1.98	0.45
19:3:640:LEU:HD23	19:3:665:LEU:HD11	1.99	0.45
25:J:238:ASN:C	25:J:240:THR:H	2.20	0.45
25:J:251:TRP:CZ2	25:J:255:LEU:HD11	2.52	0.45
42:K:47:PRO:HA	42:K:50:TYR:CD2	2.52	0.45
5:E:133:VAL:O	5:E:147:LEU:N	2.46	0.45
17:1:619:ASN:CG	17:1:624:VAL:HG21	2.37	0.45
19:3:702:PHE:HE2	19:3:715:MET:SD	2.40	0.45
32:9:137:LYS:HA	32:9:137:LYS:HD2	1.76	0.45
42:K:112:GLU:HG3	42:K:116:LEU:HD11	1.97	0.45
4:D:126:ASP:O	4:D:127:GLN:NE2	2.49	0.45
13:F:23:G:HO2'	13:F:24:U:P	2.39	0.45
19:3:185:LEU:HB3	19:3:206:GLN:NE2	2.32	0.45
19:3:675:LEU:HD23	19:3:691:THR:HA	1.99	0.45
5:E:193:THR:HG22	5:E:194:TYR:CD1	2.41	0.45
14:G:222:U:H6	30:Y:119:LYS:CE	2.23	0.45
17:1:1136:TYR:HD1	17:1:1147:VAL:CG2	2.30	0.45
17:1:1303:ILE:HD12	17:1:1303:ILE:HA	1.77	0.45
19:3:444:VAL:HG22	19:3:767:LEU:HD22	1.98	0.45
25:J:337:MET:HE3	25:J:346:TRP:CE2	2.51	0.45
1:A:959:ILE:HD11	1:A:976:MET:HE3	1.99	0.45
3:C:780:CYS:SG	3:C:782:GLU:HB2	2.57	0.45
1:A:1332:HIS:CE1	1:A:1359:HIS:HB3	2.52	0.44
1:A:2280:ASN:HB3	1:A:2309:HIS:CD2	2.52	0.44
4:D:102:TYR:HB3	4:D:103:LYS:H	1.61	0.44
4:D:1090:ARG:NH2	4:D:1090:ARG:CB	2.80	0.44
19:3:187:MET:HE3	19:3:187:MET:HB2	1.79	0.44
25:J:337:MET:HE3	25:J:346:TRP:CZ2	2.53	0.44
29:X:348:ARG:HH11	29:X:348:ARG:HG3	1.81	0.44
1:A:150:MET:O	1:A:153:ARG:HG2	2.17	0.44
2:B:39:C:C4'	2:B:40:U:OP1	2.65	0.44
17:1:641:ILE:HG12	17:1:675:MET:HE1	1.87	0.44
18:2:632:TRP:HB3	20:4:76:MET:CB	2.47	0.44
19:3:638:GLU:OE1	19:3:638:GLU:HA	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:J:223:TYR:N	25:J:226:ARG:HH21	2.15	0.44
25:J:303:ILE:HD13	25:J:313:TRP:HD1	1.81	0.44
25:J:340:GLN:N	25:J:341:PRO:CD	2.80	0.44
27:R:297:LYS:HZ1	32:9:206:GLU:HG3	1.82	0.44
27:R:404:GLU:HB3	29:X:253:ARG:NH1	2.32	0.44
29:X:364:SER:OG	29:X:365:ARG:N	2.50	0.44
1:A:203:VAL:O	1:A:203:VAL:HG13	2.17	0.44
3:C:259:LYS:HG2	44:C:1500:GTP:C6	2.53	0.44
3:C:508:LYS:HE3	3:C:510:LEU:HD21	1.99	0.44
5:E:276:ILE:O	5:E:277:PHE:HD1	2.00	0.44
14:G:210:G:N3	14:G:210:G:H2'	2.32	0.44
17:1:1109:ARG:O	17:1:1112:THR:CG2	2.63	0.44
17:1:1258:ALA:HB3	17:1:1261:VAL:HG12	1.98	0.44
19:3:1052:ASN:OD1	19:3:1052:ASN:N	2.50	0.44
25:J:375:ASP:OD1	25:J:376:VAL:N	2.50	0.44
27:R:132:LEU:O	28:T:385:TYR:HB3	2.18	0.44
1:A:2156:THR:OG1	1:A:2157:VAL:N	2.50	0.44
4:D:102:TYR:HA	4:D:137:ASP:OD2	2.18	0.44
17:1:1044:ASP:HB3	17:1:1083:TYR:CD1	2.52	0.44
17:1:1045:ARG:HH11	40:0:24:ARG:HG3	1.83	0.44
17:1:1287:ILE:HG13	23:7:32:LEU:HD21	2.00	0.44
19:3:485:LEU:HD23	19:3:491:VAL:CG1	2.47	0.44
19:3:1001:ILE:HG13	19:3:1038:LEU:HD11	2.00	0.44
25:J:313:TRP:HH2	25:J:339:TRP:CD1	2.35	0.44
29:X:294:ILE:HD12	29:X:299:CYS:SG	2.58	0.44
30:Y:16:ARG:NH1	30:Y:20:LEU:HD11	2.33	0.44
1:A:410:PRO:O	1:A:413:LEU:HG	2.18	0.44
4:D:144:LYS:HD2	4:D:144:LYS:HA	1.42	0.44
5:E:62:LEU:HD13	5:E:351:LEU:HD12	1.85	0.44
17:1:946:LYS:HA	17:1:946:LYS:HD2	1.79	0.44
17:1:1304:LEU:HD23	17:1:1304:LEU:HA	1.82	0.44
19:3:460:TRP:HZ3	19:3:505:THR:HG23	1.82	0.44
29:X:255:PRO:HB3	29:X:308:TYR:CD1	2.52	0.44
30:Y:38:ILE:O	30:Y:38:ILE:HG13	2.17	0.44
30:Y:40:LEU:HD12	30:Y:80:CYS:SG	2.58	0.44
42:K:151:SER:CB	42:K:156:LEU:HD23	2.46	0.44
1:A:543:ALA:HB3	13:F:38:G:OP1	2.18	0.44
2:B:34:U:O4	32:9:4:ARG:NH1	2.51	0.44
4:D:1308:PRO:C	4:D:1310:SER:H	2.20	0.44
17:1:446:MET:HB2	27:R:299:ARG:HG2	2.00	0.44
25:J:241:VAL:HG22	25:J:244:ASN:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:J:265:TYR:HD2	25:J:282:TYR:HD1	1.66	0.44
38:V:599:LEU:O	38:V:603:LEU:HB2	2.17	0.44
40:0:8:LYS:HB3	40:0:8:LYS:HE2	1.80	0.44
1:A:481:PHE:CG	27:R:205:ASP:HB3	2.51	0.44
1:A:662:GLY:CA	27:R:213:LYS:HZ3	2.29	0.44
1:A:1638:ASN:HB3	1:A:1652:MET:O	2.17	0.44
1:A:2078:ILE:HG23	4:D:1047:PRO:CB	2.47	0.44
3:C:590:ILE:HG22	3:C:629:ILE:HB	1.99	0.44
5:E:92:LEU:O	5:E:101:ASN:OD1	2.36	0.44
19:3:485:LEU:HD23	19:3:491:VAL:HG12	2.00	0.44
19:3:563:LEU:HD12	19:3:581:LYS:HD3	1.99	0.44
29:X:241:GLY:HA3	29:X:288:ARG:NE	2.32	0.44
29:X:262:TYR:HA	29:X:263:PRO:HD3	1.85	0.44
1:A:1421:THR:O	1:A:1424:GLN:HG2	2.18	0.44
17:1:732:TRP:HA	17:1:732:TRP:CE3	2.53	0.44
17:1:936:VAL:HG11	17:1:955:ILE:HG13	2.00	0.44
19:3:12:THR:O	19:3:34:ARG:NH1	2.50	0.44
20:4:12:ASP:CA	20:4:67:ALA:HB1	2.44	0.44
41:I:144:LYS:HB2	41:I:144:LYS:HE3	1.70	0.44
42:K:58:VAL:HG23	42:K:61:LEU:HD13	1.98	0.44
3:C:306:ASN:HA	3:C:433:MET:HG3	2.00	0.44
3:C:847:TYR:CE1	3:C:857:VAL:HG21	2.53	0.44
5:E:237:SER:HB2	5:E:255:MET:HG3	1.98	0.44
5:E:251:LEU:CG	5:E:291:CYS:SG	3.05	0.44
5:E:277:PHE:CE1	5:E:317:ARG:HG2	2.53	0.44
13:F:39:A:OP2	13:F:39:A:H8	2.01	0.44
17:1:884:ILE:HG23	17:1:888:LEU:HD23	2.00	0.44
19:3:42:ARG:HB2	19:3:53:LEU:HD11	1.99	0.44
19:3:318:ASP:HB2	19:3:323:THR:CG2	2.48	0.44
19:3:1057:ARG:HH11	19:3:1057:ARG:CG	2.13	0.44
25:J:259:GLN:OE1	25:J:259:GLN:HA	2.18	0.44
32:9:106:LEU:HD23	32:9:106:LEU:HA	1.77	0.44
1:A:41:GLN:OE1	1:A:41:GLN:HA	2.18	0.43
1:A:1574:ILE:HG22	36:M:220:LEU:HD22	2.00	0.43
3:C:497:LEU:HD23	3:C:497:LEU:HA	1.78	0.43
4:D:505:THR:CB	4:D:854:GLY:CA	2.96	0.43
4:D:1589:PHE:O	4:D:1642:GLN:N	2.49	0.43
14:G:209:U:H4'	14:G:210:G:C5	2.53	0.43
17:1:1262:ARG:NH1	23:7:24:ALA:O	2.47	0.43
18:2:630:PRO:HA	18:2:631:PRO:HD3	1.78	0.43
27:R:466:ARG:HD2	27:R:466:ARG:HA	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:330:ASP:OD1	29:X:330:ASP:O	2.36	0.43
32:9:134:LEU:O	32:9:138:ALA:HB3	2.17	0.43
42:K:75:GLU:HA	42:K:78:ILE:HG22	2.00	0.43
1:A:662:GLY:CA	27:R:213:LYS:HZ2	2.32	0.43
1:A:1344:LYS:HA	1:A:1344:LYS:HD3	1.78	0.43
1:A:1887:SER:O	1:A:1890:GLN:NE2	2.50	0.43
1:A:2306:HIS:CE1	1:A:2308:VAL:CG2	2.94	0.43
3:C:259:LYS:HD3	44:C:1500:GTP:C4	2.53	0.43
4:D:106:THR:CG2	4:D:107:LYS:H	2.30	0.43
17:1:731:LEU:HD23	17:1:731:LEU:HA	1.90	0.43
17:1:1109:ARG:CA	17:1:1112:THR:HG22	2.47	0.43
17:1:1183:VAL:HA	17:1:1186:GLN:HG2	2.00	0.43
19:3:553:GLN:NE2	19:3:619:LEU:HD13	2.32	0.43
19:3:875:ASN:OD1	19:3:875:ASN:N	2.33	0.43
26:P:189:ASP:OD1	26:P:189:ASP:N	2.34	0.43
29:X:241:GLY:O	29:X:288:ARG:NH2	2.50	0.43
30:Y:38:ILE:HG23	30:Y:90:THR:HG22	1.99	0.43
32:9:245:LYS:HD2	32:9:258:GLU:HG3	2.01	0.43
41:I:128:VAL:O	41:I:131:THR:OG1	2.27	0.43
3:C:758:LEU:HG	3:C:803:ARG:HH12	1.84	0.43
18:2:573:ASP:OD1	18:2:577:LYS:HE3	2.18	0.43
19:3:475:ILE:HD13	19:3:484:VAL:HG23	2.00	0.43
25:J:258:ILE:O	25:J:261:ALA:N	2.51	0.43
25:J:289:ASN:O	25:J:291:GLN:N	2.51	0.43
39:8:86:GLN:HB2	39:8:102:MET:HG3	2.00	0.43
40:0:89:LYS:HE2	40:0:89:LYS:HB3	1.84	0.43
41:I:91:LEU:HD11	41:I:125:PHE:CD2	2.53	0.43
4:D:140:LEU:CD2	4:D:144:LYS:HG2	2.48	0.43
17:1:150:ARG:HH21	17:1:150:ARG:HD3	1.71	0.43
19:3:520:TYR:CD1	19:3:522:ASP:HB2	2.53	0.43
19:3:566:PHE:HD1	19:3:576:GLU:HA	1.83	0.43
28:T:257:ARG:NH2	28:T:301:ASP:OD1	2.51	0.43
1:A:579:GLN:HB3	1:A:630:TRP:HB3	2.00	0.43
1:A:1551:PHE:CD2	36:M:192:THR:OG1	2.72	0.43
2:B:93:U:H4'	2:B:94:U:H5"	2.00	0.43
27:R:238:THR:OG1	27:R:241:GLU:HG3	2.18	0.43
28:T:220:VAL:HG13	28:T:230:ILE:HG12	1.99	0.43
38:V:465:SER:OG	38:V:475:LYS:NZ	2.51	0.43
41:I:36:VAL:HG23	41:I:36:VAL:O	2.19	0.43
1:A:829:PRO:HB3	21:5:86:TYR:CD2	2.52	0.43
1:A:834:HIS:CD2	1:A:1432:TYR:CE1	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:837:LYS:O	1:A:840:ILE:HG22	2.18	0.43
14:G:217:U:H6	14:G:217:U:C5'	2.29	0.43
15:H:38:G:C2'	15:H:39:G:C5'	2.97	0.43
15:H:83:G:H2'	15:H:84:C:C6	2.54	0.43
17:1:563:LEU:HB3	17:1:566:LEU:HD12	2.00	0.43
18:2:495:ARG:NH2	19:3:1026:ASP:OD2	2.52	0.43
19:3:1120:THR:HG22	19:3:1126:ILE:HG12	2.00	0.43
32:9:242:SER:HA	32:9:263:ALA:HA	2.01	0.43
42:K:28:GLN:OE1	42:K:28:GLN:N	2.50	0.43
3:C:192:ASP:OD1	3:C:195:GLY:N	2.39	0.43
3:C:854:ARG:HH21	3:C:854:ARG:HD2	1.70	0.43
17:1:563:LEU:H	17:1:563:LEU:HG	1.52	0.43
17:1:971:MET:CE	17:1:1003:VAL:CG1	2.88	0.43
27:R:403:ASN:HB2	29:X:250:PRO:C	2.39	0.43
41:I:138:ARG:HH21	42:K:83:ASN:HB2	1.83	0.43
1:A:1676:ILE:HD13	1:A:1706:ASP:HB2	2.01	0.43
1:A:1949:ARG:NE	27:R:463:LEU:HD13	2.33	0.43
3:C:323:PHE:CD2	3:C:373:ILE:HG12	2.53	0.43
4:D:123:ALA:HB1	4:D:161:LEU:CD1	2.48	0.43
4:D:1635:LEU:O	4:D:1640:ALA:N	2.51	0.43
5:E:231:MET:CE	5:E:250:LEU:HD21	2.49	0.43
14:G:218:U:H3'	30:Y:3:PRO:HG2	2.00	0.43
17:1:885:ASP:OD1	17:1:885:ASP:N	2.50	0.43
19:3:47:THR:CG2	19:3:49:LYS:CG	2.84	0.43
19:3:956:GLN:HE22	19:3:998:HIS:CE1	2.37	0.43
27:R:148:ARG:HG3	28:T:300:ILE:HG23	2.01	0.43
38:V:617:PRO:O	38:V:624:THR:OG1	2.30	0.43
41:I:67:ALA:HB2	41:I:72:ILE:HD12	2.01	0.43
1:A:1681:ARG:HG3	1:A:1715:TYR:CZ	2.53	0.43
3:C:758:LEU:HD11	3:C:798:GLN:HA	2.00	0.43
13:F:10:G:H1	14:G:10:U:H3	1.67	0.43
19:3:406:PRO:O	19:3:427:CYS:CB	2.67	0.43
19:3:603:ARG:NH1	19:3:620:ASP:HB2	2.33	0.43
19:3:669:LEU:HD12	19:3:673:VAL:CG2	2.47	0.43
25:J:358:GLU:HG2	25:J:361:ARG:HH11	1.83	0.43
42:K:53:LEU:O	42:K:58:VAL:HG12	2.18	0.43
1:A:976:MET:CE	1:A:1098:PHE:HD1	2.32	0.43
1:A:1125:ILE:CD1	32:9:35:ARG:HG3	2.49	0.43
1:A:1639:VAL:O	1:A:1654:SER:HB3	2.19	0.43
1:A:2074:ARG:H	1:A:2074:ARG:HG2	1.54	0.43
3:C:602:LYS:HD2	3:C:651:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:634:GLU:OE2	3:C:882:GLY:N	2.49	0.43
4:D:434:SER:HA	4:D:446:HIS:O	2.19	0.43
17:1:1023:ILE:O	17:1:1023:ILE:HG22	2.19	0.43
17:1:1050:VAL:HG21	17:1:1055:TRP:CZ2	2.53	0.43
18:2:632:TRP:CB	20:4:76:MET:CB	2.97	0.43
19:3:931:VAL:HG23	19:3:936:LYS:HB3	2.01	0.43
25:J:220:LEU:HD11	25:J:224:LYS:HZ3	1.84	0.43
25:J:336:TRP:HE1	25:J:341:PRO:HG3	1.83	0.43
41:I:135:LEU:HD23	41:I:135:LEU:HA	1.81	0.43
1:A:444:ARG:HG3	1:A:444:ARG:NH1	2.33	0.42
2:B:36:C:O2	37:U:11:ARG:NH2	2.51	0.42
4:D:109:THR:CG2	4:D:180:THR:OG1	2.63	0.42
4:D:406:ARG:CB	4:D:955:ASP:CB	2.97	0.42
5:E:323:LEU:HA	5:E:324:PRO:HD2	1.88	0.42
17:1:550:HIS:CG	22:6:100:TYR:CD2	3.06	0.42
17:1:1129:LEU:HD23	17:1:1129:LEU:HA	1.75	0.42
17:1:1291:ASP:N	17:1:1291:ASP:OD1	2.51	0.42
17:1:1302:TYR:OH	23:7:57:GLU:OE2	2.37	0.42
19:3:965:LYS:HG3	19:3:966:LEU:HD12	2.00	0.42
25:J:438:TYR:CE2	25:J:442:ARG:HD2	2.54	0.42
28:T:213:GLU:HG3	28:T:218:TRP:CZ2	2.54	0.42
32:9:61:PHE:CE1	32:9:66:ILE:HB	2.53	0.42
1:A:946:GLU:OE1	1:A:954:LYS:HD2	2.19	0.42
1:A:2216:CYS:HA	1:A:2225:LEU:HB3	2.01	0.42
2:B:44:A:N7	32:9:3:LYS:NZ	2.62	0.42
2:B:101:U:H6	2:B:101:U:O5'	2.02	0.42
3:C:929:LEU:HD23	3:C:929:LEU:HA	1.78	0.42
4:D:831:THR:CB	4:D:871:THR:CB	2.96	0.42
17:1:1083:TYR:CZ	40:0:13:VAL:CG2	3.02	0.42
24:L:77:LEU:O	24:L:79:PRO:HD3	2.18	0.42
25:J:246:ILE:O	25:J:250:GLN:HG2	2.19	0.42
27:R:405:VAL:HG13	27:R:405:VAL:O	2.18	0.42
30:Y:13:LEU:HD12	30:Y:13:LEU:HA	1.85	0.42
32:9:277:LYS:H	32:9:437:PRO:CB	2.32	0.42
41:I:129:GLU:HB2	41:I:133:LYS:HZ1	1.81	0.42
42:K:34:GLU:HG2	42:K:73:LEU:HD12	2.00	0.42
1:A:38:GLN:HB2	5:E:195:GLN:HE21	1.85	0.42
1:A:92:LEU:HD13	1:A:503:MET:HB3	2.00	0.42
1:A:1023:ASN:N	1:A:1023:ASN:OD1	2.50	0.42
1:A:1499:GLU:OE2	1:A:1928:SER:OG	2.34	0.42
3:C:377:LEU:HD12	3:C:377:LEU:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:480:LYS:HA	3:C:480:LYS:HD2	1.84	0.42
4:D:149:ARG:NH1	4:D:149:ARG:HG3	2.34	0.42
15:H:74:A:H5'	15:H:80:U:OP2	2.18	0.42
21:5:35:MET:HE2	21:5:35:MET:HB2	1.89	0.42
25:J:340:GLN:CG	25:J:372:VAL:HG21	2.43	0.42
30:Y:116:ARG:HH11	30:Y:116:ARG:CG	2.30	0.42
30:Y:117:ALA:HA	30:Y:118:PRO:HD3	1.86	0.42
32:9:112:ASN:HA	32:9:159:GLN:HE22	1.84	0.42
39:8:63:GLU:OE1	39:8:63:GLU:N	2.51	0.42
40:0:79:LYS:HB2	40:0:79:LYS:HE2	1.84	0.42
1:A:829:PRO:HA	21:5:86:TYR:HE2	1.83	0.42
15:H:50:A:H2'	15:H:51:A:C8	2.55	0.42
17:1:1119:VAL:HA	17:1:1122:THR:HG22	2.01	0.42
19:3:274:ARG:NH2	19:3:309:ASP:OD1	2.53	0.42
25:J:245:TRP:O	25:J:245:TRP:HE3	2.02	0.42
38:V:533:TYR:HD2	38:V:567:CYS:HG	1.68	0.42
38:V:600:ASN:OD1	38:V:604:LYS:NZ	2.53	0.42
41:I:37:LYS:CD	41:I:39:TYR:OH	2.67	0.42
41:I:65:ARG:O	41:I:68:LEU:HB3	2.19	0.42
1:A:246:LEU:HD11	1:A:411:PHE:HE2	1.82	0.42
1:A:1017:ILE:O	1:A:1023:ASN:HA	2.19	0.42
3:C:333:ASP:OD1	3:C:333:ASP:N	2.50	0.42
19:3:678:VAL:HB	19:3:687:SER:HB3	2.00	0.42
25:J:337:MET:HE3	25:J:346:TRP:CH2	2.49	0.42
1:A:404:LEU:HD23	1:A:404:LEU:HA	1.82	0.42
1:A:1320:LYS:NZ	1:A:1325:LEU:O	2.37	0.42
1:A:1678:ARG:HA	1:A:1678:ARG:HD2	1.80	0.42
1:A:1954:LEU:HA	1:A:1954:LEU:HD23	1.84	0.42
3:C:140:HIS:CD2	3:C:230:ASP:HB2	2.55	0.42
3:C:469:ASP:N	3:C:469:ASP:OD1	2.52	0.42
3:C:506:PRO:HA	3:C:526:THR:HA	2.01	0.42
3:C:737:PRO:HB3	3:C:775:ARG:HB2	2.01	0.42
5:E:321:TYR:OH	5:E:356:ILE:HG23	2.19	0.42
17:1:551:LEU:HA	17:1:551:LEU:HD23	1.87	0.42
17:1:572:HIS:HB2	17:1:612:THR:HG23	2.01	0.42
17:1:1206:ASP:N	17:1:1206:ASP:OD1	2.50	0.42
25:J:337:MET:HE3	25:J:346:TRP:CD2	2.54	0.42
25:J:358:GLU:CG	25:J:361:ARG:HD3	2.46	0.42
26:P:222:LYS:HA	26:P:222:LYS:HD2	1.89	0.42
27:R:147:THR:HG22	27:R:151:LEU:HD23	2.01	0.42
27:R:464:GLU:O	27:R:468:LYS:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:M:279:HIS:CE1	36:M:298:VAL:HB	2.55	0.42
40:0:98:GLN:H	40:0:98:GLN:HG2	1.54	0.42
3:C:454:THR:CG2	3:C:578:ARG:HG3	2.49	0.42
4:D:445:VAL:O	4:D:688:THR:CA	2.67	0.42
5:E:62:LEU:HG	5:E:351:LEU:HB2	2.01	0.42
5:E:174:GLY:O	5:E:192:ASN:CA	2.67	0.42
13:F:26:A:H2'	13:F:27:G:O4'	2.20	0.42
17:1:1125:PRO:O	17:1:1129:LEU:HB2	2.19	0.42
29:X:275:ILE:HG21	29:X:306:PHE:CE2	2.55	0.42
29:X:285:ARG:NH1	29:X:299:CYS:O	2.52	0.42
32:9:62:ASP:OD1	32:9:63:LEU:N	2.53	0.42
39:8:115:ASN:OD1	39:8:116:ILE:N	2.53	0.42
42:K:51:GLU:HG3	42:K:52:TYR:N	2.35	0.42
42:K:83:ASN:O	42:K:86:PRO:HD2	2.20	0.42
3:C:785:ARG:HH11	3:C:785:ARG:HD2	1.68	0.42
4:D:1661:VAL:O	4:D:1702:CYS:HA	2.19	0.42
18:2:710:GLU:OE2	19:3:1057:ARG:NH2	2.53	0.42
19:3:429:ARG:NH2	19:3:429:ARG:CG	2.73	0.42
25:J:274:ARG:NE	27:R:229:VAL:CG2	2.82	0.42
29:X:221:LYS:O	29:X:223:LYS:HG3	2.19	0.42
38:V:461:LEU:HD13	38:V:461:LEU:HA	1.88	0.42
1:A:1425:LYS:HD2	1:A:1425:LYS:O	2.19	0.42
1:A:1580:HIS:O	1:A:1584:LYS:HD3	2.20	0.42
1:A:2112:LYS:HE2	1:A:2112:LYS:HB3	1.67	0.42
3:C:190:LEU:O	3:C:197:SER:HA	2.19	0.42
3:C:510:LEU:HB2	3:C:564:THR:HG23	2.01	0.42
4:D:1582:ALA:C	4:D:1584:ILE:N	2.72	0.42
17:1:721:ILE:HG12	17:1:757:MET:HA	2.02	0.42
19:3:520:TYR:CE1	19:3:522:ASP:HB2	2.55	0.42
19:3:601:ARG:NH2	19:3:621:PRO:HD3	2.35	0.42
19:3:610:VAL:O	19:3:610:VAL:HG23	2.20	0.42
21:5:110:LEU:HA	21:5:110:LEU:HD13	1.87	0.42
25:J:248:TYR:CE2	25:J:264:ILE:HG12	2.54	0.42
25:J:421:LYS:O	25:J:424:GLU:HB3	2.20	0.42
30:Y:7:VAL:CG2	30:Y:108:ARG:HB3	2.49	0.42
30:Y:117:ALA:CB	31:Z:494:TYR:CE2	3.00	0.42
41:I:48:LEU:HD12	41:I:48:LEU:HA	1.89	0.42
42:K:50:TYR:CE1	42:K:84:LEU:HA	2.55	0.42
42:K:127:PRO:CG	42:K:131:SER:HB3	2.48	0.42
1:A:795:LEU:HD23	1:A:795:LEU:HA	1.89	0.42
1:A:2111:LEU:HD21	1:A:2225:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:916:ILE:HD13	3:C:928:HIS:HB3	2.02	0.42
13:F:6:G:H1'	14:G:15:C:O2	2.20	0.42
17:1:1114:VAL:O	17:1:1118:ILE:HG12	2.20	0.42
19:3:532:ARG:HE	19:3:532:ARG:HB2	1.68	0.42
32:9:276:VAL:CB	32:9:297:CYS:C	2.89	0.42
42:K:18:GLN:O	42:K:18:GLN:NE2	2.50	0.42
42:K:126:SER:HA	42:K:127:PRO:HD3	1.80	0.42
1:A:137:GLU:O	1:A:141:ILE:HG13	2.20	0.41
1:A:1501:LEU:HD22	1:A:1753:LEU:CD1	2.49	0.41
1:A:1782:ASP:N	1:A:1782:ASP:OD1	2.52	0.41
1:A:2125:ALA:O	1:A:2150:GLN:NE2	2.51	0.41
1:A:2310:ARG:CD	1:A:2313:HIS:CG	3.02	0.41
3:C:607:LEU:HD23	3:C:607:LEU:HA	1.86	0.41
3:C:799:GLU:HG3	3:C:802:HIS:H	1.85	0.41
4:D:148:LEU:HD23	4:D:152:GLU:HB2	2.02	0.41
17:1:505:LYS:HE3	17:1:505:LYS:HB3	1.87	0.41
27:R:388:ILE:HD13	29:X:350:TYR:CD1	2.55	0.41
36:M:131:GLN:O	36:M:135:GLU:HG2	2.20	0.41
38:V:469:PHE:CD1	38:V:469:PHE:C	2.93	0.41
38:V:530:LYS:HG2	38:V:567:CYS:SG	2.60	0.41
41:I:27:TYR:HE2	42:K:36:VAL:HG22	1.85	0.41
42:K:30:GLN:O	42:K:34:GLU:HG3	2.20	0.41
42:K:127:PRO:HB2	42:K:131:SER:HB3	2.02	0.41
1:A:78:ASN:HB3	1:A:80:LYS:HG2	2.01	0.41
1:A:977:LEU:CB	1:A:1175:VAL:HG22	2.48	0.41
1:A:1554:GLN:HG3	1:A:1561:PHE:CE1	2.55	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
4:D:1589:PHE:CB	4:D:1642:GLN:CB	2.98	0.41
47:F:207:G5J:O1B	41:I:39:TYR:OH	2.27	0.41
17:1:793:LYS:HG3	17:1:839:GLU:HG3	2.02	0.41
17:1:1133:MET:HG2	17:1:1172:LEU:HD22	2.02	0.41
19:3:47:THR:HG21	19:3:49:LYS:CG	2.44	0.41
19:3:628:LEU:O	36:M:309:PRO:HG3	2.20	0.41
19:3:988:ASN:HB2	19:3:1004:ASP:OD1	2.21	0.41
19:3:1099:GLU:HG3	19:3:1121:THR:HG21	2.01	0.41
25:J:423:GLU:HA	25:J:426:GLN:HB3	2.02	0.41
29:X:270:LEU:CB	29:X:271:PRO:HD2	2.47	0.41
1:A:769:LYS:HB3	1:A:1249:MET:HG2	2.01	0.41
1:A:2073:TRP:CD1	1:A:2073:TRP:O	2.73	0.41
1:A:2121:ARG:HD2	1:A:2121:ARG:HA	1.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:491:HIS:CB	3:C:551:LEU:HD22	2.50	0.41
5:E:62:LEU:HD12	5:E:351:LEU:HB2	2.02	0.41
19:3:430:GLY:HA3	19:3:431:PRO:HD2	1.84	0.41
19:3:503:THR:OG1	19:3:504:PRO:HD2	2.21	0.41
25:J:364:THR:O	25:J:367:GLU:HB3	2.20	0.41
36:M:250:GLU:OE2	40:0:88:LYS:HG2	2.20	0.41
41:I:40:THR:CG2	42:K:79:GLY:HA2	2.50	0.41
4:D:148:LEU:HD22	4:D:152:GLU:CB	2.49	0.41
4:D:722:LEU:HA	4:D:809:LEU:O	2.19	0.41
4:D:1580:CYS:O	4:D:1585:GLN:O	2.38	0.41
5:E:132:THR:HG21	5:E:146:ARG:CD	2.41	0.41
5:E:177:LYS:C	5:E:178:LEU:HD23	2.41	0.41
5:E:237:SER:HB2	5:E:255:MET:CG	2.51	0.41
13:F:6:G:N7	41:I:31:ARG:CZ	2.84	0.41
17:1:1014:LYS:HD2	40:0:91:LEU:HD21	2.02	0.41
19:3:1164:ARG:C	19:3:1170:VAL:HG22	2.41	0.41
24:L:12:ARG:HH21	24:L:12:ARG:HD3	1.75	0.41
30:Y:55:VAL:HG22	31:Z:589:ARG:CZ	2.50	0.41
3:C:130:ARG:HE	3:C:435:VAL:HA	1.84	0.41
3:C:311:SER:HB3	3:C:316:ILE:HB	2.03	0.41
3:C:676:ALA:HB1	3:C:814:ARG:HH21	1.86	0.41
5:E:147:LEU:N	5:E:147:LEU:HD23	2.35	0.41
17:1:1118:ILE:HG23	40:0:13:VAL:HG13	2.02	0.41
19:3:246:SER:O	19:3:260:ASN:ND2	2.53	0.41
19:3:642:ILE:HG22	19:3:663:LEU:HD11	2.02	0.41
21:5:27:PRO:HG3	21:5:85:ARG:CD	2.44	0.41
25:J:338:GLU:O	25:J:340:GLN:OE1	2.38	0.41
27:R:391:VAL:CG2	29:X:347:GLN:HB3	2.50	0.41
39:8:24:LEU:HD23	39:8:24:LEU:HA	1.88	0.41
1:A:384:VAL:O	3:C:354:ARG:NH2	2.50	0.41
1:A:413:LEU:C	1:A:413:LEU:HD12	2.41	0.41
1:A:537:LYS:HE2	1:A:537:LYS:HB2	1.86	0.41
3:C:781:ASP:HB2	3:C:943:LEU:HD21	2.02	0.41
4:D:140:LEU:HD23	4:D:140:LEU:C	2.40	0.41
15:H:17:A:H1'	22:6:102:ARG:HH12	1.86	0.41
17:1:929:LEU:HA	17:1:929:LEU:HD23	1.84	0.41
19:3:694:LEU:HD12	19:3:694:LEU:O	2.20	0.41
19:3:745:PHE:HB2	19:3:755:VAL:HG23	2.03	0.41
25:J:313:TRP:CE3	25:J:336:TRP:CZ2	3.08	0.41
27:R:387:ASP:H	29:X:351:GLU:CB	2.29	0.41
30:Y:37:TRP:CB	30:Y:112:VAL:HG22	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:I:139:LYS:HD2	42:K:86:PRO:HB3	2.03	0.41
42:K:49:ASN:O	42:K:53:LEU:HG	2.20	0.41
42:K:120:THR:O	42:K:124:HIS:CD2	2.73	0.41
1:A:1665:GLN:HG3	1:A:1702:LEU:HD21	2.02	0.41
3:C:412:ILE:HD13	3:C:412:ILE:HA	1.87	0.41
3:C:836:VAL:HG22	3:C:897:SER:HB3	2.02	0.41
4:D:128:PRO:HG2	4:D:131:ILE:HD12	2.02	0.41
13:F:45:A:OP2	14:G:3:A:O2'	2.34	0.41
14:G:207:A:O4'	22:6:102:ARG:HG3	2.21	0.41
15:H:79:U:C3'	15:H:80:U:H5'	2.51	0.41
17:1:1200:TYR:CD1	17:1:1239:VAL:O	2.74	0.41
17:1:1245:ARG:O	17:1:1249:TYR:HD1	2.04	0.41
19:3:834:LEU:O	19:3:837:GLU:HB3	2.21	0.41
19:3:1052:ASN:HB3	19:3:1096:HIS:HA	2.03	0.41
22:6:29:LYS:HA	22:6:35:SER:O	2.20	0.41
25:J:440:LEU:HG	25:J:445:LYS:HE2	2.02	0.41
38:V:517:LEU:HD23	38:V:517:LEU:HA	1.90	0.41
3:C:85:ASP:HB3	28:T:238:LEU:HG	2.03	0.41
17:1:619:ASN:ND2	17:1:624:VAL:HG21	2.35	0.41
19:3:138:GLN:HA	19:3:161:HIS:ND1	2.35	0.41
19:3:379:LEU:HD21	19:3:384:THR:HA	2.03	0.41
19:3:574:LEU:HA	19:3:574:LEU:HD23	1.78	0.41
21:5:83:CYS:O	21:5:83:CYS:SG	2.79	0.41
25:J:252:GLU:OE1	25:J:252:GLU:HA	2.21	0.41
25:J:337:MET:HE3	25:J:346:TRP:CE3	2.54	0.41
26:P:206:LYS:HD2	26:P:206:LYS:N	2.35	0.41
29:X:223:LYS:HG3	29:X:223:LYS:H	1.63	0.41
1:A:193:LEU:O	1:A:195:LEU:HD12	2.20	0.41
1:A:259:ASP:OD1	1:A:259:ASP:N	2.48	0.41
1:A:265:THR:HG23	1:A:327:VAL:CG2	2.35	0.41
1:A:456:LEU:HD23	1:A:456:LEU:HA	1.89	0.41
1:A:534:GLU:OE2	13:F:11:A:H5'	2.20	0.41
1:A:1112:ARG:HH11	1:A:1112:ARG:HD3	1.71	0.41
1:A:1425:LYS:HB3	27:R:416:LYS:HA	2.03	0.41
3:C:205:THR:HB	3:C:215:VAL:HG22	2.02	0.41
5:E:90:ILE:HB	5:E:105:LEU:HB2	2.03	0.41
5:E:246:GLU:HB2	5:E:248:SER:HG	1.84	0.41
5:E:274:VAL:C	5:E:275:LYS:HG3	2.39	0.41
14:G:211:U:C2'	14:G:213:C:OP2	2.69	0.41
17:1:157:ARG:NH1	21:5:103:THR:OG1	2.54	0.41
17:1:1167:TYR:CZ	18:2:581:LYS:HE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:1194:SER:HB2	19:3:1199:ARG:O	2.20	0.41
25:J:336:TRP:C	25:J:338:GLU:N	2.75	0.41
25:J:423:GLU:HB2	25:J:432:VAL:HG22	2.03	0.41
27:R:280:ILE:CG2	32:9:221:LEU:HD22	2.50	0.41
38:V:604:LYS:HE3	38:V:604:LYS:HB3	1.86	0.41
39:8:82:SER:HB3	39:8:106:TRP:CH2	2.56	0.41
41:I:98:GLN:HA	41:I:101:ARG:HD3	2.01	0.41
42:K:50:TYR:HE1	42:K:84:LEU:HA	1.86	0.41
1:A:829:PRO:HA	21:5:86:TYR:CE2	2.56	0.41
1:A:1655:THR:OG1	1:A:1656:THR:N	2.54	0.41
4:D:117:LEU:HA	4:D:120:ILE:HG22	2.03	0.41
4:D:121:GLN:HG2	4:D:132:LEU:CD2	2.48	0.41
4:D:144:LYS:HE2	4:D:179:ILE:CG2	2.51	0.41
14:G:197:U:H4'	24:L:12:ARG:CD	2.51	0.41
17:1:476:ASP:N	17:1:476:ASP:OD1	2.51	0.41
19:3:510:LEU:HG	19:3:510:LEU:O	2.20	0.41
19:3:999:ARG:NH1	19:3:1041:TYR:O	2.54	0.41
21:5:87:LEU:HA	21:5:87:LEU:HD12	1.86	0.41
22:6:42:LEU:HD11	22:6:68:ASP:HB3	2.03	0.41
24:L:72:LEU:HA	24:L:72:LEU:HD23	1.85	0.41
25:J:270:ASP:OD1	27:R:223:PRO:HD2	2.17	0.41
32:9:96:ASN:HD21	32:9:109:VAL:HG22	1.86	0.41
32:9:330:ILE:O	32:9:381:PHE:CB	2.69	0.41
36:M:288:GLN:O	36:M:291:ARG:HB2	2.21	0.41
1:A:957:GLN:OE1	1:A:957:GLN:HA	2.21	0.40
1:A:1303:LEU:HD12	1:A:1311:PHE:CE1	2.56	0.40
1:A:1753:LEU:HD23	1:A:1753:LEU:HA	1.87	0.40
1:A:2259:VAL:HG22	1:A:2260:GLN:H	1.86	0.40
4:D:686:GLU:O	4:D:866:GLU:HA	2.21	0.40
4:D:861:TYR:O	19:3:599:GLU:HG3	2.22	0.40
17:1:397:ARG:HD3	17:1:398:PRO:HD2	2.04	0.40
17:1:648:LEU:HA	17:1:648:LEU:HD12	1.90	0.40
17:1:844:VAL:HG11	17:1:848:GLU:HG2	2.03	0.40
17:1:1002:ASN:HD22	17:1:1002:ASN:HA	1.50	0.40
25:J:333:PHE:CB	25:J:349:TYR:CE1	3.04	0.40
27:R:137:GLU:HA	27:R:140:ILE:HG12	2.03	0.40
27:R:237:MET:CE	27:R:237:MET:N	2.75	0.40
28:T:468:CYS:HA	28:T:478:LEU:O	2.21	0.40
29:X:278:GLN:NE2	29:X:291:ASP:OD2	2.54	0.40
30:Y:125:ASP:O	30:Y:129:ARG:HG3	2.20	0.40
42:K:13:ARG:HD3	42:K:13:ARG:HA	1.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:200:PHE:HD1	3:C:200:PHE:HA	1.80	0.40
3:C:201:ASN:HB3	3:C:549:TRP:CE3	2.56	0.40
5:E:248:SER:HB2	5:E:249:TYR:CE1	2.53	0.40
13:F:2:U:O2'	42:K:43:PHE:CE1	2.73	0.40
13:F:33:C:H2'	13:F:34:C:O4'	2.21	0.40
17:1:403:GLU:O	17:1:406:ALA:HB3	2.20	0.40
17:1:997:LEU:HD12	17:1:997:LEU:HA	1.81	0.40
19:3:133:SER:HB2	19:3:139:LYS:HG2	2.02	0.40
19:3:500:LEU:HB2	19:3:525:ARG:HH11	1.87	0.40
19:3:673:VAL:HG12	19:3:693:TYR:HA	2.03	0.40
19:3:981:CYS:SG	19:3:981:CYS:O	2.79	0.40
19:3:1129:LEU:HD23	19:3:1129:LEU:HA	1.93	0.40
1:A:79:ARG:HH11	1:A:79:ARG:HG2	1.87	0.40
1:A:767:VAL:HG21	2:B:39:C:C2	2.56	0.40
1:A:1157:ILE:HD13	1:A:1157:ILE:HA	1.92	0.40
1:A:1256:PHE:CE2	1:A:1303:LEU:HD21	2.56	0.40
1:A:1501:LEU:HD22	1:A:1753:LEU:HD11	2.02	0.40
1:A:2320:LEU:HD21	1:A:2322:GLU:CD	2.41	0.40
3:C:461:LEU:HD23	3:C:461:LEU:HA	1.91	0.40
4:D:448:PRO:O	4:D:686:GLU:HA	2.21	0.40
4:D:577:LYS:O	4:D:581:SER:N	2.54	0.40
5:E:178:LEU:CD2	5:E:208:ILE:HD11	2.51	0.40
5:E:307:ARG:HB3	5:E:326:HIS:O	2.22	0.40
13:F:51:G:H4'	13:F:52:A:OP1	2.20	0.40
17:1:86:ALA:HB3	17:1:91:LEU:HD11	2.03	0.40
17:1:860:GLU:HG2	30:Y:26:VAL:HG11	2.03	0.40
17:1:1120:ALA:HB2	17:1:1128:VAL:HG21	2.02	0.40
25:J:228:ARG:HG3	25:J:228:ARG:HH11	1.86	0.40
29:X:329:ILE:HB	29:X:349:TYR:CE1	2.57	0.40
32:9:111:THR:HG22	32:9:112:ASN:N	2.36	0.40
39:8:110:LEU:HD23	39:8:110:LEU:HA	1.91	0.40
41:I:38:VAL:HA	42:K:42:ASN:HD21	1.86	0.40
3:C:780:CYS:SG	3:C:780:CYS:O	2.79	0.40
4:D:991:TYR:O	4:D:1090:ARG:HG2	2.22	0.40
25:J:367:GLU:O	25:J:371:LEU:HG	2.21	0.40
25:J:419:PHE:CE2	25:J:435:ILE:HG21	2.56	0.40
27:R:280:ILE:CB	32:9:221:LEU:HD22	2.48	0.40
32:9:39:PHE:HB3	32:9:159:GLN:OE1	2.21	0.40
32:9:83:LEU:HD12	32:9:84:ASP:N	2.36	0.40
38:V:603:LEU:HD12	38:V:603:LEU:HA	1.79	0.40
42:K:24:PHE:HD2	42:K:61:LEU:HD11	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:K:123:MET:O	42:K:126:SER:HB3	2.20	0.40
1:A:221:ASN:OD1	1:A:222:GLY:N	2.55	0.40
1:A:686:ARG:NH1	15:H:3:G:H4'	2.37	0.40
1:A:686:ARG:HE	1:A:710:LEU:HD13	1.86	0.40
3:C:476:CYS:HB3	3:C:565:ILE:HB	2.03	0.40
3:C:738:ASP:OD1	3:C:738:ASP:N	2.33	0.40
4:D:128:PRO:CG	4:D:131:ILE:HD12	2.51	0.40
17:1:157:ARG:O	17:1:161:LEU:HB2	2.22	0.40
17:1:675:MET:HB2	17:1:679:ILE:CG2	2.51	0.40
17:1:1045:ARG:NH1	40:0:24:ARG:HG3	2.35	0.40
19:3:137:LYS:O	19:3:137:LYS:CG	2.70	0.40
19:3:668:GLY:HA3	19:3:699:VAL:HG23	2.03	0.40
19:3:1058:LEU:HA	19:3:1059:PRO:HD3	1.98	0.40
25:J:433:ARG:HD2	25:J:433:ARG:HA	1.87	0.40
26:P:212:ASN:H	28:T:457:GLY:HA3	1.87	0.40
41:I:31:ARG:NH1	41:I:31:ARG:CG	2.80	0.40
41:I:129:GLU:HB2	41:I:133:LYS:HZ3	1.83	0.40
42:K:149:SER:HA	42:K:160:ALA:HB3	2.03	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	2213/2335 (95%)	2146 (97%)	66 (3%)	1 (0%)	100	100
3	C	900/972 (93%)	862 (96%)	38 (4%)	0	100	100
4	D	1799/2136 (84%)	1710 (95%)	84 (5%)	5 (0%)	37	66
5	E	297/357 (83%)	278 (94%)	19 (6%)	0	100	100
6	a	77/126 (61%)	76 (99%)	1 (1%)	0	100	100
6	h	76/126 (60%)	74 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	b	80/240 (33%)	78 (98%)	2 (2%)	0	100	100
7	i	84/240 (35%)	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%)	68 (94%)	4 (6%)	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	v	115/230 (50%)	113 (98%)	2 (2%)	0	100	100
17	1	977/1304 (75%)	961 (98%)	16 (2%)	0	100	100
18	2	206/895 (23%)	198 (96%)	8 (4%)	0	100	100
19	3	1184/1217 (97%)	1136 (96%)	48 (4%)	0	100	100
20	4	76/424 (18%)	71 (93%)	5 (7%)	0	100	100
21	5	107/125 (86%)	104 (97%)	3 (3%)	0	100	100
22	6	103/110 (94%)	98 (95%)	5 (5%)	0	100	100
23	7	79/86 (92%)	78 (99%)	1 (1%)	0	100	100
24	L	99/802 (12%)	93 (94%)	6 (6%)	0	100	100
25	J	483/848 (57%)	447 (92%)	36 (8%)	0	100	100
26	P	42/229 (18%)	37 (88%)	5 (12%)	0	100	100
27	R	229/536 (43%)	219 (96%)	10 (4%)	0	100	100
28	T	318/514 (62%)	310 (98%)	8 (2%)	0	100	100
29	X	154/396 (39%)	137 (89%)	16 (10%)	1 (1%)	22	52
30	Y	138/322 (43%)	135 (98%)	3 (2%)	0	100	100
31	Z	138/619 (22%)	137 (99%)	1 (1%)	0	100	100
32	9	401/520 (77%)	382 (95%)	18 (4%)	1 (0%)	44	73
33	z	175/472 (37%)	169 (97%)	6 (3%)	0	100	100
34	x	575/1041 (55%)	554 (96%)	21 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
35	y	11/476 (2%)	11 (100%)	0	0	100 100
36	M	185/343 (54%)	172 (93%)	13 (7%)	0	100 100
37	U	24/2752 (1%)	24 (100%)	0	0	100 100
38	V	464/908 (51%)	457 (98%)	7 (2%)	0	100 100
39	8	124/904 (14%)	124 (100%)	0	0	100 100
40	0	98/101 (97%)	98 (100%)	0	0	100 100
41	I	124/367 (34%)	120 (97%)	4 (3%)	0	100 100
42	K	186/198 (94%)	183 (98%)	2 (1%)	1 (0%)	25 56
All	All	13111/24253 (54%)	12617 (96%)	485 (4%)	9 (0%)	50 77

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	1584	ILE
4	D	1864	GLU
1	A	1092	ILE
29	X	263	PRO
42	K	127	PRO
4	D	1859	PRO
32	9	348	LYS
4	D	745	LYS
4	D	1583	ASP

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	1979/2108 (94%)	1924 (97%)	55 (3%)	38 73
3	C	798/866 (92%)	787 (99%)	11 (1%)	62 86
4	D	76/1908 (4%)	62 (82%)	14 (18%)	1 4
5	E	255/300 (85%)	245 (96%)	10 (4%)	27 62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	v	104/199 (52%)	99 (95%)	5 (5%)	21 54
17	1	854/1103 (77%)	820 (96%)	34 (4%)	27 61
18	2	163/776 (21%)	158 (97%)	5 (3%)	35 70
19	3	1031/1050 (98%)	997 (97%)	34 (3%)	33 68
21	5	97/109 (89%)	96 (99%)	1 (1%)	73 91
22	6	90/95 (95%)	87 (97%)	3 (3%)	33 68
23	7	72/77 (94%)	72 (100%)	0	100 100
24	L	87/709 (12%)	86 (99%)	1 (1%)	70 90
25	J	203/751 (27%)	197 (97%)	6 (3%)	36 71
26	P	42/203 (21%)	41 (98%)	1 (2%)	44 76
27	R	206/459 (45%)	194 (94%)	12 (6%)	17 46
28	T	273/441 (62%)	268 (98%)	5 (2%)	54 82
29	X	134/349 (38%)	127 (95%)	7 (5%)	19 50
30	Y	117/291 (40%)	113 (97%)	4 (3%)	32 67
31	Z	110/545 (20%)	108 (98%)	2 (2%)	54 82
32	9	195/456 (43%)	190 (97%)	5 (3%)	41 74
33	z	152/416 (36%)	152 (100%)	0	100 100
34	x	14/897 (2%)	13 (93%)	1 (7%)	12 36
35	y	11/397 (3%)	11 (100%)	0	100 100
36	M	168/294 (57%)	165 (98%)	3 (2%)	54 82
37	U	21/2432 (1%)	20 (95%)	1 (5%)	21 54
38	V	193/838 (23%)	190 (98%)	3 (2%)	58 84
39	8	111/831 (13%)	111 (100%)	0	100 100
40	0	86/87 (99%)	84 (98%)	2 (2%)	45 77
41	I	112/326 (34%)	108 (96%)	4 (4%)	30 65
42	K	119/171 (70%)	108 (91%)	11 (9%)	7 24
All	All	7873/19484 (40%)	7633 (97%)	240 (3%)	37 71

All (240) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	MET
1	A	203	VAL

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Mol	Chain	Res	Type
1	A	204	LEU
1	A	211	GLN
1	A	214	ARG
1	A	227	ARG
1	A	258	PHE
1	A	327	VAL
1	A	419	ARG
1	A	420	ARG
1	A	422	LEU
1	A	426	LEU
1	A	470	ARG
1	A	546	LEU
1	A	606	LYS
1	A	635	ARG
1	A	642	ARG
1	A	658	ARG
1	A	683	LEU
1	A	779	LEU
1	A	818	GLU
1	A	873	ASN
1	A	977	LEU
1	A	978	GLU
1	A	1017	ILE
1	A	1018	ASN
1	A	1022	MET
1	A	1131	LYS
1	A	1231	ARG
1	A	1403	LEU
1	A	1425	LYS
1	A	1499	GLU
1	A	1526	LEU
1	A	1553	VAL
1	A	1639	VAL
1	A	1693	SER
1	A	1745	GLU
1	A	1753	LEU
1	A	1762	TYR
1	A	1764	SER
1	A	1840	LYS
1	A	1889	LEU
1	A	1891	LEU
1	A	1919	LEU

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Mol	Chain	Res	Type
1	A	1921	ASP
1	A	2073	TRP
1	A	2074	ARG
1	A	2087	THR
1	A	2193	VAL
1	A	2194	THR
1	A	2254	SER
1	A	2259	VAL
1	A	2273	VAL
1	A	2329	ASP
1	A	2333	LEU
3	C	148	CYS
3	C	308	CYS
3	C	543	ARG
3	C	551	LEU
3	C	561	LYS
3	C	683	ASN
3	C	714	LEU
3	C	738	ASP
3	C	767	VAL
3	C	780	CYS
3	C	934	MET
4	D	102	TYR
4	D	103	LYS
4	D	108	GLU
4	D	110	ARG
4	D	126	ASP
4	D	148	LEU
4	D	149	ARG
4	D	153	ARG
4	D	154	ARG
4	D	157	ILE
4	D	161	LEU
4	D	167	THR
4	D	992	TYR
4	D	1090	ARG
5	E	62	LEU
5	E	74	PHE
5	E	102	TYR
5	E	152	SER
5	E	156	SER
5	E	194	TYR

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Mol	Chain	Res	Type
5	E	229	TYR
5	E	248	SER
5	E	289	LEU
5	E	290	ARG
16	v	1	MET
16	v	5	ARG
16	v	50	ARG
16	v	197	ARG
16	v	206	ARG
17	1	120	LYS
17	1	412	TYR
17	1	531	LEU
17	1	562	LYS
17	1	563	LEU
17	1	564	ASP
17	1	614	ARG
17	1	651	VAL
17	1	675	MET
17	1	677	CYS
17	1	680	LEU
17	1	721	ILE
17	1	997	LEU
17	1	1002	ASN
17	1	1024	LEU
17	1	1026	ASN
17	1	1038	LEU
17	1	1050	VAL
17	1	1058	ILE
17	1	1112	THR
17	1	1127	THR
17	1	1128	VAL
17	1	1180	ARG
17	1	1182	LEU
17	1	1184	HIS
17	1	1226	VAL
17	1	1227	ILE
17	1	1239	VAL
17	1	1260	LYS
17	1	1261	VAL
17	1	1264	VAL
17	1	1277	GLN
17	1	1301	ASP

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Mol	Chain	Res	Type
17	1	1303	ILE
18	2	498	VAL
18	2	561	MET
18	2	577	LYS
18	2	587	HIS
18	2	599	THR
19	3	86	ARG
19	3	131	MET
19	3	135	ILE
19	3	136	GLU
19	3	137	LYS
19	3	138	GLN
19	3	171	VAL
19	3	184	CYS
19	3	187	MET
19	3	295	THR
19	3	319	GLU
19	3	321	MET
19	3	322	VAL
19	3	425	VAL
19	3	429	ARG
19	3	607	VAL
19	3	609	LEU
19	3	610	VAL
19	3	612	ASN
19	3	614	VAL
19	3	686	LEU
19	3	690	ARG
19	3	691	THR
19	3	943	THR
19	3	980	LYS
19	3	981	CYS
19	3	982	GLU
19	3	1007	GLU
19	3	1013	ARG
19	3	1064	ASP
19	3	1165	SER
19	3	1166	TYR
19	3	1209	GLU
19	3	1214	ARG
21	5	85	ARG
22	6	25	LYS

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Mol	Chain	Res	Type
22	6	35	SER
22	6	95	LYS
24	L	77	LEU
25	J	236	ARG
25	J	245	TRP
25	J	247	LYS
25	J	337	MET
25	J	338	GLU
25	J	360	ASP
26	P	186	ARG
27	R	237	MET
27	R	297	LYS
27	R	323	LYS
27	R	332	ARG
27	R	384	GLU
27	R	386	ARG
27	R	388	ILE
27	R	389	SER
27	R	403	ASN
27	R	406	GLN
27	R	410	ARG
27	R	427	ASP
28	T	220	VAL
28	T	325	THR
28	T	384	HIS
28	T	418	THR
28	T	456	PRO
29	X	239	PHE
29	X	242	VAL
29	X	264	PHE
29	X	268	GLU
29	X	269	VAL
29	X	270	LEU
29	X	348	ARG
30	Y	13	LEU
30	Y	66	ASN
30	Y	80	CYS
30	Y	116	ARG
31	Z	575	ARG
31	Z	583	ARG
32	9	3	LYS
32	9	4	ARG

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Mol	Chain	Res	Type
32	9	8	LYS
32	9	35	ARG
32	9	224	THR
34	x	1028	LYS
36	M	103	THR
36	M	157	ASN
36	M	226	TYR
37	U	20	GLN
38	V	467	LEU
38	V	469	PHE
38	V	471	GLU
40	0	14	ILE
40	0	100	SER
41	I	31	ARG
41	I	37	LYS
41	I	105	ARG
41	I	139	LYS
42	K	13	ARG
42	K	54	ARG
42	K	71	GLU
42	K	74	VAL
42	K	84	LEU
42	K	91	LYS
42	K	123	MET
42	K	136	LEU
42	K	139	THR
42	K	142	VAL
42	K	155	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	704	ASN
1	A	1373	GLN
3	C	683	ASN
3	C	706	GLN
3	C	807	GLN
4	D	127	GLN
5	E	101	ASN
17	1	1252	GLN
19	3	51	HIS
28	T	283	HIS

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Mol	Chain	Res	Type
28	T	285	HIS
29	X	347	GLN
30	Y	66	ASN
39	8	88	ASN
40	0	98	GLN
42	K	70	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	F	58/124 (46%)	14 (24%)	3 (5%)
14	G	62/142 (43%)	22 (35%)	5 (8%)
15	H	61/150 (40%)	14 (22%)	0
2	B	87/117 (74%)	21 (24%)	2 (2%)
All	All	268/533 (50%)	71 (26%)	10 (3%)

All (71) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	20	G
2	B	21	A
2	B	22	U
2	B	24	G
2	B	25	C
2	B	28	A
2	B	35	U
2	B	39	C
2	B	40	U
2	B	45	C
2	B	71	C
2	B	86	C
2	B	88	A
2	B	89	U
2	B	90	U
2	B	94	U
2	B	95	G
2	B	97	G
2	B	98	G
2	B	115	C
2	B	116	U
13	F	5	U

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Mol	Chain	Res	Type
13	F	6	G
13	F	15	G
13	F	18	A
13	F	24	U
13	F	25	U
13	F	27	G
13	F	32	C
13	F	33	C
13	F	39	A
13	F	46	U
13	F	47	G
13	F	50	A
13	F	52	A
14	G	-10	C
14	G	-9	G
14	G	-5	U
14	G	-3	C
14	G	1	A
14	G	3	A
14	G	15	C
14	G	17	U
14	G	19	U
14	G	196	A
14	G	203	A
14	G	207	A
14	G	208	U
14	G	210	G
14	G	211	U
14	G	214	C
14	G	216	U
14	G	217	U
14	G	218	U
14	G	219	U
14	G	220	U
14	G	222	U
15	H	2	U
15	H	3	G
15	H	8	A
15	H	10	A
15	H	13	U
15	H	14	A
15	H	18	G

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Mol	Chain	Res	Type
15	H	29	A
15	H	31	C
15	H	32	G
15	H	39	G
15	H	44	C
15	H	45	G
15	H	83	G

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	39	C
2	B	96	A
13	F	23	G
13	F	31	U
13	F	51	G
14	G	-11	U
14	G	206	C
14	G	213	C
14	G	217	U
14	G	219	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	SEP	1	129	17	8,9,10	1.07	1 (12%)	8,12,14	1.70	3 (37%)
19	TPO	3	613	19	8,10,11	0.89	0	10,14,16	1.61	2 (20%)

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	SEP	1	129	17	-	4/5/8/10	-
19	TPO	3	613	19	-	2/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	129	SEP	P-O1P	2.12	1.57	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	3	613	TPO	P-OG1-CB	-4.43	109.83	123.21
17	1	129	SEP	P-OG-CB	-2.83	110.49	118.30
19	3	613	TPO	O-C-CA	-2.22	118.95	124.78
17	1	129	SEP	O3P-P-OG	2.17	112.52	106.73
17	1	129	SEP	OG-CB-CA	2.09	110.18	108.14

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	1	129	SEP	N-CA-CB-OG
17	1	129	SEP	CB-OG-P-O1P
17	1	129	SEP	CB-OG-P-O2P
17	1	129	SEP	CB-OG-P-O3P
19	3	613	TPO	O-C-CA-CB
19	3	613	TPO	CB-OG1-P-O1P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	1	129	SEP	2	0
19	3	613	TPO	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 14 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
44	GTP	C	1500	45	26,34,34	2.33	11 (42%)	32,54,54	1.91	9 (28%)
47	G5J	F	207	13	25,35,35	0.92	1 (4%)	31,55,55	1.41	3 (9%)
43	IHP	A	3000	-	36,36,36	1.12	3 (8%)	54,60,60	1.06	3 (5%)

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
44	GTP	C	1500	45	-	4/18/38/38	0/3/3/3
47	G5J	F	207	13	-	6/21/41/41	0/3/3/3
43	IHP	A	3000	-	-	1/30/54/54	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	C	1500	GTP	C5-C6	-6.29	1.34	1.47
44	C	1500	GTP	C5-C4	-3.87	1.33	1.43
44	C	1500	GTP	C2'-C1'	-3.54	1.48	1.53
44	C	1500	GTP	O4'-C4'	-2.59	1.39	1.45
44	C	1500	GTP	C6-N1	-2.44	1.34	1.37
44	C	1500	GTP	PG-O2G	-2.37	1.45	1.54
44	C	1500	GTP	PG-O3G	-2.33	1.45	1.54
44	C	1500	GTP	C2'-C3'	-2.19	1.47	1.53
44	C	1500	GTP	O3'-C3'	-2.17	1.37	1.43
44	C	1500	GTP	O2'-C2'	-2.08	1.38	1.43
43	A	3000	IHP	P4-O34	-2.06	1.46	1.54
43	A	3000	IHP	P5-O45	-2.04	1.47	1.54
44	C	1500	GTP	PB-O2B	-2.04	1.45	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	A	3000	IHP	P1-O31	-2.01	1.47	1.54
47	F	207	G5J	C6-N1	-2.01	1.34	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	C	1500	GTP	C5-C6-N1	4.60	122.07	113.95
47	F	207	G5J	PG-O3B-PB	-4.55	117.21	132.83
44	C	1500	GTP	C2-N1-C6	-4.29	117.20	125.10
47	F	207	G5J	PB-O3A-PA	-3.93	119.34	132.83
43	A	3000	IHP	C5-C6-C1	-3.74	102.23	110.41
44	C	1500	GTP	PB-O3B-PG	-3.32	121.42	132.83
43	A	3000	IHP	C6-C1-C2	-3.22	103.37	110.41
44	C	1500	GTP	C8-N7-C5	3.18	109.05	102.99
44	C	1500	GTP	O3'-C3'-C2'	-3.01	102.10	111.82
44	C	1500	GTP	PA-O3A-PB	-2.97	122.64	132.83
44	C	1500	GTP	O6-C6-C5	-2.83	118.84	124.37
43	A	3000	IHP	O14-C4-C5	-2.43	102.96	108.69
47	F	207	G5J	C8-N7-C5	2.39	107.55	102.99
44	C	1500	GTP	O3'-C3'-C4'	-2.11	104.95	111.05
44	C	1500	GTP	O4'-C1'-C2'	-2.09	103.88	106.93

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
44	C	1500	GTP	O4'-C4'-C5'-O5'
47	F	207	G5J	C5'-O5'-PA-O3A
47	F	207	G5J	O4'-C4'-C5'-O5'
47	F	207	G5J	C3'-C4'-C5'-O5'
44	C	1500	GTP	C3'-C4'-C5'-O5'
47	F	207	G5J	C3G-O3G-PG-O1G
44	C	1500	GTP	PG-O3B-PB-O1B
47	F	207	G5J	C5'-O5'-PA-O1A
47	F	207	G5J	C3G-O3G-PG-O2G
43	A	3000	IHP	C4-O14-P4-O44
44	C	1500	GTP	PG-O3B-PB-O2B

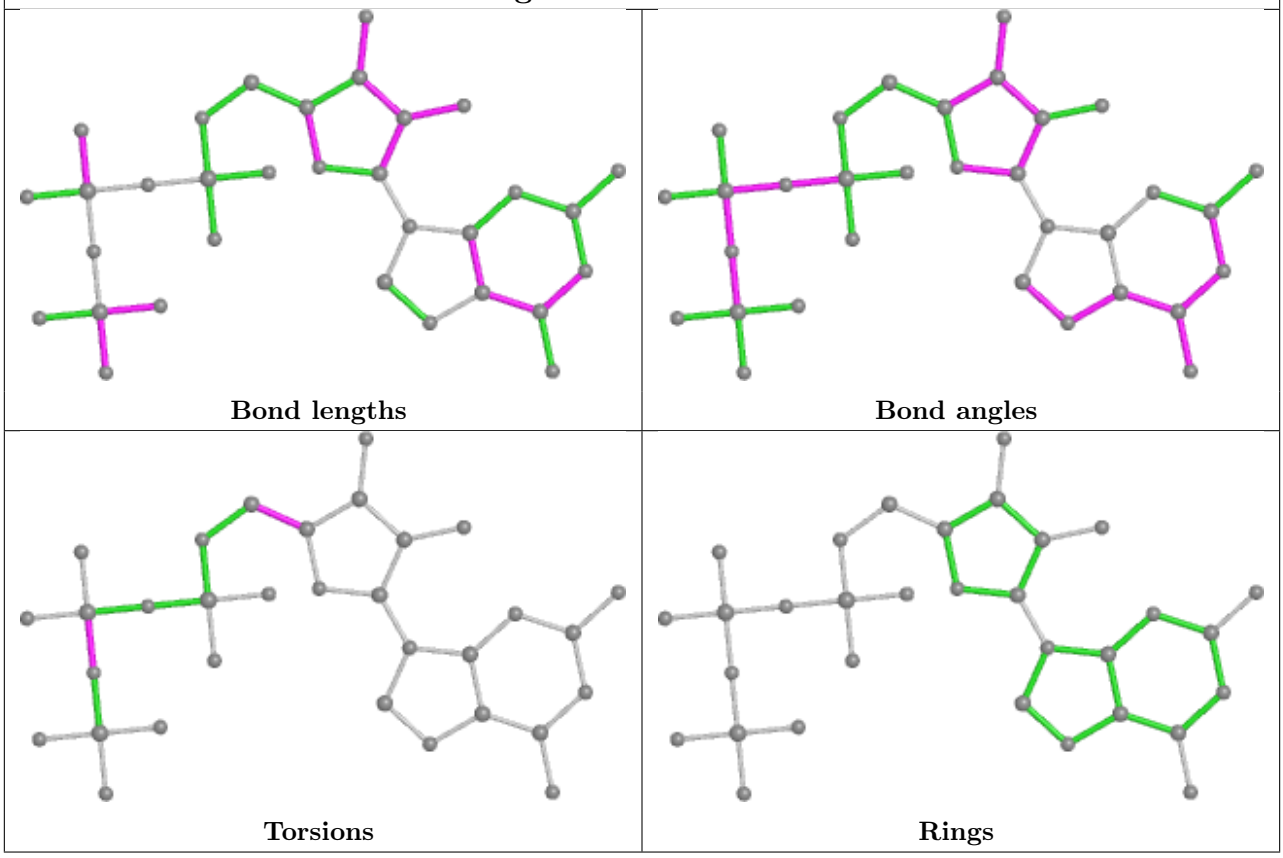
There are no ring outliers.

2 monomers are involved in 6 short contacts:

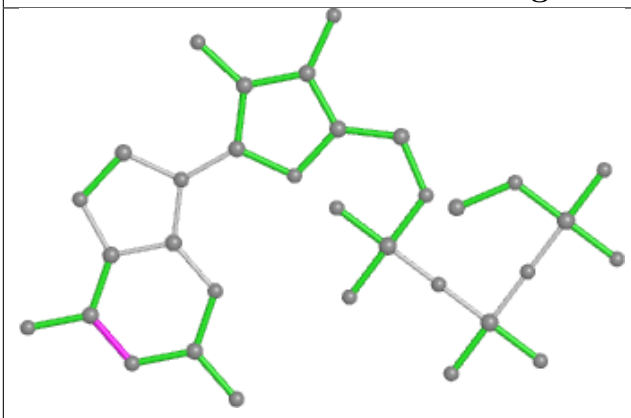
Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	C	1500	GTP	3	0
47	F	207	G5J	3	0

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

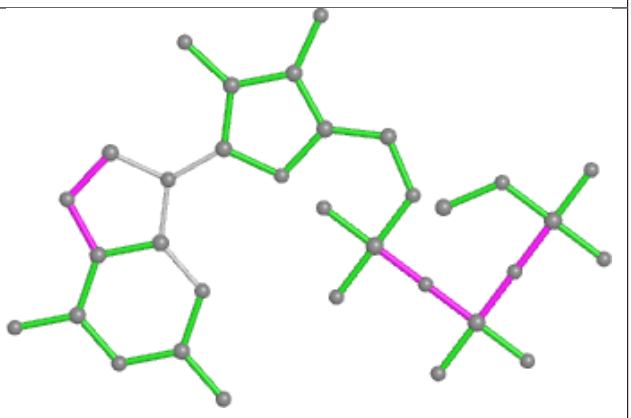
Ligand GTP C 1500



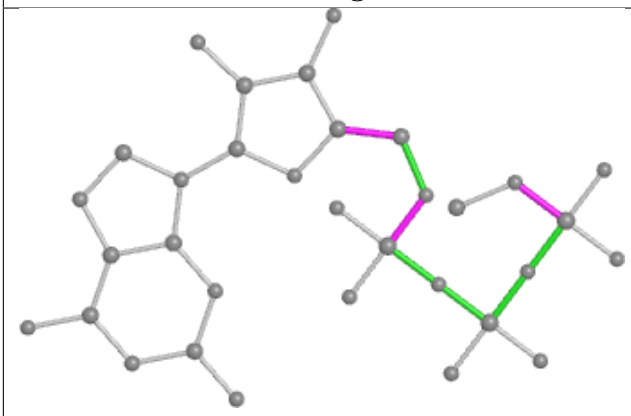
Ligand G5J F 207



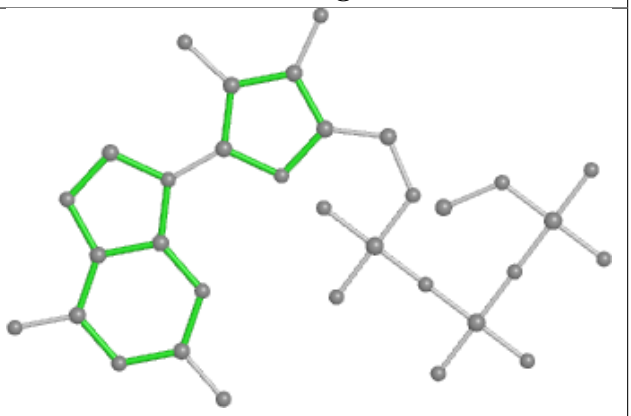
Bond lengths



Bond angles

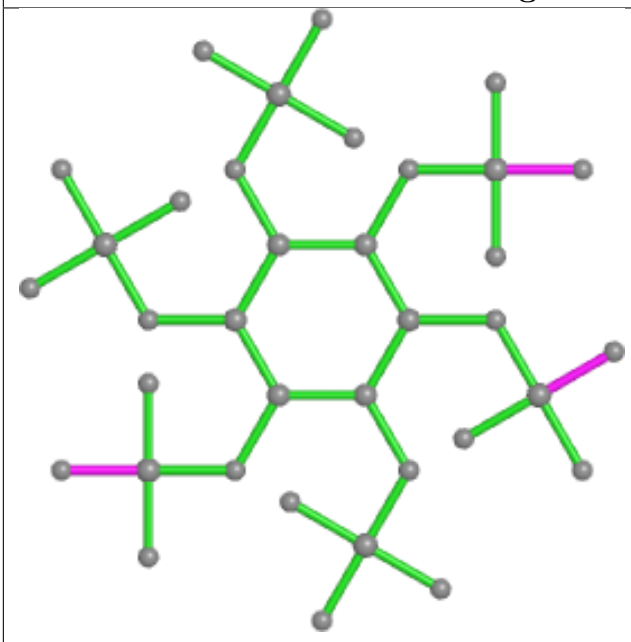


Torsions

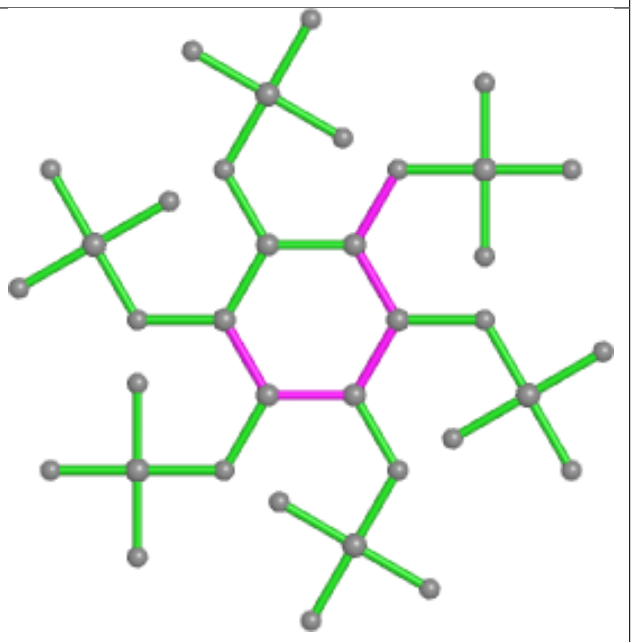


Rings

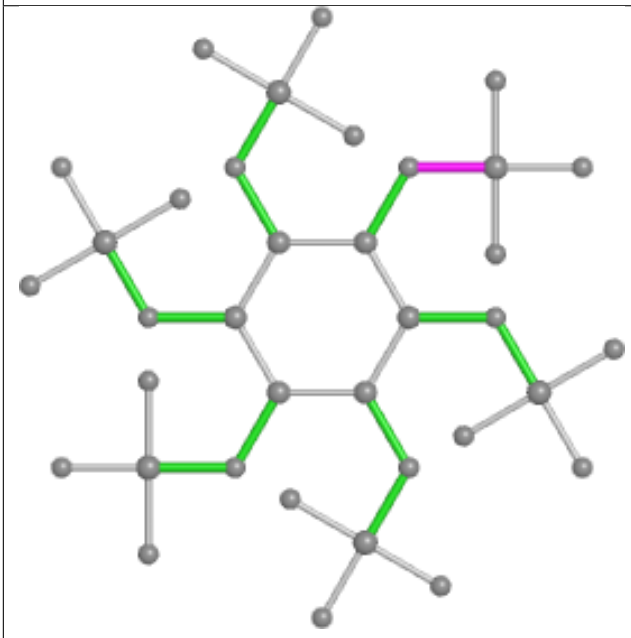
Ligand IHP A 3000



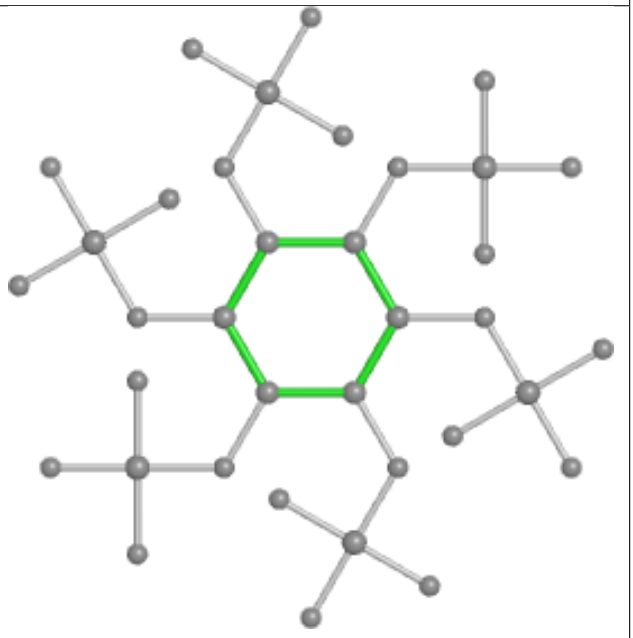
Bond lengths



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.

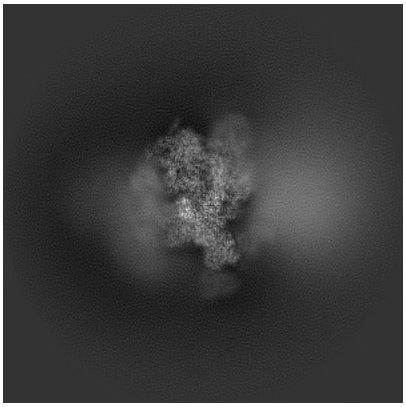
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30875. These allow visual inspection of the internal detail of the map and identification of artifacts.

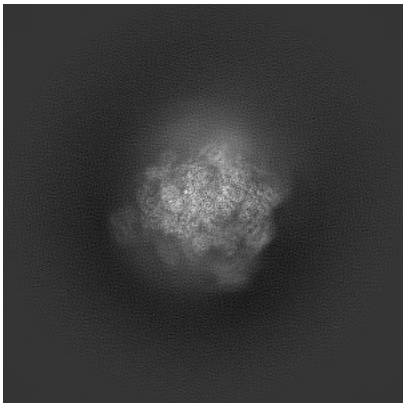
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

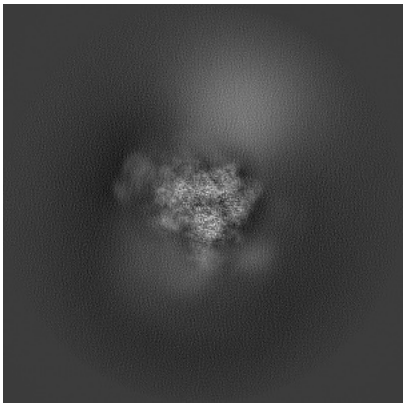
6.1.1 Primary map



X



Y

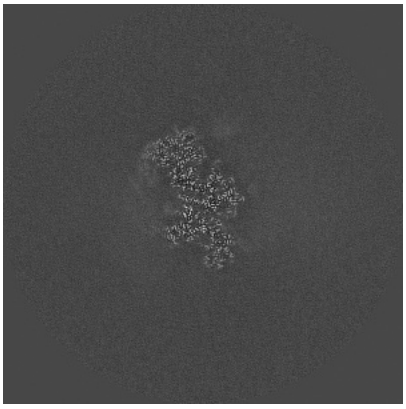


Z

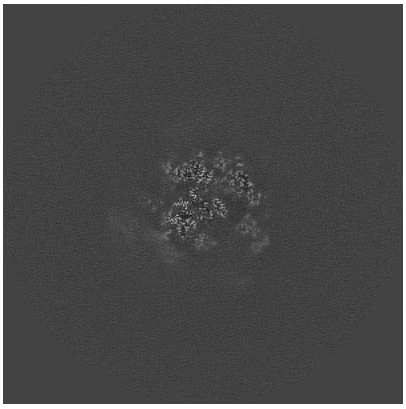
The images above show the map projected in three orthogonal directions.

6.2 Central slices

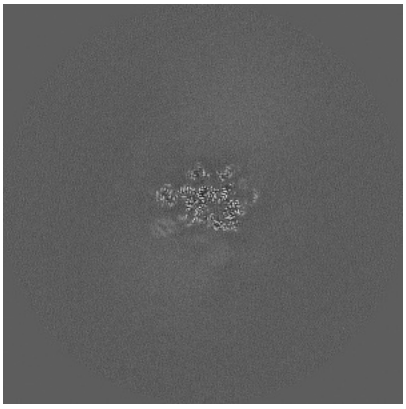
6.2.1 Primary map



X Index: 300



Y Index: 300

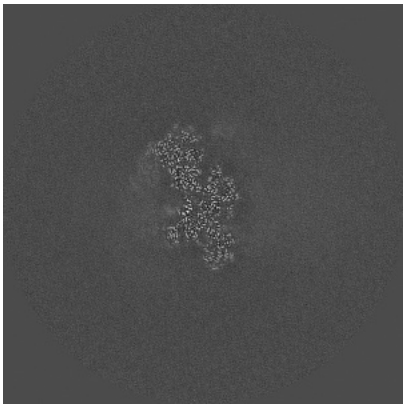


Z Index: 300

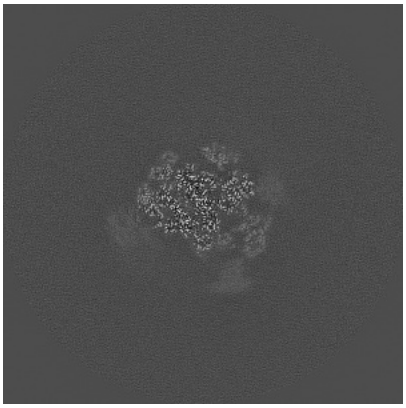
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

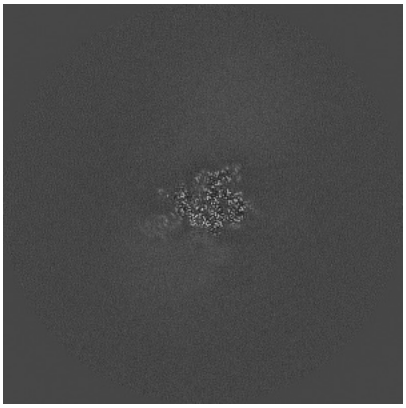
6.3.1 Primary map



X Index: 304



Y Index: 316

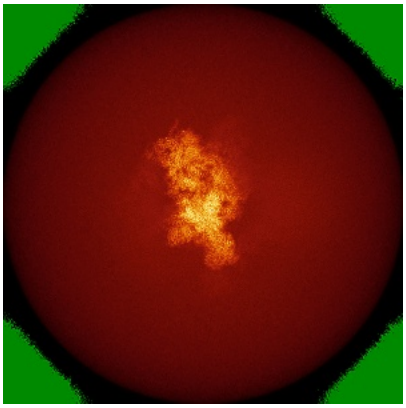


Z Index: 284

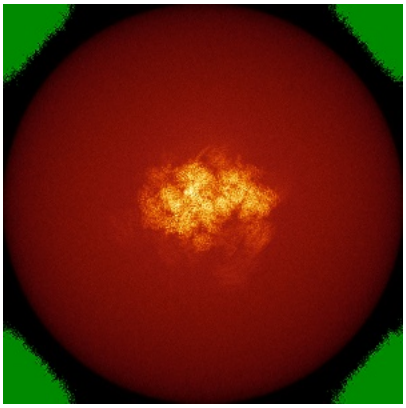
The images above show the largest variance slices of the map in three orthogonal directions.

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

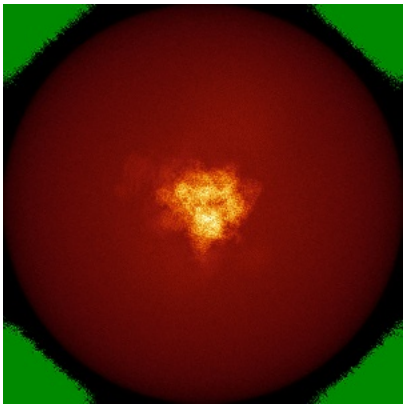
6.4.1 Primary map



X



Y



Z

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 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

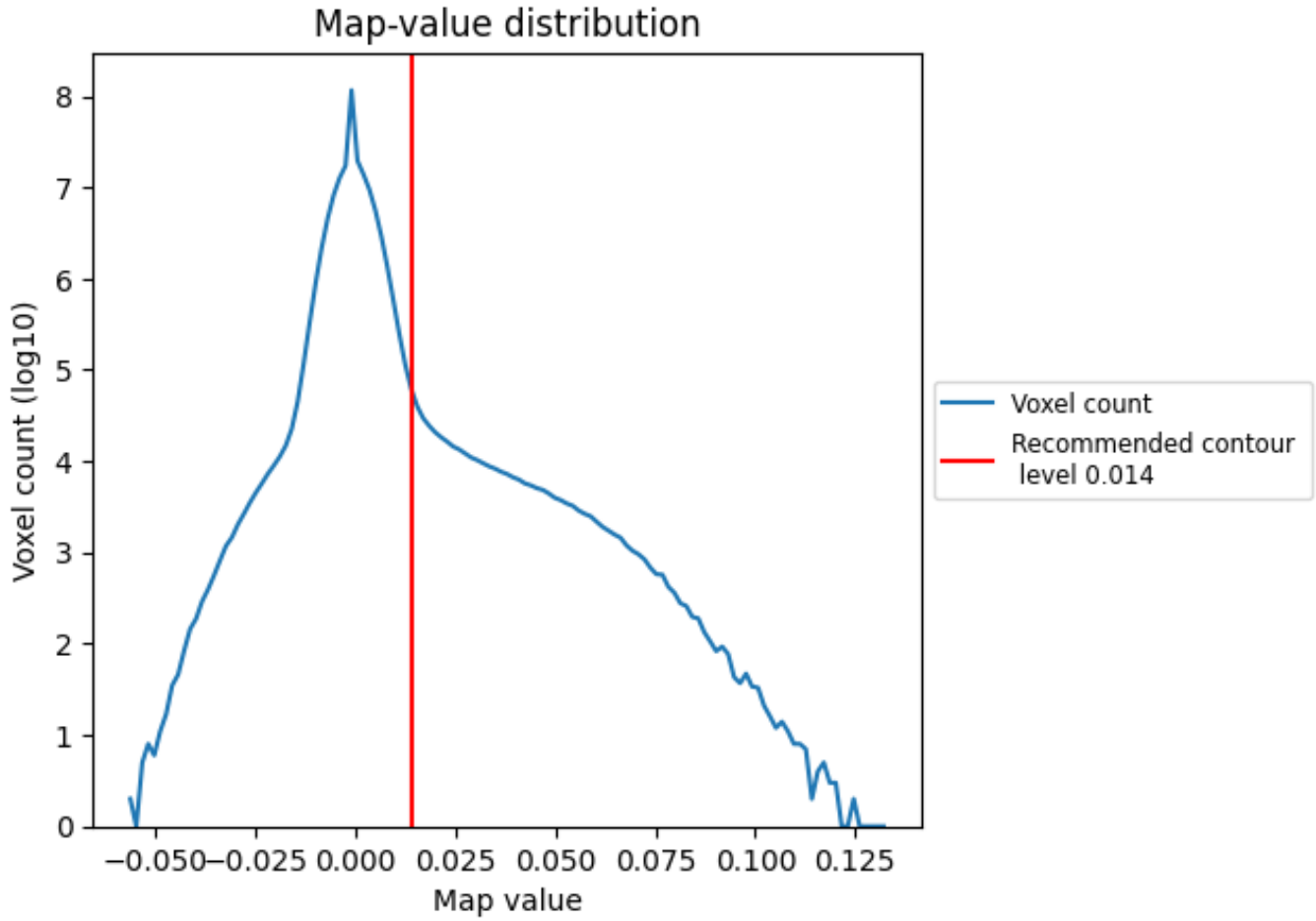
6.6 Mask visualisation (i)

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

7 Map analysis

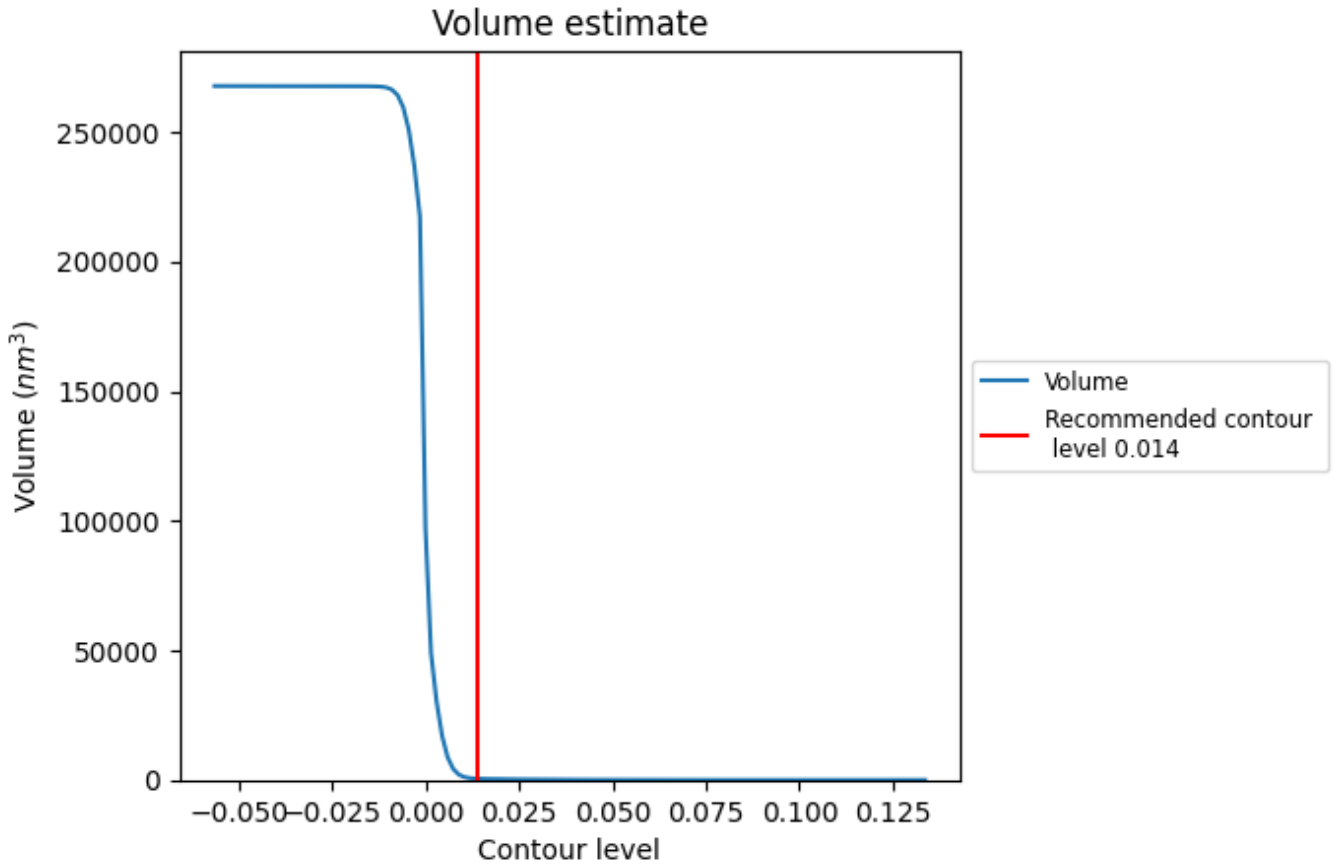
This section contains the results of statistical analysis of the map.

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.

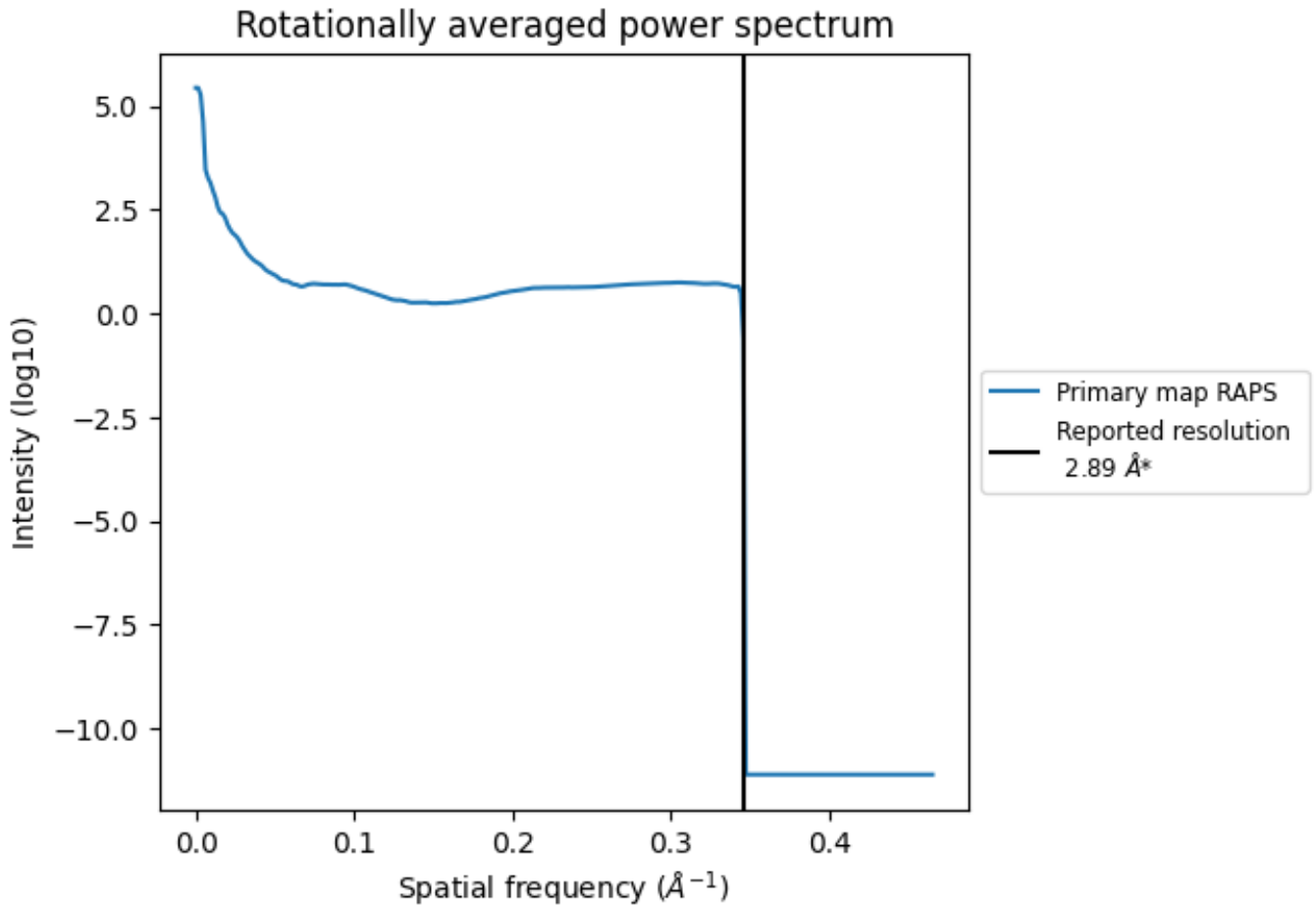
7.2 Volume estimate



The volume at the recommended contour level is 486 nm^3; this corresponds to an approximate mass of 439 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 0.346 $Å^{-1}$

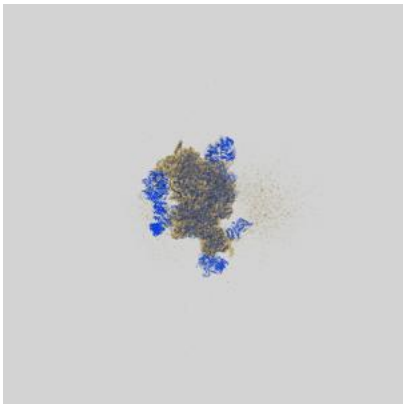
8 Fourier-Shell correlation

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

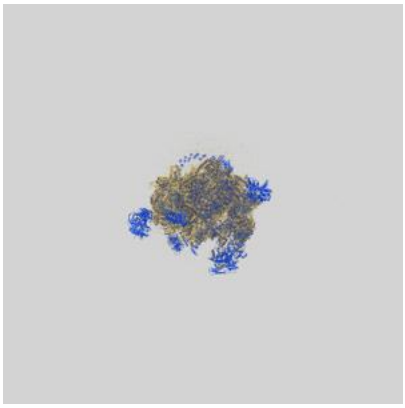
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30875 and PDB model 7DVQ. Per-residue inclusion information can be found in section 3 on page 14.

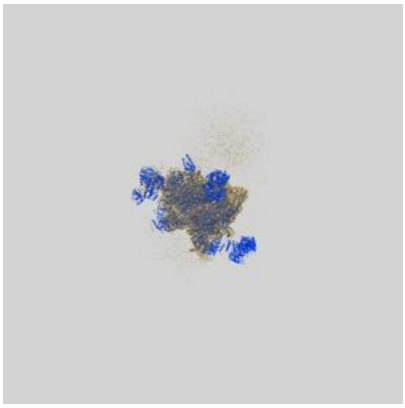
9.1 Map-model overlay



X



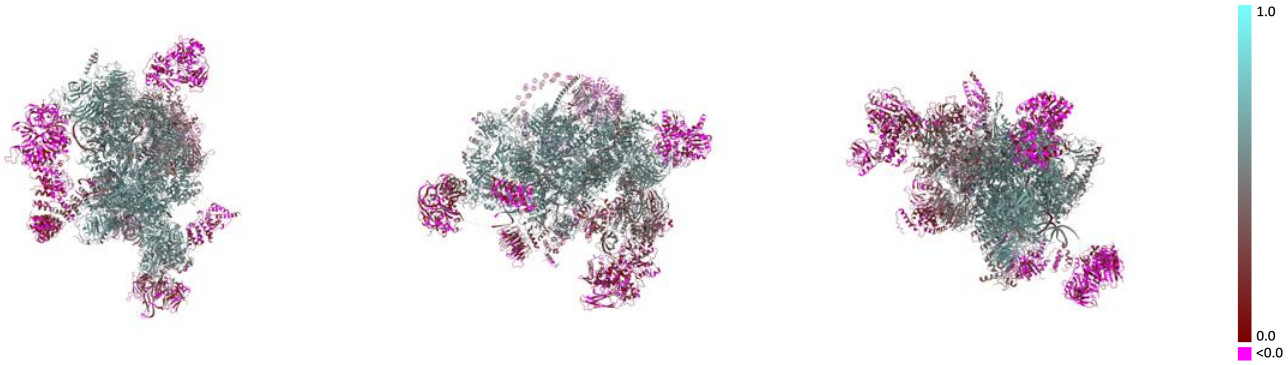
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

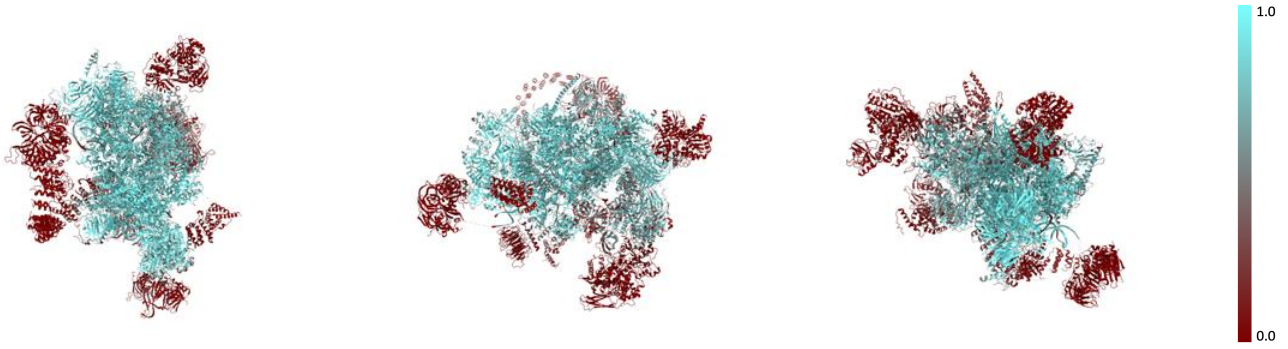
9.2 Q-score mapped to coordinate model



X Y Z

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

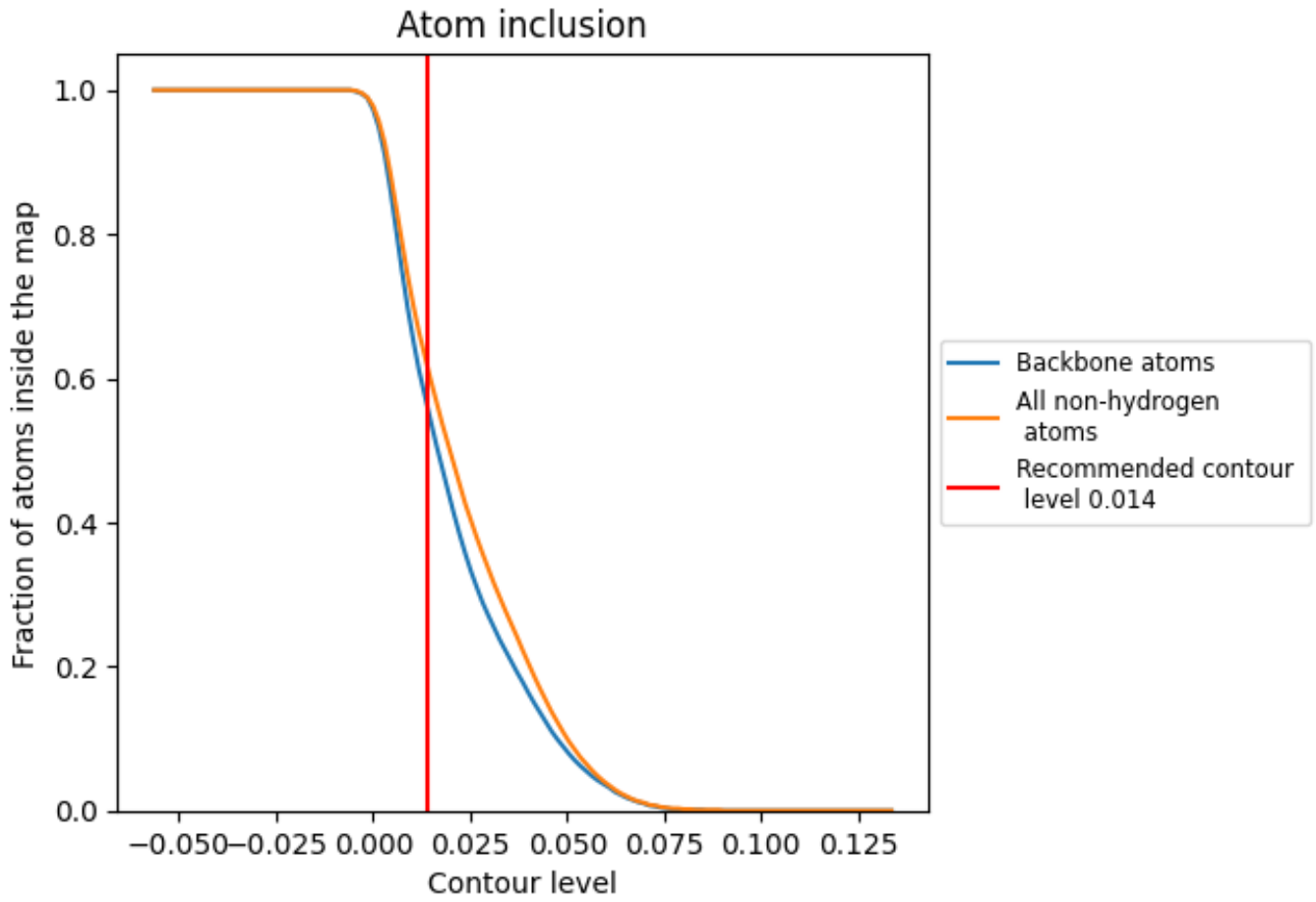
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.014).

9.4 Atom inclusion (i)



At the recommended contour level, 56% of all backbone atoms, 62% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6160	0.4320
0	0.8640	0.6050
1	0.8840	0.5900
2	0.7180	0.5030
3	0.8240	0.5400
4	0.0500	0.0180
5	0.7480	0.5010
6	0.9240	0.6120
7	0.8850	0.5890
8	0.8130	0.5490
9	0.5000	0.3510
A	0.8240	0.5630
B	0.6310	0.4010
C	0.8440	0.5630
D	0.3160	0.2360
E	0.0330	0.1220
F	0.7790	0.4750
G	0.7180	0.4570
H	0.6700	0.4050
I	0.4980	0.3360
J	0.0750	0.2170
K	0.1660	0.1400
L	0.8980	0.5950
M	0.6270	0.4630
P	0.7410	0.5350
R	0.6330	0.5000
T	0.9430	0.6110
U	0.9250	0.6080
V	0.4990	0.3300
X	0.6770	0.4420
Y	0.8180	0.5610
Z	0.7390	0.5420
a	0.0880	0.2650
b	0.0320	0.1610
c	0.0200	0.0820

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
d	0.0150	0.0700
e	0.0080	0.0930
f	0.0050	0.0620
g	0.0140	0.1750
h	0.0000	-0.0340
i	0.0020	-0.0230
j	0.0000	0.0510
k	0.0020	0.0090
l	0.0030	-0.0030
m	0.0030	0.0080
n	0.0030	-0.0330
v	0.8140	0.5130
x	0.0320	0.0370
y	0.3030	0.2890
z	0.8920	0.5800