Full wwPDB EM Validation Report ⓘ

Jul 31, 2024 – 11:44 AM JST

PDB ID	:	8I0T
EMDB ID	:	EMD-35109
Title	:	The cryo-EM structure of human Bact-III complex
Authors	:	Zhan, X.; Lu, Y.; Shi, Y.
Deposited on	:	2023-01-11
Resolution	:	3.00 Å(reported)

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

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

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

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

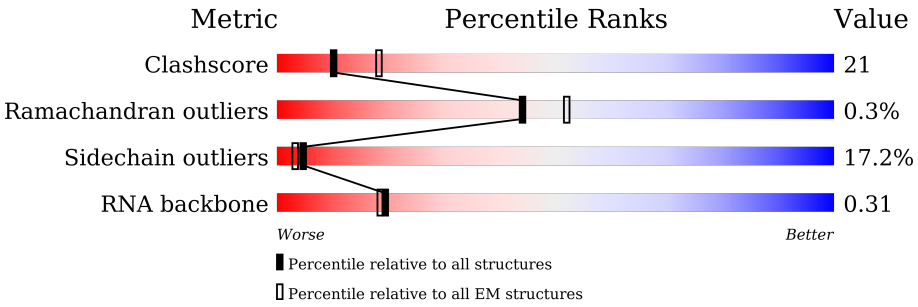
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	2335	50% 37% 8%
2	B	117	23% 42% 17% 16%
3	C	972	37% 41% 10% 12%
4	D	2136	53% 75% 5% 19%
5	E	357	28% 47% 9% 16%
6	F	107	11% 36% 36% 8% 9%
7	G	220	14% 13% 67%

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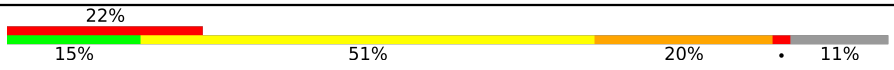
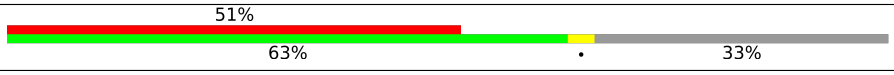
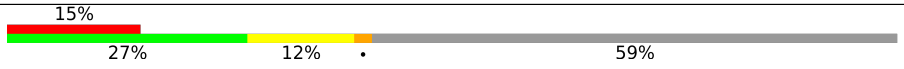
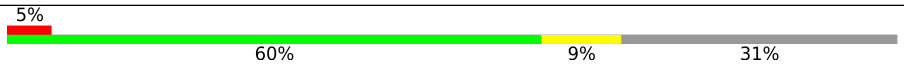
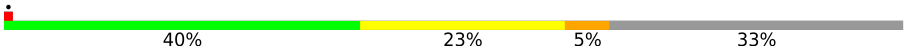
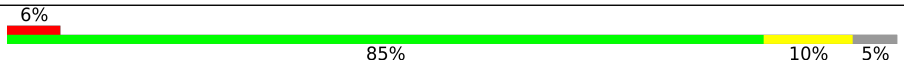
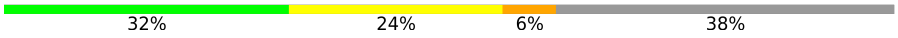
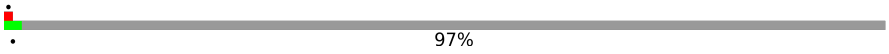
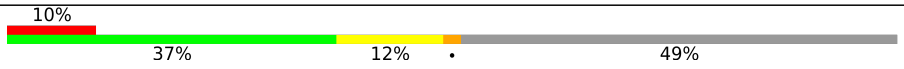
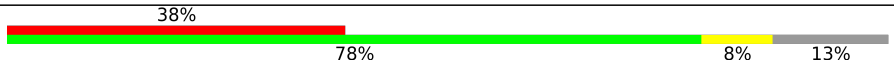
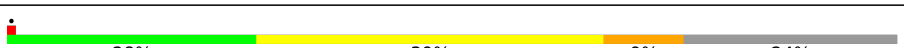
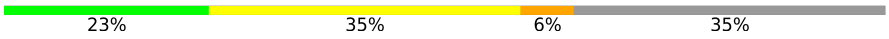
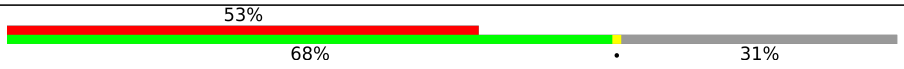
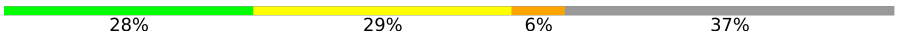
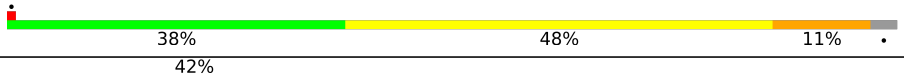
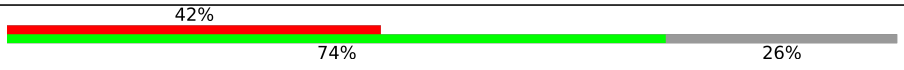
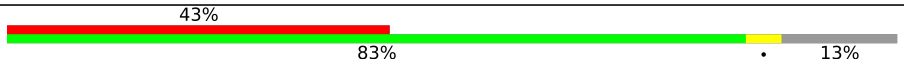
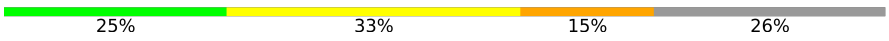
Mol	Chain	Length	Quality of chain
8	H	188	
9	I	855	
10	J	848	
11	K	343	
12	L	802	
13	N	144	
14	O	420	
15	P	229	
16	Q	1485	
17	R	536	
18	S	166	
19	T	514	
20	U	2752	
21	V	908	
22	W	579	
23	X	1041	
24	Y	492	
25	Z	225	
26	1	1304	
27	3	1217	
28	p	225	
29	w	501	
30	2	895	
31	4	424	
32	7	110	

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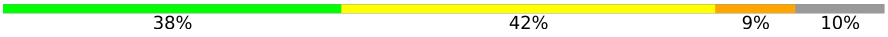
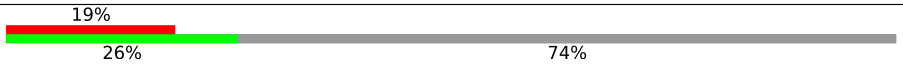
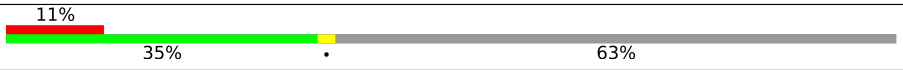
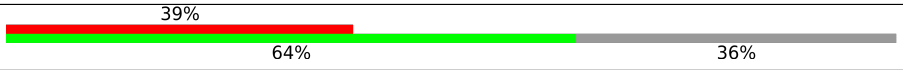
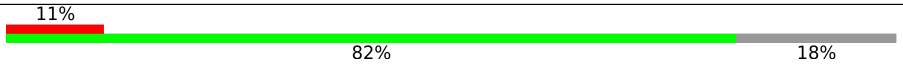
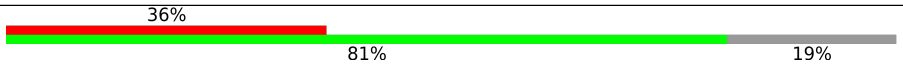
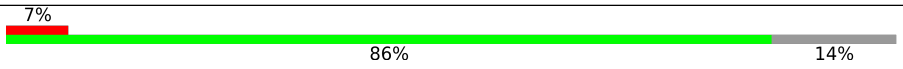
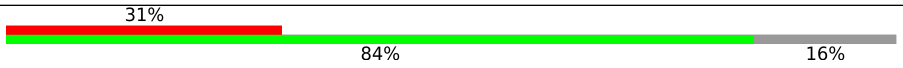
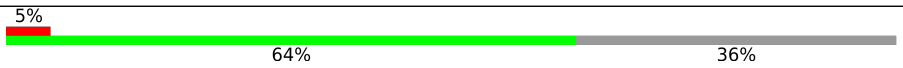
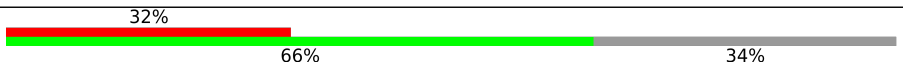
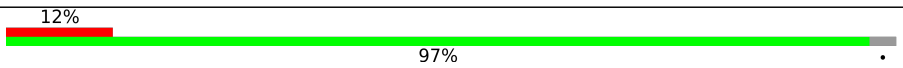
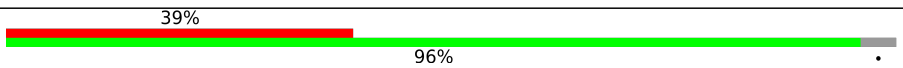
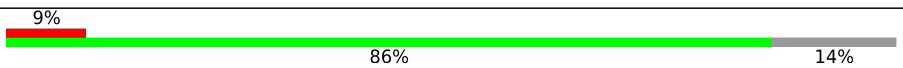
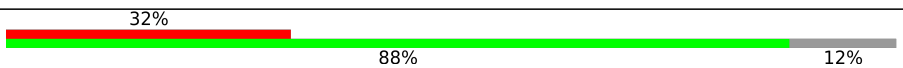
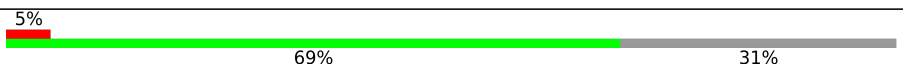
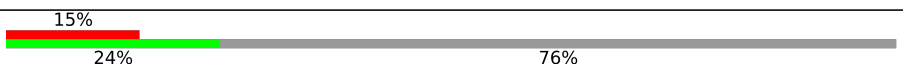
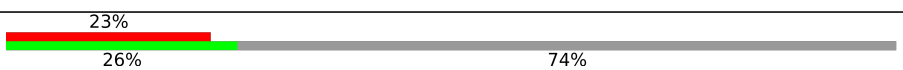
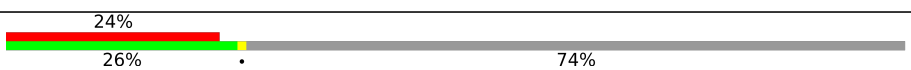
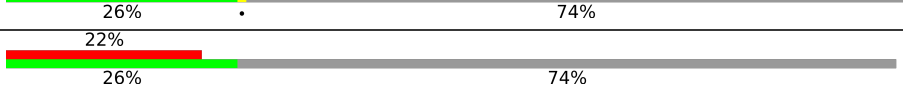
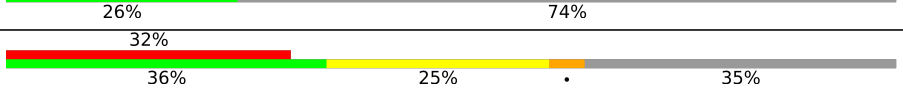
Mol	Chain	Length	Quality of chain
33	5	86	
34	y	301	
35	v	464	
36	o	255	
37	c	118	
37	h	118	
38	d	86	
38	i	86	
39	a	240	
39	m	240	
40	g	126	
40	l	126	
41	f	76	
41	k	76	
42	e	92	
42	j	92	
43	b	119	
43	n	119	
44	u	793	
45	q	504	
45	r	504	
45	s	504	
45	t	504	
46	9	520	

2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 120623 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	2242	18543	11943	3241	3280	79	0	0

- Molecule 2 is a RNA chain called U5 snRNA.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	860	6724	4298	1122	1272	32	0	0

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

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

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

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

- Molecule 6 is a RNA chain called U6 snRNA.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	72	Total	C	N	O	P	0	0
			1503	673	248	510	72		

- Molecule 8 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	167	Total	C	N	O	P	0	0
			3539	1581	607	1184	167		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	571	Total	C	N	O	0	0
			2880	1738	571	571		

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

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

- Molecule 11 is a protein called RING finger protein 113A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	49	Total	C	N	O	S	0	0
			411	258	70	80	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	328	Total	C	N	O	S	0	0
			2192	1361	421	406	4		

- Molecule 13 is a protein called Protein BUD31 homolog.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	O	290	Total 1447	C 862	N 292	O 293	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	101	Total 876	C 537	N 175	O 162	S 2	0	0

- Molecule 16 is a protein called RNA helicase aquarius.

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
17	R	361	Total 2760	C 1694	N 524	O 529	P 1	S 12	0	0

- Molecule 18 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	S	158	Total 770	C 454	N 158	O 158	0	0

- Molecule 19 is a protein called Pleiotropic regulator 1.

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

- Molecule 20 is a protein called Serine/arginine repetitive matrix protein 2.

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

- Molecule 21 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	462	Total 2959	C 1842	N 537	O 567	S 13	0	0

- Molecule 22 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	W	501	Total 2473	C 1471	N 501	O 501	0	0

- Molecule 23 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase DHX16.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	786	Total 6357	C 4010	N 1133	O 1184	S 30	0	0

- Molecule 24 is a protein called Peptidyl-prolyl cis-trans isomerase-like 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	320	Total 2556	C 1616	N 420	O 508	S 12	0	0

- Molecule 25 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Z	155	Total 772	C 462	N 155	O 155	0	0

- Molecule 26 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1	816	Total 6486	C 4163	N 1119	O 1165	S 39	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	3	1177	Total 9220	C 5854	N 1566	O 1755	S 45	0	0

- Molecule 28 is a protein called U2 small nuclear ribonucleoprotein B".

Mol	Chain	Residues	Atoms				AltConf	Trace
28	p	167	Total 841	C 507	N 167	O 167	0	0

- Molecule 29 is a protein called Splicing factor 3A subunit 3.

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

- Molecule 30 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	2	250	Total 1807	C 1134	N 340	O 326	S 7	0	0

- Molecule 31 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	4	161	Total 792	C 470	N 161	O 161	0	0

- Molecule 32 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	7	81	Total 613	C 376	N 109	O 115	S 13	0	0

- Molecule 33 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	5	77	Total 635	C 403	N 110	O 117	S 5	0	0

- Molecule 34 is a protein called Peptidyl-prolyl cis-trans isomerase E.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	v	173	Total	C	N	O	S	0	0
			1041	602	219	217	3		

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

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

- Molecule 37 is a protein called Small nuclear ribonucleoprotein Sm D2.

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

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

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

- Molecule 39 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	m	82	Total	C	N	O	0	0
			413	249	82	82		
39	a	86	Total	C	N	O	0	0
			344	172	86	86		

- Molecule 40 is a protein called Small nuclear ribonucleoprotein Sm D3.

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

- Molecule 41 is a protein called Small nuclear ribonucleoprotein G.

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

- Molecule 42 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	j	81	Total 403	C 241	N 81	O 81	0	0
42	e	79	Total 316	C 158	N 79	O 79	0	0

- Molecule 43 is a protein called Small nuclear ribonucleoprotein Sm D1.

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

- Molecule 44 is a protein called Splicing factor 3A subunit 1.

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

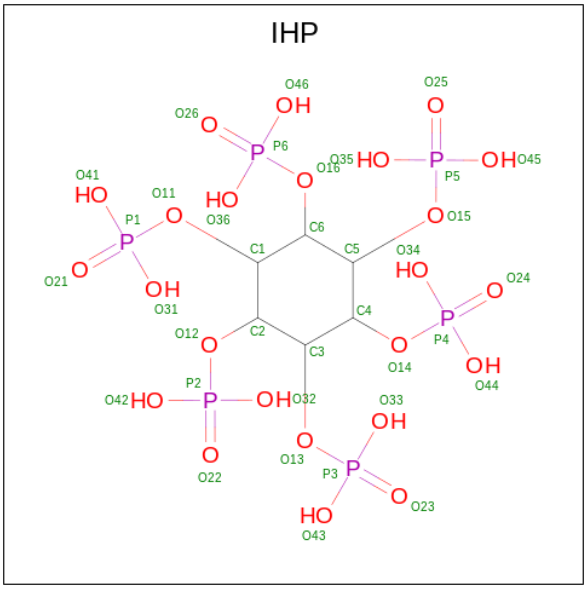
- Molecule 45 is a protein called Pre-mRNA-processing factor 19.

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

- Molecule 46 is a protein called RING-type E3 ubiquitin-protein ligase PPIL2.

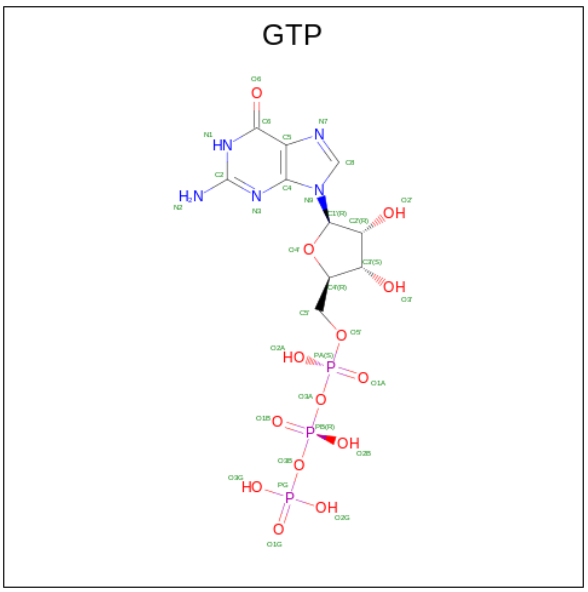
Mol	Chain	Residues	Atoms					AltConf	Trace
46	9	338	Total	C	N	O	S	0	0
			2307	1429	420	450	8		

- Molecule 47 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- Molecule 48 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 49 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
49	C	1	Total	Mg	0
			1	1	
49	F	6	Total	Mg	0
			6	6	

- Molecule 50 is ZINC ION (three-letter code: ZN) (formula: Zn).

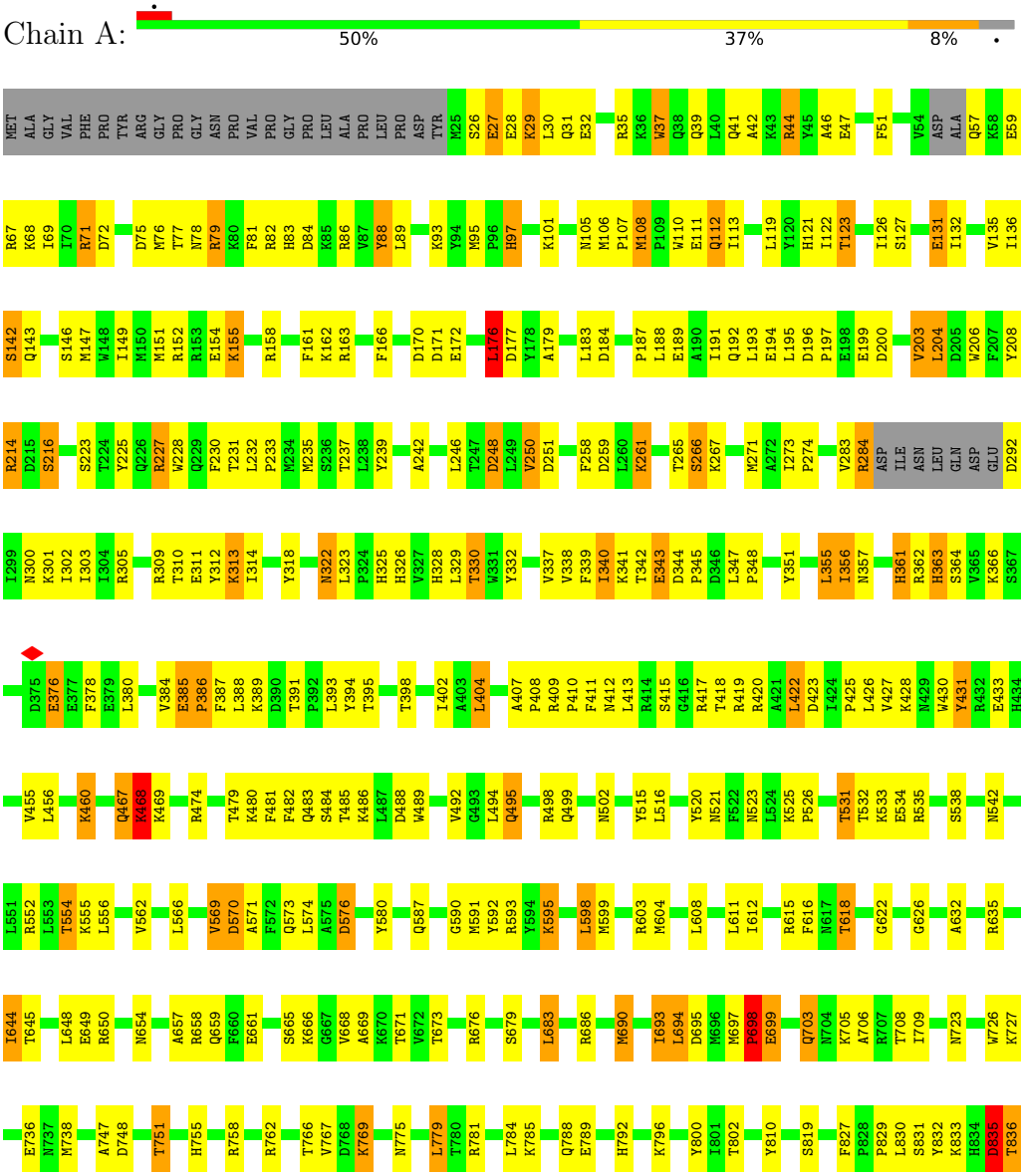
Mol	Chain	Residues	Atoms		AltConf
50	K	1	Total	Zn	0
			1	1	
50	N	3	Total	Zn	0
			3	3	
50	7	3	Total	Zn	0
			3	3	

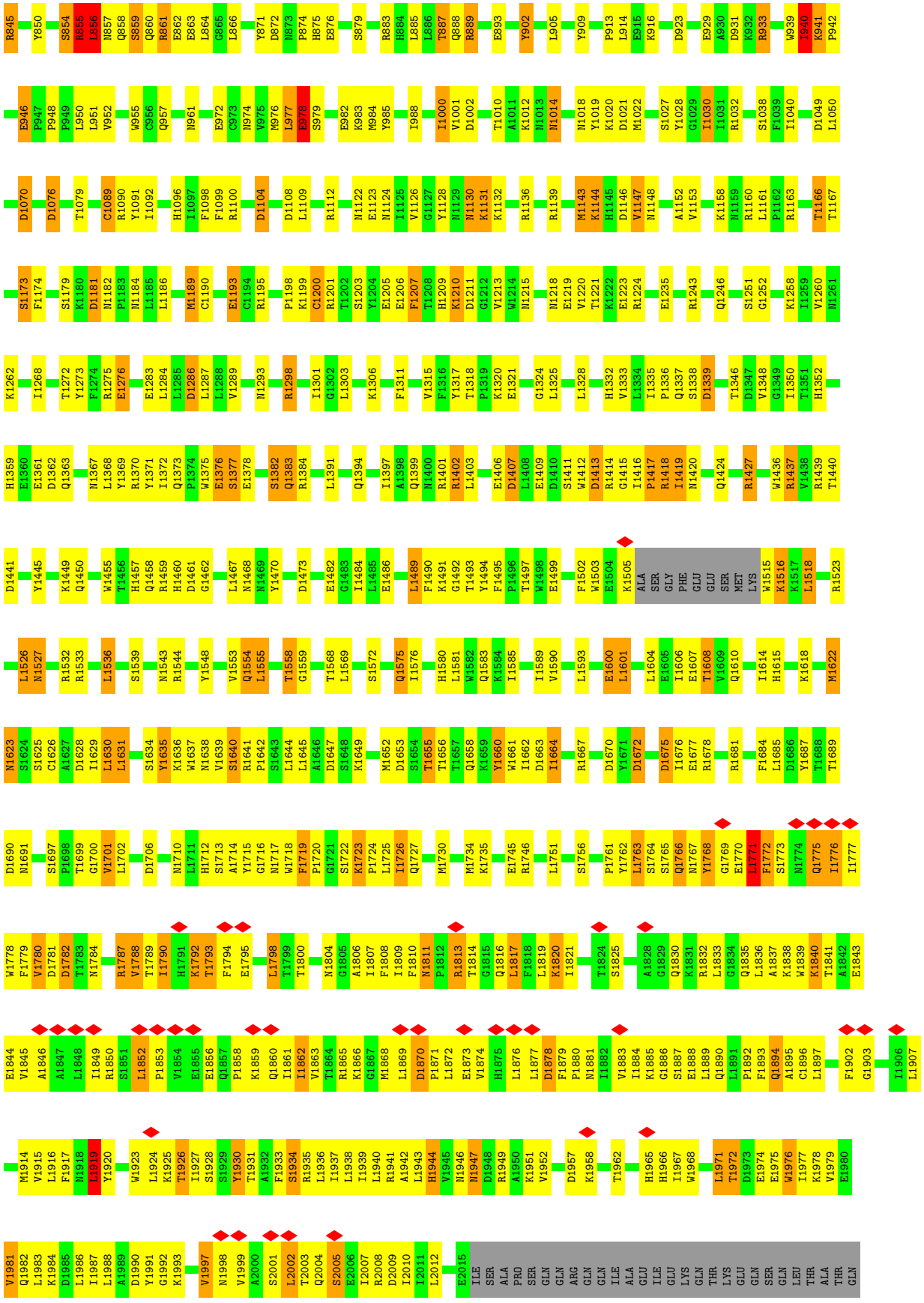
3 Residue-property plots (i)

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:

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E946 P947 P948 P949 L950 L951 V952 W955 C956 Q957 N961 E972 C973 N974 V975 M976 L977 E978 S979 E982 K983 M984 Y985 I988 I1000 V1001 D1002 T1010 A1011 K1012 N1013 N1014 N1018 Y1019 K1020 D1021 M1022 S1027 Y1028 G1029 I1030 T1031 R1032 S1038 F1039 I1040 D1049 L1050
D1070 D1076 T1079 C1089 R1090 Y1091 I1092 H1096 I1097 F1098 F1099 R1100 D1104 D1108 L1109 R1112 N1122 E1123 N1124 I1125 V1126 G1127 Y1128 N1129 N1130 K1131 K1132 R1136 R1139 M1143 K1144 H1145 D1146 V1147 N1148 A1152 V1153 K1158 N1159 R1160 L1161 P1162 R1163 T1166 T1167
S1173 F1174 S1179 K1180 D1181 N1182 P1183 N1184 I1185 L1186 M1189 C1190 E1193 C1194 R1195 P1198 K1199 C1200 R1201 T1202 S1203 Y1204 E1205 E1206 F1207 T1208 H1209 K1210 D1211 G1212 V1213 W1214 N1215 N1218 E1219 V1220 T1221 K1222 E1223 R1224 E1235 R1243 Q1246 S1251 G1252 K1258 T1259 V1260 N1261
K1262 I1268 T1272 Y1273 F1274 R1275 E1276 E1283 L1284 L1285 D1286 L1287 L1288 V1289 N1293 R1298 I1301 G1302 L1303 K1306 F1311 V1315 F1316 Y1317 T1318 P1319 K1320 E1321 G1324 L1325 L1328 H1332 V1333 L1334 I1335 P1336 Q1337 S1338 D1339 T1346 D1347 V1348 G1349 I1350 T1351 H1352
H1359 E1360 E1361 D1362 Q1363 N1367 L1368 Y1369 R1370 Y1371 I1372 Q1373 P1374 W1375 E1376 S1377 E1378 S1382 Q1383 R1384 L1391 Q1394 I1397 A1398 Q1399 N1400 R1401 R1402 L1403 E1406 D1407 L1408 E1409 D1410 S1411 W1412 D1413 R1414 G1415 I1416 P1417 R1418 I1419 N1420 Q1424 R1427 W1436 R1437 V1438 R1439 T1440
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D1690 N1691 S1697 P1698 T1699 G1700 V1701 L1702 D1706 N1710 L1711 H1712 S1713 A1714 Y1715 G1716 N1717 W1718 F1719 P1720 C1721 S1722 K1723 P1724 L1725 I1726 Q1727 M1730 M1734 K1735 E1745 R1746 L1751 S1756 P1761 Y1762 L1763 S1764 S1765 Q1766 N1767 Y1768 G1769 E1770 L1771 F1772 S1773 N1774 Q1775 I1776 I1777
W1778 F1779 V1780 D1781 D1782 T1783 N1784 R1787 V1788 T1789 I1790 H1791 K1792 T1793 F1794 E1795 L1798 T1799 T1800 N1804 G1805 A1806 I1807 F1808 I1809 F1810 N1811 P1812 R1813 T1814 G1815 Q1816 L1817 F1818 L1819 K1820 I1821 T1824 S1825 A1828 G1829 Q1830 K1831 R1832 L1833 G1834 Q1835 L1836 A1837 K1838 W1839 K1840 T1841 A1842 E1843
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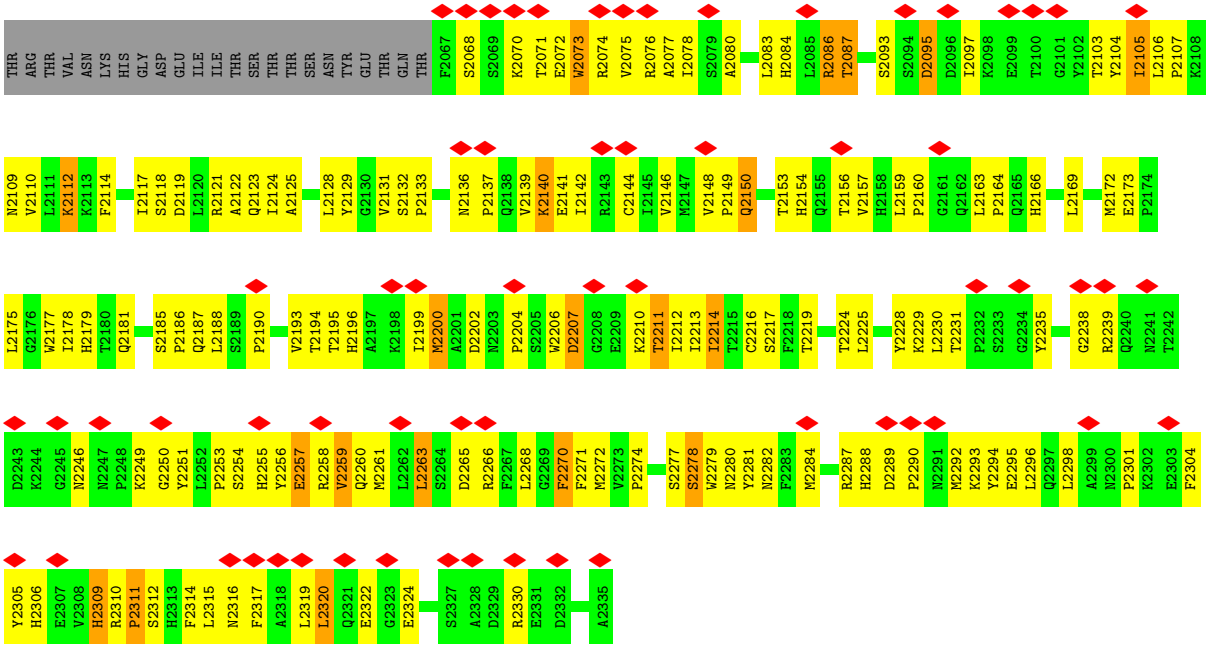
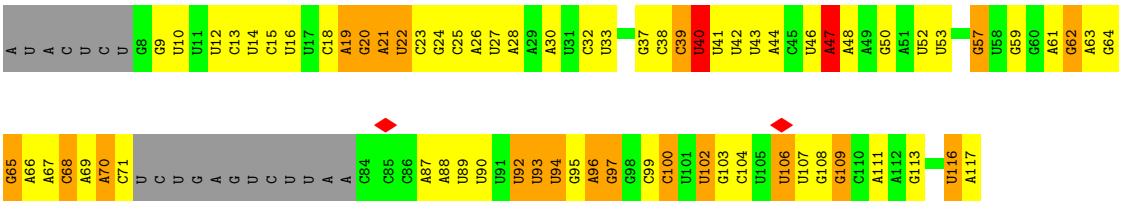
M1914 V1915 L1916 F1917 N1918 L1919 V1920 W1923 L1924 K1925 T1926 I1927 S1928 S1929 Y1930 T1931 A1932 F1933 S1934 R1935 L1936 I1937 L1938 I1939 L1940 R1941 A1942 L1943 H1944 V1945 N1946 N1947 D1948 R1949 A1950 K1951 V1952 D1957 K1958 T1962 H1965 H1966 I1967 W1968 L1971 T1972 D1973 E1974 E1975 W1976 I1977 K1978 V1979 E1980
V1981 Q1982 L1983 K1984 D1985 L1986 I1987 L1988 A1989 D1990 Y1991 G1992 K1993 V1997 N1998 V1999 A2000 S2001 L2002 T2003 Q2004 S2005 E2006 I2007 R2008 D2009 I2010 I2011 L2012 E2015 ILE SER ALA PRO SER GLN GLN ARG GLN GLN ILE ALA GLU ILE GLU LYS GLN THR LYS GLU GLN SER GLN LEU THR ALA THR GLN



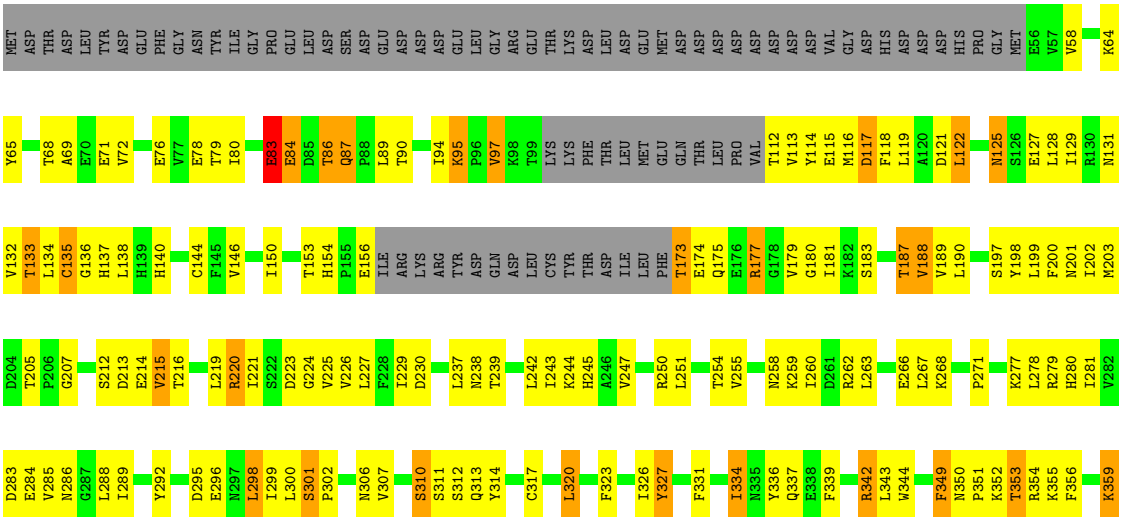
• Molecule 2: U5 snRNA

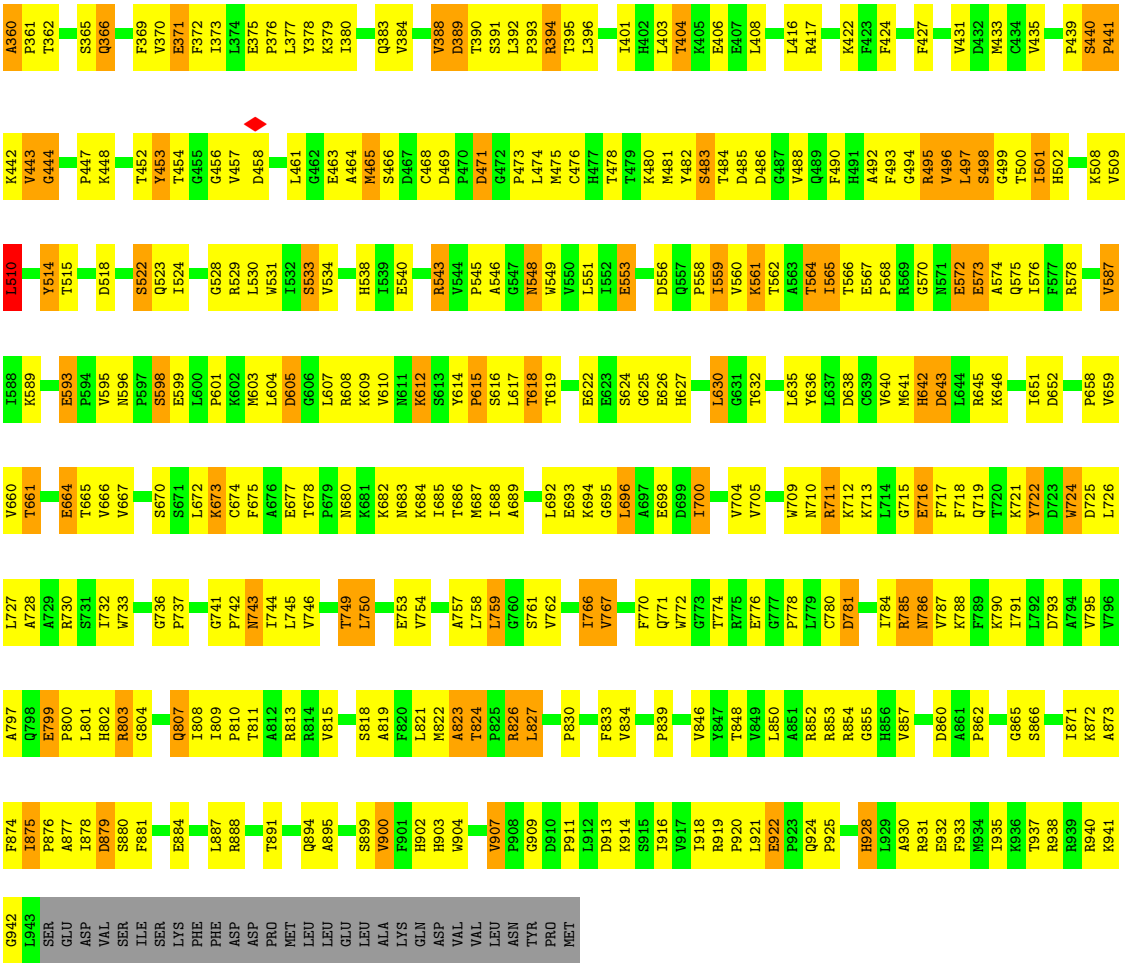
Chain B:



• Molecule 3: 116 kDa U5 small nuclear ribonucleoprotein component

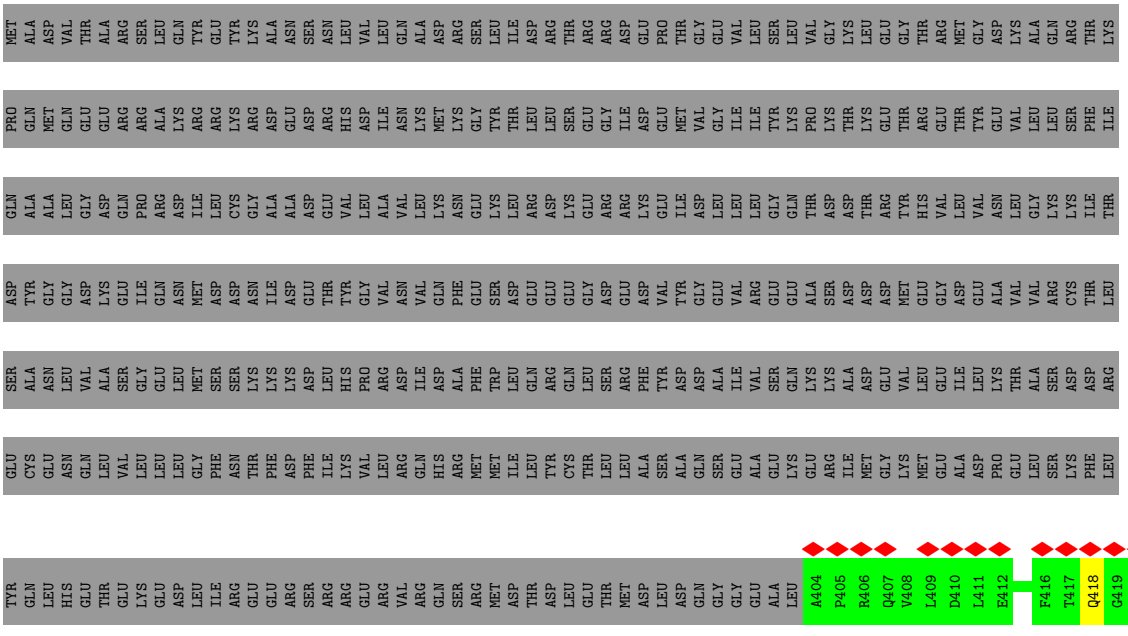
Chain C:

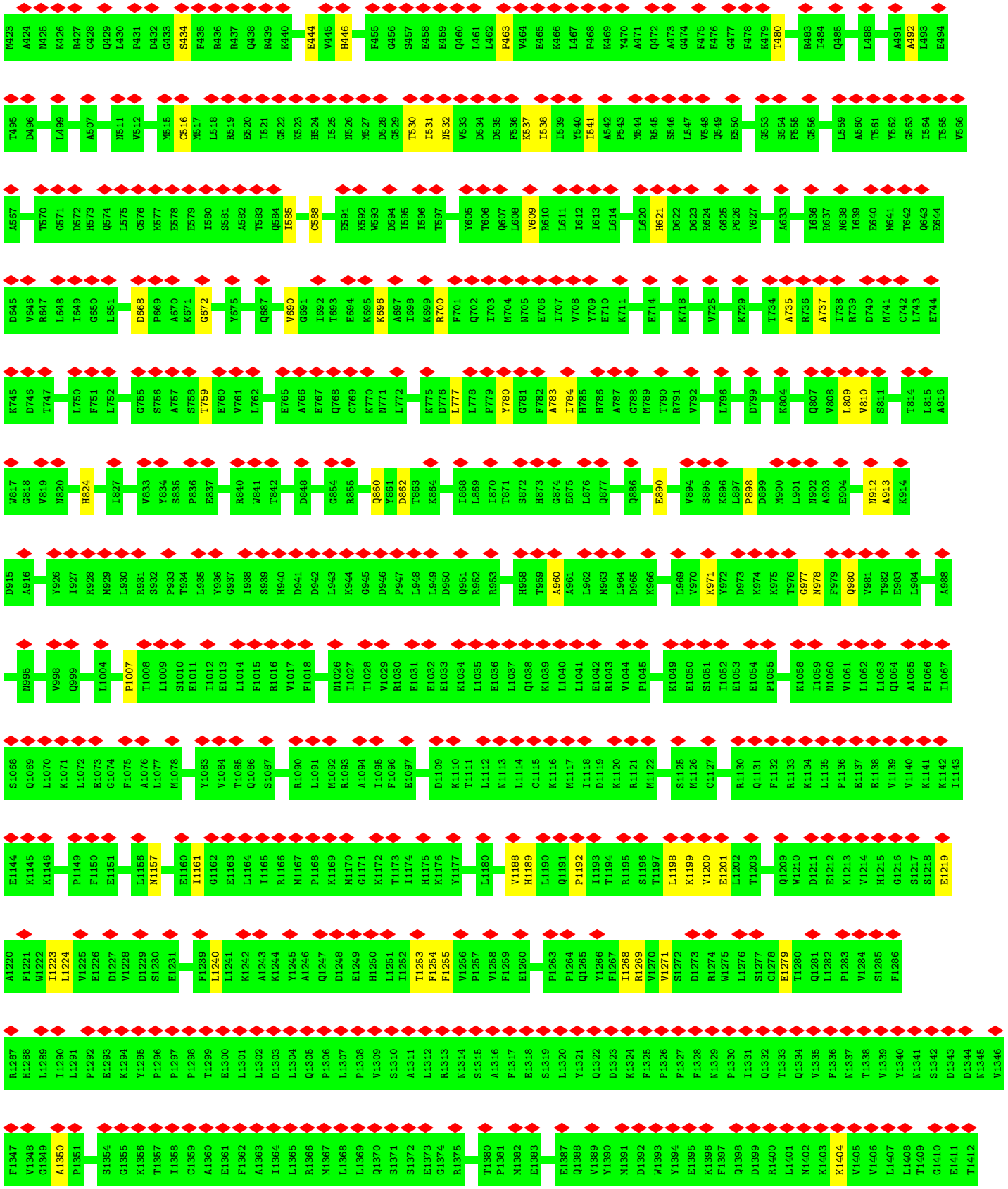




• Molecule 4: U5 small nuclear ribonucleoprotein 200 kDa helicase

Chain D:

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T495 D496 L499 A507 N511 V512 M515 C516 M517 L518 R519 E520 I521 G522 K523 H524 I525 N526 M527 D528 G529 T530 I531 N532 V533 D534 D535 F536 K537 I538 I539 Y540 I541 A542 P543 M544 R545 S546 L547 V548 Q549 E550 G553 S554 F555 G556 L559 A560 T561 Y562 G563 I564 T565 V566
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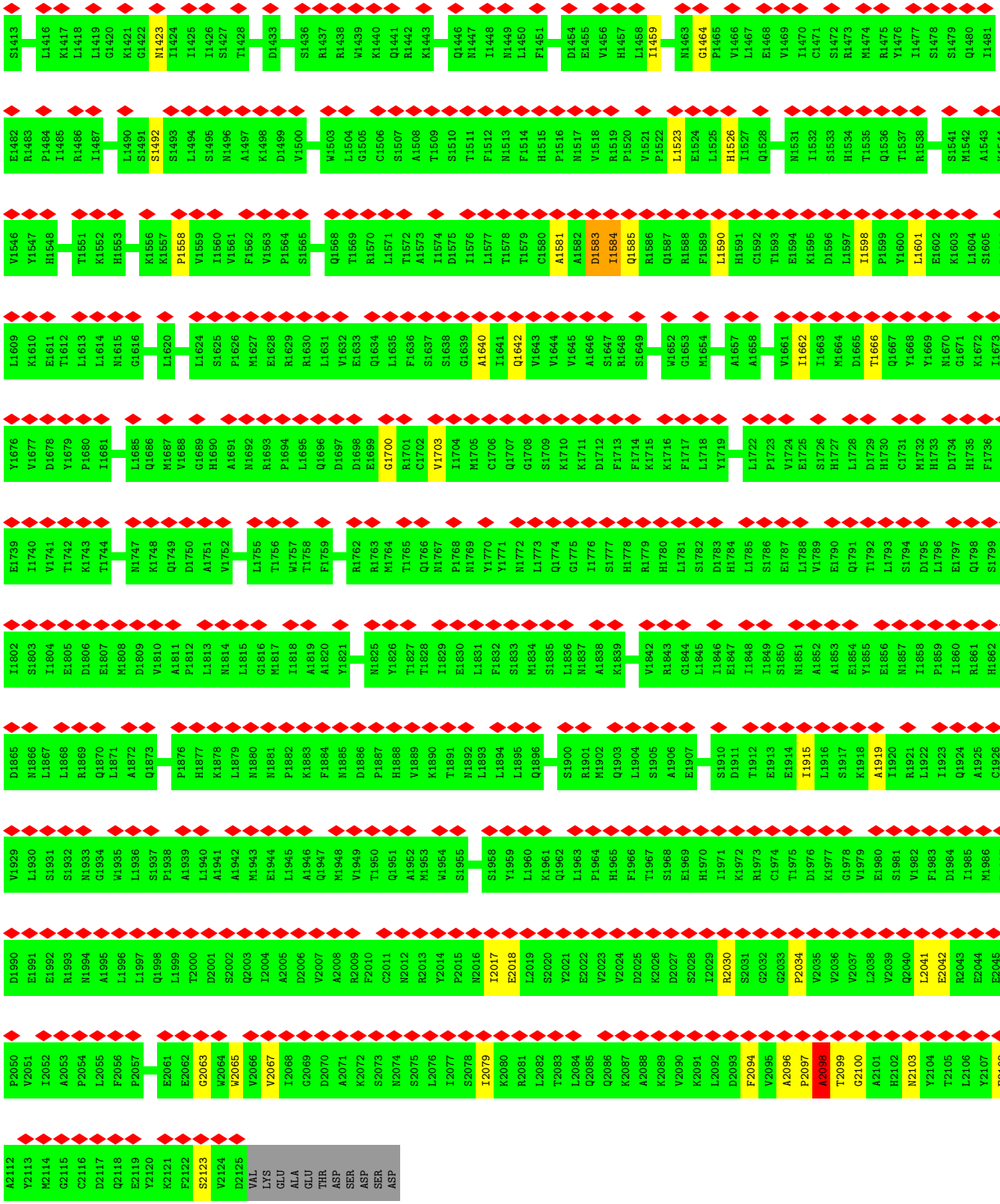
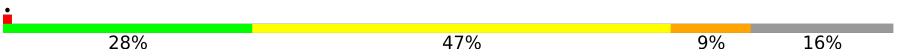
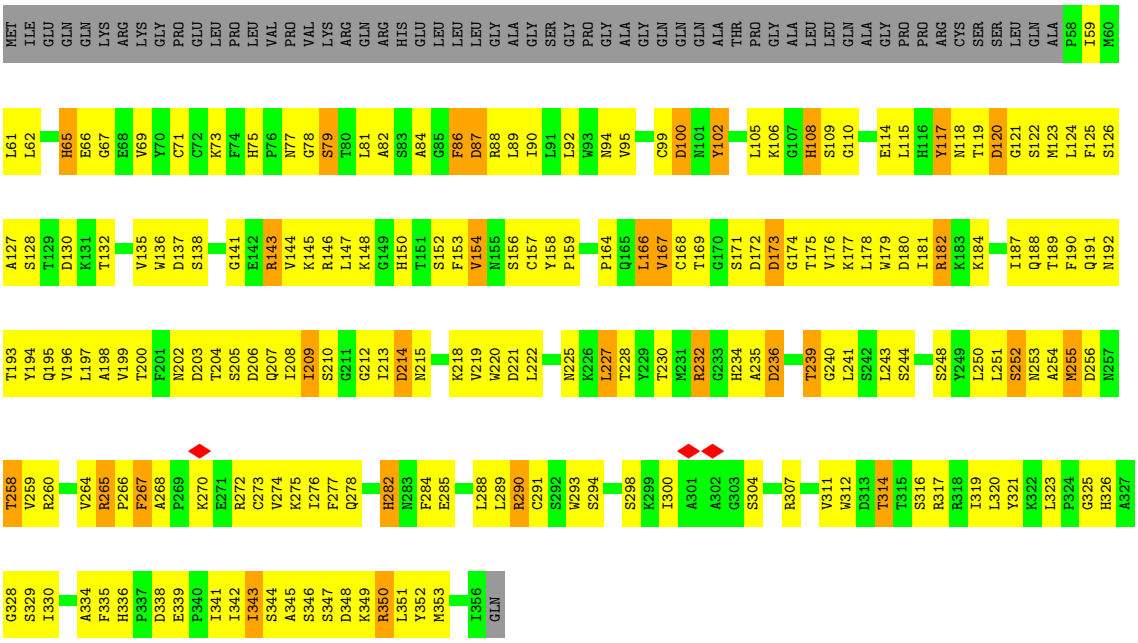


• Molecule 5: U5 small nuclear ribonucleoprotein 40 kDa protein

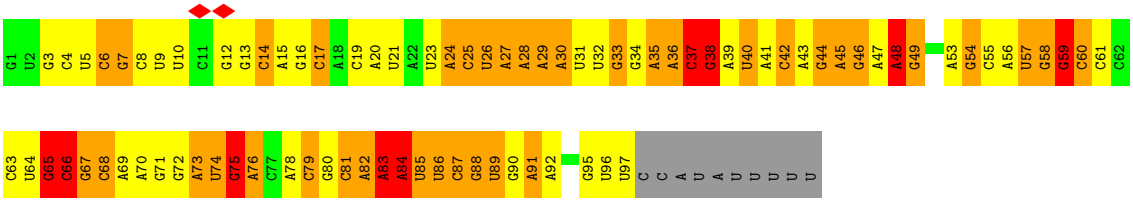
Chain E:





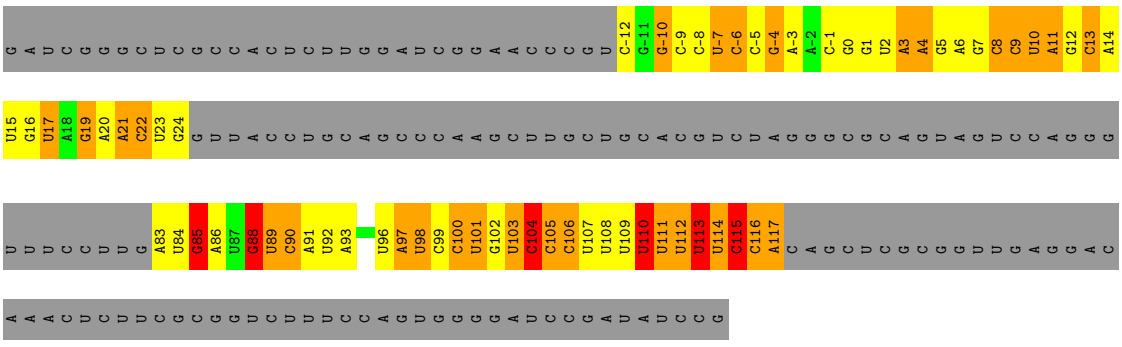
• Molecule 6: U6 snRNA

Chain F:



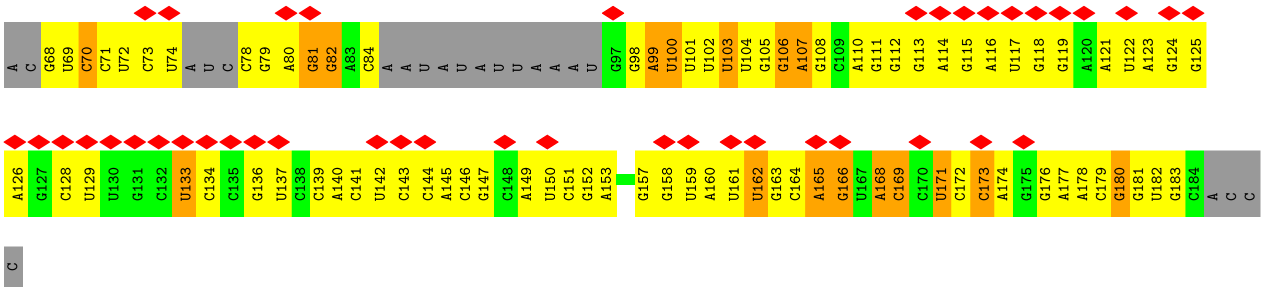
• Molecule 7: Pre-mRNA

Chain G:



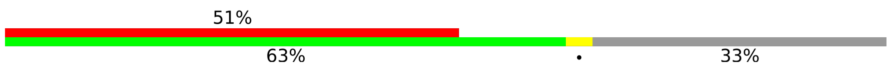
• Molecule 8: U2 snRNA

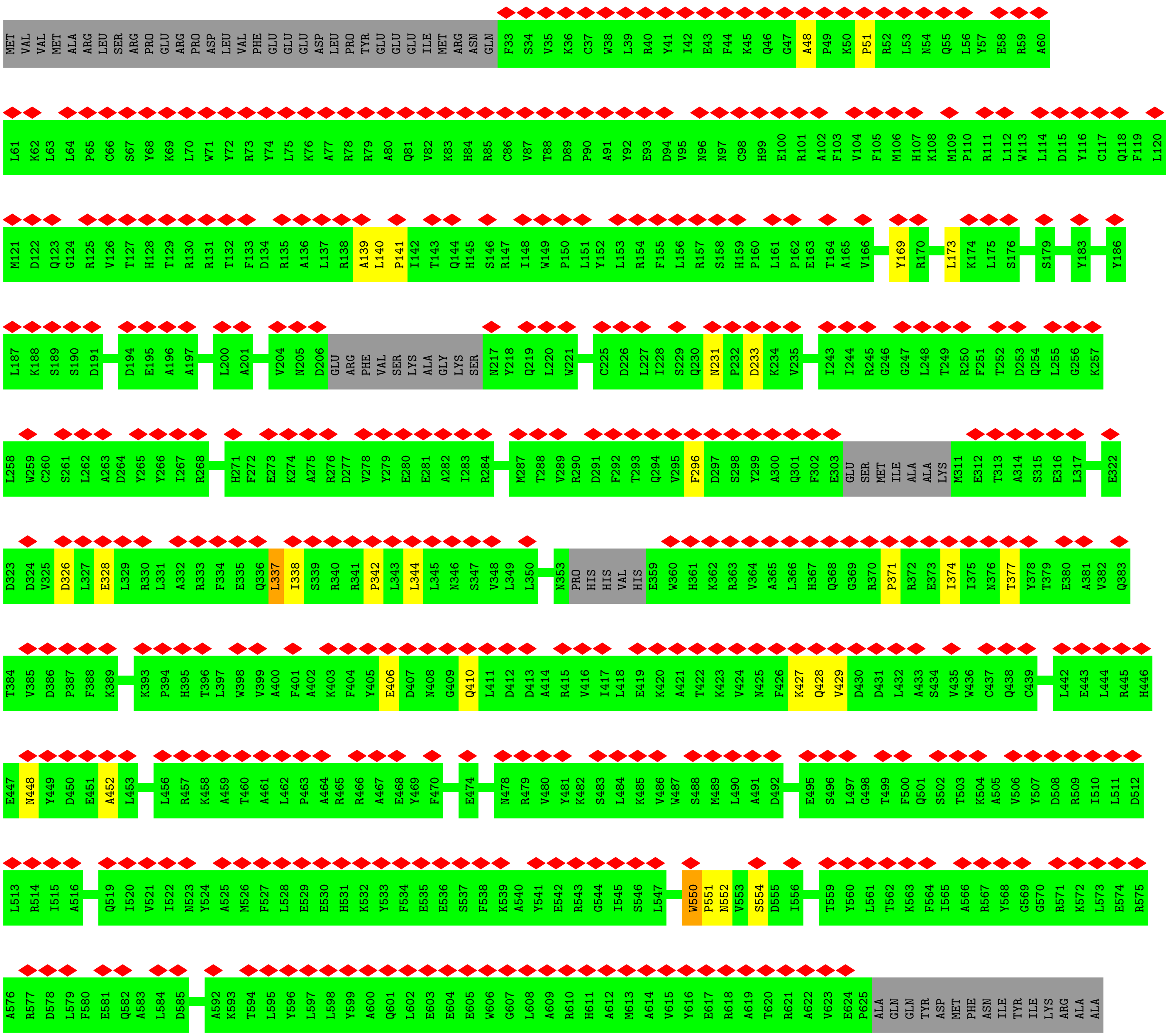
Chain H:

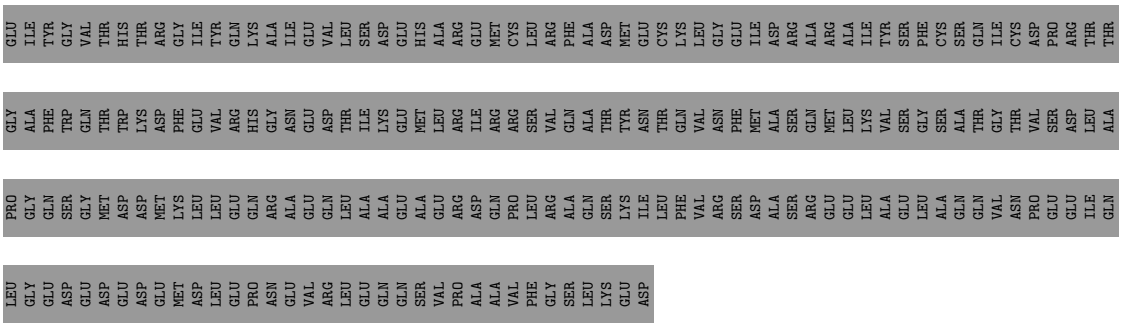


• Molecule 9: Pre-mRNA-splicing factor SYF1

Chain I:

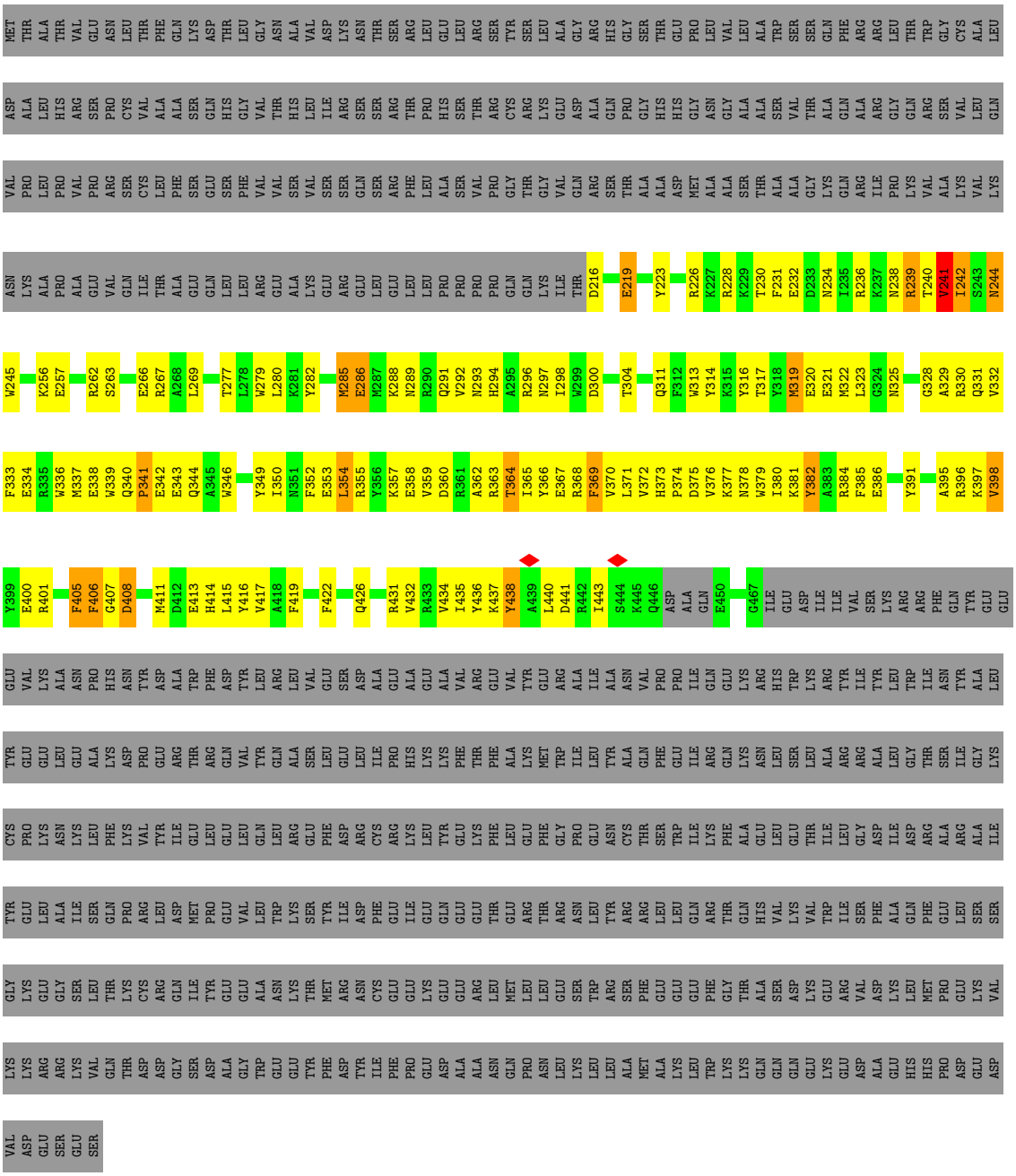






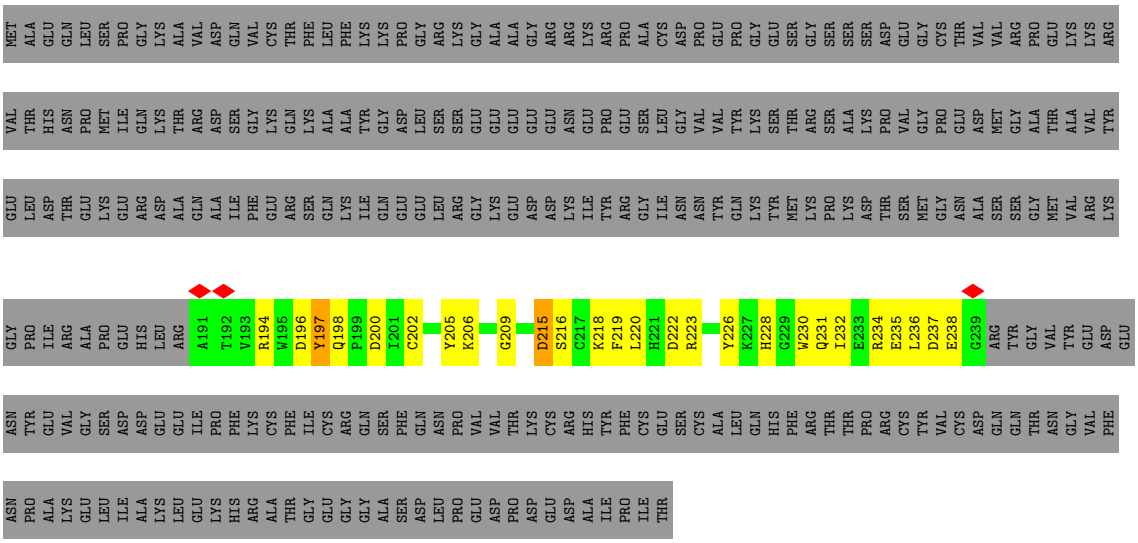
• Molecule 10: Crooked neck-like protein 1

Chain J: 14% 14% 71%



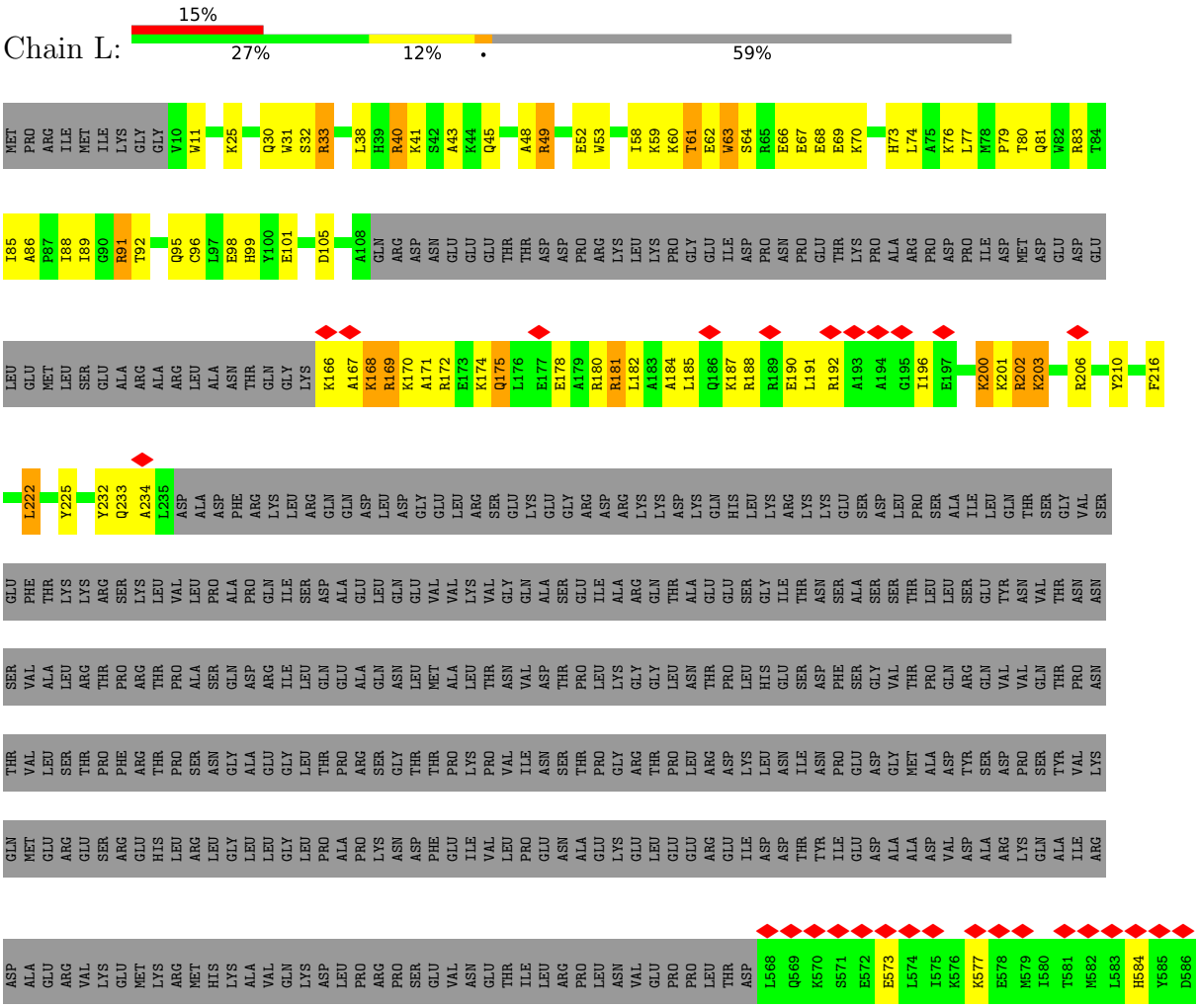
• Molecule 11: RING finger protein 113A

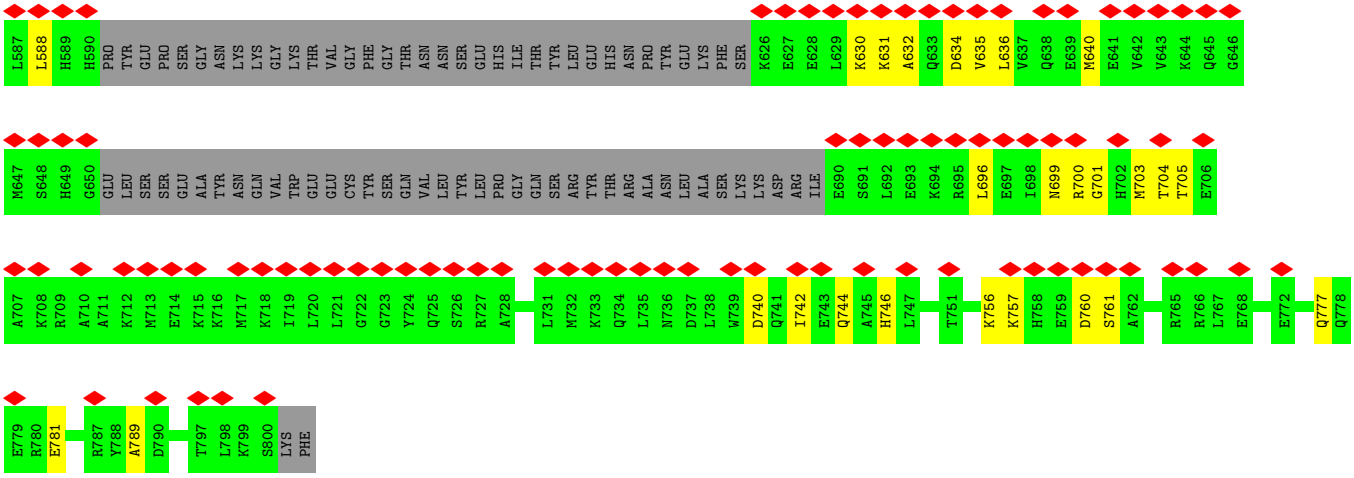
Chain K:



• Molecule 12: Cell division cycle 5-like protein

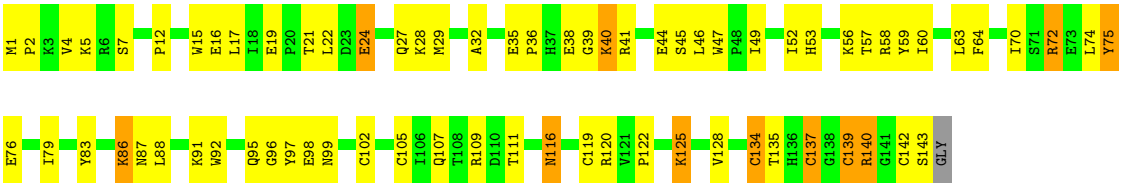
Chain L:





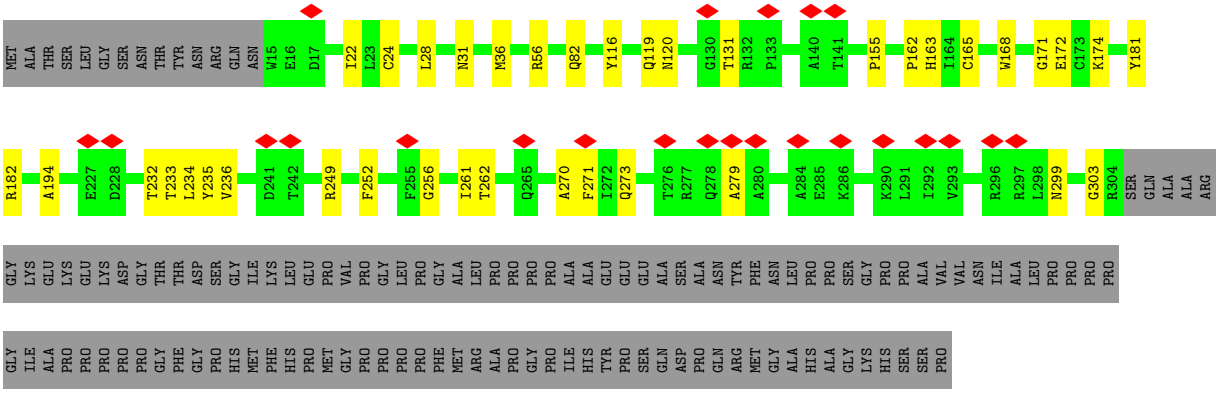
• Molecule 13: Protein BUD31 homolog

Chain N:



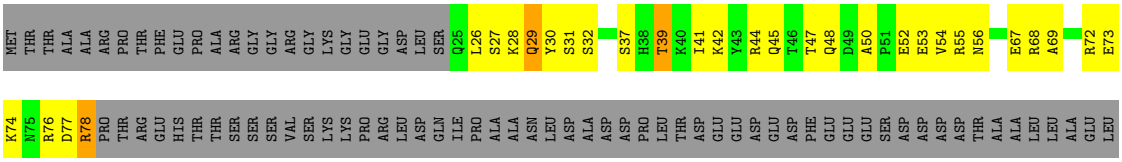
• Molecule 14: Pre-mRNA-splicing factor RBM22

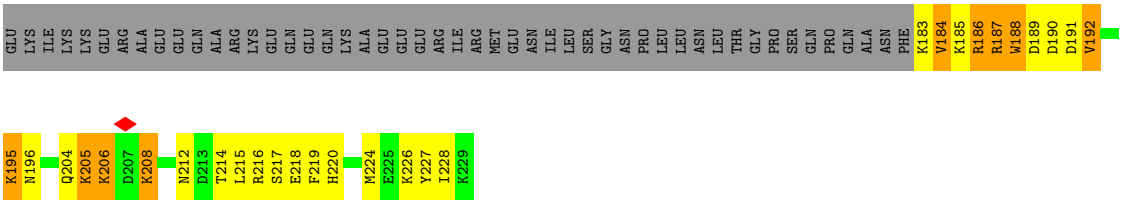
Chain O:



• Molecule 15: Spliceosome-associated protein CWC15 homolog

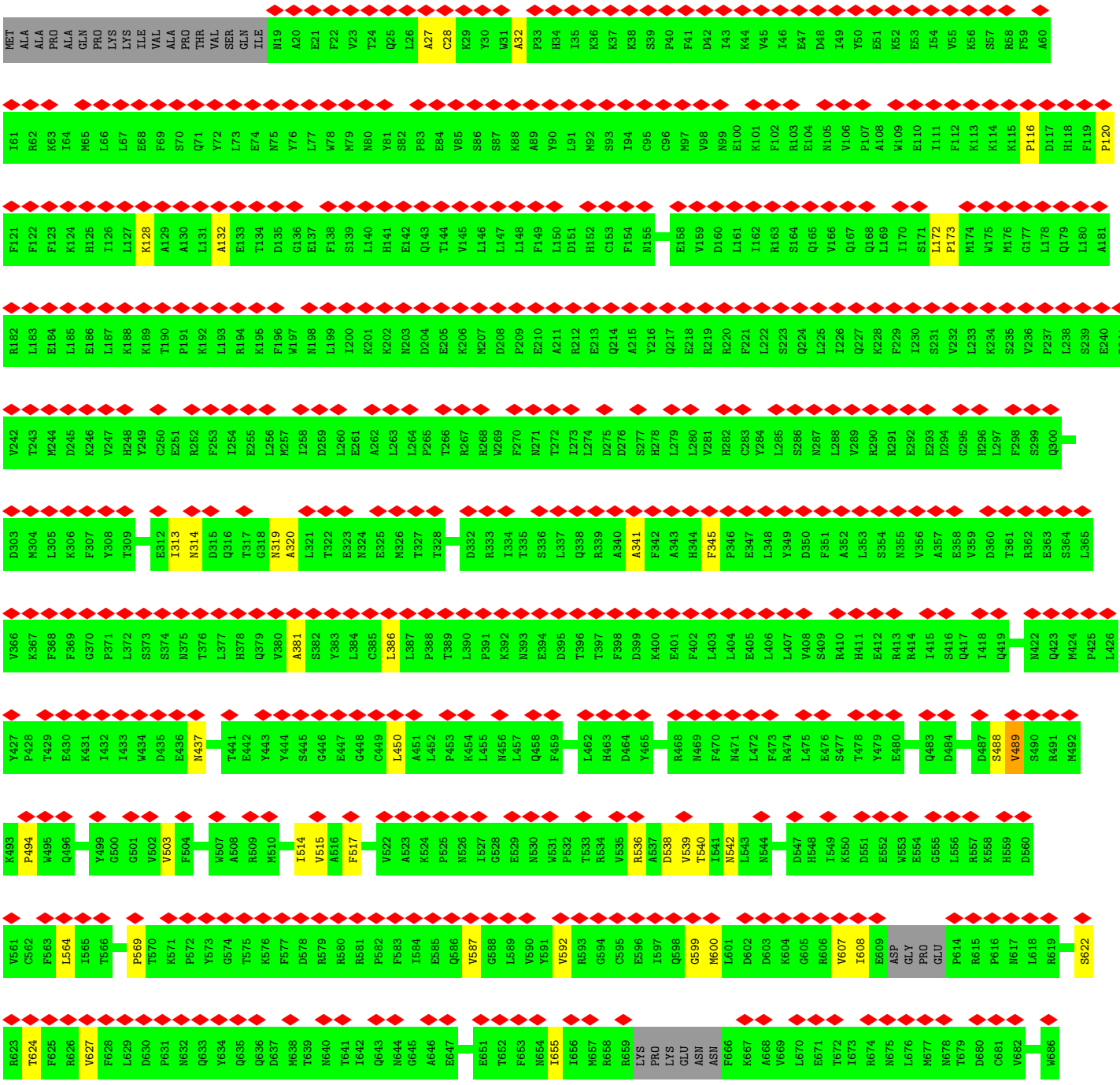
Chain P:

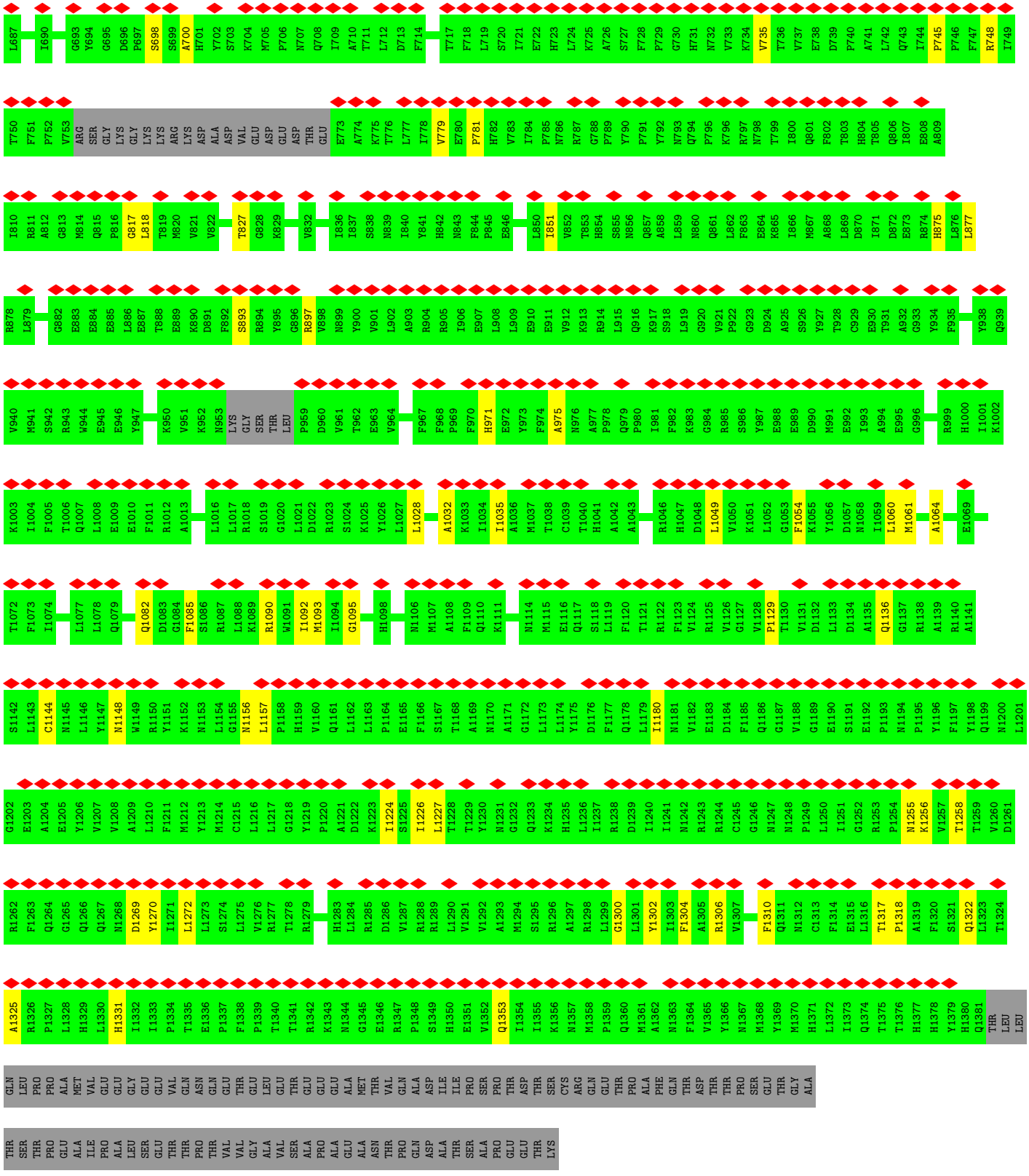




- Molecule 16: RNA helicase aquarius

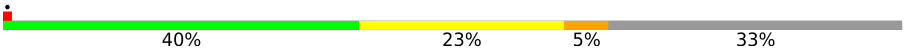
Chain Q:

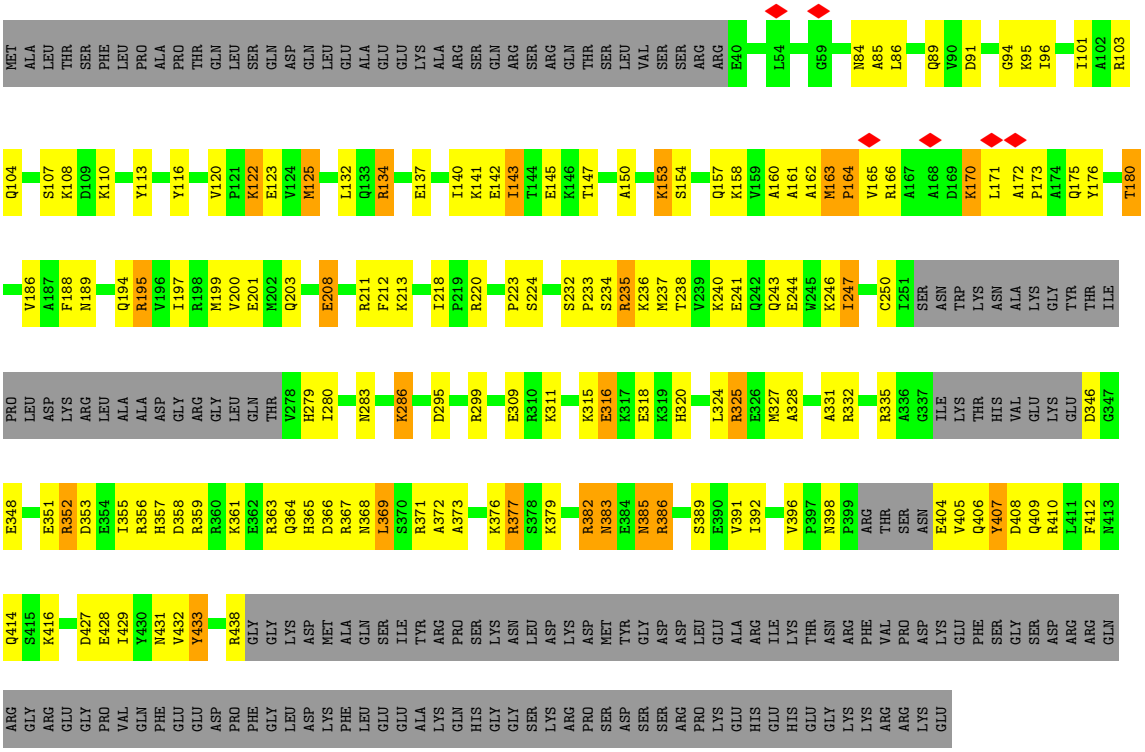




• Molecule 17: SNW domain-containing protein 1

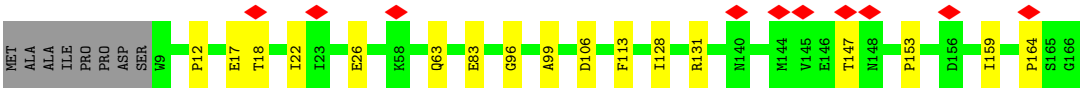
Chain R:





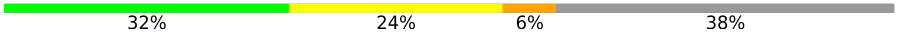
• Molecule 18: Peptidyl-prolyl cis-trans isomerase-like 1

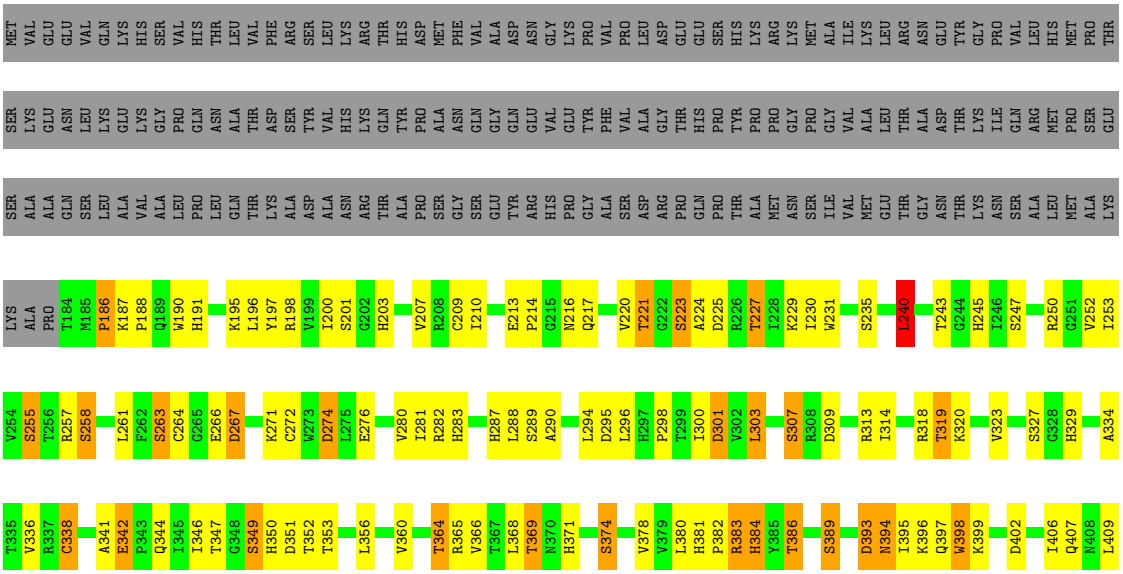
Chain S:

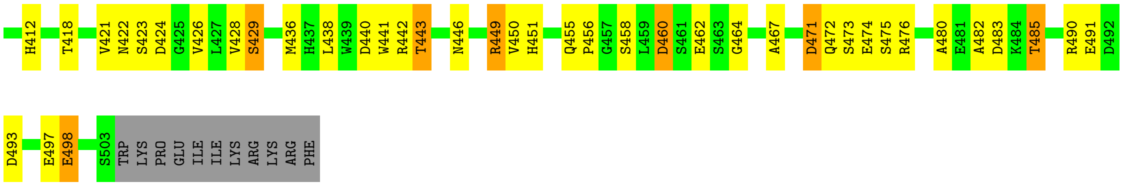


• Molecule 19: Pleiotropic regulator 1

Chain T:

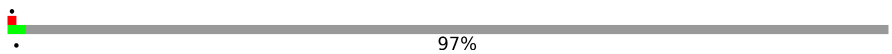


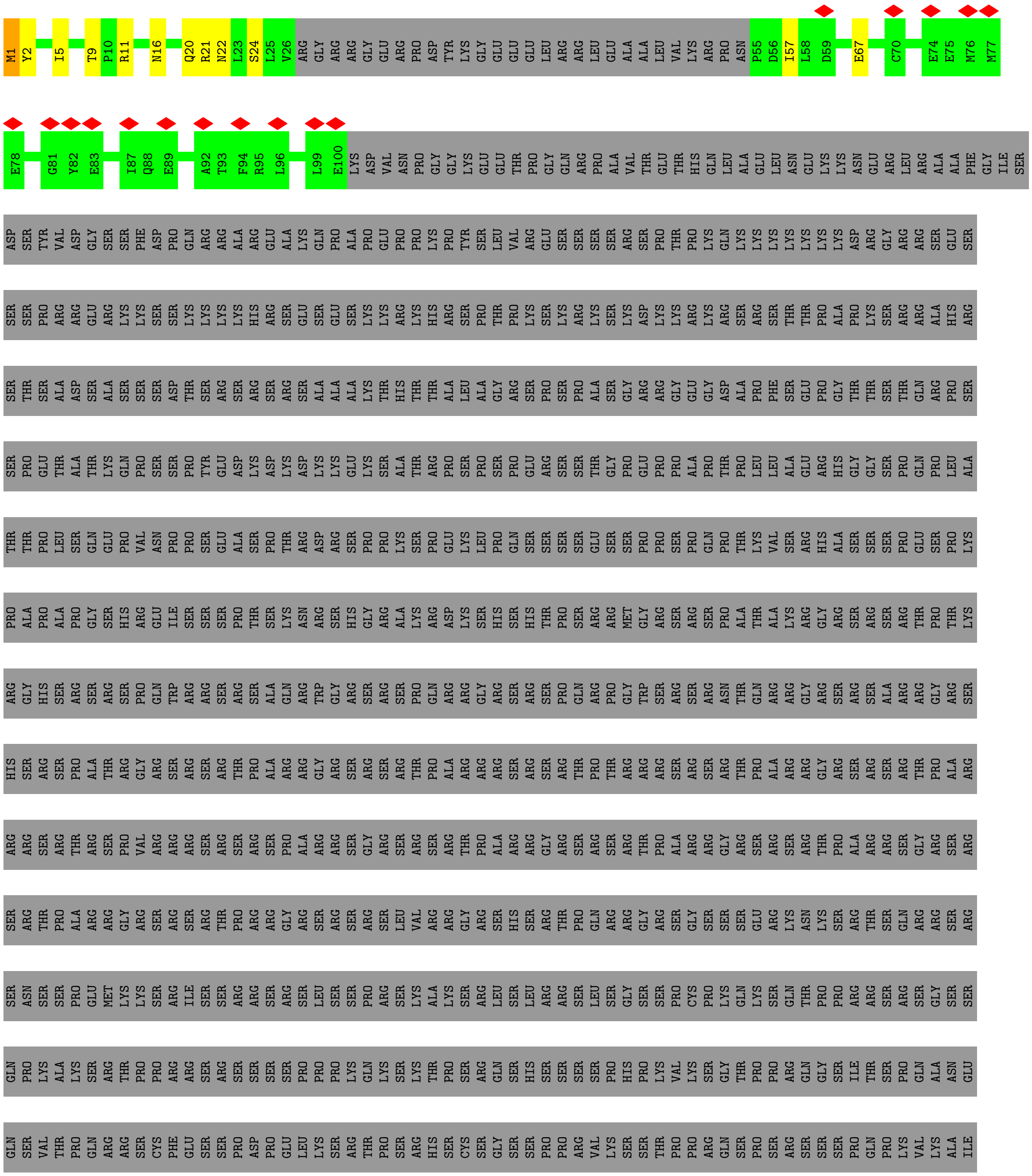




- Molecule 20: Serine/arginine repetitive matrix protein 2

Chain U:





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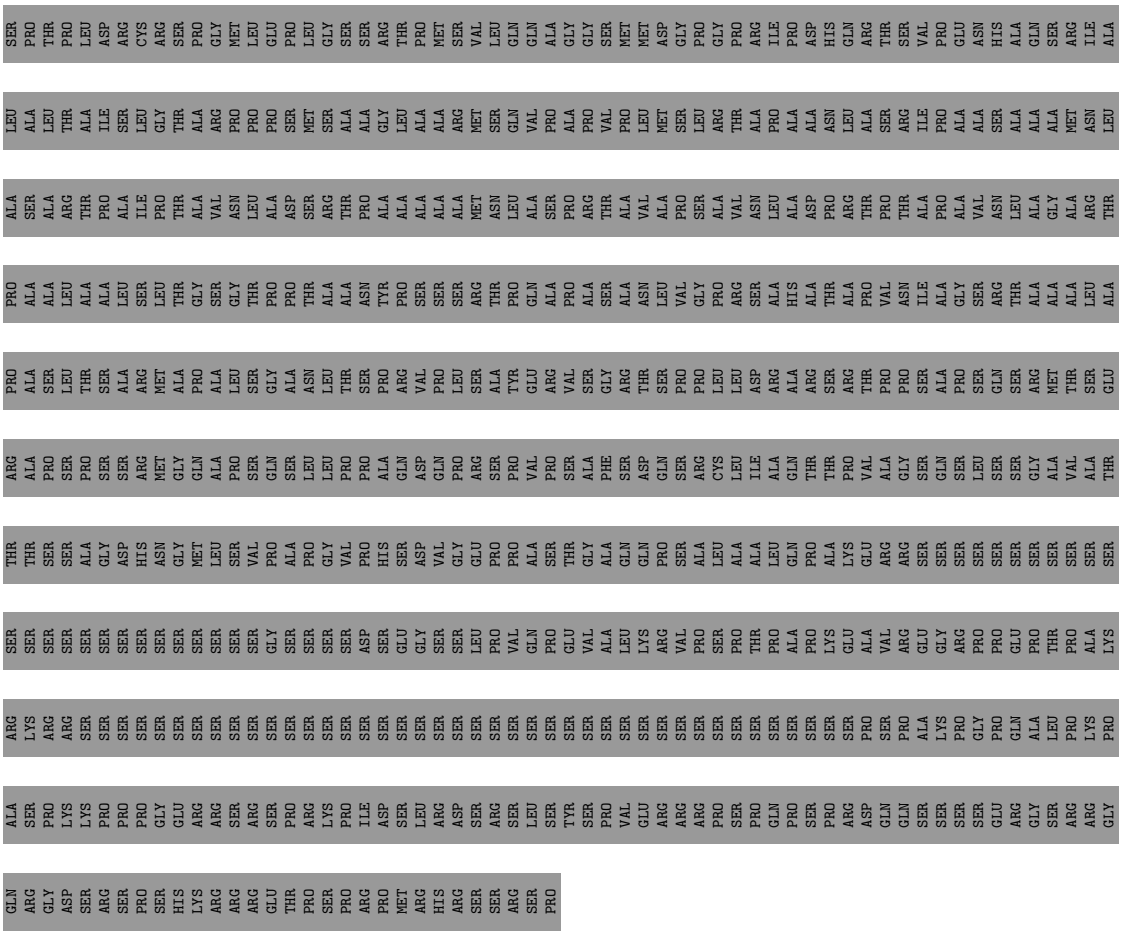
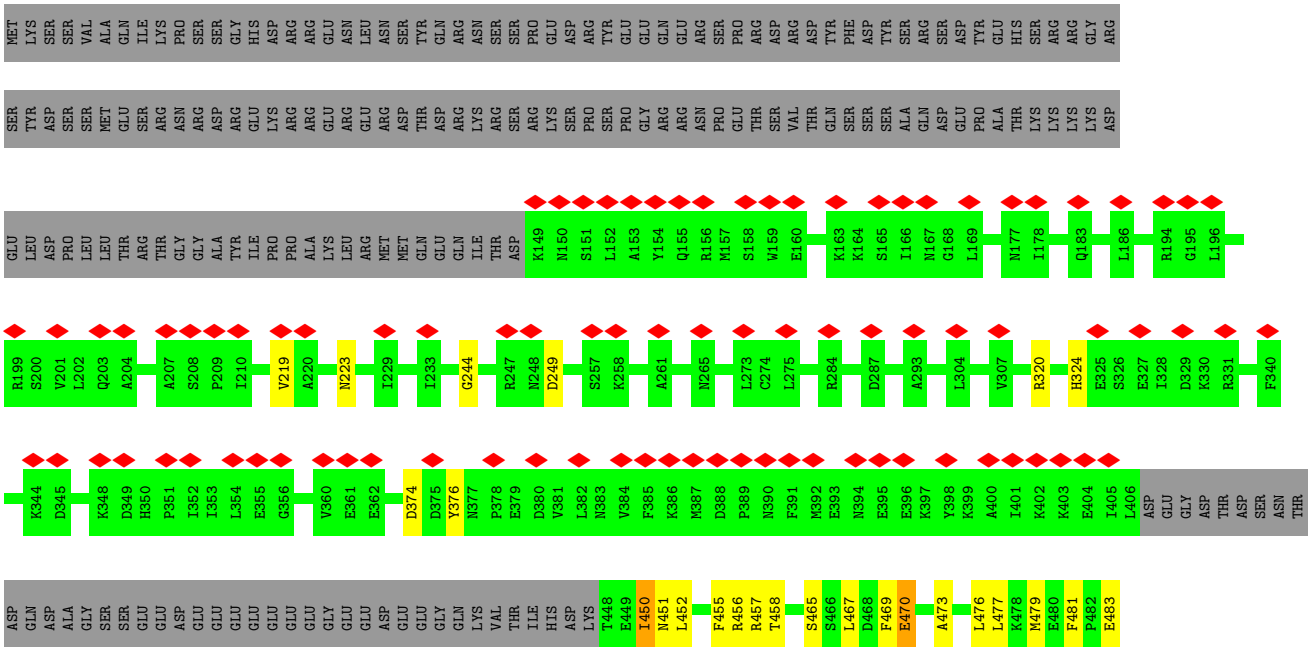
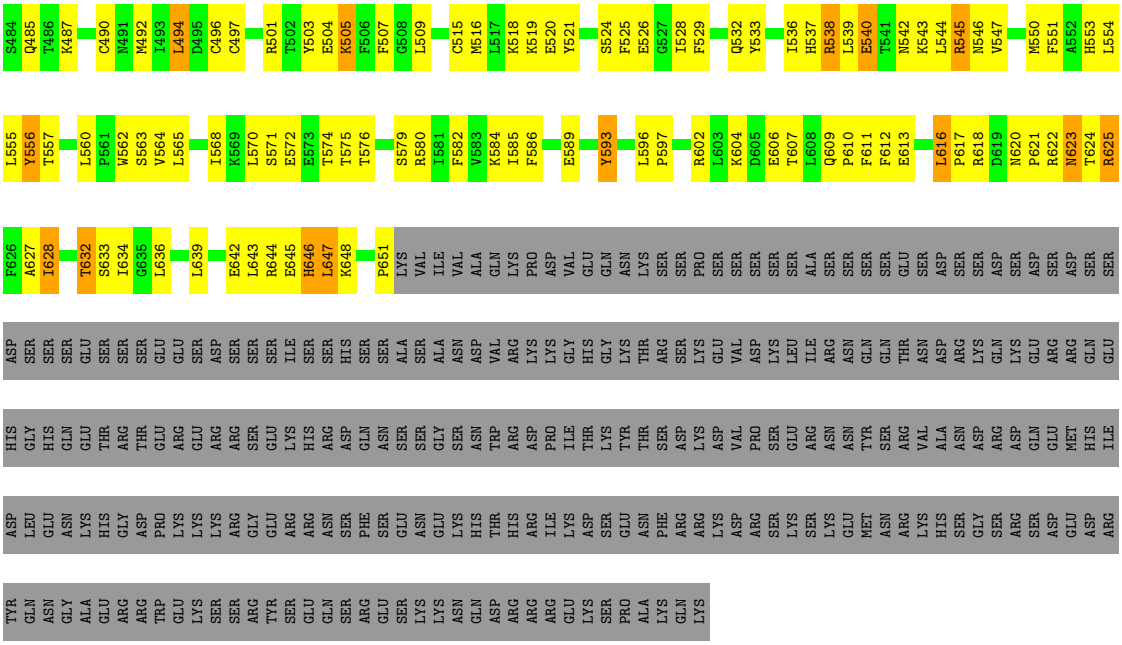


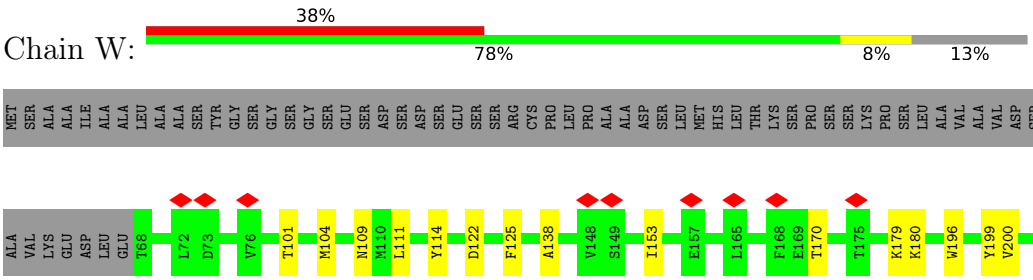
• Molecule 21: Pre-mRNA-splicing factor CWC22 homolog

Chain V:



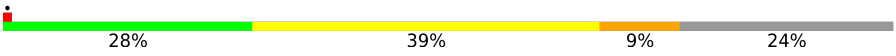


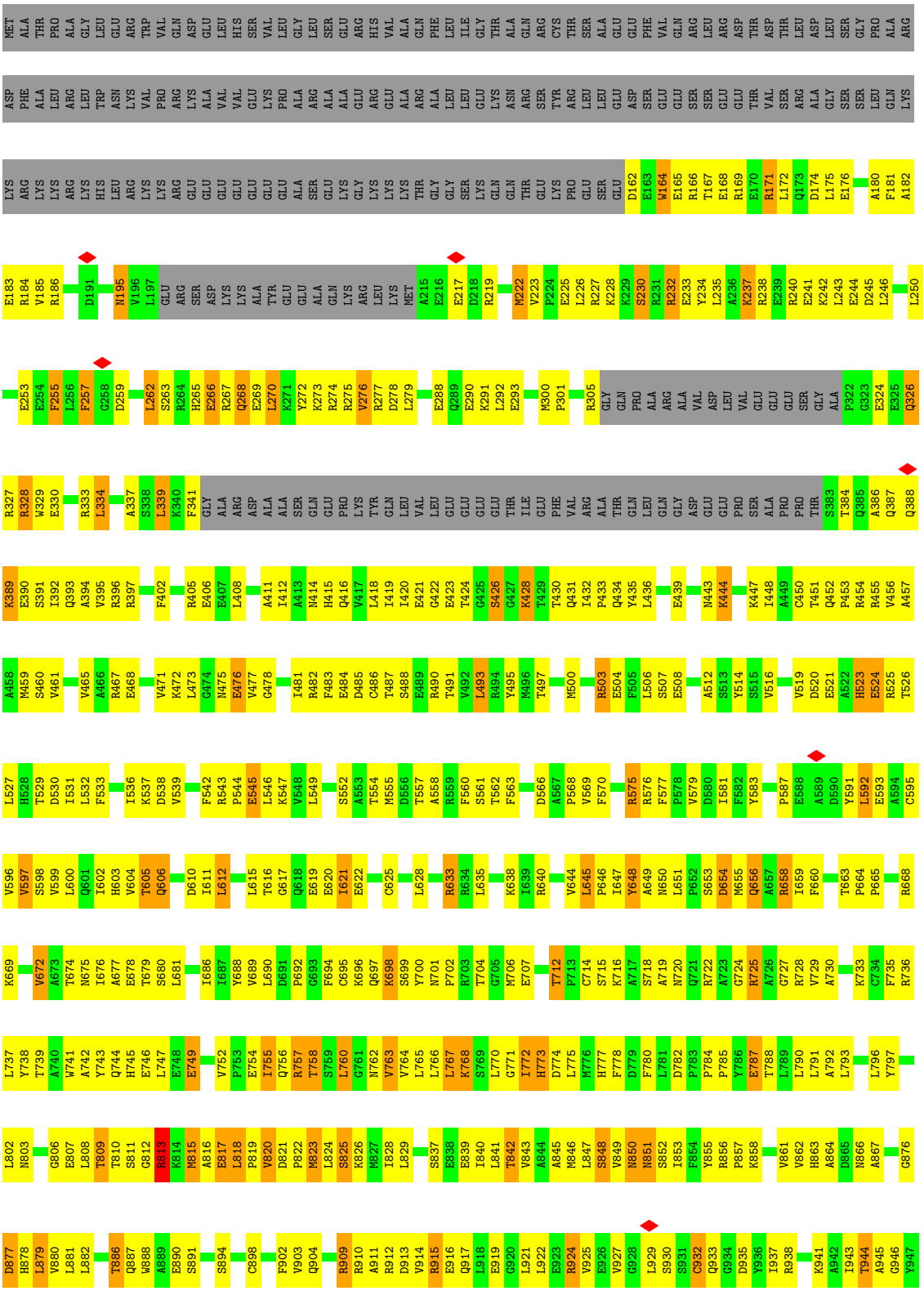
• Molecule 22: Pre-mRNA-processing factor 17

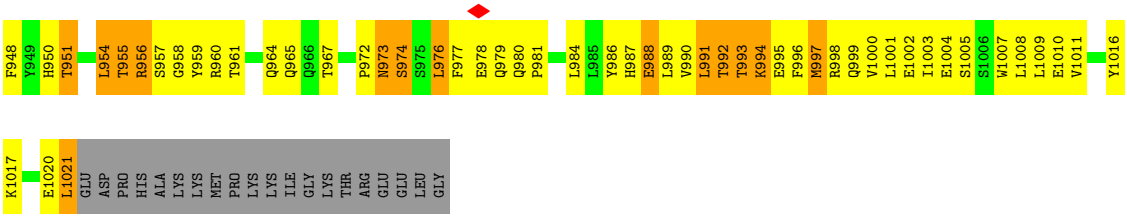


• Molecule 23: Pre-mRNA-splicing factor ATP-dependent RNA helicase DHX16

Chain X:

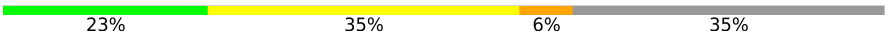


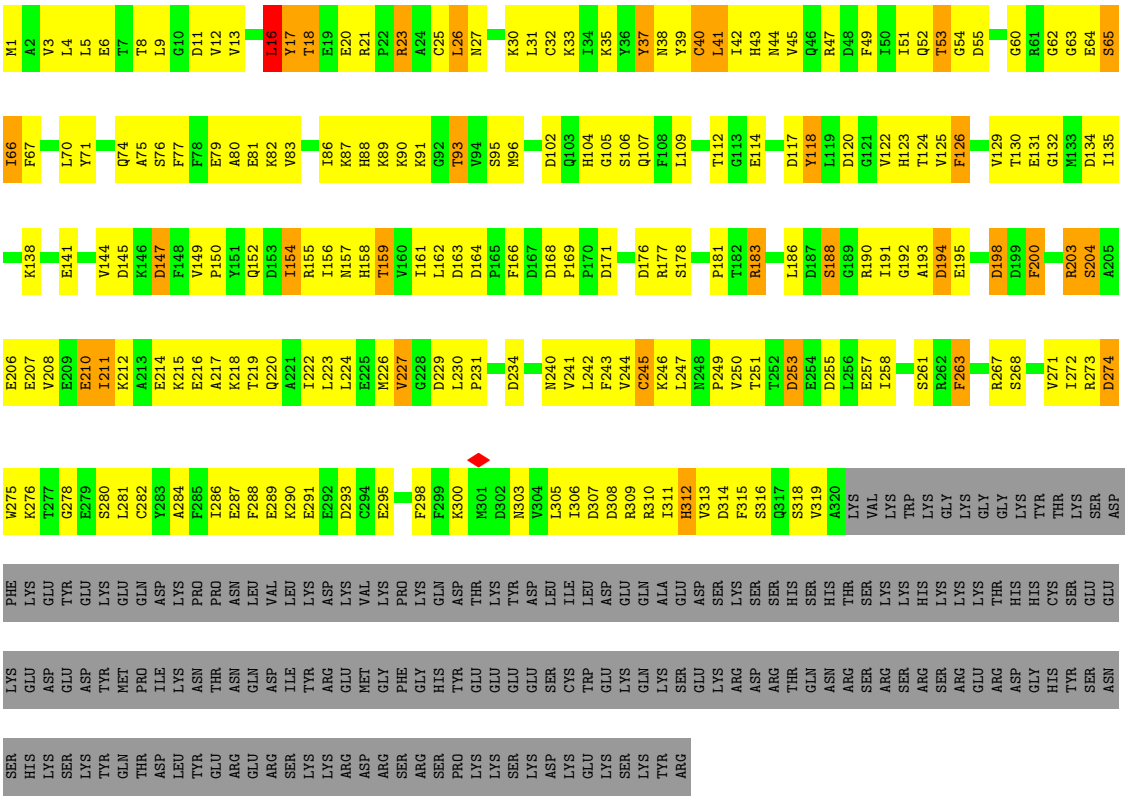




• Molecule 24: Peptidyl-prolyl cis-trans isomerase-like 4

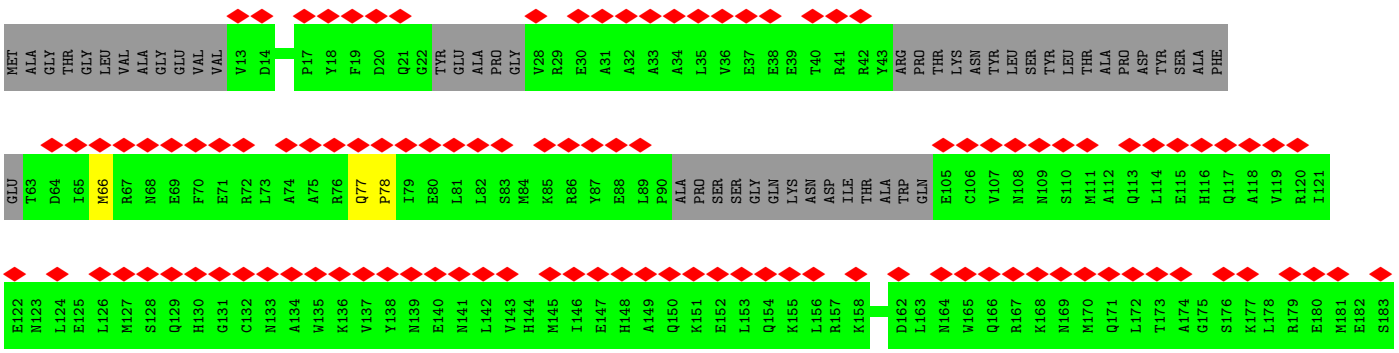
Chain Y:

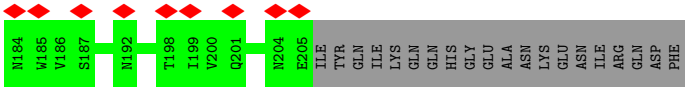




• Molecule 25: Pre-mRNA-splicing factor SPF27

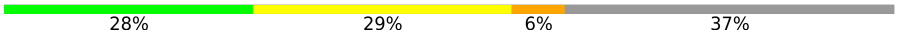
Chain Z:

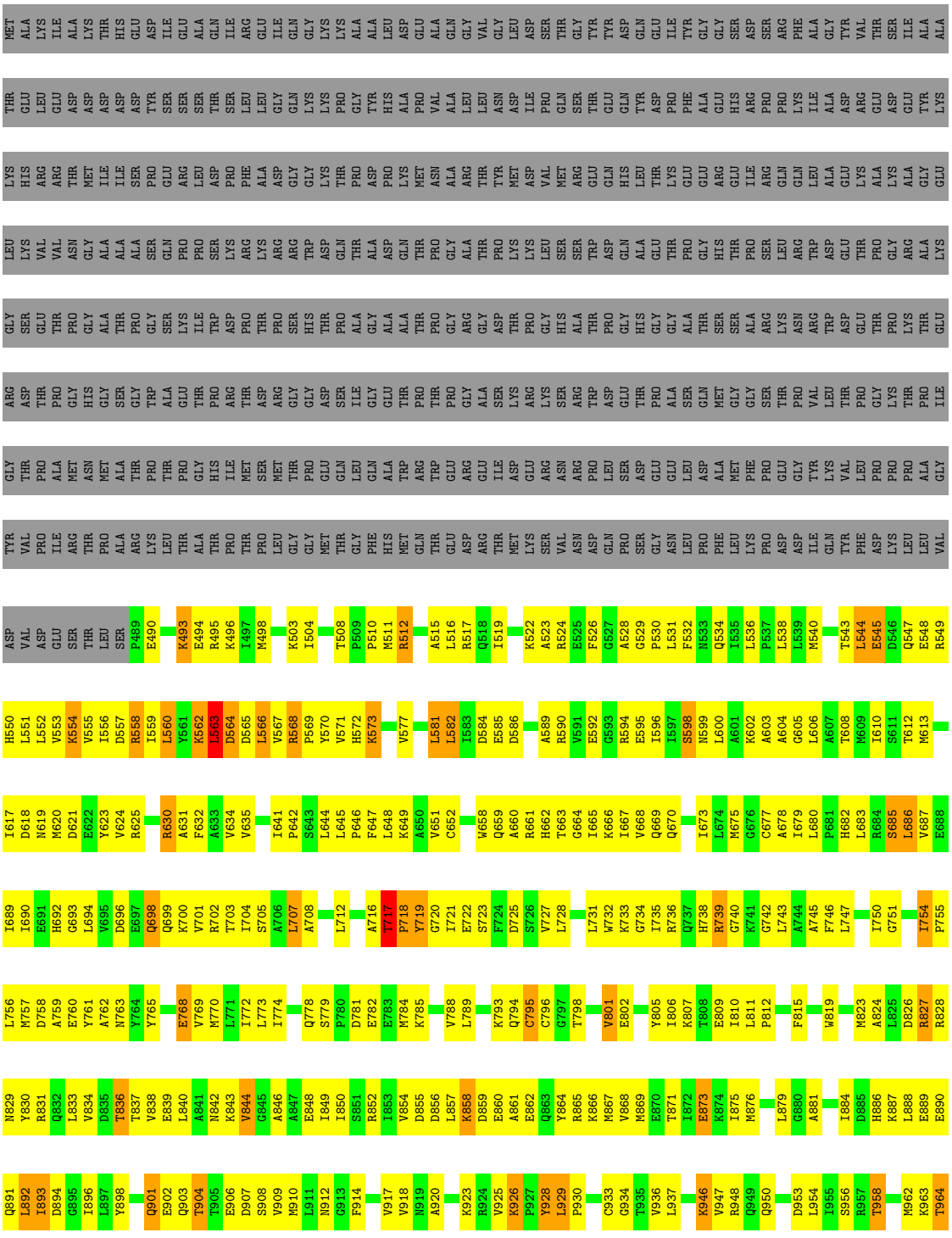


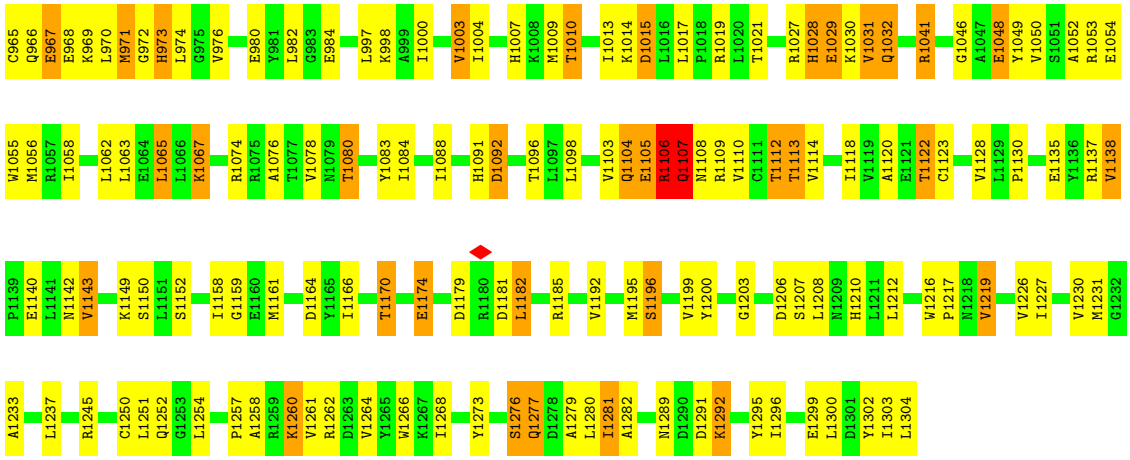


• Molecule 26: Splicing factor 3B subunit 1

Chain 1:

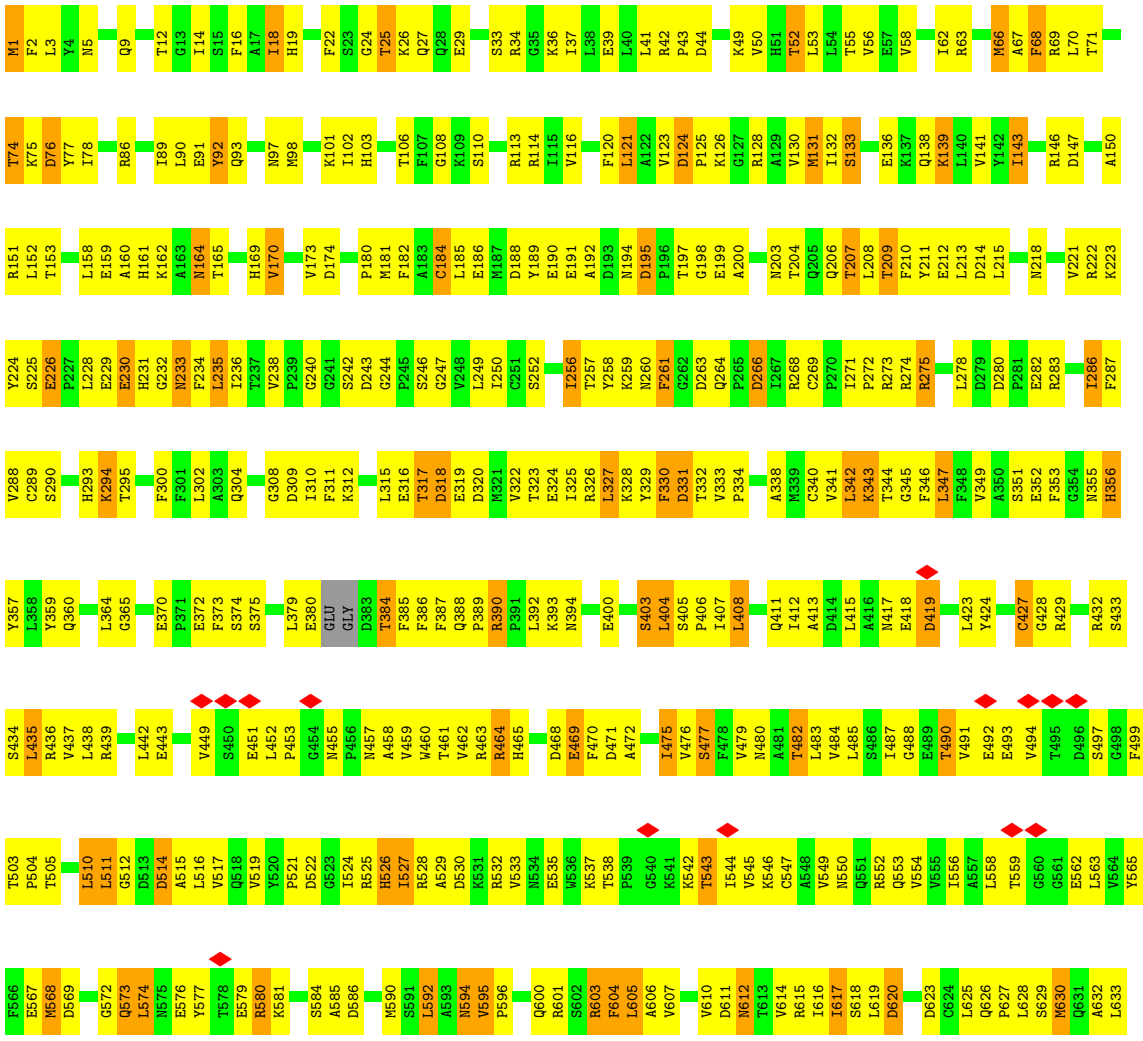


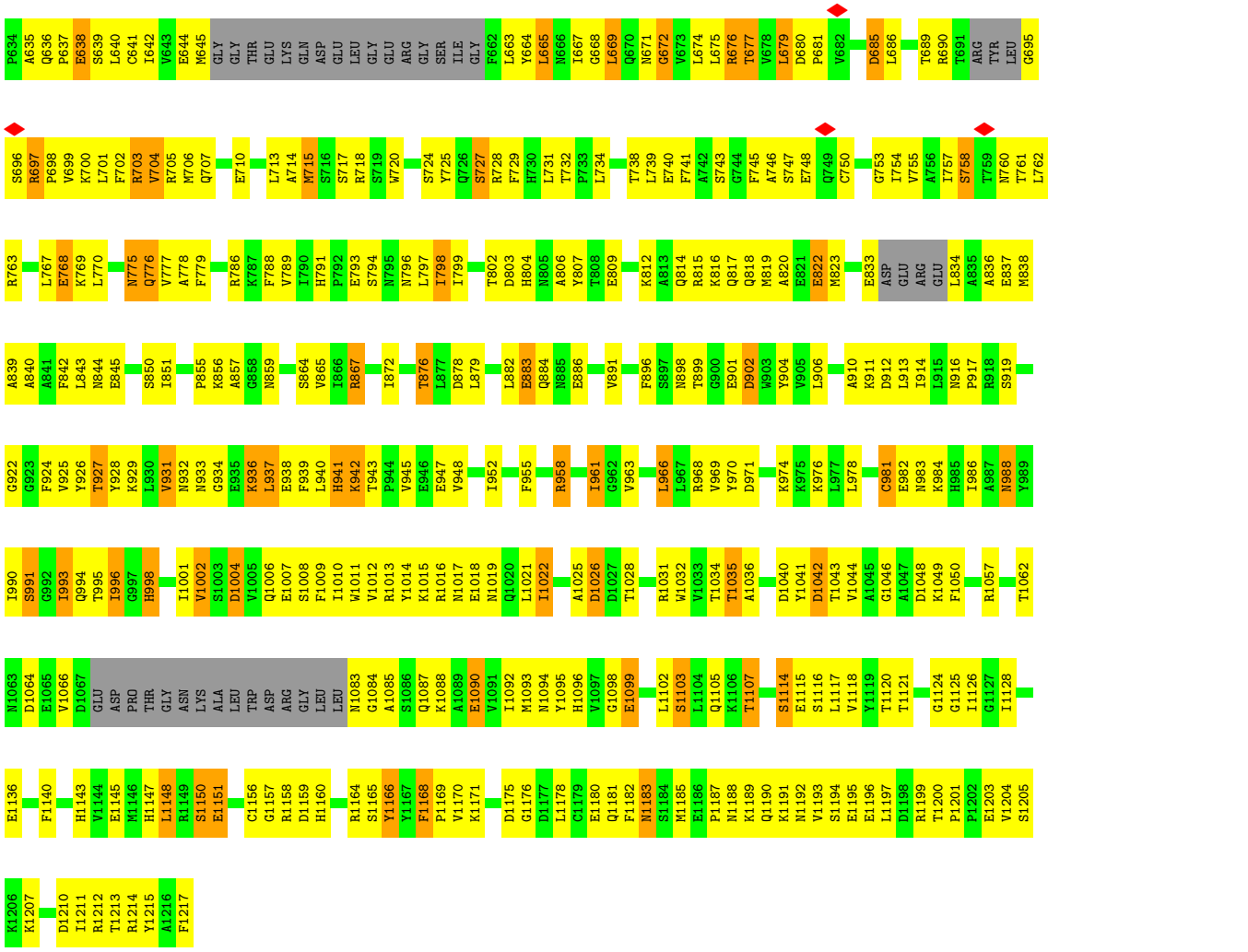




• Molecule 27: Splicing factor 3B subunit 3

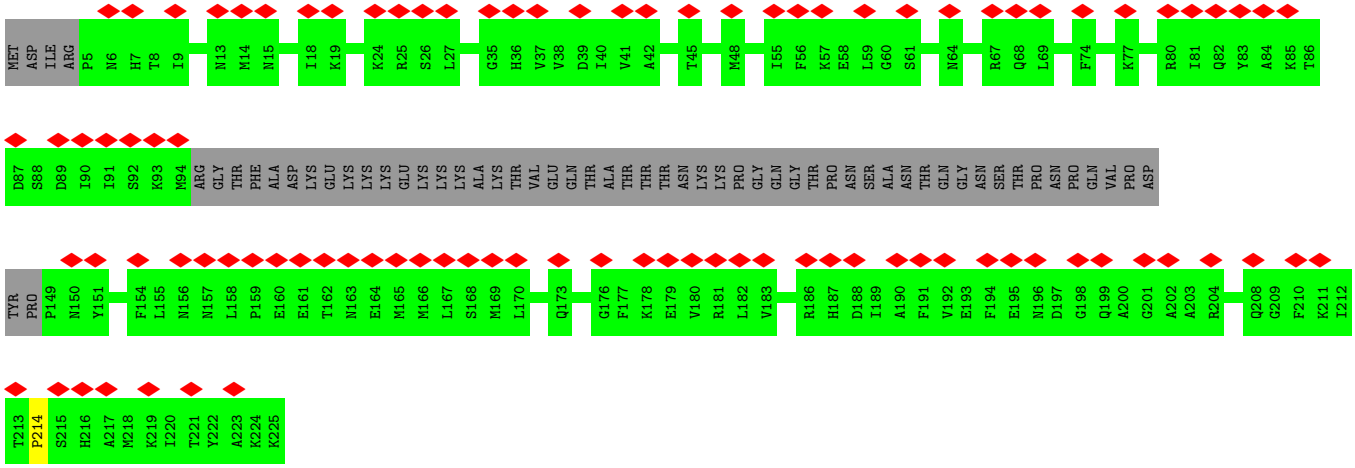
Chain 3:





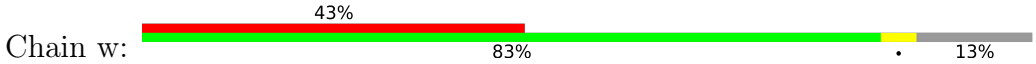
• Molecule 28: U2 small nuclear ribonucleoprotein B"

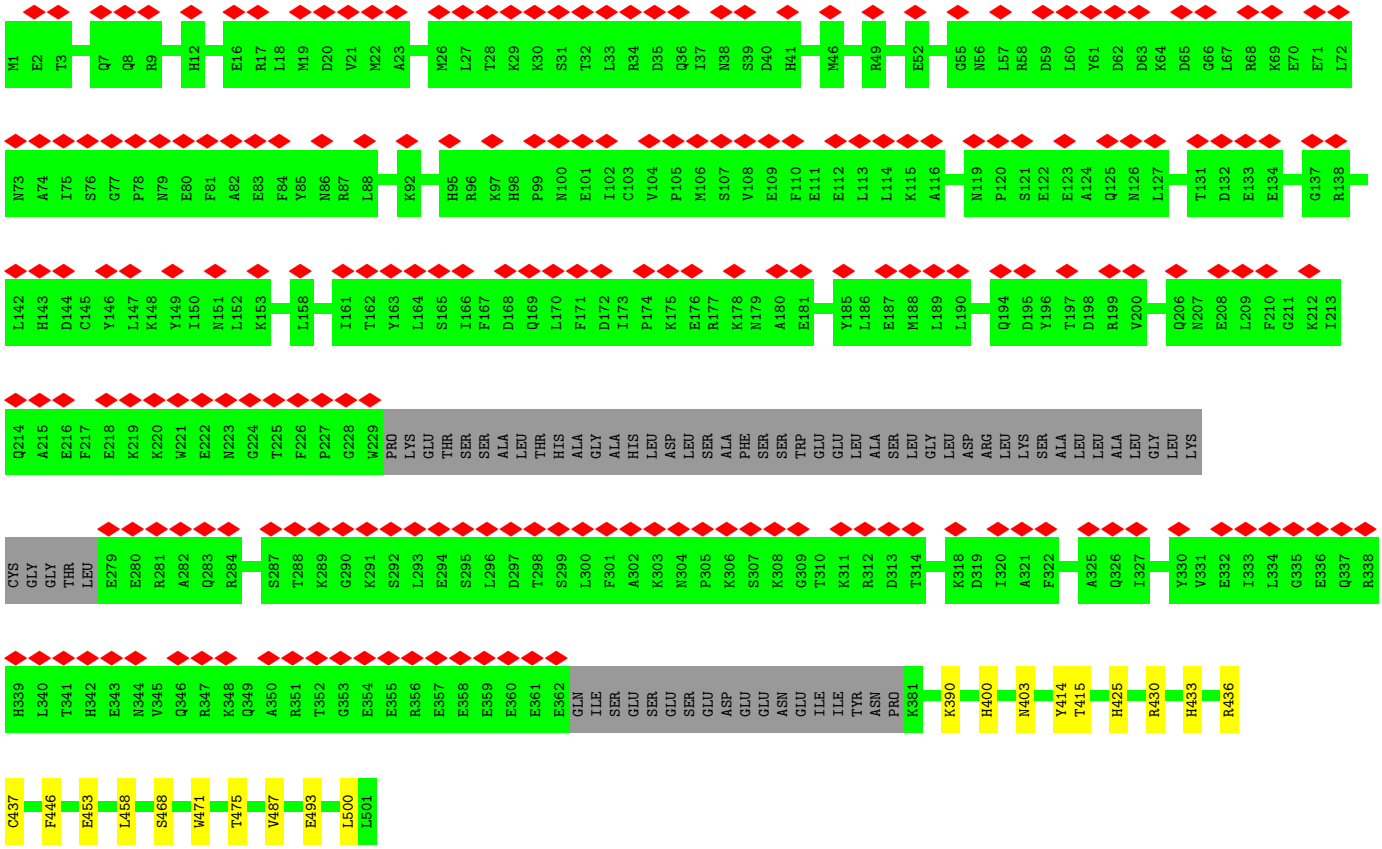
Chain p:



• Molecule 29: Splicing factor 3A subunit 3

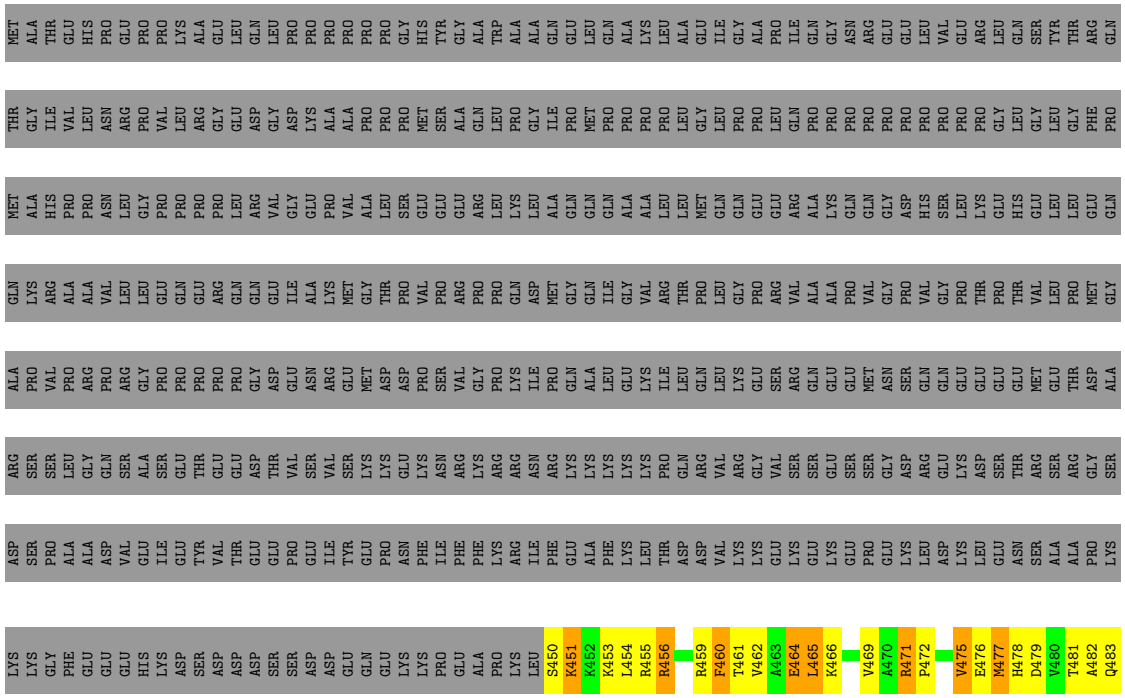
Chain w:

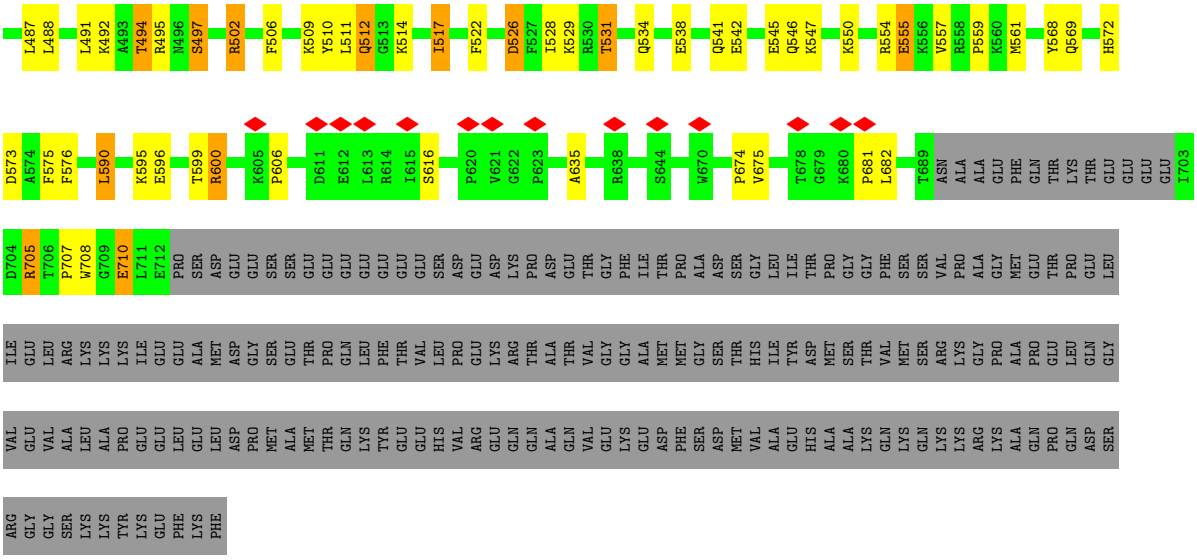




• Molecule 30: Splicing factor 3B subunit 2

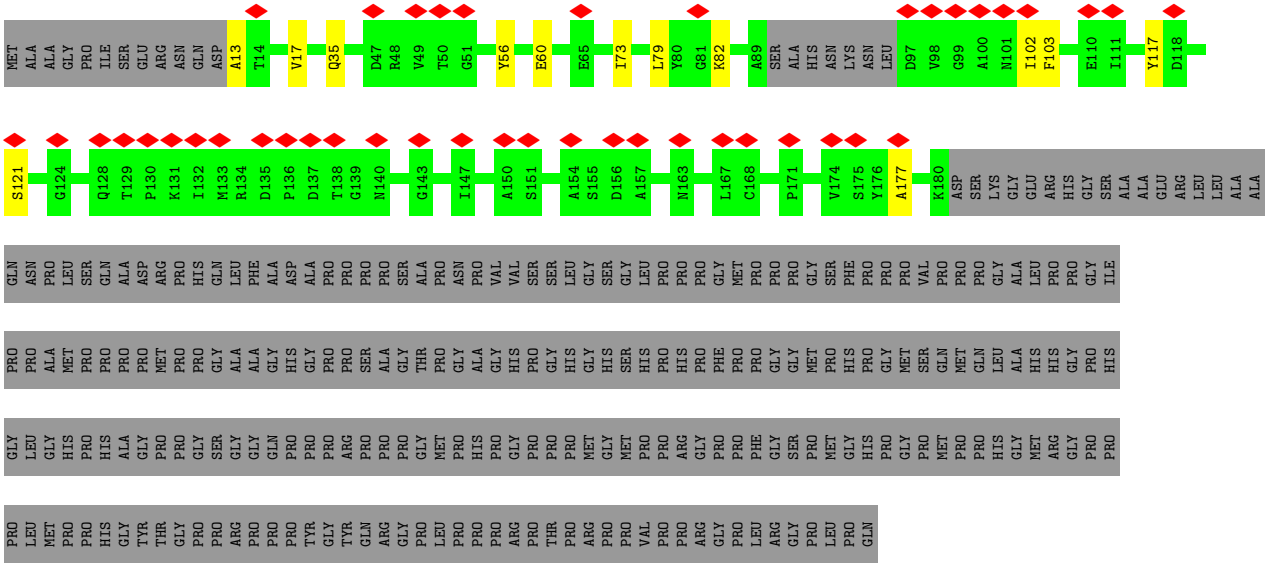
Chain 2:





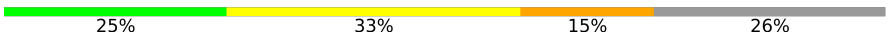
• Molecule 31: Splicing factor 3B subunit 4

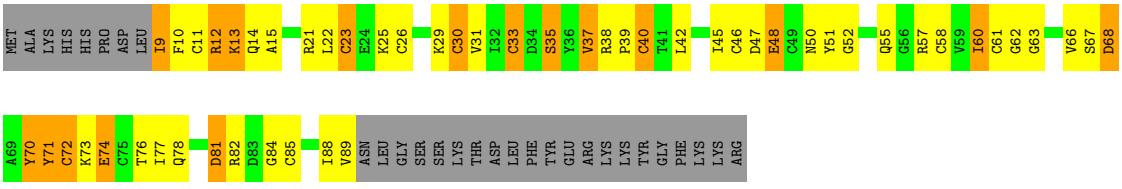
Chain 4:



• Molecule 32: PHD finger-like domain-containing protein 5A

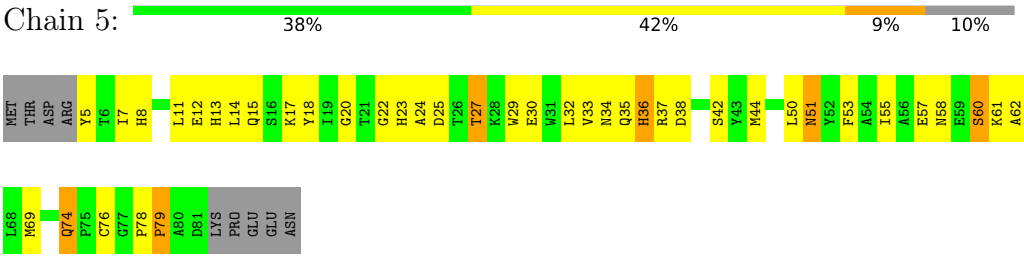
Chain 7:





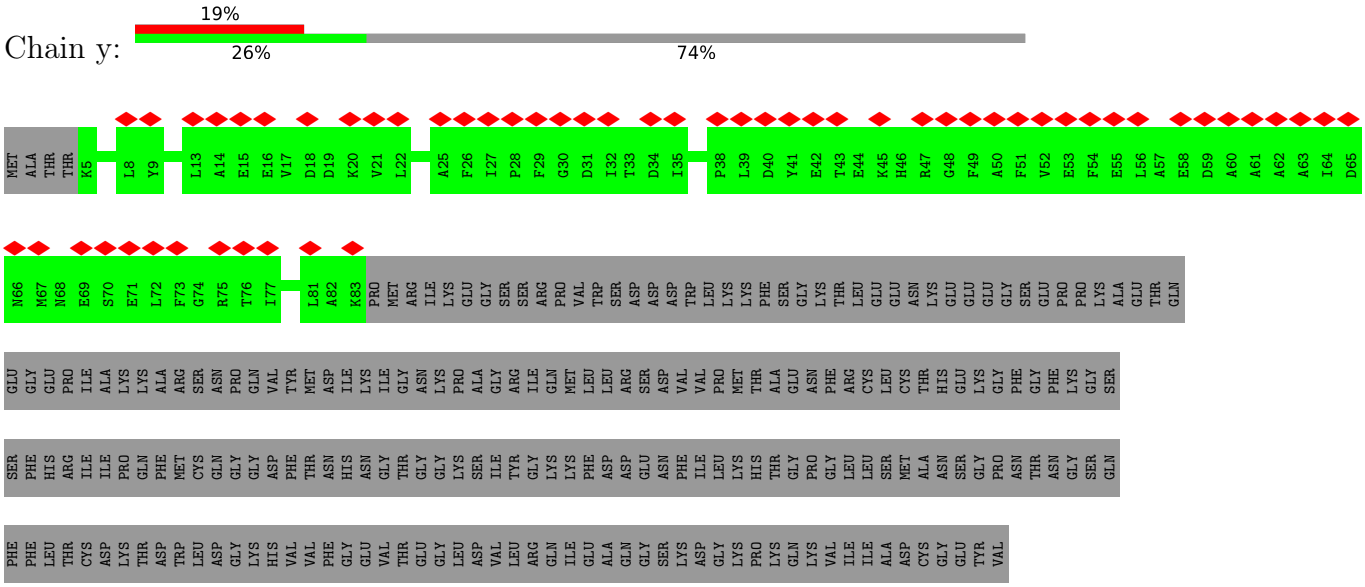
• Molecule 33: Splicing factor 3B subunit 5

Chain 5:



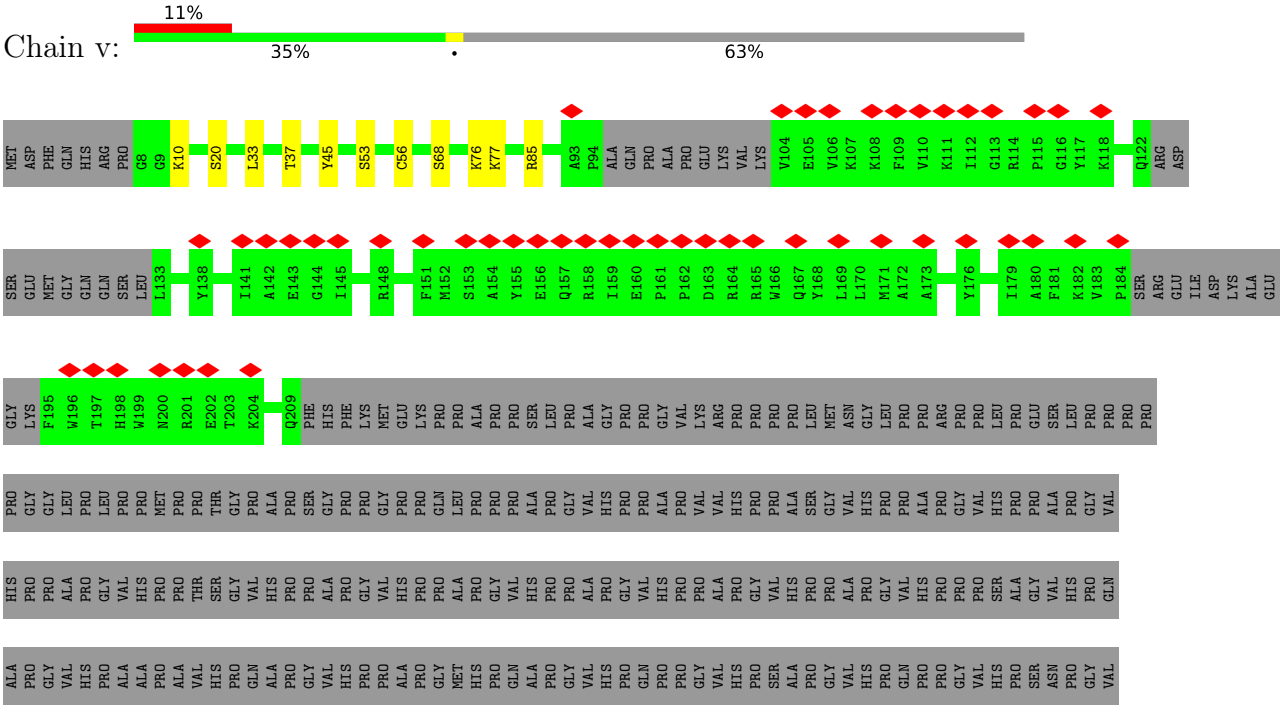
• Molecule 34: Peptidyl-prolyl cis-trans isomerase E

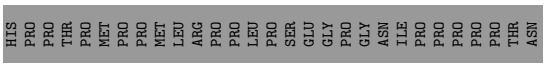
Chain y:



• Molecule 35: Splicing factor 3A subunit 2

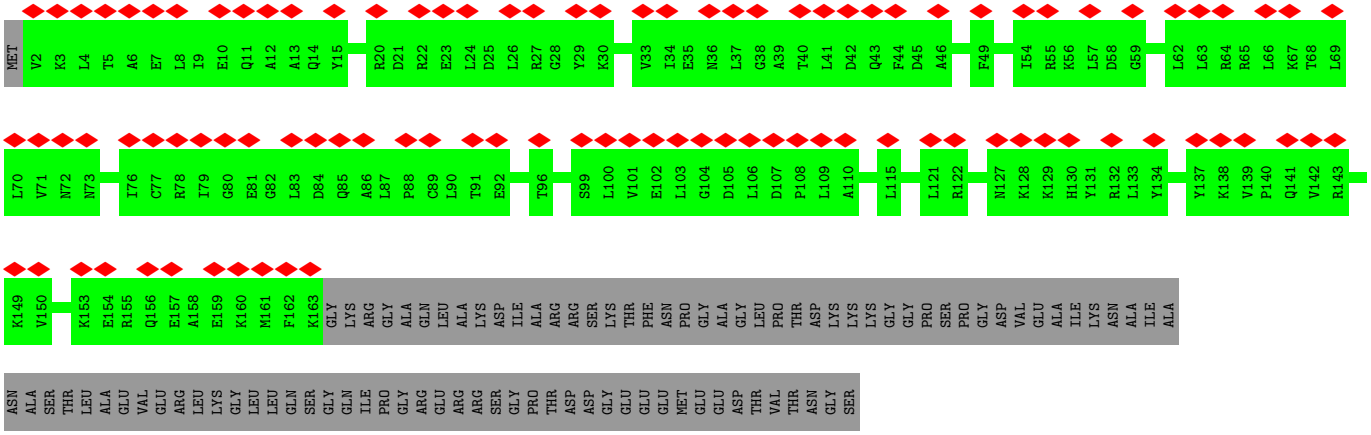
Chain v:





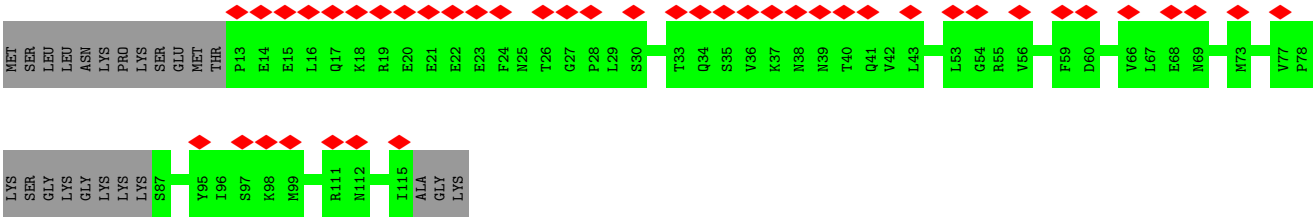
• Molecule 36: U2 small nuclear ribonucleoprotein A'

Chain o:



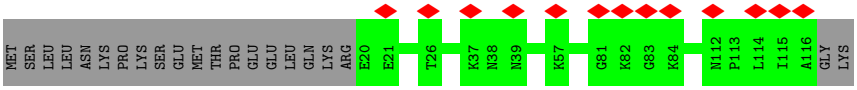
• Molecule 37: Small nuclear ribonucleoprotein Sm D2

Chain h:



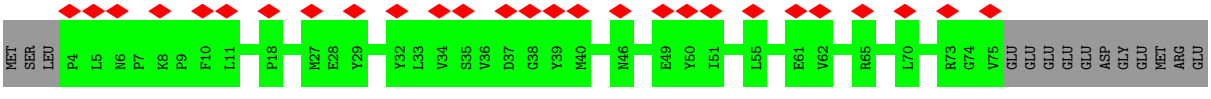
• Molecule 37: Small nuclear ribonucleoprotein Sm D2

Chain c:



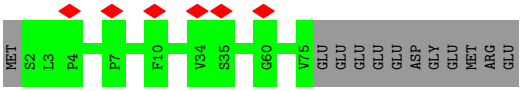
• Molecule 38: Small nuclear ribonucleoprotein F

Chain i:



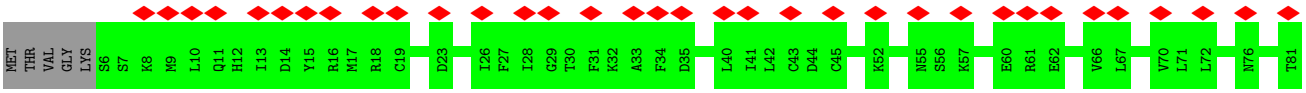
• Molecule 38: Small nuclear ribonucleoprotein F

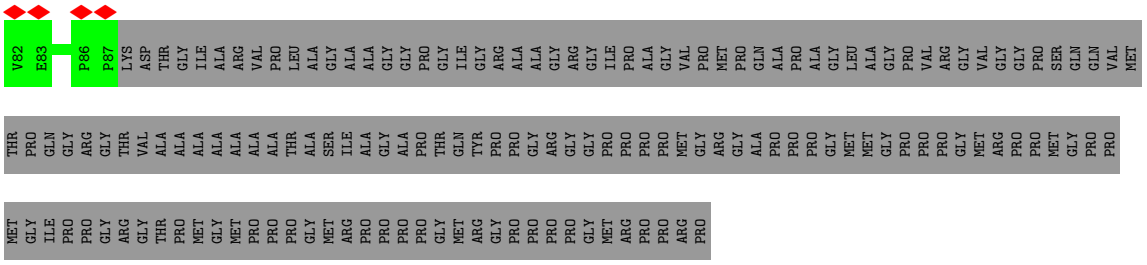
Chain d:



• Molecule 39: Small nuclear ribonucleoprotein-associated proteins B and B'

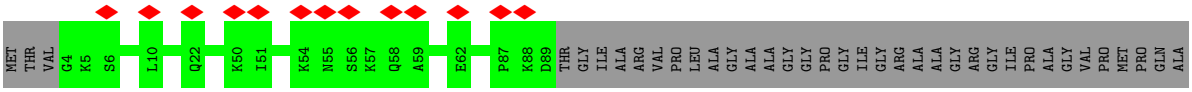
Chain m:





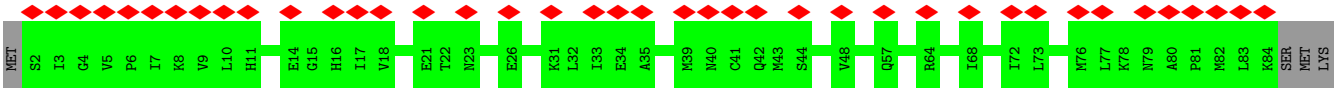
• Molecule 39: Small nuclear ribonucleoprotein-associated proteins B and B'

Chain a:



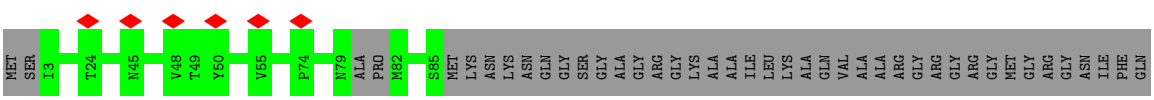
• Molecule 40: Small nuclear ribonucleoprotein Sm D3

Chain l:



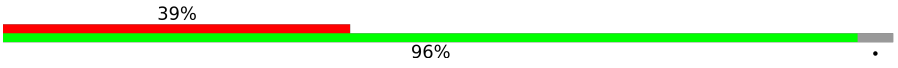
• Molecule 40: Small nuclear ribonucleoprotein Sm D3

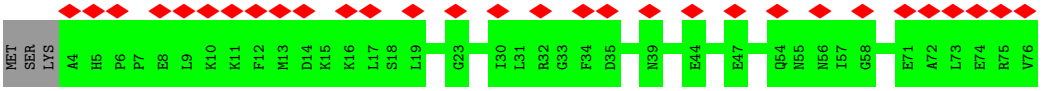
Chain g:



• Molecule 41: Small nuclear ribonucleoprotein G

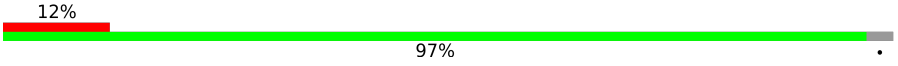
Chain k:

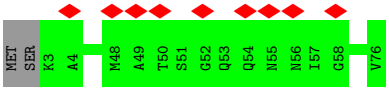




• Molecule 41: Small nuclear ribonucleoprotein G

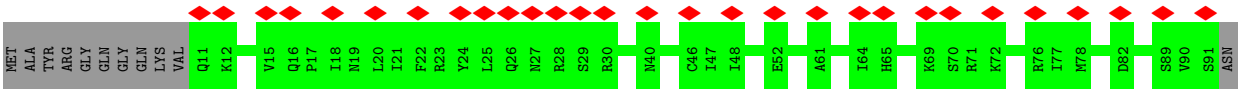
Chain f:





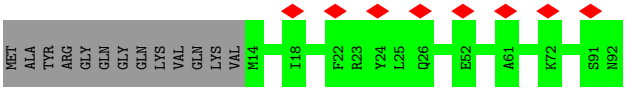
• Molecule 42: Small nuclear ribonucleoprotein E

Chain j:



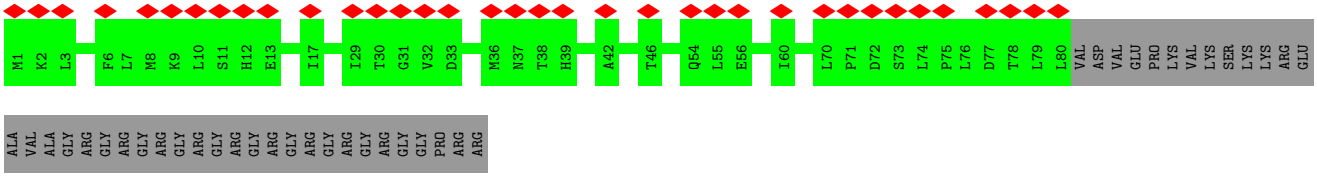
• Molecule 42: Small nuclear ribonucleoprotein E

Chain e:



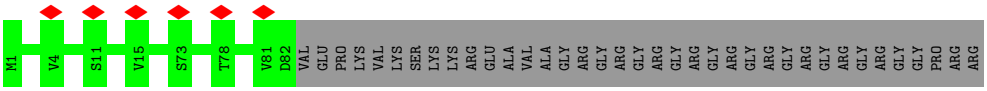
• Molecule 43: Small nuclear ribonucleoprotein Sm D1

Chain n:



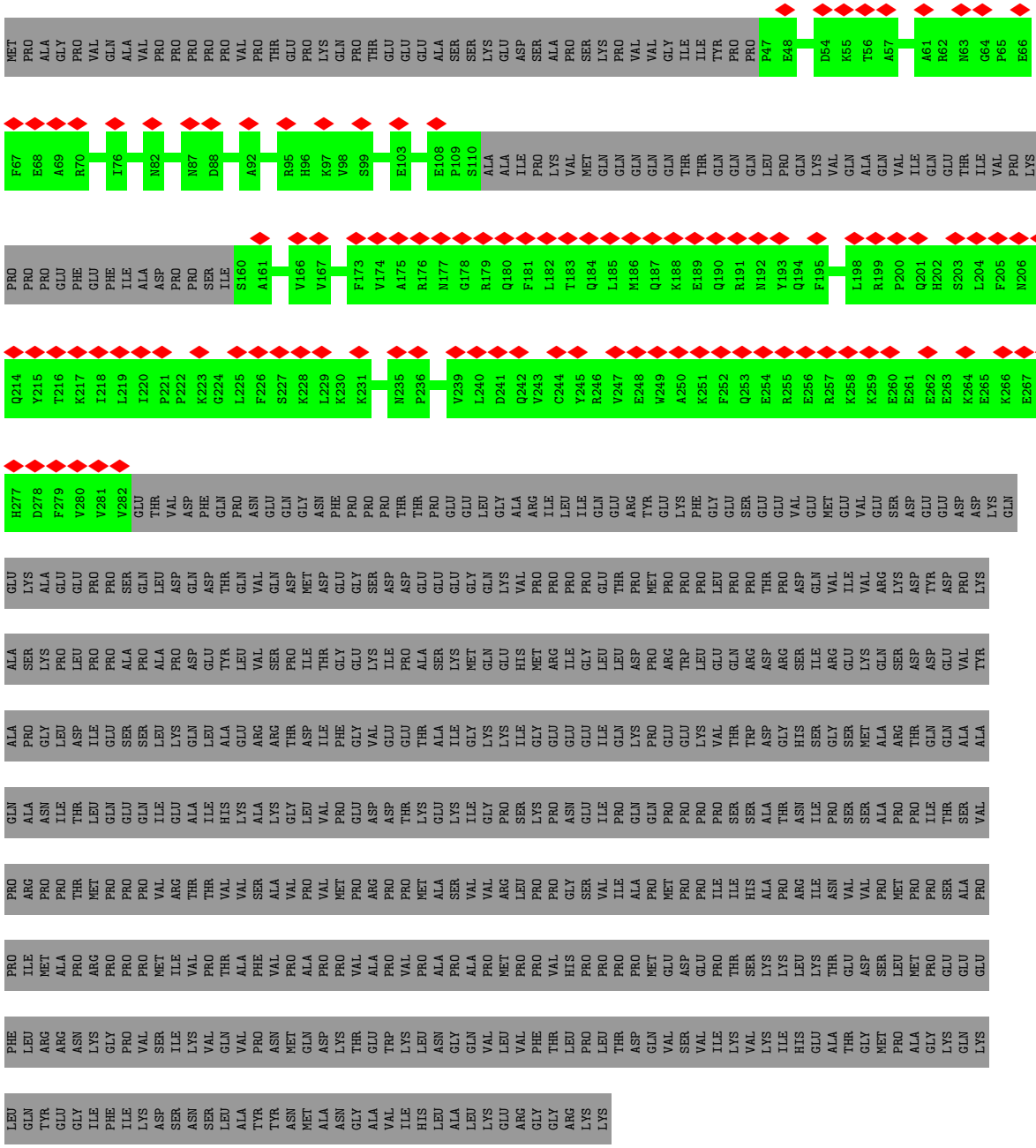
• Molecule 43: Small nuclear ribonucleoprotein Sm D1

Chain b:



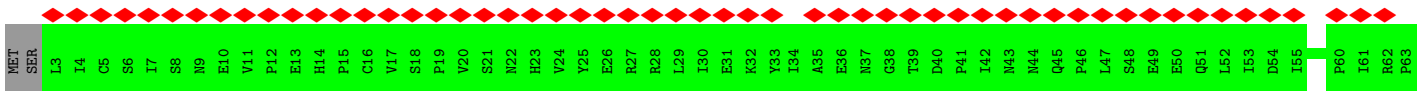
• Molecule 44: Splicing factor 3A subunit 1

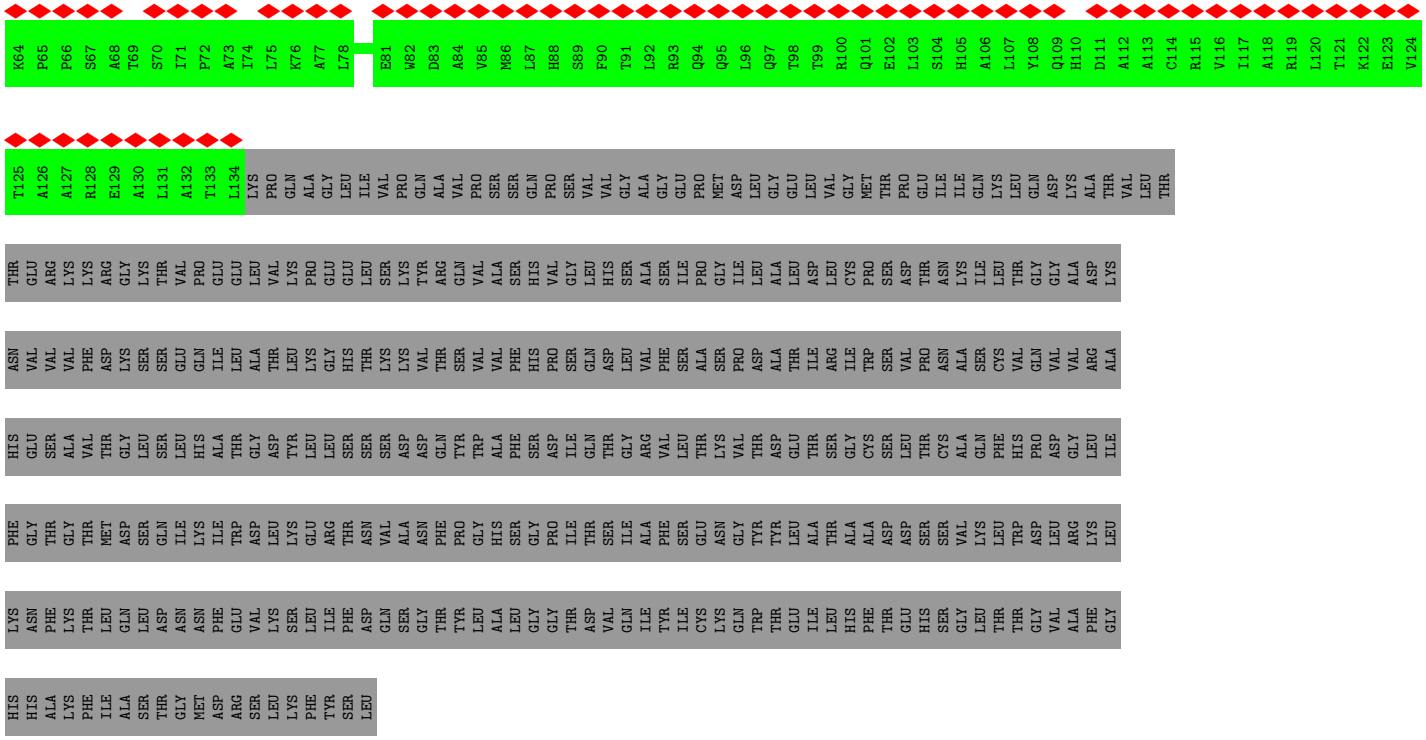
Chain u:



• Molecule 45: Pre-mRNA-processing factor 19

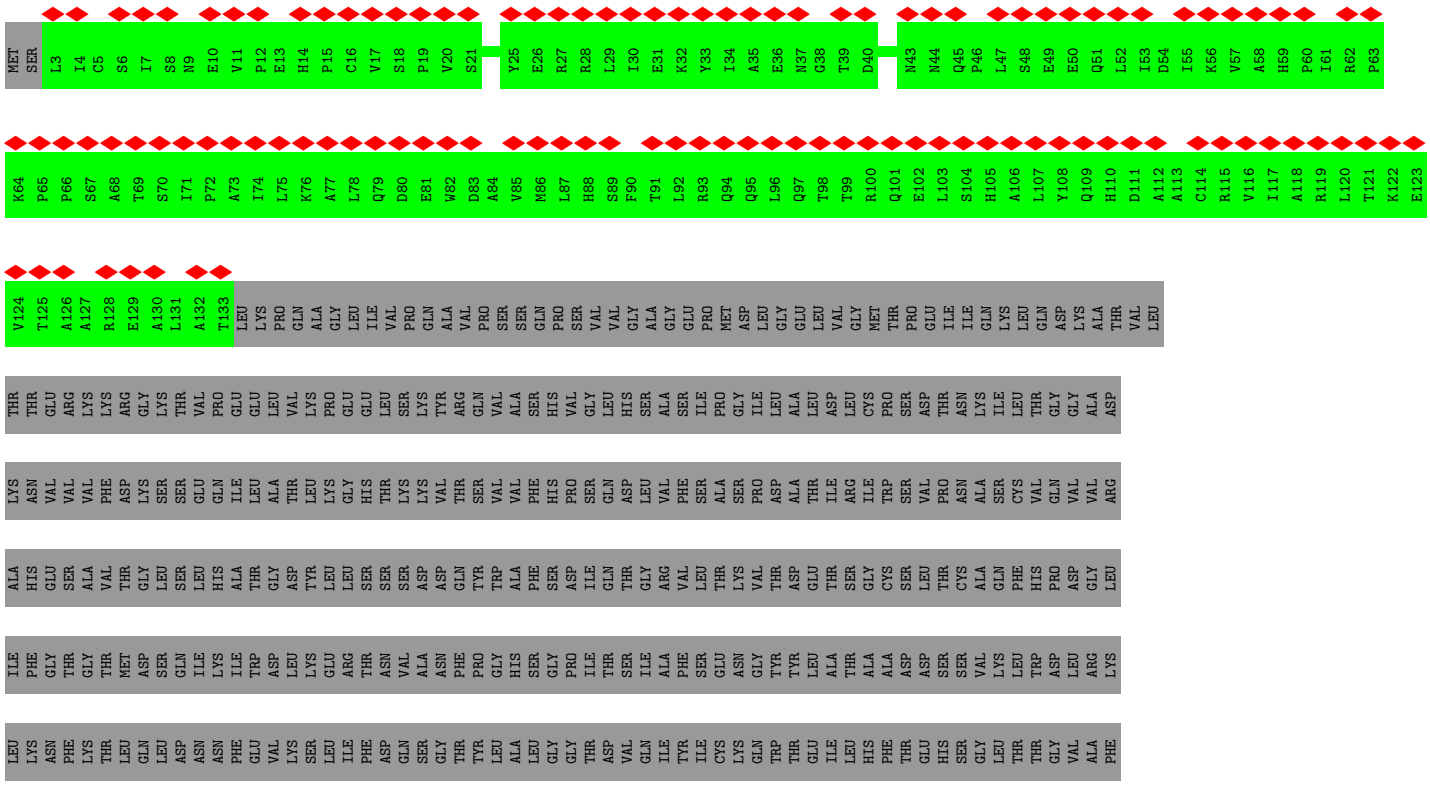
Chain q:





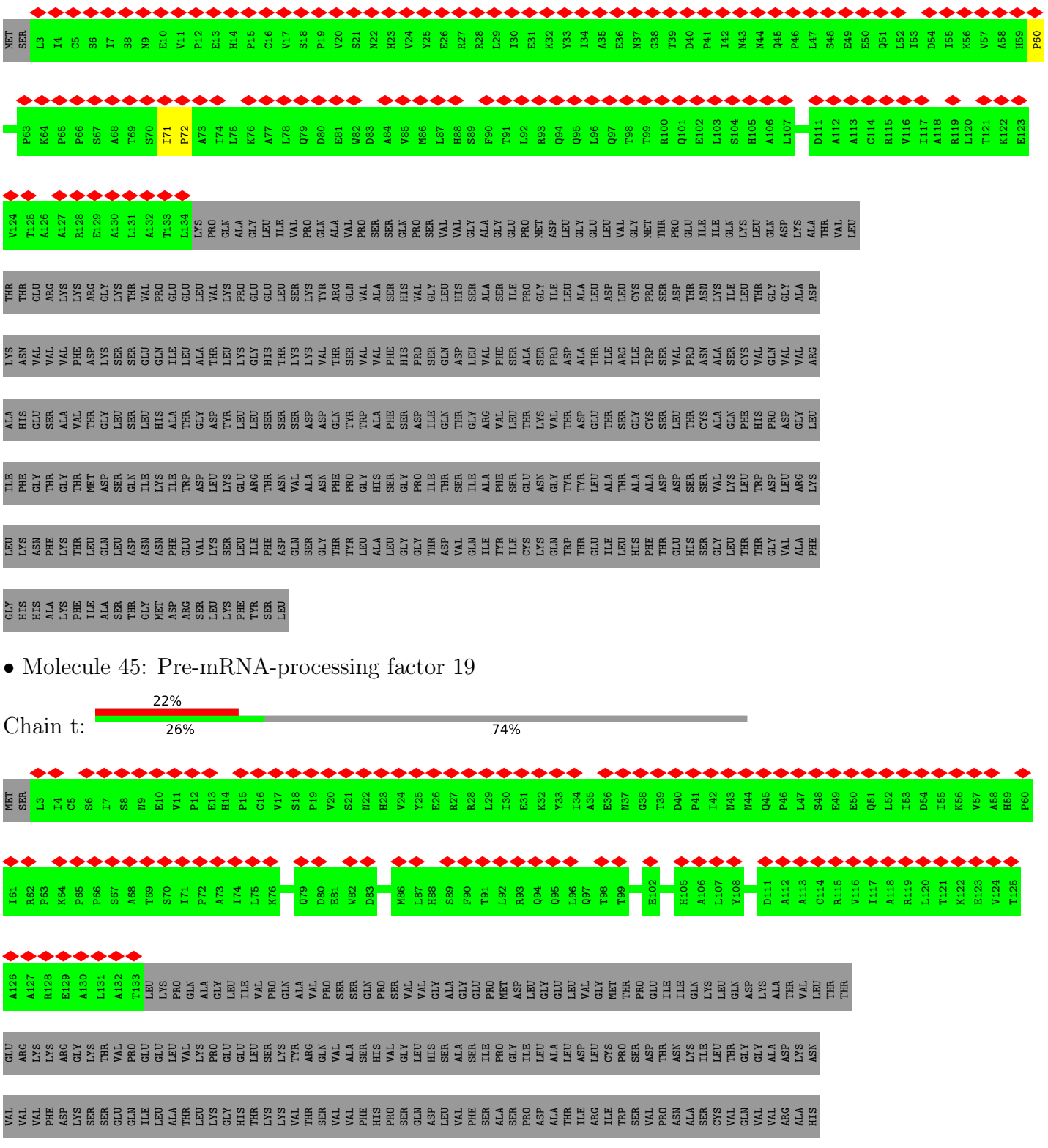
- Molecule 45: Pre-mRNA-processing factor 19

Chain r:



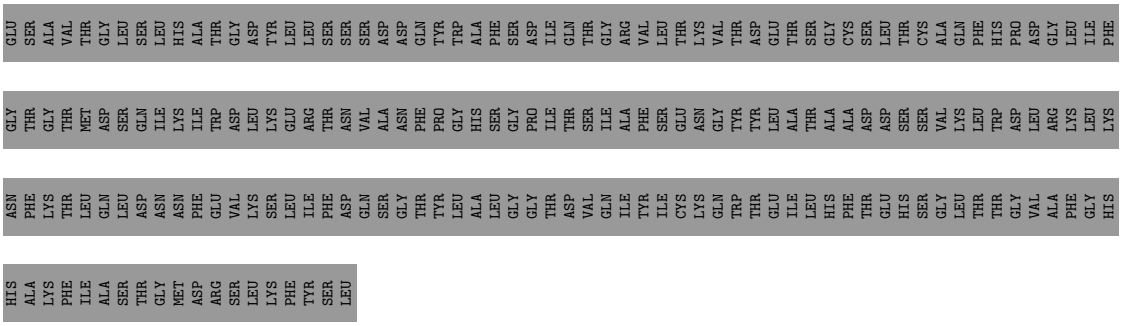
• Molecule 45: Pre-mRNA-processing factor 19

Chain s:



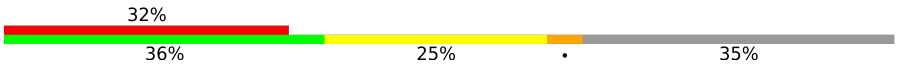
• Molecule 45: Pre-mRNA-processing factor 19

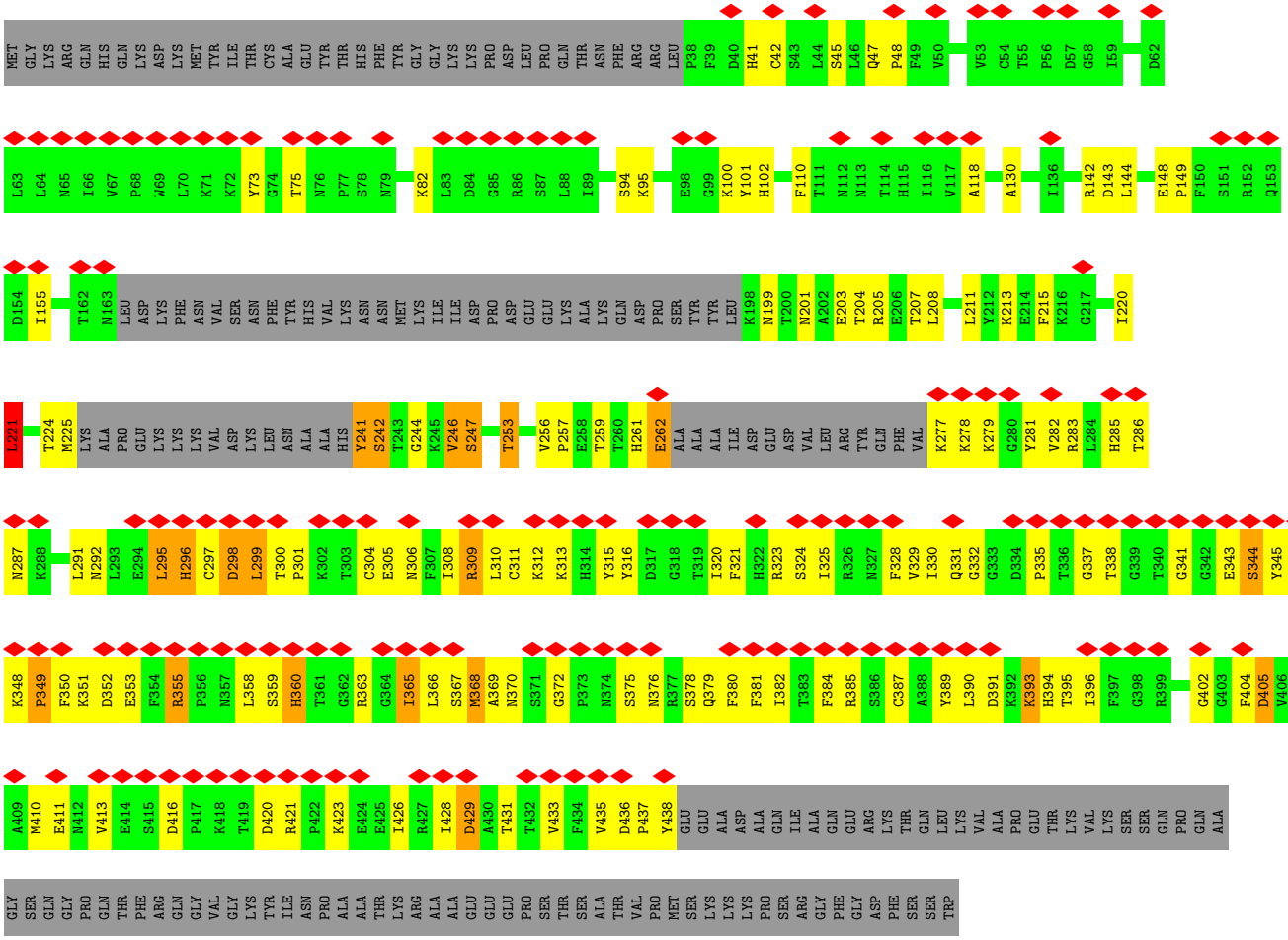
Chain t:



• Molecule 46: RING-type E3 ubiquitin-protein ligase PPIL2

Chain 9:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	111205	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.975	Depositor
Minimum map value	-2.446	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.082	Depositor
Recommended contour level	0.22	Depositor
Map size (Å)	516.96, 516.96, 516.96	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.077, 1.077, 1.077	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.91	22/19056 (0.1%)	0.70	12/25857 (0.0%)
2	B	1.14	7/2303 (0.3%)	1.16	8/3579 (0.2%)
3	C	0.39	0/6873	0.59	2/9346 (0.0%)
4	D	0.25	0/8527	0.45	0/11887
5	E	0.32	0/2392	0.60	1/3242 (0.0%)
6	F	1.51	38/2323 (1.6%)	1.32	20/3619 (0.6%)
7	G	1.00	4/1673 (0.2%)	1.29	17/2597 (0.7%)
8	H	0.79	14/3947 (0.4%)	1.08	7/6138 (0.1%)
9	I	0.25	0/2898	0.44	0/4057
10	J	0.44	0/2171	0.55	0/2929
11	K	0.59	0/423	0.60	0/568
12	L	0.48	1/2216 (0.0%)	0.54	0/3007
13	N	0.39	0/1210	0.57	0/1622
14	O	0.27	0/1447	0.49	0/2013
15	P	0.81	3/888 (0.3%)	0.72	1/1177 (0.1%)
16	Q	0.25	0/6796	0.45	0/9527
17	R	0.52	0/2789	0.57	0/3747
18	S	0.27	0/769	0.52	0/1063
19	T	0.86	0/2574	0.71	2/3511 (0.1%)
20	U	0.55	0/424	0.49	0/582
21	V	0.42	0/2993	0.55	1/4088 (0.0%)
22	W	0.26	0/2471	0.48	0/3437
23	X	0.43	1/6479 (0.0%)	0.64	2/8747 (0.0%)
24	Y	0.38	0/2605	0.60	2/3522 (0.1%)
25	Z	0.27	0/768	0.41	0/1067
26	1	0.63	0/6609	0.65	4/8947 (0.0%)
27	3	0.53	0/9408	0.66	1/12767 (0.0%)
28	p	0.25	0/847	0.47	0/1181
29	w	0.31	0/2311	0.49	0/3008
30	2	0.49	0/1837	0.60	0/2473
31	4	0.27	0/790	0.48	0/1095
32	7	0.56	0/621	0.61	0/833

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	5	0.72	0/654	0.64	0/885
34	y	0.26	0/389	0.49	0/540
35	v	0.38	0/1054	0.57	0/1385
36	o	0.24	0/821	0.48	0/1149
37	c	0.25	0/387	0.54	0/482
37	h	0.24	0/485	0.48	0/677
38	d	0.25	0/295	0.55	0/367
38	i	0.27	0/362	0.53	0/502
39	a	0.26	0/343	0.57	0/427
39	m	0.26	0/416	0.54	0/581
40	g	0.24	0/322	0.56	0/399
40	l	0.26	0/417	0.51	0/581
41	f	0.25	0/295	0.57	0/367
41	k	0.26	0/366	0.53	0/509
42	e	0.23	0/315	0.52	0/392
42	j	0.25	0/403	0.46	0/561
43	b	0.24	0/327	0.53	0/407
43	n	0.24	0/404	0.50	0/564
44	u	0.24	0/842	0.42	0/1110
45	q	0.25	0/658	0.40	0/919
45	r	0.26	0/653	0.41	0/912
45	s	0.27	0/658	0.44	0/919
45	t	0.26	0/653	0.40	0/912
46	9	0.32	0/2342	0.55	1/3182 (0.0%)
All	All	0.61	90/123299 (0.1%)	0.67	81/169962 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	16
3	C	0	6
4	D	0	2
9	I	0	3
10	J	0	3
11	K	0	1
12	L	0	2
13	N	0	2
15	P	0	2
16	Q	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
17	R	0	1
18	S	0	1
23	X	0	1
24	Y	0	3
25	Z	0	1
26	1	0	4
27	3	0	5
30	2	0	1
32	7	0	1
33	5	0	1
46	9	0	2
All	All	0	60

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	109	U	O3'-P	9.45	1.72	1.61
6	F	67	G	C5-C4	-7.50	1.33	1.38
8	H	22	U	N1-C2	-7.49	1.31	1.38
8	H	25	G	C5-C4	-7.15	1.33	1.38
6	F	65	G	C5-C4	-7.11	1.33	1.38
6	F	65	G	N9-C8	-6.84	1.33	1.37
6	F	75	G	N7-C5	-6.65	1.35	1.39
6	F	67	G	N9-C4	-6.61	1.32	1.38
8	H	22	U	C2-N3	-6.48	1.33	1.37
1	A	1028	TYR	CD1-CE1	-6.45	1.29	1.39
6	F	65	G	C6-N1	-6.36	1.35	1.39
1	A	1273	TYR	CE2-CZ	-6.33	1.30	1.38
6	F	65	G	N1-C2	-6.27	1.32	1.37
6	F	66	C	N3-C4	-6.21	1.29	1.33
8	H	21	C	N1-C6	-6.13	1.33	1.37
6	F	55	C	C4-C5	-6.10	1.38	1.43
6	F	71	G	N9-C8	-6.08	1.33	1.37
6	F	72	G	C5-C4	-6.08	1.34	1.38
15	P	188	TRP	C-O	-6.05	1.11	1.23
6	F	71	G	C5-C4	-6.01	1.34	1.38
6	F	69	A	C5-C4	-6.00	1.34	1.38
8	H	23	A	C5-C4	-6.00	1.34	1.38
2	B	42	U	N1-C2	-5.96	1.33	1.38
8	H	22	U	C4-C5	-5.96	1.38	1.43
6	F	71	G	N7-C5	-5.90	1.35	1.39
8	H	23	A	N7-C5	-5.89	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1470	TYR	CD1-CE1	-5.84	1.30	1.39
6	F	55	C	N1-C6	-5.83	1.33	1.37
6	F	56	A	N9-C4	-5.83	1.34	1.37
6	F	56	A	C5-C4	-5.79	1.34	1.38
6	F	70	A	C5-C4	-5.77	1.34	1.38
12	L	81	GLN	CA-CB	-5.76	1.41	1.53
6	F	74	U	C2-N3	-5.69	1.33	1.37
1	A	1317	TYR	CD1-CE1	-5.69	1.30	1.39
1	A	909	TYR	CD1-CE1	-5.68	1.30	1.39
1	A	1470	TYR	CE1-CZ	-5.63	1.31	1.38
1	A	1503	TRP	CB-CG	-5.63	1.40	1.50
1	A	902	TYR	CD2-CE2	-5.62	1.30	1.39
1	A	1193	GLU	CB-CG	-5.58	1.41	1.52
8	H	21	C	N3-C4	-5.56	1.30	1.33
8	H	21	C	C4-C5	-5.55	1.38	1.43
8	H	22	U	N3-C4	-5.54	1.33	1.38
6	F	53	A	C6-N1	-5.54	1.31	1.35
6	F	54	G	C5-C4	-5.54	1.34	1.38
2	B	42	U	C4-C5	-5.53	1.38	1.43
15	P	227	TYR	CE1-CZ	-5.51	1.31	1.38
2	B	43	U	C2-N3	-5.50	1.33	1.37
6	F	53	A	C5-C4	-5.46	1.34	1.38
1	A	810	TYR	CD1-CE1	-5.44	1.31	1.39
6	F	67	G	N3-C4	-5.43	1.31	1.35
7	G	-4	G	C6-N1	-5.41	1.35	1.39
8	H	25	G	N3-C4	-5.38	1.31	1.35
6	F	69	A	C6-N1	-5.36	1.31	1.35
8	H	25	G	C2-N3	-5.32	1.28	1.32
6	F	64	U	C2-N3	-5.32	1.34	1.37
7	G	-3	A	C6-N1	-5.30	1.31	1.35
1	A	1371	TYR	CD1-CE1	-5.29	1.31	1.39
6	F	63	C	N1-C6	-5.28	1.33	1.37
15	P	227	TYR	CD1-CE1	-5.28	1.31	1.39
6	F	70	A	C6-N1	-5.28	1.31	1.35
1	A	1315	VAL	CB-CG2	-5.27	1.41	1.52
6	F	65	G	N7-C5	-5.25	1.36	1.39
2	B	32	C	N1-C6	-5.24	1.34	1.37
2	B	50	G	C5-C4	-5.24	1.34	1.38
8	H	20	G	C5-C4	-5.22	1.34	1.38
6	F	54	G	N7-C5	-5.22	1.36	1.39
1	A	1153	VAL	CB-CG1	-5.21	1.42	1.52
1	A	902	TYR	CD1-CE1	-5.20	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	-4	G	C5-C4	-5.20	1.34	1.38
8	H	25	G	N9-C4	-5.20	1.33	1.38
1	A	1371	TYR	CD2-CE2	-5.17	1.31	1.39
1	A	1371	TYR	CE2-CZ	-5.17	1.31	1.38
6	F	56	A	N7-C5	-5.17	1.36	1.39
6	F	53	A	N9-C4	-5.16	1.34	1.37
6	F	75	G	N9-C8	-5.16	1.34	1.37
1	A	800	TYR	CD1-CE1	-5.14	1.31	1.39
1	A	1260	VAL	CB-CG1	-5.13	1.42	1.52
2	B	33	U	C2-N3	-5.13	1.34	1.37
6	F	76	A	N3-C4	-5.11	1.31	1.34
1	A	1445	TYR	CD2-CE2	-5.09	1.31	1.39
1	A	1470	TYR	CD2-CE2	-5.08	1.31	1.39
6	F	55	C	N3-C4	-5.08	1.30	1.33
1	A	978	GLU	CB-CG	-5.07	1.42	1.52
6	F	67	G	N1-C2	-5.05	1.33	1.37
6	F	56	A	N3-C4	-5.05	1.31	1.34
6	F	55	C	C2-N3	-5.03	1.31	1.35
23	X	605	THR	C-N	-5.02	1.22	1.34
6	F	56	A	C6-N1	-5.02	1.32	1.35
2	B	26	A	N9-C4	-5.01	1.34	1.37
1	A	1099	PHE	CD1-CE1	-5.01	1.29	1.39

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	104	C	N1-C2-O2	9.23	124.44	118.90
19	T	186	PRO	C-N-CA	-8.88	99.51	121.70
1	A	1771	LEU	CA-CB-CG	8.78	135.50	115.30
7	G	110	U	C4'-C3'-O3'	-8.39	91.77	109.40
7	G	109	U	P-O3'-C3'	8.38	129.75	119.70
7	G	104	C	N3-C2-O2	-8.10	116.23	121.90
7	G	104	C	C2-N1-C1'	7.76	127.34	118.80
7	G	103	U	C2-N1-C1'	7.74	126.99	117.70
7	G	-1	C	C2-N3-C4	-7.59	116.11	119.90
1	A	176	LEU	CA-CB-CG	7.13	131.69	115.30
7	G	103	U	N1-C2-O2	7.04	127.72	122.80
3	C	94	ILE	C-N-CA	-6.87	104.53	121.70
2	B	40	U	C2-N1-C1'	6.72	125.76	117.70
6	F	48	A	C8-N9-C4	-6.62	103.15	105.80
6	F	14	C	C6-N1-C2	-6.37	117.75	120.30
26	1	1107	GLN	C-N-CA	-6.32	105.90	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	95	G	N3-C4-N9	-6.22	122.27	126.00
8	H	173	C	N1-C2-O2	6.03	122.52	118.90
8	H	15	U	C2-N1-C1'	-5.98	110.52	117.70
7	G	115	C	N1-C2-O2	5.95	122.47	118.90
6	F	14	C	N3-C2-O2	-5.92	117.75	121.90
7	G	103	U	N3-C2-O2	-5.92	118.06	122.20
6	F	36	A	N7-C8-N9	5.87	116.74	113.80
6	F	38	G	N7-C8-N9	5.84	116.02	113.10
2	B	40	U	N1-C2-O2	5.81	126.87	122.80
2	B	40	U	C5-C6-N1	5.80	125.60	122.70
24	Y	16	LEU	CA-CB-CG	5.79	128.62	115.30
1	A	1751	LEU	CB-CG-CD2	-5.78	101.17	111.00
6	F	76	A	N9-C4-C5	5.78	108.11	105.80
8	H	64	A	C5-C6-N6	-5.78	119.08	123.70
6	F	67	G	N3-C4-C5	5.77	131.48	128.60
7	G	113	U	P-O3'-C3'	5.72	126.56	119.70
8	H	20	G	C4-C5-N7	5.70	113.08	110.80
2	B	47	A	O4'-C1'-N9	5.68	112.74	108.20
2	B	19	A	N9-C4-C5	-5.68	103.53	105.80
7	G	104	C	C6-N1-C1'	-5.67	113.99	120.80
23	X	813	ARG	CB-CA-C	-5.66	99.07	110.40
15	P	188	TRP	C-N-CA	5.62	135.75	121.70
19	T	240	LEU	CA-CB-CG	5.59	128.16	115.30
1	A	598	LEU	CB-CG-CD2	-5.56	101.56	111.00
6	F	83	A	N1-C6-N6	5.55	121.93	118.60
6	F	59	G	C5-N7-C8	-5.54	101.53	104.30
6	F	68	C	N1-C2-O2	-5.53	115.58	118.90
1	A	835	ASP	CB-CG-OD1	-5.52	113.33	118.30
6	F	37	C	N1-C2-O2	5.50	122.20	118.90
6	F	95	G	N3-C4-C5	5.49	131.35	128.60
2	B	100	C	C5-C6-N1	5.46	123.73	121.00
27	3	235	LEU	CA-CB-CG	5.39	127.69	115.30
5	E	227	LEU	CA-CB-CG	5.37	127.66	115.30
6	F	36	A	C5-N7-C8	-5.37	101.22	103.90
6	F	83	A	C5-C6-N6	-5.37	119.41	123.70
1	A	1763	LEU	CA-CB-CG	5.34	127.59	115.30
7	G	85	G	C4-N9-C1'	-5.33	119.57	126.50
1	A	1601	LEU	CA-CB-CG	5.32	127.54	115.30
8	H	13	C	P-O3'-C3'	5.30	126.06	119.70
21	V	494	LEU	CA-CB-CG	5.28	127.44	115.30
1	A	1252	GLY	N-CA-C	-5.27	99.92	113.10
7	G	88	G	OP1-P-O3'	5.25	116.75	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	103	U	C6-N1-C1'	-5.25	113.85	121.20
8	H	43	U	N1-C2-O2	-5.25	119.13	122.80
6	F	57	U	C2-N1-C1'	5.22	123.97	117.70
26	1	929	LEU	CA-CB-CG	-5.22	103.30	115.30
6	F	37	C	C2-N1-C1'	5.21	124.53	118.80
8	H	43	U	C2-N3-C4	-5.20	123.88	127.00
26	1	563	LEU	CA-CB-CG	5.19	127.23	115.30
3	C	510	LEU	CA-CB-CG	5.18	127.22	115.30
1	A	1919	LEU	CA-CB-CG	5.18	127.21	115.30
6	F	84	A	N3-C4-N9	-5.17	123.26	127.40
2	B	40	U	C6-N1-C1'	-5.17	113.97	121.20
7	G	-1	C	N3-C4-C5	5.16	123.97	121.90
6	F	59	G	N7-C8-N9	5.13	115.67	113.10
23	X	592	LEU	CA-CB-CG	5.12	127.08	115.30
24	Y	26	LEU	CA-CB-CG	5.10	127.04	115.30
1	A	1328	LEU	CA-CB-CG	5.09	127.01	115.30
26	1	1280	LEU	CB-CG-CD2	-5.09	102.35	111.00
1	A	779	LEU	CB-CG-CD1	-5.04	102.42	111.00
2	B	37	G	N9-C4-C5	5.04	107.42	105.40
6	F	84	A	C6-C5-N7	5.03	135.82	132.30
46	9	221	LEU	CA-CB-CG	-5.02	103.75	115.30
1	A	951	LEU	CB-CG-CD2	-5.02	102.47	111.00
7	G	110	U	C3'-C2'-O2'	5.02	127.85	113.30

There are no chirality outliers.

All (60) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	1	1105	GLU	Peptide
26	1	1107	GLN	Peptide
26	1	1179	ASP	Peptide
26	1	717	THR	Peptide
30	2	502	ARG	Peptide
27	3	268	ARG	Peptide
27	3	342	LEU	Peptide
27	3	490	THR	Peptide
27	3	916	ASN	Peptide
27	3	971	ASP	Peptide
33	5	79	PRO	Peptide
32	7	13	LYS	Peptide
46	9	329	VAL	Peptide
46	9	349	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	A	108	MET	Peptide
1	A	1338	SER	Peptide
1	A	1416	ILE	Peptide
1	A	187	PRO	Peptide
1	A	203	VAL	Peptide
1	A	2150	GLN	Peptide
1	A	376	GLU	Peptide
1	A	386	PRO	Peptide
1	A	467	GLN	Peptide
1	A	468	LYS	Peptide
1	A	698	PRO	Peptide
1	A	703	GLN	Peptide
1	A	855	ARG	Peptide
1	A	940	ILE	Peptide
1	A	941	LYS	Peptide
1	A	982	GLU	Peptide
3	C	360	ALA	Peptide
3	C	427	PHE	Peptide
3	C	443	VAL	Peptide
3	C	533	SER	Peptide
3	C	534	VAL	Peptide
3	C	823	ALA	Peptide
4	D	1583	ASP	Peptide
4	D	2098	ALA	Peptide
9	I	337	LEU	Peptide
9	I	338	ILE	Peptide
9	I	550	TRP	Peptide
10	J	241	VAL	Peptide
10	J	354	LEU	Peptide
10	J	413	GLU	Peptide
11	K	196	ASP	Peptide
12	L	200	LYS	Peptide
12	L	202	ARG	Peptide
13	N	12	PRO	Peptide
13	N	36	PRO	Peptide
15	P	29	GLN	Peptide
15	P	56	ASN	Peptide
16	Q	488	SER	Peptide
16	Q	489	VAL	Peptide
17	R	163	MET	Peptide
18	S	164	PRO	Peptide
23	X	326	GLN	Peptide

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Mol	Chain	Res	Type	Group
24	Y	204	SER	Peptide
24	Y	274	ASP	Peptide
24	Y	37	TYR	Peptide
25	Z	77	GLN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	18543	0	18403	835	0
2	B	2066	0	1047	58	0
3	C	6724	0	6696	430	0
4	D	8528	0	3745	58	0
5	E	2338	0	2275	170	0
6	F	2075	0	1048	124	0
7	G	1503	0	766	137	0
8	H	3539	0	1791	134	0
9	I	2880	0	1411	16	0
10	J	2116	0	1977	109	0
11	K	411	0	362	19	0
12	L	2192	0	1775	83	0
13	N	1184	0	1190	59	0
14	O	1447	0	638	26	0
15	P	876	0	875	59	0
16	Q	6730	0	3268	56	0
17	R	2760	0	2639	129	0
18	S	770	0	356	8	0
19	T	2507	0	2451	114	0
20	U	422	0	291	11	0
21	V	2959	0	2237	106	0
22	W	2473	0	1096	30	0
23	X	6357	0	6349	480	0
24	Y	2556	0	2492	181	0
25	Z	772	0	342	0	0
26	1	6486	0	6690	382	0
27	3	9220	0	9139	604	0
28	p	841	0	420	0	0
29	w	2275	0	1347	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	2	1807	0	1622	65	0
31	4	792	0	367	9	0
32	7	613	0	597	43	0
33	5	635	0	595	37	0
34	y	390	0	190	0	0
35	v	1041	0	800	0	0
36	o	816	0	386	0	0
37	c	388	0	102	0	0
37	h	482	0	220	0	0
38	d	296	0	87	0	0
38	i	359	0	179	0	0
39	a	344	0	93	0	0
39	m	413	0	194	0	0
40	g	324	0	89	0	0
40	l	415	0	198	0	0
41	f	296	0	84	0	0
41	k	364	0	176	0	0
42	e	316	0	85	0	0
42	j	403	0	173	0	0
43	b	328	0	89	0	0
43	n	402	0	184	0	0
44	u	834	0	325	0	0
45	q	659	0	296	0	0
45	r	654	0	294	0	0
45	s	659	0	296	0	0
45	t	654	0	294	0	0
46	9	2307	0	1898	126	0
47	A	36	0	6	2	0
48	C	32	0	12	2	0
49	C	1	0	0	0	0
49	F	6	0	0	0	0
50	7	3	0	0	0	0
50	K	1	0	0	0	0
50	N	3	0	0	0	0
All	All	120623	0	93047	4334	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 21.

All (4334) 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)
23:X:819:PRO:HD3	23:X:921:LEU:CD1	1.48	1.39
15:P:184:VAL:HG22	24:Y:123:HIS:CE1	1.61	1.33
23:X:819:PRO:CD	23:X:921:LEU:CD1	2.11	1.28
15:P:184:VAL:CG2	24:Y:123:HIS:HE1	1.46	1.26
23:X:819:PRO:CD	23:X:921:LEU:HD12	1.66	1.24
15:P:184:VAL:CG2	24:Y:123:HIS:CE1	2.19	1.21
21:V:532:GLN:O	21:V:536:ILE:HB	1.47	1.13
23:X:815:MET:SD	23:X:829:LEU:HD11	1.89	1.12
23:X:242:LYS:O	23:X:246:LEU:HB2	1.53	1.07
23:X:818:LEU:HD22	23:X:819:PRO:HD2	1.34	1.06
27:3:616:ILE:HB	27:3:629:SER:O	1.54	1.06
7:G:99:C:N4	8:H:32:U:H3	1.50	1.06
2:B:40:U:O4	7:G:0:G:N2	1.88	1.05
24:Y:246:LYS:HE3	24:Y:312:HIS:HB2	1.36	1.04
16:Q:1331:HIS:HA	16:Q:1353:GLN:O	1.59	1.02
6:F:38:G:H2'	6:F:39:A:H8	1.25	1.00
1:A:1768:TYR:HA	1:A:1771:LEU:HB3	1.43	0.99
23:X:819:PRO:HD2	23:X:921:LEU:HD12	1.44	0.99
27:3:477:SER:HB2	27:3:505:THR:H	1.28	0.98
3:C:255:VAL:O	3:C:307:VAL:HA	1.64	0.97
6:F:59:G:N2	6:F:76:A:N1	2.12	0.97
33:5:36:HIS:HD1	33:5:76:CYS:HG	1.06	0.97
7:G:112:U:O4	23:X:503:ARG:NH2	1.96	0.96
6:F:36:A:H3'	6:F:37:C:H5"	1.44	0.96
23:X:819:PRO:HD3	23:X:921:LEU:HD13	1.46	0.96
7:G:111:U:O4	23:X:820:VAL:HA	1.65	0.96
6:F:59:G:H1	6:F:76:A:N6	1.64	0.94
27:3:114:ARG:NH1	33:5:38:ASP:OD1	2.00	0.94
23:X:760:LEU:HB2	23:X:764:VAL:HG23	1.49	0.94
7:G:99:C:H42	8:H:32:U:H3	0.95	0.92
27:3:516:LEU:O	27:3:527:ILE:HB	1.70	0.92
27:3:459:VAL:HG21	27:3:757:ILE:HG21	1.51	0.92
19:T:257:ARG:NH2	19:T:301:ASP:OD1	2.03	0.91
4:D:1224:LEU:O	4:D:1268:ILE:HA	1.69	0.91
16:Q:851:ILE:HA	16:Q:1060:LEU:O	1.70	0.91
23:X:819:PRO:HD3	23:X:921:LEU:HD11	1.50	0.91
1:A:26:SER:HB2	1:A:29:LYS:HB2	1.51	0.90
32:7:33:CYS:HG	32:7:35:SER:HG	0.98	0.90
6:F:85:U:H3	8:H:14:C:H42	1.20	0.90
23:X:506:LEU:CD2	23:X:770:LEU:HD21	2.02	0.89
27:3:463:ARG:H	27:3:510:LEU:HD22	1.35	0.89
46:9:321:PHE:HA	46:9:332:GLY:HA3	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:35:LYS:NZ	24:Y:159:THR:O	2.04	0.89
15:P:185:LYS:O	24:Y:49:PHE:HE1	1.56	0.89
26:1:564:ASP:O	26:1:568:ARG:NH2	2.06	0.89
1:A:435:CYS:HG	7:G:-10:G:H1	1.13	0.88
2:B:18:C:N3	2:B:59:G:N1	2.20	0.88
18:S:18:THR:HA	18:S:159:ILE:HA	1.56	0.88
46:9:352:ASP:OD1	46:9:376:ASN:ND2	2.07	0.88
17:R:348:GLU:O	17:R:352:ARG:HB2	1.74	0.88
23:X:527:LEU:HD13	23:X:763:VAL:HG11	1.56	0.88
23:X:650:ASN:O	23:X:904:GLN:NE2	2.07	0.87
1:A:1637:TRP:O	1:A:1656:THR:HA	1.73	0.87
27:3:668:GLY:HA3	27:3:699:VAL:HG11	1.57	0.87
27:3:1008:SER:OG	27:3:1009:PHE:N	2.07	0.87
8:H:19:G:N2	8:H:20:G:O6	2.08	0.86
27:3:139:LYS:HG3	27:3:160:ALA:HB3	1.57	0.86
13:N:58:ARG:NH2	13:N:98:GLU:O	2.08	0.86
1:A:2003:THR:HA	26:1:858:LYS:HD3	1.56	0.86
3:C:480:LYS:HB2	3:C:493:PHE:HB3	1.58	0.86
17:R:134:ARG:NH1	19:T:382:PRO:O	2.09	0.85
23:X:725:ARG:HD3	23:X:728:ARG:HH12	1.42	0.85
1:A:957:GLN:O	1:A:961:ASN:ND2	2.08	0.85
4:D:1558:PRO:HA	4:D:1642:GLN:O	1.75	0.85
1:A:325:HIS:HD2	1:A:326:HIS:HD2	1.25	0.85
27:3:806:ALA:HA	27:3:856:LYS:HB3	1.58	0.85
1:A:1581:LEU:HD22	1:A:1746:ARG:HH11	1.41	0.85
19:T:483:ASP:OD2	19:T:485:THR:OG1	1.95	0.85
14:O:236:VAL:HA	14:O:299:ASN:O	1.77	0.84
23:X:878:HIS:HA	23:X:881:LEU:HD12	1.59	0.84
7:G:19:G:N2	14:O:194:ALA:O	2.09	0.84
32:7:40:CYS:SG	32:7:73:LYS:NZ	2.51	0.84
17:R:103:ARG:NH1	17:R:110:LYS:O	2.11	0.84
46:9:305:GLU:OE1	46:9:309:ARG:NH1	2.11	0.84
3:C:605:ASP:HA	3:C:608:ARG:HD2	1.59	0.84
1:A:888:GLN:O	1:A:889:ARG:NH1	2.10	0.83
2:B:46:U:O2	20:U:11:ARG:NH2	2.10	0.83
2:B:18:C:N4	2:B:59:G:O6	2.10	0.83
3:C:529:ARG:HH22	3:C:540:GLU:HB2	1.42	0.83
24:Y:245:CYS:SG	24:Y:246:LYS:N	2.51	0.83
17:R:359:ARG:HB3	17:R:363:ARG:HH21	1.42	0.83
27:3:280:ASP:HB3	27:3:283:ARG:HG3	1.60	0.83
24:Y:246:LYS:HB2	24:Y:311:ILE:HA	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2146:VAL:HG13	1:A:2272:MET:HB3	1.59	0.83
26:1:734:GLY:O	26:1:738:HIS:HB2	1.77	0.83
3:C:301:SER:H	3:C:306:ASN:HD22	1.27	0.83
3:C:670:SER:HA	3:C:823:ALA:HB3	1.60	0.83
27:3:352:GLU:OE2	27:3:429:ARG:NH1	2.12	0.83
1:A:385:GLU:O	3:C:327:TYR:OH	1.95	0.82
10:J:431:ARG:HA	10:J:434:VAL:HG12	1.59	0.82
27:3:585:ALA:HB1	27:3:610:VAL:HG12	1.59	0.82
15:P:44:ARG:NH2	19:T:255:SER:O	2.12	0.82
33:5:36:HIS:ND1	33:5:76:CYS:SG	2.49	0.82
27:3:568:MET:HB3	27:3:574:LEU:HD12	1.60	0.82
17:R:175:GLN:HB2	17:R:199:MET:HB2	1.61	0.82
26:1:665:ILE:HD13	26:1:705:SER:HB2	1.61	0.82
1:A:214:ARG:NH2	1:A:223:SER:O	2.11	0.82
6:F:91:A:H2'	6:F:92:A:H8	1.43	0.82
5:E:240:GLY:O	5:E:252:SER:HA	1.80	0.82
1:A:875:HIS:HE1	23:X:866:ASN:HB3	1.42	0.82
7:G:112:U:C5	23:X:506:LEU:HD12	2.15	0.82
26:1:725:ASP:HA	26:1:728:LEU:HG	1.61	0.82
1:A:858:GLN:OE1	1:A:861:ARG:NH1	2.13	0.82
1:A:946:GLU:HB3	1:A:950:LEU:HD23	1.61	0.81
21:V:624:THR:HG21	21:V:647:LEU:HD13	1.61	0.81
15:P:186:ARG:NE	15:P:190:ASP:OD2	2.14	0.81
26:1:652:CYS:HB2	26:1:692:HIS:HE1	1.46	0.81
1:A:1819:LEU:HB3	1:A:1915:VAL:HG23	1.62	0.81
1:A:2320:LEU:HD23	1:A:2322:GLU:H	1.44	0.81
14:O:234:LEU:O	14:O:271:PHE:HA	1.81	0.81
1:A:1962:THR:HG23	1:A:1966:HIS:HB2	1.61	0.81
17:R:233:PRO:O	17:R:235:ARG:NH2	2.14	0.81
13:N:15:TRP:HZ3	13:N:22:LEU:HD12	1.46	0.80
17:R:369:LEU:HA	17:R:376:LYS:HE3	1.64	0.80
23:X:234:TYR:OH	23:X:238:ARG:NH1	2.14	0.80
24:Y:135:ILE:HA	24:Y:138:LYS:HD2	1.63	0.80
27:3:29:GLU:HG3	27:3:42:ARG:HG3	1.63	0.80
1:A:1518:LEU:O	1:A:1523:ARG:NH1	2.12	0.80
27:3:108:GLY:O	32:7:82:ARG:NH1	2.14	0.80
5:E:239:THR:HG23	5:E:254:ALA:HA	1.63	0.80
6:F:85:U:H3	8:H:14:C:N4	1.78	0.80
23:X:760:LEU:H	23:X:760:LEU:HD12	1.45	0.80
23:X:821:ASP:HB2	23:X:822:PRO:HD2	1.61	0.80
5:E:61:LEU:HD21	5:E:350:ARG:HD3	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:521:TYR:HA	21:V:524:SER:HB2	1.63	0.80
3:C:561:LYS:NZ	3:C:614:TYR:O	2.15	0.80
6:F:41:A:N1	7:G:6:A:N6	2.29	0.80
19:T:245:HIS:HE2	19:T:263:SER:HG	1.26	0.80
27:3:170:VAL:HG23	27:3:184:CYS:HB3	1.64	0.80
3:C:488:VAL:HG13	3:C:609:LYS:HD3	1.64	0.79
23:X:819:PRO:CD	23:X:921:LEU:HD11	2.05	0.79
27:3:412:ILE:HG12	27:3:423:LEU:HD22	1.63	0.79
1:A:310:THR:HA	1:A:313:LYS:HG3	1.64	0.79
7:G:112:U:OP1	23:X:503:ARG:HG2	1.81	0.79
19:T:191:HIS:NE2	19:T:440:ASP:OD1	2.15	0.79
1:A:1412:TRP:O	1:A:1420:ASN:ND2	2.14	0.79
3:C:464:ALA:HB1	3:C:473:PRO:HG3	1.65	0.79
3:C:686:THR:HB	3:C:793:ASP:HB3	1.63	0.79
15:P:67:GLU:OE2	19:T:476:ARG:NH2	2.16	0.79
27:3:162:LYS:HE3	27:3:165:THR:HG21	1.62	0.79
1:A:155:LYS:NZ	1:A:622:GLY:O	2.15	0.79
26:1:963:LYS:O	26:1:966:GLN:N	2.14	0.79
6:F:38:G:H2'	6:F:39:A:C8	2.15	0.79
26:1:598:SER:O	26:1:602:LYS:HB2	1.83	0.79
3:C:255:VAL:HB	3:C:307:VAL:HG12	1.65	0.79
13:N:120:ARG:NH1	13:N:142:CYS:SG	2.55	0.79
19:T:307:SER:OG	19:T:309:ASP:OD1	2.00	0.79
23:X:961:THR:O	23:X:965:GLN:NE2	2.15	0.79
26:1:805:TYR:O	26:1:809:GLU:HB2	1.82	0.79
27:3:412:ILE:HD12	27:3:1107:THR:HG21	1.64	0.79
3:C:396:LEU:HD21	3:C:403:LEU:HB2	1.63	0.79
3:C:495:ARG:HD2	3:C:497:LEU:HG	1.62	0.79
23:X:263:SER:O	23:X:267:ARG:HB2	1.83	0.79
1:A:1320:LYS:NZ	1:A:1325:LEU:O	2.15	0.78
6:F:59:G:H1	6:F:76:A:H61	0.84	0.78
11:K:206:LYS:O	11:K:223:ARG:NH1	2.16	0.78
26:1:1137:ARG:NH1	30:2:522:PHE:O	2.16	0.78
23:X:819:PRO:CG	23:X:921:LEU:HD11	2.14	0.78
26:1:757:MET:HB3	26:1:762:ALA:HB2	1.64	0.78
1:A:318:TYR:O	3:C:645:ARG:NH2	2.16	0.78
3:C:674:CYS:HB3	3:C:818:SER:HB2	1.66	0.78
10:J:293:ASN:HA	10:J:296:ARG:HD2	1.64	0.78
23:X:324:GLU:OE1	23:X:327:ARG:NH2	2.16	0.78
23:X:653:SER:HA	23:X:656:GLN:HG3	1.65	0.78
27:3:228:LEU:HD21	27:3:250:ILE:HG21	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:266:GLU:OE2	10:J:282:TYR:OH	2.00	0.78
16:Q:1272:LEU:HA	16:Q:1302:TYR:O	1.84	0.78
23:X:526:THR:HG23	23:X:529:THR:H	1.46	0.78
26:1:544:LEU:HD21	26:1:549:ARG:HG3	1.64	0.78
27:3:136:GLU:OE2	27:3:189:TYR:OH	2.00	0.78
27:3:592:LEU:HD22	27:3:605:LEU:HD13	1.65	0.78
26:1:834:VAL:HG22	26:1:871:THR:HG23	1.65	0.77
1:A:1014:ASN:ND2	1:A:1014:ASN:O	2.16	0.77
3:C:300:LEU:HD23	3:C:306:ASN:HB3	1.64	0.77
3:C:510:LEU:HB2	3:C:564:THR:O	1.82	0.77
21:V:518:LYS:HD3	21:V:519:LYS:H	1.49	0.77
23:X:610:ASP:HB3	23:X:686:ILE:HD13	1.66	0.77
23:X:882:LEU:O	23:X:886:THR:OG1	2.01	0.77
3:C:677:GLU:HA	3:C:683:ASN:O	1.83	0.77
19:T:267:ASP:N	19:T:267:ASP:OD1	2.17	0.77
19:T:349:SER:OG	19:T:351:ASP:OD1	1.99	0.77
1:A:155:LYS:HG3	1:A:626:GLY:HA3	1.66	0.77
1:A:1497:THR:OG1	1:A:1499:GLU:OE1	2.02	0.77
1:A:1631:LEU:HB2	1:A:1660:TYR:HB3	1.67	0.77
23:X:617:GLY:O	23:X:621:ILE:HB	1.84	0.77
23:X:819:PRO:HG3	23:X:921:LEU:HD11	1.64	0.77
10:J:354:LEU:HD21	10:J:362:ALA:HB2	1.67	0.77
1:A:2188:LEU:O	1:A:2251:TYR:OH	2.01	0.77
19:T:406:ILE:HG22	19:T:407:GLN:HG2	1.67	0.77
23:X:263:SER:HA	23:X:267:ARG:HH21	1.49	0.77
23:X:434:GLN:NE2	23:X:468:GLU:OE2	2.18	0.77
26:1:972:GLY:HA2	26:1:1010:THR:HG21	1.64	0.77
1:A:325:HIS:CD2	1:A:326:HIS:HD2	2.02	0.77
5:E:255:MET:HB2	5:E:282:HIS:HB3	1.67	0.77
6:F:84:A:H1'	6:F:85:U:H5'	1.67	0.77
15:P:42:LYS:NZ	19:T:276:GLU:OE1	2.18	0.77
23:X:768:LYS:HE3	23:X:773:HIS:HA	1.65	0.77
6:F:36:A:N1	7:G:10:U:N3	2.32	0.77
27:3:878:ASP:OD1	27:3:879:LEU:N	2.18	0.77
27:3:1013:ARG:NH2	27:3:1064:ASP:OD1	2.19	0.77
1:A:1014:ASN:HD21	12:L:83:ARG:HB2	1.51	0.76
6:F:31:U:O4	7:G:15:U:N3	2.17	0.76
27:3:351:SER:H	27:3:356:HIS:HB3	1.50	0.76
6:F:45:A:OP2	30:2:554:ARG:NH1	2.18	0.76
26:1:565:ASP:HA	26:1:568:ARG:HE	1.51	0.76
26:1:861:ALA:O	26:1:864:TYR:N	2.17	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:929:LYS:HE3	27:3:938:GLU:HB2	1.65	0.76
23:X:605:THR:OG1	23:X:606:GLN:NE2	2.19	0.76
26:1:524:ARG:NH1	26:1:562:LYS:O	2.18	0.76
30:2:635:ALA:HB3	31:4:73:ILE:HA	1.67	0.76
32:7:22:LEU:N	32:7:67:SER:O	2.18	0.76
23:X:765:LEU:HD12	23:X:765:LEU:O	1.85	0.76
26:1:554:LYS:HA	26:1:558:ARG:HH21	1.50	0.76
27:3:464:ARG:HG2	27:3:516:LEU:HD11	1.67	0.76
6:F:28:A:O2'	13:N:39:GLY:O	2.02	0.76
13:N:32:ALA:HA	13:N:35:GLU:HG3	1.67	0.76
16:Q:1136:GLN:H	16:Q:1156:ASN:HA	1.50	0.76
17:R:160:ALA:HA	17:R:163:MET:HG2	1.68	0.75
23:X:527:LEU:CD1	23:X:763:VAL:HG11	2.16	0.75
1:A:79:ARG:HH11	1:A:82:ARG:HH21	1.35	0.75
24:Y:145:ASP:OD2	24:Y:190:ARG:NH2	2.18	0.75
1:A:163:ARG:NH2	1:A:576:ASP:OD1	2.19	0.75
1:A:1407:ASP:OD1	1:A:1407:ASP:N	2.18	0.75
1:A:1892:PRO:HG2	1:A:1940:LEU:HB2	1.67	0.75
26:1:793:LYS:HE2	26:1:839:GLU:HG3	1.67	0.75
1:A:171:ASP:OD1	1:A:521:ASN:ND2	2.17	0.75
3:C:154:HIS:HB3	3:C:156:GLU:HB3	1.67	0.75
23:X:620:GLU:OE1	23:X:696:LYS:NZ	2.19	0.75
7:G:107:U:OP1	23:X:696:LYS:NZ	2.19	0.75
27:3:463:ARG:HB2	27:3:510:LEU:HD13	1.66	0.75
5:E:90:ILE:HD12	5:E:105:LEU:HD22	1.68	0.75
12:L:701:GLY:O	12:L:705:THR:N	2.17	0.75
26:1:838:VAL:HG13	26:1:875:ILE:HG12	1.67	0.75
27:3:89:ILE:HD12	27:3:103:HIS:HB2	1.67	0.75
27:3:902:ASP:OD1	27:3:902:ASP:N	2.19	0.75
27:3:1026:ASP:OD1	27:3:1026:ASP:N	2.18	0.75
21:V:490:CYS:HB2	21:V:525:PHE:HE2	1.51	0.75
27:3:525:ARG:HG3	27:3:533:VAL:HG13	1.67	0.75
1:A:972:GLU:N	1:A:972:GLU:OE1	2.19	0.75
1:A:2272:MET:HG3	1:A:2296:LEU:HD22	1.69	0.75
21:V:589:GLU:O	21:V:593:TYR:HB2	1.86	0.75
23:X:819:PRO:CG	23:X:921:LEU:CD1	2.65	0.75
27:3:459:VAL:HG22	27:3:476:VAL:HA	1.68	0.75
27:3:969:VAL:HB	27:3:981:CYS:HB2	1.69	0.75
10:J:228:ARG:HG2	12:L:210:TYR:HB3	1.67	0.74
1:A:789:GLU:HB2	46:9:253:THR:HB	1.69	0.74
3:C:392:LEU:O	3:C:396:LEU:HB2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:932:ASN:HB2	27:3:936:LYS:HE3	1.69	0.74
1:A:366:LYS:HE3	21:V:324:HIS:HA	1.69	0.74
1:A:532:THR:OG1	7:G:3:A:OP1	2.05	0.74
7:G:112:U:H5	23:X:506:LEU:HD12	1.49	0.74
23:X:164:TRP:HB2	23:X:538:ASP:HB3	1.70	0.74
1:A:1201:ARG:O	1:A:1203:SER:N	2.20	0.74
3:C:177:ARG:NH2	3:C:638:ASP:OD2	2.20	0.74
23:X:822:PRO:HA	23:X:825:SER:OG	1.88	0.74
24:Y:12:VAL:HG22	24:Y:132:GLY:HA3	1.68	0.74
30:2:491:LEU:O	30:2:494:THR:OG1	2.06	0.74
7:G:115:C:H3'	7:G:116:C:H4'	1.70	0.74
27:3:511:LEU:HD23	27:3:512:GLY:H	1.52	0.74
1:A:762:ARG:HH12	15:P:226:LYS:HZ1	1.33	0.74
6:F:91:A:H2'	6:F:92:A:C8	2.22	0.74
46:9:390:LEU:HD22	46:9:393:LYS:HE2	1.68	0.74
1:A:402:ILE:HG21	3:C:268:LYS:HE3	1.70	0.74
11:K:200:ASP:HB3	11:K:219:PHE:HD1	1.53	0.74
23:X:288:GLU:HA	23:X:291:LYS:HD3	1.70	0.74
23:X:815:MET:HG3	23:X:825:SER:HB3	1.70	0.74
1:A:419:ARG:NH2	1:A:423:ASP:O	2.20	0.74
22:W:555:GLY:O	22:W:568:THR:HA	1.87	0.74
23:X:164:TRP:HE1	23:X:539:VAL:HG22	1.52	0.74
23:X:167:THR:HG23	23:X:771:GLY:HA3	1.68	0.74
23:X:850:ASN:O	23:X:852:SER:N	2.21	0.74
1:A:1784:ASN:HD21	1:A:1894:GLN:HB2	1.51	0.73
3:C:277:LYS:HD2	3:C:865:GLY:HA3	1.70	0.73
3:C:349:PHE:HE1	3:C:354:ARG:HA	1.53	0.73
6:F:90:G:H2'	6:F:91:A:C8	2.22	0.73
6:F:42:C:H2'	6:F:43:A:O4'	1.88	0.73
27:3:206:GLN:HG3	27:3:231:HIS:HD2	1.52	0.73
46:9:298:ASP:N	46:9:298:ASP:OD1	2.19	0.73
3:C:262:ARG:NH2	3:C:266:GLU:OE2	2.21	0.73
16:Q:515:VAL:N	16:Q:540:THR:O	2.21	0.73
23:X:506:LEU:HD21	23:X:770:LEU:HD21	1.70	0.73
27:3:228:LEU:HD12	27:3:229:GLU:H	1.52	0.73
5:E:172:ASP:HA	5:E:195:GLN:HB3	1.70	0.73
8:H:43:U:O2'	8:H:44:U:O5'	2.04	0.73
21:V:616:LEU:HB2	21:V:643:LEU:HD12	1.71	0.73
3:C:476:CYS:HB2	3:C:565:ILE:HB	1.71	0.73
32:7:73:LYS:O	32:7:77:ILE:HG13	1.88	0.73
1:A:498:ARG:O	1:A:502:ASN:ND2	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1778:TRP:HH2	1:A:1852:LEU:HD21	1.52	0.73
7:G:111:U:H5	23:X:820:VAL:H	1.35	0.73
1:A:835:ASP:N	1:A:835:ASP:OD1	2.19	0.73
1:A:1638:ASN:HA	1:A:1655:THR:O	1.88	0.73
1:A:1713:SER:OG	1:A:1714:ALA:N	2.21	0.73
3:C:183:SER:HB3	3:C:205:THR:HA	1.70	0.73
10:J:414:HIS:HA	10:J:417:VAL:HG22	1.71	0.73
15:P:186:ARG:HB2	15:P:186:ARG:HH11	1.53	0.73
17:R:161:ALA:HA	17:R:166:ARG:HH22	1.52	0.73
27:3:565:TYR:HE1	27:3:619:LEU:HB2	1.54	0.73
15:P:185:LYS:O	24:Y:49:PHE:CE1	2.42	0.73
21:V:622:ARG:HA	21:V:625:ARG:HH21	1.54	0.73
27:3:412:ILE:H	27:3:1105:GLN:HE22	1.34	0.73
5:E:87:ASP:N	5:E:87:ASP:OD1	2.19	0.73
23:X:715:SER:OG	23:X:749:GLU:O	2.07	0.73
27:3:325:ILE:N	27:3:375:SER:OG	2.20	0.73
27:3:487:ILE:HA	27:3:491:VAL:HG13	1.69	0.73
27:3:1040:ASP:OD2	27:3:1043:THR:N	2.20	0.73
30:2:526:ASP:OD1	30:2:526:ASP:N	2.17	0.73
32:7:21:ARG:NH1	32:7:68:ASP:OD1	2.21	0.73
19:T:349:SER:OG	19:T:350:HIS:N	2.17	0.73
1:A:1771:LEU:HD21	1:A:1779:PHE:HZ	1.54	0.72
1:A:2080:ALA:HA	1:A:2083:LEU:HG	1.70	0.72
3:C:131:ASN:HD22	3:C:495:ARG:HH22	1.36	0.72
23:X:815:MET:HG2	23:X:825:SER:HB2	1.70	0.72
3:C:132:VAL:HG11	3:C:226:VAL:HG23	1.70	0.72
15:P:184:VAL:HG23	24:Y:123:HIS:HE1	1.49	0.72
27:3:581:LYS:HD2	27:3:625:LEU:HD22	1.71	0.72
6:F:30:A:H61	7:G:16:G:H1'	1.53	0.72
24:Y:251:THR:OG1	24:Y:307:ASP:OD2	2.08	0.72
27:3:208:LEU:HD13	27:3:250:ILE:HD11	1.71	0.72
1:A:784:LEU:O	1:A:788:GLN:HG3	1.89	0.72
12:L:188:ARG:HA	12:L:191:LEU:HB2	1.71	0.72
1:A:1160:ARG:HD3	15:P:192:VAL:HG21	1.72	0.72
1:A:2068:SER:HB3	1:A:2072:GLU:HB3	1.69	0.72
3:C:496:VAL:HB	3:C:546:ALA:HA	1.71	0.72
26:1:498:MET:HE1	26:1:530:PRO:HB2	1.71	0.72
1:A:428:LYS:NZ	2:B:27:U:OP2	2.23	0.72
19:T:201:SER:OG	19:T:455:GLN:NE2	2.23	0.72
1:A:119:LEU:HD11	1:A:482:PHE:HB3	1.72	0.72
1:A:979:SER:HB3	1:A:1173:SER:HB2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1104:ASP:OD1	1:A:1104:ASP:N	2.22	0.72
3:C:313:GLN:O	3:C:417:ARG:NE	2.22	0.72
7:G:111:U:C5	23:X:819:PRO:HA	2.25	0.72
26:1:553:VAL:HA	26:1:556:ILE:HG22	1.72	0.72
26:1:600:LEU:O	26:1:604:ALA:HB2	1.90	0.72
1:A:51:PHE:HB3	5:E:88:ARG:HH11	1.55	0.71
1:A:64:GLU:N	1:A:64:GLU:OE1	2.22	0.71
3:C:642:HIS:O	3:C:646:LYS:HB2	1.90	0.71
8:H:43:U:H2'	8:H:44:U:C6	2.25	0.71
26:1:717:THR:HB	26:1:718:PRO:HD3	1.72	0.71
26:1:1299:GLU:HA	26:1:1302:TYR:HE2	1.55	0.71
5:E:153:PHE:HB2	5:E:172:ASP:HB2	1.72	0.71
7:G:110:U:H5"	23:X:455:ARG:HG3	1.72	0.71
1:A:658:ARG:NH1	6:F:67:G:OP2	2.24	0.71
15:P:212:ASN:ND2	19:T:458:SER:OG	2.23	0.71
23:X:760:LEU:HD12	23:X:760:LEU:N	2.05	0.71
24:Y:40:CYS:O	24:Y:155:ARG:HA	1.90	0.71
26:1:802:GLU:HB2	26:1:805:TYR:H	1.55	0.71
46:9:300:THR:HA	46:9:353:GLU:HG2	1.72	0.71
17:R:367:ARG:HD3	17:R:371:ARG:HD2	1.71	0.71
22:W:291:VAL:HA	22:W:308:SER:HA	1.71	0.71
24:Y:71:TYR:O	24:Y:74:GLN:NE2	2.23	0.71
24:Y:122:VAL:HB	24:Y:123:HIS:HD2	1.55	0.71
27:3:487:ILE:HG13	27:3:491:VAL:HG22	1.73	0.71
1:A:531:THR:OG1	1:A:534:GLU:OE1	2.04	0.71
1:A:1558:THR:OG1	1:A:1559:GLY:N	2.20	0.71
10:J:350:ILE:HD11	10:J:365:ILE:HB	1.72	0.71
17:R:371:ARG:HH12	24:Y:282:CYS:HB2	1.55	0.71
23:X:232:ARG:HA	23:X:235:LEU:HG	1.73	0.71
23:X:991:LEU:HA	23:X:995:GLU:HA	1.72	0.71
26:1:528:ALA:HA	26:1:531:LEU:HB2	1.72	0.71
27:3:642:ILE:O	27:3:703:ARG:NE	2.24	0.71
7:G:111:U:OP2	23:X:482:ARG:HB2	1.91	0.71
8:H:53:U:OP1	30:2:450:SER:OG	2.05	0.71
23:X:646:PRO:HA	23:X:672:VAL:HG12	1.71	0.71
1:A:135:VAL:O	1:A:418:THR:OG1	2.08	0.71
6:F:86:U:N3	8:H:12:G:O6	2.23	0.71
16:Q:875:HIS:HA	16:Q:1032:ALA:HA	1.72	0.71
17:R:163:MET:O	17:R:165:VAL:N	2.23	0.71
17:R:373:ALA:HB3	17:R:376:LYS:HB2	1.71	0.71
27:3:22:PHE:O	27:3:75:LYS:NZ	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1640:SER:OG	1:A:1641:ARG:N	2.21	0.71
16:Q:971:HIS:O	16:Q:975:ALA:HB2	1.90	0.71
23:X:846:MET:HG3	23:X:881:LEU:HB3	1.71	0.71
23:X:862:VAL:O	23:X:866:ASN:ND2	2.24	0.71
26:1:503:LYS:HE2	26:1:511:MET:HG2	1.72	0.71
33:5:62:ALA:HA	33:5:65:ARG:HH12	1.55	0.71
19:T:471:ASP:OD2	19:T:472:GLN:N	2.23	0.71
3:C:711:ARG:NH2	3:C:732:ILE:O	2.23	0.71
26:1:1108:ASN:O	26:1:1112:THR:HG22	1.91	0.71
1:A:658:ARG:NH2	6:F:65:G:OP2	2.23	0.70
1:A:1835:GLN:HA	1:A:1838:LYS:HG3	1.72	0.70
26:1:1273:TYR:OH	33:5:38:ASP:OD2	2.09	0.70
16:Q:536:ARG:HA	16:Q:627:VAL:O	1.91	0.70
23:X:257:PHE:HA	23:X:262:LEU:HD21	1.73	0.70
23:X:772:ILE:HG21	23:X:775:LEU:HD23	1.73	0.70
27:3:1048:ASP:OD1	27:3:1049:LYS:N	2.24	0.70
1:A:1132:LYS:HG3	1:A:1139:ARG:HH21	1.55	0.70
6:F:81:C:H1'	6:F:82:A:C5	2.25	0.70
8:H:12:G:O2'	8:H:13:C:O4'	2.05	0.70
27:3:384:THR:OG1	27:3:385:PHE:O	2.08	0.70
27:3:565:TYR:HB3	27:3:577:TYR:HB3	1.72	0.70
12:L:632:ALA:O	12:L:636:LEU:N	2.24	0.70
19:T:371:HIS:NE2	19:T:389:SER:OG	2.23	0.70
23:X:246:LEU:HG	23:X:277:ARG:HE	1.56	0.70
46:9:143:ASP:N	46:9:148:GLU:O	2.23	0.70
1:A:1618:LYS:NZ	1:A:1663:ASP:OD1	2.24	0.70
3:C:394:ARG:NH1	3:C:395:THR:OG1	2.25	0.70
26:1:586:ASP:OD1	26:1:589:ALA:N	2.24	0.70
1:A:31:GLN:OE1	5:E:194:TYR:OH	2.08	0.70
1:A:1130:ASN:OD1	1:A:1130:ASN:N	2.22	0.70
3:C:117:ASP:N	3:C:117:ASP:OD1	2.14	0.70
3:C:818:SER:O	3:C:822:MET:HB2	1.91	0.70
6:F:48:A:O3'	12:L:33:ARG:NH1	2.24	0.70
8:H:28:C:O2'	8:H:29:A:N3	2.25	0.70
19:T:342:GLU:OE1	19:T:365:ARG:NH1	2.20	0.70
23:X:785:PRO:O	23:X:788:THR:OG1	2.09	0.70
26:1:582:LEU:HG	26:1:634:VAL:HG21	1.72	0.70
32:7:71:TYR:CE2	32:7:81:ASP:HB2	2.25	0.70
1:A:1070:ASP:OD1	1:A:1070:ASP:N	2.25	0.70
13:N:107:GLN:OE1	13:N:109:ARG:NH1	2.25	0.70
15:P:205:LYS:HB2	15:P:208:LYS:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1056:MET:HE2	26:1:1096:THR:HG21	1.73	0.70
23:X:423:GLU:O	23:X:426:SER:OG	2.08	0.70
23:X:701:ASN:ND2	23:X:704:THR:OG1	2.24	0.70
2:B:12:U:O2	2:B:65:G:N2	2.19	0.70
19:T:455:GLN:HG2	19:T:456:PRO:HD2	1.74	0.70
24:Y:6:GLU:O	24:Y:157:ASN:N	2.24	0.70
26:1:630:ARG:HE	26:1:670:GLN:CD	1.95	0.70
3:C:854:ARG:NH1	3:C:879:ASP:OD2	2.25	0.70
6:F:38:G:OP1	6:F:38:G:H8	1.74	0.70
6:F:46:G:O3'	12:L:166:LYS:NZ	2.23	0.70
13:N:120:ARG:O	13:N:143:SER:OG	2.09	0.70
26:1:699:GLN:HE22	26:1:738:HIS:HE1	1.40	0.70
1:A:1181:ASP:OD1	1:A:1181:ASP:N	2.24	0.69
23:X:839:GLU:N	23:X:839:GLU:OE2	2.22	0.69
26:1:1181:ASP:OD1	26:1:1182:LEU:N	2.24	0.69
27:3:1182:PHE:O	27:3:1190:GLN:NE2	2.24	0.69
3:C:667:VAL:HG22	3:C:824:THR:HG21	1.74	0.69
6:F:41:A:H2'	6:F:42:C:C6	2.28	0.69
1:A:494:LEU:HD21	1:A:562:VAL:HG21	1.74	0.69
1:A:857:ASN:ND2	1:A:860:GLN:OE1	2.25	0.69
1:A:1146:ASP:OD2	1:A:1182:ASN:ND2	2.25	0.69
1:A:1251:SER:O	1:A:1251:SER:OG	2.07	0.69
7:G:98:U:OP2	26:1:1106:ARG:NH2	2.25	0.69
23:X:695:CYS:HB3	23:X:722:ARG:HH22	1.58	0.69
23:X:765:LEU:HD11	23:X:816:ALA:HB2	1.74	0.69
11:K:223:ARG:NH2	26:1:1054:GLU:OE2	2.25	0.69
23:X:225:GLU:HA	23:X:228:LYS:HG2	1.73	0.69
27:3:1194:SER:OG	27:3:1199:ARG:O	2.10	0.69
32:7:33:CYS:SG	32:7:35:SER:OG	2.31	0.69
1:A:1838:LYS:HD3	1:A:1868:MET:HG3	1.73	0.69
2:B:66:A:H2'	2:B:67:A:C8	2.27	0.69
5:E:274:VAL:HG12	5:E:275:LYS:HG3	1.74	0.69
1:A:105:ASN:O	1:A:489:TRP:NE1	2.26	0.69
1:A:1427:ARG:NE	23:X:326:GLN:OE1	2.17	0.69
3:C:933:PHE:O	3:C:937:THR:OG1	2.07	0.69
17:R:382:ARG:HH21	17:R:385:ASN:HD22	1.40	0.69
27:3:833:GLU:O	27:3:836:ALA:N	2.23	0.69
7:G:106:C:OP2	23:X:998:ARG:NH2	2.26	0.69
27:3:328:LYS:NZ	27:3:370:GLU:OE2	2.26	0.69
32:7:46:CYS:H	32:7:85:CYS:HB2	1.58	0.69
3:C:509:VAL:O	3:C:522:SER:OG	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:158:TYR:CE1	5:E:200:THR:HG22	2.28	0.69
6:F:36:A:C3'	6:F:37:C:H5"	2.21	0.69
6:F:81:C:H1'	6:F:82:A:C4	2.27	0.69
18:S:83:GLU:HA	18:S:106:ASP:HA	1.74	0.69
19:T:423:SER:OG	19:T:424:ASP:OD1	2.09	0.69
23:X:226:LEU:HD22	24:Y:315:PHE:HE2	1.56	0.69
23:X:554:THR:HG22	23:X:555:MET:H	1.58	0.69
24:Y:30:LYS:HE3	24:Y:168:ASP:HA	1.74	0.69
26:1:621:ASP:HB3	26:1:624:VAL:HG22	1.75	0.69
26:1:680:LEU:HA	26:1:683:LEU:HB2	1.75	0.69
26:1:948:ARG:NH2	26:1:984:GLU:OE2	2.25	0.69
30:2:675:VAL:HA	30:2:681:PRO:HA	1.73	0.69
3:C:495:ARG:HB2	3:C:495:ARG:HH11	1.58	0.69
19:T:188:PRO:HB3	19:T:443:THR:HG21	1.74	0.69
23:X:1009:LEU:HD23	23:X:1021:LEU:HD11	1.73	0.69
26:1:1252:GLN:NE2	30:2:497:SER:OG	2.26	0.69
26:1:1262:ARG:NH1	33:5:24:ALA:O	2.18	0.69
33:5:62:ALA:HA	33:5:65:ARG:NH1	2.07	0.69
1:A:2289:ASP:HB2	1:A:2292:MET:HB3	1.73	0.69
14:O:165:CYS:O	14:O:168:TRP:N	2.26	0.69
4:D:913:ALA:N	4:D:977:GLY:O	2.23	0.68
23:X:516:VAL:HG22	23:X:547:LYS:HB2	1.75	0.68
23:X:654:ASP:OD1	23:X:654:ASP:N	2.25	0.68
1:A:1676:ILE:HD12	1:A:1706:ASP:HB2	1.74	0.68
3:C:188:VAL:HG23	3:C:190:LEU:HD11	1.75	0.68
5:E:209:ILE:HG21	5:E:250:LEU:HD11	1.75	0.68
10:J:285:MET:O	10:J:289:ASN:ND2	2.26	0.68
24:Y:53:THR:OG1	24:Y:54:GLY:N	2.24	0.68
27:3:745:PHE:HB2	27:3:755:VAL:HG23	1.75	0.68
27:3:968:ARG:HB2	27:3:970:TYR:HE2	1.57	0.68
32:7:37:VAL:HB	32:7:38:ARG:HG3	1.75	0.68
3:C:604:LEU:HA	3:C:607:LEU:HG	1.74	0.68
4:D:971:LYS:O	4:D:980:GLN:N	2.26	0.68
5:E:202:ASN:ND2	5:E:204:THR:OG1	2.26	0.68
23:X:822:PRO:O	23:X:826:LYS:N	2.23	0.68
26:1:734:GLY:O	26:1:738:HIS:CB	2.40	0.68
3:C:737:PRO:HD2	3:C:741:GLY:HA3	1.74	0.68
5:E:202:ASN:ND2	5:E:207:GLN:OE1	2.26	0.68
23:X:422:GLY:O	23:X:428:LYS:NZ	2.22	0.68
1:A:1516:LYS:H	1:A:1516:LYS:HD3	1.57	0.68
1:A:1807:ILE:HD11	1:A:1841:THR:HG22	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:188:GLN:NE2	5:E:189:THR:H	1.91	0.68
6:F:26:U:H5'	6:F:27:A:H8	1.59	0.68
23:X:595:CYS:O	23:X:598:SER:OG	2.12	0.68
27:3:981:CYS:SG	27:3:1019:ASN:ND2	2.66	0.68
1:A:1866:LYS:HG3	1:A:1886:GLY:HA3	1.76	0.68
1:A:2105:ILE:HB	1:A:2141:GLU:HG3	1.76	0.68
6:F:30:A:H2'	6:F:31:U:O4'	1.94	0.68
8:H:173:C:H2'	8:H:174:A:C8	2.28	0.68
23:X:387:GLN:NE2	23:X:390:GLU:OE2	2.26	0.68
23:X:659:ILE:O	23:X:669:LYS:NZ	2.27	0.68
27:3:449:VAL:HG13	27:3:763:ARG:HG2	1.76	0.68
27:3:485:LEU:HD23	27:3:491:VAL:HG12	1.76	0.68
27:3:775:ASN:HD22	27:3:775:ASN:H	1.40	0.68
1:A:57:GLN:O	13:N:107:GLN:NE2	2.24	0.68
3:C:144:CYS:SG	3:C:312:SER:OG	2.52	0.68
22:W:432:ARG:HA	22:W:446:GLU:HA	1.74	0.68
27:3:812:LYS:HD2	27:3:856:LYS:HE3	1.74	0.68
1:A:2235:TYR:OH	1:A:2239:ARG:NH2	2.24	0.68
15:P:208:LYS:O	15:P:208:LYS:NZ	2.20	0.68
23:X:845:ALA:HB2	23:X:915:ARG:HB2	1.76	0.68
1:A:296:PHE:HZ	3:C:593:GLU:HB2	1.59	0.68
10:J:330:ARG:NE	10:J:353:GLU:OE2	2.25	0.68
27:3:427:CYS:SG	27:3:428:GLY:N	2.66	0.68
9:I:448:ASN:O	9:I:452:ALA:CB	2.42	0.67
16:Q:1028:LEU:HA	16:Q:1032:ALA:HB3	1.74	0.67
27:3:603:ARG:HG3	27:3:604:PHE:CE1	2.29	0.67
27:3:840:ALA:O	27:3:844:ASN:ND2	2.27	0.67
30:2:674:PRO:O	30:2:682:LEU:N	2.24	0.67
1:A:1719:PHE:HB2	1:A:1720:PRO:HD2	1.75	0.67
3:C:480:LYS:NZ	3:C:482:TYR:OH	2.26	0.67
22:W:535:TRP:HA	22:W:542:LEU:HA	1.76	0.67
1:A:1768:TYR:HA	1:A:1771:LEU:CB	2.23	0.67
7:G:111:U:C5	23:X:820:VAL:N	2.58	0.67
26:1:1052:ALA:HA	26:1:1088:ILE:HD11	1.75	0.67
26:1:1276:SER:O	26:1:1276:SER:OG	2.07	0.67
1:A:1735:LYS:NZ	1:A:1763:LEU:O	2.28	0.67
17:R:325:ARG:HH11	24:Y:222:ILE:HG23	1.59	0.67
21:V:609:GLN:HE22	21:V:616:LEU:HD21	1.58	0.67
27:3:700:LYS:HB3	27:3:702:PHE:CZ	2.30	0.67
46:9:300:THR:OG1	46:9:304:CYS:SG	2.39	0.67
5:E:209:ILE:HG12	5:E:219:VAL:HG22	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:732:TRP:NE1	26:1:768:GLU:OE2	2.27	0.67
27:3:147:ASP:OD1	27:3:151:ARG:N	2.28	0.67
1:A:1782:ASP:OD2	1:A:1782:ASP:N	2.28	0.67
3:C:221:ILE:HD13	3:C:493:PHE:HE1	1.59	0.67
12:L:89:ILE:HD11	12:L:96:CYS:SG	2.34	0.67
23:X:808:LEU:HD23	23:X:813:ARG:HD3	1.75	0.67
1:A:1792:LYS:HA	1:A:1798:LEU:HA	1.75	0.67
21:V:636:LEU:HB3	21:V:639:LEU:HD12	1.77	0.67
24:Y:42:ILE:HB	24:Y:154:ILE:HD12	1.76	0.67
27:3:697:ARG:NH2	27:3:717:SER:OG	2.28	0.67
46:9:323:ARG:HB3	46:9:331:GLN:HB3	1.76	0.67
1:A:875:HIS:CE1	23:X:866:ASN:HB3	2.29	0.67
1:A:1622:MET:O	1:A:1687:TYR:OH	2.12	0.67
27:3:39:GLU:OE2	27:3:55:THR:OG1	2.12	0.67
27:3:434:SER:OG	27:3:436:ARG:NE	2.25	0.67
27:3:926:TYR:HB3	27:3:928:TYR:HE2	1.60	0.67
16:Q:517:PHE:HA	16:Q:538:ASP:O	1.94	0.67
46:9:416:ASP:O	46:9:420:ASP:N	2.28	0.67
1:A:384:VAL:HG12	3:C:331:PHE:HB3	1.76	0.67
1:A:2093:SER:OG	1:A:2095:ASP:OD2	2.11	0.67
27:3:499:PHE:HZ	27:3:516:LEU:HD22	1.57	0.67
27:3:665:LEU:HD11	27:3:667:ILE:HG13	1.77	0.67
27:3:876:THR:O	27:3:876:THR:OG1	2.12	0.67
27:3:1160:HIS:NE2	27:3:1175:ASP:OD2	2.20	0.67
1:A:142:SER:HA	1:A:242:ALA:HB2	1.76	0.66
1:A:2123:GLN:HB3	1:A:2157:VAL:HB	1.78	0.66
1:A:2263:LEU:HD23	1:A:2263:LEU:H	1.59	0.66
19:T:336:VAL:HG23	19:T:347:THR:HG22	1.77	0.66
1:A:1286:ASP:OD1	1:A:1286:ASP:N	2.26	0.66
3:C:80:ILE:HD11	19:T:198:ARG:HD3	1.77	0.66
5:E:312:TRP:HD1	5:E:319:ILE:HA	1.60	0.66
7:G:110:U:OP1	23:X:455:ARG:HG3	1.95	0.66
12:L:79:PRO:O	12:L:80:THR:OG1	2.13	0.66
23:X:957:SER:OG	23:X:960:ARG:NH2	2.28	0.66
27:3:521:PRO:O	27:3:543:THR:OG1	2.12	0.66
46:9:142:ARG:HA	46:9:149:PRO:HA	1.77	0.66
8:H:125:G:H2'	8:H:126:A:C8	2.30	0.66
27:3:288:VAL:HG23	27:3:289:CYS:H	1.59	0.66
1:A:37:TRP:NE1	1:A:41:GLN:OE1	2.27	0.66
1:A:762:ARG:HH22	15:P:226:LYS:HZ3	1.44	0.66
1:A:1764:SER:O	1:A:1766:GLN:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:774:THR:HG22	3:C:784:ILE:HD11	1.78	0.66
23:X:276:VAL:HG13	24:Y:227:VAL:HG12	1.78	0.66
21:V:604:LYS:HZ2	21:V:639:LEU:HD23	1.60	0.66
23:X:592:LEU:HD12	23:X:593:GLU:H	1.61	0.66
1:A:1878:ASP:OD1	1:A:1878:ASP:N	2.21	0.66
3:C:146:VAL:O	3:C:150:ILE:HG13	1.94	0.66
3:C:887:LEU:O	3:C:891:THR:HG22	1.95	0.66
5:E:146:ARG:HD2	5:E:148:LYS:HE2	1.76	0.66
10:J:434:VAL:O	10:J:438:TYR:HB3	1.96	0.66
19:T:203:HIS:CE1	19:T:229:LYS:HG3	2.29	0.66
27:3:215:LEU:H	27:3:215:LEU:HD12	1.59	0.66
27:3:705:ARG:HA	27:3:710:GLU:HA	1.76	0.66
27:3:983:ASN:ND2	27:3:1021:LEU:O	2.25	0.66
1:A:1780:VAL:HB	1:A:1863:VAL:HG23	1.77	0.66
5:E:135:VAL:HG21	5:E:181:ILE:HD13	1.77	0.66
7:G:111:U:O4	23:X:820:VAL:CA	2.41	0.66
12:L:73:HIS:HD2	46:9:220:ILE:HB	1.60	0.66
26:1:923:LYS:HG2	26:1:926:LYS:HE3	1.78	0.66
27:3:169:HIS:HD2	27:3:170:VAL:H	1.44	0.66
27:3:1188:ASN:OD1	27:3:1189:LYS:N	2.28	0.66
4:D:2065:TRP:O	4:D:2108:PHE:HA	1.95	0.66
4:D:2098:ALA:O	4:D:2100:GLY:N	2.29	0.66
24:Y:244:VAL:HG12	24:Y:247:LEU:HD21	1.77	0.66
46:9:286:THR:HG22	46:9:428:ILE:HD13	1.76	0.66
1:A:1790:ILE:HG23	1:A:1800:THR:HB	1.77	0.66
2:B:63:A:H2'	2:B:64:G:C8	2.31	0.66
3:C:515:THR:HG22	3:C:518:ASP:HB2	1.77	0.66
3:C:778:PRO:HB2	3:C:821:LEU:HD21	1.78	0.66
5:E:75:HIS:HB3	5:E:78:GLY:H	1.60	0.66
5:E:135:VAL:O	5:E:144:VAL:N	2.28	0.66
24:Y:183:ARG:HA	24:Y:183:ARG:HE	1.61	0.66
27:3:185:LEU:HG	27:3:235:LEU:HD11	1.77	0.66
27:3:206:GLN:HG3	27:3:231:HIS:CD2	2.31	0.66
27:3:1009:PHE:HE1	27:3:1036:ALA:HB2	1.61	0.66
1:A:2076:ARG:NH1	1:A:2305:TYR:OH	2.29	0.66
7:G:112:U:H5	23:X:506:LEU:CD1	2.08	0.66
12:L:696:LEU:O	12:L:700:ARG:N	2.26	0.66
23:X:698:LYS:HZ1	23:X:758:THR:HA	1.61	0.66
24:Y:17:TYR:HB3	24:Y:20:GLU:HG3	1.78	0.66
26:1:758:ASP:O	26:1:762:ALA:N	2.15	0.66
26:1:796:CYS:HA	26:1:801:VAL:HG11	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:862:GLU:OE1	26:1:904:THR:OG1	2.14	0.66
1:A:2001:SER:HA	26:1:855:ASP:HB3	1.77	0.65
13:N:29:MET:HB2	13:N:52:ILE:HG21	1.78	0.65
14:O:36:MET:HA	14:O:56:ARG:O	1.96	0.65
26:1:1299:GLU:HA	26:1:1302:TYR:CE2	2.30	0.65
27:3:191:GLU:HA	27:3:194:ASN:HD22	1.59	0.65
27:3:586:ASP:HB3	27:3:610:VAL:HB	1.77	0.65
27:3:777:VAL:HG22	27:3:779:PHE:HE1	1.61	0.65
26:1:694:LEU:HD12	26:1:694:LEU:H	1.59	0.65
3:C:713:LYS:HA	3:C:716:GLU:CD	2.15	0.65
27:3:169:HIS:ND1	27:3:234:PHE:HB2	2.10	0.65
27:3:620:ASP:N	27:3:620:ASP:OD1	2.27	0.65
1:A:2207:ASP:HB2	1:A:2210:LYS:HD2	1.79	0.65
7:G:99:C:N4	8:H:32:U:N3	2.25	0.65
26:1:712:LEU:O	26:1:716:ALA:HB3	1.97	0.65
27:3:511:LEU:HD21	27:3:517:VAL:HG23	1.78	0.65
27:3:1117:LEU:O	27:3:1128:ILE:HA	1.96	0.65
22:W:179:LYS:O	22:W:200:VAL:N	2.28	0.65
32:7:26:CYS:SG	32:7:61:CYS:HB2	2.36	0.65
46:9:341:GLY:O	46:9:379:GLN:NE2	2.28	0.65
8:H:12:G:H2'	8:H:13:C:C6	2.31	0.65
10:J:300:ASP:O	10:J:304:THR:OG1	2.15	0.65
15:P:184:VAL:HG21	24:Y:123:HIS:CE1	2.26	0.65
1:A:139:VAL:O	1:A:143:GLN:HG3	1.97	0.65
1:A:325:HIS:HD2	1:A:326:HIS:CD2	2.12	0.65
3:C:140:HIS:CD2	3:C:230:ASP:HB2	2.32	0.65
5:E:321:TYR:HB3	5:E:323:LEU:HG	1.79	0.65
6:F:35:A:H8	7:G:12:G:C6	2.15	0.65
9:I:448:ASN:O	9:I:452:ALA:HB2	1.96	0.65
22:W:101:THR:O	22:W:104:MET:N	2.30	0.65
23:X:822:PRO:O	23:X:825:SER:N	2.29	0.65
26:1:696:ASP:O	26:1:702:ARG:NH1	2.29	0.65
30:2:476:GLU:HG2	30:2:477:MET:H	1.61	0.65
46:9:118:ALA:O	46:9:155:ILE:HA	1.96	0.65
1:A:176:LEU:H	1:A:176:LEU:HD23	1.61	0.65
12:L:636:LEU:O	12:L:640:MET:N	2.26	0.65
23:X:850:ASN:O	23:X:853:ILE:HG13	1.97	0.65
26:1:662:HIS:CE1	26:1:700:LYS:HB3	2.32	0.65
1:A:850:TYR:OH	1:A:863:GLU:OE1	2.13	0.65
24:Y:39:TYR:N	24:Y:156:ILE:O	2.29	0.65
27:3:911:LYS:HB3	27:3:922:GLY:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:PRO:O	1:A:142:SER:OG	2.14	0.64
1:A:2125:ALA:HB2	1:A:2157:VAL:HG11	1.79	0.64
1:A:2128:LEU:HD22	1:A:2142:ILE:HG21	1.79	0.64
3:C:709:TRP:HB3	3:C:713:LYS:HB2	1.78	0.64
3:C:759:LEU:HA	3:C:762:VAL:HG12	1.79	0.64
7:G:88:G:O2'	7:G:89:U:H5'	1.98	0.64
7:G:98:U:O4	8:H:33:G:N1	2.25	0.64
17:R:408:ASP:OD1	17:R:409:GLN:N	2.30	0.64
24:Y:87:LYS:NZ	24:Y:120:ASP:OD2	2.30	0.64
27:3:734:LEU:HD12	27:3:767:LEU:HD22	1.79	0.64
1:A:82:ARG:NH1	7:G:15:U:O4	2.29	0.64
1:A:248:ASP:OD1	1:A:248:ASP:N	2.27	0.64
5:E:153:PHE:O	5:E:172:ASP:N	2.30	0.64
8:H:119:G:H8	8:H:119:G:O5'	1.80	0.64
10:J:334:GLU:OE2	10:J:349:TYR:OH	2.11	0.64
26:1:1174:GLU:OE2	26:1:1210:HIS:NE2	2.26	0.64
46:9:360:HIS:HB2	46:9:387:CYS:O	1.97	0.64
1:A:955:TRP:HE1	1:A:976:MET:HE1	1.63	0.64
5:E:260:ARG:HD3	5:E:276:ILE:HG12	1.79	0.64
12:L:630:LYS:O	12:L:634:ASP:N	2.29	0.64
14:O:232:THR:O	14:O:273:GLN:HA	1.97	0.64
27:3:121:LEU:HB2	27:3:132:ILE:HD12	1.78	0.64
1:A:857:ASN:OD1	1:A:860:GLN:N	2.24	0.64
1:A:1941:ARG:NH2	1:A:2012:LEU:O	2.23	0.64
1:A:2281:TYR:O	1:A:2284:MET:N	2.24	0.64
3:C:492:ALA:O	3:C:551:LEU:HA	1.97	0.64
26:1:662:HIS:CD2	26:1:704:ILE:HG21	2.33	0.64
27:3:1017:ASN:OD1	27:3:1018:GLU:N	2.31	0.64
1:A:60:ASP:OD1	1:A:60:ASP:N	2.30	0.64
1:A:1660:TYR:OH	1:A:1717:ASN:O	2.06	0.64
3:C:227:LEU:HD11	3:C:239:THR:HG22	1.80	0.64
3:C:925:PRO:HG2	3:C:928:HIS:CE1	2.33	0.64
6:F:60:C:H2'	10:J:236:ARG:HH21	1.62	0.64
19:T:223:SER:OG	19:T:225:ASP:OD2	2.09	0.64
23:X:483:PHE:CE1	23:X:917:GLN:HG3	2.32	0.64
27:3:1031:ARG:HG2	27:3:1031:ARG:HH11	1.63	0.64
9:I:406:GLU:HA	9:I:410:GLN:HA	1.79	0.64
19:T:351:ASP:O	19:T:352:THR:OG1	2.15	0.64
23:X:523:HIS:O	23:X:525:ARG:HG2	1.97	0.64
26:1:843:LYS:HB3	26:1:844:VAL:HG22	1.80	0.64
27:3:260:ASN:OD1	27:3:261:PHE:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:512:GLY:HA3	27:3:515:ALA:HB3	1.79	0.64
27:3:747:SER:N	27:3:750:CYS:O	2.31	0.64
5:E:105:LEU:HD11	5:E:136:TRP:CD2	2.32	0.64
12:L:757:LYS:O	12:L:761:SER:N	2.28	0.64
30:2:606:PRO:HA	31:4:35:GLN:HA	1.78	0.64
46:9:75:THR:HA	46:9:82:LYS:HA	1.79	0.64
3:C:223:ASP:OD1	3:C:495:ARG:NH2	2.31	0.64
26:1:568:ARG:NH1	26:1:605:GLY:H	1.96	0.64
1:A:1575:GLN:HB2	11:K:220:LEU:HD21	1.79	0.64
1:A:1581:LEU:HD22	1:A:1746:ARG:NH1	2.13	0.64
3:C:137:HIS:HB3	3:C:140:HIS:CE1	2.33	0.64
8:H:18:U:O2'	8:H:19:G:O5'	2.16	0.64
16:Q:700:ALA:O	16:Q:818:LEU:N	2.31	0.64
21:V:509:LEU:HG	21:V:553:HIS:HE1	1.62	0.64
23:X:171:ARG:O	23:X:174:ASP:HB3	1.98	0.64
26:1:1120:ALA:HB2	26:1:1128:VAL:HG21	1.80	0.64
30:2:469:VAL:HG12	30:2:471:ARG:H	1.62	0.64
2:B:12:U:H2'	2:B:13:C:C6	2.33	0.64
3:C:877:ALA:O	3:C:880:SER:OG	2.16	0.64
26:1:717:THR:O	26:1:719:TYR:N	2.30	0.64
27:3:568:MET:HA	27:3:574:LEU:HA	1.79	0.64
23:X:878:HIS:CE1	23:X:1001:LEU:HB2	2.33	0.63
26:1:859:ASP:O	26:1:865:ARG:NE	2.27	0.63
27:3:635:ALA:HB3	27:3:669:LEU:HD13	1.78	0.63
1:A:1544:ARG:NE	1:A:1672:ASP:OD2	2.31	0.63
3:C:286:ASN:HD21	3:C:300:LEU:H	1.44	0.63
23:X:715:SER:O	23:X:718:SER:OG	2.10	0.63
27:3:794:SER:O	27:3:796:ASN:ND2	2.31	0.63
27:3:1201:PRO:HA	27:3:1204:VAL:HG22	1.80	0.63
7:G:112:U:C4	23:X:503:ARG:NH2	2.64	0.63
19:T:329:HIS:HE2	19:T:347:THR:HG1	1.46	0.63
27:3:1004:ASP:OD1	27:3:1006:GLN:N	2.28	0.63
32:7:10:PHE:HB3	32:7:12:ARG:HG2	1.79	0.63
1:A:2153:THR:HG22	1:A:2154:HIS:H	1.63	0.63
3:C:173:THR:O	3:C:177:ARG:HB2	1.98	0.63
23:X:625:CYS:HA	23:X:628:LEU:HD12	1.80	0.63
23:X:815:MET:CE	23:X:829:LEU:CD1	2.75	0.63
24:Y:62:GLY:O	24:Y:107:GLN:NE2	2.30	0.63
26:1:826:ASP:OD1	26:1:827:ARG:N	2.32	0.63
27:3:384:THR:OG1	27:3:385:PHE:N	2.31	0.63
46:9:221:LEU:HA	46:9:224:THR:HB	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1892:PRO:HG3	1:A:1941:ARG:HE	1.64	0.63
4:D:1583:ASP:O	4:D:1585:GLN:N	2.31	0.63
17:R:170:LYS:H	17:R:170:LYS:HD2	1.64	0.63
21:V:525:PHE:HB3	21:V:560:LEU:HD21	1.81	0.63
24:Y:230:LEU:HD13	24:Y:231:PRO:HD2	1.81	0.63
26:1:625:ARG:NH1	26:1:659:GLN:OE1	2.31	0.63
26:1:967:GLU:HG3	26:1:970:LEU:HB3	1.81	0.63
27:3:1010:ILE:HG12	27:3:1026:ASP:HB3	1.80	0.63
1:A:68:LYS:O	1:A:72:ASP:HB2	1.98	0.63
1:A:1553:VAL:HG22	11:K:194:ARG:HB3	1.80	0.63
3:C:685:ILE:HD11	3:C:808:ILE:HD11	1.81	0.63
12:L:61:THR:OG1	12:L:62:GLU:N	2.32	0.63
23:X:937:ILE:HG22	23:X:941:LYS:HD2	1.81	0.63
26:1:699:GLN:HE22	26:1:738:HIS:CE1	2.15	0.63
27:3:233:ASN:ND2	27:3:233:ASN:H	1.95	0.63
1:A:988:ILE:HD12	1:A:1030:ILE:HD12	1.81	0.63
21:V:490:CYS:HB2	21:V:525:PHE:CE2	2.32	0.63
21:V:621:PRO:O	21:V:625:ARG:NE	2.32	0.63
32:7:39:PRO:HB2	32:7:70:TYR:HD1	1.63	0.63
46:9:211:LEU:O	46:9:215:PHE:HB3	1.99	0.63
1:A:615:ARG:O	1:A:618:THR:OG1	2.16	0.63
13:N:38:GLU:C	13:N:40:LYS:H	2.02	0.63
27:3:958:ARG:NH2	27:3:1014:TYR:OH	2.31	0.63
32:7:30:CYS:SG	32:7:31:VAL:N	2.72	0.63
32:7:52:GLY:H	32:7:55:GLN:HE21	1.47	0.63
1:A:1681:ARG:NH1	1:A:1681:ARG:HB3	2.14	0.63
2:B:99:C:H2'	2:B:100:C:C6	2.33	0.63
18:S:17:GLU:HA	18:S:22:ILE:HA	1.79	0.63
23:X:276:VAL:HG22	24:Y:227:VAL:HA	1.79	0.63
23:X:784:PRO:HB2	23:X:788:THR:OG1	1.98	0.63
12:L:777:GLN:O	12:L:781:GLU:N	2.31	0.62
13:N:140:ARG:H	22:W:196:TRP:HA	1.64	0.62
23:X:615:LEU:HB2	23:X:621:ILE:HG13	1.81	0.62
27:3:884:GLN:NE2	27:3:884:GLN:O	2.32	0.62
27:3:1193:VAL:HA	27:3:1196:GLU:HG2	1.81	0.62
1:A:858:GLN:O	1:A:862:GLU:HG3	1.98	0.62
8:H:46:U:O2'	8:H:47:U:OP2	2.16	0.62
23:X:815:MET:SD	23:X:829:LEU:CD1	2.77	0.62
24:Y:244:VAL:HG22	24:Y:313:VAL:HG13	1.82	0.62
26:1:742:GLY:O	26:1:746:PHE:HB2	1.99	0.62
27:3:545:VAL:HG12	27:3:546:LYS:HG2	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:PRO:O	3:C:342:ARG:NH2	2.31	0.62
1:A:595:LYS:NZ	2:B:30:A:OP1	2.32	0.62
4:D:1192:PRO:HA	4:D:1198:LEU:HA	1.81	0.62
5:E:69:VAL:HG11	5:E:351:LEU:HD21	1.80	0.62
19:T:195:LYS:NZ	19:T:490:ARG:HH21	1.96	0.62
32:7:33:CYS:HB3	32:7:72:CYS:SG	2.39	0.62
46:9:279:LYS:HA	46:9:295:LEU:O	2.00	0.62
1:A:361:HIS:O	1:A:362:ARG:NH1	2.32	0.62
1:A:467:GLN:HG2	2:B:19:A:H62	1.64	0.62
10:J:375:ASP:OD2	10:J:378:ASN:ND2	2.31	0.62
21:V:620:ASN:ND2	21:V:623:ASN:OD1	2.31	0.62
23:X:648:TYR:CE2	23:X:651:LEU:HB3	2.34	0.62
27:3:70:LEU:HD11	27:3:152:LEU:HD13	1.80	0.62
27:3:207:THR:O	27:3:209:THR:HG22	1.98	0.62
27:3:966:LEU:HB2	27:3:968:ARG:HD2	1.81	0.62
27:3:1009:PHE:HZ	27:3:1046:GLY:HA3	1.65	0.62
3:C:201:ASN:HB3	3:C:549:TRP:CZ3	2.33	0.62
4:D:912:ASN:HA	4:D:978:ASN:HA	1.81	0.62
13:N:116:ASN:OD1	13:N:116:ASN:N	2.31	0.62
26:1:683:LEU:O	26:1:723:SER:OG	2.15	0.62
26:1:1013:ILE:HD11	26:1:1049:TYR:CD2	2.34	0.62
27:3:452:LEU:HD12	27:3:453:PRO:HD2	1.80	0.62
1:A:340:ILE:HG22	1:A:355:LEU:HD13	1.81	0.62
5:E:176:VAL:HG22	5:E:196:VAL:HG21	1.80	0.62
15:P:187:ARG:O	15:P:187:ARG:HG2	1.95	0.62
23:X:645:LEU:HD11	23:X:669:LYS:HD2	1.82	0.62
24:Y:244:VAL:HG13	24:Y:313:VAL:HG22	1.80	0.62
32:7:46:CYS:O	32:7:50:ASN:HB2	1.99	0.62
46:9:306:ASN:OD1	46:9:345:TYR:N	2.27	0.62
1:A:1346:THR:O	1:A:1346:THR:OG1	2.15	0.62
3:C:384:VAL:HA	3:C:392:LEU:HD11	1.82	0.62
5:E:114:GLU:OE2	5:E:290:ARG:NH2	2.32	0.62
12:L:105:ASP:OD1	23:X:305:ARG:NH1	2.32	0.62
23:X:250:LEU:HA	23:X:253:GLU:HG2	1.82	0.62
23:X:419:ILE:HG22	23:X:569:VAL:HG13	1.81	0.62
1:A:1143:MET:O	1:A:1147:VAL:HG13	1.98	0.62
3:C:665:THR:OG1	3:C:666:VAL:N	2.33	0.62
5:E:120:ASP:OD1	5:E:120:ASP:N	2.28	0.62
16:Q:28:CYS:HA	16:Q:32:ALA:HB3	1.80	0.62
17:R:315:LYS:O	17:R:318:GLU:HG3	1.99	0.62
23:X:230:SER:O	23:X:234:TYR:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:550:HIS:HD2	26:1:551:LEU:HD22	1.64	0.62
26:1:1292:LYS:NZ	33:5:79:PRO:O	2.33	0.62
27:3:1136:GLU:OE1	27:3:1136:GLU:N	2.27	0.62
1:A:2324:GLU:O	1:A:2330:ARG:NH1	2.33	0.62
3:C:112:THR:HB	3:C:115:GLU:HB2	1.81	0.62
3:C:281:ILE:O	3:C:285:VAL:HG12	1.99	0.62
3:C:604:LEU:HD23	3:C:607:LEU:HD21	1.80	0.62
8:H:99:A:O2'	8:H:100:U:OP2	2.18	0.62
10:J:328:GLY:O	10:J:332:VAL:HG13	2.00	0.62
23:X:488:SER:O	23:X:491:THR:OG1	2.10	0.62
27:3:387:PHE:HE1	27:3:389:PRO:HG3	1.64	0.62
27:3:758:SER:N	27:3:761:THR:O	2.25	0.62
1:A:348:PRO:HG2	1:A:351:TYR:HB2	1.80	0.62
3:C:116:MET:HA	3:C:119:LEU:HG	1.82	0.62
12:L:192:ARG:HA	12:L:196:ILE:O	1.99	0.62
21:V:544:LEU:HD21	21:V:582:PHE:HB2	1.82	0.62
26:1:490:GLU:O	26:1:494:GLU:HG2	1.98	0.62
14:O:256:GLY:HA3	14:O:279:ALA:HB1	1.82	0.61
15:P:184:VAL:HG22	24:Y:123:HIS:NE2	2.11	0.61
23:X:846:MET:HB3	23:X:881:LEU:HD22	1.82	0.61
46:9:306:ASN:HD21	46:9:344:SER:HA	1.65	0.61
1:A:44:ARG:NH2	5:E:285:GLU:O	2.26	0.61
1:A:1000:ILE:HG22	1:A:1001:VAL:HG13	1.82	0.61
3:C:510:LEU:HD13	3:C:514:TYR:CE2	2.34	0.61
24:Y:207:GLU:HA	24:Y:210:GLU:HB3	1.82	0.61
26:1:617:ILE:HD12	26:1:660:ALA:HB1	1.81	0.61
27:3:25:THR:OG1	27:3:27:GLN:N	2.31	0.61
24:Y:21:ARG:NH1	24:Y:83:VAL:O	2.33	0.61
26:1:743:LEU:O	26:1:747:LEU:HB2	2.01	0.61
27:3:293:HIS:NE2	27:3:295:THR:HB	2.15	0.61
27:3:928:TYR:HB3	27:3:937:LEU:HB3	1.81	0.61
46:9:42:CYS:N	46:9:47:GLN:O	2.33	0.61
46:9:349:PRO:HB2	46:9:375:SER:HA	1.82	0.61
1:A:1949:ARG:HA	1:A:1952:VAL:HG12	1.83	0.61
4:D:2063:GLY:O	4:D:2110:SER:HA	1.99	0.61
17:R:408:ASP:OD1	17:R:410:ARG:N	2.24	0.61
19:T:250:ARG:HD2	19:T:266:GLU:HG3	1.81	0.61
26:1:1091:HIS:HE2	30:2:568:TYR:HE1	1.49	0.61
27:3:214:ASP:O	27:3:218:ASN:N	2.33	0.61
27:3:325:ILE:O	27:3:374:SER:HA	2.00	0.61
27:3:680:ASP:CG	27:3:681:PRO:HD2	2.21	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:9:358:LEU:HD22	46:9:396:ILE:HB	1.83	0.61
3:C:614:TYR:OH	3:C:643:ASP:OD2	2.17	0.61
5:E:300:ILE:HD11	5:E:314:THR:HG23	1.82	0.61
6:F:90:G:H2'	6:F:91:A:H8	1.65	0.61
17:R:110:LYS:NZ	19:T:364:THR:O	2.32	0.61
23:X:525:ARG:NH1	23:X:530:ASP:OD1	2.33	0.61
26:1:595:GLU:O	26:1:599:ASN:ND2	2.33	0.61
27:3:12:THR:O	27:3:34:ARG:NH1	2.34	0.61
1:A:1298:ARG:HH11	1:A:1298:ARG:HB2	1.65	0.61
1:A:2117:ILE:HD13	1:A:2301:PRO:HB2	1.82	0.61
5:E:208:ILE:O	5:E:219:VAL:HA	2.01	0.61
9:I:550:TRP:O	9:I:552:ASN:N	2.32	0.61
10:J:262:ARG:O	10:J:266:GLU:HG2	2.01	0.61
21:V:606:GLU:OE2	21:V:609:GLN:HG3	1.99	0.61
26:1:669:GLN:HB2	26:1:708:ALA:HA	1.83	0.61
26:1:1212:LEU:HD13	26:1:1237:LEU:HD13	1.81	0.61
27:3:207:THR:O	27:3:207:THR:OG1	2.15	0.61
1:A:641:MET:O	1:A:645:THR:HG23	2.01	0.61
4:D:1223:ILE:HA	4:D:1269:ARG:O	2.00	0.61
5:E:277:PHE:CE2	5:E:300:ILE:HG13	2.36	0.61
23:X:557:THR:HA	23:X:560:PHE:HB2	1.82	0.61
27:3:318:ASP:OD1	27:3:319:GLU:N	2.33	0.61
1:A:343:GLU:HG3	1:A:344:ASP:H	1.62	0.61
1:A:1554:GLN:NE2	1:A:1558:THR:O	2.34	0.61
3:C:216:THR:HG22	3:C:245:HIS:HE1	1.65	0.61
3:C:609:LYS:HA	3:C:612:LYS:HD2	1.82	0.61
3:C:811:THR:O	3:C:815:VAL:HG23	1.99	0.61
4:D:1404:LYS:O	4:D:1423:ASN:N	2.33	0.61
4:D:1662:ILE:HA	4:D:1703:VAL:O	2.01	0.61
6:F:96:U:H2'	6:F:97:U:C6	2.36	0.61
16:Q:313:ILE:HA	16:Q:320:ALA:HA	1.83	0.61
21:V:620:ASN:HB3	21:V:623:ASN:HD21	1.64	0.61
23:X:418:LEU:HD13	23:X:568:PRO:HG2	1.82	0.61
46:9:316:TYR:HE1	46:9:378:SER:HB2	1.66	0.61
1:A:1610:GLN:HB3	1:A:1630:LEU:HB3	1.83	0.61
5:E:264:VAL:HA	5:E:272:ARG:NH1	2.16	0.61
23:X:619:GLU:HA	23:X:622:GLU:OE1	2.01	0.61
23:X:621:ILE:HG12	23:X:672:VAL:HG13	1.82	0.61
23:X:803:ASN:OD1	23:X:806:GLY:N	2.32	0.61
27:3:565:TYR:CE1	27:3:619:LEU:HB2	2.33	0.61
27:3:807:TYR:H	27:3:856:LYS:HD2	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:883:GLU:OE2	27:3:884:GLN:N	2.33	0.61
1:A:2306:HIS:O	1:A:2310:ARG:HB2	2.00	0.61
3:C:137:HIS:CD2	3:C:138:LEU:H	2.18	0.61
3:C:855:GLY:HA2	3:C:875:ILE:HD12	1.83	0.61
4:D:668:ASP:O	4:D:672:GLY:N	2.34	0.61
4:D:1201:GLU:HA	4:D:1253:THR:HA	1.83	0.61
15:P:186:ARG:HH11	15:P:186:ARG:CB	2.13	0.61
17:R:137:GLU:HA	17:R:140:ILE:HB	1.83	0.61
17:R:382:ARG:NH2	17:R:385:ASN:HD22	1.99	0.61
26:1:495:ARG:HH21	26:1:530:PRO:HB3	1.66	0.61
26:1:664:GLY:HA2	26:1:667:ILE:HD12	1.82	0.61
26:1:834:VAL:O	26:1:838:VAL:HG23	2.01	0.61
1:A:1935:ARG:O	1:A:1939:ILE:HG13	2.01	0.60
3:C:133:THR:HG22	3:C:225:VAL:HG23	1.81	0.60
3:C:560:VAL:HG12	3:C:561:LYS:H	1.65	0.60
7:G:112:U:C6	23:X:503:ARG:HG3	2.36	0.60
16:Q:27:ALA:O	16:Q:32:ALA:N	2.28	0.60
27:3:71:THR:O	27:3:146:ARG:NH2	2.33	0.60
27:3:330:PHE:O	27:3:390:ARG:NH2	2.32	0.60
3:C:712:LYS:O	3:C:716:GLU:HG3	2.01	0.60
15:P:206:LYS:O	15:P:218:GLU:HG3	2.01	0.60
23:X:754:GLU:HA	23:X:757:ARG:NH2	2.16	0.60
1:A:1089:CYS:SG	1:A:1096:HIS:HD2	2.24	0.60
1:A:2131:VAL:HG12	1:A:2132:SER:H	1.66	0.60
3:C:476:CYS:O	3:C:564:THR:HA	2.01	0.60
6:F:36:A:N6	7:G:10:U:O4	2.33	0.60
19:T:356:LEU:HD13	19:T:366:VAL:HB	1.82	0.60
1:A:762:ARG:NH1	15:P:226:LYS:HZ1	1.99	0.60
4:D:1219:GLU:O	4:D:1240:LEU:HA	2.02	0.60
8:H:16:U:H1'	8:H:17:U:H5'	1.82	0.60
26:1:508:THR:HB	26:1:510:PRO:HD2	1.83	0.60
26:1:1028:HIS:O	26:1:1032:GLN:HB2	2.01	0.60
30:2:477:MET:SD	30:2:478:HIS:ND1	2.75	0.60
19:T:446:ASN:HD21	19:T:449:ARG:HE	1.49	0.60
46:9:315:TYR:CE1	46:9:335:PRO:HG2	2.36	0.60
2:B:96:A:H4'	2:B:97:G:H5"	1.82	0.60
6:F:36:A:H3'	6:F:37:C:C5'	2.28	0.60
18:S:147:THR:HA	18:S:153:PRO:HA	1.82	0.60
26:1:1166:ILE:O	26:1:1170:THR:HG22	2.01	0.60
26:1:1192:VAL:O	26:1:1196:SER:OG	2.20	0.60
27:3:138:GLN:HG2	27:3:161:HIS:CE1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:139:LYS:NZ	27:3:160:ALA:O	2.34	0.60
31:4:17:VAL:O	31:4:56:TYR:HA	2.01	0.60
32:7:13:LYS:NZ	32:7:48:GLU:OE1	2.26	0.60
1:A:261:LYS:HB2	1:A:330:THR:HB	1.82	0.60
3:C:444:GLY:O	3:C:447:PRO:HD2	2.01	0.60
3:C:687:MET:HE2	3:C:791:ILE:HG12	1.84	0.60
8:H:29:A:N6	12:L:32:SER:OG	2.34	0.60
12:L:740:ASP:O	12:L:744:GLN:N	2.33	0.60
26:1:590:ARG:O	26:1:594:ARG:HB2	2.02	0.60
1:A:1837:ALA:O	1:A:1841:THR:HG23	2.02	0.60
3:C:125:ASN:OD1	3:C:128:LEU:N	2.25	0.60
8:H:48:A:C2	8:H:65:U:H2'	2.37	0.60
16:Q:489:VAL:O	16:Q:494:PRO:HD3	2.02	0.60
27:3:947:GLU:HB3	27:3:963:VAL:HG13	1.82	0.60
46:9:330:ILE:HD13	46:9:410:MET:HB3	1.84	0.60
1:A:570:ASP:OD1	1:A:571:ALA:N	2.34	0.60
1:A:1457:HIS:ND1	1:A:1460:HIS:HD2	2.00	0.60
19:T:295:ASP:OD1	19:T:296:LEU:N	2.31	0.60
23:X:837:SER:O	23:X:841:LEU:HG	2.02	0.60
26:1:619:ASN:OD1	26:1:620:MET:N	2.32	0.60
27:3:695:GLY:O	27:3:697:ARG:NE	2.30	0.60
12:L:584:HIS:O	12:L:588:LEU:N	2.32	0.60
23:X:810:THR:HA	23:X:813:ARG:HE	1.66	0.60
24:Y:192:GLY:N	24:Y:195:GLU:OE2	2.35	0.60
27:3:246:SER:OG	27:3:247:GLY:N	2.35	0.60
27:3:615:ARG:NH2	27:3:630:MET:HB3	2.17	0.60
1:A:1189:MET:CG	1:A:1190:CYS:H	2.14	0.59
1:A:1644:LEU:HD23	1:A:1715:TYR:HD1	1.67	0.59
3:C:630:LEU:HD21	3:C:661:THR:HG21	1.84	0.59
17:R:86:LEU:HD23	17:R:86:LEU:H	1.66	0.59
23:X:164:TRP:NE1	23:X:539:VAL:HG22	2.17	0.59
26:1:495:ARG:HA	26:1:498:MET:HE3	1.84	0.59
26:1:617:ILE:HD13	26:1:651:VAL:HB	1.83	0.59
26:1:1110:VAL:O	26:1:1113:THR:HG22	2.02	0.59
1:A:1303:LEU:HD12	1:A:1311:PHE:CE1	2.37	0.59
8:H:125:G:H2'	8:H:126:A:H8	1.67	0.59
1:A:467:GLN:HE21	1:A:469:LYS:HG2	1.67	0.59
1:A:1581:LEU:O	1:A:1585:ILE:HG13	2.03	0.59
1:A:1819:LEU:HD22	1:A:1902:PHE:HD1	1.67	0.59
19:T:255:SER:OG	19:T:258:SER:O	2.19	0.59
23:X:405:ARG:HG3	23:X:435:TYR:CE2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:424:THR:HG21	23:X:728:ARG:HH21	1.67	0.59
3:C:724:TRP:HE1	3:C:732:ILE:HD11	1.66	0.59
5:E:174:GLY:HA2	5:E:194:TYR:C	2.23	0.59
5:E:259:VAL:HG22	5:E:277:PHE:HB2	1.84	0.59
5:E:330:ILE:HA	5:E:346:SER:HA	1.83	0.59
5:E:345:ALA:HA	5:E:351:LEU:HD23	1.84	0.59
10:J:289:ASN:HB3	12:L:232:TYR:CE2	2.38	0.59
17:R:150:ALA:O	17:R:153:LYS:HG3	2.02	0.59
19:T:383:ARG:O	19:T:384:HIS:ND1	2.31	0.59
24:Y:3:VAL:HG23	24:Y:16:LEU:HD21	1.85	0.59
26:1:1258:ALA:HB3	26:1:1261:VAL:HG13	1.83	0.59
27:3:680:ASP:OD2	27:3:681:PRO:HD2	2.02	0.59
1:A:693:ILE:O	1:A:695:ASP:N	2.34	0.59
1:A:1925:LYS:HE2	21:V:457:ARG:HH21	1.67	0.59
6:F:85:U:O2	8:H:14:C:N3	2.36	0.59
23:X:698:LYS:NZ	23:X:758:THR:HA	2.17	0.59
26:1:677:CYS:O	26:1:680:LEU:HD12	2.01	0.59
27:3:435:LEU:HD13	27:3:799:ILE:HD11	1.84	0.59
27:3:910:ALA:HB1	27:3:913:LEU:HD11	1.83	0.59
46:9:366:LEU:HD11	46:9:380:PHE:HB2	1.84	0.59
2:B:107:U:H2'	2:B:108:G:O4'	2.03	0.59
3:C:531:TRP:CE3	3:C:540:GLU:HB3	2.37	0.59
7:G:111:U:OP2	23:X:482:ARG:HD3	2.03	0.59
21:V:613:GLU:OE1	21:V:618:ARG:NH2	2.36	0.59
22:W:359:TRP:HA	22:W:366:CYS:HA	1.85	0.59
23:X:537:LYS:HD2	23:X:563:PHE:CE1	2.38	0.59
23:X:877:ASP:OD1	23:X:877:ASP:N	2.36	0.59
24:Y:42:ILE:HG21	24:Y:51:ILE:HG22	1.84	0.59
1:A:1124:ASN:ND2	1:A:1148:ASN:OD1	2.32	0.59
1:A:1211:ASP:O	1:A:1213:VAL:N	2.36	0.59
1:A:1502:PHE:HZ	1:A:1505:LYS:HB2	1.68	0.59
1:A:2149:PRO:HD3	1:A:2274:PRO:HG3	1.84	0.59
17:R:147:THR:HG23	19:T:360:VAL:HG22	1.85	0.59
3:C:493:PHE:HD2	3:C:551:LEU:HG	1.67	0.59
6:F:41:A:H2	7:G:6:A:N1	2.01	0.59
13:N:72:ARG:O	13:N:76:GLU:HG3	2.02	0.59
15:P:190:ASP:OD1	24:Y:118:TYR:OH	2.21	0.59
17:R:240:LYS:O	17:R:244:GLU:HG3	2.03	0.59
26:1:630:ARG:HG3	26:1:670:GLN:HG3	1.83	0.59
26:1:698:GLN:HB3	26:1:701:VAL:HG12	1.84	0.59
27:3:69:ARG:NH1	27:3:74:THR:HA	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:212:GLU:HB2	27:3:223:LYS:HG3	1.84	0.59
27:3:528:ARG:HG2	27:3:532:ARG:HH21	1.67	0.59
27:3:706:MET:HG3	27:3:707:GLN:HG2	1.83	0.59
1:A:274:PRO:HG3	20:U:1:MET:HG3	1.85	0.59
15:P:39:THR:O	19:T:318:ARG:HD3	2.03	0.59
15:P:188:TRP:O	15:P:188:TRP:CG	2.56	0.59
23:X:587:PRO:HB2	26:1:827:ARG:HH12	1.67	0.59
23:X:591:TYR:HD2	23:X:692:PRO:HB2	1.68	0.59
23:X:694:PHE:O	23:X:722:ARG:NH1	2.26	0.59
27:3:700:LYS:HE2	27:3:715:MET:HB3	1.84	0.59
27:3:982:GLU:HG2	27:3:984:LYS:HE3	1.84	0.59
33:5:65:ARG:HB3	33:5:65:ARG:CZ	2.32	0.59
1:A:179:ALA:HA	1:A:183:LEU:HB2	1.84	0.59
1:A:378:PHE:O	3:C:355:LYS:HG3	2.03	0.59
14:O:116:TYR:O	14:O:120:ASN:ND2	2.35	0.59
16:Q:1306:ARG:O	16:Q:1310:PHE:CB	2.51	0.59
26:1:1217:PRO:HD3	30:2:590:LEU:HD13	1.85	0.59
1:A:1209:HIS:CG	1:A:1210:LYS:N	2.71	0.58
7:G:85:G:H2'	7:G:86:A:C8	2.38	0.58
8:H:13:C:H1'	8:H:14:C:H5'	1.84	0.58
16:Q:1322:GLN:HA	16:Q:1325:ALA:HB2	1.85	0.58
17:R:91:ASP:OD1	17:R:94:GLY:N	2.36	0.58
23:X:815:MET:CE	23:X:829:LEU:HD12	2.33	0.58
24:Y:30:LYS:NZ	24:Y:168:ASP:OD1	2.29	0.58
24:Y:51:ILE:O	24:Y:109:LEU:HA	2.03	0.58
26:1:759:ALA:O	26:1:763:ASN:N	2.35	0.58
26:1:854:VAL:HG23	26:1:855:ASP:H	1.68	0.58
27:3:195:ASP:OD2	27:3:198:GLY:N	2.36	0.58
27:3:329:TYR:CE2	27:3:389:PRO:HA	2.37	0.58
1:A:727:LYS:HG3	46:9:244:GLY:HA3	1.86	0.58
3:C:379:LYS:O	3:C:383:GLN:HG2	2.04	0.58
6:F:89:U:H2'	6:F:90:G:O4'	2.03	0.58
21:V:542:ASN:OD1	21:V:545:ARG:NH2	2.35	0.58
23:X:524:GLU:OE2	23:X:529:THR:OG1	2.20	0.58
23:X:960:ARG:HG3	23:X:967:THR:HA	1.84	0.58
23:X:1004:GLU:HB2	23:X:1007:TRP:CD2	2.38	0.58
26:1:1203:GLY:HA2	27:3:1171:LYS:HG3	1.84	0.58
27:3:25:THR:OG1	27:3:26:LYS:N	2.35	0.58
27:3:803:ASP:OD2	33:5:58:ASN:ND2	2.36	0.58
1:A:1502:PHE:CZ	1:A:1505:LYS:HB2	2.37	0.58
2:B:93:U:O2'	2:B:94:U:O4'	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:108:HIS:CD2	5:E:128:SER:HB3	2.38	0.58
5:E:334:ALA:HB3	5:E:343:ILE:HG23	1.85	0.58
8:H:180:G:H2'	8:H:181:G:C8	2.38	0.58
23:X:797:TYR:HA	23:X:802:LEU:HB2	1.84	0.58
24:Y:90:LYS:HB2	24:Y:93:THR:HG23	1.84	0.58
26:1:605:GLY:O	26:1:608:THR:OG1	2.16	0.58
26:1:1110:VAL:O	26:1:1114:VAL:HG23	2.04	0.58
27:3:387:PHE:CE1	27:3:389:PRO:HG3	2.38	0.58
2:B:63:A:H2'	2:B:64:G:H8	1.67	0.58
6:F:43:A:H2	7:G:4:A:H61	1.50	0.58
17:R:137:GLU:OE1	17:R:137:GLU:N	2.32	0.58
26:1:1104:GLN:O	26:1:1105:GLU:HB3	2.03	0.58
27:3:1147:HIS:O	27:3:1151:GLU:HG3	2.03	0.58
1:A:736:GLU:OE2	46:9:247:SER:OG	2.16	0.58
1:A:1817:LEU:HD11	1:A:1819:LEU:HD13	1.84	0.58
3:C:352:LYS:HE2	3:C:352:LYS:H	1.67	0.58
3:C:500:THR:HG22	3:C:545:PRO:HA	1.83	0.58
4:D:759:THR:N	27:3:680:ASP:OD2	2.31	0.58
7:G:7:G:C5	7:G:8:C:C4	2.92	0.58
26:1:850:ILE:O	26:1:854:VAL:HG13	2.04	0.58
26:1:898:TYR:OH	26:1:902:GLU:HG2	2.03	0.58
27:3:326:ARG:NE	27:3:372:GLU:OE2	2.19	0.58
8:H:6:U:H2'	8:H:7:U:C6	2.38	0.58
8:H:50:C:H2'	8:H:51:A:C8	2.38	0.58
21:V:456:ARG:NE	21:V:492:MET:SD	2.76	0.58
23:X:219:ARG:HA	23:X:222:MET:SD	2.43	0.58
24:Y:87:LYS:O	24:Y:89:LYS:N	2.36	0.58
26:1:512:ARG:O	26:1:516:LEU:HB2	2.04	0.58
26:1:815:PHE:HZ	26:1:849:ILE:HG23	1.67	0.58
27:3:642:ILE:H	27:3:703:ARG:HE	1.52	0.58
1:A:83:HIS:NE2	7:G:16:G:O6	2.37	0.58
1:A:1251:SER:OG	1:A:1298:ARG:HD3	2.04	0.58
1:A:2086:ARG:NH1	1:A:2219:THR:O	2.36	0.58
3:C:673:LYS:HE2	20:U:57:ILE:HA	1.86	0.58
3:C:925:PRO:O	3:C:928:HIS:ND1	2.36	0.58
23:X:815:MET:CE	23:X:829:LEU:HD11	2.34	0.58
24:Y:33:LYS:HG3	24:Y:161:ILE:HG13	1.85	0.58
27:3:462:VAL:O	27:3:472:ALA:N	2.30	0.58
1:A:357:ASN:HD22	3:C:862:PRO:HB3	1.69	0.58
1:A:1992:GLY:HA2	1:A:1997:VAL:HG23	1.85	0.58
2:B:53:U:OP1	15:P:39:THR:OG1	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:115:GLU:OE1	3:C:115:GLU:N	2.37	0.58
23:X:987:HIS:HB3	23:X:999:GLN:HB2	1.85	0.58
26:1:747:LEU:HA	26:1:750:ILE:HG12	1.85	0.58
26:1:1074:ARG:O	26:1:1078:VAL:HG23	2.03	0.58
27:3:141:VAL:HB	27:3:158:LEU:HD12	1.86	0.58
27:3:191:GLU:O	27:3:194:ASN:N	2.26	0.58
30:2:542:GLU:O	30:2:546:GLN:HG2	2.03	0.58
33:5:7:ILE:HG13	33:5:8:HIS:N	2.18	0.58
2:B:20:G:O6	2:B:57:G:N2	2.37	0.58
3:C:441:PRO:HA	3:C:444:GLY:HA3	1.86	0.58
5:E:102:TYR:HD1	5:E:102:TYR:H	1.51	0.58
6:F:37:C:H4'	6:F:38:G:OP2	2.00	0.58
23:X:451:THR:HG22	23:X:519:VAL:HA	1.86	0.58
23:X:543:ARG:NE	23:X:545:GLU:OE1	2.34	0.58
24:Y:263:PHE:HE1	24:Y:300:LYS:HD2	1.69	0.58
27:3:525:ARG:HD3	27:3:533:VAL:HG22	1.85	0.58
27:3:638:GLU:OE2	27:3:698:PRO:HB3	2.04	0.58
46:9:363:ARG:HG3	46:9:384:PHE:HA	1.86	0.58
1:A:1862:ILE:HG23	1:A:1885:LYS:HB3	1.86	0.58
1:A:2004:GLN:OE1	26:1:898:TYR:HB2	2.04	0.58
3:C:78:GLU:HG3	3:C:79:THR:N	2.18	0.58
5:E:206:ASP:C	5:E:222:LEU:HG	2.24	0.58
14:O:233:THR:O	14:O:303:GLY:N	2.29	0.58
23:X:948:PHE:O	23:X:1016:TYR:OH	2.21	0.58
26:1:675:MET:HB3	26:1:678:ALA:HB3	1.84	0.58
27:3:538:THR:OG1	27:3:542:LYS:O	2.22	0.58
5:E:180:ASP:HB2	5:E:187:ILE:HD11	1.84	0.57
6:F:82:A:H1'	6:F:83:A:H2'	1.85	0.57
7:G:105:C:O2'	23:X:619:GLU:OE2	2.21	0.57
7:G:116:C:H5"	17:R:371:ARG:NE	2.19	0.57
23:X:257:PHE:CZ	23:X:270:LEU:HB2	2.39	0.57
23:X:772:ILE:HD12	23:X:778:PHE:HD2	1.69	0.57
24:Y:5:LEU:HD22	24:Y:156:ILE:HG23	1.85	0.57
26:1:1262:ARG:HD2	33:5:24:ALA:O	2.04	0.57
27:3:449:VAL:HG22	27:3:763:ARG:HB3	1.85	0.57
32:7:33:CYS:HB2	32:7:74:GLU:OE1	2.04	0.57
46:9:316:TYR:CE1	46:9:378:SER:HB2	2.39	0.57
1:A:1870:ASP:OD1	1:A:1870:ASP:N	2.26	0.57
1:A:2074:ARG:HD2	1:A:2078:ILE:HG23	1.86	0.57
3:C:803:ARG:O	3:C:807:GLN:HG2	2.04	0.57
7:G:88:G:H4'	7:G:89:U:OP1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:369:LEU:HD23	17:R:377:ARG:HA	1.85	0.57
24:Y:268:SER:OG	24:Y:287:GLU:OE2	2.16	0.57
27:3:479:VAL:HG23	27:3:480:ASN:ND2	2.20	0.57
1:A:1762:TYR:CE2	1:A:2008:ARG:HG3	2.39	0.57
7:G:116:C:H6	17:R:371:ARG:HG2	1.69	0.57
10:J:408:ASP:OD1	10:J:408:ASP:N	2.36	0.57
19:T:450:VAL:C	19:T:451:HIS:HD1	2.06	0.57
23:X:583:TYR:HB3	23:X:739:THR:HA	1.86	0.57
23:X:815:MET:CG	23:X:825:SER:CB	2.82	0.57
23:X:910:ARG:O	23:X:914:VAL:HG13	2.03	0.57
24:Y:141:GLU:OE1	46:9:205:ARG:NH1	2.37	0.57
26:1:1078:VAL:HG12	26:1:1118:ILE:HD12	1.85	0.57
46:9:366:LEU:HD13	46:9:382:ILE:HG13	1.86	0.57
1:A:1220:VAL:HG23	1:A:1221:THR:HG23	1.87	0.57
10:J:230:THR:OG1	10:J:231:PHE:N	2.37	0.57
13:N:63:LEU:HB3	13:N:70:ILE:HD12	1.85	0.57
21:V:515:CYS:HA	21:V:521:TYR:HB2	1.84	0.57
23:X:521:GLU:HB3	23:X:523:HIS:CE1	2.38	0.57
24:Y:152:GLN:NE2	24:Y:193:ALA:HA	2.19	0.57
26:1:703:THR:HG22	26:1:745:ALA:HB3	1.87	0.57
1:A:171:ASP:O	1:A:520:TYR:HB2	2.04	0.57
1:A:393:LEU:HD12	3:C:379:LYS:HE2	1.87	0.57
5:E:255:MET:HB2	5:E:282:HIS:CB	2.35	0.57
12:L:742:ILE:O	12:L:746:HIS:N	2.37	0.57
13:N:97:TYR:HD1	13:N:120:ARG:HH21	1.53	0.57
23:X:238:ARG:HH21	24:Y:224:LEU:HD12	1.70	0.57
27:3:345:GLY:O	27:3:360:GLN:HG3	2.04	0.57
27:3:607:VAL:HB	27:3:615:ARG:HB2	1.85	0.57
27:3:1200:THR:O	27:3:1203:GLU:N	2.38	0.57
46:9:278:LYS:HG2	46:9:279:LYS:H	1.69	0.57
1:A:1639:VAL:HG22	1:A:1719:PHE:HB3	1.86	0.57
1:A:2196:HIS:CE1	1:A:2211:THR:HB	2.40	0.57
2:B:97:G:H1	2:B:116:U:H3	1.50	0.57
3:C:216:THR:HG22	3:C:245:HIS:CE1	2.40	0.57
10:J:333:PHE:O	10:J:337:MET:HG2	2.05	0.57
23:X:707:GLU:O	23:X:990:VAL:HA	2.05	0.57
27:3:310:ILE:O	27:3:311:PHE:HD2	1.87	0.57
1:A:827:PHE:HB2	1:A:1002:ASP:OD2	2.04	0.57
1:A:1773:SER:HB2	1:A:1775:GLN:HG3	1.87	0.57
1:A:2228:TYR:HA	1:A:2258:ARG:HA	1.86	0.57
3:C:439:PRO:O	3:C:443:VAL:HB	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:560:VAL:HG12	3:C:561:LYS:HG2	1.87	0.57
3:C:704:VAL:HG12	3:C:717:PHE:HE1	1.68	0.57
5:E:75:HIS:ND1	5:E:77:ASN:HB2	2.19	0.57
5:E:197:LEU:HD21	5:E:213:ILE:HD11	1.87	0.57
5:E:208:ILE:HG13	5:E:222:LEU:HD21	1.86	0.57
24:Y:118:TYR:N	24:Y:118:TYR:CD1	2.72	0.57
26:1:631:ALA:O	26:1:635:VAL:HG13	2.05	0.57
27:3:329:TYR:HE2	27:3:389:PRO:HA	1.69	0.57
27:3:791:HIS:HD2	27:3:794:SER:OG	1.87	0.57
32:7:68:ASP:OD1	32:7:68:ASP:N	2.38	0.57
1:A:872:ASP:O	1:A:874:PRO:HD3	2.04	0.57
1:A:1978:LYS:O	1:A:1981:VAL:HG12	2.05	0.57
4:D:668:ASP:O	4:D:672:GLY:CA	2.53	0.57
8:H:68:G:H2'	8:H:69:U:C6	2.39	0.57
10:J:406:PHE:HD1	10:J:411:MET:HA	1.69	0.57
12:L:756:LYS:O	12:L:760:ASP:N	2.35	0.57
17:R:335:ARG:CB	23:X:272:TYR:HB2	2.35	0.57
46:9:360:HIS:HB3	46:9:365:ILE:HG21	1.85	0.57
1:A:265:THR:OG1	1:A:328:HIS:O	2.23	0.57
1:A:1275:ARG:O	1:A:1369:TYR:HE1	1.88	0.57
1:A:1971:LEU:HD22	1:A:1972:THR:H	1.70	0.57
3:C:543:ARG:CZ	3:C:543:ARG:HB2	2.34	0.57
3:C:670:SER:HB2	3:C:689:ALA:H	1.70	0.57
5:E:81:LEU:O	5:E:92:LEU:HA	2.04	0.57
11:K:205:TYR:O	11:K:209:GLY:N	2.36	0.57
21:V:532:GLN:O	21:V:536:ILE:CB	2.39	0.57
21:V:576:THR:O	21:V:579:SER:OG	2.16	0.57
21:V:609:GLN:HA	21:V:612:PHE:HB2	1.85	0.57
24:Y:30:LYS:HE3	24:Y:169:PRO:HD2	1.86	0.57
26:1:720:GLY:HA2	26:1:756:LEU:HD23	1.86	0.57
3:C:258:ASN:OD1	3:C:259:LYS:N	2.37	0.57
3:C:928:HIS:ND1	3:C:928:HIS:N	2.53	0.57
8:H:41:U:H2'	8:H:42:G:C8	2.39	0.57
8:H:70:C:H2'	8:H:71:C:C6	2.39	0.57
23:X:598:SER:O	23:X:602:ILE:HG13	2.05	0.57
24:Y:55:ASP:OD2	24:Y:60:GLY:N	2.37	0.57
26:1:716:ALA:O	26:1:756:LEU:HD21	2.05	0.57
27:3:365:GLY:HA2	27:3:394:ASN:ND2	2.19	0.57
1:A:250:VAL:HG23	1:A:251:ASP:OD2	2.05	0.56
5:E:251:LEU:HD21	5:E:300:ILE:HG23	1.87	0.56
12:L:38:LEU:HB3	12:L:41:LYS:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:41:ARG:O	13:N:45:SER:OG	2.23	0.56
17:R:389:SER:HA	17:R:392:ILE:HD12	1.87	0.56
19:T:247:SER:OG	19:T:267:ASP:OD1	2.20	0.56
23:X:265:HIS:O	23:X:268:GLN:HG2	2.04	0.56
24:Y:8:THR:HG23	24:Y:155:ARG:HB2	1.86	0.56
26:1:557:ASP:HB2	26:1:558:ARG:NH2	2.20	0.56
27:3:616:ILE:HG22	27:3:628:LEU:HB3	1.86	0.56
27:3:1148:LEU:HA	27:3:1151:GLU:OE2	2.05	0.56
46:9:323:ARG:HB3	46:9:331:GLN:HE21	1.70	0.56
1:A:123:THR:O	1:A:123:THR:OG1	2.23	0.56
1:A:1771:LEU:HD13	1:A:1777:ILE:HD12	1.86	0.56
4:D:434:SER:HA	4:D:446:HIS:O	2.05	0.56
6:F:89:U:H3	8:H:9:U:H3	1.52	0.56
10:J:360:ASP:O	10:J:364:THR:OG1	2.22	0.56
14:O:116:TYR:HA	17:R:218:ILE:HD13	1.87	0.56
17:R:353:ASP:O	17:R:357:HIS:HB2	2.05	0.56
24:Y:272:ILE:HG22	24:Y:281:LEU:HD12	1.86	0.56
26:1:784:MET:O	26:1:788:VAL:HG12	2.05	0.56
1:A:170:ASP:OD1	1:A:171:ASP:N	2.38	0.56
1:A:2144:CYS:HB2	1:A:2270:PHE:HE1	1.69	0.56
3:C:136:GLY:HA2	3:C:227:LEU:HD12	1.86	0.56
3:C:286:ASN:HD21	3:C:300:LEU:N	2.02	0.56
3:C:380:ILE:O	3:C:384:VAL:HG23	2.05	0.56
4:D:530:THR:C	4:D:532:ASN:H	2.09	0.56
5:E:197:LEU:HD11	5:E:213:ILE:HD13	1.87	0.56
6:F:21:U:N3	13:N:125:LYS:HE3	2.20	0.56
6:F:87:C:C2	6:F:88:G:C8	2.94	0.56
12:L:631:LYS:O	12:L:635:VAL:N	2.37	0.56
13:N:49:ILE:H	13:N:49:ILE:HD12	1.70	0.56
17:R:180:THR:HG23	17:R:194:GLN:HE21	1.71	0.56
21:V:604:LYS:NZ	21:V:639:LEU:HD23	2.21	0.56
24:Y:257:GLU:O	24:Y:261:SER:HB3	2.05	0.56
27:3:169:HIS:CD2	27:3:170:VAL:H	2.22	0.56
27:3:1140:PHE:HE1	27:3:1197:LEU:HD13	1.67	0.56
27:3:1180:GLU:CD	27:3:1212:ARG:HH21	2.08	0.56
2:B:13:C:H2'	2:B:14:U:O4'	2.05	0.56
19:T:272:CYS:HB3	19:T:282:ARG:HB3	1.86	0.56
23:X:171:ARG:NH2	23:X:506:LEU:O	2.38	0.56
23:X:457:ALA:O	23:X:460:SER:OG	2.21	0.56
27:3:418:GLU:OE1	27:3:419:ASP:N	2.28	0.56
27:3:552:ARG:HH21	27:3:567:GLU:HB3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:592:LEU:HD11	27:3:619:LEU:HD21	1.88	0.56
1:A:435:CYS:SG	7:G:-10:G:N1	2.60	0.56
1:A:1482:GLU:O	1:A:1486:GLU:HG2	2.05	0.56
3:C:350:ASN:ND2	3:C:353:THR:OG1	2.38	0.56
17:R:172:ALA:HB1	17:R:173:PRO:HD2	1.86	0.56
23:X:596:VAL:O	23:X:600:LEU:HG	2.05	0.56
23:X:681:LEU:H	23:X:725:ARG:HH22	1.52	0.56
24:Y:65:SER:N	24:Y:76:SER:O	2.33	0.56
24:Y:253:ASP:OD1	24:Y:253:ASP:N	2.30	0.56
26:1:754:ILE:HG22	26:1:755:PRO:HD3	1.88	0.56
26:1:954:LEU:O	26:1:958:THR:HG22	2.05	0.56
2:B:12:U:H2'	2:B:13:C:H6	1.70	0.56
19:T:227:THR:HG22	19:T:243:THR:HG22	1.88	0.56
19:T:381:HIS:HD2	19:T:441:TRP:CE2	2.23	0.56
21:V:570:LEU:HD13	21:V:627:ALA:HB1	1.87	0.56
23:X:716:LYS:N	23:X:747:LEU:HD12	2.20	0.56
26:1:739:ARG:HA	26:1:743:LEU:HD22	1.88	0.56
33:5:14:LEU:HA	33:5:17:LYS:HB2	1.86	0.56
1:A:693:ILE:HB	1:A:738:MET:SD	2.46	0.56
1:A:1014:ASN:ND2	12:L:83:ARG:HB2	2.18	0.56
1:A:1359:HIS:HD2	1:A:1361:GLU:O	1.89	0.56
1:A:1629:ILE:HB	1:A:1662:ILE:HB	1.88	0.56
1:A:1655:THR:OG1	1:A:1656:THR:N	2.38	0.56
1:A:1670:ASP:N	1:A:1670:ASP:OD1	2.37	0.56
1:A:1787:ARG:NH1	1:A:1788:VAL:O	2.39	0.56
8:H:72:U:H2'	8:H:73:C:C6	2.41	0.56
13:N:97:TYR:HA	13:N:120:ARG:HH21	1.71	0.56
24:Y:67:PHE:HB2	24:Y:75:ALA:O	2.05	0.56
26:1:970:LEU:O	26:1:973:HIS:HB2	2.06	0.56
26:1:1098:LEU:HD12	26:1:1135:GLU:HG2	1.87	0.56
27:3:607:VAL:N	27:3:615:ARG:O	2.29	0.56
1:A:1923:TRP:HB3	1:A:1927:ILE:HD11	1.87	0.56
1:A:2076:ARG:NH1	1:A:2119:ASP:OD2	2.39	0.56
2:B:99:C:H2'	2:B:100:C:H6	1.71	0.56
3:C:68:THR:OG1	3:C:69:ALA:N	2.37	0.56
3:C:463:GLU:H	3:C:463:GLU:CD	2.08	0.56
3:C:510:LEU:HB2	3:C:564:THR:HG23	1.87	0.56
5:E:221:ASP:HB2	5:E:228:THR:OG1	2.06	0.56
24:Y:263:PHE:CE1	24:Y:300:LYS:HD2	2.40	0.56
26:1:807:LYS:HG3	26:1:844:VAL:HG11	1.88	0.56
27:3:69:ARG:HH12	27:3:74:THR:HA	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:86:ARG:NH1	27:3:1157:GLY:O	2.38	0.56
27:3:510:LEU:HD23	27:3:510:LEU:H	1.70	0.56
27:3:703:ARG:HH11	27:3:703:ARG:HB2	1.70	0.56
1:A:940:ILE:HD13	1:A:1090:ARG:HH12	1.71	0.56
1:A:1984:LYS:HA	1:A:1987:ILE:HD12	1.88	0.56
3:C:375:GLU:O	3:C:379:LYS:HG3	2.06	0.56
3:C:587:VAL:HG11	3:C:830:PRO:HG3	1.87	0.56
12:L:187:LYS:O	12:L:191:LEU:N	2.35	0.56
13:N:16:GLU:CD	13:N:16:GLU:H	2.09	0.56
23:X:388:GLN:O	23:X:392:ILE:HG13	2.06	0.56
23:X:405:ARG:NH1	23:X:406:GLU:OE1	2.39	0.56
23:X:819:PRO:HG3	23:X:921:LEU:CD1	2.30	0.56
27:3:206:GLN:NE2	27:3:231:HIS:HA	2.21	0.56
27:3:717:SER:HB2	27:3:718:ARG:NH1	2.21	0.56
27:3:1083:ASN:OD1	27:3:1084:GLY:N	2.39	0.56
46:9:382:ILE:HG21	46:9:407:LEU:HD12	1.88	0.56
1:A:1339:ASP:OD1	1:A:1339:ASP:N	2.38	0.56
1:A:1782:ASP:HB3	1:A:1807:ILE:HD13	1.88	0.56
1:A:1861:ILE:HG23	1:A:1884:ILE:HG23	1.86	0.56
3:C:461:LEU:HA	3:C:464:ALA:HB3	1.86	0.56
3:C:478:THR:HA	3:C:494:GLY:HA3	1.87	0.56
3:C:875:ILE:HG13	3:C:876:PRO:HD2	1.89	0.56
7:G:85:G:H1	8:H:45:C:H42	1.53	0.56
17:R:372:ALA:HB3	17:R:376:LYS:HE2	1.87	0.56
24:Y:91:LYS:HG3	24:Y:114:GLU:HG3	1.88	0.56
24:Y:217:ALA:O	24:Y:220:GLN:HG3	2.05	0.56
27:3:68:PHE:CE2	27:3:77:TYR:HB2	2.41	0.56
1:A:172:GLU:OE1	1:A:172:GLU:N	2.39	0.55
1:A:525:LYS:HB2	1:A:525:LYS:HZ3	1.71	0.55
1:A:591:MET:HB3	1:A:598:LEU:HD21	1.87	0.55
1:A:876:GLU:O	1:A:879:SER:OG	2.23	0.55
1:A:1184:ASN:OD1	1:A:1195:ARG:NH1	2.36	0.55
3:C:913:ASP:O	3:C:931:ARG:NE	2.39	0.55
10:J:416:TYR:HE2	10:J:443:ILE:HD13	1.71	0.55
19:T:220:VAL:HG23	19:T:230:ILE:HG12	1.87	0.55
23:X:821:ASP:O	23:X:825:SER:OG	2.23	0.55
27:3:288:VAL:HG12	33:5:62:ALA:HB3	1.89	0.55
27:3:527:ILE:HG12	27:3:532:ARG:O	2.06	0.55
27:3:1115:GLU:HG2	30:2:708:TRP:HE1	1.70	0.55
46:9:297:CYS:SG	46:9:437:PRO:HG3	2.46	0.55
1:A:1336:PRO:HB2	1:A:1350:ILE:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1813:ARG:HE	1:A:1814:THR:HG23	1.71	0.55
1:A:2305:TYR:O	1:A:2310:ARG:NH1	2.37	0.55
3:C:827:LEU:HD12	3:C:911:PRO:HB3	1.88	0.55
9:I:169:TYR:O	9:I:173:LEU:CB	2.54	0.55
13:N:140:ARG:NE	22:W:196:TRP:O	2.36	0.55
17:R:348:GLU:HG2	23:X:266:GLU:OE1	2.05	0.55
23:X:772:ILE:HG21	23:X:775:LEU:CD2	2.36	0.55
23:X:992:THR:HG1	23:X:996:PHE:HD2	1.52	0.55
27:3:926:TYR:HB3	27:3:928:TYR:CE2	2.41	0.55
27:3:1191:LYS:O	27:3:1195:GLU:HG3	2.07	0.55
1:A:296:PHE:CZ	3:C:593:GLU:HB2	2.41	0.55
1:A:341:LYS:HA	1:A:341:LYS:HE2	1.87	0.55
1:A:939:TRP:NE1	1:A:1049:ASP:OD2	2.33	0.55
1:A:1836:LEU:HA	1:A:1839:TRP:HD1	1.70	0.55
3:C:694:LYS:HA	3:C:786:ASN:OD1	2.06	0.55
5:E:326:HIS:CE1	5:E:344:SER:HG	2.21	0.55
6:F:83:A:N6	8:H:16:U:C4	2.74	0.55
10:J:376:VAL:HA	10:J:379:TRP:HD1	1.71	0.55
12:L:48:ALA:O	12:L:52:GLU:HG2	2.07	0.55
23:X:226:LEU:HD22	24:Y:315:PHE:CE2	2.39	0.55
27:3:226:GLU:OE1	27:3:259:LYS:HD3	2.07	0.55
27:3:373:PHE:HE1	27:3:385:PHE:HB3	1.70	0.55
1:A:84:ASP:O	1:A:88:TYR:HB2	2.07	0.55
1:A:1131:LYS:HG2	1:A:1193:GLU:OE2	2.06	0.55
1:A:2129:TYR:CD2	1:A:2172:MET:HE3	2.40	0.55
5:E:227:LEU:O	5:E:227:LEU:HD12	2.07	0.55
6:F:21:U:C4	13:N:125:LYS:HE3	2.41	0.55
8:H:28:C:O2'	8:H:29:A:O5'	2.25	0.55
10:J:226:ARG:O	10:J:230:THR:HG23	2.06	0.55
10:J:262:ARG:HH22	10:J:291:GLN:HG2	1.70	0.55
10:J:342:GLU:OE2	10:J:344:GLN:N	2.37	0.55
19:T:274:ASP:HB2	19:T:281:ILE:HD13	1.88	0.55
21:V:518:LYS:HD2	21:V:520:GLU:OE1	2.06	0.55
21:V:543:LYS:HA	21:V:546:ASN:ND2	2.22	0.55
21:V:618:ARG:HB3	21:V:646:HIS:CE1	2.42	0.55
21:V:622:ARG:CA	21:V:625:ARG:HH21	2.19	0.55
24:Y:181:PRO:HB2	24:Y:186:LEU:HG	1.89	0.55
24:Y:271:VAL:HG22	24:Y:284:ALA:HB2	1.88	0.55
26:1:826:ASP:HB3	26:1:829:ASN:HB2	1.87	0.55
27:3:567:GLU:OE2	27:3:601:ARG:NH2	2.40	0.55
46:9:324:SER:O	46:9:420:ASP:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ASN:N	1:A:322:ASN:OD1	2.38	0.55
1:A:2005:SER:HB2	1:A:2008:ARG:HH22	1.70	0.55
3:C:759:LEU:O	3:C:762:VAL:N	2.38	0.55
7:G:85:G:N2	8:H:45:C:N3	2.51	0.55
7:G:111:U:H5	23:X:819:PRO:HA	1.69	0.55
26:1:549:ARG:NH2	26:1:592:GLU:OE1	2.30	0.55
27:3:1015:LYS:O	27:3:1019:ASN:N	2.40	0.55
1:A:81:PHE:O	1:A:83:HIS:N	2.39	0.55
1:A:292:ASP:CG	1:A:293:TRP:H	2.10	0.55
1:A:2072:GLU:HA	1:A:2075:VAL:HG22	1.87	0.55
3:C:746:VAL:O	3:C:791:ILE:HG13	2.06	0.55
3:C:772:TRP:HH2	46:9:130:ALA:HA	1.71	0.55
8:H:50:C:H2'	8:H:51:A:H8	1.71	0.55
17:R:113:TYR:OH	19:T:402:ASP:O	2.20	0.55
21:V:497:CYS:HB2	21:V:507:PHE:CB	2.36	0.55
21:V:553:HIS:CD2	21:V:556:TYR:HE1	2.25	0.55
27:3:791:HIS:NE2	27:3:934:GLY:HA3	2.22	0.55
27:3:1143:HIS:O	27:3:1147:HIS:ND1	2.39	0.55
33:5:27:THR:HG23	33:5:30:GLU:HG3	1.88	0.55
46:9:375:SER:O	46:9:375:SER:OG	2.22	0.55
1:A:1787:ARG:HD3	1:A:1788:VAL:N	2.22	0.55
5:E:268:ALA:O	5:E:270:LYS:HD2	2.07	0.55
6:F:16:G:H2'	6:F:17:C:C6	2.41	0.55
8:H:107:A:H2'	8:H:108:G:C8	2.42	0.55
10:J:368:ARG:HA	10:J:368:ARG:NE	2.22	0.55
17:R:280:ILE:H	46:9:225:MET:HA	1.72	0.55
19:T:213:GLU:OE1	19:T:217:GLN:N	2.30	0.55
23:X:600:LEU:O	23:X:604:VAL:HG23	2.06	0.55
26:1:1252:GLN:NE2	30:2:492:LYS:HA	2.22	0.55
30:2:451:LYS:HB2	30:2:455:ARG:NH1	2.22	0.55
1:A:27:GLU:O	1:A:31:GLN:HG2	2.07	0.55
3:C:189:VAL:HA	3:C:198:TYR:O	2.06	0.55
3:C:390:THR:O	3:C:393:PRO:HD2	2.07	0.55
21:V:529:PHE:CE1	21:V:564:VAL:HB	2.42	0.55
22:W:138:ALA:N	22:W:153:ILE:O	2.37	0.55
23:X:837:SER:HB3	23:X:930:SER:H	1.71	0.55
27:3:526:HIS:CG	27:3:573:GLN:HE21	2.25	0.55
27:3:1145:GLU:HA	27:3:1148:LEU:HB2	1.88	0.55
46:9:308:ILE:HA	46:9:311:CYS:HB2	1.87	0.55
1:A:608:LEU:HD13	1:A:632:ALA:HB1	1.89	0.55
1:A:1303:LEU:HD12	1:A:1311:PHE:HE1	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1947:ASN:O	1:A:1951:LYS:HG3	2.07	0.55
5:E:330:ILE:H	5:E:330:ILE:HD12	1.72	0.55
7:G:90:C:O5'	7:G:90:C:H6	1.88	0.55
8:H:57:A:H5'	30:2:481:THR:HG21	1.88	0.55
13:N:120:ARG:CZ	13:N:143:SER:HB3	2.37	0.55
23:X:593:GLU:O	23:X:597:VAL:HG22	2.06	0.55
27:3:233:ASN:HD21	27:3:286:ILE:CG2	2.19	0.55
27:3:406:PRO:HG2	27:3:408:LEU:HD11	1.89	0.55
27:3:994:GLN:HE22	27:3:1036:ALA:C	2.10	0.55
1:A:176:LEU:H	1:A:176:LEU:CD2	2.20	0.55
1:A:2163:LEU:HD11	1:A:2206:TRP:HE1	1.71	0.55
3:C:441:PRO:O	3:C:444:GLY:HA3	2.07	0.55
3:C:465:MET:O	3:C:468:CYS:N	2.37	0.55
8:H:36:G:H2'	8:H:37:U:C6	2.42	0.55
16:Q:514:ILE:H	16:Q:655:ILE:HA	1.71	0.55
23:X:475:ASN:HB3	23:X:490:ARG:HD3	1.89	0.55
26:1:819:TRP:HZ2	26:1:837:THR:HG21	1.71	0.55
26:1:1062:LEU:HA	26:1:1065:LEU:HD12	1.88	0.55
27:3:911:LYS:CB	27:3:922:GLY:O	2.55	0.55
31:4:13:ALA:O	31:4:60:GLU:HA	2.06	0.55
46:9:368:MET:O	46:9:394:HIS:ND1	2.40	0.55
1:A:305:ARG:NH1	3:C:924:GLN:O	2.37	0.54
1:A:389:LYS:HA	3:C:379:LYS:NZ	2.22	0.54
1:A:705:LYS:O	1:A:708:THR:HG22	2.07	0.54
1:A:1787:ARG:HD3	1:A:1788:VAL:H	1.71	0.54
1:A:2188:LEU:HD13	1:A:2228:TYR:CD1	2.42	0.54
1:A:2311:PRO:O	1:A:2315:LEU:N	2.37	0.54
3:C:118:PHE:O	3:C:122:LEU:HD12	2.07	0.54
4:D:418:GLN:O	4:D:422:PHE:N	2.40	0.54
8:H:165:A:O2'	8:H:166:G:O5'	2.24	0.54
10:J:238:ASN:C	10:J:240:THR:H	2.11	0.54
14:O:249:ARG:O	14:O:252:PHE:N	2.39	0.54
14:O:261:ILE:HA	14:O:271:PHE:O	2.07	0.54
16:Q:1049:LEU:O	16:Q:1054:PHE:N	2.39	0.54
16:Q:1136:GLN:N	16:Q:1156:ASN:HA	2.21	0.54
23:X:822:PRO:HA	23:X:825:SER:CB	2.37	0.54
24:Y:21:ARG:NH2	24:Y:81:GLU:O	2.41	0.54
27:3:342:LEU:HB3	27:3:343:LYS:O	2.06	0.54
27:3:542:LYS:HB2	27:3:558:LEU:HD11	1.88	0.54
30:2:531:THR:O	30:2:531:THR:OG1	2.25	0.54
46:9:301:PRO:O	46:9:305:GLU:HB2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:854:SER:OG	1:A:855:ARG:N	2.39	0.54
1:A:1761:PRO:O	1:A:1930:TYR:OH	2.25	0.54
3:C:260:ILE:HG13	3:C:310:SER:O	2.05	0.54
7:G:85:G:N1	8:H:44:U:N3	2.55	0.54
11:K:209:GLY:HA2	11:K:223:ARG:HD3	1.89	0.54
19:T:223:SER:OG	19:T:224:ALA:N	2.38	0.54
19:T:243:THR:O	19:T:243:THR:OG1	2.24	0.54
23:X:815:MET:CG	23:X:825:SER:HB3	2.36	0.54
26:1:735:ILE:HD12	26:1:747:LEU:HD12	1.88	0.54
26:1:1206:ASP:OD1	26:1:1207:SER:N	2.41	0.54
1:A:65:HIS:CD2	13:N:46:LEU:HD13	2.43	0.54
1:A:1224:ARG:HG3	1:A:1224:ARG:HH11	1.73	0.54
3:C:224:GLY:HA2	3:C:251:LEU:HB3	1.89	0.54
3:C:719:GLN:HG3	3:C:724:TRP:O	2.06	0.54
5:E:214:ASP:N	5:E:214:ASP:OD1	2.39	0.54
10:J:407:GLY:O	10:J:411:MET:HB3	2.07	0.54
13:N:21:THR:O	13:N:24:GLU:HG3	2.06	0.54
13:N:122:PRO:HG2	13:N:125:LYS:HE2	1.89	0.54
17:R:143:ILE:O	17:R:147:THR:OG1	2.18	0.54
23:X:597:VAL:HA	23:X:600:LEU:HD12	1.89	0.54
24:Y:210:GLU:O	24:Y:214:GLU:HG3	2.08	0.54
26:1:769:VAL:HA	26:1:772:ILE:HD13	1.89	0.54
27:3:747:SER:OG	27:3:748:GLU:N	2.40	0.54
27:3:883:GLU:HB3	27:3:886:GLU:HG3	1.89	0.54
27:3:943:THR:HG23	27:3:976:LYS:HB3	1.89	0.54
32:7:57:ARG:NH1	32:7:62:GLY:O	2.39	0.54
1:A:380:LEU:HB2	3:C:354:ARG:HB3	1.89	0.54
7:G:83:A:P	7:G:83:A:H8	2.31	0.54
23:X:561:SER:O	23:X:566:ASP:N	2.32	0.54
24:Y:70:LEU:HD23	24:Y:171:ASP:HB2	1.89	0.54
26:1:728:LEU:HB3	26:1:765:TYR:OH	2.08	0.54
1:A:233:PRO:O	1:A:237:THR:HG23	2.07	0.54
1:A:1536:LEU:HG	1:A:1572:SER:HB3	1.89	0.54
3:C:404:THR:O	3:C:408:LEU:HD12	2.08	0.54
6:F:89:U:H2'	6:F:90:G:C8	2.42	0.54
11:K:200:ASP:HB3	11:K:219:PHE:CD1	2.40	0.54
26:1:785:LYS:O	26:1:789:LEU:HD12	2.07	0.54
27:3:718:ARG:HB2	27:3:720:TRP:NE1	2.21	0.54
1:A:657:ALA:O	1:A:661:GLU:HG3	2.08	0.54
3:C:213:ASP:OD2	3:C:616:SER:OG	2.17	0.54
3:C:857:VAL:HA	3:C:873:ALA:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:294:SER:HB2	5:E:298:SER:H	1.73	0.54
23:X:195:ASN:HD21	24:Y:310:ARG:HH12	1.55	0.54
26:1:953:ASP:O	26:1:956:SER:OG	2.18	0.54
27:3:234:PHE:CE1	27:3:236:ILE:HG12	2.42	0.54
46:9:321:PHE:N	46:9:426:ILE:O	2.38	0.54
1:A:467:GLN:HG2	2:B:19:A:N6	2.23	0.54
1:A:703:GLN:O	1:A:705:LYS:N	2.41	0.54
3:C:692:LEU:HB2	3:C:786:ASN:ND2	2.23	0.54
3:C:772:TRP:CH2	46:9:130:ALA:HA	2.42	0.54
26:1:1122:THR:OG1	26:1:1123:CYS:N	2.41	0.54
26:1:1257:PRO:HD3	30:2:482:ALA:HB2	1.90	0.54
1:A:39:GLN:HE22	22:W:170:THR:H	1.55	0.54
1:A:792:HIS:HE1	17:R:279:HIS:HD2	1.56	0.54
1:A:1777:ILE:HG23	1:A:1860:GLN:HG3	1.89	0.54
3:C:715:GLY:HA2	3:C:719:GLN:HE22	1.73	0.54
15:P:41:ILE:HG13	19:T:318:ARG:HG3	1.89	0.54
23:X:481:ILE:HD11	23:X:484:GLU:HB3	1.90	0.54
24:Y:21:ARG:HH12	24:Y:83:VAL:N	2.06	0.54
26:1:565:ASP:OD1	26:1:566:LEU:N	2.41	0.54
26:1:778:GLN:N	26:1:778:GLN:OE1	2.41	0.54
31:4:79:LEU:N	31:4:82:LYS:O	2.41	0.54
1:A:1979:VAL:HA	1:A:1982:GLN:HB2	1.89	0.54
3:C:215:VAL:HG11	3:C:242:LEU:HD21	1.89	0.54
3:C:719:GLN:NE2	3:C:726:LEU:HA	2.23	0.54
3:C:891:THR:HG21	3:C:895:ALA:HB3	1.90	0.54
6:F:38:G:H8	6:F:38:G:P	2.31	0.54
7:G:7:G:H2’	7:G:8:C:C6	2.42	0.54
7:G:100:C:H4’	7:G:101:U:C6	2.42	0.54
12:L:74:LEU:O	12:L:77:LEU:N	2.41	0.54
23:X:454:ARG:NH1	23:X:680:SER:OG	2.40	0.54
23:X:932:CYS:HB2	23:X:938:ARG:HD2	1.90	0.54
26:1:652:CYS:SG	26:1:689:ILE:HG23	2.48	0.54
26:1:1092:ASP:O	26:1:1096:THR:HG23	2.08	0.54
30:2:495:ARG:O	30:2:497:SER:N	2.41	0.54
33:5:8:HIS:NE2	33:5:12:GLU:OE2	2.37	0.54
33:5:14:LEU:HD23	33:5:17:LYS:HD2	1.88	0.54
1:A:1819:LEU:HB3	1:A:1915:VAL:CG2	2.37	0.54
1:A:2125:ALA:HB2	1:A:2179:HIS:HB3	1.89	0.54
1:A:2148:VAL:HG13	1:A:2149:PRO:O	2.07	0.54
3:C:658:PRO:HB2	3:C:881:PHE:CZ	2.43	0.54
5:E:78:GLY:HA3	5:E:336:HIS:CE1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:197:LEU:HG	5:E:212:GLY:HA2	1.89	0.54
5:E:334:ALA:HB3	5:E:343:ILE:CG2	2.38	0.54
19:T:329:HIS:CE1	19:T:349:SER:HB3	2.43	0.54
26:1:933:CYS:O	26:1:936:VAL:N	2.41	0.54
27:3:164:ASN:HA	27:3:189:TYR:CZ	2.43	0.54
1:A:1780:VAL:HA	1:A:1808:PHE:O	2.09	0.53
1:A:2177:TRP:CZ3	1:A:2179:HIS:HD2	2.26	0.53
1:A:2181:GLN:O	1:A:2217:SER:HA	2.09	0.53
1:A:2246:ASN:OD1	1:A:2246:ASN:N	2.40	0.53
3:C:884:GLU:O	3:C:888:ARG:HG3	2.07	0.53
5:E:62:LEU:HB2	5:E:351:LEU:HB2	1.89	0.53
12:L:11:TRP:CD2	12:L:49:ARG:HD3	2.43	0.53
13:N:139:CYS:SG	13:N:140:ARG:N	2.82	0.53
16:Q:564:LEU:O	16:Q:592:VAL:HA	2.07	0.53
26:1:896:ILE:HD12	26:1:917:VAL:HG11	1.90	0.53
27:3:289:CYS:SG	27:3:338:ALA:HA	2.48	0.53
1:A:1661:TRP:HH2	1:A:1684:PHE:HE1	1.56	0.53
1:A:1771:LEU:HD21	1:A:1779:PHE:CZ	2.40	0.53
1:A:1811:ASN:HB3	1:A:1814:THR:OG1	2.09	0.53
1:A:2095:ASP:OD2	1:A:2258:ARG:NH2	2.42	0.53
3:C:529:ARG:NH2	3:C:540:GLU:HB2	2.19	0.53
3:C:558:PRO:HG2	3:C:559:ILE:HG23	1.91	0.53
6:F:49:G:N7	12:L:33:ARG:HB3	2.23	0.53
23:X:767:LEU:O	23:X:767:LEU:HD13	2.08	0.53
26:1:933:CYS:SG	26:1:970:LEU:HD21	2.48	0.53
27:3:777:VAL:HG22	27:3:779:PHE:CE1	2.43	0.53
33:5:63:ARG:O	33:5:67:ASN:ND2	2.42	0.53
46:9:94:SER:O	46:9:101:TYR:HA	2.09	0.53
1:A:37:TRP:O	1:A:41:GLN:HG2	2.08	0.53
3:C:320:LEU:HD22	3:C:343:LEU:HB2	1.90	0.53
3:C:622:GLU:O	3:C:625:GLY:N	2.41	0.53
8:H:151:C:H2'	8:H:152:G:C8	2.43	0.53
17:R:125:MET:HB2	19:T:186:PRO:HG2	1.90	0.53
17:R:427:ASP:OD1	17:R:428:GLU:N	2.41	0.53
24:Y:267:ARG:N	24:Y:287:GLU:O	2.34	0.53
27:3:269:CYS:SG	27:3:327:LEU:HD11	2.48	0.53
27:3:623:ASP:OD2	27:3:626:GLN:NE2	2.41	0.53
27:3:642:ILE:N	27:3:703:ARG:HE	2.06	0.53
32:7:46:CYS:N	32:7:85:CYS:HB2	2.22	0.53
1:A:550:VAL:O	1:A:554:THR:HG23	2.09	0.53
1:A:1778:TRP:CH2	1:A:1852:LEU:HD21	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2164:PRO:HB3	1:A:2296:LEU:HD11	1.88	0.53
3:C:928:HIS:N	3:C:928:HIS:HD1	2.07	0.53
5:E:75:HIS:CE1	5:E:121:GLY:HA3	2.43	0.53
8:H:36:G:H2'	8:H:37:U:H6	1.73	0.53
17:R:361:LYS:HA	17:R:364:GLN:HG3	1.90	0.53
21:V:505:LYS:NZ	21:V:593:TYR:OH	2.35	0.53
27:3:18:ILE:HG21	27:3:67:ALA:H	1.72	0.53
27:3:477:SER:CB	27:3:505:THR:H	2.11	0.53
46:9:323:ARG:O	46:9:331:GLN:N	2.36	0.53
1:A:699:GLU:OE1	1:A:699:GLU:HA	2.08	0.53
1:A:1333:VAL:HG11	21:V:467:LEU:HD13	1.90	0.53
1:A:1793:THR:HB	1:A:1795:GLU:H	1.73	0.53
4:D:2018:GLU:O	4:D:2041:LEU:HA	2.09	0.53
7:G:88:G:O6	8:H:40:C:N4	2.41	0.53
8:H:78:C:H2'	8:H:79:G:H8	1.72	0.53
9:I:374:ILE:O	9:I:377:THR:N	2.42	0.53
21:V:555:LEU:HG	21:V:586:PHE:HZ	1.73	0.53
24:Y:104:HIS:CD2	24:Y:124:THR:HG1	2.23	0.53
24:Y:255:ASP:O	24:Y:258:ILE:HB	2.09	0.53
26:1:693:GLY:HA2	26:1:696:ASP:HB2	1.90	0.53
26:1:806:ILE:HG23	26:1:810:ILE:HB	1.90	0.53
46:9:296:HIS:H	46:9:296:HIS:CD2	2.26	0.53
1:A:2129:TYR:HB3	1:A:2172:MET:HE3	1.91	0.53
3:C:298:LEU:HD21	3:C:300:LEU:HG	1.89	0.53
3:C:323:PHE:CE2	3:C:373:ILE:HG12	2.44	0.53
3:C:711:ARG:HB3	3:C:730:ARG:HH22	1.74	0.53
17:R:91:ASP:OD1	17:R:95:LYS:N	2.26	0.53
17:R:383:ASN:HA	17:R:386:ARG:NH1	2.23	0.53
19:T:245:HIS:NE2	19:T:263:SER:OG	2.23	0.53
21:V:244:GLY:O	21:V:249:ASP:N	2.30	0.53
23:X:180:ALA:O	23:X:184:ARG:HG3	2.09	0.53
26:1:833:LEU:O	26:1:837:THR:OG1	2.23	0.53
27:3:92:TYR:OH	27:3:97:ASN:OD1	2.18	0.53
27:3:769:LYS:HD3	27:3:769:LYS:N	2.24	0.53
46:9:360:HIS:ND1	46:9:396:ILE:HD11	2.23	0.53
3:C:604:LEU:HD21	3:C:627:HIS:HE1	1.73	0.53
5:E:117:TYR:HB3	5:E:118:ASN:O	2.09	0.53
5:E:253:ASN:ND2	5:E:291:CYS:HB3	2.23	0.53
7:G:116:C:C6	17:R:371:ARG:HG2	2.44	0.53
12:L:573:GLU:O	12:L:577:LYS:N	2.37	0.53
12:L:699:ASN:O	12:L:703:MET:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:599:GLY:HA3	16:Q:608:ILE:H	1.74	0.53
17:R:352:ARG:HG3	17:R:355:ILE:HD12	1.90	0.53
26:1:1058:ILE:O	26:1:1062:LEU:HG	2.08	0.53
27:3:939:PHE:CZ	27:3:942:LYS:HG2	2.44	0.53
1:A:35:ARG:HG2	1:A:35:ARG:HH11	1.72	0.53
1:A:697:MET:N	1:A:698:PRO:HD3	2.24	0.53
1:A:2284:MET:HE2	1:A:2287:ARG:HH21	1.74	0.53
7:G:112:U:C4	23:X:503:ARG:NE	2.76	0.53
19:T:423:SER:HB3	19:T:474:GLU:OE1	2.08	0.53
23:X:741:TRP:CH2	26:1:782:GLU:HB3	2.44	0.53
23:X:815:MET:CG	23:X:825:SER:HB2	2.39	0.53
24:Y:9:LEU:O	24:Y:135:ILE:HD13	2.08	0.53
24:Y:147:ASP:OD2	24:Y:147:ASP:N	2.40	0.53
26:1:731:LEU:O	26:1:735:ILE:HG12	2.08	0.53
26:1:1103:VAL:O	26:1:1109:ARG:HD3	2.08	0.53
27:3:34:ARG:HB2	27:3:37:ILE:HB	1.91	0.53
27:3:266:ASP:OD1	27:3:266:ASP:N	2.40	0.53
27:3:632:ALA:O	27:3:633:LEU:HD23	2.09	0.53
27:3:1168:PHE:N	27:3:1168:PHE:CD2	2.77	0.53
30:2:460:PHE:HB3	30:2:464:GLU:HG2	1.91	0.53
46:9:296:HIS:HE1	46:9:358:LEU:HD21	1.74	0.53
1:A:283:VAL:HG13	1:A:284:ARG:H	1.74	0.53
1:A:1108:ASP:O	1:A:1112:ARG:HG3	2.09	0.53
1:A:1427:ARG:HB3	23:X:329:TRP:CE3	2.44	0.53
1:A:1926:THR:O	1:A:1926:THR:OG1	2.24	0.53
3:C:572:GLU:CD	3:C:573:GLU:H	2.11	0.53
3:C:682:LYS:HB3	3:C:797:ALA:HB2	1.90	0.53
7:G:116:C:H3'	7:G:117:A:H8	1.73	0.53
10:J:377:LYS:NZ	10:J:381:LYS:HE3	2.23	0.53
12:L:68:GLU:OE2	12:L:99:HIS:NE2	2.38	0.53
12:L:73:HIS:CD2	46:9:220:ILE:HB	2.44	0.53
17:R:137:GLU:HB2	17:R:141:LYS:HE3	1.89	0.53
17:R:369:LEU:HD12	17:R:376:LYS:NZ	2.24	0.53
23:X:913:ASP:O	23:X:916:GLU:HG3	2.09	0.53
24:Y:203:ARG:HH21	24:Y:203:ARG:HA	1.74	0.53
26:1:515:ALA:O	26:1:519:ILE:HG22	2.09	0.53
27:3:530:ASP:O	27:3:532:ARG:N	2.40	0.53
27:3:803:ASP:OD1	27:3:804:HIS:N	2.41	0.53
27:3:1025:ALA:HA	27:3:1087:GLN:O	2.09	0.53
1:A:75:ASP:O	1:A:77:THR:N	2.41	0.53
3:C:879:ASP:OD1	3:C:879:ASP:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1157:ASN:O	4:D:1161:ILE:N	2.31	0.53
5:E:191:GLN:HE21	5:E:193:THR:HA	1.74	0.53
5:E:239:THR:OG1	5:E:289:LEU:HB3	2.09	0.53
6:F:20:A:O4'	13:N:96:GLY:HA3	2.08	0.53
7:G:15:U:H3'	7:G:16:G:H8	1.73	0.53
7:G:112:U:C5	23:X:503:ARG:NE	2.77	0.53
19:T:418:THR:HG21	19:T:467:ALA:HA	1.90	0.53
23:X:476:GLU:HA	23:X:491:THR:HA	1.90	0.53
23:X:743:TYR:O	23:X:747:LEU:HB2	2.08	0.53
23:X:879:LEU:HD23	23:X:879:LEU:H	1.73	0.53
24:Y:3:VAL:HG11	24:Y:32:CYS:SG	2.48	0.53
27:3:206:GLN:NE2	27:3:232:GLY:H	2.07	0.53
27:3:390:ARG:HD3	27:3:393:LYS:HE3	1.91	0.53
27:3:940:LEU:HB3	27:3:941:HIS:CE1	2.43	0.53
1:A:1436:TRP:O	1:A:1440:THR:HG23	2.08	0.52
1:A:1767:ASN:O	1:A:1770:GLU:HB3	2.09	0.52
3:C:227:LEU:HD21	3:C:229:ILE:HD11	1.91	0.52
3:C:490:PHE:HB2	3:C:556:ASP:HB3	1.91	0.52
4:D:2103:ASN:HA	4:D:2123:SER:HA	1.91	0.52
8:H:118:G:H2'	8:H:119:G:C8	2.43	0.52
10:J:292:VAL:HG12	10:J:296:ARG:HE	1.75	0.52
17:R:348:GLU:HG3	23:X:262:LEU:HB2	1.89	0.52
24:Y:126:PHE:C	24:Y:126:PHE:CD2	2.82	0.52
26:1:815:PHE:HA	26:1:819:TRP:CD1	2.43	0.52
46:9:282:VAL:HG22	46:9:433:VAL:HG13	1.90	0.52
1:A:1649:LYS:HB3	1:A:1880:PRO:HB2	1.92	0.52
3:C:480:LYS:HB3	3:C:482:TYR:CE1	2.44	0.52
5:E:65:HIS:CE1	5:E:84:ALA:HA	2.44	0.52
6:F:31:U:H3'	6:F:32:U:H6	1.74	0.52
7:G:8:C:H2'	7:G:9:C:C6	2.45	0.52
16:Q:735:VAL:HA	16:Q:779:VAL:O	2.08	0.52
17:R:320:HIS:NE2	17:R:324:LEU:HD11	2.24	0.52
26:1:846:ALA:HB1	26:1:850:ILE:HG12	1.91	0.52
27:3:550:ASN:HD22	27:3:553:GLN:HB2	1.75	0.52
27:3:639:SER:OG	27:3:699:VAL:O	2.14	0.52
27:3:642:ILE:HB	27:3:703:ARG:HH21	1.73	0.52
1:A:65:HIS:O	1:A:69:ILE:HG13	2.10	0.52
1:A:305:ARG:HG3	3:C:878:ILE:HG21	1.92	0.52
1:A:1437:ARG:NH1	1:A:1455:TRP:O	2.43	0.52
1:A:2196:HIS:NE2	1:A:2211:THR:HB	2.24	0.52
6:F:13:G:H2'	6:F:14:C:C6	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:328:GLY:HA2	10:J:331:GLN:HE21	1.74	0.52
12:L:175:GLN:O	12:L:178:GLU:N	2.42	0.52
19:T:207:VAL:HG12	19:T:480:ALA:HB1	1.90	0.52
21:V:642:GLU:O	21:V:645:GLU:HB3	2.10	0.52
23:X:954:LEU:HG	23:X:956:ARG:NH1	2.25	0.52
24:Y:23:ARG:O	24:Y:26:LEU:HG	2.09	0.52
24:Y:198:ASP:HA	24:Y:200:PHE:CE2	2.43	0.52
27:3:120:PHE:HB2	27:3:133:SER:OG	2.09	0.52
30:2:453:LYS:HB3	30:2:456:ARG:HH21	1.74	0.52
1:A:361:HIS:HB2	3:C:280:HIS:ND1	2.24	0.52
1:A:857:ASN:OD1	1:A:859:SER:N	2.42	0.52
1:A:1189:MET:HG3	1:A:1190:CYS:H	1.75	0.52
1:A:1352:HIS:CE1	20:U:21:ARG:HB2	2.43	0.52
3:C:442:LYS:HZ3	3:C:469:ASP:HA	1.73	0.52
7:G:85:G:O6	8:H:44:U:O4	2.28	0.52
14:O:172:GLU:O	14:O:174:LYS:N	2.42	0.52
15:P:186:ARG:CD	15:P:190:ASP:OD2	2.57	0.52
16:Q:381:ALA:O	16:Q:386:LEU:N	2.30	0.52
23:X:257:PHE:CE1	23:X:270:LEU:HB2	2.44	0.52
23:X:803:ASN:OD1	23:X:807:GLU:N	2.37	0.52
26:1:842:ASN:OD1	26:1:879:LEU:HD11	2.10	0.52
26:1:1260:LYS:O	26:1:1264:VAL:HG22	2.10	0.52
27:3:519:VAL:HB	27:3:524:ILE:HG23	1.92	0.52
46:9:413:VAL:HG11	46:9:426:ILE:HD11	1.90	0.52
1:A:362:ARG:HA	1:A:362:ARG:HH11	1.74	0.52
3:C:125:ASN:OD1	3:C:127:GLU:N	2.39	0.52
3:C:314:TYR:CD2	3:C:416:LEU:HD22	2.44	0.52
4:D:2017:ILE:HA	4:D:2042:GLU:O	2.10	0.52
5:E:191:GLN:NE2	5:E:193:THR:HA	2.24	0.52
10:J:267:ARG:HD3	12:L:216:PHE:O	2.10	0.52
15:P:205:LYS:CB	15:P:208:LYS:HB3	2.39	0.52
16:Q:748:ARG:O	16:Q:779:VAL:HA	2.08	0.52
23:X:957:SER:OG	23:X:957:SER:O	2.19	0.52
1:A:1983:LEU:O	1:A:1987:ILE:HG13	2.08	0.52
3:C:89:LEU:HD12	19:T:240:LEU:HD11	1.90	0.52
12:L:178:GLU:O	12:L:181:ARG:HG3	2.09	0.52
24:Y:33:LYS:NZ	24:Y:168:ASP:OD1	2.29	0.52
27:3:442:LEU:HD13	27:3:770:LEU:HD23	1.91	0.52
27:3:700:LYS:HB3	27:3:702:PHE:HZ	1.74	0.52
27:3:872:ILE:HD12	27:3:872:ILE:H	1.75	0.52
1:A:212:PRO:HD2	1:A:225:TYR:OH	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:84:A:C1'	6:F:85:U:H5'	2.37	0.52
6:F:87:C:H2'	6:F:88:G:O4'	2.08	0.52
10:J:376:VAL:HG13	10:J:415:LEU:HB2	1.92	0.52
23:X:240:ARG:O	23:X:243:LEU:HB3	2.10	0.52
23:X:257:PHE:HZ	23:X:267:ARG:HA	1.74	0.52
23:X:991:LEU:HB2	23:X:995:GLU:OE1	2.10	0.52
26:1:886:HIS:HD2	26:1:887:LYS:HD3	1.74	0.52
27:3:605:LEU:O	27:3:617:ILE:N	2.42	0.52
27:3:698:PRO:O	27:3:700:LYS:NZ	2.34	0.52
46:9:320:ILE:HD11	46:9:337:GLY:O	2.10	0.52
1:A:1590:VAL:HG12	1:A:1664:ILE:HG13	1.92	0.52
3:C:693:GLU:HB3	3:C:696:LEU:HD21	1.92	0.52
3:C:742:PRO:HG2	3:C:785:ARG:HA	1.92	0.52
10:J:314:TYR:CE1	10:J:336:TRP:HH2	2.28	0.52
17:R:369:LEU:HG	17:R:376:LYS:HG2	1.91	0.52
19:T:371:HIS:CE1	19:T:396:LYS:HG3	2.45	0.52
21:V:555:LEU:HD22	21:V:560:LEU:HB2	1.91	0.52
23:X:558:ALA:O	23:X:562:THR:OG1	2.21	0.52
23:X:973:ASN:OD1	23:X:973:ASN:N	2.42	0.52
26:1:1289:ASN:HB3	26:1:1295:TYR:H	1.75	0.52
27:3:233:ASN:HD21	27:3:286:ILE:HG22	1.75	0.52
27:3:312:LYS:HB2	27:3:330:PHE:HD1	1.72	0.52
32:7:58:CYS:HB3	32:7:62:GLY:N	2.25	0.52
1:A:650:ARG:O	1:A:654:ASN:ND2	2.40	0.52
2:B:102:U:H2'	2:B:103:G:C8	2.44	0.52
3:C:223:ASP:HA	3:C:448:LYS:NZ	2.25	0.52
3:C:311:SER:OG	3:C:314:TYR:HB2	2.09	0.52
5:E:203:ASP:N	5:E:203:ASP:OD1	2.43	0.52
11:K:228:HIS:HB2	11:K:231:GLN:NE2	2.25	0.52
17:R:170:LYS:H	17:R:170:LYS:CD	2.20	0.52
23:X:242:LYS:HD2	23:X:246:LEU:HD22	1.92	0.52
27:3:229:GLU:HB2	27:3:230:GLU:OE1	2.09	0.52
31:4:117:TYR:O	31:4:121:SER:CB	2.58	0.52
1:A:758:ARG:HH21	1:A:775:ASN:HD22	1.58	0.52
1:A:2279:TRP:CD1	1:A:2301:PRO:HB3	2.44	0.52
5:E:166:LEU:HD12	5:E:178:LEU:HD11	1.91	0.52
6:F:35:A:C8	7:G:12:G:C6	2.97	0.52
17:R:414:GLN:HG2	23:X:633:ARG:NH1	2.24	0.52
21:V:539:LEU:HB3	21:V:543:LYS:HB2	1.91	0.52
22:W:294:VAL:HA	22:W:305:LEU:O	2.10	0.52
23:X:504:GLU:O	23:X:507:SER:OG	2.21	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:527:LEU:N	23:X:754:GLU:OE2	2.38	0.52
23:X:714:CYS:SG	23:X:722:ARG:NH1	2.84	0.52
26:1:661:ARG:HG2	26:1:692:HIS:NE2	2.25	0.52
26:1:1007:HIS:HB3	26:1:1049:TYR:OH	2.10	0.52
1:A:121:HIS:HD2	1:A:482:PHE:CE1	2.29	0.51
1:A:209:ASP:HB2	1:A:212:PRO:HA	1.92	0.51
1:A:1580:HIS:HD2	1:A:1583:GLN:NE2	2.08	0.51
1:A:2002:LEU:HB2	1:A:2007:ILE:HG23	1.92	0.51
1:A:2148:VAL:HG22	1:A:2149:PRO:HD2	1.93	0.51
1:A:2231:THR:HG22	1:A:2257:GLU:HG2	1.92	0.51
5:E:218:LYS:HG3	5:E:230:THR:HG22	1.92	0.51
8:H:172:C:N4	8:H:173:C:H41	2.07	0.51
10:J:377:LYS:HA	10:J:380:ILE:HB	1.92	0.51
14:O:31:ASN:O	17:R:195:ARG:NH2	2.43	0.51
16:Q:827:THR:HA	16:Q:1136:GLN:HA	1.93	0.51
23:X:257:PHE:CZ	23:X:267:ARG:HA	2.45	0.51
26:1:740:GLY:H	26:1:743:LEU:HD22	1.74	0.51
27:3:1008:SER:HG	27:3:1009:PHE:N	2.06	0.51
1:A:417:ARG:HB3	1:A:417:ARG:NH1	2.24	0.51
1:A:599:MET:O	1:A:603:ARG:HG3	2.10	0.51
1:A:1076:ASP:N	1:A:1076:ASP:OD2	2.43	0.51
1:A:1406:GLU:N	1:A:1406:GLU:OE1	2.43	0.51
1:A:2074:ARG:HD3	1:A:2077:ALA:HB3	1.92	0.51
5:E:190:PHE:HE1	5:E:225:ASN:HA	1.75	0.51
7:G:85:G:H2'	7:G:86:A:N9	2.25	0.51
15:P:186:ARG:CG	15:P:186:ARG:NH1	2.72	0.51
23:X:790:LEU:HA	23:X:793:LEU:HD12	1.92	0.51
24:Y:74:GLN:CD	24:Y:74:GLN:H	2.13	0.51
27:3:644:GLU:HG2	27:3:645:MET:N	2.25	0.51
1:A:1838:LYS:HA	1:A:1868:MET:SD	2.50	0.51
1:A:1895:ALA:HB1	1:A:1943:LEU:HB2	1.92	0.51
2:B:65:G:H2'	2:B:66:A:H8	1.75	0.51
3:C:131:ASN:ND2	3:C:495:ARG:HH12	2.09	0.51
3:C:673:LYS:HZ2	3:C:688:ILE:HG21	1.74	0.51
3:C:724:TRP:HA	3:C:724:TRP:CE3	2.45	0.51
4:D:1523:LEU:HA	4:D:1700:GLY:O	2.10	0.51
5:E:219:VAL:O	5:E:228:THR:N	2.42	0.51
6:F:36:A:H5"	6:F:37:C:OP2	2.10	0.51
10:J:286:GLU:HG2	10:J:298:ILE:HD12	1.91	0.51
10:J:431:ARG:HD2	10:J:434:VAL:HG11	1.93	0.51
10:J:431:ARG:HH11	10:J:434:VAL:HG11	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:57:THR:HG21	13:N:88:LEU:HD23	1.91	0.51
16:Q:1136:GLN:O	16:Q:1157:LEU:N	2.42	0.51
26:1:641:ILE:N	26:1:642:PRO:HD2	2.26	0.51
26:1:652:CYS:HB2	26:1:692:HIS:CE1	2.35	0.51
26:1:1291:ASP:OD1	26:1:1292:LYS:N	2.43	0.51
27:3:91:GLU:HG2	27:3:92:TYR:N	2.25	0.51
1:A:79:ARG:HD2	1:A:82:ARG:HE	1.76	0.51
1:A:1211:ASP:C	1:A:1213:VAL:H	2.14	0.51
1:A:1957:ASP:OD1	1:A:1958:LYS:N	2.43	0.51
3:C:396:LEU:HG	3:C:401:ILE:O	2.11	0.51
5:E:328:GLY:N	5:E:348:ASP:HB3	2.26	0.51
7:G:6:A:C6	7:G:7:G:C5	2.98	0.51
23:X:164:TRP:HE3	23:X:165:GLU:HA	1.75	0.51
23:X:430:THR:O	23:X:433:PRO:HD2	2.10	0.51
23:X:611:ILE:HG12	23:X:688:TYR:HB2	1.92	0.51
26:1:545:GLU:HG2	26:1:548:GLU:HG3	1.91	0.51
26:1:648:LEU:HA	26:1:651:VAL:HG22	1.92	0.51
27:3:147:ASP:OD1	27:3:150:ALA:N	2.43	0.51
27:3:720:TRP:CE3	27:3:731:LEU:HG	2.45	0.51
27:3:1114:SER:HB2	27:3:1215:TYR:CE1	2.46	0.51
1:A:984:MET:O	1:A:988:ILE:HG13	2.11	0.51
1:A:1284:LEU:O	1:A:1287:LEU:N	2.43	0.51
1:A:1645:LEU:HD13	1:A:1718:TRP:CH2	2.46	0.51
8:H:41:U:H2'	8:H:42:G:H8	1.75	0.51
10:J:336:TRP:CD1	10:J:341:PRO:HG3	2.45	0.51
10:J:386:GLU:O	10:J:391:TYR:N	2.40	0.51
16:Q:1180:ILE:O	16:Q:1304:PHE:HA	2.10	0.51
17:R:160:ALA:O	17:R:166:ARG:NH1	2.43	0.51
17:R:243:GLN:HA	17:R:243:GLN:OE1	2.11	0.51
23:X:168:GLU:O	23:X:172:LEU:HG	2.11	0.51
23:X:603:HIS:HA	23:X:668:ARG:CZ	2.40	0.51
23:X:635:LEU:O	23:X:638:LYS:HB2	2.11	0.51
26:1:906:GLU:N	26:1:906:GLU:OE1	2.44	0.51
26:1:1080:THR:HA	26:1:1083:TYR:HD2	1.74	0.51
27:3:628:LEU:HD21	27:3:681:PRO:HA	1.92	0.51
27:3:991:SER:O	27:3:991:SER:OG	2.28	0.51
46:9:95:LYS:HA	46:9:100:LYS:O	2.11	0.51
7:G:108:U:H5"	23:X:676:ILE:HB	1.93	0.51
8:H:133:U:H2'	8:H:134:C:C6	2.46	0.51
10:J:357:LYS:O	10:J:359:VAL:N	2.43	0.51
12:L:30:GLN:HB3	12:L:33:ARG:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:28:LYS:HD2	17:R:164:PRO:HB3	1.91	0.51
15:P:186:ARG:NH1	15:P:186:ARG:HG2	2.25	0.51
19:T:203:HIS:HE1	19:T:229:LYS:HG3	1.73	0.51
23:X:263:SER:HA	23:X:267:ARG:NH2	2.22	0.51
23:X:272:TYR:O	23:X:276:VAL:HB	2.11	0.51
23:X:411:ALA:HA	23:X:414:ASN:HD22	1.75	0.51
27:3:43:PRO:HB3	27:3:50:VAL:HG22	1.93	0.51
27:3:181:MET:HB3	27:3:212:GLU:HA	1.92	0.51
27:3:413:ALA:HB1	27:3:415:LEU:HD13	1.92	0.51
27:3:515:ALA:HB2	27:3:528:ARG:CZ	2.40	0.51
27:3:695:GLY:HA3	27:3:717:SER:OG	2.10	0.51
32:7:71:TYR:CD2	32:7:81:ASP:HB2	2.46	0.51
1:A:1401:ARG:HB2	1:A:1401:ARG:NH1	2.25	0.51
1:A:1817:LEU:HD22	1:A:1917:PHE:HB2	1.93	0.51
1:A:2188:LEU:HD23	1:A:2193:VAL:HG12	1.92	0.51
3:C:737:PRO:HD3	3:C:743:ASN:ND2	2.26	0.51
3:C:750:LEU:O	3:C:754:VAL:HG23	2.10	0.51
7:G:117:A:H3'	24:Y:246:LYS:HE2	1.93	0.51
16:Q:1061:MET:O	16:Q:1093:MET:HA	2.11	0.51
17:R:237:MET:HE3	17:R:241:GLU:HB3	1.93	0.51
19:T:396:LYS:HB2	19:T:398:TRP:HE1	1.76	0.51
19:T:429:SER:O	19:T:429:SER:OG	2.29	0.51
21:V:628:ILE:O	21:V:632:THR:OG1	2.27	0.51
23:X:911:ALA:O	23:X:914:VAL:HG22	2.10	0.51
24:Y:306:ILE:HD12	24:Y:311:ILE:HD11	1.93	0.51
26:1:687:VAL:O	26:1:690:ILE:HG13	2.11	0.51
26:1:731:LEU:HD23	26:1:746:PHE:CD1	2.46	0.51
27:3:1011:TRP:HB2	27:3:1025:ALA:O	2.11	0.51
1:A:348:PRO:HB3	1:A:394:TYR:CZ	2.45	0.51
1:A:1179:SER:O	1:A:1201:ARG:NH1	2.29	0.51
1:A:1209:HIS:CG	1:A:1210:LYS:H	2.28	0.51
1:A:1397:ILE:HG13	17:R:405:VAL:HG22	1.93	0.51
1:A:1988:LEU:HD12	1:A:2002:LEU:HD13	1.92	0.51
15:P:73:GLU:HG2	15:P:76:ARG:HH21	1.76	0.51
24:Y:18:THR:HB	24:Y:166:PHE:CE2	2.46	0.51
24:Y:126:PHE:C	24:Y:126:PHE:HD2	2.14	0.51
27:3:317:THR:HB	27:3:322:VAL:HA	1.92	0.51
27:3:819:MET:HA	27:3:822:GLU:CD	2.31	0.51
46:9:370:ASN:HB2	46:9:375:SER:O	2.10	0.51
1:A:474:ARG:HH21	1:A:474:ARG:HB2	1.76	0.51
1:A:1868:MET:O	1:A:1871:PRO:HD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1946:ASN:HD22	1:A:1949:ARG:HB2	1.76	0.51
2:B:66:A:H2'	2:B:67:A:H8	1.73	0.51
3:C:187:THR:HA	3:C:200:PHE:O	2.11	0.51
3:C:203:MET:HG3	3:C:221:ILE:HD11	1.92	0.51
6:F:31:U:H3'	6:F:32:U:C6	2.46	0.51
8:H:103:U:H4'	8:H:104:U:H5'	1.92	0.51
16:Q:893:SER:O	16:Q:897:ARG:CB	2.59	0.51
23:X:386:ALA:O	23:X:390:GLU:HG3	2.11	0.51
24:Y:21:ARG:HH12	24:Y:83:VAL:H	1.58	0.51
27:3:379:LEU:HD12	27:3:380:GLU:H	1.76	0.51
46:9:323:ARG:HE	46:9:325:ILE:HD11	1.76	0.51
1:A:35:ARG:O	1:A:39:GLN:HG3	2.11	0.51
1:A:767:VAL:HG21	2:B:39:C:O2'	2.11	0.51
1:A:1814:THR:OG1	1:A:1816:GLN:HB2	2.11	0.51
1:A:2114:PHE:O	1:A:2118:SER:OG	2.27	0.51
3:C:285:VAL:O	3:C:289:ILE:HG13	2.10	0.51
3:C:369:PHE:CE1	3:C:373:ILE:HD12	2.46	0.51
3:C:510:LEU:HD12	3:C:576:ILE:HG22	1.92	0.51
3:C:854:ARG:NH1	3:C:876:PRO:HG2	2.26	0.51
8:H:165:A:O2'	8:H:166:G:O4'	2.29	0.51
14:O:119:GLN:CD	17:R:218:ILE:HD11	2.32	0.51
17:R:325:ARG:HE	24:Y:222:ILE:HD12	1.76	0.51
19:T:213:GLU:HG2	19:T:214:PRO:N	2.26	0.51
21:V:620:ASN:HB3	21:V:623:ASN:ND2	2.25	0.51
24:Y:64:GLU:HB3	24:Y:76:SER:HB2	1.93	0.51
26:1:547:GLN:HA	26:1:550:HIS:HB3	1.92	0.51
26:1:573:LYS:H	26:1:573:LYS:HD2	1.75	0.51
26:1:712:LEU:O	26:1:716:ALA:CB	2.58	0.51
27:3:185:LEU:HD13	27:3:206:GLN:OE1	2.11	0.51
27:3:477:SER:HB2	27:3:505:THR:N	2.11	0.51
27:3:642:ILE:H	27:3:703:ARG:NE	2.09	0.51
27:3:819:MET:HA	27:3:822:GLU:OE1	2.10	0.51
1:A:1661:TRP:CE3	1:A:1700:GLY:HA3	2.46	0.50
1:A:1858:PRO:C	1:A:1859:LYS:HD2	2.31	0.50
5:E:66:GLU:N	5:E:87:ASP:OD2	2.44	0.50
5:E:248:SER:OG	5:E:265:ARG:NH2	2.44	0.50
5:E:312:TRP:CD1	5:E:319:ILE:HA	2.42	0.50
7:G:12:G:H3'	7:G:13:C:C6	2.46	0.50
7:G:111:U:C4	23:X:820:VAL:N	2.77	0.50
16:Q:128:LYS:O	16:Q:132:ALA:HB2	2.10	0.50
17:R:408:ASP:OD2	17:R:410:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:305:LEU:HD21	24:Y:308:ASP:HA	1.93	0.50
26:1:663:THR:HA	26:1:666:LYS:HE3	1.93	0.50
27:3:606:ALA:HA	27:3:616:ILE:HA	1.92	0.50
27:3:776:GLN:HG2	27:3:777:VAL:N	2.27	0.50
27:3:929:LYS:HG3	27:3:931:VAL:HG22	1.93	0.50
27:3:932:ASN:O	27:3:933:ASN:ND2	2.44	0.50
46:9:315:TYR:OH	46:9:343:GLU:OE1	2.26	0.50
1:A:136:ILE:HG22	1:A:138:PRO:HD2	1.93	0.50
3:C:440:SER:O	3:C:442:LYS:N	2.44	0.50
6:F:73:A:OP1	6:F:75:G:O2'	2.28	0.50
8:H:151:C:H2'	8:H:152:G:H8	1.76	0.50
10:J:314:TYR:CD1	10:J:336:TRP:HH2	2.29	0.50
10:J:374:PRO:HB3	10:J:405:PHE:HZ	1.76	0.50
17:R:283:ASN:N	17:R:283:ASN:OD1	2.44	0.50
19:T:428:VAL:HG22	19:T:438:LEU:HD22	1.92	0.50
23:X:397:ARG:HA	23:X:402:PHE:CG	2.47	0.50
23:X:454:ARG:HH12	23:X:679:THR:CB	2.25	0.50
23:X:531:ILE:HD13	23:X:767:LEU:HD23	1.93	0.50
24:Y:247:LEU:HB2	24:Y:282:CYS:C	2.32	0.50
26:1:831:ARG:O	26:1:834:VAL:HB	2.11	0.50
27:3:2:PHE:C	27:3:3:LEU:HD23	2.32	0.50
32:7:39:PRO:HB2	32:7:70:TYR:CD1	2.45	0.50
1:A:1275:ARG:C	1:A:1276:GLU:HG3	2.32	0.50
1:A:1942:ALA:HB2	1:A:1983:LEU:HD23	1.93	0.50
1:A:2073:TRP:CD1	1:A:2074:ARG:HB2	2.47	0.50
3:C:135:CYS:SG	3:C:242:LEU:HD13	2.52	0.50
3:C:694:LYS:O	3:C:698:GLU:HG2	2.11	0.50
6:F:81:C:H4'	6:F:82:A:H5'	1.92	0.50
7:G:104:C:O2'	7:G:105:C:OP2	2.26	0.50
8:H:181:G:H2'	8:H:182:U:C6	2.46	0.50
16:Q:1060:LEU:HA	16:Q:1092:ILE:O	2.12	0.50
19:T:386:THR:HG22	19:T:398:TRP:O	2.11	0.50
26:1:560:LEU:HD23	26:1:603:ALA:HB3	1.92	0.50
26:1:618:ASP:HA	26:1:660:ALA:HB2	1.92	0.50
26:1:972:GLY:O	26:1:976:VAL:HG12	2.10	0.50
27:3:42:ARG:HB2	27:3:53:LEU:HD11	1.93	0.50
27:3:663:LEU:HD23	27:3:679:LEU:HB3	1.92	0.50
27:3:823:MET:SD	27:3:838:MET:HG3	2.52	0.50
27:3:1040:ASP:OD2	27:3:1042:ASP:N	2.45	0.50
46:9:350:PHE:CE1	46:9:376:ASN:HB3	2.46	0.50
1:A:298:ASP:CG	1:A:300:ASN:HD22	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:LEU:O	1:A:455:VAL:HG23	2.11	0.50
1:A:516:LEU:HD11	1:A:538:SER:HB2	1.92	0.50
1:A:2095:ASP:CG	1:A:2258:ARG:HH21	2.14	0.50
3:C:559:ILE:HD12	3:C:560:VAL:O	2.10	0.50
5:E:122:SER:O	5:E:138:SER:OG	2.28	0.50
5:E:268:ALA:O	5:E:270:LYS:N	2.44	0.50
7:G:85:G:H2'	7:G:86:A:C4	2.47	0.50
8:H:57:A:OP1	30:2:459:ARG:NH1	2.32	0.50
20:U:20:GLN:HG2	20:U:21:ARG:H	1.75	0.50
27:3:233:ASN:ND2	27:3:233:ASN:N	2.59	0.50
27:3:424:TYR:CD1	27:3:437:VAL:HG22	2.46	0.50
27:3:451:GLU:HA	27:3:761:THR:HG22	1.92	0.50
46:9:292:ASN:HB2	46:9:402:GLY:H	1.75	0.50
1:A:146:SER:HA	1:A:149:ILE:HD12	1.94	0.50
1:A:196:ASP:OD2	1:A:199:GLU:N	2.29	0.50
1:A:948:PRO:O	1:A:952:VAL:HG23	2.11	0.50
1:A:2166:HIS:H	1:A:2169:LEU:HB2	1.76	0.50
3:C:283:ASP:OD2	3:C:284:GLU:N	2.45	0.50
3:C:531:TRP:CZ3	3:C:540:GLU:HB3	2.47	0.50
5:E:167:VAL:O	5:E:178:LEU:HD12	2.11	0.50
16:Q:1082:GLN:N	16:Q:1085:PHE:O	2.29	0.50
17:R:386:ARG:O	23:X:909:ARG:NH1	2.45	0.50
23:X:774:ASP:OD2	23:X:777:HIS:ND1	2.45	0.50
24:Y:117:ASP:N	24:Y:117:ASP:OD1	2.44	0.50
26:1:830:TYR:O	26:1:834:VAL:HG23	2.11	0.50
26:1:898:TYR:CZ	26:1:902:GLU:HG2	2.47	0.50
26:1:908:SER:OG	26:1:912:ASN:OD1	2.28	0.50
1:A:154:GLU:OE2	1:A:158:ARG:NE	2.32	0.50
1:A:266:SER:OG	1:A:267:LYS:N	2.42	0.50
1:A:542:ASN:O	1:A:546:LEU:HB2	2.11	0.50
1:A:2253:PRO:HA	1:A:2256:TYR:CE2	2.47	0.50
3:C:144:CYS:HB2	48:C:1500:GTP:H5"	1.94	0.50
3:C:474:LEU:O	3:C:566:THR:HA	2.12	0.50
3:C:692:LEU:HB2	3:C:786:ASN:HD22	1.77	0.50
5:E:118:ASN:ND2	5:E:121:GLY:H	2.09	0.50
7:G:106:C:H42	23:X:988:GLU:CD	2.14	0.50
10:J:313:TRP:HB3	10:J:336:TRP:CZ3	2.46	0.50
16:Q:1269:ASP:O	16:Q:1300:GLY:N	2.45	0.50
17:R:367:ARG:O	17:R:371:ARG:HG3	2.10	0.50
19:T:190:TRP:CG	19:T:497:GLU:HG3	2.46	0.50
23:X:472:LYS:HB3	23:X:475:ASN:ND2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:824:ALA:HB3	26:1:864:TYR:HD1	1.77	0.50
26:1:1003:VAL:HG22	26:1:1004:ILE:N	2.27	0.50
27:3:22:PHE:N	27:3:29:GLU:OE1	2.45	0.50
27:3:616:ILE:O	27:3:628:LEU:N	2.45	0.50
27:3:677:THR:HA	27:3:685:ASP:O	2.12	0.50
30:2:451:LYS:O	30:2:455:ARG:HD2	2.11	0.50
1:A:47:GLU:OE1	1:A:47:GLU:N	2.42	0.50
1:A:1628:ASP:OD2	1:A:1663:ASP:HA	2.12	0.50
1:A:1874:VAL:O	1:A:1877:LEU:HG	2.12	0.50
1:A:2142:ILE:HG12	1:A:2175:LEU:HD13	1.93	0.50
3:C:243:ILE:HD11	3:C:288:LEU:HB3	1.94	0.50
3:C:918:ILE:HG22	3:C:920:PRO:HA	1.93	0.50
5:E:110:GLY:H	5:E:130:ASP:CG	2.15	0.50
6:F:58:G:O2'	6:F:59:G:H5'	2.11	0.50
12:L:222:LEU:H	12:L:222:LEU:HD22	1.77	0.50
21:V:490:CYS:SG	21:V:524:SER:HB3	2.51	0.50
21:V:617:PRO:HB3	21:V:623:ASN:HD22	1.77	0.50
26:1:699:GLN:NE2	26:1:738:HIS:HE1	2.08	0.50
27:3:353:PHE:CE1	33:5:55:ILE:HD11	2.47	0.50
27:3:458:ALA:HB1	27:3:460:TRP:HZ3	1.76	0.50
1:A:216:SER:O	1:A:216:SER:OG	2.24	0.50
1:A:570:ASP:HB3	1:A:573:GLN:HB2	1.93	0.50
3:C:300:LEU:HA	3:C:306:ASN:ND2	2.27	0.50
3:C:508:LYS:HB2	3:C:524:ILE:HD13	1.93	0.50
5:E:346:SER:HB3	5:E:348:ASP:OD1	2.12	0.50
6:F:7:G:C6	6:F:15:A:C6	3.00	0.50
6:F:41:A:C2	7:G:7:G:N1	2.80	0.50
7:G:111:U:C5	23:X:819:PRO:CA	2.95	0.50
8:H:152:G:H2'	8:H:153:A:C8	2.47	0.50
13:N:119:CYS:HB2	13:N:134:CYS:HB3	1.93	0.50
17:R:351:GLU:O	17:R:355:ILE:HG13	2.11	0.50
23:X:745:HIS:HB2	23:X:746:GLU:OE2	2.11	0.50
23:X:1005:SER:HA	23:X:1008:LEU:HG	1.94	0.50
24:Y:44:ASN:HD22	24:Y:52:GLN:CB	2.24	0.50
27:3:259:LYS:HE2	27:3:266:ASP:HB3	1.94	0.50
27:3:665:LEU:HD21	27:3:667:ILE:HD11	1.94	0.50
27:3:700:LYS:O	27:3:714:ALA:HA	2.11	0.50
27:3:757:ILE:HA	27:3:762:LEU:HA	1.94	0.50
27:3:945:VAL:HG21	27:3:963:VAL:HG21	1.94	0.50
3:C:377:LEU:HA	3:C:380:ILE:HB	1.94	0.50
3:C:810:PRO:HA	3:C:813:ARG:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:313:TRP:HB3	10:J:336:TRP:CE3	2.47	0.50
10:J:382:TYR:O	10:J:386:GLU:HG2	2.11	0.50
15:P:186:ARG:HH11	15:P:186:ARG:CG	2.23	0.50
19:T:221:THR:HG1	19:T:231:TRP:HE1	1.57	0.50
22:W:531:LYS:HA	22:W:546:PHE:O	2.11	0.50
23:X:592:LEU:HD12	23:X:593:GLU:N	2.27	0.50
23:X:612:LEU:HD23	23:X:686:ILE:HG13	1.94	0.50
27:3:275:ARG:HB3	27:3:275:ARG:HH21	1.75	0.50
30:2:534:GLN:O	30:2:538:GLU:HG3	2.11	0.50
30:2:616:SER:O	31:4:79:LEU:HA	2.12	0.50
46:9:102:HIS:HA	46:9:110:PHE:H	1.77	0.50
1:A:1091:TYR:O	1:A:1092:ILE:C	2.48	0.49
1:A:1817:LEU:HD23	1:A:1917:PHE:H	1.77	0.49
3:C:709:TRP:HZ3	3:C:717:PHE:HB2	1.76	0.49
4:D:538:ILE:O	4:D:585:ILE:HA	2.12	0.49
6:F:88:G:C2	8:H:11:G:C2	3.00	0.49
16:Q:817:GLY:O	16:Q:1090:ARG:HA	2.12	0.49
23:X:752:VAL:O	23:X:757:ARG:NH2	2.44	0.49
24:Y:74:GLN:OE1	24:Y:74:GLN:N	2.45	0.49
27:3:1165:SER:HB2	27:3:1169:PRO:HA	1.94	0.49
1:A:1218:ASN:OD1	1:A:1220:VAL:HG22	2.12	0.49
3:C:389:ASP:OD2	3:C:389:ASP:N	2.29	0.49
3:C:530:LEU:O	3:C:540:GLU:HA	2.12	0.49
3:C:850:LEU:O	3:C:855:GLY:N	2.45	0.49
8:H:173:C:H2'	8:H:174:A:H8	1.76	0.49
27:3:463:ARG:HD3	27:3:468:ASP:HB3	1.94	0.49
46:9:323:ARG:HD2	46:9:324:SER:H	1.77	0.49
1:A:845:ARG:HH12	1:A:1440:THR:HG22	1.77	0.49
1:A:1850:ARG:HG2	1:A:1879:PHE:HE2	1.77	0.49
2:B:87:A:H61	2:B:92:U:P	2.35	0.49
3:C:302:PRO:HG2	3:C:320:LEU:HD11	1.94	0.49
17:R:243:GLN:OE1	17:R:246:LYS:HD2	2.11	0.49
19:T:221:THR:OG1	19:T:231:TRP:NE1	2.36	0.49
19:T:399:LYS:HB2	19:T:406:ILE:HD11	1.94	0.49
23:X:162:ASP:O	23:X:165:GLU:N	2.45	0.49
23:X:443:ASN:O	23:X:444:LYS:HB2	2.12	0.49
23:X:485:ASP:OD1	23:X:487:THR:OG1	2.25	0.49
23:X:772:ILE:HD12	23:X:778:PHE:CD2	2.46	0.49
23:X:842:THR:HB	23:X:882:LEU:HD12	1.94	0.49
23:X:888:TRP:O	23:X:891:SER:OG	2.25	0.49
26:1:522:LYS:HD3	26:1:526:PHE:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:614:VAL:HG23	27:3:633:LEU:HD11	1.93	0.49
27:3:713:LEU:HD13	27:3:714:ALA:N	2.27	0.49
27:3:940:LEU:HB3	27:3:941:HIS:ND1	2.26	0.49
27:3:1187:PRO:O	27:3:1191:LYS:HG3	2.12	0.49
46:9:281:TYR:H	46:9:435:VAL:HG22	1.77	0.49
1:A:137:GLU:O	1:A:141:ILE:HG13	2.12	0.49
1:A:347:LEU:HD22	1:A:351:TYR:CZ	2.47	0.49
1:A:1402:ARG:HD2	23:X:664:PRO:CB	2.42	0.49
1:A:1902:PHE:CE2	1:A:1967:ILE:HD12	2.47	0.49
8:H:105:G:O2'	8:H:107:A:OP1	2.23	0.49
19:T:422:ASN:OD1	19:T:474:GLU:HB3	2.11	0.49
23:X:651:LEU:HD13	23:X:655:MET:HB2	1.94	0.49
23:X:736:ARG:HB3	23:X:738:TYR:CE1	2.48	0.49
26:1:563:LEU:HB2	26:1:567:VAL:HG13	1.95	0.49
26:1:569:PRO:HD2	26:1:570:TYR:CE2	2.48	0.49
27:3:146:ARG:HB3	27:3:150:ALA:HA	1.93	0.49
27:3:294:LYS:HZ2	27:3:294:LYS:C	2.15	0.49
1:A:197:PRO:HA	1:A:204:LEU:HD13	1.94	0.49
1:A:1089:CYS:SG	1:A:1096:HIS:CD2	3.05	0.49
2:B:21:A:H2'	2:B:21:A:N3	2.26	0.49
4:D:537:LYS:O	4:D:609:VAL:HA	2.13	0.49
7:G:7:G:O2'	7:G:8:C:H5'	2.13	0.49
10:J:320:GLU:OE1	10:J:325:ASN:HB3	2.12	0.49
12:L:196:ILE:HD13	22:W:509:GLY:HA3	1.95	0.49
19:T:319:THR:O	19:T:319:THR:OG1	2.30	0.49
21:V:620:ASN:HD22	21:V:623:ASN:H	1.60	0.49
23:X:655:MET:O	23:X:658:ARG:HG2	2.12	0.49
23:X:932:CYS:HA	23:X:938:ARG:HH11	1.77	0.49
24:Y:224:LEU:HD11	24:Y:229:ASP:HB2	1.94	0.49
26:1:581:LEU:O	26:1:584:ASP:HB3	2.12	0.49
26:1:663:THR:HA	26:1:666:LYS:CE	2.43	0.49
27:3:238:VAL:HB	27:3:247:GLY:O	2.12	0.49
27:3:1207:LYS:O	27:3:1211:ILE:HG12	2.12	0.49
1:A:223:SER:N	2:B:12:U:OP1	2.44	0.49
1:A:332:TYR:O	3:C:888:ARG:NH2	2.41	0.49
1:A:590:GLY:HA2	1:A:592:TYR:CE2	2.47	0.49
1:A:671:THR:O	1:A:676:ARG:NH1	2.46	0.49
1:A:2178:ILE:HG13	1:A:2214:ILE:O	2.13	0.49
3:C:670:SER:OG	3:C:819:ALA:O	2.31	0.49
3:C:711:ARG:HH22	3:C:733:TRP:HA	1.78	0.49
6:F:19:C:H2'	6:F:20:A:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:70:ILE:HG23	13:N:74:LEU:HD23	1.94	0.49
24:Y:13:VAL:HB	24:Y:131:GLU:HG3	1.95	0.49
27:3:968:ARG:HG2	27:3:982:GLU:OE1	2.12	0.49
32:7:73:LYS:HA	32:7:76:THR:HG22	1.95	0.49
1:A:498:ARG:HG2	1:A:502:ASN:HD21	1.77	0.49
1:A:1642:PRO:HA	1:A:1716:GLY:O	2.13	0.49
3:C:129:ILE:HG22	3:C:199:LEU:HB3	1.93	0.49
3:C:475:MET:HA	3:C:565:ILE:O	2.12	0.49
5:E:110:GLY:N	5:E:130:ASP:OD1	2.35	0.49
8:H:7:U:H2'	8:H:8:C:C6	2.47	0.49
8:H:33:G:C6	8:H:34:U:C4	3.01	0.49
8:H:54:U:H2'	8:H:55:U:C6	2.48	0.49
10:J:366:TYR:O	10:J:370:VAL:HG23	2.13	0.49
12:L:52:GLU:O	12:L:58:ILE:HD13	2.12	0.49
19:T:497:GLU:OE1	19:T:497:GLU:N	2.29	0.49
23:X:478:GLY:HA3	23:X:487:THR:HG22	1.94	0.49
27:3:18:ILE:HD12	27:3:67:ALA:HB2	1.95	0.49
27:3:740:GLU:HB2	27:3:758:SER:HA	1.95	0.49
1:A:384:VAL:HA	3:C:331:PHE:HD2	1.77	0.49
1:A:1131:LYS:HE2	1:A:1174:PHE:CE2	2.48	0.49
1:A:1382:SER:HB2	1:A:1415:GLY:HA2	1.93	0.49
1:A:1649:LYS:HG2	1:A:1877:LEU:HD22	1.94	0.49
2:B:14:U:H2'	2:B:15:C:H6	1.78	0.49
3:C:500:THR:HB	3:C:502:HIS:CE1	2.48	0.49
10:J:411:MET:CE	10:J:415:LEU:HB3	2.41	0.49
15:P:68:ARG:HB3	15:P:68:ARG:HH11	1.77	0.49
17:R:414:GLN:HG2	23:X:633:ARG:HH12	1.77	0.49
23:X:416:GLN:NE2	23:X:546:LEU:O	2.29	0.49
23:X:855:TYR:CE2	23:X:857:PRO:HG3	2.48	0.49
26:1:1076:ALA:O	26:1:1080:THR:HG23	2.12	0.49
33:5:60:SER:O	33:5:63:ARG:N	2.46	0.49
1:A:176:LEU:HD11	1:A:566:LEU:HD11	1.94	0.49
1:A:1413:ASP:O	1:A:1414:ARG:HG3	2.13	0.49
1:A:1635:TYR:O	1:A:1636:LYS:HG3	2.12	0.49
1:A:1649:LYS:HD2	1:A:1649:LYS:HA	1.58	0.49
1:A:1845:VAL:O	1:A:1849:ILE:HG13	2.13	0.49
1:A:1860:GLN:HA	1:A:1883:VAL:O	2.13	0.49
1:A:1894:GLN:HE21	1:A:1944:HIS:CE1	2.31	0.49
1:A:1902:PHE:HE2	1:A:1967:ILE:HD12	1.77	0.49
3:C:528:GLY:HA3	3:C:553:GLU:HG2	1.95	0.49
5:E:236:ASP:HB2	5:E:256:ASP:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:86:U:C4	8:H:12:G:O6	2.66	0.49
10:J:352:PHE:HA	10:J:355:ARG:NE	2.27	0.49
13:N:46:LEU:HA	13:N:49:ILE:HD13	1.95	0.49
17:R:376:LYS:HA	17:R:379:LYS:HB2	1.94	0.49
19:T:395:ILE:HD12	19:T:395:ILE:H	1.78	0.49
26:1:523:ALA:C	26:1:563:LEU:HD11	2.33	0.49
27:3:388:GLN:NE2	27:3:845:GLU:OE1	2.46	0.49
32:7:42:LEU:HG	32:7:70:TYR:CE2	2.47	0.49
46:9:312:LYS:NZ	46:9:436:ASP:OD2	2.37	0.49
1:A:369:GLU:HB2	1:A:371:LEU:HD13	1.95	0.49
1:A:485:THR:HG22	1:A:486:LYS:N	2.27	0.49
1:A:976:MET:HE2	1:A:1098:PHE:HD1	1.78	0.49
1:A:1144:LYS:HD3	46:9:45:SER:O	2.13	0.49
1:A:1402:ARG:HB2	17:R:407:TYR:HA	1.95	0.49
1:A:1846:ALA:O	1:A:1850:ARG:HG3	2.13	0.49
1:A:2087:THR:OG1	1:A:2112:LYS:HD3	2.13	0.49
3:C:64:LYS:HE2	15:P:206:LYS:HD2	1.94	0.49
3:C:201:ASN:HB3	3:C:549:TRP:CE3	2.48	0.49
3:C:301:SER:H	3:C:306:ASN:ND2	2.04	0.49
4:D:1188:VAL:HA	4:D:1201:GLU:O	2.13	0.49
5:E:171:SER:OG	5:E:173:ASP:OD2	2.25	0.49
10:J:346:TRP:CD1	10:J:369:PHE:HD1	2.30	0.49
23:X:715:SER:OG	23:X:716:LYS:N	2.45	0.49
23:X:811:SER:O	23:X:815:MET:SD	2.71	0.49
26:1:796:CYS:HB3	26:1:806:ILE:HG12	1.95	0.49
27:3:234:PHE:C	27:3:235:LEU:HD12	2.33	0.49
27:3:952:ILE:HG12	27:3:961:ILE:HG12	1.95	0.49
30:2:462:VAL:O	30:2:466:LYS:HG3	2.12	0.49
1:A:246:LEU:HD11	1:A:411:PHE:HE1	1.78	0.48
1:A:1836:LEU:HA	1:A:1839:TRP:CD1	2.48	0.48
3:C:250:ARG:NH1	3:C:447:PRO:O	2.46	0.48
3:C:496:VAL:HG13	3:C:501:ILE:HD11	1.94	0.48
3:C:693:GLU:OE1	3:C:695:GLY:N	2.45	0.48
3:C:938:ARG:HG2	3:C:942:GLY:HA3	1.95	0.48
4:D:860:GLN:O	27:3:601:ARG:NH1	2.46	0.48
8:H:182:U:H2'	8:H:183:G:C8	2.48	0.48
21:V:320:ARG:O	21:V:324:HIS:CB	2.61	0.48
22:W:434:VAL:HA	22:W:443:ARG:O	2.13	0.48
23:X:716:LYS:O	23:X:720:ASN:ND2	2.46	0.48
23:X:932:CYS:SG	23:X:935:ASP:N	2.86	0.48
26:1:717:THR:HB	26:1:718:PRO:CD	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:796:CYS:HA	26:1:801:VAL:HG21	1.94	0.48
27:3:49:LYS:HD3	27:3:49:LYS:HA	1.59	0.48
27:3:209:THR:OG1	27:3:210:PHE:N	2.45	0.48
27:3:356:HIS:CD2	27:3:403:SER:HG	2.30	0.48
32:7:30:CYS:SG	32:7:33:CYS:HB3	2.53	0.48
1:A:214:ARG:NH2	1:A:223:SER:OG	2.46	0.48
1:A:1199:LYS:HE2	1:A:1206:GLU:CD	2.34	0.48
1:A:1268:ILE:O	1:A:1272:THR:OG1	2.25	0.48
3:C:509:VAL:HG22	3:C:523:GLN:O	2.13	0.48
8:H:64:A:H2'	8:H:65:U:C6	2.48	0.48
8:H:139:C:H2'	8:H:140:A:H8	1.78	0.48
16:Q:600:MET:O	16:Q:607:VAL:HA	2.13	0.48
17:R:154:SER:O	17:R:157:GLN:HG2	2.12	0.48
21:V:647:LEU:O	21:V:651:PRO:HD3	2.13	0.48
26:1:862:GLU:HA	26:1:865:ARG:NH1	2.27	0.48
26:1:970:LEU:O	26:1:974:LEU:HG	2.13	0.48
27:3:477:SER:HA	27:3:482:THR:HG23	1.95	0.48
1:A:427:VAL:HG12	1:A:430:TRP:CE3	2.49	0.48
1:A:1258:LYS:O	1:A:1262:LYS:HG3	2.13	0.48
1:A:1649:LYS:CB	1:A:1880:PRO:HB2	2.44	0.48
3:C:823:ALA:O	3:C:824:THR:OG1	2.26	0.48
5:E:137:ASP:O	5:E:141:GLY:N	2.26	0.48
6:F:5:U:H5'	6:F:6:C:H4'	1.94	0.48
10:J:232:GLU:HG3	12:L:210:TYR:CE1	2.48	0.48
12:L:70:LYS:HG3	46:9:220:ILE:HG21	1.93	0.48
17:R:162:ALA:C	17:R:164:PRO:HD3	2.33	0.48
17:R:201:GLU:H	17:R:201:GLU:CD	2.16	0.48
19:T:195:LYS:HZ1	19:T:490:ARG:HH21	1.60	0.48
21:V:616:LEU:HD12	21:V:616:LEU:O	2.13	0.48
23:X:772:ILE:CD1	23:X:778:PHE:HD2	2.26	0.48
24:Y:43:HIS:O	24:Y:149:VAL:HG22	2.13	0.48
26:1:933:CYS:SG	26:1:970:LEU:HD11	2.52	0.48
27:3:469:GLU:HG2	27:3:470:PHE:CD1	2.47	0.48
27:3:1095:TYR:CE1	27:3:1164:ARG:HD2	2.48	0.48
1:A:57:GLN:HG3	2:B:13:C:O2'	2.13	0.48
1:A:693:ILE:HG22	1:A:694:LEU:HD23	1.94	0.48
1:A:1862:ILE:HG21	1:A:1885:LYS:HE2	1.95	0.48
3:C:366:GLN:HG3	3:C:371:GLU:HG3	1.96	0.48
5:E:176:VAL:O	5:E:189:THR:HA	2.14	0.48
6:F:39:A:C5	6:F:40:U:C5	3.02	0.48
10:J:364:THR:O	10:J:367:GLU:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:406:PHE:HB3	10:J:411:MET:SD	2.54	0.48
14:O:162:PRO:CB	14:O:181:TYR:HA	2.43	0.48
17:R:315:LYS:NZ	24:Y:191:ILE:HG12	2.28	0.48
19:T:257:ARG:HD3	19:T:298:PRO:O	2.14	0.48
21:V:551:PHE:O	21:V:555:LEU:HD23	2.14	0.48
23:X:235:LEU:HD22	24:Y:220:GLN:HG2	1.94	0.48
24:Y:274:ASP:O	24:Y:278:GLY:N	2.41	0.48
26:1:770:MET:HA	26:1:773:LEU:HG	1.95	0.48
26:1:795:CYS:O	26:1:798:THR:HG23	2.13	0.48
26:1:967:GLU:CG	26:1:970:LEU:HB3	2.43	0.48
26:1:1300:LEU:HB3	27:3:1032:TRP:CZ3	2.48	0.48
27:3:249:LEU:HA	27:3:257:THR:O	2.12	0.48
27:3:484:VAL:O	27:3:485:LEU:HD12	2.13	0.48
27:3:503:THR:HG22	27:3:504:PRO:HD2	1.95	0.48
27:3:804:HIS:NE2	27:3:859:ASN:O	2.46	0.48
31:4:102:ILE:C	31:4:177:ALA:HB2	2.33	0.48
32:7:15:ALA:HB2	32:7:84:GLY:HA2	1.94	0.48
1:A:420:ARG:NH2	1:A:423:ASP:OD1	2.47	0.48
1:A:1384:ARG:HH22	1:A:1414:ARG:NH1	2.11	0.48
3:C:286:ASN:ND2	3:C:300:LEU:O	2.46	0.48
3:C:561:LYS:NZ	3:C:615:PRO:O	2.41	0.48
3:C:666:VAL:HG12	3:C:667:VAL:N	2.29	0.48
3:C:799:GLU:O	3:C:801:LEU:N	2.46	0.48
3:C:850:LEU:HB3	3:C:855:GLY:HA3	1.95	0.48
9:I:326:ASP:C	9:I:328:GLU:H	2.17	0.48
10:J:269:LEU:HD21	10:J:279:TRP:CZ3	2.47	0.48
13:N:53:HIS:O	13:N:57:THR:HG22	2.13	0.48
15:P:45:GLN:HA	15:P:45:GLN:HE21	1.79	0.48
24:Y:246:LYS:HD2	24:Y:310:ARG:O	2.14	0.48
26:1:1159:GLY:O	26:1:1161:MET:N	2.46	0.48
27:3:143:ILE:H	27:3:143:ILE:HD12	1.79	0.48
27:3:357:TYR:HE1	27:3:400:GLU:HG3	1.77	0.48
27:3:603:ARG:HD2	27:3:603:ARG:O	2.13	0.48
27:3:706:MET:HG2	27:3:770:LEU:HD12	1.94	0.48
27:3:833:GLU:C	27:3:836:ALA:H	2.14	0.48
1:A:612:ILE:O	1:A:616:PHE:HB2	2.13	0.48
1:A:1809:ILE:O	1:A:1817:LEU:HA	2.13	0.48
2:B:97:G:H2'	2:B:97:G:N3	2.28	0.48
2:B:103:G:C6	2:B:111:A:N1	2.82	0.48
2:B:106:U:H2'	2:B:107:U:C6	2.48	0.48
3:C:69:ALA:HA	3:C:72:VAL:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:212:SER:O	3:C:216:THR:HG23	2.13	0.48
3:C:313:GLN:HG3	3:C:417:ARG:HH21	1.78	0.48
6:F:15:A:H2'	6:F:16:G:C8	2.48	0.48
17:R:369:LEU:HA	17:R:376:LYS:CE	2.41	0.48
21:V:451:ASN:O	21:V:455:PHE:HB2	2.13	0.48
23:X:391:SER:O	23:X:395:VAL:HG23	2.13	0.48
23:X:450:CYS:HB2	23:X:495:TYR:CD1	2.48	0.48
23:X:592:LEU:O	23:X:595:CYS:HB2	2.14	0.48
26:1:815:PHE:O	26:1:819:TRP:HB2	2.13	0.48
26:1:914:PHE:O	26:1:918:VAL:HG23	2.14	0.48
27:3:642:ILE:H	27:3:703:ARG:HH21	1.61	0.48
27:3:745:PHE:CB	27:3:755:VAL:HG23	2.43	0.48
1:A:30:LEU:HD22	5:E:214:ASP:HA	1.94	0.48
1:A:42:ALA:O	1:A:46:ALA:HB2	2.14	0.48
1:A:762:ARG:NH2	15:P:226:LYS:HZ3	2.10	0.48
1:A:781:ARG:HH21	8:H:24:A:H5"	1.78	0.48
1:A:1019:TYR:O	1:A:1020:LYS:C	2.51	0.48
1:A:1209:HIS:ND1	1:A:1210:LYS:HE2	2.29	0.48
1:A:2202:ASP:O	1:A:2204:PRO:HD3	2.14	0.48
3:C:618:THR:HG23	3:C:630:LEU:HB3	1.94	0.48
4:D:463:PRO:HA	4:D:480:THR:HA	1.95	0.48
5:E:136:TRP:CZ3	5:E:143:ARG:HB3	2.48	0.48
6:F:48:A:O2'	12:L:33:ARG:NH1	2.39	0.48
19:T:369:THR:O	19:T:369:THR:OG1	2.27	0.48
21:V:584:LYS:HG3	21:V:634:ILE:HG22	1.96	0.48
23:X:606:GLN:HB2	23:X:668:ARG:HH22	1.79	0.48
23:X:964:GLN:HG3	26:1:543:THR:HG21	1.96	0.48
24:Y:214:GLU:O	24:Y:218:LYS:HG3	2.13	0.48
26:1:796:CYS:C	26:1:801:VAL:HG21	2.34	0.48
27:3:757:ILE:HG22	27:3:762:LEU:HG	1.94	0.48
27:3:820:ALA:HA	27:3:823:MET:HE1	1.96	0.48
2:B:103:G:C6	2:B:104:C:C4	3.02	0.48
3:C:938:ARG:HA	3:C:942:GLY:H	1.76	0.48
5:E:75:HIS:O	5:E:78:GLY:N	2.46	0.48
7:G:90:C:H42	8:H:40:C:H42	1.60	0.48
8:H:106:G:H1'	8:H:107:A:N7	2.29	0.48
10:J:396:ARG:HH22	10:J:426:GLN:HG3	1.79	0.48
12:L:178:GLU:HB3	12:L:181:ARG:HH11	1.79	0.48
18:S:96:GLY:O	18:S:131:ARG:HA	2.14	0.48
19:T:271:LYS:HG2	19:T:280:VAL:HG11	1.96	0.48
21:V:505:LYS:HE3	21:V:553:HIS:NE2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:689:VAL:C	23:X:690:LEU:HD23	2.34	0.48
24:Y:9:LEU:HD23	24:Y:138:LYS:HD3	1.95	0.48
24:Y:37:TYR:OH	24:Y:106:SER:HB3	2.13	0.48
26:1:517:ARG:HB3	26:1:517:ARG:CZ	2.43	0.48
26:1:972:GLY:CA	26:1:1010:THR:HG21	2.41	0.48
27:3:484:VAL:C	27:3:485:LEU:HD12	2.34	0.48
27:3:581:LYS:HB2	27:3:625:LEU:HD22	1.94	0.48
27:3:664:TYR:CG	27:3:729:PHE:HZ	2.32	0.48
27:3:926:TYR:CZ	27:3:942:LYS:HD2	2.48	0.48
1:A:122:ILE:HD13	1:A:483:GLN:HG2	1.96	0.48
1:A:723:ASN:HD22	1:A:788:GLN:NE2	2.12	0.48
1:A:1375:TRP:O	1:A:1378:GLU:N	2.46	0.48
1:A:1852:LEU:HD23	1:A:1858:PRO:HD3	1.96	0.48
3:C:183:SER:OG	3:C:214:GLU:OE1	2.31	0.48
3:C:607:LEU:HA	3:C:610:VAL:HG22	1.96	0.48
3:C:624:SER:HB2	3:C:626:GLU:HG2	1.96	0.48
3:C:725:ASP:HB3	3:C:728:ALA:H	1.79	0.48
4:D:898:PRO:HA	4:D:960:ALA:HB1	1.96	0.48
5:E:118:ASN:HD21	5:E:122:SER:H	1.61	0.48
5:E:164:PRO:O	5:E:166:LEU:HD23	2.14	0.48
6:F:23:U:H2'	6:F:24:A:O4'	2.14	0.48
6:F:82:A:H2'	6:F:82:A:OP2	2.14	0.48
7:G:5:G:N1	7:G:6:A:N6	2.62	0.48
23:X:929:LEU:H	23:X:929:LEU:HD12	1.78	0.48
26:1:524:ARG:HD3	26:1:563:LEU:HD12	1.96	0.48
26:1:1041:ARG:HD2	26:1:1041:ARG:HA	1.48	0.48
27:3:19:HIS:ND1	27:3:19:HIS:O	2.46	0.48
27:3:407:ILE:HD11	27:3:1124:GLY:CA	2.44	0.48
27:3:415:LEU:HB2	27:3:424:TYR:CE2	2.49	0.48
27:3:914:ILE:HD12	27:3:919:SER:HB3	1.95	0.48
30:2:705:ARG:N	30:2:705:ARG:HD2	2.28	0.48
1:A:273:ILE:HD11	1:A:314:ILE:HG21	1.96	0.48
1:A:523:ASN:OD1	1:A:552:ARG:NH1	2.43	0.48
1:A:1289:VAL:HG21	1:A:1335:ILE:HD11	1.95	0.48
1:A:1382:SER:HA	1:A:1415:GLY:HA2	1.96	0.48
1:A:1417:PRO:HD2	23:X:337:ALA:HB2	1.95	0.48
1:A:1490:PHE:O	1:A:1493:THR:OG1	2.30	0.48
1:A:2129:TYR:HD2	1:A:2172:MET:HB2	1.79	0.48
3:C:749:THR:O	3:C:753:GLU:HB2	2.13	0.48
3:C:891:THR:O	3:C:894:GLN:HG2	2.14	0.48
4:D:1199:LYS:HA	4:D:1255:PHE:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:126:SER:OG	5:E:136:TRP:NE1	2.46	0.48
5:E:150:HIS:NE2	5:E:169:THR:OG1	2.32	0.48
5:E:178:LEU:HB3	5:E:187:ILE:HB	1.96	0.48
7:G:7:G:C2	7:G:8:C:C2	3.02	0.48
8:H:176:G:H8	8:H:176:G:O5'	1.97	0.48
10:J:219:GLU:HB3	12:L:185:LEU:HD11	1.96	0.48
21:V:529:PHE:CD1	21:V:564:VAL:HB	2.49	0.48
23:X:411:ALA:HA	23:X:414:ASN:ND2	2.28	0.48
26:1:789:LEU:HB3	26:1:836:THR:HG21	1.96	0.48
26:1:823:MET:O	26:1:829:ASN:HB2	2.14	0.48
27:3:181:MET:HB2	27:3:211:TYR:O	2.13	0.48
27:3:449:VAL:HG11	27:3:763:ARG:NH1	2.29	0.48
27:3:605:LEU:HD23	27:3:617:ILE:HG22	1.95	0.48
46:9:203:GLU:O	46:9:207:THR:OG1	2.12	0.48
46:9:365:ILE:HG23	46:9:396:ILE:HD13	1.95	0.48
1:A:1361:GLU:OE1	1:A:1361:GLU:HA	2.14	0.47
1:A:1647:ASP:OD1	1:A:1881:ASN:HB2	2.14	0.47
3:C:441:PRO:C	3:C:444:GLY:HA3	2.34	0.47
4:D:777:LEU:O	4:D:780:TYR:N	2.40	0.47
5:E:244:SER:HB2	5:E:293:TRP:CE2	2.49	0.47
6:F:49:G:H8	6:F:49:G:OP1	1.97	0.47
7:G:9:C:O2'	7:G:10:U:O4'	2.12	0.47
8:H:106:G:N3	8:H:107:A:C6	2.81	0.47
13:N:15:TRP:NE1	13:N:19:GLU:OE1	2.47	0.47
13:N:102:CYS:SG	13:N:137:CYS:HB2	2.54	0.47
22:W:180:LYS:HA	22:W:200:VAL:H	1.78	0.47
23:X:864:ALA:HA	23:X:902:PHE:CD2	2.48	0.47
23:X:955:THR:OG1	23:X:958:GLY:O	2.15	0.47
23:X:961:THR:HG21	23:X:964:GLN:NE2	2.29	0.47
27:3:346:PHE:HA	27:3:360:GLN:HA	1.95	0.47
27:3:636:GLN:HG2	27:3:637:PRO:HD2	1.96	0.47
27:3:1125:GLY:C	27:3:1126:ILE:HG13	2.35	0.47
31:4:103:PHE:N	31:4:177:ALA:HB2	2.29	0.47
32:7:52:GLY:N	32:7:55:GLN:HE21	2.10	0.47
46:9:73:TYR:O	46:9:75:THR:N	2.47	0.47
1:A:1019:TYR:O	1:A:1021:ASP:N	2.47	0.47
1:A:1645:LEU:HD13	1:A:1718:TRP:HH2	1.79	0.47
1:A:1675:ASP:OD1	1:A:1678:ARG:N	2.40	0.47
1:A:2097:ILE:HD13	1:A:2260:GLN:HG3	1.96	0.47
1:A:2122:ALA:HB1	1:A:2282:ASN:OD1	2.15	0.47
2:B:102:U:H2'	2:B:103:G:H8	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:384:VAL:HG11	3:C:416:LEU:HG	1.97	0.47
3:C:495:ARG:HB2	3:C:495:ARG:NH1	2.27	0.47
6:F:29:A:H2'	6:F:30:A:C8	2.49	0.47
7:G:117:A:O5'	24:Y:246:LYS:HE2	2.14	0.47
10:J:257:GLU:OE1	10:J:257:GLU:N	2.47	0.47
16:Q:341:ALA:O	16:Q:345:PHE:N	2.36	0.47
21:V:537:HIS:CE1	21:V:538:ARG:HG2	2.49	0.47
23:X:487:THR:HG22	23:X:491:THR:HG21	1.94	0.47
23:X:516:VAL:HG13	23:X:549:LEU:HD13	1.95	0.47
24:Y:1:MET:HG2	24:Y:163:ASP:OD2	2.13	0.47
24:Y:45:VAL:HG22	24:Y:51:ILE:HG23	1.95	0.47
26:1:570:TYR:HA	26:1:573:LYS:HD3	1.96	0.47
26:1:1299:GLU:O	26:1:1302:TYR:HD2	1.97	0.47
27:3:114:ARG:NH1	33:5:37:ARG:HB2	2.30	0.47
1:A:1427:ARG:HB3	23:X:329:TRP:CZ3	2.49	0.47
4:D:1459:ILE:HA	4:D:1464:GLY:HA3	1.96	0.47
8:H:34:U:H2'	8:H:35:A:C8	2.49	0.47
10:J:406:PHE:HB3	10:J:411:MET:HB2	1.97	0.47
12:L:86:ALA:HB1	12:L:91:ARG:O	2.14	0.47
19:T:412:HIS:ND1	19:T:429:SER:OG	2.44	0.47
23:X:431:GLN:HA	23:X:434:GLN:NE2	2.30	0.47
23:X:702:PRO:HB2	23:X:791:LEU:HD13	1.97	0.47
24:Y:214:GLU:HB3	24:Y:218:LYS:NZ	2.29	0.47
24:Y:291:GLU:O	24:Y:295:GLU:HG3	2.14	0.47
26:1:495:ARG:HA	26:1:498:MET:HB3	1.95	0.47
26:1:632:PHE:O	26:1:635:VAL:HG22	2.13	0.47
26:1:770:MET:O	26:1:774:ILE:HG12	2.14	0.47
27:3:22:PHE:HA	27:3:76:ASP:HB2	1.95	0.47
27:3:169:HIS:CD2	27:3:170:VAL:N	2.82	0.47
27:3:1034:THR:HG22	27:3:1049:LYS:HG3	1.96	0.47
32:7:58:CYS:HB3	32:7:62:GLY:H	1.79	0.47
1:A:425:PRO:HB3	1:A:635:ARG:NH1	2.30	0.47
1:A:1527:ASN:ND2	11:K:215:ASP:HB3	2.29	0.47
1:A:1764:SER:C	1:A:1766:GLN:H	2.17	0.47
1:A:1776:ILE:H	1:A:1776:ILE:HG12	1.49	0.47
1:A:1939:ILE:HG21	1:A:1968:TRP:CE2	2.49	0.47
3:C:483:SER:HA	3:C:490:PHE:HA	1.96	0.47
3:C:589:LYS:HB3	3:C:659:VAL:HG23	1.96	0.47
5:E:168:CYS:SG	5:E:199:VAL:HG21	2.54	0.47
7:G:85:G:N2	8:H:45:C:C2	2.80	0.47
15:P:217:SER:OG	15:P:218:GLU:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:617:PRO:HG2	21:V:623:ASN:O	2.14	0.47
23:X:981:PRO:HB3	23:X:1002:GLU:OE1	2.14	0.47
26:1:720:GLY:HA2	26:1:756:LEU:HB3	1.97	0.47
26:1:854:VAL:HG11	26:1:891:GLN:HE21	1.79	0.47
27:3:169:HIS:HD2	27:3:170:VAL:N	2.09	0.47
27:3:511:LEU:HD21	27:3:517:VAL:CG2	2.44	0.47
32:7:13:LYS:HD2	32:7:48:GLU:OE2	2.14	0.47
33:5:51:ASN:OD1	33:5:51:ASN:N	2.46	0.47
46:9:246:VAL:HG21	46:9:261:HIS:CG	2.50	0.47
1:A:121:HIS:ND1	1:A:123:THR:HG23	2.30	0.47
1:A:902:TYR:HE2	1:A:1246:GLN:HB3	1.79	0.47
1:A:929:GLU:OE1	1:A:933:ARG:NH2	2.40	0.47
1:A:1332:HIS:CE1	1:A:1359:HIS:HB3	2.50	0.47
1:A:1473:ASP:OD1	1:A:1473:ASP:N	2.46	0.47
1:A:2200:MET:HG3	1:A:2206:TRP:HB2	1.95	0.47
5:E:198:ALA:O	5:E:210:SER:HA	2.14	0.47
7:G:15:U:H3'	7:G:16:G:C8	2.49	0.47
8:H:171:U:N3	8:H:172:C:C4	2.83	0.47
21:V:452:LEU:O	21:V:456:ARG:HG3	2.14	0.47
23:X:842:THR:HA	23:X:915:ARG:HD2	1.97	0.47
24:Y:27:ASN:OD1	24:Y:66:ILE:N	2.28	0.47
26:1:625:ARG:HH21	26:1:662:HIS:HB3	1.79	0.47
26:1:666:LYS:HB3	26:1:704:ILE:HD13	1.96	0.47
26:1:1140:GLU:HB2	26:1:1143:VAL:CG1	2.44	0.47
27:3:75:LYS:HE3	27:3:76:ASP:H	1.79	0.47
27:3:347:LEU:CD2	27:3:359:TYR:HB2	2.44	0.47
27:3:1181:GLN:O	27:3:1185:MET:HG3	2.14	0.47
32:7:21:ARG:NH1	32:7:66:VAL:O	2.27	0.47
46:9:300:THR:HA	46:9:353:GLU:CG	2.43	0.47
1:A:211:GLN:HB3	1:A:225:TYR:CE1	2.49	0.47
1:A:386:PRO:HG2	1:A:389:LYS:HD2	1.97	0.47
1:A:569:VAL:O	1:A:570:ASP:HB2	2.14	0.47
1:A:1928:SER:HB2	1:A:1931:THR:H	1.80	0.47
2:B:21:A:O3'	2:B:22:U:H4'	2.14	0.47
5:E:312:TRP:HE1	5:E:319:ILE:HG12	1.80	0.47
6:F:36:A:N6	6:F:38:G:O6	2.48	0.47
6:F:41:A:C2	7:G:7:G:C2	3.03	0.47
7:G:112:U:O2	7:G:112:U:H2'	2.14	0.47
10:J:376:VAL:O	10:J:379:TRP:HB2	2.15	0.47
12:L:202:ARG:O	12:L:203:LYS:HE3	2.14	0.47
13:N:24:GLU:HB2	13:N:28:LYS:HE2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:1224:ILE:O	16:Q:1255:ASN:N	2.46	0.47
17:R:325:ARG:NH1	24:Y:222:ILE:O	2.48	0.47
17:R:391:VAL:HG13	17:R:396:VAL:HB	1.96	0.47
21:V:563:SER:HA	21:V:611:PHE:CD2	2.50	0.47
23:X:919:GLU:O	23:X:922:LEU:HB2	2.15	0.47
26:1:647:PHE:O	26:1:651:VAL:HG13	2.15	0.47
27:3:604:PHE:HA	27:3:618:SER:HA	1.96	0.47
27:3:612:ASN:HA	27:3:636:GLN:HA	1.95	0.47
27:3:1031:ARG:HG2	27:3:1031:ARG:NH1	2.27	0.47
33:5:13:HIS:ND1	33:5:17:LYS:HE3	2.30	0.47
1:A:110:TRP:O	1:A:192:GLN:NE2	2.47	0.47
1:A:1019:TYR:CG	1:A:1020:LYS:N	2.79	0.47
1:A:1206:GLU:HG2	1:A:1207:PHE:N	2.28	0.47
1:A:1401:ARG:HB2	1:A:1401:ARG:CZ	2.44	0.47
1:A:1771:LEU:HD11	1:A:1779:PHE:CE2	2.49	0.47
1:A:1885:LYS:HG2	1:A:1886:GLY:N	2.30	0.47
1:A:1920:TYR:HD2	1:A:1924:LEU:HD11	1.80	0.47
1:A:2107:PRO:HB2	1:A:2109:ASN:OD1	2.14	0.47
1:A:2319:LEU:HD13	1:A:2319:LEU:HA	1.75	0.47
3:C:238:ASN:O	3:C:242:LEU:HB2	2.15	0.47
3:C:514:TYR:CE2	3:C:522:SER:HB2	2.49	0.47
3:C:595:VAL:HG13	3:C:652:ASP:O	2.15	0.47
3:C:636:TYR:O	3:C:640:VAL:HG23	2.15	0.47
3:C:678:THR:OG1	3:C:680:ASN:O	2.19	0.47
3:C:719:GLN:OE1	3:C:724:TRP:HB3	2.13	0.47
4:D:1598:ILE:O	4:D:1601:LEU:N	2.46	0.47
5:E:100:ASP:N	5:E:100:ASP:OD1	2.48	0.47
5:E:193:THR:HG23	5:E:194:TYR:CG	2.50	0.47
5:E:288:LEU:HD21	5:E:290:ARG:HE	1.79	0.47
6:F:84:A:H4'	6:F:85:U:OP1	2.13	0.47
8:H:14:C:H1'	8:H:15:U:H5'	1.97	0.47
12:L:233:GLN:HG3	12:L:234:ALA:H	1.79	0.47
16:Q:542:ASN:HA	16:Q:622:SER:HA	1.96	0.47
19:T:253:ILE:O	19:T:261:LEU:HD12	2.15	0.47
21:V:473:ALA:O	21:V:477:LEU:HG	2.15	0.47
23:X:787:GLU:O	23:X:791:LEU:HD12	2.15	0.47
26:1:573:LYS:O	26:1:577:VAL:HG23	2.15	0.47
26:1:858:LYS:HE2	26:1:858:LYS:HB3	1.67	0.47
27:3:436:ARG:HD3	27:3:776:GLN:OE1	2.14	0.47
27:3:524:ILE:O	27:3:535:GLU:HA	2.15	0.47
27:3:563:LEU:O	27:3:580:ARG:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:565:TYR:HE1	27:3:619:LEU:HD12	1.80	0.47
27:3:839:ALA:O	27:3:843:LEU:HD12	2.14	0.47
27:3:864:SER:O	27:3:865:VAL:HG23	2.15	0.47
32:7:23:CYS:N	32:7:58:CYS:SG	2.73	0.47
46:9:325:ILE:HD13	46:9:328:PHE:HD1	1.79	0.47
1:A:309:ARG:HD3	1:A:311:GLU:OE1	2.15	0.47
1:A:312:TYR:N	1:A:312:TYR:CD1	2.83	0.47
1:A:644:ILE:HD12	1:A:644:ILE:HA	1.73	0.47
1:A:1373:GLN:NE2	1:A:1377:SER:OG	2.48	0.47
1:A:1661:TRP:HH2	1:A:1684:PHE:CE1	2.33	0.47
1:A:1865:ARG:NH2	1:A:1865:ARG:HA	2.29	0.47
2:B:64:G:C4	2:B:65:G:C8	3.02	0.47
5:E:177:LYS:HB3	5:E:179:TRP:NE1	2.30	0.47
8:H:107:A:C6	8:H:108:G:C6	3.02	0.47
12:L:168:LYS:HD3	12:L:171:ALA:HB3	1.96	0.47
17:R:328:ALA:HB2	24:Y:226:MET:SD	2.55	0.47
23:X:976:LEU:HD12	23:X:1000:VAL:HG23	1.96	0.47
24:Y:211:ILE:O	24:Y:215:LYS:HG2	2.15	0.47
26:1:529:GLY:HA2	26:1:570:TYR:CZ	2.49	0.47
26:1:840:LEU:HD13	26:1:840:LEU:HA	1.80	0.47
26:1:854:VAL:HG12	26:1:892:LEU:CD2	2.45	0.47
26:1:860:GLU:O	26:1:865:ARG:NH2	2.48	0.47
26:1:1233:ALA:O	26:1:1237:LEU:HB2	2.15	0.47
26:1:1279:ALA:O	26:1:1281:ILE:N	2.48	0.47
27:3:70:LEU:HD13	27:3:146:ARG:HG2	1.96	0.47
27:3:302:LEU:HA	27:3:311:PHE:O	2.14	0.47
27:3:457:ASN:ND2	27:3:479:VAL:HG12	2.29	0.47
27:3:617:ILE:HG12	27:3:627:PRO:HA	1.95	0.47
27:3:910:ALA:CB	27:3:913:LEU:HD11	2.45	0.47
27:3:1199:ARG:HH21	27:3:1207:LYS:HD3	1.80	0.47
30:2:466:LYS:HG2	30:2:475:VAL:HG21	1.97	0.47
1:A:79:ARG:HH11	1:A:82:ARG:NH2	2.09	0.47
1:A:93:LYS:O	1:A:649:GLU:HG2	2.15	0.47
1:A:1283:GLU:OE1	1:A:1283:GLU:N	2.48	0.47
1:A:1788:VAL:HB	1:A:1800:THR:OG1	2.14	0.47
1:A:1860:GLN:HB3	1:A:1883:VAL:HB	1.97	0.47
1:A:2132:SER:HB3	1:A:2137:PRO:HA	1.97	0.47
1:A:2149:PRO:HD3	1:A:2274:PRO:CG	2.45	0.47
3:C:350:ASN:ND2	3:C:353:THR:H	2.13	0.47
3:C:826:ARG:HA	3:C:911:PRO:HG3	1.97	0.47
26:1:582:LEU:HA	26:1:590:ARG:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:998:LYS:HZ1	26:1:1041:ARG:NH1	2.12	0.47
26:1:1135:GLU:HG3	26:1:1135:GLU:O	2.15	0.47
27:3:164:ASN:HA	27:3:189:TYR:OH	2.15	0.47
27:3:404:LEU:HD12	27:3:404:LEU:HA	1.77	0.47
27:3:674:LEU:C	27:3:675:LEU:HD12	2.34	0.47
1:A:112:GLN:O	1:A:113:ILE:HG13	2.15	0.47
1:A:196:ASP:HB3	1:A:199:GLU:HB2	1.97	0.47
1:A:388:LEU:HD23	1:A:388:LEU:HA	1.75	0.47
1:A:1275:ARG:NH1	1:A:1373:GLN:O	2.43	0.47
1:A:2212:ILE:HG21	1:A:2259:VAL:HG11	1.96	0.47
6:F:88:G:H2'	6:F:89:U:H5'	1.96	0.47
21:V:496:CYS:HG	21:V:507:PHE:HE1	1.62	0.47
21:V:540:GLU:H	21:V:540:GLU:HG3	1.51	0.47
23:X:172:LEU:O	23:X:175:LEU:HG	2.15	0.47
23:X:576:ARG:HA	23:X:576:ARG:NH2	2.30	0.47
23:X:754:GLU:HA	23:X:757:ARG:HH22	1.78	0.47
23:X:817:GLU:H	23:X:817:GLU:HG2	1.38	0.47
24:Y:9:LEU:CD2	24:Y:138:LYS:HD3	2.45	0.47
26:1:503:LYS:HE2	26:1:511:MET:CG	2.44	0.47
27:3:333:VAL:HG21	27:3:349:VAL:HG21	1.97	0.47
27:3:558:LEU:HG	27:3:559:THR:N	2.30	0.47
1:A:747:ALA:O	1:A:751:THR:OG1	2.29	0.46
1:A:1869:LEU:O	1:A:1873:GLU:HB2	2.14	0.46
1:A:1925:LYS:HE2	21:V:457:ARG:NH2	2.30	0.46
1:A:2103:THR:HB	1:A:2260:GLN:CD	2.36	0.46
3:C:122:LEU:O	3:C:125:ASN:HB3	2.15	0.46
3:C:175:GLN:OE1	3:C:175:GLN:N	2.47	0.46
3:C:302:PRO:HD2	3:C:344:TRP:CD1	2.50	0.46
8:H:51:A:H2'	8:H:52:G:O4'	2.15	0.46
10:J:256:LYS:HE2	12:L:232:TYR:CE1	2.50	0.46
10:J:289:ASN:O	10:J:291:GLN:NE2	2.48	0.46
12:L:166:LYS:HB3	12:L:167:ALA:H	1.59	0.46
17:R:386:ARG:HG2	23:X:909:ARG:HH22	1.80	0.46
21:V:543:LYS:HA	21:V:546:ASN:HD21	1.81	0.46
24:Y:224:LEU:CD1	24:Y:229:ASP:HB2	2.45	0.46
26:1:554:LYS:HD2	26:1:558:ARG:HE	1.80	0.46
26:1:568:ARG:HG3	26:1:568:ARG:HH11	1.79	0.46
26:1:746:PHE:O	26:1:750:ILE:HG23	2.15	0.46
26:1:869:MET:O	26:1:873:GLU:HB3	2.15	0.46
26:1:881:ALA:HB1	26:1:884:ILE:HG12	1.97	0.46
26:1:898:TYR:HA	26:1:901:GLN:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:929:LEU:N	26:1:930:PRO:HD2	2.30	0.46
27:3:24:GLY:HA2	27:3:74:THR:O	2.14	0.46
27:3:69:ARG:HG3	27:3:75:LYS:O	2.15	0.46
27:3:159:GLU:CD	27:3:161:HIS:H	2.19	0.46
27:3:867:ARG:NH1	27:3:879:LEU:HD13	2.30	0.46
27:3:1085:ALA:HB3	27:3:1088:LYS:HE2	1.97	0.46
32:7:12:ARG:NH1	32:7:84:GLY:O	2.48	0.46
1:A:1685:LEU:O	1:A:1689:THR:HG23	2.14	0.46
3:C:366:GLN:H	3:C:366:GLN:HG2	1.37	0.46
3:C:601:PRO:HA	3:C:604:LEU:HD12	1.97	0.46
4:D:2034:PRO:HA	4:D:2094:PHE:O	2.15	0.46
5:E:75:HIS:HB3	5:E:78:GLY:N	2.29	0.46
8:H:13:C:H1'	8:H:14:C:OP2	2.15	0.46
8:H:166:G:N3	8:H:166:G:H2'	2.29	0.46
9:I:551:PRO:HB3	9:I:554:SER:CB	2.46	0.46
10:J:328:GLY:HA2	10:J:331:GLN:NE2	2.30	0.46
12:L:92:THR:OG1	12:L:95:GLN:HG3	2.15	0.46
17:R:383:ASN:N	17:R:383:ASN:OD1	2.48	0.46
19:T:266:GLU:HG2	19:T:290:ALA:HB1	1.98	0.46
19:T:287:HIS:CE1	19:T:313:ARG:HG3	2.50	0.46
22:W:530:GLY:O	22:W:547:LYS:HA	2.16	0.46
23:X:182:ALA:HB2	23:X:924:ARG:HH11	1.80	0.46
23:X:273:LYS:HA	23:X:276:VAL:HG12	1.96	0.46
23:X:394:ALA:HA	23:X:397:ARG:HD2	1.96	0.46
23:X:503:ARG:O	23:X:506:LEU:HB2	2.16	0.46
23:X:876:GLY:O	23:X:880:VAL:HG23	2.16	0.46
24:Y:31:LEU:HG	24:Y:66:ILE:HB	1.98	0.46
32:7:12:ARG:HD2	32:7:12:ARG:HA	1.68	0.46
1:A:1131:LYS:NZ	1:A:1193:GLU:OE2	2.29	0.46
1:A:1417:PRO:O	1:A:1461:ASP:O	2.33	0.46
1:A:2185:SER:HB3	1:A:2187:GLN:HE22	1.81	0.46
2:B:103:G:H2'	2:B:104:C:O4'	2.16	0.46
3:C:807:GLN:HE22	46:9:144:LEU:HA	1.80	0.46
13:N:38:GLU:C	13:N:40:LYS:N	2.69	0.46
13:N:57:THR:HG23	13:N:92:TRP:CH2	2.51	0.46
19:T:210:ILE:HG22	19:T:467:ALA:HB1	1.98	0.46
22:W:384:ASP:O	22:W:388:GLN:N	2.48	0.46
23:X:452:GLN:O	23:X:497:THR:HA	2.15	0.46
23:X:700:TYR:HB3	23:X:757:ARG:O	2.15	0.46
23:X:727:GLY:HA2	23:X:730:ALA:O	2.15	0.46
26:1:516:LEU:HD12	26:1:516:LEU:HA	1.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:848:GLU:O	26:1:852:ARG:HG3	2.15	0.46
26:1:967:GLU:HB3	26:1:970:LEU:HB3	1.98	0.46
27:3:304:GLN:HE21	27:3:308:GLY:HA2	1.80	0.46
27:3:809:GLU:O	27:3:812:LYS:HB2	2.15	0.46
33:5:8:HIS:HA	33:5:11:LEU:HB2	1.97	0.46
1:A:340:ILE:H	1:A:340:ILE:HG12	1.37	0.46
2:B:38:C:C5	2:B:39:C:C4	3.03	0.46
3:C:226:VAL:HG22	3:C:254:THR:HB	1.98	0.46
3:C:377:LEU:HD12	3:C:380:ILE:HD12	1.97	0.46
3:C:510:LEU:HD13	3:C:514:TYR:CD2	2.50	0.46
7:G:112:U:C6	23:X:503:ARG:CG	2.98	0.46
9:I:427:LYS:O	9:I:429:VAL:N	2.48	0.46
10:J:289:ASN:HB3	12:L:232:TYR:CZ	2.50	0.46
10:J:339:TRP:HA	17:R:116:TYR:HD2	1.80	0.46
10:J:411:MET:HE3	10:J:415:LEU:HB3	1.98	0.46
16:Q:1144:CYS:O	16:Q:1148:ASN:N	2.47	0.46
21:V:550:MET:O	21:V:554:LEU:HG	2.15	0.46
23:X:454:ARG:HH12	23:X:679:THR:HB	1.81	0.46
23:X:508:GLU:OE1	23:X:512:ALA:N	2.48	0.46
23:X:575:ARG:HH22	23:X:724:GLY:HA2	1.79	0.46
24:Y:298:PHE:CE2	24:Y:314:ASP:HA	2.50	0.46
27:3:272:PRO:HD3	27:3:327:LEU:HD13	1.97	0.46
27:3:665:LEU:CB	27:3:679:LEU:HD23	2.45	0.46
27:3:1102:LEU:HD12	27:3:1102:LEU:HA	1.66	0.46
32:7:47:ASP:HA	32:7:50:ASN:HB3	1.96	0.46
46:9:323:ARG:HD2	46:9:420:ASP:HB2	1.97	0.46
46:9:363:ARG:HB3	46:9:363:ARG:CZ	2.45	0.46
1:A:409:ARG:N	1:A:410:PRO:HD2	2.30	0.46
1:A:796:LYS:HB3	1:A:796:LYS:HE3	1.76	0.46
1:A:2144:CYS:HB2	1:A:2270:PHE:CE1	2.49	0.46
1:A:2280:ASN:ND2	1:A:2304:PHE:O	2.47	0.46
3:C:95:LYS:HE2	3:C:95:LYS:HB2	1.58	0.46
4:D:621:HIS:HA	4:D:890:GLU:O	2.16	0.46
8:H:15:U:O2'	8:H:16:U:OP2	2.26	0.46
23:X:223:VAL:O	23:X:227:ARG:HG3	2.16	0.46
23:X:675:ASN:O	23:X:678:GLU:HB2	2.16	0.46
23:X:823:MET:HE3	23:X:823:MET:HB2	1.82	0.46
24:Y:30:LYS:CE	24:Y:169:PRO:HD2	2.45	0.46
24:Y:215:LYS:O	24:Y:218:LYS:N	2.48	0.46
26:1:864:TYR:O	26:1:868:VAL:HG13	2.15	0.46
26:1:903:GLN:HG2	26:1:910:MET:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1277:GLN:NE2	26:1:1277:GLN:O	2.48	0.46
27:3:226:GLU:HB3	27:3:261:PHE:CE2	2.51	0.46
27:3:451:GLU:HG3	27:3:760:ASN:O	2.16	0.46
27:3:594:ASN:OD1	27:3:594:ASN:N	2.46	0.46
27:3:604:PHE:CE1	27:3:681:PRO:HD3	2.51	0.46
27:3:745:PHE:CG	27:3:755:VAL:HG23	2.51	0.46
1:A:155:LYS:HE3	1:A:626:GLY:O	2.16	0.46
1:A:344:ASP:OD2	1:A:347:LEU:HD12	2.15	0.46
1:A:549:GLU:HB2	1:A:591:MET:HG3	1.97	0.46
1:A:1411:SER:O	1:A:1419:ILE:HG12	2.15	0.46
1:A:2187:GLN:HB2	1:A:2256:TYR:OH	2.16	0.46
3:C:220:ARG:HA	3:C:220:ARG:HE	1.81	0.46
5:E:311:VAL:HB	5:E:321:TYR:HB2	1.97	0.46
6:F:29:A:H61	7:G:17:U:P	2.39	0.46
8:H:14:C:OP2	8:H:14:C:H2'	2.16	0.46
10:J:411:MET:SD	10:J:415:LEU:HD23	2.56	0.46
10:J:432:VAL:O	10:J:435:ILE:HG13	2.16	0.46
19:T:301:ASP:OD1	19:T:301:ASP:N	2.48	0.46
21:V:374:ASP:O	21:V:376:TYR:N	2.45	0.46
24:Y:88:HIS:CE1	24:Y:125:VAL:HG22	2.51	0.46
24:Y:242:LEU:HD23	24:Y:315:PHE:HA	1.96	0.46
26:1:1000:ILE:O	26:1:1003:VAL:HG13	2.16	0.46
26:1:1015:ASP:OD1	26:1:1015:ASP:N	2.49	0.46
27:3:259:LYS:HE3	27:3:259:LYS:HB2	1.68	0.46
27:3:528:ARG:NH1	27:3:572:GLY:O	2.49	0.46
27:3:945:VAL:HG23	27:3:968:ARG:HH12	1.80	0.46
27:3:1158:ARG:HG3	27:3:1159:ASP:H	1.79	0.46
1:A:79:ARG:HD2	1:A:82:ARG:NE	2.31	0.46
1:A:259:ASP:OD1	1:A:259:ASP:N	2.39	0.46
1:A:310:THR:O	1:A:314:ILE:HG22	2.16	0.46
1:A:726:TRP:O	46:9:247:SER:HB2	2.14	0.46
1:A:1778:TRP:C	1:A:1779:PHE:HD2	2.19	0.46
1:A:2278:SER:HG	1:A:2309:HIS:CE1	2.33	0.46
2:B:69:A:H3'	2:B:70:A:C8	2.51	0.46
3:C:118:PHE:CE2	3:C:122:LEU:HD11	2.51	0.46
3:C:721:LYS:HD3	3:C:722:TYR:CZ	2.50	0.46
9:I:231:ASN:O	9:I:233:ASP:N	2.47	0.46
10:J:367:GLU:O	10:J:371:LEU:HG	2.16	0.46
10:J:395:ALA:O	10:J:398:VAL:HG12	2.16	0.46
12:L:40:ARG:O	12:L:40:ARG:HG2	2.16	0.46
12:L:188:ARG:HD2	12:L:191:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:120:ARG:HA	13:N:120:ARG:HD2	1.51	0.46
16:Q:314:ASN:N	16:Q:319:ASN:O	2.43	0.46
23:X:415:HIS:CD2	23:X:568:PRO:HG3	2.50	0.46
24:Y:38:ASN:OD1	24:Y:158:HIS:HA	2.14	0.46
26:1:612:THR:HB	26:1:613:MET:HE2	1.97	0.46
27:3:373:PHE:CE1	27:3:385:PHE:HB3	2.48	0.46
27:3:676:ARG:HD2	27:3:729:PHE:CD2	2.51	0.46
27:3:725:TYR:O	27:3:728:ARG:HB2	2.16	0.46
32:7:48:GLU:H	32:7:48:GLU:HG3	1.32	0.46
1:A:411:PHE:C	1:A:413:LEU:H	2.19	0.46
1:A:758:ARG:HD3	1:A:779:LEU:HD11	1.97	0.46
1:A:1580:HIS:CD2	1:A:1583:GLN:NE2	2.84	0.46
1:A:2194:THR:OG1	1:A:2238:GLY:HA2	2.16	0.46
3:C:388:VAL:HA	3:C:392:LEU:CD1	2.46	0.46
4:D:492:ALA:O	4:D:516:CYS:HA	2.16	0.46
10:J:339:TRP:HA	17:R:116:TYR:CD2	2.51	0.46
12:L:11:TRP:CZ2	12:L:41:LYS:HD2	2.51	0.46
13:N:64:PHE:CZ	13:N:72:ARG:HD2	2.51	0.46
17:R:367:ARG:CD	17:R:371:ARG:HD2	2.42	0.46
23:X:389:LYS:HE2	23:X:389:LYS:O	2.16	0.46
23:X:456:VAL:HA	23:X:459:MET:HG3	1.97	0.46
23:X:612:LEU:HB2	23:X:686:ILE:HG21	1.97	0.46
24:Y:204:SER:OG	24:Y:206:GLU:N	2.49	0.46
24:Y:241:VAL:HA	24:Y:286:ILE:O	2.16	0.46
26:1:871:THR:O	26:1:875:ILE:HG13	2.15	0.46
26:1:1216:TRP:O	26:1:1219:VAL:HB	2.16	0.46
27:3:312:LYS:HB2	27:3:330:PHE:CD1	2.50	0.46
30:2:542:GLU:HA	30:2:545:GLU:HG2	1.98	0.46
30:2:599:THR:O	30:2:600:ARG:HG3	2.16	0.46
46:9:306:ASN:CG	46:9:345:TYR:H	2.17	0.46
46:9:369:ALA:HA	46:9:394:HIS:CE1	2.51	0.46
1:A:108:MET:O	1:A:110:TRP:N	2.48	0.46
1:A:755:HIS:HE1	15:P:220:HIS:CE1	2.34	0.46
1:A:836:THR:HG21	23:X:866:ASN:ND2	2.31	0.46
1:A:1189:MET:HG3	1:A:1190:CYS:N	2.31	0.46
1:A:1352:HIS:CD2	20:U:5:ILE:HG13	2.50	0.46
1:A:1644:LEU:HD23	1:A:1644:LEU:HA	1.71	0.46
1:A:2289:ASP:CB	1:A:2292:MET:HB3	2.42	0.46
2:B:18:C:O2	2:B:59:G:N2	2.33	0.46
2:B:65:G:H2'	2:B:66:A:C8	2.51	0.46
3:C:86:THR:OG1	3:C:87:GLN:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:114:TYR:N	3:C:115:GLU:OE1	2.49	0.46
5:E:342:ILE:O	5:E:353:MET:HA	2.16	0.46
23:X:676:ILE:HG12	23:X:681:LEU:HD11	1.97	0.46
26:1:830:TYR:CG	26:1:867:MET:HG3	2.51	0.46
27:3:334:PRO:HB3	27:3:432:ARG:NH1	2.30	0.46
27:3:798:ILE:H	27:3:798:ILE:HG12	1.47	0.46
1:A:97:HIS:ND1	1:A:649:GLU:OE2	2.47	0.46
1:A:977:LEU:HG	1:A:978:GLU:N	2.30	0.46
1:A:1634:SER:OG	1:A:1635:TYR:N	2.50	0.46
1:A:1974:GLU:O	1:A:1978:LYS:HG3	2.15	0.46
3:C:700:ILE:HG13	3:C:705:VAL:HG11	1.98	0.46
6:F:36:A:C6	6:F:38:G:C6	3.04	0.46
6:F:88:G:C2	6:F:89:U:C6	3.04	0.46
16:Q:116:PRO:O	16:Q:120:PRO:HD2	2.16	0.46
16:Q:172:LEU:N	16:Q:173:PRO:HD2	2.31	0.46
17:R:189:ASN:ND2	17:R:195:ARG:HG2	2.30	0.46
17:R:286:LYS:HB2	46:9:215:PHE:CZ	2.50	0.46
17:R:315:LYS:HG2	17:R:316:GLU:N	2.31	0.46
21:V:450:ILE:HD12	21:V:450:ILE:HA	1.83	0.46
22:W:122:ASP:O	22:W:125:PHE:N	2.49	0.46
23:X:290:GLU:O	23:X:293:GLU:HG3	2.16	0.46
23:X:765:LEU:HD12	23:X:765:LEU:C	2.33	0.46
24:Y:144:VAL:HA	24:Y:150:PRO:HA	1.98	0.46
27:3:5:ASN:O	27:3:1176:GLY:HA3	2.16	0.46
27:3:185:LEU:O	27:3:186:GLU:HG3	2.16	0.46
27:3:592:LEU:HD11	27:3:619:LEU:HD11	1.97	0.46
27:3:788:PHE:HB2	27:3:799:ILE:HA	1.98	0.46
1:A:693:ILE:C	1:A:695:ASP:N	2.70	0.45
1:A:1030:ILE:HD11	1:A:1040:ILE:HG21	1.98	0.45
1:A:1903:GLY:O	1:A:1907:LEU:HG	2.16	0.45
1:A:2004:GLN:CD	26:1:898:TYR:HB2	2.36	0.45
2:B:14:U:H2'	2:B:15:C:C6	2.51	0.45
3:C:237:LEU:HD21	3:C:900:VAL:HG13	1.98	0.45
3:C:339:PHE:HE1	3:C:356:PHE:HZ	1.62	0.45
3:C:651:ILE:HG22	3:C:652:ASP:N	2.31	0.45
3:C:857:VAL:HA	3:C:873:ALA:CB	2.46	0.45
5:E:329:SER:N	5:E:347:SER:OG	2.49	0.45
7:G:9:C:H2'	7:G:10:U:C2	2.51	0.45
8:H:150:U:H3	8:H:181:G:H22	1.64	0.45
10:J:296:ARG:HD3	12:L:225:TYR:CE1	2.50	0.45
12:L:201:LYS:HD2	12:L:201:LYS:HA	1.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:334:ALA:HB2	19:T:350:HIS:CE1	2.51	0.45
23:X:989:LEU:HD12	23:X:989:LEU:HA	1.84	0.45
26:1:662:HIS:HB2	26:1:701:VAL:HB	1.98	0.45
26:1:907:ASP:OD2	26:1:909:VAL:HB	2.16	0.45
26:1:1135:GLU:O	26:1:1138:VAL:HG12	2.16	0.45
27:3:817:GLN:HG3	27:3:818:GLN:OE1	2.15	0.45
27:3:910:ALA:HB2	27:3:948:VAL:HG23	1.98	0.45
30:2:514:LYS:NZ	30:2:596:GLU:OE1	2.43	0.45
46:9:285:HIS:O	46:9:429:ASP:HB2	2.16	0.45
1:A:246:LEU:HD11	1:A:411:PHE:CE1	2.51	0.45
1:A:2133:PRO:HD2	1:A:2136:ASN:O	2.16	0.45
3:C:360:ALA:H	3:C:361:PRO:HD3	1.82	0.45
3:C:442:LYS:CD	3:C:468:CYS:HB3	2.46	0.45
5:E:125:PHE:N	5:E:125:PHE:CD2	2.83	0.45
5:E:251:LEU:HB2	5:E:293:TRP:NE1	2.31	0.45
5:E:266:PRO:HG3	12:L:789:ALA:HB2	1.99	0.45
6:F:85:U:H1'	6:F:86:U:C6	2.51	0.45
7:G:5:G:H2'	7:G:5:G:N3	2.31	0.45
7:G:99:C:N4	8:H:32:U:C4	2.84	0.45
8:H:43:U:H2'	8:H:44:U:C5	2.51	0.45
10:J:334:GLU:O	10:J:338:GLU:HG3	2.16	0.45
12:L:63:TRP:HB3	12:L:68:GLU:HG3	1.99	0.45
12:L:178:GLU:HB3	12:L:181:ARG:NH1	2.32	0.45
13:N:64:PHE:HZ	13:N:72:ARG:HD2	1.81	0.45
15:P:26:LEU:HD12	15:P:26:LEU:HA	1.62	0.45
15:P:27:SER:HB2	15:P:29:GLN:OE1	2.15	0.45
17:R:213:LYS:HB3	17:R:213:LYS:HE3	1.62	0.45
17:R:364:GLN:O	17:R:368:ASN:ND2	2.50	0.45
19:T:394:ASN:N	19:T:394:ASN:OD1	2.48	0.45
24:Y:188:SER:HB2	24:Y:190:ARG:HB2	1.98	0.45
26:1:572:HIS:NE2	26:1:613:MET:HE3	2.31	0.45
26:1:586:ASP:O	26:1:590:ARG:HG3	2.16	0.45
26:1:854:VAL:HG11	26:1:891:GLN:HG3	1.97	0.45
27:3:278:LEU:HD21	27:3:816:LYS:NZ	2.32	0.45
27:3:528:ARG:HG3	27:3:529:ALA:N	2.32	0.45
1:A:526:PRO:HD2	11:K:197:TYR:CD2	2.51	0.45
1:A:531:THR:O	1:A:535:ARG:HB2	2.16	0.45
1:A:643:GLY:HA3	2:B:28:A:O2'	2.16	0.45
1:A:1536:LEU:HD11	1:A:1576:ILE:HD11	1.97	0.45
1:A:2278:SER:OG	1:A:2279:TRP:N	2.49	0.45
3:C:453:TYR:CE2	3:C:575:GLN:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:105:LEU:HD11	5:E:136:TRP:CE3	2.50	0.45
6:F:38:G:C4	6:F:39:A:N7	2.84	0.45
14:O:119:GLN:OE1	17:R:218:ILE:HD11	2.17	0.45
19:T:422:ASN:HB2	19:T:426:VAL:HB	1.98	0.45
21:V:562:TRP:CD2	21:V:602:ARG:HD3	2.51	0.45
23:X:436:LEU:CD2	23:X:516:VAL:HG11	2.46	0.45
23:X:447:LYS:HB2	23:X:514:TYR:CD1	2.51	0.45
23:X:867:ALA:HB3	23:X:902:PHE:HD2	1.80	0.45
26:1:536:LEU:O	26:1:540:MET:HG2	2.16	0.45
26:1:1226:VAL:O	26:1:1230:VAL:HG23	2.17	0.45
27:3:1204:VAL:HG23	27:3:1205:SER:N	2.30	0.45
1:A:122:ILE:HB	1:A:481:PHE:O	2.17	0.45
1:A:929:GLU:O	1:A:933:ARG:HG3	2.16	0.45
1:A:1108:ASP:OD1	1:A:1108:ASP:N	2.49	0.45
1:A:1607:GLU:OE2	1:A:1608:THR:OG1	2.34	0.45
1:A:1934:SER:O	1:A:1938:LEU:HG	2.17	0.45
3:C:711:ARG:HB3	3:C:730:ARG:NH2	2.31	0.45
3:C:902:HIS:ND1	3:C:903:HIS:HD2	2.14	0.45
9:I:296:PHE:CB	9:I:337:LEU:HA	2.46	0.45
16:Q:437:ASN:O	16:Q:450:LEU:HA	2.17	0.45
17:R:158:LYS:O	17:R:161:ALA:HB3	2.17	0.45
21:V:646:HIS:C	21:V:646:HIS:ND1	2.69	0.45
23:X:725:ARG:HD3	23:X:728:ARG:NH1	2.21	0.45
23:X:858:LYS:O	23:X:861:VAL:HG23	2.16	0.45
24:Y:70:LEU:HD22	24:Y:169:PRO:HB2	1.98	0.45
26:1:769:VAL:HG13	26:1:773:LEU:HD21	1.99	0.45
27:3:232:GLY:HA3	27:3:252:SER:HA	1.97	0.45
27:3:404:LEU:HB3	27:3:407:ILE:HG12	1.99	0.45
27:3:515:ALA:HA	27:3:528:ARG:HA	1.97	0.45
27:3:633:LEU:HD12	27:3:637:PRO:HG3	1.97	0.45
27:3:996:ILE:HG21	27:3:1041:TYR:CD1	2.52	0.45
27:3:1015:LYS:HD2	27:3:1015:LYS:HA	1.78	0.45
27:3:1188:ASN:HA	27:3:1191:LYS:HZ2	1.81	0.45
46:9:370:ASN:ND2	46:9:375:SER:H	2.15	0.45
1:A:1719:PHE:CD1	1:A:1719:PHE:C	2.90	0.45
1:A:2107:PRO:HG2	1:A:2110:VAL:HG22	1.99	0.45
3:C:113:VAL:HG23	3:C:114:TYR:H	1.82	0.45
3:C:121:ASP:OD1	3:C:122:LEU:N	2.49	0.45
3:C:510:LEU:CB	3:C:564:THR:HG23	2.47	0.45
3:C:574:ALA:O	3:C:575:GLN:NE2	2.46	0.45
3:C:718:PHE:HB3	3:C:724:TRP:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:783:ALA:O	4:D:809:LEU:HA	2.17	0.45
5:E:71:CYS:HB2	5:E:115:LEU:HG	1.99	0.45
17:R:348:GLU:HG3	23:X:262:LEU:CB	2.47	0.45
21:V:533:TYR:CE2	21:V:568:ILE:HG23	2.52	0.45
23:X:396:ARG:NE	23:X:431:GLN:HE22	2.15	0.45
23:X:525:ARG:O	23:X:754:GLU:HB2	2.16	0.45
26:1:856:ASP:HB3	26:1:864:TYR:CE2	2.51	0.45
26:1:857:LEU:HA	26:1:865:ARG:HB3	1.98	0.45
26:1:1195:MET:O	26:1:1199:VAL:HG23	2.16	0.45
26:1:1266:TRP:CZ3	33:5:22:GLY:HA3	2.51	0.45
27:3:93:GLN:O	27:3:97:ASN:N	2.50	0.45
27:3:124:ASP:OD2	27:3:128:ARG:HG3	2.17	0.45
27:3:458:ALA:O	27:3:459:VAL:HG23	2.17	0.45
27:3:485:LEU:HA	27:3:494:VAL:HB	1.99	0.45
27:3:642:ILE:H	27:3:703:ARG:NH2	2.14	0.45
27:3:1159:ASP:OD1	27:3:1160:HIS:N	2.50	0.45
27:3:1210:ASP:HA	27:3:1213:THR:OG1	2.15	0.45
46:9:312:LYS:HB2	46:9:312:LYS:HE2	1.76	0.45
1:A:1368:LEU:HA	1:A:1368:LEU:HD23	1.57	0.45
1:A:1418:ARG:HB2	1:A:1462:GLY:HA3	1.98	0.45
1:A:1625:SER:OG	1:A:1687:TYR:HD2	1.99	0.45
1:A:2188:LEU:HD12	1:A:2188:LEU:HA	1.81	0.45
3:C:403:LEU:HD23	3:C:403:LEU:HA	1.87	0.45
3:C:568:PRO:C	3:C:570:GLY:H	2.20	0.45
4:D:668:ASP:O	4:D:672:GLY:HA3	2.16	0.45
8:H:70:C:H2'	8:H:71:C:H6	1.80	0.45
10:J:262:ARG:NH2	10:J:291:GLN:HG2	2.32	0.45
17:R:171:LEU:HD11	17:R:203:GLN:OE1	2.16	0.45
23:X:263:SER:O	23:X:267:ARG:CB	2.60	0.45
23:X:444:LYS:N	23:X:444:LYS:HD2	2.32	0.45
23:X:698:LYS:HD3	23:X:707:GLU:HB2	1.99	0.45
24:Y:80:ALA:HB2	24:Y:102:ASP:O	2.16	0.45
24:Y:186:LEU:HD23	24:Y:186:LEU:HA	1.79	0.45
26:1:1063:LEU:HA	26:1:1063:LEU:HD23	1.64	0.45
26:1:1130:PRO:HD3	30:2:575:PHE:CE2	2.52	0.45
26:1:1142:ASN:H	26:1:1142:ASN:HD22	1.64	0.45
26:1:1276:SER:H	27:3:113:ARG:NH2	2.14	0.45
27:3:424:TYR:HD1	27:3:437:VAL:HG22	1.82	0.45
27:3:565:TYR:CE1	27:3:619:LEU:HD12	2.51	0.45
30:2:541:GLN:O	30:2:545:GLU:HG2	2.17	0.45
46:9:241:TYR:HB2	46:9:242:SER:H	1.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ILE:HG12	1:A:571:ALA:HB1	1.99	0.45
1:A:273:ILE:HG23	1:A:274:PRO:HD2	1.99	0.45
3:C:247:VAL:HG11	3:C:292:TYR:HB3	1.98	0.45
4:D:1581:ALA:O	4:D:1584:ILE:HA	2.17	0.45
6:F:39:A:C2'	6:F:40:U:H5'	2.47	0.45
6:F:83:A:H1'	6:F:84:A:C8	2.52	0.45
7:G:-7:U:H5'	7:G:-6:C:OP2	2.17	0.45
8:H:160:A:C2	8:H:171:U:C2	3.05	0.45
14:O:235:TYR:HA	14:O:270:ALA:O	2.17	0.45
17:R:429:ILE:CD1	17:R:431:ASN:HD22	2.30	0.45
21:V:553:HIS:CD2	21:V:556:TYR:CE1	3.05	0.45
21:V:596:LEU:N	21:V:597:PRO:HD2	2.32	0.45
26:1:974:LEU:HG	26:1:974:LEU:H	1.46	0.45
27:3:52:THR:O	27:3:52:THR:OG1	2.34	0.45
30:2:471:ARG:HE	30:2:471:ARG:HB3	1.49	0.45
46:9:437:PRO:HG2	46:9:438:TYR:CE2	2.52	0.45
1:A:1000:ILE:HA	1:A:1000:ILE:HD12	1.58	0.45
3:C:567:GLU:H	3:C:567:GLU:HG2	1.50	0.45
3:C:684:LYS:HB3	3:C:795:VAL:HB	1.98	0.45
3:C:776:GLU:O	3:C:781:ASP:HA	2.16	0.45
3:C:801:LEU:HD23	3:C:801:LEU:HA	1.76	0.45
3:C:827:LEU:O	3:C:907:VAL:HG23	2.17	0.45
3:C:852:ARG:HD2	7:G:-12:C:H5'	1.98	0.45
5:E:188:GLN:CD	5:E:189:THR:H	2.21	0.45
6:F:25:C:H4'	6:F:26:U:OP2	2.17	0.45
6:F:40:U:H2'	6:F:41:A:C8	2.51	0.45
7:G:90:C:H42	8:H:40:C:N4	2.14	0.45
7:G:105:C:H5'	7:G:105:C:O2	2.17	0.45
8:H:105:G:N2	8:H:107:A:H5'	2.32	0.45
9:I:342:PRO:C	9:I:344:LEU:H	2.20	0.45
16:Q:599:GLY:HA3	16:Q:608:ILE:N	2.31	0.45
18:S:99:ALA:HB2	18:S:128:ILE:HA	1.99	0.45
21:V:219:VAL:O	21:V:223:ASN:CB	2.65	0.45
21:V:570:LEU:HD23	21:V:575:THR:HG21	1.98	0.45
23:X:257:PHE:O	23:X:259:ASP:N	2.49	0.45
23:X:421:GLU:HB2	23:X:557:THR:HG21	1.99	0.45
23:X:620:GLU:OE2	23:X:620:GLU:N	2.44	0.45
23:X:1017:LYS:HB2	23:X:1020:GLU:OE2	2.17	0.45
24:Y:276:LYS:HB3	24:Y:276:LYS:HE2	1.75	0.45
26:1:560:LEU:HD11	26:1:600:LEU:HD12	1.99	0.45
26:1:1017:LEU:HD22	26:1:1050:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1282:ALA:HB2	27:3:1050:PHE:CE1	2.52	0.45
27:3:185:LEU:HD23	27:3:185:LEU:HA	1.69	0.45
27:3:704:VAL:C	27:3:710:GLU:HG3	2.37	0.45
30:2:596:GLU:N	30:2:596:GLU:OE2	2.50	0.45
46:9:221:LEU:HD23	46:9:221:LEU:H	1.81	0.45
46:9:355:ARG:HB3	46:9:358:LEU:HD12	1.99	0.45
1:A:228:TRP:O	1:A:415:SER:HA	2.16	0.45
1:A:426:LEU:H	1:A:426:LEU:HG	1.64	0.45
1:A:839:LEU:O	1:A:843:LEU:HG	2.17	0.45
1:A:1361:GLU:HG3	1:A:1362:ASP:OD2	2.17	0.45
1:A:1526:LEU:O	11:K:216:SER:HB3	2.16	0.45
1:A:1838:LYS:HB3	1:A:1868:MET:HG3	1.99	0.45
1:A:2193:VAL:HB	1:A:2230:LEU:HD21	1.99	0.45
3:C:262:ARG:HE	3:C:262:ARG:HB3	1.66	0.45
3:C:349:PHE:CZ	3:C:351:PRO:HA	2.52	0.45
3:C:853:ARG:HD3	3:C:879:ASP:O	2.17	0.45
6:F:65:G:H5"	6:F:66:C:OP2	2.17	0.45
7:G:6:A:H2'	7:G:7:G:C8	2.52	0.45
14:O:256:GLY:HA3	14:O:279:ALA:CB	2.47	0.45
15:P:52:GLU:HB2	15:P:53:GLU:OE1	2.17	0.45
21:V:593:TYR:HD1	21:V:593:TYR:HA	1.73	0.45
23:X:246:LEU:HG	23:X:277:ARG:NE	2.27	0.45
26:1:644:LEU:HB3	26:1:648:LEU:CD1	2.46	0.45
26:1:658:TRP:CZ3	26:1:698:GLN:HG2	2.52	0.45
27:3:27:GLN:OE1	27:3:42:ARG:NH1	2.50	0.45
27:3:147:ASP:OD2	27:3:151:ARG:HG2	2.16	0.45
27:3:184:CYS:SG	27:3:211:TYR:HE1	2.40	0.45
27:3:595:VAL:HG22	27:3:596:PRO:O	2.17	0.45
27:3:601:ARG:HD3	27:3:620:ASP:HB3	1.98	0.45
30:2:517:ILE:H	30:2:517:ILE:HG13	1.27	0.45
32:7:9:ILE:O	32:7:88:ILE:HG22	2.17	0.45
33:5:33:VAL:CG2	33:5:76:CYS:HB2	2.47	0.45
46:9:242:SER:HB2	46:9:262:GLU:C	2.37	0.45
46:9:423:LYS:HB3	46:9:423:LYS:HE3	1.68	0.45
1:A:361:HIS:HB2	3:C:280:HIS:CG	2.52	0.45
1:A:1457:HIS:ND1	1:A:1460:HIS:CD2	2.84	0.45
1:A:1933:PHE:O	1:A:1937:ILE:HG13	2.17	0.45
1:A:2190:PRO:HG3	1:A:2251:TYR:CD2	2.52	0.45
3:C:118:PHE:CZ	3:C:122:LEU:HD11	2.52	0.45
3:C:122:LEU:HD21	3:C:197:SER:OG	2.16	0.45
5:E:75:HIS:HB3	5:E:79:SER:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:125:PHE:CE2	5:E:135:VAL:HG13	2.52	0.45
6:F:84:A:O2'	6:F:85:U:H2'	2.17	0.45
15:P:50:ALA:O	15:P:54:VAL:HG23	2.17	0.45
15:P:186:ARG:HD2	15:P:190:ASP:OD2	2.17	0.45
17:R:299:ARG:NH2	23:X:301:PRO:O	2.26	0.45
22:W:463:SER:O	22:W:481:MET:N	2.29	0.45
23:X:242:LYS:HE3	23:X:242:LYS:HB3	1.48	0.45
23:X:448:ILE:HB	23:X:493:LEU:HD22	1.98	0.45
23:X:620:GLU:H	23:X:620:GLU:CD	2.17	0.45
27:3:249:LEU:HD23	27:3:256:ILE:HD11	1.98	0.45
27:3:325:ILE:HB	27:3:375:SER:HB3	1.99	0.45
27:3:331:ASP:OD2	27:3:393:LYS:N	2.39	0.45
27:3:331:ASP:CG	27:3:390:ARG:HH21	2.20	0.45
27:3:407:ILE:HD11	27:3:1124:GLY:HA2	1.99	0.45
27:3:753:GLY:O	27:3:754:ILE:HD13	2.17	0.45
46:9:325:ILE:HB	46:9:328:PHE:HB3	1.98	0.45
1:A:1614:ILE:H	1:A:1614:ILE:HG13	1.59	0.44
1:A:1645:LEU:HD11	1:A:1727:GLN:HG3	1.99	0.44
1:A:1712:HIS:ND1	1:A:1734:MET:HG3	2.32	0.44
1:A:2004:GLN:NE2	26:1:898:TYR:HB2	2.32	0.44
1:A:2074:ARG:HD3	1:A:2074:ARG:HA	1.69	0.44
3:C:129:ILE:HA	3:C:199:LEU:O	2.16	0.44
5:E:270:LYS:HA	5:E:270:LYS:HE3	1.98	0.44
6:F:81:C:N4	8:H:17:U:H3	2.15	0.44
7:G:99:C:N3	8:H:33:G:C4	2.85	0.44
10:J:285:MET:HE3	10:J:286:GLU:OE2	2.17	0.44
17:R:153:LYS:HD2	17:R:154:SER:N	2.32	0.44
19:T:341:ALA:O	19:T:344:GLN:HG3	2.17	0.44
23:X:644:VAL:O	23:X:645:LEU:HD23	2.18	0.44
23:X:826:LYS:HA	23:X:826:LYS:HD2	1.68	0.44
24:Y:298:PHE:HE2	24:Y:314:ASP:HA	1.82	0.44
24:Y:303:ASN:HA	24:Y:311:ILE:O	2.18	0.44
26:1:781:ASP:O	26:1:785:LYS:HG3	2.17	0.44
27:3:14:ILE:HD11	27:3:356:HIS:CD2	2.51	0.44
27:3:485:LEU:CD2	27:3:491:VAL:HG12	2.46	0.44
27:3:569:ASP:O	27:3:572:GLY:N	2.45	0.44
27:3:739:LEU:HD23	27:3:739:LEU:HA	1.71	0.44
27:3:988:ASN:ND2	27:3:1004:ASP:OD1	2.50	0.44
27:3:1098:GLY:C	27:3:1099:GLU:HG3	2.37	0.44
30:2:477:MET:SD	30:2:478:HIS:CE1	3.10	0.44
46:9:366:LEU:HD11	46:9:380:PHE:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:LYS:NZ	17:R:165:VAL:HG22	2.32	0.44
1:A:232:LEU:N	1:A:233:PRO:HD2	2.32	0.44
1:A:325:HIS:CD2	1:A:326:HIS:CD2	2.93	0.44
1:A:407:ALA:O	1:A:412:ASN:HB3	2.17	0.44
1:A:485:THR:HG22	1:A:486:LYS:H	1.83	0.44
1:A:683:LEU:HD21	6:F:57:U:H5'	1.99	0.44
1:A:974:ASN:OD1	1:A:1100:ARG:NH1	2.50	0.44
1:A:1219:GLU:HG3	23:X:341:PHE:HD1	1.80	0.44
1:A:1681:ARG:HB3	1:A:1681:ARG:HH11	1.82	0.44
3:C:83:GLU:H	3:C:83:GLU:HG2	1.34	0.44
3:C:138:LEU:HA	3:C:207:GLY:HA3	1.98	0.44
3:C:296:GLU:H	3:C:296:GLU:CD	2.21	0.44
3:C:938:ARG:O	3:C:942:GLY:N	2.49	0.44
7:G:99:C:C4	8:H:33:G:C5	3.05	0.44
10:J:231:PHE:HA	10:J:234:ASN:HD22	1.82	0.44
17:R:211:ARG:HB2	17:R:212:PHE:CE2	2.52	0.44
23:X:419:ILE:O	23:X:569:VAL:HA	2.17	0.44
26:1:581:LEU:HD13	26:1:589:ALA:HB1	1.98	0.44
26:1:761:TYR:O	26:1:765:TYR:HB2	2.17	0.44
30:2:526:ASP:O	30:2:528:ILE:N	2.50	0.44
33:5:50:LEU:HD12	33:5:50:LEU:HA	1.54	0.44
46:9:282:VAL:HG13	46:9:433:VAL:HG22	1.98	0.44
1:A:591:MET:HB3	1:A:598:LEU:CD2	2.48	0.44
1:A:1362:ASP:CG	1:A:1363:GLN:H	2.16	0.44
3:C:137:HIS:HB3	3:C:140:HIS:ND1	2.32	0.44
5:E:267:PHE:HD2	5:E:268:ALA:N	2.16	0.44
5:E:343:ILE:HA	5:E:352:TYR:O	2.17	0.44
6:F:7:G:H2'	6:F:8:C:C6	2.52	0.44
6:F:83:A:H1'	6:F:84:A:C4	2.53	0.44
7:G:12:G:H3'	7:G:13:C:C5	2.51	0.44
7:G:110:U:OP1	23:X:455:ARG:CG	2.65	0.44
10:J:346:TRP:CG	10:J:369:PHE:HD1	2.35	0.44
10:J:381:LYS:O	10:J:384:ARG:HB3	2.17	0.44
15:P:74:LYS:HA	15:P:77:ASP:HB3	1.99	0.44
16:Q:698:SER:HA	16:Q:1129:PRO:HD3	1.98	0.44
19:T:295:ASP:O	19:T:303:LEU:HD23	2.18	0.44
21:V:636:LEU:HD23	21:V:636:LEU:HA	1.57	0.44
23:X:242:LYS:HG3	24:Y:227:VAL:HG21	1.98	0.44
23:X:497:THR:H	23:X:500:MET:HB2	1.81	0.44
23:X:898:CYS:SG	23:X:903:VAL:HB	2.57	0.44
23:X:988:GLU:CB	23:X:998:ARG:HB2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1046:GLY:O	26:1:1048:GLU:N	2.50	0.44
26:1:1149:LYS:O	26:1:1152:SER:HB3	2.17	0.44
26:1:1251:LEU:HD23	26:1:1251:LEU:HA	1.68	0.44
27:3:243:ASP:OD1	27:3:244:GLY:N	2.50	0.44
30:2:569:GLN:O	30:2:573:ASP:HB2	2.17	0.44
1:A:364:SER:O	1:A:366:LYS:HD3	2.17	0.44
1:A:599:MET:H	1:A:599:MET:HG2	1.55	0.44
1:A:779:LEU:HD12	1:A:905:LEU:HD11	2.00	0.44
1:A:872:ASP:C	1:A:874:PRO:HD3	2.38	0.44
1:A:1318:THR:HB	1:A:1324:GLY:HA3	2.00	0.44
1:A:1660:TYR:CE1	1:A:1699:THR:HG22	2.53	0.44
1:A:1687:TYR:HA	1:A:1690:ASP:OD2	2.17	0.44
1:A:1723:LYS:HB3	1:A:1724:PRO:HD3	1.98	0.44
1:A:1889:LEU:HD12	1:A:1889:LEU:HA	1.80	0.44
3:C:485:ASP:OD1	3:C:486:ASP:N	2.51	0.44
3:C:742:PRO:CG	3:C:785:ARG:HG2	2.48	0.44
3:C:788:LYS:HE2	3:C:790:LYS:HE3	1.98	0.44
3:C:802:HIS:CE1	3:C:803:ARG:HH11	2.36	0.44
4:D:759:THR:H	27:3:680:ASP:CG	2.20	0.44
5:E:235:ALA:HB3	5:E:256:ASP:HB2	1.99	0.44
6:F:40:U:H3	7:G:7:G:H1	1.65	0.44
6:F:82:A:O2'	6:F:83:A:H2'	2.17	0.44
7:G:88:G:H1'	8:H:42:G:N2	2.33	0.44
7:G:99:C:N3	8:H:33:G:C5	2.86	0.44
13:N:75:TYR:O	13:N:79:ILE:HD12	2.18	0.44
16:Q:494:PRO:HB2	16:Q:503:VAL:O	2.17	0.44
24:Y:26:LEU:HB3	24:Y:166:PHE:CE1	2.53	0.44
26:1:750:ILE:HG13	26:1:751:GLY:N	2.32	0.44
26:1:963:LYS:O	26:1:965:CYS:N	2.50	0.44
26:1:1017:LEU:HD21	26:1:1058:ILE:HD11	1.99	0.44
27:3:275:ARG:HH21	27:3:275:ARG:CB	2.31	0.44
27:3:288:VAL:HG23	27:3:289:CYS:N	2.30	0.44
27:3:986:ILE:HG21	27:3:990:ILE:HG12	1.99	0.44
1:A:863:GLU:HG3	1:A:913:PRO:HB3	2.00	0.44
1:A:1914:MET:HE1	1:A:1916:LEU:HB2	2.00	0.44
3:C:743:ASN:HB3	3:C:787:VAL:HG13	2.00	0.44
3:C:921:LEU:HD23	3:C:921:LEU:HA	1.68	0.44
4:D:824:HIS:HA	4:D:862:ASP:CB	2.47	0.44
6:F:5:U:N3	6:F:7:G:N7	2.65	0.44
6:F:19:C:H4'	13:N:95:GLN:NE2	2.32	0.44
7:G:105:C:OP1	23:X:993:THR:OG1	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:158:G:H2'	8:H:159:U:O4'	2.16	0.44
15:P:45:GLN:HA	15:P:45:GLN:NE2	2.33	0.44
23:X:181:PHE:O	23:X:185:VAL:HG23	2.16	0.44
23:X:576:ARG:HB3	23:X:577:PHE:CD2	2.52	0.44
23:X:992:THR:O	23:X:994:LYS:N	2.51	0.44
23:X:1003:ILE:HD12	23:X:1008:LEU:HD21	1.99	0.44
26:1:781:ASP:HB3	26:1:784:MET:HB2	2.00	0.44
26:1:946:LYS:O	26:1:950:GLN:HG3	2.17	0.44
27:3:228:LEU:HD12	27:3:229:GLU:N	2.28	0.44
27:3:543:THR:O	27:3:558:LEU:HD12	2.17	0.44
27:3:554:VAL:HG12	27:3:556:ILE:HG23	2.00	0.44
27:3:568:MET:H	27:3:568:MET:HG2	1.58	0.44
27:3:768:GLU:HB3	27:3:769:LYS:H	1.63	0.44
1:A:39:GLN:NE2	22:W:170:THR:H	2.16	0.44
1:A:246:LEU:HA	1:A:246:LEU:HD23	1.68	0.44
1:A:246:LEU:HD22	1:A:408:PRO:HG2	1.99	0.44
1:A:731:LEU:O	46:9:241:TYR:HB3	2.17	0.44
1:A:923:ASP:OD2	1:A:1439:ARG:NH1	2.49	0.44
1:A:1383:GLN:OE1	23:X:339:LEU:HB3	2.17	0.44
1:A:1403:LEU:O	17:R:407:TYR:HB2	2.17	0.44
1:A:1555:LEU:HA	1:A:1555:LEU:HD22	1.67	0.44
1:A:1661:TRP:CH2	1:A:1684:PHE:HE1	2.36	0.44
1:A:2187:GLN:HB2	1:A:2256:TYR:CE1	2.52	0.44
3:C:219:LEU:HD23	3:C:219:LEU:HA	1.67	0.44
3:C:219:LEU:HD22	3:C:251:LEU:HG	2.00	0.44
3:C:267:LEU:HD23	3:C:267:LEU:HA	1.74	0.44
4:D:1526:HIS:O	4:D:1703:VAL:HA	2.18	0.44
5:E:114:GLU:O	5:E:126:SER:HA	2.18	0.44
6:F:43:A:N6	6:F:44:G:O6	2.50	0.44
6:F:60:C:H2'	10:J:236:ARG:NH2	2.32	0.44
19:T:203:HIS:CD2	19:T:207:VAL:HG22	2.52	0.44
19:T:320:LYS:HE2	19:T:320:LYS:HB2	1.72	0.44
23:X:327:ARG:NH1	23:X:327:ARG:HB3	2.32	0.44
23:X:819:PRO:CG	23:X:921:LEU:HD12	2.35	0.44
27:3:1151:GLU:OE2	27:3:1193:VAL:HG21	2.18	0.44
27:3:1211:ILE:HD12	27:3:1214:ARG:HE	1.82	0.44
30:2:512:GLN:N	30:2:512:GLN:OE1	2.51	0.44
46:9:41:HIS:HA	46:9:48:PRO:HA	1.99	0.44
46:9:295:LEU:HD13	46:9:308:ILE:HD11	1.99	0.44
46:9:370:ASN:HD22	46:9:375:SER:H	1.66	0.44
1:A:298:ASP:HB3	1:A:301:LYS:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:HIS:HB2	1:A:366:LYS:NZ	2.31	0.44
1:A:2249:LYS:HE3	1:A:2249:LYS:HB3	1.64	0.44
3:C:280:HIS:HA	3:C:283:ASP:OD1	2.17	0.44
3:C:502:HIS:CE1	3:C:543:ARG:HH12	2.35	0.44
4:D:1915:ILE:O	4:D:1919:ALA:HB2	2.17	0.44
7:G:99:C:C4	8:H:33:G:C6	3.05	0.44
8:H:106:G:N3	8:H:107:A:N6	2.65	0.44
10:J:342:GLU:O	10:J:346:TRP:CD1	2.71	0.44
12:L:76:LYS:NZ	12:L:76:LYS:HB3	2.31	0.44
12:L:169:ARG:HE	12:L:169:ARG:HB2	1.57	0.44
13:N:56:LYS:HB3	13:N:56:LYS:HE2	1.84	0.44
14:O:163:HIS:O	14:O:182:ARG:N	2.51	0.44
17:R:325:ARG:HH11	24:Y:222:ILE:CG2	2.28	0.44
20:U:24:SER:O	20:U:24:SER:OG	2.28	0.44
21:V:525:PHE:HA	21:V:528:ILE:HB	1.99	0.44
21:V:571:SER:HB3	21:V:574:THR:OG1	2.17	0.44
21:V:628:ILE:HG21	21:V:644:ARG:HD2	1.98	0.44
23:X:408:LEU:HB2	23:X:570:PHE:CZ	2.52	0.44
23:X:686:ILE:HD13	23:X:686:ILE:HA	1.87	0.44
24:Y:64:GLU:HG2	24:Y:77:PHE:CE1	2.52	0.44
24:Y:240:ASN:ND2	24:Y:289:GLU:O	2.51	0.44
24:Y:246:LYS:O	24:Y:311:ILE:HG22	2.17	0.44
26:1:967:GLU:HB3	26:1:971:MET:H	1.83	0.44
26:1:1080:THR:HA	26:1:1083:TYR:CD2	2.52	0.44
27:3:341:VAL:HG12	27:3:347:LEU:HB2	2.00	0.44
27:3:558:LEU:HD23	27:3:562:GLU:HB3	1.99	0.44
27:3:741:PHE:HB3	27:3:757:ILE:HG13	1.99	0.44
27:3:769:LYS:HD3	27:3:769:LYS:H	1.81	0.44
27:3:955:PHE:HZ	27:3:1014:TYR:CD2	2.36	0.44
30:2:528:ILE:O	30:2:531:THR:HG23	2.18	0.44
46:9:292:ASN:HB2	46:9:402:GLY:N	2.33	0.44
1:A:35:ARG:HG2	1:A:35:ARG:NH1	2.33	0.44
1:A:75:ASP:O	1:A:77:THR:HG22	2.18	0.44
1:A:1866:LYS:HE2	1:A:1866:LYS:HB2	1.83	0.44
1:A:1917:PHE:HD1	1:A:1967:ILE:HD11	1.83	0.44
3:C:203:MET:CG	3:C:221:ILE:HD11	2.48	0.44
3:C:686:THR:CB	3:C:793:ASP:HB3	2.42	0.44
8:H:30:A:H2'	8:H:30:A:N3	2.32	0.44
8:H:161:U:H2'	8:H:163:G:N2	2.32	0.44
12:L:62:GLU:N	12:L:62:GLU:OE1	2.51	0.44
13:N:58:ARG:HA	13:N:58:ARG:HD3	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:1317:THR:N	16:Q:1318:PRO:HD2	2.33	0.44
17:R:382:ARG:HH12	17:R:386:ARG:NE	2.16	0.44
21:V:572:GLU:OE1	21:V:580:ARG:NH2	2.51	0.44
23:X:587:PRO:CB	26:1:827:ARG:HH12	2.29	0.44
23:X:809:THR:HB	23:X:812:GLY:H	1.82	0.44
27:3:164:ASN:HD22	27:3:190:GLU:HG2	1.82	0.44
27:3:249:LEU:HD12	27:3:249:LEU:N	2.33	0.44
27:3:592:LEU:HA	27:3:592:LEU:HD13	1.64	0.44
27:3:611:ASP:O	27:3:612:ASN:HB2	2.17	0.44
27:3:717:SER:HB2	27:3:718:ARG:HH12	1.81	0.44
1:A:121:HIS:CD2	1:A:482:PHE:CE1	3.06	0.44
1:A:858:GLN:OE1	1:A:858:GLN:HA	2.17	0.44
1:A:984:MET:HG3	1:A:985:TYR:CD1	2.53	0.44
1:A:1109:LEU:HG	1:A:1152:ALA:HB1	2.00	0.44
1:A:1301:ILE:HA	1:A:1301:ILE:HD13	1.67	0.44
1:A:1337:GLN:HA	1:A:1337:GLN:HE21	1.83	0.44
1:A:1457:HIS:CE1	1:A:1460:HIS:HD2	2.35	0.44
1:A:2001:SER:CA	26:1:855:ASP:HB3	2.47	0.44
2:B:64:G:C6	2:B:65:G:C5	3.05	0.44
3:C:474:LEU:HD11	3:C:501:ILE:HG23	1.99	0.44
3:C:608:ARG:HB3	3:C:612:LYS:HE3	2.00	0.44
5:E:81:LEU:HB2	5:E:95:VAL:HG22	1.99	0.44
5:E:125:PHE:N	5:E:125:PHE:HD2	2.16	0.44
5:E:180:ASP:OD1	5:E:182:ARG:N	2.24	0.44
5:E:326:HIS:CE1	5:E:346:SER:HB2	2.53	0.44
7:G:88:G:H2'	7:G:88:G:N3	2.33	0.44
8:H:5:C:H2'	8:H:6:U:C6	2.53	0.44
10:J:375:ASP:HB2	10:J:378:ASN:CG	2.38	0.44
10:J:436:TYR:O	10:J:440:LEU:HD23	2.18	0.44
12:L:200:LYS:O	12:L:201:LYS:HB2	2.18	0.44
15:P:216:ARG:NH1	46:9:257:PRO:HG3	2.33	0.44
18:S:12:PRO:O	18:S:26:GLU:HA	2.17	0.44
19:T:195:LYS:HZ3	19:T:490:ARG:HH21	1.64	0.44
19:T:467:ALA:HB3	19:T:480:ALA:HB3	2.00	0.44
22:W:314:LYS:HA	22:W:326:ARG:O	2.17	0.44
23:X:482:ARG:NH2	23:X:914:VAL:HG12	2.33	0.44
23:X:581:ILE:HG21	23:X:736:ARG:NH1	2.33	0.44
23:X:764:VAL:HG11	23:X:792:ALA:HB1	1.99	0.44
24:Y:8:THR:CG2	24:Y:155:ARG:HB2	2.47	0.44
24:Y:27:ASN:HD21	24:Y:65:SER:HA	1.83	0.44
24:Y:37:TYR:CE1	24:Y:106:SER:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:184:CYS:HG	27:3:211:TYR:HE1	1.66	0.44
46:9:300:THR:O	46:9:304:CYS:HB2	2.18	0.44
1:A:983:LYS:HE2	1:A:983:LYS:HB2	1.53	0.43
1:A:1050:LEU:HA	1:A:1050:LEU:HD23	1.80	0.43
1:A:2310:ARG:HE	1:A:2314:PHE:HE1	1.66	0.43
2:B:61:A:H2'	2:B:62:G:O4'	2.18	0.43
3:C:848:THR:O	3:C:852:ARG:HG3	2.18	0.43
3:C:909:GLY:HA3	3:C:930:ALA:HB3	1.99	0.43
5:E:328:GLY:O	5:E:346:SER:OG	2.36	0.43
14:O:171:GLY:O	22:W:207:LYS:HA	2.18	0.43
17:R:376:LYS:HE3	17:R:376:LYS:HB3	1.75	0.43
19:T:498:GLU:H	19:T:498:GLU:HG3	1.42	0.43
21:V:497:CYS:HG	21:V:503:TYR:HE2	1.63	0.43
21:V:609:GLN:N	21:V:610:PRO:HD2	2.33	0.43
23:X:269:GLU:HA	23:X:272:TYR:HB3	2.00	0.43
23:X:808:LEU:HD21	23:X:813:ARG:HA	2.00	0.43
23:X:921:LEU:O	23:X:925:VAL:HG22	2.17	0.43
23:X:950:HIS:CG	23:X:986:TYR:CE2	3.06	0.43
24:Y:44:ASN:HD22	24:Y:52:GLN:HB3	1.82	0.43
26:1:532:PHE:HD2	26:1:570:TYR:CD2	2.35	0.43
26:1:645:LEU:HD13	26:1:682:HIS:CD2	2.52	0.43
26:1:694:LEU:HD13	26:1:727:VAL:HG21	2.00	0.43
26:1:770:MET:HE3	26:1:770:MET:HB2	1.72	0.43
26:1:893:ILE:HD13	26:1:893:ILE:HA	1.68	0.43
26:1:1185:ARG:HE	26:1:1185:ARG:HB2	1.43	0.43
27:3:125:PRO:HG2	27:3:174:ASP:HA	1.98	0.43
27:3:526:HIS:HB2	27:3:574:LEU:CD2	2.48	0.43
27:3:993:ILE:HG23	27:3:1002:VAL:HG23	1.99	0.43
46:9:315:TYR:CZ	46:9:335:PRO:HG2	2.52	0.43
1:A:694:LEU:HD22	1:A:709:ILE:HD12	2.00	0.43
1:A:748:ASP:OD1	15:P:214:THR:HB	2.19	0.43
1:A:1224:ARG:HG3	1:A:1224:ARG:NH1	2.33	0.43
1:A:1276:GLU:OE1	1:A:1375:TRP:N	2.37	0.43
1:A:1623:ASN:HD22	1:A:1623:ASN:C	2.19	0.43
1:A:1853:PRO:HD2	1:A:1856:GLU:OE2	2.17	0.43
1:A:1991:TYR:CD2	1:A:2010:ILE:HG12	2.53	0.43
1:A:2144:CYS:HA	1:A:2270:PHE:O	2.19	0.43
2:B:63:A:C2	2:B:64:G:C5	3.06	0.43
3:C:243:ILE:HG13	3:C:244:LYS:N	2.32	0.43
3:C:471:ASP:O	3:C:499:GLY:HA2	2.18	0.43
3:C:745:LEU:HB2	3:C:770:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:67:GLY:C	5:E:349:LYS:HG2	2.39	0.43
5:E:145:LYS:HD2	5:E:184:LYS:HE2	1.98	0.43
6:F:36:A:N6	6:F:38:G:C6	2.86	0.43
7:G:6:A:C4	7:G:7:G:C8	3.06	0.43
16:Q:1226:ILE:N	16:Q:1256:LYS:O	2.51	0.43
21:V:451:ASN:OD1	21:V:452:LEU:N	2.51	0.43
21:V:537:HIS:CE1	21:V:538:ARG:HE	2.36	0.43
23:X:416:GLN:NE2	23:X:544:PRO:HA	2.32	0.43
23:X:482:ARG:HH21	23:X:914:VAL:HG12	1.83	0.43
23:X:591:TYR:CD2	23:X:692:PRO:HB2	2.50	0.43
23:X:697:GLN:HB2	23:X:712:THR:HG21	1.99	0.43
23:X:849:VAL:O	23:X:851:ASN:N	2.51	0.43
24:Y:26:LEU:HB3	24:Y:166:PHE:CD1	2.53	0.43
24:Y:47:ARG:NH2	24:Y:141:GLU:O	2.51	0.43
26:1:666:LYS:HB3	26:1:704:ILE:CD1	2.48	0.43
26:1:685:SER:O	26:1:689:ILE:HG12	2.17	0.43
26:1:806:ILE:HA	26:1:810:ILE:HD12	2.00	0.43
26:1:969:LYS:HD2	26:1:969:LYS:H	1.83	0.43
27:3:705:ARG:NH2	27:3:746:ALA:HB2	2.34	0.43
30:2:465:LEU:HB3	30:2:475:VAL:HG11	2.01	0.43
46:9:321:PHE:HB2	46:9:426:ILE:HB	2.00	0.43
46:9:370:ASN:ND2	46:9:372:GLY:O	2.45	0.43
1:A:75:ASP:OD1	1:A:75:ASP:N	2.52	0.43
1:A:408:PRO:C	1:A:410:PRO:HD2	2.38	0.43
1:A:1012:LYS:O	1:A:1012:LYS:HG3	2.19	0.43
1:A:1375:TRP:O	1:A:1377:SER:N	2.51	0.43
1:A:1725:LEU:HD12	1:A:1725:LEU:HA	1.75	0.43
1:A:1769:GLY:HA2	1:A:1772:PHE:CE1	2.53	0.43
1:A:1998:ASN:HB3	1:A:2001:SER:HB3	2.00	0.43
1:A:2004:GLN:CD	1:A:2004:GLN:H	2.21	0.43
47:A:3000:IHP:O31	47:A:3000:IHP:P6	2.76	0.43
5:E:84:ALA:HB2	5:E:90:ILE:HG12	1.99	0.43
5:E:150:HIS:CE1	5:E:177:LYS:HD2	2.53	0.43
5:E:156:SER:OG	5:E:197:LEU:O	2.33	0.43
5:E:316:SER:O	5:E:317:ARG:HG3	2.18	0.43
6:F:96:U:OP1	10:J:384:ARG:NH2	2.51	0.43
8:H:10:C:H2'	8:H:11:G:C8	2.52	0.43
8:H:114:A:H2'	8:H:115:G:C8	2.53	0.43
10:J:372:VAL:HG12	10:J:373:HIS:CE1	2.53	0.43
13:N:15:TRP:CZ3	13:N:22:LEU:HD12	2.38	0.43
16:Q:569:PRO:HA	16:Q:587:VAL:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:22:ASN:ND2	21:V:470:GLU:OE2	2.43	0.43
23:X:972:PRO:HA	23:X:977:PHE:CD2	2.52	0.43
24:Y:21:ARG:O	24:Y:25:CYS:HB2	2.18	0.43
24:Y:177:ARG:HG2	24:Y:178:SER:H	1.83	0.43
24:Y:223:LEU:O	24:Y:226:MET:HB3	2.18	0.43
26:1:830:TYR:HA	26:1:867:MET:SD	2.57	0.43
26:1:963:LYS:HG3	26:1:964:THR:N	2.33	0.43
26:1:1053:ARG:NH1	30:2:559:PRO:O	2.52	0.43
27:3:514:ASP:OD1	27:3:514:ASP:N	2.52	0.43
27:3:696:SER:O	27:3:696:SER:OG	2.32	0.43
30:2:451:LYS:O	30:2:454:LEU:HG	2.19	0.43
1:A:371:LEU:HD12	1:A:371:LEU:HA	1.81	0.43
1:A:1593:LEU:HD23	1:A:1593:LEU:HA	1.55	0.43
1:A:1726:ILE:O	1:A:1727:GLN:C	2.54	0.43
1:A:1781:ASP:HB2	1:A:1808:PHE:HB3	1.99	0.43
1:A:1839:TRP:CE3	1:A:1871:PRO:HB3	2.53	0.43
1:A:1893:PHE:O	1:A:1896:CYS:HB2	2.17	0.43
3:C:259:LYS:H	3:C:311:SER:HA	1.83	0.43
3:C:502:HIS:CE1	3:C:543:ARG:NH1	2.86	0.43
3:C:724:TRP:HA	3:C:724:TRP:HE3	1.80	0.43
3:C:914:LYS:HD2	3:C:931:ARG:NH2	2.33	0.43
4:D:1189:HIS:O	4:D:1200:VAL:HA	2.18	0.43
5:E:176:VAL:HG21	5:E:220:TRP:HE1	1.83	0.43
7:G:90:C:H2'	7:G:91:A:C8	2.53	0.43
9:I:140:LEU:N	9:I:141:PRO:HD3	2.34	0.43
10:J:242:ILE:HA	10:J:245:TRP:HD1	1.83	0.43
10:J:291:GLN:HB3	10:J:294:HIS:ND1	2.33	0.43
19:T:288:LEU:O	19:T:289:SER:OG	2.31	0.43
19:T:473:SER:OG	19:T:475:SER:HB3	2.18	0.43
23:X:269:GLU:HA	23:X:269:GLU:OE2	2.19	0.43
23:X:792:ALA:O	23:X:796:LEU:HG	2.19	0.43
23:X:877:ASP:O	23:X:880:VAL:HB	2.19	0.43
24:Y:208:VAL:O	24:Y:212:LYS:HG3	2.18	0.43
26:1:997:LEU:HD23	26:1:997:LEU:HA	1.84	0.43
27:3:101:LYS:HB2	27:3:101:LYS:HE3	1.65	0.43
27:3:373:PHE:HD1	27:3:385:PHE:CD2	2.36	0.43
27:3:595:VAL:HG21	27:3:600:GLN:C	2.39	0.43
30:2:483:GLN:OE1	30:2:483:GLN:N	2.51	0.43
1:A:131:GLU:HG3	1:A:132:ILE:N	2.33	0.43
1:A:785:LYS:HE3	1:A:785:LYS:HB3	1.56	0.43
3:C:530:LEU:HD23	3:C:530:LEU:HA	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:643:ASP:N	3:C:643:ASP:OD1	2.52	0.43
3:C:745:LEU:HD22	3:C:770:PHE:HB2	1.99	0.43
3:C:766:ILE:HD12	3:C:766:ILE:HA	1.87	0.43
3:C:909:GLY:HA3	3:C:930:ALA:H	1.83	0.43
5:E:145:LYS:CD	5:E:184:LYS:HE2	2.49	0.43
5:E:154:VAL:HG13	5:E:171:SER:HB3	2.00	0.43
5:E:326:HIS:NE2	5:E:344:SER:OG	2.26	0.43
8:H:7:U:H2'	8:H:8:C:O4'	2.18	0.43
12:L:225:TYR:O	17:R:85:ALA:HB2	2.19	0.43
15:P:74:LYS:O	15:P:77:ASP:HB3	2.18	0.43
19:T:346:ILE:HD13	19:T:380:LEU:HD21	1.99	0.43
23:X:737:LEU:O	23:X:737:LEU:HD23	2.17	0.43
24:Y:275:TRP:CG	24:Y:276:LYS:N	2.86	0.43
26:1:508:THR:HB	26:1:510:PRO:CD	2.46	0.43
26:1:551:LEU:O	26:1:555:VAL:HG23	2.18	0.43
26:1:889:GLU:OE2	26:1:928:TYR:OH	2.31	0.43
26:1:1158:ILE:HG13	26:1:1159:GLY:N	2.32	0.43
27:3:234:PHE:CD1	27:3:235:LEU:N	2.86	0.43
27:3:278:LEU:HD21	27:3:816:LYS:HZ3	1.83	0.43
27:3:549:VAL:HG12	27:3:550:ASN:O	2.18	0.43
27:3:604:PHE:CZ	27:3:681:PRO:HD3	2.53	0.43
27:3:715:MET:HE3	27:3:739:LEU:H	1.84	0.43
27:3:1117:LEU:HD12	27:3:1117:LEU:HA	1.60	0.43
1:A:101:LYS:HD3	1:A:101:LYS:HA	1.65	0.43
1:A:888:GLN:C	1:A:889:ARG:HG2	2.39	0.43
1:A:1636:LYS:HG3	1:A:1658:GLN:HE21	1.84	0.43
1:A:2107:PRO:O	1:A:2110:VAL:HG22	2.18	0.43
3:C:366:GLN:HB2	3:C:370:VAL:HB	2.00	0.43
3:C:721:LYS:HB2	3:C:722:TYR:CE2	2.54	0.43
3:C:839:PRO:HG2	3:C:894:GLN:HB3	1.99	0.43
5:E:202:ASN:OD1	5:E:207:GLN:N	2.38	0.43
6:F:24:A:P	13:N:111:THR:HG1	2.42	0.43
7:G:21:A:H4'	7:G:22:C:OP1	2.18	0.43
7:G:100:C:H3'	7:G:100:C:OP2	2.19	0.43
19:T:462:GLU:O	19:T:483:ASP:HB3	2.18	0.43
21:V:497:CYS:HB2	21:V:507:PHE:HB2	1.99	0.43
21:V:563:SER:O	21:V:565:LEU:N	2.52	0.43
23:X:327:ARG:HH12	23:X:328:ARG:NH2	2.17	0.43
23:X:390:GLU:O	23:X:393:GLN:HG3	2.18	0.43
23:X:412:ILE:HB	23:X:418:LEU:HD23	2.01	0.43
23:X:516:VAL:HG22	23:X:547:LYS:CB	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:647:ILE:HA	23:X:651:LEU:HD21	2.01	0.43
26:1:668:VAL:HG22	26:1:686:LEU:HD23	1.99	0.43
27:3:182:PHE:O	27:3:210:PHE:HA	2.19	0.43
27:3:925:VAL:O	27:3:942:LYS:HA	2.18	0.43
30:2:707:PRO:HG2	30:2:710:GLU:HG2	2.00	0.43
33:5:63:ARG:HD3	33:5:63:ARG:HA	1.77	0.43
1:A:71:ARG:HG3	1:A:71:ARG:HH11	1.83	0.43
1:A:384:VAL:HA	3:C:331:PHE:CD2	2.54	0.43
1:A:1189:MET:CG	1:A:1190:CYS:N	2.80	0.43
1:A:1777:ILE:HA	1:A:1860:GLN:O	2.18	0.43
1:A:1781:ASP:OD2	1:A:1893:PHE:HB2	2.18	0.43
3:C:226:VAL:HG13	3:C:254:THR:HG22	2.00	0.43
3:C:632:THR:H	3:C:636:TYR:HD2	1.66	0.43
5:E:125:PHE:CD1	5:E:159:PRO:HG3	2.54	0.43
5:E:175:THR:HB	5:E:189:THR:CG2	2.49	0.43
6:F:24:A:OP2	13:N:111:THR:OG1	2.35	0.43
7:G:6:A:C6	7:G:7:G:C6	3.06	0.43
7:G:90:C:N4	8:H:40:C:H42	2.16	0.43
7:G:104:C:O2	7:G:104:C:H2'	2.18	0.43
10:J:241:VAL:O	10:J:244:ASN:ND2	2.51	0.43
10:J:363:ARG:HB2	10:J:382:TYR:OH	2.18	0.43
13:N:91:LYS:HD3	13:N:91:LYS:HA	1.72	0.43
23:X:529:THR:O	23:X:532:LEU:HG	2.19	0.43
23:X:845:ALA:CB	23:X:915:ARG:HB2	2.46	0.43
24:Y:21:ARG:HH22	24:Y:82:LYS:C	2.21	0.43
27:3:123:VAL:HG22	27:3:124:ASP:H	1.84	0.43
27:3:329:TYR:HB3	27:3:370:GLU:CD	2.39	0.43
27:3:488:GLY:C	27:3:490:THR:H	2.20	0.43
27:3:499:PHE:CZ	27:3:516:LEU:HD22	2.46	0.43
27:3:924:PHE:HA	27:3:943:THR:O	2.18	0.43
46:9:404:PHE:O	46:9:407:LEU:HD23	2.19	0.43
46:9:405:ASP:OD1	46:9:405:ASP:N	2.38	0.43
1:A:709:ILE:HG12	17:R:247:ILE:HD12	2.00	0.43
1:A:1210:LYS:HE2	1:A:1210:LYS:HB2	1.75	0.43
1:A:1391:LEU:HD23	1:A:1391:LEU:HA	1.73	0.43
1:A:1585:ILE:O	1:A:1589:ILE:HD12	2.18	0.43
1:A:1719:PHE:C	1:A:1719:PHE:HD1	2.22	0.43
3:C:69:ALA:O	3:C:72:VAL:N	2.45	0.43
3:C:453:TYR:HB3	3:C:456:GLY:H	1.83	0.43
3:C:757:ALA:O	3:C:761:SER:HB2	2.18	0.43
3:C:833:PHE:CZ	3:C:872:LYS:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:319:MET:HG3	10:J:320:GLU:N	2.33	0.43
13:N:56:LYS:HD2	13:N:83:TYR:HB3	2.01	0.43
21:V:571:SER:HA	21:V:623:ASN:HB3	2.01	0.43
23:X:733:LYS:HB3	23:X:735:PHE:HE2	1.84	0.43
23:X:765:LEU:CD1	23:X:816:ALA:HB2	2.44	0.43
26:1:630:ARG:O	26:1:634:VAL:HG23	2.19	0.43
26:1:936:VAL:HG12	26:1:937:LEU:HD12	2.01	0.43
27:3:462:VAL:HG11	27:3:516:LEU:HD23	2.00	0.43
27:3:543:THR:C	27:3:558:LEU:HD12	2.38	0.43
27:3:590:MET:HB2	27:3:606:ALA:O	2.18	0.43
30:2:472:PRO:O	30:2:475:VAL:HG23	2.19	0.43
30:2:529:LYS:HB2	30:2:529:LYS:HE2	1.61	0.43
32:7:74:GLU:O	32:7:78:GLN:HG3	2.18	0.43
1:A:67:ARG:HE	1:A:67:ARG:HB2	1.46	0.43
1:A:1768:TYR:CA	1:A:1771:LEU:HB3	2.31	0.43
1:A:2142:ILE:HG23	1:A:2175:LEU:HD13	2.01	0.43
3:C:137:HIS:CD2	3:C:238:ASN:HB2	2.54	0.43
3:C:463:GLU:HA	3:C:466:SER:HB3	2.01	0.43
3:C:493:PHE:HB2	3:C:551:LEU:HD23	2.01	0.43
3:C:710:ASN:OD1	3:C:713:LYS:HG3	2.19	0.43
7:G:86:A:H2	8:H:44:U:O2	2.02	0.43
10:J:397:LYS:O	10:J:401:ARG:HD3	2.19	0.43
11:K:232:ILE:O	11:K:236:LEU:HG	2.18	0.43
23:X:974:SER:HB3	23:X:977:PHE:HB2	2.00	0.43
23:X:1004:GLU:HG3	23:X:1007:TRP:CZ2	2.54	0.43
26:1:666:LYS:O	26:1:670:GLN:HG2	2.19	0.43
26:1:1108:ASN:N	26:1:1108:ASN:OD1	2.51	0.43
26:1:1273:TYR:O	26:1:1277:GLN:HB3	2.19	0.43
27:3:16:PHE:HE2	27:3:63:ARG:C	2.22	0.43
27:3:316:GLU:O	27:3:323:THR:OG1	2.29	0.43
27:3:528:ARG:HG3	27:3:529:ALA:H	1.83	0.43
27:3:898:ASN:OD1	27:3:899:THR:N	2.52	0.43
27:3:1156:CYS:O	27:3:1158:ARG:N	2.50	0.43
1:A:407:ALA:HB1	1:A:411:PHE:HB2	2.01	0.43
1:A:690:MET:SD	1:A:706:ALA:HB1	2.59	0.43
1:A:864:LEU:HD12	1:A:864:LEU:HA	1.52	0.43
1:A:1806:ALA:HA	1:A:1821:ILE:HA	2.01	0.43
1:A:2178:ILE:HG13	1:A:2214:ILE:HB	2.00	0.43
2:B:40:U:H5'	2:B:41:U:OP2	2.19	0.43
3:C:298:LEU:O	3:C:299:ILE:HD13	2.19	0.43
3:C:664:GLU:HG3	3:C:784:ILE:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1271:VAL:HA	4:D:1279:GLU:HA	2.00	0.43
5:E:207:GLN:HB3	5:E:219:VAL:HG12	2.01	0.43
5:E:251:LEU:HB2	5:E:293:TRP:CE2	2.54	0.43
7:G:13:C:H2'	7:G:14:A:O4'	2.19	0.43
8:H:118:G:C6	8:H:140:A:N6	2.87	0.43
14:O:155:PRO:N	17:R:188:PHE:HE1	2.16	0.43
15:P:69:ALA:HA	15:P:72:ARG:NH1	2.34	0.43
23:X:164:TRP:CE3	23:X:165:GLU:HA	2.53	0.43
23:X:235:LEU:HD22	24:Y:220:GLN:CG	2.49	0.43
27:3:58:VAL:HG21	27:3:62:ILE:CD1	2.49	0.43
27:3:436:ARG:HG2	27:3:778:ALA:CB	2.49	0.43
27:3:483:LEU:HD11	27:3:493:GLU:OE2	2.19	0.43
27:3:638:GLU:O	27:3:638:GLU:HG3	2.19	0.43
27:3:641:CYS:H	27:3:701:LEU:HD23	1.83	0.43
27:3:791:HIS:NE2	27:3:793:GLU:HB2	2.34	0.43
27:3:1158:ARG:HG3	27:3:1159:ASP:N	2.34	0.43
27:3:1183:ASN:OD1	27:3:1183:ASN:N	2.51	0.43
32:7:58:CYS:N	32:7:63:GLY:O	2.52	0.43
33:5:11:LEU:O	33:5:14:LEU:HB2	2.19	0.43
33:5:20:GLY:HA2	33:5:34:ASN:ND2	2.33	0.43
1:A:298:ASP:O	1:A:302:ILE:HG12	2.19	0.42
1:A:456:LEU:O	1:A:460:LYS:HG2	2.18	0.42
1:A:858:GLN:HA	1:A:861:ARG:NH1	2.34	0.42
1:A:1784:ASN:CG	1:A:1897:LEU:HD11	2.39	0.42
2:B:67:A:H2'	2:B:68:C:O4'	2.19	0.42
3:C:474:LEU:HA	3:C:498:SER:O	2.19	0.42
4:D:1590:LEU:HA	4:D:1640:ALA:O	2.19	0.42
5:E:171:SER:O	5:E:196:VAL:N	2.44	0.42
7:G:11:A:H2'	7:G:12:G:O4'	2.19	0.42
7:G:90:C:H2'	7:G:91:A:C4	2.54	0.42
8:H:8:C:H2'	8:H:9:U:C6	2.54	0.42
8:H:152:G:C6	8:H:153:A:N6	2.87	0.42
8:H:162:U:H4'	8:H:163:G:O4'	2.18	0.42
17:R:122:LYS:HE2	19:T:399:LYS:NZ	2.34	0.42
19:T:423:SER:N	19:T:474:GLU:OE2	2.52	0.42
23:X:482:ARG:HE	23:X:483:PHE:HE2	1.65	0.42
26:1:823:MET:SD	26:1:829:ASN:ND2	2.92	0.42
27:3:169:HIS:HD2	27:3:170:VAL:O	2.02	0.42
27:3:199:GLU:OE2	27:3:199:GLU:HA	2.19	0.42
27:3:595:VAL:HG21	27:3:601:ARG:N	2.34	0.42
27:3:779:PHE:N	27:3:779:PHE:CD1	2.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:9:351:LYS:H	46:9:351:LYS:HG2	1.68	0.42
1:A:366:LYS:HG3	21:V:324:HIS:O	2.18	0.42
1:A:2250:GLY:O	1:A:2255:HIS:HE1	2.02	0.42
3:C:481:MET:HB3	3:C:490:PHE:CD2	2.55	0.42
3:C:529:ARG:O	3:C:530:LEU:HD23	2.19	0.42
3:C:604:LEU:HD21	3:C:627:HIS:CE1	2.53	0.42
3:C:692:LEU:CD2	3:C:788:LYS:HB2	2.50	0.42
3:C:834:VAL:HG22	3:C:899:SER:HB2	2.01	0.42
3:C:852:ARG:HD2	7:G:-12:C:O5'	2.19	0.42
4:D:444:GLU:HA	4:D:690:VAL:HA	2.02	0.42
4:D:735:ALA:C	4:D:737:ALA:H	2.22	0.42
4:D:784:ILE:HA	4:D:810:VAL:O	2.19	0.42
5:E:325:GLY:O	5:E:352:TYR:OH	2.34	0.42
6:F:21:U:H3	13:N:125:LYS:HG2	1.84	0.42
6:F:36:A:C8	6:F:36:A:O5'	2.72	0.42
8:H:43:U:HO2'	8:H:44:U:P	2.38	0.42
9:I:139:ALA:C	9:I:141:PRO:HD3	2.40	0.42
9:I:448:ASN:O	9:I:452:ALA:HB3	2.18	0.42
17:R:407:TYR:HE2	17:R:412:PHE:HZ	1.66	0.42
23:X:238:ARG:HH12	24:Y:319:VAL:HG23	1.83	0.42
23:X:527:LEU:HD21	23:X:755:ILE:HA	2.01	0.42
23:X:959:TYR:OH	23:X:980:GLN:O	2.37	0.42
24:Y:96:MET:HE1	24:Y:105:GLY:O	2.19	0.42
26:1:493:LYS:O	26:1:496:LYS:N	2.52	0.42
26:1:722:GLU:OE1	26:1:722:GLU:N	2.38	0.42
26:1:1199:VAL:HG12	26:1:1199:VAL:O	2.19	0.42
26:1:1227:ILE:O	26:1:1231:MET:HG2	2.19	0.42
27:3:131:MET:HB2	27:3:141:VAL:HG22	2.01	0.42
27:3:690:ARG:HH12	27:3:696:SER:H	1.67	0.42
1:A:147:MET:O	1:A:151:MET:HG2	2.19	0.42
1:A:206:TRP:HA	1:A:209:ASP:OD2	2.19	0.42
1:A:468:LYS:HA	1:A:468:LYS:HD3	1.53	0.42
1:A:875:HIS:CE1	23:X:866:ASN:CB	3.01	0.42
1:A:1198:PRO:HG2	1:A:1201:ARG:HB2	2.00	0.42
1:A:1268:ILE:HD11	17:R:432:VAL:HG13	2.01	0.42
1:A:1384:ARG:NH1	1:A:1384:ARG:HB2	2.35	0.42
1:A:1424:GLN:O	1:A:1427:ARG:NH2	2.45	0.42
1:A:1600:GLU:OE1	1:A:1604:LEU:HG	2.19	0.42
1:A:1832:ARG:O	1:A:1836:LEU:HD13	2.20	0.42
1:A:1840:LYS:O	1:A:1844:GLU:HG2	2.18	0.42
1:A:1935:ARG:HA	1:A:1938:LEU:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2122:ALA:O	1:A:2124:ILE:HG23	2.19	0.42
1:A:2229:LYS:O	1:A:2257:GLU:HG3	2.19	0.42
3:C:125:ASN:CG	3:C:127:GLU:H	2.23	0.42
3:C:336:TYR:CE1	3:C:337:GLN:HG2	2.54	0.42
3:C:351:PRO:O	3:C:354:ARG:HD3	2.19	0.42
3:C:508:LYS:O	3:C:566:THR:HG22	2.19	0.42
3:C:830:PRO:HA	3:C:904:TRP:HA	2.00	0.42
6:F:6:C:O2'	6:F:7:G:OP1	2.34	0.42
10:J:416:TYR:CE2	10:J:443:ILE:HD13	2.52	0.42
13:N:86:LYS:HG3	13:N:87:ASN:N	2.33	0.42
15:P:68:ARG:HB3	15:P:68:ARG:NH1	2.33	0.42
19:T:300:ILE:H	19:T:300:ILE:HG13	1.65	0.42
21:V:556:TYR:CE1	21:V:557:THR:HG23	2.54	0.42
22:W:109:ASN:H	22:W:114:TYR:HA	1.84	0.42
23:X:408:LEU:HD13	23:X:570:PHE:CD2	2.55	0.42
23:X:428:LYS:H	23:X:428:LYS:HG3	1.58	0.42
23:X:546:LEU:HD12	23:X:546:LEU:HA	1.87	0.42
24:Y:249:PRO:HA	24:Y:280:SER:HB2	2.01	0.42
24:Y:290:LYS:HB2	24:Y:293:ASP:OD2	2.19	0.42
26:1:548:GLU:O	26:1:552:LEU:HG	2.19	0.42
26:1:551:LEU:O	26:1:554:LYS:HB3	2.19	0.42
26:1:1212:LEU:HD12	26:1:1212:LEU:HA	1.75	0.42
26:1:1295:TYR:HH	33:5:29:TRP:HD1	1.67	0.42
27:3:311:PHE:HZ	27:3:387:PHE:CE2	2.38	0.42
30:2:534:GLN:HG2	30:2:538:GLU:OE1	2.18	0.42
1:A:113:ILE:HG23	1:A:488:ASP:OD1	2.19	0.42
1:A:940:ILE:HD13	1:A:1090:ARG:NH1	2.34	0.42
1:A:1014:ASN:ND2	1:A:1014:ASN:C	2.73	0.42
2:B:46:U:C2'	2:B:47:A:H5'	2.49	0.42
3:C:263:LEU:HA	3:C:267:LEU:HB2	1.99	0.42
3:C:561:LYS:H	3:C:561:LYS:HG2	1.48	0.42
3:C:716:GLU:HG3	3:C:716:GLU:H	1.72	0.42
3:C:767:VAL:O	3:C:771:GLN:HG3	2.19	0.42
5:E:124:LEU:HD21	5:E:138:SER:HB3	2.01	0.42
5:E:177:LYS:HB3	5:E:179:TRP:HE1	1.83	0.42
5:E:258:THR:HG23	5:E:278:GLN:HE22	1.84	0.42
6:F:39:A:C4	6:F:40:U:C6	3.07	0.42
10:J:396:ARG:NH2	10:J:426:GLN:HG3	2.35	0.42
11:K:198:GLN:NE2	11:K:198:GLN:HA	2.34	0.42
17:R:365:HIS:O	17:R:369:LEU:HD13	2.20	0.42
17:R:404:GLU:HG3	17:R:405:VAL:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:330:GLU:O	23:X:334:LEU:HD12	2.19	0.42
23:X:430:THR:O	23:X:434:GLN:HG3	2.19	0.42
23:X:577:PHE:HB2	23:X:727:GLY:O	2.19	0.42
26:1:592:GLU:O	26:1:596:ILE:HG23	2.18	0.42
26:1:632:PHE:HA	26:1:635:VAL:HG22	2.02	0.42
26:1:1254:LEU:O	26:1:1262:ARG:HG2	2.19	0.42
27:3:192:ALA:HA	27:3:200:ALA:HB3	2.01	0.42
27:3:234:PHE:HE1	27:3:236:ILE:HG12	1.81	0.42
27:3:405:SER:HA	27:3:406:PRO:HA	1.90	0.42
33:5:61:LYS:HB3	33:5:65:ARG:HH22	1.84	0.42
46:9:299:LEU:H	46:9:299:LEU:HD23	1.85	0.42
1:A:356:ILE:H	1:A:356:ILE:HG13	1.19	0.42
1:A:1298:ARG:O	1:A:1298:ARG:HG3	2.20	0.42
1:A:1495:PHE:HD1	1:A:1495:PHE:HA	1.74	0.42
1:A:2295:GLU:N	1:A:2295:GLU:OE2	2.52	0.42
1:A:2312:SER:O	1:A:2316:ASN:HB2	2.19	0.42
3:C:680:ASN:O	3:C:682:LYS:N	2.53	0.42
3:C:846:VAL:HG11	3:C:871:ILE:HD12	1.99	0.42
6:F:43:A:C2	7:G:5:G:C6	3.07	0.42
6:F:83:A:C5	6:F:84:A:C6	3.08	0.42
16:Q:1227:LEU:HA	16:Q:1258:THR:O	2.20	0.42
17:R:392:ILE:HD13	23:X:660:PHE:CE2	2.54	0.42
19:T:393:ASP:OD2	19:T:393:ASP:N	2.53	0.42
22:W:532:LEU:CB	22:W:548:ALA:HB2	2.49	0.42
23:X:238:ARG:HH22	24:Y:230:LEU:HG	1.83	0.42
23:X:815:MET:HG3	23:X:825:SER:CB	2.41	0.42
24:Y:195:GLU:H	24:Y:195:GLU:HG3	1.43	0.42
26:1:606:LEU:HA	26:1:606:LEU:HD12	1.76	0.42
26:1:933:CYS:O	26:1:934:GLY:C	2.58	0.42
26:1:1266:TRP:CE3	33:5:22:GLY:HA3	2.54	0.42
27:3:665:LEU:HB2	27:3:679:LEU:HD23	2.00	0.42
27:3:789:VAL:HG13	27:3:891:VAL:HG13	2.00	0.42
27:3:896:PHE:H	27:3:896:PHE:HD2	1.68	0.42
30:2:451:LYS:HA	30:2:454:LEU:HD23	2.02	0.42
30:2:526:ASP:HA	30:2:529:LYS:NZ	2.34	0.42
46:9:408:THR:O	46:9:411:GLU:HB3	2.20	0.42
1:A:71:ARG:HG3	1:A:71:ARG:NH1	2.35	0.42
1:A:166:PHE:CE2	1:A:580:TYR:HD2	2.38	0.42
1:A:235:MET:HB3	1:A:404:LEU:HD11	2.01	0.42
1:A:1215:ASN:HB3	1:A:1224:ARG:NH1	2.34	0.42
1:A:1784:ASN:ND2	1:A:1894:GLN:HB2	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1833:LEU:H	1:A:1833:LEU:HG	1.69	0.42
1:A:1975:GLU:O	1:A:1979:VAL:HG22	2.19	0.42
1:A:1990:ASP:HA	1:A:1993:LYS:HD3	2.00	0.42
1:A:2070:LYS:HG3	1:A:2071:THR:N	2.34	0.42
1:A:2121:ARG:HA	1:A:2121:ARG:HD2	1.79	0.42
1:A:2187:GLN:HB2	1:A:2256:TYR:CZ	2.55	0.42
3:C:78:GLU:HG3	3:C:79:THR:H	1.83	0.42
3:C:598:SER:OG	3:C:599:GLU:HG2	2.20	0.42
3:C:852:ARG:HD2	7:G:-12:C:C5'	2.49	0.42
5:E:215:ASN:HB2	5:E:232:ARG:NH1	2.34	0.42
5:E:244:SER:HB2	5:E:293:TRP:CD2	2.54	0.42
6:F:88:G:H2'	6:F:89:U:C5'	2.50	0.42
8:H:27:U:O2'	8:H:28:C:H5'	2.20	0.42
8:H:35:A:H3'	8:H:36:G:H8	1.83	0.42
9:I:48:ALA:O	9:I:51:PRO:HD2	2.20	0.42
10:J:329:ALA:O	10:J:332:VAL:HG22	2.19	0.42
23:X:477:VAL:HG22	23:X:493:LEU:HB2	2.02	0.42
24:Y:12:VAL:HG13	24:Y:131:GLU:O	2.20	0.42
24:Y:290:LYS:HB2	24:Y:293:ASP:CG	2.40	0.42
26:1:962:MET:O	26:1:967:GLU:HB2	2.18	0.42
26:1:1027:ARG:HD3	26:1:1027:ARG:HA	1.82	0.42
26:1:1109:ARG:O	26:1:1112:THR:HG23	2.20	0.42
27:3:212:GLU:HG2	27:3:213:LEU:N	2.35	0.42
27:3:576:GLU:OE1	27:3:580:ARG:NH2	2.52	0.42
27:3:671:ASN:HB3	27:3:696:SER:HA	2.01	0.42
27:3:996:ILE:O	27:3:998:HIS:N	2.53	0.42
27:3:1191:LYS:O	27:3:1192:ASN:C	2.57	0.42
30:2:547:LYS:NZ	30:2:555:GLU:HG2	2.35	0.42
1:A:196:ASP:N	1:A:200:ASP:OD2	2.50	0.42
1:A:344:ASP:HB2	1:A:345:PRO:HD2	2.01	0.42
1:A:549:GLU:CB	1:A:591:MET:HG3	2.50	0.42
1:A:1200:CYS:SG	1:A:1201:ARG:N	2.92	0.42
1:A:2114:PHE:HE1	1:A:2178:ILE:HG23	1.84	0.42
3:C:481:MET:CE	3:C:612:LYS:HB3	2.50	0.42
3:C:660:VAL:HG22	3:C:661:THR:O	2.20	0.42
3:C:860:ASP:N	3:C:860:ASP:OD1	2.53	0.42
4:D:1200:VAL:N	4:D:1254:PHE:O	2.45	0.42
5:E:343:ILE:HD11	5:E:351:LEU:HD13	2.01	0.42
10:J:292:VAL:HG12	10:J:296:ARG:NE	2.35	0.42
10:J:317:THR:O	10:J:320:GLU:N	2.52	0.42
11:K:228:HIS:HD2	11:K:230:TRP:CE2	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:169:ARG:O	12:L:172:ARG:N	2.48	0.42
21:V:542:ASN:HA	21:V:545:ARG:NH2	2.34	0.42
21:V:543:LYS:O	21:V:547:VAL:HG23	2.20	0.42
21:V:585:ILE:H	21:V:585:ILE:HG13	1.71	0.42
23:X:741:TRP:NE1	26:1:781:ASP:HA	2.34	0.42
23:X:743:TYR:CD1	23:X:744:GLN:HG3	2.55	0.42
23:X:976:LEU:HD11	23:X:1001:LEU:HA	2.01	0.42
24:Y:4:LEU:HD11	24:Y:11:ASP:HB3	2.01	0.42
24:Y:194:ASP:N	24:Y:194:ASP:OD2	2.53	0.42
26:1:1106:ARG:H	26:1:1109:ARG:HG3	1.83	0.42
27:3:164:ASN:ND2	27:3:190:GLU:HG2	2.35	0.42
27:3:1022:ILE:HD13	27:3:1022:ILE:HA	1.77	0.42
27:3:1175:ASP:OD1	27:3:1178:LEU:N	2.52	0.42
33:5:12:GLU:HA	33:5:15:GLN:HB3	2.01	0.42
46:9:285:HIS:N	46:9:285:HIS:CD2	2.87	0.42
1:A:79:ARG:NH1	1:A:82:ARG:HH21	2.10	0.42
1:A:193:LEU:HG	1:A:194:GLU:N	2.35	0.42
1:A:203:VAL:HG12	1:A:206:TRP:CZ2	2.55	0.42
1:A:210:HIS:CE1	1:A:211:GLN:HG3	2.55	0.42
1:A:1337:GLN:HA	1:A:1337:GLN:NE2	2.35	0.42
1:A:1484:ILE:HD13	1:A:1484:ILE:HG21	1.78	0.42
2:B:15:C:H2'	2:B:16:U:H6	1.83	0.42
3:C:369:PHE:HE1	3:C:373:ILE:HD12	1.84	0.42
3:C:666:VAL:HG12	3:C:667:VAL:H	1.84	0.42
3:C:678:THR:HG21	3:C:683:ASN:HD22	1.84	0.42
5:E:94:ASN:O	5:E:99:CYS:HA	2.19	0.42
6:F:32:U:H2'	6:F:33:G:C8	2.54	0.42
6:F:38:G:C4	6:F:39:A:C8	3.08	0.42
6:F:82:A:C4	6:F:83:A:C8	3.07	0.42
8:H:12:G:H2'	8:H:13:C:N1	2.34	0.42
11:K:234:ARG:HA	11:K:234:ARG:HD3	1.89	0.42
12:L:184:ALA:O	12:L:188:ARG:HB2	2.20	0.42
17:R:141:LYS:O	17:R:145:GLU:HG2	2.20	0.42
23:X:165:GLU:HG2	23:X:169:ARG:NH2	2.35	0.42
23:X:233:GLU:O	23:X:237:LYS:HB3	2.19	0.42
23:X:268:GLN:HE21	23:X:268:GLN:HB3	1.66	0.42
23:X:648:TYR:O	23:X:656:GLN:NE2	2.51	0.42
23:X:718:SER:OG	23:X:719:ALA:N	2.52	0.42
24:Y:63:GLY:O	24:Y:105:GLY:HA3	2.19	0.42
26:1:733:LYS:HB3	26:1:733:LYS:HE3	1.80	0.42
27:3:469:GLU:OE1	27:3:469:GLU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:484:VAL:O	27:3:494:VAL:HB	2.19	0.42
27:3:675:LEU:HB3	27:3:686:LEU:HD12	2.02	0.42
27:3:791:HIS:CB	27:3:796:ASN:O	2.68	0.42
30:2:456:ARG:HA	30:2:459:ARG:HB2	2.02	0.42
1:A:659:GLN:O	1:A:659:GLN:NE2	2.53	0.42
1:A:694:LEU:HD23	1:A:694:LEU:N	2.34	0.42
1:A:694:LEU:HD22	1:A:709:ILE:CD1	2.49	0.42
1:A:1268:ILE:HD13	1:A:1268:ILE:HG21	1.77	0.42
1:A:1810:PHE:CE1	1:A:1919:LEU:HG	2.55	0.42
1:A:1939:ILE:HG21	1:A:1968:TRP:NE1	2.35	0.42
2:B:109:G:H8	2:B:109:G:OP2	2.03	0.42
3:C:366:GLN:HG3	3:C:371:GLU:CG	2.50	0.42
3:C:567:GLU:HG3	3:C:570:GLY:O	2.19	0.42
8:H:63:G:N1	8:H:64:A:N6	2.67	0.42
10:J:285:MET:HE3	10:J:285:MET:HB3	1.98	0.42
12:L:188:ARG:O	12:L:192:ARG:HG2	2.20	0.42
21:V:617:PRO:HB2	21:V:624:THR:HA	2.02	0.42
23:X:242:LYS:HG2	23:X:246:LEU:HD13	2.01	0.42
23:X:485:ASP:OD1	23:X:486:CYS:N	2.53	0.42
23:X:527:LEU:HD13	23:X:763:VAL:HG21	2.00	0.42
23:X:610:ASP:OD2	23:X:669:LYS:HB3	2.19	0.42
23:X:677:ALA:O	23:X:725:ARG:NE	2.53	0.42
23:X:948:PHE:O	23:X:951:THR:OG1	2.35	0.42
24:Y:30:LYS:CE	24:Y:168:ASP:HA	2.48	0.42
26:1:534:GLN:O	26:1:538:LEU:HD12	2.20	0.42
26:1:679:ILE:O	26:1:682:HIS:N	2.46	0.42
26:1:903:GLN:OE1	26:1:910:MET:HB2	2.19	0.42
27:3:212:GLU:CB	27:3:223:LYS:HG3	2.49	0.42
27:3:274:ARG:NH1	27:3:309:ASP:OD1	2.32	0.42
27:3:275:ARG:HB3	27:3:386:PHE:HB3	2.02	0.42
27:3:408:LEU:HD12	27:3:427:CYS:HA	2.02	0.42
27:3:610:VAL:HA	27:3:636:GLN:HE21	1.85	0.42
27:3:1147:HIS:O	27:3:1150:SER:OG	2.33	0.42
27:3:1199:ARG:HH21	27:3:1207:LYS:NZ	2.18	0.42
46:9:331:GLN:HG3	46:9:381:PHE:HB3	2.00	0.42
1:A:193:LEU:HB3	1:A:208:TYR:OH	2.20	0.42
1:A:283:VAL:O	1:A:284:ARG:HG2	2.20	0.42
1:A:1489:LEU:HD23	1:A:1489:LEU:HA	1.85	0.42
47:A:3000:IHP:O26	47:A:3000:IHP:P1	2.78	0.42
3:C:198:TYR:CZ	3:C:435:VAL:HG11	2.55	0.42
3:C:461:LEU:HB3	3:C:465:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:833:PHE:HD1	3:C:874:PHE:CE1	2.38	0.42
5:E:168:CYS:SG	5:E:208:ILE:HD13	2.60	0.42
5:E:199:VAL:HA	5:E:209:ILE:O	2.20	0.42
6:F:3:G:H2'	6:F:4:C:C6	2.55	0.42
6:F:58:G:O2'	6:F:59:G:OP1	2.35	0.42
19:T:464:GLY:O	19:T:482:ALA:N	2.49	0.42
23:X:543:ARG:NH2	23:X:546:LEU:HD13	2.35	0.42
27:3:459:VAL:CG2	27:3:476:VAL:HA	2.45	0.42
27:3:565:TYR:HB3	27:3:577:TYR:CB	2.46	0.42
27:3:577:TYR:HE2	27:3:579:GLU:HB3	1.85	0.42
27:3:1015:LYS:NZ	27:3:1016:ARG:H	2.18	0.42
30:2:510:TYR:O	30:2:511:LEU:HD23	2.20	0.42
30:2:511:LEU:HD23	30:2:511:LEU:HA	1.72	0.42
30:2:550:LYS:HG2	30:2:554:ARG:HH21	1.84	0.42
46:9:350:PHE:O	46:9:376:ASN:HB2	2.20	0.42
1:A:378:PHE:CG	3:C:342:ARG:HD2	2.55	0.41
1:A:875:HIS:HE1	23:X:866:ASN:CB	2.24	0.41
1:A:1298:ARG:NH2	2:B:39:C:O3'	2.49	0.41
1:A:1637:TRP:O	1:A:1656:THR:CA	2.56	0.41
1:A:2112:LYS:HB2	1:A:2112:LYS:HE2	1.89	0.41
1:A:2150:GLN:O	1:A:2281:TYR:HB2	2.19	0.41
3:C:97:VAL:HG11	15:P:47:THR:HG21	2.01	0.41
3:C:153:THR:HG21	3:C:188:VAL:HG12	2.02	0.41
5:E:259:VAL:CG2	5:E:277:PHE:HB2	2.48	0.41
6:F:13:G:H8	6:F:13:G:O5'	2.03	0.41
7:G:104:C:HO2'	7:G:105:C:P	2.42	0.41
7:G:112:U:C4	23:X:503:ARG:CZ	3.03	0.41
8:H:160:A:H2'	8:H:161:U:O4'	2.20	0.41
10:J:289:ASN:HB2	10:J:291:GLN:OE1	2.20	0.41
10:J:321:GLU:OE1	10:J:329:ALA:HB2	2.20	0.41
11:K:230:TRP:CZ3	11:K:231:GLN:HG3	2.55	0.41
12:L:31:TRP:HB3	12:L:43:ALA:HB1	2.02	0.41
12:L:66:GLU:HA	12:L:69:GLU:HG3	2.02	0.41
14:O:262:THR:O	14:O:270:ALA:HA	2.21	0.41
16:Q:1224:ILE:HA	16:Q:1270:TYR:O	2.19	0.41
17:R:110:LYS:NZ	19:T:365:ARG:O	2.35	0.41
21:V:643:LEU:HD23	21:V:643:LEU:HA	1.48	0.41
23:X:228:LYS:HE3	23:X:232:ARG:NH2	2.35	0.41
23:X:393:GLN:O	23:X:397:ARG:HG3	2.19	0.41
23:X:742:ALA:O	23:X:747:LEU:HD23	2.20	0.41
27:3:206:GLN:HE22	27:3:232:GLY:H	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:605:LEU:HB3	27:3:619:LEU:HD22	2.02	0.41
46:9:437:PRO:HG2	46:9:438:TYR:CD2	2.55	0.41
1:A:106:MET:HA	1:A:107:PRO:HD3	1.77	0.41
1:A:126:ILE:HA	1:A:499:GLN:OE1	2.20	0.41
1:A:1166:THR:HG23	1:A:1167:THR:N	2.35	0.41
1:A:1235:GLU:O	1:A:1235:GLU:HG2	2.19	0.41
1:A:1779:PHE:HB3	1:A:1893:PHE:HE2	1.84	0.41
3:C:928:HIS:HD1	3:C:928:HIS:H	1.67	0.41
7:G:113:U:H1'	7:G:114:U:OP2	2.19	0.41
13:N:140:ARG:NH2	22:W:196:TRP:O	2.52	0.41
14:O:24:CYS:O	14:O:28:LEU:CB	2.68	0.41
16:Q:539:VAL:O	16:Q:624:THR:HA	2.19	0.41
17:R:241:GLU:HA	17:R:244:GLU:OE2	2.21	0.41
19:T:209:CYS:SG	19:T:252:VAL:HG13	2.60	0.41
19:T:352:THR:HG22	19:T:374:SER:N	2.35	0.41
21:V:476:LEU:HD23	21:V:476:LEU:HA	1.77	0.41
22:W:180:LYS:HA	22:W:199:TYR:HA	2.03	0.41
23:X:416:GLN:HE22	23:X:544:PRO:HA	1.86	0.41
23:X:621:ILE:HG12	23:X:672:VAL:CG1	2.50	0.41
26:1:826:ASP:OD1	26:1:828:ARG:N	2.42	0.41
26:1:892:LEU:HD22	26:1:892:LEU:HA	1.70	0.41
26:1:1142:ASN:HD22	26:1:1142:ASN:N	2.19	0.41
27:3:128:ARG:HH21	27:3:180:PRO:HG3	1.85	0.41
27:3:343:LYS:C	27:3:345:GLY:H	2.24	0.41
27:3:423:LEU:HB2	27:3:438:LEU:HB2	2.02	0.41
27:3:855:PRO:O	27:3:856:LYS:HD3	2.20	0.41
27:3:947:GLU:HG3	27:3:948:VAL:H	1.84	0.41
1:A:46:ALA:HB1	1:A:47:GLU:OE1	2.20	0.41
1:A:227:ARG:HE	1:A:227:ARG:HB2	1.70	0.41
1:A:668:VAL:HG23	1:A:669:ALA:H	1.84	0.41
1:A:1376:GLU:O	1:A:1376:GLU:HG3	2.14	0.41
1:A:1745:GLU:OE1	26:1:980:GLU:HG2	2.20	0.41
1:A:2177:TRP:O	1:A:2213:ILE:HA	2.20	0.41
1:A:2207:ASP:O	1:A:2211:THR:OG1	2.38	0.41
1:A:2284:MET:HB3	1:A:2287:ARG:HB3	2.03	0.41
3:C:453:TYR:CZ	3:C:575:GLN:HB2	2.55	0.41
4:D:696:LYS:O	4:D:700:ARG:CB	2.69	0.41
4:D:2030:ARG:O	4:D:2096:ALA:HB3	2.20	0.41
5:E:135:VAL:HG21	5:E:181:ILE:CD1	2.45	0.41
5:E:241:LEU:HA	5:E:251:LEU:O	2.19	0.41
10:J:297:ASN:OD1	12:L:225:TYR:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:362:ALA:O	10:J:366:TYR:HD2	2.03	0.41
13:N:1:MET:H3	13:N:2:PRO:HD2	1.85	0.41
13:N:47:TRP:NE1	13:N:135:THR:O	2.48	0.41
17:R:352:ARG:HG2	17:R:356:ARG:HH21	1.85	0.41
19:T:424:ASP:OD1	19:T:424:ASP:N	2.53	0.41
23:X:164:TRP:HE3	23:X:165:GLU:CA	2.33	0.41
23:X:756:GLN:NE2	23:X:782:ASP:OD2	2.53	0.41
23:X:760:LEU:HA	23:X:763:VAL:HG13	2.01	0.41
23:X:815:MET:HE1	23:X:829:LEU:HD12	2.02	0.41
23:X:819:PRO:O	23:X:819:PRO:HG2	2.19	0.41
23:X:840:ILE:HD13	23:X:840:ILE:HA	1.95	0.41
23:X:994:LYS:HD2	23:X:996:PHE:CZ	2.56	0.41
27:3:43:PRO:HA	27:3:50:VAL:HA	2.01	0.41
27:3:724:SER:HB2	27:3:727:SER:HA	2.01	0.41
1:A:368:GLN:HA	1:A:368:GLN:OE1	2.21	0.41
1:A:769:LYS:HA	1:A:769:LYS:HD2	1.44	0.41
1:A:883:ARG:O	1:A:887:THR:HG23	2.20	0.41
1:A:1677:GLU:HA	1:A:1677:GLU:OE2	2.19	0.41
1:A:1936:LEU:HG	1:A:1940:LEU:HD21	2.02	0.41
1:A:2140:LYS:NZ	1:A:2210:LYS:HG2	2.35	0.41
1:A:2148:VAL:HG23	1:A:2294:TYR:CZ	2.56	0.41
1:A:2160:PRO:HD3	1:A:2288:HIS:CE1	2.56	0.41
1:A:2188:LEU:HD13	1:A:2228:TYR:CE1	2.55	0.41
3:C:736:GLY:O	3:C:771:GLN:HG2	2.21	0.41
3:C:919:ARG:HB2	3:C:922:GLU:HG2	2.03	0.41
3:C:940:ARG:HG2	3:C:941:LYS:HG3	2.01	0.41
5:E:118:ASN:ND2	5:E:122:SER:H	2.17	0.41
5:E:124:LEU:C	5:E:125:PHE:HD2	2.24	0.41
6:F:88:G:N3	8:H:11:G:C2	2.88	0.41
7:G:7:G:C6	7:G:8:C:N3	2.88	0.41
7:G:111:U:O4	23:X:820:VAL:N	2.53	0.41
8:H:44:U:OP2	8:H:44:U:H6	2.02	0.41
10:J:328:GLY:O	10:J:331:GLN:HG2	2.20	0.41
10:J:331:GLN:HA	10:J:334:GLU:HG2	2.02	0.41
16:Q:1064:ALA:HB3	16:Q:1095:GLY:HA3	2.02	0.41
17:R:358:ASP:OD2	23:X:255:PHE:HZ	2.03	0.41
23:X:408:LEU:HD13	23:X:570:PHE:CG	2.55	0.41
23:X:497:THR:HG23	23:X:500:MET:HG3	2.01	0.41
23:X:563:PHE:HE2	23:X:780:PHE:O	2.04	0.41
23:X:648:TYR:HB2	23:X:649:ALA:H	1.79	0.41
23:X:664:PRO:HA	23:X:665:PRO:HD2	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:1007:TRP:HA	23:X:1010:GLU:HB2	2.02	0.41
26:1:555:VAL:HG12	26:1:559:ILE:HD13	2.02	0.41
26:1:703:THR:HG23	26:1:742:GLY:HA2	2.03	0.41
27:3:1:MET:HG3	27:3:1092:ILE:HD12	2.02	0.41
27:3:91:GLU:OE1	27:3:102:ILE:HD11	2.20	0.41
27:3:914:ILE:HG22	27:3:917:PRO:HD2	2.02	0.41
27:3:969:VAL:HB	27:3:981:CYS:CB	2.45	0.41
27:3:1001:ILE:HG21	27:3:1044:VAL:HG21	2.03	0.41
30:2:456:ARG:HE	30:2:456:ARG:HB3	1.79	0.41
1:A:76:MET:HE1	1:A:84:ASP:HB2	2.03	0.41
1:A:648:LEU:HD23	1:A:648:LEU:HA	1.86	0.41
1:A:1661:TRP:CD2	1:A:1700:GLY:HA3	2.55	0.41
1:A:1764:SER:C	1:A:1766:GLN:N	2.73	0.41
1:A:2185:SER:HA	1:A:2186:PRO:HD3	1.92	0.41
1:A:2277:SER:HB3	1:A:2281:TYR:HE1	1.86	0.41
3:C:223:ASP:HA	3:C:448:LYS:HZ1	1.85	0.41
3:C:258:ASN:HD21	3:C:312:SER:HB3	1.85	0.41
3:C:334:ILE:HD11	3:C:339:PHE:CD2	2.55	0.41
3:C:349:PHE:CE1	3:C:354:ARG:HA	2.43	0.41
4:D:2067:VAL:HA	4:D:2079:ILE:HA	2.02	0.41
6:F:79:C:O2'	12:L:170:LYS:HD2	2.21	0.41
7:G:93:A:C2	8:H:38:A:C2	3.08	0.41
7:G:111:U:OP2	23:X:482:ARG:CB	2.63	0.41
12:L:63:TRP:HD1	12:L:67:GLU:HB3	1.85	0.41
15:P:195:LYS:O	15:P:196:ASN:C	2.59	0.41
16:Q:877:LEU:O	16:Q:1035:ILE:HA	2.21	0.41
19:T:460:ASP:N	46:9:259:THR:O	2.46	0.41
23:X:275:ARG:O	23:X:279:LEU:HG	2.21	0.41
24:Y:95:SER:OG	24:Y:109:LEU:HD21	2.20	0.41
24:Y:267:ARG:HB3	24:Y:287:GLU:HG2	2.03	0.41
26:1:914:PHE:O	26:1:917:VAL:HG12	2.21	0.41
27:3:66:MET:HE3	27:3:123:VAL:HG12	2.03	0.41
27:3:164:ASN:N	27:3:164:ASN:OD1	2.53	0.41
27:3:289:CYS:SG	27:3:290:SER:N	2.94	0.41
27:3:1035:THR:HG21	27:3:1103:SER:HA	2.01	0.41
46:9:300:THR:OG1	46:9:300:THR:O	2.37	0.41
46:9:350:PHE:CZ	46:9:376:ASN:HB3	2.55	0.41
46:9:360:HIS:CE1	46:9:391:ASP:HB2	2.54	0.41
1:A:845:ARG:HH12	1:A:1440:THR:CG2	2.32	0.41
1:A:855:ARG:NH1	1:A:1523:ARG:HB3	2.35	0.41
1:A:1352:HIS:ND1	20:U:21:ARG:HA	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1402:ARG:HD2	23:X:664:PRO:HB2	2.02	0.41
1:A:1971:LEU:HD23	1:A:1971:LEU:HA	1.82	0.41
3:C:221:ILE:O	3:C:549:TRP:NE1	2.53	0.41
5:E:192:ASN:CG	5:E:193:THR:H	2.24	0.41
5:E:193:THR:HG23	5:E:194:TYR:CD2	2.55	0.41
7:G:111:U:OP1	23:X:500:MET:HG2	2.20	0.41
8:H:41:U:C2	8:H:42:G:C8	3.08	0.41
8:H:42:G:C6	8:H:43:U:C4	3.09	0.41
8:H:55:U:H2'	8:H:57:A:OP2	2.21	0.41
12:L:168:LYS:HA	12:L:168:LYS:HE3	2.01	0.41
13:N:27:GLN:OE1	13:N:27:GLN:HA	2.21	0.41
13:N:63:LEU:O	13:N:70:ILE:HB	2.21	0.41
23:X:453:PRO:HB3	23:X:524:GLU:CD	2.40	0.41
24:Y:64:GLU:HG2	24:Y:77:PHE:CZ	2.56	0.41
24:Y:96:MET:HE2	24:Y:104:HIS:HB3	2.02	0.41
26:1:504:ILE:HG13	26:1:515:ALA:HB3	2.03	0.41
26:1:556:ILE:O	26:1:560:LEU:HB2	2.21	0.41
26:1:769:VAL:O	26:1:772:ILE:HB	2.21	0.41
27:3:412:ILE:H	27:3:1105:GLN:NE2	2.09	0.41
27:3:637:PRO:HB3	27:3:640:LEU:HD21	2.03	0.41
27:3:1015:LYS:HZ2	27:3:1016:ARG:N	2.19	0.41
27:3:1096:HIS:ND1	27:3:1166:TYR:HB2	2.36	0.41
27:3:1180:GLU:OE2	27:3:1212:ARG:NH2	2.45	0.41
30:2:572:HIS:O	30:2:576:PHE:HB2	2.20	0.41
33:5:74:GLN:NE2	33:5:78:PRO:HA	2.36	0.41
1:A:533:LYS:NZ	7:G:5:G:OP2	2.25	0.41
1:A:755:HIS:CD2	15:P:219:PHE:HE2	2.38	0.41
1:A:1638:ASN:O	1:A:1652:MET:HB3	2.21	0.41
1:A:1701:VAL:HA	1:A:1716:GLY:HA3	2.02	0.41
1:A:1820:LYS:O	1:A:1820:LYS:HG3	2.21	0.41
1:A:1850:ARG:NH1	1:A:1878:ASP:OD2	2.54	0.41
1:A:1938:LEU:HD22	1:A:1984:LYS:HG3	2.02	0.41
1:A:2166:HIS:HB3	1:A:2169:LEU:HG	2.02	0.41
1:A:2228:TYR:CD2	1:A:2258:ARG:HG3	2.56	0.41
3:C:311:SER:OG	3:C:311:SER:O	2.32	0.41
3:C:810:PRO:HG3	3:C:813:ARG:HH22	1.85	0.41
5:E:82:ALA:HA	5:E:92:LEU:HD23	2.03	0.41
5:E:90:ILE:HB	5:E:105:LEU:HB3	2.01	0.41
5:E:127:ALA:HB2	5:E:157:CYS:HB2	2.03	0.41
5:E:243:LEU:HD23	5:E:243:LEU:HA	1.95	0.41
7:G:12:G:H8	7:G:12:G:O5'	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:5:C:O2'	8:H:6:U:H5'	2.20	0.41
16:Q:745:PRO:HG2	16:Q:781:PRO:HA	2.03	0.41
17:R:125:MET:HA	19:T:442:ARG:HH12	1.85	0.41
17:R:125:MET:HA	19:T:442:ARG:NH1	2.35	0.41
17:R:160:ALA:O	17:R:163:MET:HB2	2.21	0.41
21:V:562:TRP:CE2	21:V:602:ARG:HD3	2.55	0.41
23:X:754:GLU:HG3	23:X:757:ARG:HH12	1.84	0.41
24:Y:27:ASN:ND2	24:Y:65:SER:HB2	2.36	0.41
26:1:802:GLU:HG2	26:1:805:TYR:HB2	2.02	0.41
26:1:876:MET:HE3	26:1:920:ALA:HB3	2.02	0.41
27:3:280:ASP:H	27:3:857:ALA:CB	2.33	0.41
27:3:1001:ILE:HD12	27:3:1011:TRP:NE1	2.36	0.41
27:3:1004:ASP:OD2	27:3:1007:GLU:HB2	2.21	0.41
32:7:26:CYS:SG	32:7:60:ILE:HG13	2.61	0.41
1:A:32:GLU:HA	1:A:35:ARG:HB3	2.03	0.41
1:A:152:ARG:HG3	1:A:616:PHE:CE2	2.56	0.41
1:A:611:LEU:HD12	1:A:611:LEU:HA	1.83	0.41
1:A:727:LYS:HE2	1:A:727:LYS:HB3	1.74	0.41
1:A:1161:LEU:HD22	1:A:1166:THR:HG22	2.03	0.41
1:A:1220:VAL:HG23	1:A:1221:THR:N	2.36	0.41
1:A:1287:LEU:HD12	1:A:1287:LEU:HA	1.83	0.41
1:A:1468:ASN:OD1	17:R:433:TYR:HB3	2.20	0.41
1:A:1610:GLN:HB3	1:A:1630:LEU:CB	2.51	0.41
3:C:69:ALA:O	3:C:72:VAL:HG12	2.20	0.41
3:C:259:LYS:HE3	48:C:1500:GTP:C4	2.56	0.41
3:C:695:GLY:O	3:C:698:GLU:HB2	2.20	0.41
3:C:700:ILE:HG21	3:C:742:PRO:HA	2.02	0.41
3:C:727:LEU:HA	3:C:730:ARG:HG2	2.03	0.41
3:C:758:LEU:HD22	3:C:800:PRO:HD3	2.02	0.41
3:C:932:GLU:HA	3:C:935:ILE:HD12	2.03	0.41
5:E:69:VAL:HG12	5:E:345:ALA:HB1	2.03	0.41
10:J:239:ARG:O	10:J:239:ARG:HG2	2.21	0.41
10:J:342:GLU:CD	10:J:343:GLU:N	2.74	0.41
11:K:232:ILE:HA	11:K:235:GLU:HG2	2.03	0.41
12:L:25:LYS:HZ2	12:L:25:LYS:HG3	1.80	0.41
14:O:131:THR:O	22:W:111:LEU:HA	2.20	0.41
19:T:350:HIS:HA	19:T:374:SER:HB3	2.03	0.41
23:X:431:GLN:HA	23:X:434:GLN:HE21	1.86	0.41
23:X:606:GLN:HG3	23:X:688:TYR:CE1	2.56	0.41
23:X:845:ALA:O	23:X:848:SER:OG	2.38	0.41
24:Y:49:PHE:N	24:Y:112:THR:OG1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:664:GLY:O	26:1:668:VAL:HG23	2.20	0.41
26:1:1067:LYS:HB3	26:1:1067:LYS:HE2	1.67	0.41
27:3:77:TYR:HE2	27:3:152:LEU:HD22	1.85	0.41
27:3:497:SER:OG	27:3:499:PHE:HB2	2.21	0.41
27:3:615:ARG:O	27:3:616:ILE:HD12	2.21	0.41
27:3:664:TYR:HA	27:3:677:THR:O	2.21	0.41
27:3:966:LEU:H	27:3:966:LEU:HG	1.72	0.41
33:5:53:PHE:O	33:5:57:GLU:HG2	2.21	0.41
1:A:59:GLU:HA	1:A:59:GLU:OE2	2.20	0.41
1:A:136:ILE:HG13	1:A:225:TYR:HE2	1.85	0.41
1:A:225:TYR:O	1:A:418:THR:HG21	2.21	0.41
1:A:303:ILE:HG22	1:A:305:ARG:HG2	2.03	0.41
1:A:547:CYS:O	1:A:548:ARG:C	2.58	0.41
1:A:1173:SER:OG	1:A:1174:PHE:N	2.52	0.41
1:A:1403:LEU:HB2	17:R:407:TYR:HB3	2.03	0.41
1:A:1543:ASN:HB2	1:A:1569:LEU:HD21	2.02	0.41
1:A:1872:LEU:HD12	1:A:1884:ILE:HD13	2.02	0.41
1:A:1927:ILE:HD12	1:A:1931:THR:HG22	2.03	0.41
1:A:1936:LEU:O	1:A:1940:LEU:HG	2.21	0.41
1:A:1976:TRP:HA	1:A:1979:VAL:HG22	2.03	0.41
1:A:2294:TYR:HD2	1:A:2295:GLU:O	2.03	0.41
1:A:2298:LEU:HA	1:A:2298:LEU:HD23	1.88	0.41
3:C:83:GLU:HB2	3:C:84:GLU:H	1.75	0.41
3:C:174:GLU:CD	3:C:180:GLY:HA2	2.41	0.41
3:C:336:TYR:CZ	3:C:337:GLN:HG2	2.56	0.41
3:C:556:ASP:OD1	3:C:556:ASP:N	2.54	0.41
3:C:678:THR:HG23	3:C:683:ASN:HB2	2.03	0.41
3:C:750:LEU:HG	20:U:67:GLU:CB	2.50	0.41
4:D:541:ILE:HA	4:D:588:CYS:O	2.21	0.41
4:D:1350:ALA:O	4:D:1492:SER:HA	2.21	0.41
5:E:94:ASN:N	5:E:100:ASP:O	2.40	0.41
5:E:147:LEU:HD21	5:E:179:TRP:HB3	2.02	0.41
5:E:339:GLU:HB3	5:E:341:ILE:HG13	2.02	0.41
7:G:85:G:H1	8:H:45:C:N4	2.18	0.41
7:G:90:C:N3	8:H:40:C:N3	2.68	0.41
7:G:96:U:H5”	7:G:97:A:OP2	2.21	0.41
8:H:142:U:C2	8:H:143:C:C5	3.09	0.41
8:H:182:U:H2’	8:H:183:G:H8	1.85	0.41
10:J:319:MET:O	10:J:323:LEU:HD13	2.20	0.41
10:J:431:ARG:CA	10:J:434:VAL:HG12	2.41	0.41
19:T:314:ILE:O	19:T:323:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:469:PHE:CE1	21:V:509:LEU:HD13	2.56	0.41
23:X:326:GLN:O	23:X:326:GLN:HG2	2.21	0.41
23:X:482:ARG:O	23:X:483:PHE:HB2	2.21	0.41
23:X:616:THR:HB	23:X:696:LYS:HE2	2.03	0.41
23:X:716:LYS:HG3	23:X:747:LEU:HB3	2.03	0.41
23:X:822:PRO:O	23:X:825:SER:CA	2.68	0.41
23:X:843:VAL:HG23	23:X:882:LEU:HD13	2.02	0.41
23:X:856:ARG:CZ	23:X:856:ARG:HB3	2.51	0.41
23:X:887:GLN:O	23:X:890:GLU:HB3	2.20	0.41
23:X:941:LYS:HA	23:X:944:THR:OG1	2.21	0.41
23:X:1007:TRP:HA	23:X:1010:GLU:OE2	2.20	0.41
24:Y:183:ARG:HH21	24:Y:186:LEU:HB3	1.85	0.41
24:Y:242:LEU:HD13	24:Y:313:VAL:HG11	2.01	0.41
24:Y:242:LEU:HD12	24:Y:288:PHE:CZ	2.56	0.41
26:1:641:ILE:H	26:1:641:ILE:HG13	1.56	0.41
26:1:834:VAL:HG22	26:1:871:THR:CG2	2.44	0.41
26:1:926:LYS:HE2	26:1:965:CYS:HA	2.03	0.41
26:1:1028:HIS:HB3	26:1:1031:VAL:HG13	2.02	0.41
26:1:1029:GLU:H	26:1:1029:GLU:HG3	1.73	0.41
27:3:70:LEU:HD23	27:3:70:LEU:HA	1.78	0.41
27:3:174:ASP:HB3	27:3:240:GLY:H	1.86	0.41
27:3:526:HIS:HB2	27:3:574:LEU:HD21	2.03	0.41
27:3:542:LYS:H	27:3:542:LYS:HG3	1.45	0.41
27:3:926:TYR:CD1	27:3:942:LYS:HB3	2.56	0.41
30:2:469:VAL:HG12	30:2:471:ARG:N	2.31	0.41
46:9:220:ILE:HG22	46:9:221:LEU:N	2.36	0.41
46:9:221:LEU:H	46:9:221:LEU:CD2	2.32	0.41
46:9:281:TYR:HB3	46:9:283:ARG:HH12	1.86	0.41
46:9:320:ILE:HG13	46:9:337:GLY:HA2	2.01	0.41
1:A:615:ARG:HE	1:A:615:ARG:HB2	1.62	0.41
1:A:1189:MET:HE2	1:A:1189:MET:HB2	1.77	0.41
1:A:2188:LEU:HD22	1:A:2228:TYR:CB	2.51	0.41
3:C:372:PHE:O	3:C:376:PRO:HG3	2.20	0.41
3:C:718:PHE:HB3	3:C:724:TRP:HD1	1.86	0.41
6:F:84:A:C4	6:F:85:U:C6	3.09	0.41
8:H:168:A:H5"	8:H:169:C:C6	2.56	0.41
13:N:59:TYR:CZ	13:N:63:LEU:HD11	2.56	0.41
19:T:213:GLU:OE1	19:T:216:ASN:N	2.54	0.41
19:T:338:CYS:HA	19:T:344:GLN:O	2.20	0.41
21:V:636:LEU:HD13	21:V:639:LEU:HD11	2.03	0.41
23:X:826:LYS:HB3	23:X:946:GLY:HA2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:997:MET:C	23:X:998:ARG:HD2	2.42	0.41
24:Y:41:LEU:HB3	24:Y:155:ARG:NH1	2.36	0.41
26:1:550:HIS:CD2	26:1:551:LEU:HD22	2.49	0.41
26:1:1208:LEU:HB3	26:1:1237:LEU:HD21	2.03	0.41
27:3:224:TYR:HB3	27:3:261:PHE:CD1	2.56	0.41
27:3:941:HIS:CE1	27:3:974:LYS:HA	2.56	0.41
30:2:487:LEU:HD12	30:2:487:LEU:HA	1.85	0.41
1:A:162:LYS:HE2	1:A:163:ARG:O	2.21	0.40
1:A:699:GLU:HB3	17:R:237:MET:SD	2.60	0.40
1:A:1284:LEU:HD23	1:A:1284:LEU:HA	1.77	0.40
1:A:1492:GLY:HA2	1:A:1710:ASN:ND2	2.34	0.40
1:A:1949:ARG:NH2	1:A:1986:LEU:HD21	2.36	0.40
1:A:2071:THR:O	1:A:2075:VAL:HG13	2.21	0.40
1:A:2073:TRP:HH2	1:A:2310:ARG:NE	2.19	0.40
1:A:2195:THR:O	1:A:2199:ILE:HG13	2.21	0.40
3:C:258:ASN:HA	3:C:310:SER:O	2.21	0.40
3:C:286:ASN:OD1	3:C:300:LEU:HD12	2.21	0.40
3:C:496:VAL:HG23	3:C:548:ASN:H	1.86	0.40
7:G:112:U:O2	7:G:112:U:C2'	2.68	0.40
7:G:117:A:O3'	24:Y:312:HIS:HD2	2.03	0.40
8:H:34:U:H2'	8:H:35:A:C1'	2.51	0.40
8:H:81:G:H2'	8:H:82:G:O4'	2.21	0.40
10:J:280:LEU:HD23	10:J:280:LEU:HA	1.75	0.40
15:P:188:TRP:O	15:P:188:TRP:CD1	2.74	0.40
17:R:208:GLU:OE2	17:R:211:ARG:NH2	2.50	0.40
21:V:501:ARG:HH11	21:V:501:ARG:HB2	1.86	0.40
23:X:887:GLN:HA	23:X:890:GLU:HB3	2.03	0.40
26:1:646:PRO:O	26:1:649:LYS:HB2	2.20	0.40
26:1:862:GLU:O	26:1:866:LYS:HB2	2.21	0.40
26:1:953:ASP:O	26:1:956:SER:N	2.55	0.40
27:3:195:ASP:OD1	27:3:197:THR:OG1	2.35	0.40
27:3:503:THR:OG1	27:3:522:ASP:OD2	2.21	0.40
27:3:686:LEU:HD13	27:3:686:LEU:HA	1.96	0.40
27:3:706:MET:HG2	27:3:770:LEU:CD1	2.51	0.40
27:3:911:LYS:HG3	27:3:912:ASP:CG	2.42	0.40
32:7:51:TYR:CG	32:7:52:GLY:N	2.90	0.40
1:A:829:PRO:HD2	1:A:832:TYR:CG	2.56	0.40
1:A:1352:HIS:HB2	20:U:5:ILE:HG21	2.03	0.40
1:A:2104:TYR:HB3	1:A:2142:ILE:HD11	2.03	0.40
2:B:113:G:O5'	2:B:113:G:H8	2.04	0.40
3:C:930:ALA:HA	3:C:933:PHE:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:40:U:H3'	6:F:41:A:C8	2.56	0.40
7:G:111:U:P	23:X:482:ARG:HB2	2.60	0.40
12:L:701:GLY:O	12:L:704:THR:N	2.55	0.40
15:P:74:LYS:HA	15:P:77:ASP:CB	2.52	0.40
17:R:116:TYR:HD1	17:R:120:VAL:HG13	1.86	0.40
19:T:280:VAL:H	19:T:280:VAL:HG23	1.67	0.40
19:T:368:LEU:HD13	19:T:398:TRP:CE3	2.56	0.40
21:V:520:GLU:O	21:V:524:SER:OG	2.27	0.40
23:X:428:LYS:HE2	23:X:428:LYS:HB2	1.94	0.40
23:X:506:LEU:HD23	23:X:770:LEU:HD21	1.97	0.40
23:X:532:LEU:O	23:X:536:ILE:HG13	2.21	0.40
23:X:747:LEU:HA	23:X:747:LEU:HD13	1.86	0.40
23:X:978:GLU:OE1	23:X:978:GLU:HA	2.21	0.40
24:Y:40:CYS:O	24:Y:155:ARG:CA	2.66	0.40
24:Y:161:ILE:HG21	24:Y:164:ASP:HB2	2.03	0.40
26:1:686:LEU:HA	26:1:689:ILE:HG12	2.03	0.40
26:1:1216:TRP:CH2	26:1:1268:ILE:HD13	2.56	0.40
27:3:184:CYS:SG	27:3:211:TYR:CE1	3.14	0.40
27:3:258:TYR:CG	27:3:259:LYS:N	2.90	0.40
27:3:328:LYS:NZ	27:3:370:GLU:HB3	2.36	0.40
27:3:334:PRO:HG2	27:3:357:TYR:CD2	2.56	0.40
27:3:459:VAL:HA	27:3:475:ILE:O	2.21	0.40
27:3:510:LEU:HG	27:3:510:LEU:O	2.21	0.40
27:3:610:VAL:HG23	27:3:636:GLN:NE2	2.36	0.40
27:3:615:ARG:C	27:3:616:ILE:HD12	2.41	0.40
27:3:1057:ARG:O	27:3:1090:GLU:HG3	2.22	0.40
30:2:506:PHE:N	30:2:506:PHE:CD1	2.88	0.40
1:A:431:TYR:HB3	1:A:611:LEU:HD21	2.02	0.40
1:A:495:GLN:HE21	1:A:495:GLN:HB2	1.62	0.40
1:A:1362:ASP:OD1	1:A:1363:GLN:N	2.34	0.40
1:A:1518:LEU:HD23	1:A:1518:LEU:N	2.36	0.40
1:A:1618:LYS:HG3	1:A:1626:CYS:HB2	2.02	0.40
2:B:14:U:C2	2:B:15:C:C5	3.10	0.40
3:C:271:PRO:HG3	3:C:378:TYR:CD2	2.57	0.40
6:F:38:G:P	6:F:38:G:C8	3.14	0.40
7:G:7:G:C5	7:G:8:C:N4	2.90	0.40
7:G:111:U:C6	23:X:819:PRO:HA	2.55	0.40
8:H:28:C:N4	12:L:32:SER:OG	2.54	0.40
11:K:237:ASP:OD1	11:K:238:GLU:N	2.54	0.40
17:R:352:ARG:O	17:R:355:ILE:HB	2.22	0.40
21:V:503:TYR:OH	21:V:550:MET:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:290:GLY:O	22:W:309:MET:N	2.42	0.40
23:X:941:LYS:HE2	23:X:1007:TRP:NE1	2.37	0.40
23:X:984:LEU:HD23	23:X:984:LEU:HA	1.96	0.40
26:1:893:ILE:HG22	26:1:894:ASP:OD2	2.22	0.40
26:1:1055:TRP:CE3	26:1:1055:TRP:HA	2.56	0.40
27:3:316:GLU:HG3	27:3:324:GLU:OE1	2.22	0.40
27:3:672:GLY:H	27:3:696:SER:CA	2.34	0.40
27:3:838:MET:H	27:3:838:MET:HG2	1.73	0.40
27:3:896:PHE:CD2	27:3:896:PHE:N	2.90	0.40
27:3:927:THR:HG23	27:3:940:LEU:HB2	2.04	0.40
27:3:998:HIS:HE1	27:3:1041:TYR:OH	2.04	0.40
33:5:44:MET:HE2	33:5:44:MET:HB2	1.88	0.40
46:9:323:ARG:CB	46:9:331:GLN:HE21	2.32	0.40
1:A:422:LEU:HD22	1:A:638:LEU:HD13	2.02	0.40
1:A:520:TYR:O	1:A:555:LYS:NZ	2.26	0.40
1:A:781:ARG:NH2	8:H:24:A:H5"	2.36	0.40
1:A:856:LEU:H	1:A:856:LEU:HG	1.38	0.40
1:A:1136:ARG:HG2	1:A:1139:ARG:NH1	2.36	0.40
1:A:1839:TRP:CZ3	1:A:1871:PRO:HB3	2.56	0.40
1:A:1865:ARG:HA	1:A:1865:ARG:HD2	1.86	0.40
2:B:99:C:C2	2:B:100:C:C5	3.09	0.40
3:C:242:LEU:HA	3:C:242:LEU:HD23	1.50	0.40
3:C:366:GLN:NE2	3:C:375:GLU:OE1	2.53	0.40
3:C:749:THR:O	3:C:753:GLU:N	2.53	0.40
3:C:804:GLY:O	3:C:808:ILE:HB	2.22	0.40
3:C:834:VAL:HG22	3:C:899:SER:CB	2.52	0.40
5:E:260:ARG:HD2	5:E:273:CYS:SG	2.62	0.40
6:F:85:U:C2	8:H:14:C:N3	2.89	0.40
12:L:98:GLU:O	12:L:101:GLU:HG3	2.21	0.40
13:N:75:TYR:CZ	13:N:79:ILE:HD11	2.57	0.40
14:O:22:ILE:O	14:O:82:GLN:N	2.43	0.40
17:R:331:ALA:HA	23:X:275:ARG:HH12	1.87	0.40
18:S:63:GLN:HA	18:S:113:PHE:HA	2.03	0.40
22:W:239:THR:HA	22:W:327:THR:O	2.21	0.40
23:X:257:PHE:CD1	23:X:270:LEU:HG	2.57	0.40
23:X:741:TRP:HE1	26:1:781:ASP:CG	2.25	0.40
23:X:822:PRO:C	23:X:825:SER:H	2.25	0.40
24:Y:134:ASP:O	24:Y:138:LYS:HG3	2.20	0.40
26:1:517:ARG:HB3	26:1:517:ARG:NH1	2.37	0.40
26:1:811:LEU:HB2	26:1:812:PRO:HD3	2.03	0.40
26:1:1080:THR:O	26:1:1084:ILE:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:9:204:THR:O	46:9:208:LEU:HG	2.22	0.40
46:9:367:SER:HA	46:9:395:THR:O	2.21	0.40
1:A:435:CYS:HA	7:G:-10:G:H22	1.87	0.40
1:A:902:TYR:CE2	1:A:1246:GLN:HB3	2.57	0.40
1:A:2133:PRO:HD3	1:A:2139:VAL:O	2.22	0.40
3:C:732:ILE:HG12	3:C:744:ILE:HG21	2.03	0.40
5:E:86:PHE:HD2	5:E:86:PHE:O	2.04	0.40
12:L:85:ILE:O	12:L:88:ILE:HG13	2.22	0.40
15:P:77:ASP:O	15:P:78:ARG:HG2	2.21	0.40
19:T:395:ILE:HB	19:T:409:LEU:HB2	2.03	0.40
21:V:555:LEU:HG	21:V:586:PHE:CZ	2.53	0.40
21:V:618:ARG:HE	21:V:618:ARG:HB2	1.78	0.40
23:X:432:ILE:HB	23:X:433:PRO:HD3	2.02	0.40
23:X:439:GLU:OE1	23:X:439:GLU:N	2.55	0.40
23:X:461:VAL:O	23:X:465:VAL:HG23	2.22	0.40
23:X:762:ASN:HB2	23:X:821:ASP:HA	2.03	0.40
23:X:766:LEU:HD12	23:X:766:LEU:HA	1.81	0.40
23:X:796:LEU:HB2	23:X:802:LEU:CD1	2.51	0.40
23:X:945:ALA:HA	23:X:1011:VAL:HG11	2.04	0.40
26:1:549:ARG:O	26:1:553:VAL:HG22	2.22	0.40
26:1:669:GLN:NE2	26:1:707:LEU:HD22	2.37	0.40
26:1:758:ASP:OD2	26:1:761:TYR:HB2	2.21	0.40
26:1:840:LEU:O	26:1:844:VAL:HG23	2.21	0.40
26:1:850:ILE:HG22	26:1:888:LEU:HD11	2.02	0.40
26:1:912:ASN:OD1	26:1:912:ASN:N	2.53	0.40
27:3:180:PRO:HD2	27:3:215:LEU:HD11	2.03	0.40
27:3:346:PHE:HB3	27:3:359:TYR:O	2.22	0.40
27:3:1114:SER:HB2	27:3:1215:TYR:HE1	1.83	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	2232/2335 (96%)	1971 (88%)	250 (11%)	11 (0%)	29	68
3	C	854/972 (88%)	737 (86%)	110 (13%)	7 (1%)	19	57
4	D	1720/2136 (80%)	1589 (92%)	124 (7%)	7 (0%)	34	72
5	E	297/357 (83%)	271 (91%)	26 (9%)	0	100	100
9	I	563/855 (66%)	481 (85%)	80 (14%)	2 (0%)	34	72
10	J	245/848 (29%)	215 (88%)	27 (11%)	3 (1%)	13	48
11	K	47/343 (14%)	41 (87%)	6 (13%)	0	100	100
12	L	318/802 (40%)	294 (92%)	24 (8%)	0	100	100
13	N	141/144 (98%)	119 (84%)	21 (15%)	1 (1%)	22	60
14	O	288/420 (69%)	242 (84%)	46 (16%)	0	100	100
15	P	97/229 (42%)	85 (88%)	11 (11%)	1 (1%)	15	53
16	Q	1319/1485 (89%)	1207 (92%)	112 (8%)	0	100	100
17	R	352/536 (66%)	314 (89%)	36 (10%)	2 (1%)	25	64
18	S	156/166 (94%)	147 (94%)	9 (6%)	0	100	100
19	T	318/514 (62%)	289 (91%)	29 (9%)	0	100	100
20	U	68/2752 (2%)	62 (91%)	6 (9%)	0	100	100
21	V	458/908 (50%)	430 (94%)	28 (6%)	0	100	100
22	W	497/579 (86%)	442 (89%)	55 (11%)	0	100	100
23	X	778/1041 (75%)	691 (89%)	82 (10%)	5 (1%)	25	64
24	Y	318/492 (65%)	277 (87%)	41 (13%)	0	100	100
25	Z	147/225 (65%)	132 (90%)	13 (9%)	2 (1%)	11	43
26	1	814/1304 (62%)	705 (87%)	105 (13%)	4 (0%)	29	68
27	3	1165/1217 (96%)	991 (85%)	173 (15%)	1 (0%)	51	85
28	p	163/225 (72%)	147 (90%)	15 (9%)	1 (1%)	25	64
29	w	428/501 (85%)	380 (89%)	48 (11%)	0	100	100
30	2	246/895 (28%)	212 (86%)	33 (13%)	1 (0%)	34	72
31	4	157/424 (37%)	138 (88%)	19 (12%)	0	100	100
32	7	79/110 (72%)	65 (82%)	14 (18%)	0	100	100
33	5	75/86 (87%)	64 (85%)	11 (15%)	0	100	100
34	y	77/301 (26%)	64 (83%)	13 (17%)	0	100	100
35	v	165/464 (36%)	149 (90%)	16 (10%)	0	100	100
36	o	160/255 (63%)	136 (85%)	24 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	c	95/118 (80%)	85 (90%)	10 (10%)	0	100	100
37	h	91/118 (77%)	82 (90%)	9 (10%)	0	100	100
38	d	72/86 (84%)	63 (88%)	9 (12%)	0	100	100
38	i	70/86 (81%)	64 (91%)	6 (9%)	0	100	100
39	a	84/240 (35%)	71 (84%)	13 (16%)	0	100	100
39	m	80/240 (33%)	72 (90%)	8 (10%)	0	100	100
40	g	77/126 (61%)	69 (90%)	8 (10%)	0	100	100
40	l	81/126 (64%)	70 (86%)	11 (14%)	0	100	100
41	f	72/76 (95%)	61 (85%)	11 (15%)	0	100	100
41	k	71/76 (93%)	63 (89%)	8 (11%)	0	100	100
42	e	77/92 (84%)	71 (92%)	6 (8%)	0	100	100
42	j	79/92 (86%)	73 (92%)	6 (8%)	0	100	100
43	b	80/119 (67%)	65 (81%)	15 (19%)	0	100	100
43	n	78/119 (66%)	67 (86%)	11 (14%)	0	100	100
44	u	183/793 (23%)	170 (93%)	13 (7%)	0	100	100
45	q	130/504 (26%)	116 (89%)	14 (11%)	0	100	100
45	r	129/504 (26%)	119 (92%)	10 (8%)	0	100	100
45	s	130/504 (26%)	107 (82%)	20 (15%)	3 (2%)	6	30
45	t	129/504 (26%)	120 (93%)	9 (7%)	0	100	100
46	9	330/520 (64%)	292 (88%)	38 (12%)	0	100	100
All	All	16880/28964 (58%)	14987 (89%)	1842 (11%)	51 (0%)	44	76

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	R	164	PRO
17	R	223	PRO
23	X	820	VAL
1	A	699	GLU
1	A	1417	PRO
3	C	83	GLU
3	C	824	THR
4	D	2098	ALA
4	D	2099	THR
10	J	241	VAL

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Mol	Chain	Res	Type
23	X	851	ASN
26	1	1107	GLN
1	A	698	PRO
1	A	856	LEU
1	A	1548	TYR
1	A	1765	SER
3	C	359	LYS
4	D	1584	ILE
9	I	371	PRO
13	N	40	LYS
23	X	993	THR
26	1	718	PRO
26	1	1106	ARG
1	A	1418	ARG
4	D	1007	PRO
10	J	358	GLU
23	X	523	HIS
23	X	992	THR
25	Z	66	MET
25	Z	78	PRO
26	1	717	THR
1	A	570	ASP
1	A	942	PRO
3	C	440	SER
4	D	1666	THR
9	I	428	GLN
30	2	600	ARG
45	s	60	PRO
1	A	189	GLU
3	C	441	PRO
15	P	48	GLN
28	p	214	PRO
45	s	71	ILE
3	C	444	GLY
4	D	2097	PRO
10	J	341	PRO
27	3	672	GLY
4	D	531	ILE
1	A	2311	PRO
3	C	615	PRO
45	s	72	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	2012/2108 (95%)	1683 (84%)	329 (16%)	2 11
3	C	747/866 (86%)	612 (82%)	135 (18%)	1 9
5	E	256/300 (85%)	209 (82%)	47 (18%)	1 9
9	I	22/749 (3%)	22 (100%)	0	100 100
10	J	205/751 (27%)	175 (85%)	30 (15%)	3 15
11	K	43/294 (15%)	37 (86%)	6 (14%)	3 16
12	L	141/709 (20%)	119 (84%)	22 (16%)	2 13
13	N	130/130 (100%)	111 (85%)	19 (15%)	3 15
14	O	3/361 (1%)	3 (100%)	0	100 100
15	P	95/203 (47%)	73 (77%)	22 (23%)	1 4
16	Q	71/1336 (5%)	71 (100%)	0	100 100
17	R	268/458 (58%)	214 (80%)	54 (20%)	1 6
19	T	273/441 (62%)	224 (82%)	49 (18%)	2 9
20	U	21/2432 (1%)	17 (81%)	4 (19%)	1 8
21	V	188/838 (22%)	159 (85%)	29 (15%)	2 13
23	X	682/897 (76%)	560 (82%)	122 (18%)	2 9
24	Y	286/451 (63%)	243 (85%)	43 (15%)	3 14
26	1	700/1104 (63%)	598 (85%)	102 (15%)	3 15
27	3	1018/1051 (97%)	809 (80%)	209 (20%)	1 6
28	p	8/195 (4%)	8 (100%)	0	100 100
29	w	112/446 (25%)	93 (83%)	19 (17%)	2 10
30	2	152/776 (20%)	126 (83%)	26 (17%)	2 10
32	7	69/95 (73%)	47 (68%)	22 (32%)	0 1
33	5	68/77 (88%)	53 (78%)	15 (22%)	1 4
35	v	78/382 (20%)	67 (86%)	11 (14%)	3 16
36	o	6/218 (3%)	6 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
37	h	5/110 (4%)	5 (100%)	0	100 100
38	i	4/74 (5%)	4 (100%)	0	100 100
39	m	4/177 (2%)	4 (100%)	0	100 100
40	l	3/101 (3%)	3 (100%)	0	100 100
41	k	3/66 (4%)	3 (100%)	0	100 100
42	j	1/84 (1%)	1 (100%)	0	100 100
43	n	3/101 (3%)	3 (100%)	0	100 100
44	u	10/709 (1%)	10 (100%)	0	100 100
46	9	185/456 (41%)	147 (80%)	38 (20%)	1 6
All	All	7872/19546 (40%)	6519 (83%)	1353 (17%)	5 10

All (1353) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	GLU
1	A	28	GLU
1	A	29	LYS
1	A	37	TRP
1	A	44	ARG
1	A	60	ASP
1	A	66	VAL
1	A	71	ARG
1	A	78	ASN
1	A	79	ARG
1	A	86	ARG
1	A	88	TYR
1	A	89	LEU
1	A	95	MET
1	A	97	HIS
1	A	111	GLU
1	A	112	GLN
1	A	123	THR
1	A	127	SER
1	A	131	GLU
1	A	142	SER
1	A	155	LYS
1	A	161	PHE
1	A	176	LEU
1	A	177	ASP

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Mol	Chain	Res	Type
1	A	184	ASP
1	A	188	LEU
1	A	195	LEU
1	A	204	LEU
1	A	214	ARG
1	A	216	SER
1	A	227	ARG
1	A	230	PHE
1	A	231	THR
1	A	239	TYR
1	A	248	ASP
1	A	250	VAL
1	A	258	PHE
1	A	261	LYS
1	A	266	SER
1	A	271	MET
1	A	284	ARG
1	A	313	LYS
1	A	322	ASN
1	A	323	LEU
1	A	329	LEU
1	A	330	THR
1	A	337	VAL
1	A	338	VAL
1	A	339	PHE
1	A	340	ILE
1	A	342	THR
1	A	343	GLU
1	A	355	LEU
1	A	356	ILE
1	A	361	HIS
1	A	363	HIS
1	A	376	GLU
1	A	385	GLU
1	A	387	PHE
1	A	391	THR
1	A	395	THR
1	A	398	THR
1	A	404	LEU
1	A	422	LEU
1	A	431	TYR
1	A	433	GLU

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Mol	Chain	Res	Type
1	A	439	GLN
1	A	460	LYS
1	A	468	LYS
1	A	479	THR
1	A	480	LYS
1	A	484	SER
1	A	492	VAL
1	A	495	GLN
1	A	515	TYR
1	A	531	THR
1	A	546	LEU
1	A	554	THR
1	A	556	LEU
1	A	569	VAL
1	A	574	LEU
1	A	576	ASP
1	A	587	GLN
1	A	593	ARG
1	A	595	LYS
1	A	604	MET
1	A	618	THR
1	A	644	ILE
1	A	665	SER
1	A	666	LYS
1	A	673	THR
1	A	679	SER
1	A	683	LEU
1	A	686	ARG
1	A	690	MET
1	A	693	ILE
1	A	694	LEU
1	A	728	VAL
1	A	733	THR
1	A	751	THR
1	A	766	THR
1	A	769	LYS
1	A	802	THR
1	A	819	SER
1	A	830	LEU
1	A	831	SER
1	A	833	LYS
1	A	835	ASP

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Mol	Chain	Res	Type
1	A	836	THR
1	A	839	LEU
1	A	845	ARG
1	A	854	SER
1	A	855	ARG
1	A	856	LEU
1	A	859	SER
1	A	861	ARG
1	A	866	LEU
1	A	871	TYR
1	A	885	LEU
1	A	887	THR
1	A	889	ARG
1	A	893	GLU
1	A	914	LEU
1	A	916	LYS
1	A	931	ASP
1	A	933	ARG
1	A	940	ILE
1	A	941	LYS
1	A	946	GLU
1	A	977	LEU
1	A	978	GLU
1	A	1000	ILE
1	A	1010	THR
1	A	1014	ASN
1	A	1018	ASN
1	A	1022	MET
1	A	1027	SER
1	A	1030	ILE
1	A	1032	ARG
1	A	1038	SER
1	A	1070	ASP
1	A	1076	ASP
1	A	1079	THR
1	A	1089	CYS
1	A	1104	ASP
1	A	1122	ASN
1	A	1123	GLU
1	A	1126	VAL
1	A	1128	TYR
1	A	1130	ASN

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Mol	Chain	Res	Type
1	A	1131	LYS
1	A	1143	MET
1	A	1144	LYS
1	A	1147	VAL
1	A	1158	LYS
1	A	1163	ARG
1	A	1166	THR
1	A	1173	SER
1	A	1181	ASP
1	A	1186	LEU
1	A	1189	MET
1	A	1200	CYS
1	A	1205	GLU
1	A	1207	PHE
1	A	1210	LYS
1	A	1223	GLU
1	A	1243	ARG
1	A	1276	GLU
1	A	1286	ASP
1	A	1293	ASN
1	A	1298	ARG
1	A	1306	LYS
1	A	1321	GLU
1	A	1339	ASP
1	A	1348	VAL
1	A	1367	ASN
1	A	1370	ARG
1	A	1372	ILE
1	A	1376	GLU
1	A	1377	SER
1	A	1382	SER
1	A	1383	GLN
1	A	1394	GLN
1	A	1399	GLN
1	A	1402	ARG
1	A	1407	ASP
1	A	1409	GLU
1	A	1413	ASP
1	A	1419	ILE
1	A	1427	ARG
1	A	1437	ARG
1	A	1441	ASP

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Mol	Chain	Res	Type
1	A	1449	LYS
1	A	1450	GLN
1	A	1458	GLN
1	A	1459	ARG
1	A	1467	LEU
1	A	1489	LEU
1	A	1491	LYS
1	A	1494	TYR
1	A	1515	TRP
1	A	1516	LYS
1	A	1518	LEU
1	A	1526	LEU
1	A	1527	ASN
1	A	1532	ARG
1	A	1533	ARG
1	A	1536	LEU
1	A	1539	SER
1	A	1554	GLN
1	A	1555	LEU
1	A	1558	THR
1	A	1568	THR
1	A	1575	GLN
1	A	1600	GLU
1	A	1601	LEU
1	A	1606	ILE
1	A	1608	THR
1	A	1615	HIS
1	A	1622	MET
1	A	1623	ASN
1	A	1630	LEU
1	A	1631	LEU
1	A	1635	TYR
1	A	1640	SER
1	A	1653	ASP
1	A	1655	THR
1	A	1660	TYR
1	A	1664	ILE
1	A	1667	ARG
1	A	1672	ASP
1	A	1675	ASP
1	A	1691	ASN
1	A	1697	SER

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Mol	Chain	Res	Type
1	A	1701	VAL
1	A	1702	LEU
1	A	1719	PHE
1	A	1722	SER
1	A	1723	LYS
1	A	1726	ILE
1	A	1730	MET
1	A	1756	SER
1	A	1766	GLN
1	A	1768	TYR
1	A	1771	LEU
1	A	1772	PHE
1	A	1775	GLN
1	A	1776	ILE
1	A	1780	VAL
1	A	1782	ASP
1	A	1787	ARG
1	A	1788	VAL
1	A	1789	THR
1	A	1790	ILE
1	A	1792	LYS
1	A	1793	THR
1	A	1794	PHE
1	A	1798	LEU
1	A	1804	ASN
1	A	1811	ASN
1	A	1813	ARG
1	A	1817	LEU
1	A	1820	LYS
1	A	1825	SER
1	A	1830	GLN
1	A	1840	LYS
1	A	1843	GLU
1	A	1852	LEU
1	A	1862	ILE
1	A	1870	ASP
1	A	1876	LEU
1	A	1878	ASP
1	A	1887	SER
1	A	1888	GLU
1	A	1890	GLN
1	A	1894	GLN

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Mol	Chain	Res	Type
1	A	1919	LEU
1	A	1926	THR
1	A	1930	TYR
1	A	1934	SER
1	A	1944	HIS
1	A	1947	ASN
1	A	1965	HIS
1	A	1971	LEU
1	A	1972	THR
1	A	1976	TRP
1	A	1977	ILE
1	A	1981	VAL
1	A	1997	VAL
1	A	1999	VAL
1	A	2002	LEU
1	A	2005	SER
1	A	2009	ASP
1	A	2073	TRP
1	A	2084	HIS
1	A	2086	ARG
1	A	2087	THR
1	A	2095	ASP
1	A	2105	ILE
1	A	2106	LEU
1	A	2112	LYS
1	A	2140	LYS
1	A	2156	THR
1	A	2159	LEU
1	A	2173	GLU
1	A	2200	MET
1	A	2207	ASP
1	A	2211	THR
1	A	2214	ILE
1	A	2216	CYS
1	A	2224	THR
1	A	2225	LEU
1	A	2254	SER
1	A	2257	GLU
1	A	2259	VAL
1	A	2261	MET
1	A	2263	LEU
1	A	2265	ASP

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Mol	Chain	Res	Type
1	A	2266	ARG
1	A	2268	LEU
1	A	2270	PHE
1	A	2271	PHE
1	A	2278	SER
1	A	2290	PRO
1	A	2293	LYS
1	A	2309	HIS
1	A	2317	PHE
1	A	2320	LEU
3	C	58	VAL
3	C	65	TYR
3	C	71	GLU
3	C	76	GLU
3	C	83	GLU
3	C	84	GLU
3	C	86	THR
3	C	87	GLN
3	C	90	THR
3	C	95	LYS
3	C	97	VAL
3	C	117	ASP
3	C	122	LEU
3	C	125	ASN
3	C	133	THR
3	C	134	LEU
3	C	135	CYS
3	C	173	THR
3	C	177	ARG
3	C	179	VAL
3	C	181	ILE
3	C	187	THR
3	C	188	VAL
3	C	202	ILE
3	C	215	VAL
3	C	220	ARG
3	C	278	LEU
3	C	279	ARG
3	C	295	ASP
3	C	298	LEU
3	C	301	SER
3	C	310	SER

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Mol	Chain	Res	Type
3	C	317	CYS
3	C	320	LEU
3	C	326	ILE
3	C	327	TYR
3	C	334	ILE
3	C	342	ARG
3	C	349	PHE
3	C	353	THR
3	C	359	LYS
3	C	362	THR
3	C	365	SER
3	C	366	GLN
3	C	371	GLU
3	C	388	VAL
3	C	389	ASP
3	C	391	SER
3	C	394	ARG
3	C	404	THR
3	C	406	GLU
3	C	422	LYS
3	C	424	PHE
3	C	431	VAL
3	C	433	MET
3	C	452	THR
3	C	453	TYR
3	C	454	THR
3	C	457	VAL
3	C	458	ASP
3	C	465	MET
3	C	471	ASP
3	C	483	SER
3	C	484	THR
3	C	495	ARG
3	C	496	VAL
3	C	497	LEU
3	C	498	SER
3	C	501	ILE
3	C	510	LEU
3	C	514	TYR
3	C	522	SER
3	C	533	SER
3	C	538	HIS

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Mol	Chain	Res	Type
3	C	543	ARG
3	C	548	ASN
3	C	553	GLU
3	C	559	ILE
3	C	561	LYS
3	C	562	THR
3	C	564	THR
3	C	565	ILE
3	C	572	GLU
3	C	573	GLU
3	C	578	ARG
3	C	587	VAL
3	C	593	GLU
3	C	596	ASN
3	C	598	SER
3	C	603	MET
3	C	605	ASP
3	C	612	LYS
3	C	617	LEU
3	C	618	THR
3	C	619	THR
3	C	630	LEU
3	C	635	LEU
3	C	641	MET
3	C	642	HIS
3	C	643	ASP
3	C	661	THR
3	C	664	GLU
3	C	672	LEU
3	C	673	LYS
3	C	675	PHE
3	C	696	LEU
3	C	700	ILE
3	C	711	ARG
3	C	716	GLU
3	C	722	TYR
3	C	724	TRP
3	C	743	ASN
3	C	749	THR
3	C	750	LEU
3	C	759	LEU
3	C	766	ILE

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Mol	Chain	Res	Type
3	C	767	VAL
3	C	780	CYS
3	C	781	ASP
3	C	785	ARG
3	C	786	ASN
3	C	799	GLU
3	C	803	ARG
3	C	807	GLN
3	C	809	ILE
3	C	826	ARG
3	C	827	LEU
3	C	866	SER
3	C	875	ILE
3	C	879	ASP
3	C	900	VAL
3	C	907	VAL
3	C	916	ILE
3	C	922	GLU
3	C	928	HIS
5	E	59	ILE
5	E	65	HIS
5	E	73	LYS
5	E	79	SER
5	E	86	PHE
5	E	87	ASP
5	E	89	LEU
5	E	100	ASP
5	E	102	TYR
5	E	106	LYS
5	E	108	HIS
5	E	109	SER
5	E	117	TYR
5	E	119	THR
5	E	120	ASP
5	E	123	MET
5	E	132	THR
5	E	143	ARG
5	E	152	SER
5	E	154	VAL
5	E	166	LEU
5	E	167	VAL
5	E	173	ASP

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Mol	Chain	Res	Type
5	E	182	ARG
5	E	205	SER
5	E	209	ILE
5	E	214	ASP
5	E	232	ARG
5	E	234	HIS
5	E	236	ASP
5	E	239	THR
5	E	252	SER
5	E	255	MET
5	E	258	THR
5	E	265	ARG
5	E	267	PHE
5	E	282	HIS
5	E	284	PHE
5	E	290	ARG
5	E	304	SER
5	E	307	ARG
5	E	314	THR
5	E	320	LEU
5	E	335	PHE
5	E	338	ASP
5	E	343	ILE
5	E	350	ARG
10	J	216	ASP
10	J	219	GLU
10	J	223	TYR
10	J	239	ARG
10	J	242	ILE
10	J	244	ASN
10	J	263	SER
10	J	277	THR
10	J	285	MET
10	J	286	GLU
10	J	288	LYS
10	J	311	GLN
10	J	316	TYR
10	J	319	MET
10	J	322	MET
10	J	340	GLN
10	J	364	THR
10	J	369	PHE

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Mol	Chain	Res	Type
10	J	382	TYR
10	J	385	PHE
10	J	398	VAL
10	J	400	GLU
10	J	405	PHE
10	J	406	PHE
10	J	408	ASP
10	J	419	PHE
10	J	422	PHE
10	J	437	LYS
10	J	438	TYR
10	J	441	ASP
11	K	197	TYR
11	K	202	CYS
11	K	215	ASP
11	K	218	LYS
11	K	222	ASP
11	K	226	TYR
12	L	33	ARG
12	L	40	ARG
12	L	45	GLN
12	L	49	ARG
12	L	53	TRP
12	L	59	LYS
12	L	60	LYS
12	L	61	THR
12	L	63	TRP
12	L	64	SER
12	L	91	ARG
12	L	168	LYS
12	L	169	ARG
12	L	174	LYS
12	L	175	GLN
12	L	180	ARG
12	L	181	ARG
12	L	182	LEU
12	L	190	GLU
12	L	203	LYS
12	L	206	ARG
12	L	222	LEU
13	N	4	VAL
13	N	5	LYS

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Mol	Chain	Res	Type
13	N	7	SER
13	N	17	LEU
13	N	24	GLU
13	N	44	GLU
13	N	60	ILE
13	N	72	ARG
13	N	75	TYR
13	N	86	LYS
13	N	99	ASN
13	N	105	CYS
13	N	116	ASN
13	N	125	LYS
13	N	128	VAL
13	N	134	CYS
13	N	137	CYS
13	N	139	CYS
13	N	140	ARG
15	P	30	TYR
15	P	31	SER
15	P	32	SER
15	P	37	SER
15	P	39	THR
15	P	55	ARG
15	P	78	ARG
15	P	183	LYS
15	P	184	VAL
15	P	186	ARG
15	P	187	ARG
15	P	189	ASP
15	P	191	ASP
15	P	192	VAL
15	P	195	LYS
15	P	204	GLN
15	P	205	LYS
15	P	206	LYS
15	P	208	LYS
15	P	215	LEU
15	P	224	MET
15	P	228	ILE
17	R	84	ASN
17	R	89	GLN
17	R	96	ILE

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Mol	Chain	Res	Type
17	R	101	ILE
17	R	104	GLN
17	R	107	SER
17	R	108	LYS
17	R	122	LYS
17	R	123	GLU
17	R	125	MET
17	R	132	LEU
17	R	134	ARG
17	R	142	GLU
17	R	143	ILE
17	R	153	LYS
17	R	170	LYS
17	R	176	TYR
17	R	180	THR
17	R	186	VAL
17	R	195	ARG
17	R	197	ILE
17	R	200	VAL
17	R	208	GLU
17	R	220	ARG
17	R	232	SER
17	R	234	SER
17	R	235	ARG
17	R	236	LYS
17	R	238	THR
17	R	247	ILE
17	R	250	CYS
17	R	286	LYS
17	R	295	ASP
17	R	309	GLU
17	R	311	LYS
17	R	316	GLU
17	R	325	ARG
17	R	327	MET
17	R	332	ARG
17	R	346	ASP
17	R	352	ARG
17	R	366	ASP
17	R	369	LEU
17	R	377	ARG
17	R	382	ARG

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Mol	Chain	Res	Type
17	R	383	ASN
17	R	385	ASN
17	R	386	ARG
17	R	398	ASN
17	R	406	GLN
17	R	407	TYR
17	R	416	LYS
17	R	433	TYR
17	R	438	ARG
19	T	187	LYS
19	T	196	LEU
19	T	197	TYR
19	T	200	ILE
19	T	221	THR
19	T	223	SER
19	T	227	THR
19	T	235	SER
19	T	240	LEU
19	T	255	SER
19	T	258	SER
19	T	263	SER
19	T	264	CYS
19	T	267	ASP
19	T	274	ASP
19	T	283	HIS
19	T	294	LEU
19	T	301	ASP
19	T	303	LEU
19	T	307	SER
19	T	319	THR
19	T	327	SER
19	T	338	CYS
19	T	342	GLU
19	T	349	SER
19	T	353	THR
19	T	364	THR
19	T	369	THR
19	T	374	SER
19	T	378	VAL
19	T	383	ARG
19	T	384	HIS
19	T	386	THR

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Mol	Chain	Res	Type
19	T	389	SER
19	T	393	ASP
19	T	394	ASN
19	T	397	GLN
19	T	398	TRP
19	T	421	VAL
19	T	429	SER
19	T	436	MET
19	T	443	THR
19	T	449	ARG
19	T	460	ASP
19	T	471	ASP
19	T	485	THR
19	T	491	GLU
19	T	493	ASP
19	T	498	GLU
20	U	1	MET
20	U	2	TYR
20	U	9	THR
20	U	16	ASN
21	V	450	ILE
21	V	458	THR
21	V	465	SER
21	V	470	GLU
21	V	479	MET
21	V	481	PHE
21	V	483	GLU
21	V	485	GLN
21	V	487	LYS
21	V	494	LEU
21	V	504	GLU
21	V	505	LYS
21	V	516	MET
21	V	526	GLU
21	V	538	ARG
21	V	540	GLU
21	V	545	ARG
21	V	556	TYR
21	V	593	TYR
21	V	607	THR
21	V	616	LEU
21	V	623	ASN

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Mol	Chain	Res	Type
21	V	625	ARG
21	V	628	ILE
21	V	632	THR
21	V	633	SER
21	V	646	HIS
21	V	647	LEU
21	V	648	LYS
23	X	164	TRP
23	X	166	ARG
23	X	171	ARG
23	X	176	GLU
23	X	183	GLU
23	X	186	ARG
23	X	195	ASN
23	X	217	GLU
23	X	222	MET
23	X	230	SER
23	X	232	ARG
23	X	237	LYS
23	X	241	GLU
23	X	244	GLU
23	X	245	ASP
23	X	255	PHE
23	X	257	PHE
23	X	262	LEU
23	X	266	GLU
23	X	268	GLN
23	X	270	LEU
23	X	274	ARG
23	X	276	VAL
23	X	278	ASP
23	X	292	LEU
23	X	300	MET
23	X	328	ARG
23	X	333	ARG
23	X	334	LEU
23	X	339	LEU
23	X	384	THR
23	X	389	LYS
23	X	420	ILE
23	X	426	SER
23	X	428	LYS

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Mol	Chain	Res	Type
23	X	444	LYS
23	X	467	ARG
23	X	471	VAL
23	X	473	LEU
23	X	476	GLU
23	X	493	LEU
23	X	503	ARG
23	X	520	ASP
23	X	524	GLU
23	X	533	PHE
23	X	542	PHE
23	X	545	GLU
23	X	552	SER
23	X	575	ARG
23	X	579	VAL
23	X	597	VAL
23	X	599	VAL
23	X	606	GLN
23	X	612	LEU
23	X	621	ILE
23	X	633	ARG
23	X	640	ARG
23	X	645	LEU
23	X	648	TYR
23	X	654	ASP
23	X	656	GLN
23	X	658	ARG
23	X	663	THR
23	X	672	VAL
23	X	674	THR
23	X	698	LYS
23	X	699	SER
23	X	706	MET
23	X	712	THR
23	X	725	ARG
23	X	729	VAL
23	X	749	GLU
23	X	755	ILE
23	X	757	ARG
23	X	758	THR
23	X	760	LEU
23	X	763	VAL

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Mol	Chain	Res	Type
23	X	767	LEU
23	X	768	LYS
23	X	772	ILE
23	X	773	HIS
23	X	787	GLU
23	X	809	THR
23	X	813	ARG
23	X	815	MET
23	X	817	GLU
23	X	818	LEU
23	X	823	MET
23	X	824	LEU
23	X	825	SER
23	X	828	ILE
23	X	842	THR
23	X	847	LEU
23	X	848	SER
23	X	850	ASN
23	X	863	HIS
23	X	877	ASP
23	X	879	LEU
23	X	886	THR
23	X	894	SER
23	X	909	ARG
23	X	912	ARG
23	X	915	ARG
23	X	924	ARG
23	X	927	VAL
23	X	932	CYS
23	X	933	GLN
23	X	943	ILE
23	X	944	THR
23	X	951	THR
23	X	954	LEU
23	X	955	THR
23	X	956	ARG
23	X	973	ASN
23	X	974	SER
23	X	976	LEU
23	X	979	GLN
23	X	988	GLU
23	X	991	LEU

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Mol	Chain	Res	Type
23	X	994	LYS
23	X	997	MET
23	X	1021	LEU
24	Y	16	LEU
24	Y	17	TYR
24	Y	18	THR
24	Y	23	ARG
24	Y	40	CYS
24	Y	41	LEU
24	Y	53	THR
24	Y	65	SER
24	Y	66	ILE
24	Y	79	GLU
24	Y	86	ILE
24	Y	93	THR
24	Y	118	TYR
24	Y	126	PHE
24	Y	129	VAL
24	Y	130	THR
24	Y	147	ASP
24	Y	154	ILE
24	Y	159	THR
24	Y	162	LEU
24	Y	176	ASP
24	Y	183	ARG
24	Y	188	SER
24	Y	194	ASP
24	Y	198	ASP
24	Y	200	PHE
24	Y	203	ARG
24	Y	210	GLU
24	Y	211	ILE
24	Y	216	GLU
24	Y	219	THR
24	Y	227	VAL
24	Y	234	ASP
24	Y	243	PHE
24	Y	245	CYS
24	Y	250	VAL
24	Y	253	ASP
24	Y	263	PHE
24	Y	273	ARG

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Mol	Chain	Res	Type
24	Y	309	ARG
24	Y	312	HIS
24	Y	316	SER
24	Y	318	SER
26	1	493	LYS
26	1	512	ARG
26	1	544	LEU
26	1	545	GLU
26	1	554	LYS
26	1	558	ARG
26	1	560	LEU
26	1	562	LYS
26	1	563	LEU
26	1	564	ASP
26	1	566	LEU
26	1	568	ARG
26	1	571	VAL
26	1	573	LYS
26	1	581	LEU
26	1	582	LEU
26	1	585	GLU
26	1	598	SER
26	1	610	ILE
26	1	623	TYR
26	1	630	ARG
26	1	673	ILE
26	1	685	SER
26	1	686	LEU
26	1	698	GLN
26	1	707	LEU
26	1	719	TYR
26	1	721	ILE
26	1	736	ARG
26	1	739	ARG
26	1	754	ILE
26	1	760	GLU
26	1	768	GLU
26	1	779	SER
26	1	794	GLN
26	1	795	CYS
26	1	801	VAL
26	1	827	ARG

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Mol	Chain	Res	Type
26	1	836	THR
26	1	844	VAL
26	1	858	LYS
26	1	873	GLU
26	1	890	GLU
26	1	892	LEU
26	1	893	ILE
26	1	901	GLN
26	1	904	THR
26	1	925	VAL
26	1	926	LYS
26	1	928	TYR
26	1	946	LYS
26	1	947	VAL
26	1	958	THR
26	1	964	THR
26	1	967	GLU
26	1	968	GLU
26	1	971	MET
26	1	973	HIS
26	1	982	LEU
26	1	1003	VAL
26	1	1009	MET
26	1	1010	THR
26	1	1014	LYS
26	1	1015	ASP
26	1	1019	ARG
26	1	1021	THR
26	1	1028	HIS
26	1	1029	GLU
26	1	1030	LYS
26	1	1031	VAL
26	1	1032	GLN
26	1	1041	ARG
26	1	1048	GLU
26	1	1065	LEU
26	1	1067	LYS
26	1	1080	THR
26	1	1092	ASP
26	1	1104	GLN
26	1	1106	ARG
26	1	1112	THR

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Mol	Chain	Res	Type
26	1	1113	THR
26	1	1122	THR
26	1	1138	VAL
26	1	1143	VAL
26	1	1150	SER
26	1	1164	ASP
26	1	1170	THR
26	1	1174	GLU
26	1	1182	LEU
26	1	1196	SER
26	1	1200	TYR
26	1	1219	VAL
26	1	1245	ARG
26	1	1250	CYS
26	1	1260	LYS
26	1	1276	SER
26	1	1277	GLN
26	1	1281	ILE
26	1	1292	LYS
26	1	1296	ILE
26	1	1303	ILE
26	1	1304	LEU
27	3	1	MET
27	3	9	GLN
27	3	18	ILE
27	3	25	THR
27	3	33	SER
27	3	36	LYS
27	3	41	LEU
27	3	44	ASP
27	3	52	THR
27	3	56	VAL
27	3	66	MET
27	3	68	PHE
27	3	74	THR
27	3	76	ASP
27	3	78	ILE
27	3	90	LEU
27	3	92	TYR
27	3	98	MET
27	3	106	THR
27	3	110	SER

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Mol	Chain	Res	Type
27	3	116	VAL
27	3	121	LEU
27	3	124	ASP
27	3	126	LYS
27	3	130	VAL
27	3	131	MET
27	3	133	SER
27	3	139	LYS
27	3	143	ILE
27	3	153	THR
27	3	164	ASN
27	3	170	VAL
27	3	173	VAL
27	3	184	CYS
27	3	188	ASP
27	3	195	ASP
27	3	203	ASN
27	3	204	THR
27	3	207	THR
27	3	209	THR
27	3	221	VAL
27	3	222	ARG
27	3	225	SER
27	3	226	GLU
27	3	230	GLU
27	3	233	ASN
27	3	242	SER
27	3	256	ILE
27	3	261	PHE
27	3	263	ASP
27	3	264	GLN
27	3	266	ASP
27	3	271	ILE
27	3	273	ARG
27	3	275	ARG
27	3	282	GLU
27	3	286	ILE
27	3	287	PHE
27	3	294	LYS
27	3	300	PHE
27	3	315	LEU
27	3	317	THR

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Mol	Chain	Res	Type
27	3	318	ASP
27	3	320	ASP
27	3	327	LEU
27	3	330	PHE
27	3	331	ASP
27	3	332	THR
27	3	340	CYS
27	3	343	LYS
27	3	344	THR
27	3	347	LEU
27	3	355	ASN
27	3	356	HIS
27	3	364	LEU
27	3	384	THR
27	3	390	ARG
27	3	392	LEU
27	3	403	SER
27	3	404	LEU
27	3	408	LEU
27	3	411	GLN
27	3	417	ASN
27	3	419	ASP
27	3	427	CYS
27	3	433	SER
27	3	435	LEU
27	3	439	ARG
27	3	443	GLU
27	3	455	ASN
27	3	461	THR
27	3	464	ARG
27	3	465	HIS
27	3	469	GLU
27	3	471	ASP
27	3	475	ILE
27	3	477	SER
27	3	482	THR
27	3	492	GLU
27	3	510	LEU
27	3	511	LEU
27	3	514	ASP
27	3	526	HIS
27	3	527	ILE

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Mol	Chain	Res	Type
27	3	537	LYS
27	3	543	THR
27	3	544	ILE
27	3	547	CYS
27	3	568	MET
27	3	573	GLN
27	3	574	LEU
27	3	580	ARG
27	3	584	SER
27	3	592	LEU
27	3	594	ASN
27	3	595	VAL
27	3	603	ARG
27	3	604	PHE
27	3	605	LEU
27	3	612	ASN
27	3	617	ILE
27	3	620	ASP
27	3	630	MET
27	3	638	GLU
27	3	665	LEU
27	3	669	LEU
27	3	676	ARG
27	3	677	THR
27	3	679	LEU
27	3	685	ASP
27	3	689	THR
27	3	697	ARG
27	3	703	ARG
27	3	704	VAL
27	3	715	MET
27	3	727	SER
27	3	732	THR
27	3	738	THR
27	3	743	SER
27	3	758	SER
27	3	768	GLU
27	3	775	ASN
27	3	776	GLN
27	3	786	ARG
27	3	797	LEU
27	3	798	ILE

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Mol	Chain	Res	Type
27	3	802	THR
27	3	814	GLN
27	3	815	ARG
27	3	822	GLU
27	3	834	LEU
27	3	837	GLU
27	3	842	PHE
27	3	850	SER
27	3	851	ILE
27	3	867	ARG
27	3	876	THR
27	3	882	LEU
27	3	883	GLU
27	3	901	GLU
27	3	902	ASP
27	3	904	TYR
27	3	906	LEU
27	3	927	THR
27	3	931	VAL
27	3	936	LYS
27	3	937	LEU
27	3	941	HIS
27	3	942	LYS
27	3	958	ARG
27	3	961	ILE
27	3	966	LEU
27	3	978	LEU
27	3	981	CYS
27	3	988	ASN
27	3	991	SER
27	3	993	ILE
27	3	995	THR
27	3	996	ILE
27	3	998	HIS
27	3	1002	VAL
27	3	1004	ASP
27	3	1012	VAL
27	3	1022	ILE
27	3	1026	ASP
27	3	1028	THR
27	3	1035	THR
27	3	1042	ASP

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Mol	Chain	Res	Type
27	3	1062	THR
27	3	1066	VAL
27	3	1090	GLU
27	3	1093	MET
27	3	1094	ASN
27	3	1099	GLU
27	3	1103	SER
27	3	1107	THR
27	3	1114	SER
27	3	1116	SER
27	3	1118	VAL
27	3	1120	THR
27	3	1121	THR
27	3	1148	LEU
27	3	1150	SER
27	3	1151	GLU
27	3	1166	TYR
27	3	1168	PHE
27	3	1170	VAL
27	3	1183	ASN
27	3	1217	PHE
29	w	390	LYS
29	w	400	HIS
29	w	403	ASN
29	w	414	TYR
29	w	415	THR
29	w	425	HIS
29	w	430	ARG
29	w	433	HIS
29	w	436	ARG
29	w	437	CYS
29	w	446	PHE
29	w	453	GLU
29	w	458	LEU
29	w	468	SER
29	w	471	TRP
29	w	475	THR
29	w	487	VAL
29	w	493	GLU
29	w	500	LEU
30	2	451	LYS
30	2	456	ARG

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Mol	Chain	Res	Type
30	2	460	PHE
30	2	461	THR
30	2	464	GLU
30	2	465	LEU
30	2	471	ARG
30	2	475	VAL
30	2	477	MET
30	2	479	ASP
30	2	488	LEU
30	2	494	THR
30	2	497	SER
30	2	502	ARG
30	2	509	LYS
30	2	512	GLN
30	2	517	ILE
30	2	526	ASP
30	2	531	THR
30	2	555	GLU
30	2	557	VAL
30	2	561	MET
30	2	590	LEU
30	2	595	LYS
30	2	705	ARG
30	2	710	GLU
32	7	9	ILE
32	7	11	CYS
32	7	12	ARG
32	7	14	GLN
32	7	23	CYS
32	7	25	LYS
32	7	29	LYS
32	7	30	CYS
32	7	33	CYS
32	7	35	SER
32	7	37	VAL
32	7	40	CYS
32	7	45	ILE
32	7	48	GLU
32	7	60	ILE
32	7	68	ASP
32	7	70	TYR
32	7	71	TYR

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Mol	Chain	Res	Type
32	7	72	CYS
32	7	74	GLU
32	7	81	ASP
32	7	89	VAL
33	5	5	TYR
33	5	18	TYR
33	5	23	HIS
33	5	25	ASP
33	5	27	THR
33	5	32	LEU
33	5	35	GLN
33	5	36	HIS
33	5	42	SER
33	5	51	ASN
33	5	60	SER
33	5	63	ARG
33	5	65	ARG
33	5	69	MET
33	5	74	GLN
35	v	10	LYS
35	v	20	SER
35	v	33	LEU
35	v	37	THR
35	v	45	TYR
35	v	53	SER
35	v	56	CYS
35	v	68	SER
35	v	76	LYS
35	v	77	LYS
35	v	85	ARG
46	9	199	ASN
46	9	201	ASN
46	9	213	LYS
46	9	221	LEU
46	9	241	TYR
46	9	242	SER
46	9	246	VAL
46	9	247	SER
46	9	253	THR
46	9	256	VAL
46	9	262	GLU
46	9	277	LYS

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Mol	Chain	Res	Type
46	9	287	ASN
46	9	291	LEU
46	9	295	LEU
46	9	296	HIS
46	9	298	ASP
46	9	299	LEU
46	9	309	ARG
46	9	310	LEU
46	9	313	LYS
46	9	338	THR
46	9	344	SER
46	9	346	TRP
46	9	348	LYS
46	9	355	ARG
46	9	359	SER
46	9	360	HIS
46	9	365	ILE
46	9	368	MET
46	9	385	ARG
46	9	389	TYR
46	9	393	LYS
46	9	405	ASP
46	9	407	LEU
46	9	421	ARG
46	9	429	ASP
46	9	431	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (171) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	78	ASN
1	A	121	HIS
1	A	210	HIS
1	A	300	ASN
1	A	325	HIS
1	A	326	HIS
1	A	328	HIS
1	A	357	ASN
1	A	439	GLN
1	A	467	GLN
1	A	502	ASN

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Mol	Chain	Res	Type
1	A	584	HIS
1	A	659	GLN
1	A	675	GLN
1	A	755	HIS
1	A	775	ASN
1	A	788	GLN
1	A	792	HIS
1	A	1096	HIS
1	A	1293	ASN
1	A	1337	GLN
1	A	1345	GLN
1	A	1428	HIS
1	A	1460	HIS
1	A	1527	ASN
1	A	1552	GLN
1	A	1580	HIS
1	A	1583	GLN
1	A	1623	ASN
1	A	1658	GLN
1	A	1784	ASN
1	A	1811	ASN
1	A	1830	GLN
1	A	1965	HIS
1	A	2138	GLN
1	A	2155	GLN
1	A	2241	ASN
1	A	2255	HIS
1	A	2276	GLN
3	C	82	GLN
3	C	131	ASN
3	C	140	HIS
3	C	210	ASN
3	C	245	HIS
3	C	286	ASN
3	C	306	ASN
3	C	313	GLN
3	C	350	ASN
3	C	411	ASN
3	C	548	ASN
3	C	627	HIS
3	C	706	GLN
3	C	743	ASN

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Mol	Chain	Res	Type
3	C	802	HIS
5	E	116	HIS
5	E	188	GLN
5	E	287	ASN
10	J	234	ASN
10	J	238	ASN
10	J	244	ASN
10	J	289	ASN
10	J	331	GLN
10	J	347	HIS
10	J	351	ASN
11	K	198	GLN
11	K	228	HIS
12	L	29	ASN
12	L	45	GLN
12	L	175	GLN
13	N	87	ASN
13	N	95	GLN
14	O	120	ASN
15	P	45	GLN
15	P	204	GLN
15	P	212	ASN
17	R	104	GLN
17	R	175	GLN
17	R	184	GLN
17	R	279	HIS
17	R	385	ASN
17	R	398	ASN
17	R	431	ASN
19	T	203	HIS
19	T	269	GLN
19	T	381	HIS
19	T	407	GLN
19	T	446	ASN
19	T	455	GLN
20	U	20	GLN
21	V	474	HIS
21	V	491	ASN
21	V	553	HIS
21	V	609	GLN
21	V	620	ASN
23	X	195	ASN

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Mol	Chain	Res	Type
23	X	265	HIS
23	X	268	GLN
23	X	414	ASN
23	X	475	ASN
23	X	606	GLN
23	X	656	GLN
23	X	701	ASN
23	X	720	ASN
23	X	745	HIS
23	X	866	ASN
23	X	870	ASN
23	X	904	GLN
23	X	964	GLN
23	X	971	HIS
23	X	979	GLN
23	X	987	HIS
24	Y	44	ASN
24	Y	123	HIS
24	Y	158	HIS
24	Y	312	HIS
26	1	534	GLN
26	1	550	HIS
26	1	599	ASN
26	1	682	HIS
26	1	692	HIS
26	1	763	ASN
26	1	817	HIS
26	1	829	ASN
26	1	886	HIS
26	1	1028	HIS
26	1	1032	GLN
26	1	1069	HIS
26	1	1104	GLN
26	1	1256	HIS
26	1	1277	GLN
27	3	5	ASN
27	3	19	HIS
27	3	46	ASN
27	3	145	ASN
27	3	169	HIS
27	3	179	ASN
27	3	194	ASN

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Mol	Chain	Res	Type
27	3	205	GLN
27	3	206	GLN
27	3	231	HIS
27	3	233	ASN
27	3	264	GLN
27	3	411	GLN
27	3	480	ASN
27	3	550	ASN
27	3	573	GLN
27	3	612	ASN
27	3	636	GLN
27	3	709	GLN
27	3	730	HIS
27	3	775	ASN
27	3	791	HIS
27	3	796	ASN
27	3	817	GLN
27	3	844	ASN
27	3	861	GLN
27	3	994	GLN
27	3	1019	ASN
27	3	1052	ASN
27	3	1105	GLN
27	3	1172	ASN
29	w	413	ASN
29	w	423	GLN
30	2	546	GLN
32	7	14	GLN
32	7	55	GLN
35	v	50	HIS
35	v	65	ASN
46	9	331	GLN
46	9	412	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	96/117 (82%)	33 (34%)	1 (1%)
6	F	96/107 (89%)	48 (50%)	4 (4%)
7	G	70/220 (31%)	46 (65%)	9 (12%)
8	H	163/188 (86%)	73 (44%)	6 (3%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	425/632 (67%)	200 (47%)	20 (4%)

All (200) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	9	G
2	B	10	U
2	B	20	G
2	B	21	A
2	B	22	U
2	B	23	C
2	B	24	G
2	B	25	C
2	B	40	U
2	B	44	A
2	B	47	A
2	B	48	A
2	B	52	U
2	B	57	G
2	B	62	G
2	B	65	G
2	B	68	C
2	B	70	A
2	B	71	C
2	B	88	A
2	B	89	U
2	B	90	U
2	B	92	U
2	B	93	U
2	B	94	U
2	B	95	G
2	B	96	A
2	B	97	G
2	B	102	U
2	B	106	U
2	B	109	G
2	B	116	U
2	B	117	A
6	F	6	C
6	F	7	G
6	F	9	U
6	F	10	U

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Mol	Chain	Res	Type
6	F	12	G
6	F	17	C
6	F	24	A
6	F	25	C
6	F	26	U
6	F	27	A
6	F	28	A
6	F	29	A
6	F	30	A
6	F	33	G
6	F	34	G
6	F	35	A
6	F	37	C
6	F	38	G
6	F	40	U
6	F	42	C
6	F	44	G
6	F	45	A
6	F	46	G
6	F	48	A
6	F	49	G
6	F	54	G
6	F	59	G
6	F	60	C
6	F	61	C
6	F	65	G
6	F	66	C
6	F	68	C
6	F	73	A
6	F	74	U
6	F	75	G
6	F	78	A
6	F	79	C
6	F	80	G
6	F	81	C
6	F	82	A
6	F	83	A
6	F	84	A
6	F	85	U
6	F	86	U
6	F	87	C
6	F	88	G

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Mol	Chain	Res	Type
6	F	89	U
6	F	91	A
7	G	-10	G
7	G	-9	C
7	G	-8	C
7	G	-7	U
7	G	-6	C
7	G	-5	C
7	G	-4	G
7	G	1	G
7	G	2	U
7	G	3	A
7	G	4	A
7	G	8	C
7	G	9	C
7	G	10	U
7	G	11	A
7	G	13	C
7	G	17	U
7	G	19	G
7	G	20	A
7	G	21	A
7	G	22	C
7	G	23	U
7	G	24	G
7	G	84	U
7	G	85	G
7	G	88	G
7	G	89	U
7	G	90	C
7	G	92	U
7	G	97	A
7	G	98	U
7	G	100	C
7	G	101	U
7	G	102	G
7	G	103	U
7	G	104	C
7	G	105	C
7	G	106	C
7	G	110	U
7	G	111	U

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Mol	Chain	Res	Type
7	G	112	U
7	G	113	U
7	G	114	U
7	G	115	C
7	G	116	C
7	G	117	A
8	H	2	U
8	H	13	C
8	H	14	C
8	H	15	U
8	H	16	U
8	H	17	U
8	H	18	U
8	H	19	G
8	H	23	A
8	H	24	A
8	H	29	A
8	H	30	A
8	H	31	G
8	H	33	G
8	H	34	U
8	H	35	A
8	H	44	U
8	H	45	C
8	H	46	U
8	H	47	U
8	H	48	A
8	H	49	U
8	H	53	U
8	H	63	G
8	H	64	A
8	H	65	U
8	H	70	C
8	H	74	U
8	H	80	A
8	H	81	G
8	H	82	G
8	H	84	C
8	H	98	G
8	H	99	A
8	H	100	U
8	H	101	U

Continued on next page...

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Mol	Chain	Res	Type
8	H	102	U
8	H	103	U
8	H	106	G
8	H	107	A
8	H	110	A
8	H	111	G
8	H	112	G
8	H	113	G
8	H	116	A
8	H	117	U
8	H	121	A
8	H	122	U
8	H	123	A
8	H	124	G
8	H	128	C
8	H	129	U
8	H	133	U
8	H	136	G
8	H	137	U
8	H	141	C
8	H	144	C
8	H	145	A
8	H	146	C
8	H	147	G
8	H	149	A
8	H	157	G
8	H	162	U
8	H	164	C
8	H	165	A
8	H	166	G
8	H	168	A
8	H	169	C
8	H	171	U
8	H	177	A
8	H	178	A
8	H	179	C
8	H	180	G

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	39	C

Continued on next page...

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Mol	Chain	Res	Type
6	F	37	C
6	F	47	A
6	F	48	A
6	F	58	G
7	G	21	A
7	G	84	U
7	G	88	G
7	G	89	U
7	G	101	U
7	G	105	C
7	G	110	U
7	G	111	U
7	G	113	U
8	H	13	C
8	H	18	U
8	H	43	U
8	H	45	C
8	H	47	U
8	H	165	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	SEP	R	224	17	8,9,10	1.42	1 (12%)	8,12,14	2.10	2 (25%)

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	R	224	17	-	0/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	R	224	SEP	P-O1P	3.12	1.60	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	R	224	SEP	P-OG-CB	-4.46	106.02	118.30
17	R	224	SEP	OG-CB-CA	3.47	111.52	108.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 14 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
48	GTP	C	1500	49	26,34,34	1.14	1 (3%)	32,54,54	1.91	7 (21%)
47	IHP	A	3000	-	36,36,36	1.44	6 (16%)	54,60,60	1.91	18 (33%)

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
48	GTP	C	1500	49	-	4/18/38/38	0/3/3/3
47	IHP	A	3000	-	-	8/30/54/54	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	C	1500	GTP	C5-C6	-4.13	1.39	1.47
47	A	3000	IHP	P6-O16	4.02	1.66	1.59
47	A	3000	IHP	P5-O15	2.73	1.64	1.59
47	A	3000	IHP	C5-C4	2.41	1.57	1.52
47	A	3000	IHP	C6-C5	2.31	1.57	1.52
47	A	3000	IHP	P1-O41	-2.18	1.46	1.54
47	A	3000	IHP	P2-O12	2.18	1.63	1.59

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	C	1500	GTP	PA-O3A-PB	-5.10	115.31	132.83
48	C	1500	GTP	PB-O3B-PG	-5.09	115.36	132.83
47	A	3000	IHP	O46-P6-O26	-4.04	94.87	110.68
47	A	3000	IHP	O14-C4-C5	3.70	117.41	108.69
48	C	1500	GTP	C5-C6-N1	3.42	119.98	113.95
47	A	3000	IHP	C4-C3-C2	3.39	117.83	110.41
47	A	3000	IHP	O41-P1-O21	3.37	123.88	110.68
48	C	1500	GTP	C3'-C2'-C1'	3.32	105.98	100.98
47	A	3000	IHP	C6-C1-C2	3.18	117.38	110.41
48	C	1500	GTP	C2-N1-C6	-3.14	119.32	125.10
47	A	3000	IHP	O31-P1-O21	-3.13	98.43	110.68
47	A	3000	IHP	O12-C2-C3	3.10	115.98	108.69
47	A	3000	IHP	O43-P3-O33	3.03	119.22	107.64
48	C	1500	GTP	C8-N7-C5	2.99	108.69	102.99
47	A	3000	IHP	O14-C4-C3	-2.92	101.80	108.69
47	A	3000	IHP	O12-C2-C1	2.68	114.99	108.69
47	A	3000	IHP	O36-P6-O26	2.58	120.76	110.68
47	A	3000	IHP	O41-P1-O31	2.51	117.22	107.64
47	A	3000	IHP	O13-C3-C4	2.43	114.41	108.69
47	A	3000	IHP	O15-P5-O25	-2.41	100.07	109.39
47	A	3000	IHP	O16-P6-O26	-2.31	100.47	109.39
47	A	3000	IHP	O44-P4-O34	2.31	116.47	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	C	1500	GTP	O6-C6-C5	-2.27	119.93	124.37
47	A	3000	IHP	O16-C6-C5	2.16	113.77	108.69
47	A	3000	IHP	O15-C5-C4	2.02	113.45	108.69

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
47	A	3000	IHP	C1-C6-O16-P6
47	A	3000	IHP	C5-C6-O16-P6
48	C	1500	GTP	C4'-C5'-O5'-PA
48	C	1500	GTP	C3'-C4'-C5'-O5'
48	C	1500	GTP	O4'-C4'-C5'-O5'
47	A	3000	IHP	C1-O11-P1-O41
47	A	3000	IHP	C3-O13-P3-O23
47	A	3000	IHP	C6-O16-P6-O26
47	A	3000	IHP	C2-O12-P2-O42
47	A	3000	IHP	C6-O16-P6-O36
47	A	3000	IHP	C6-O16-P6-O46
48	C	1500	GTP	C5'-O5'-PA-O1A

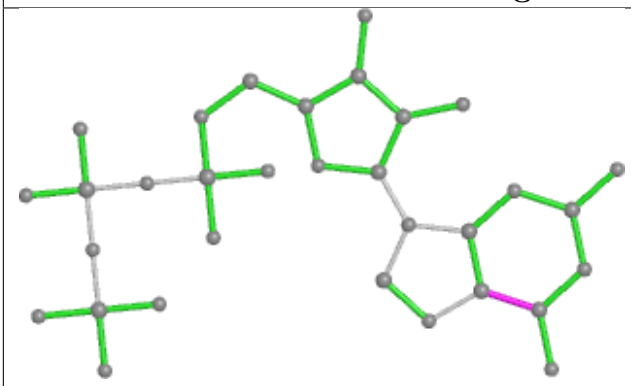
There are no ring outliers.

2 monomers are involved in 4 short contacts:

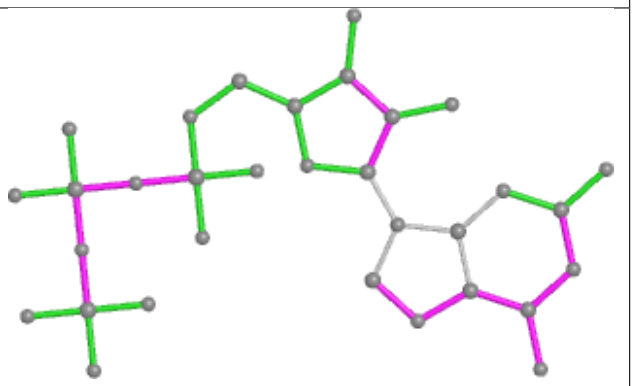
Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	C	1500	GTP	2	0
47	A	3000	IHP	2	0

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

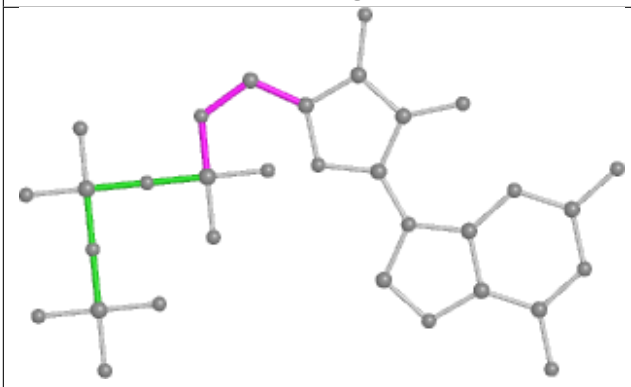
Ligand GTP C 1500



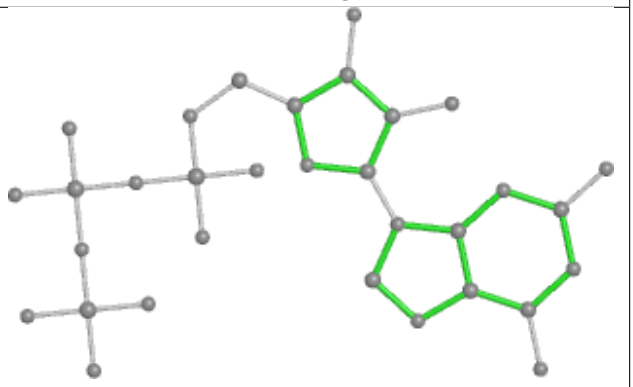
Bond lengths



Bond angles

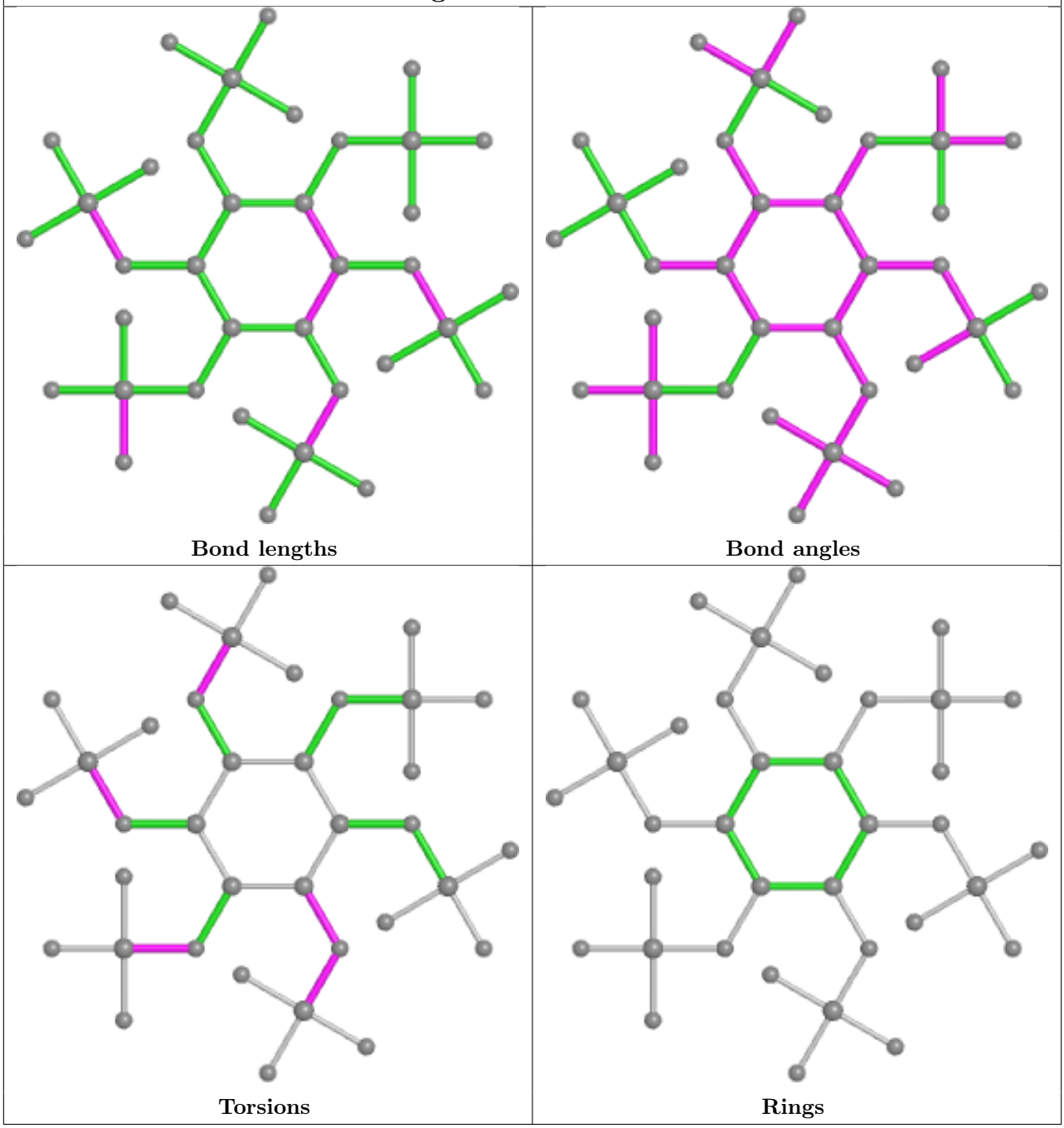


Torsions



Rings

Ligand IHP A 3000



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

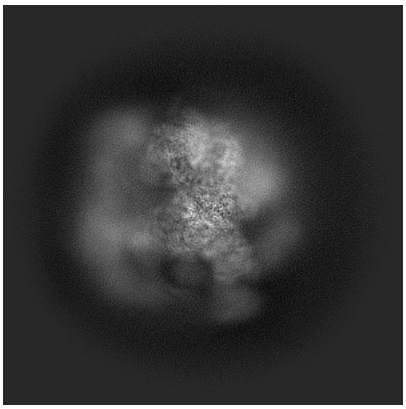
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35109. These allow visual inspection of the internal detail of the map and identification of artifacts.

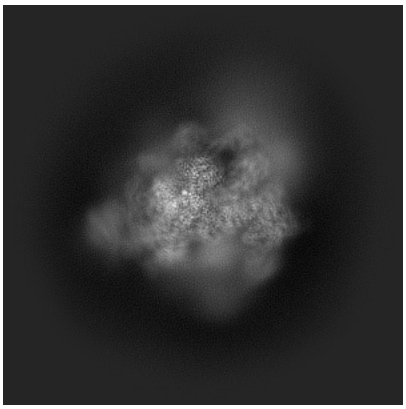
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

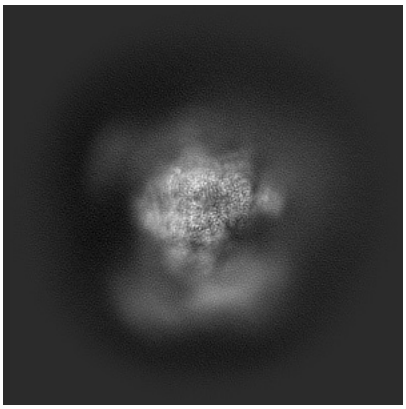
6.1.1 Primary map



X

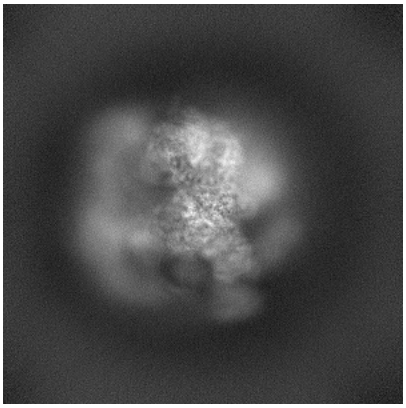


Y

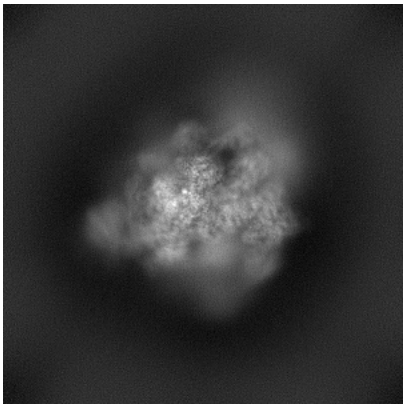


Z

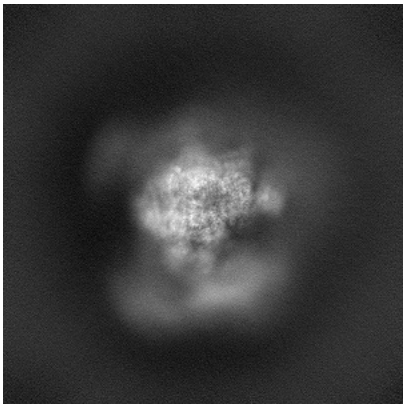
6.1.2 Raw map



X



Y

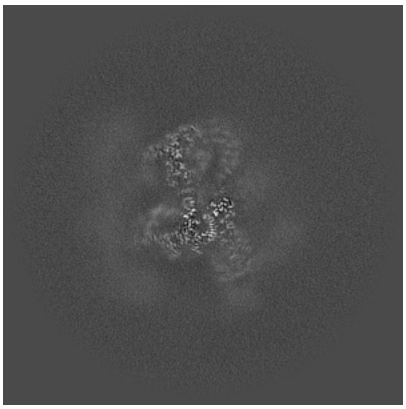


Z

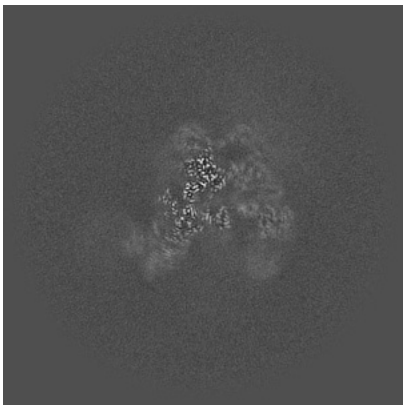
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

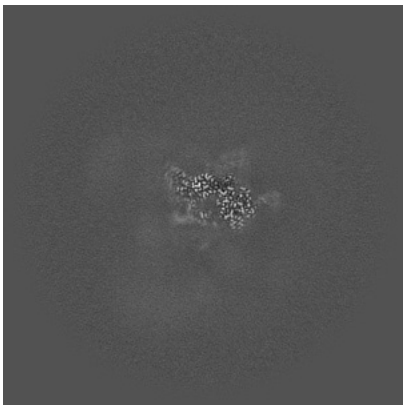
6.2.1 Primary map



X Index: 240

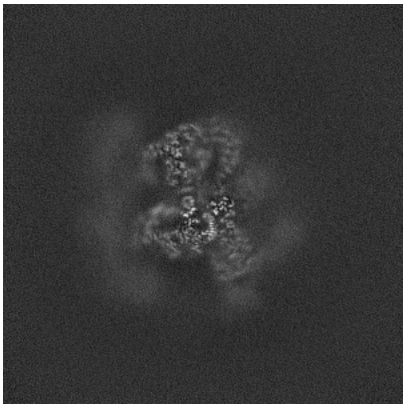


Y Index: 240

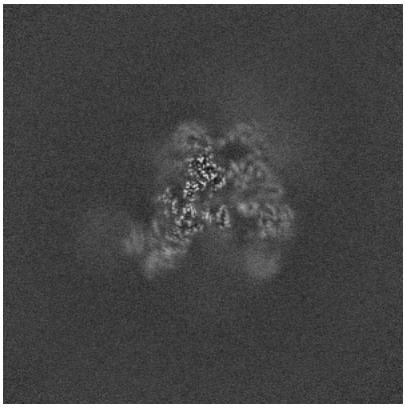


Z Index: 240

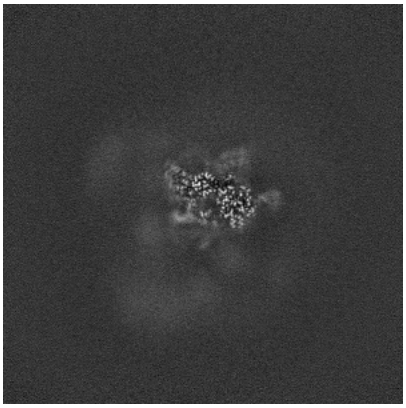
6.2.2 Raw map



X Index: 240



Y Index: 240

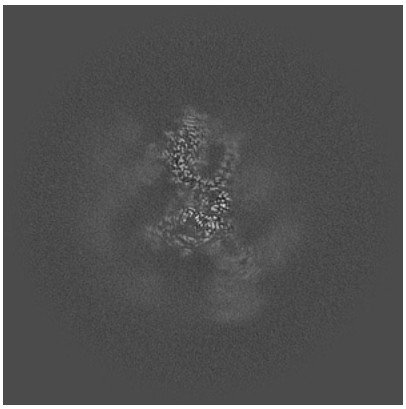


Z Index: 240

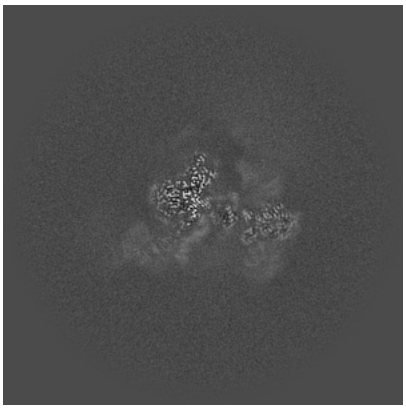
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

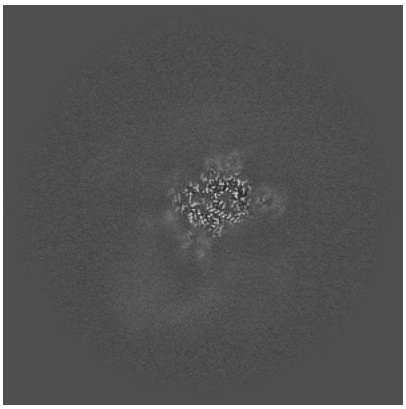
6.3.1 Primary map



X Index: 227

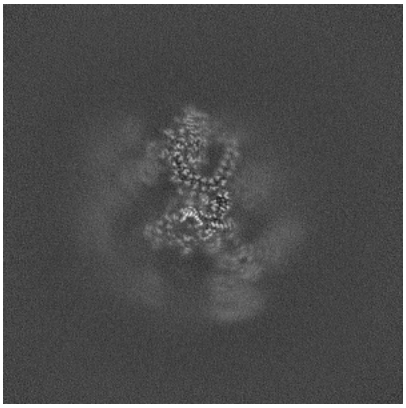


Y Index: 226

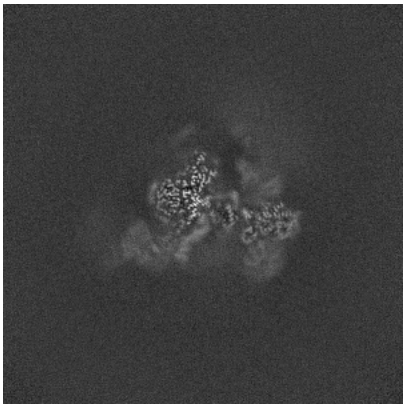


Z Index: 227

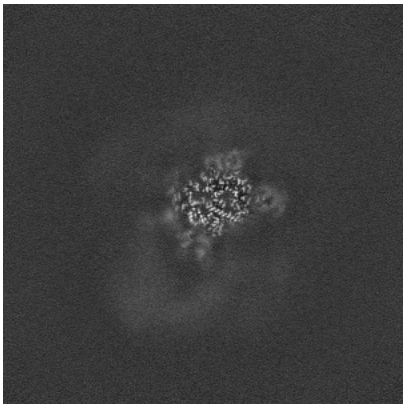
6.3.2 Raw map



X Index: 226



Y Index: 226

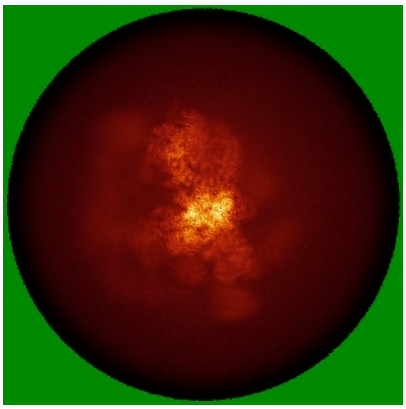


Z Index: 227

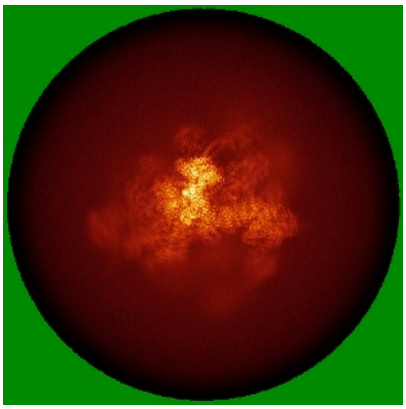
The images above show the largest variance slices of the map in three orthogonal directions.

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

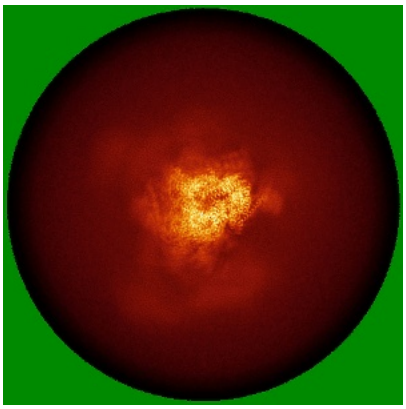
6.4.1 Primary map



X

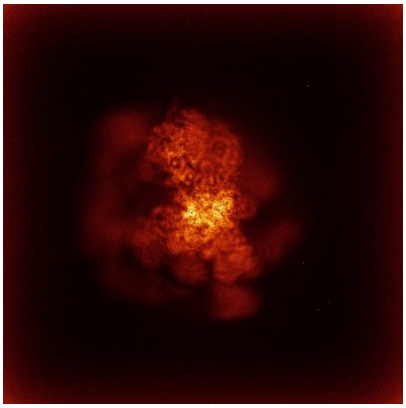


Y

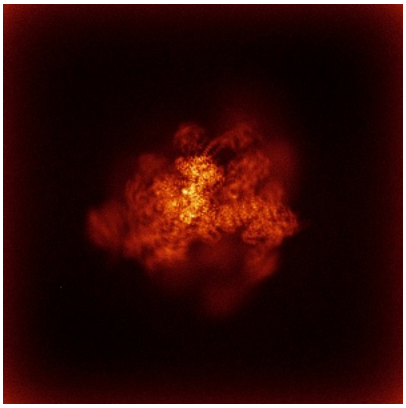


Z

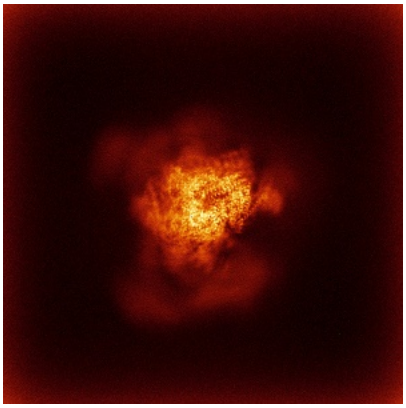
6.4.2 Raw map



X



Y

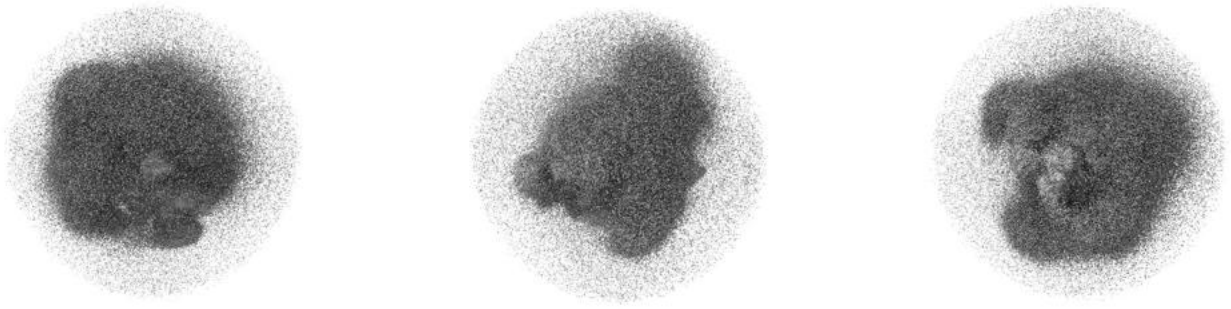


Z

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

6.5 Orthogonal surface views (i)

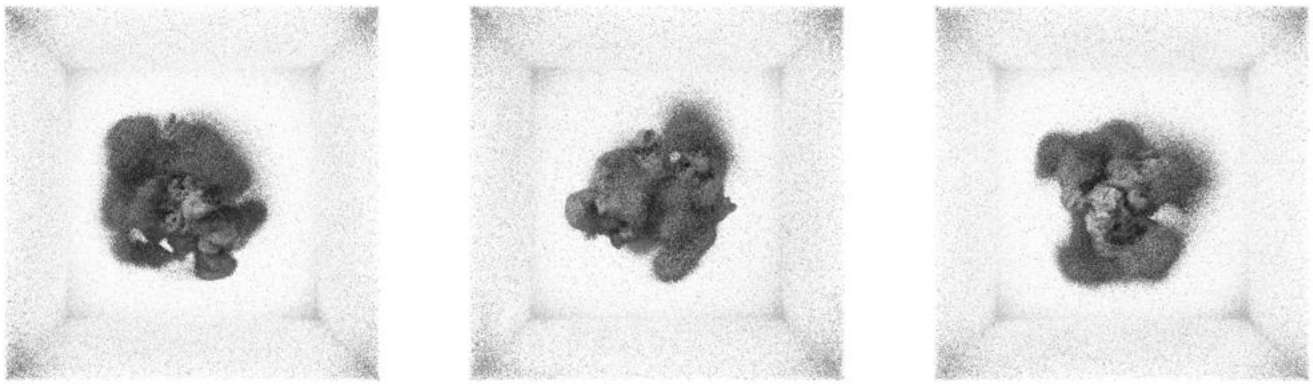
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.22. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

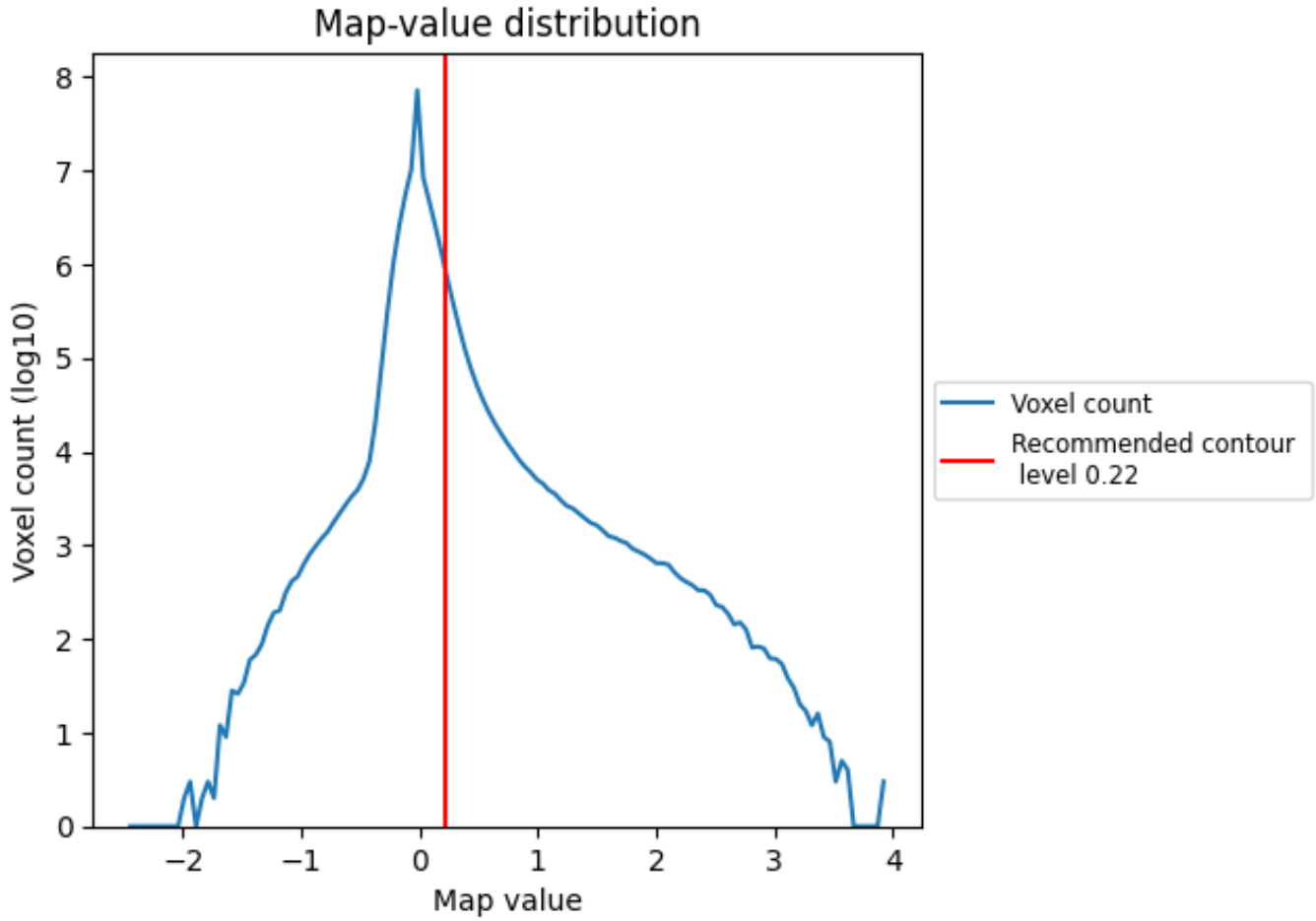
6.6 Mask visualisation (i)

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

7 Map analysis

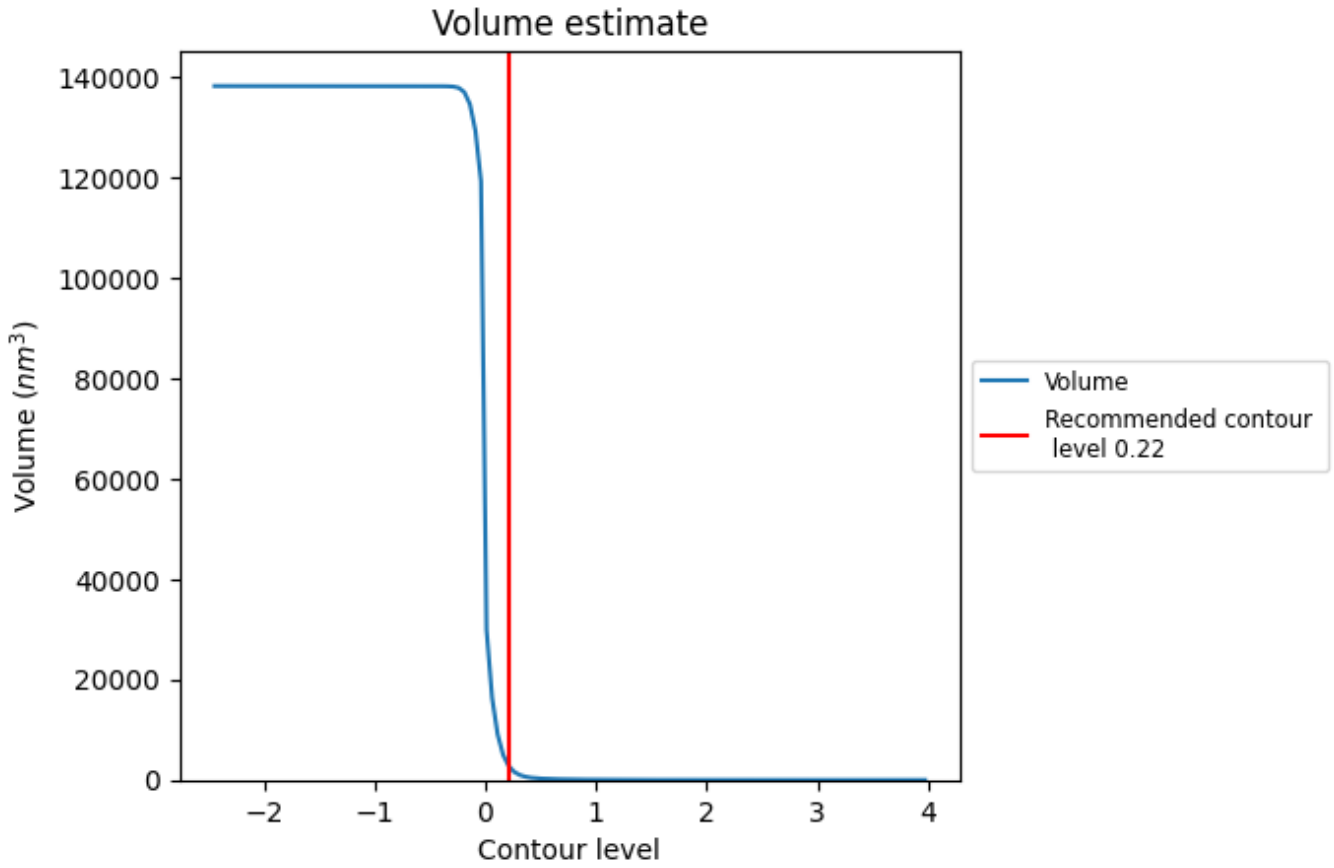
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

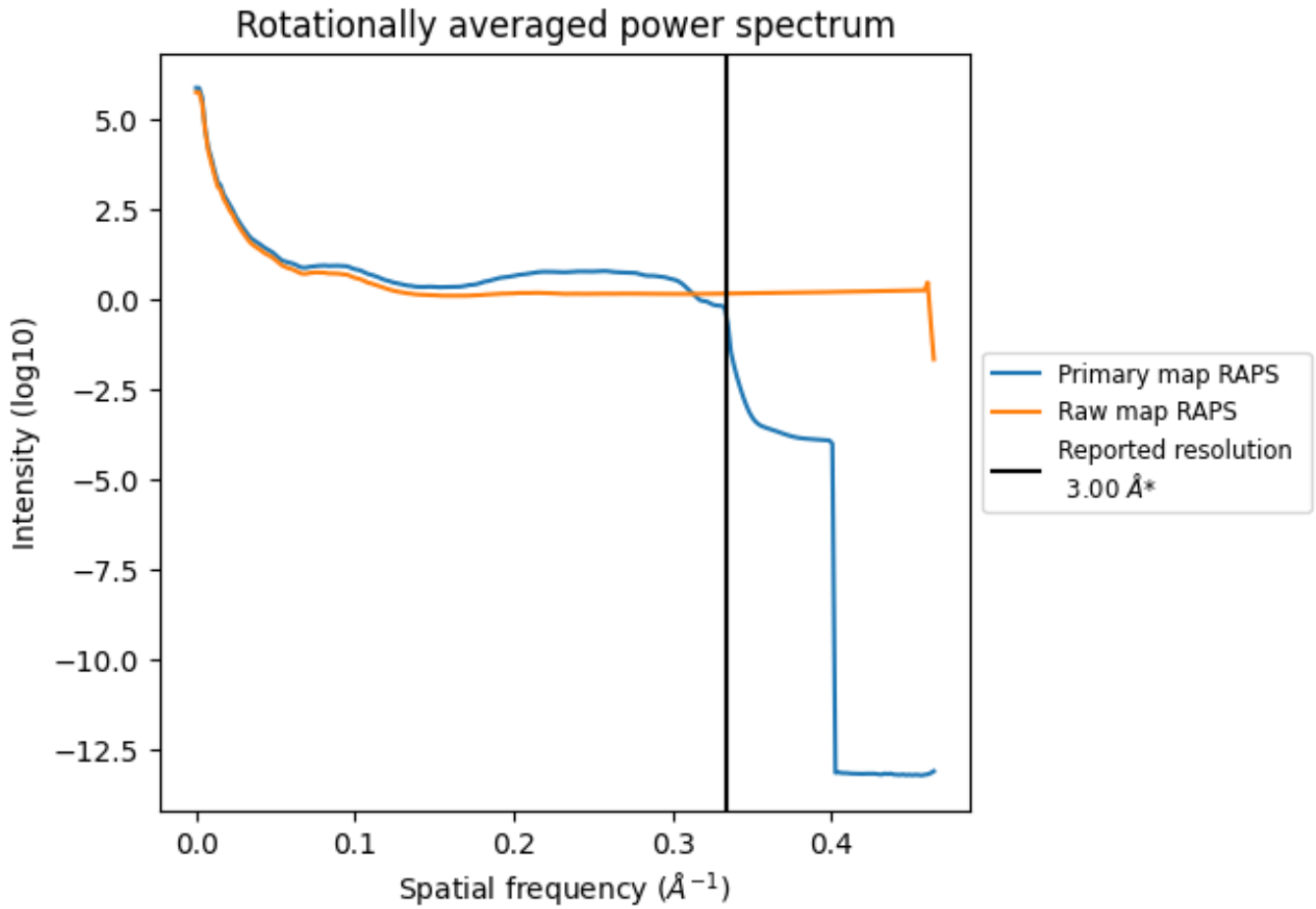
7.2 Volume estimate



The volume at the recommended contour level is 2586 nm^3; this corresponds to an approximate mass of 2336 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

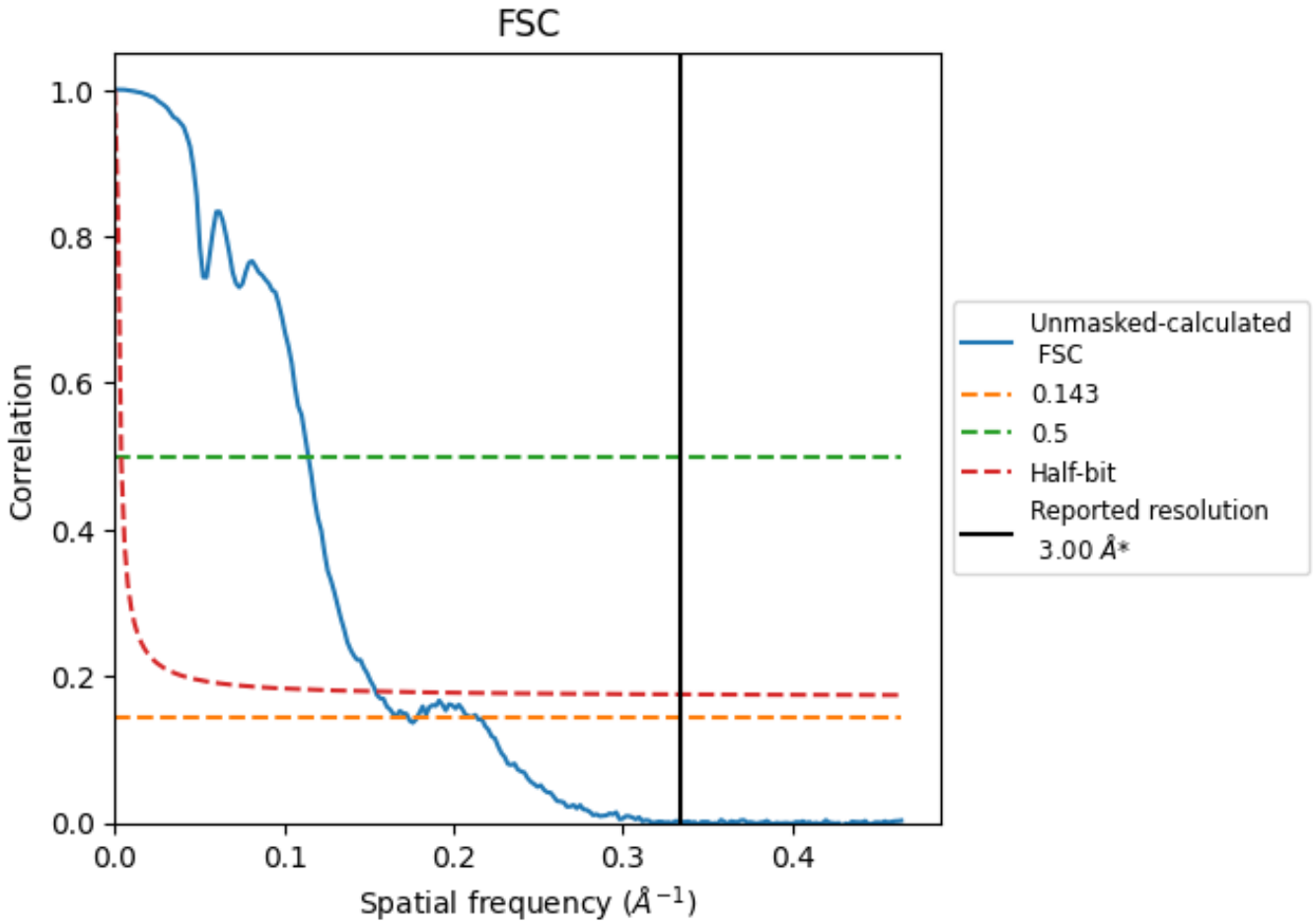


*Reported resolution corresponds to spatial frequency of 0.333 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates (i)

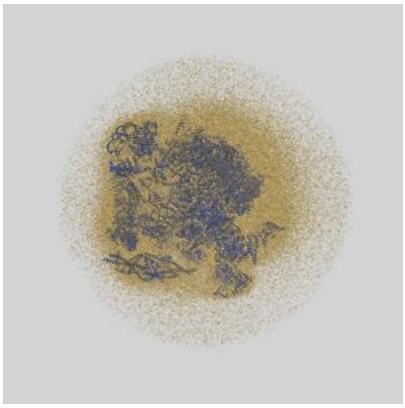
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.77	8.75	6.49

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.77 differs from the reported value 3.0 by more than 10 %

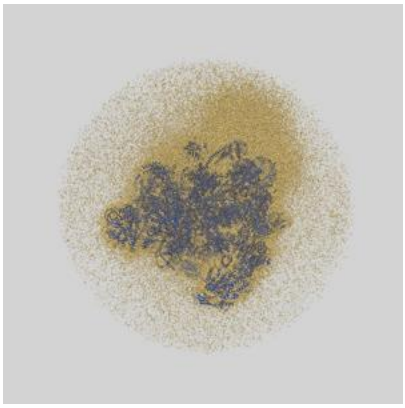
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35109 and PDB model 8I0T. Per-residue inclusion information can be found in section 3 on page 14.

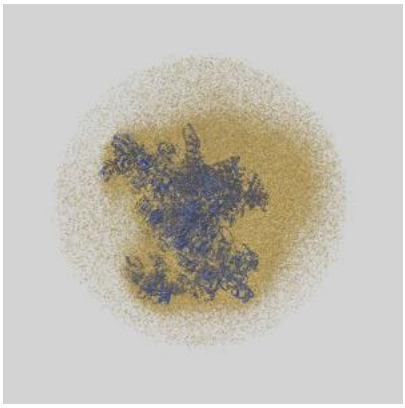
9.1 Map-model overlay



X



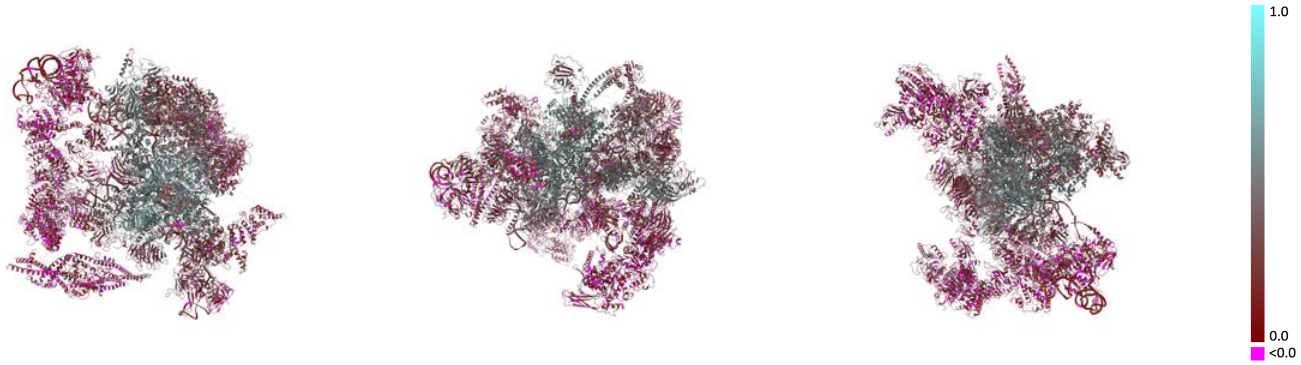
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.22 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

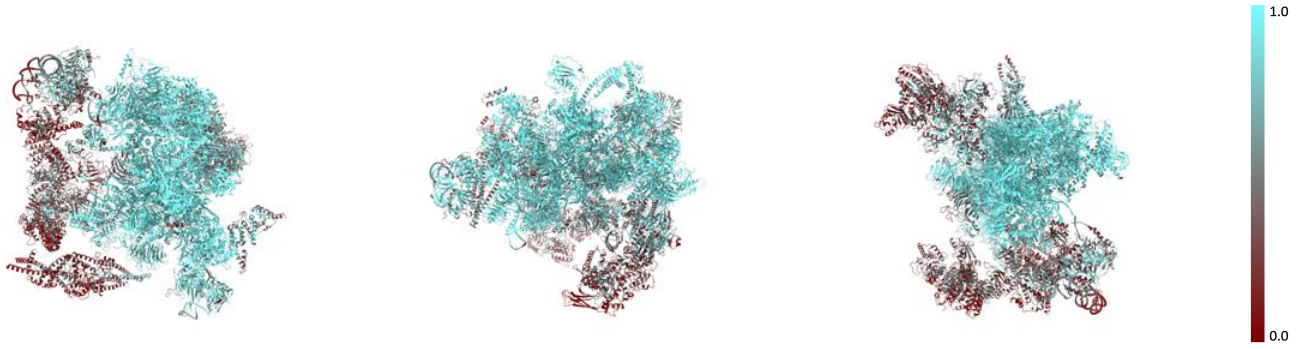
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

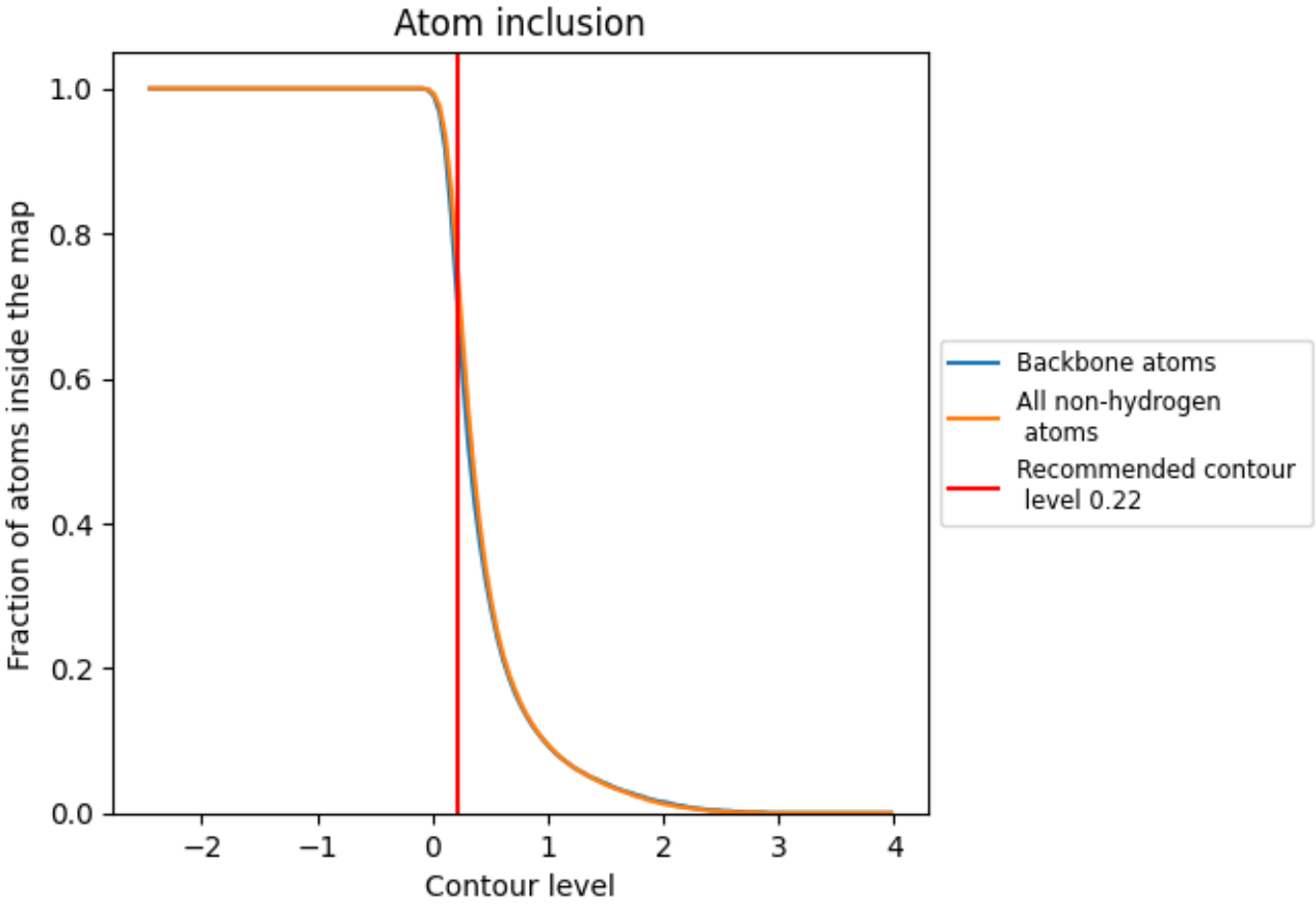
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.22).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 75% 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 (0.22) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7470	0.3400
1	0.9470	0.4170
2	0.9040	0.4390
3	0.9370	0.4190
4	0.6830	0.2090
5	0.9520	0.5020
7	0.9570	0.4140
9	0.4520	0.2830
A	0.8920	0.4820
B	0.9000	0.3660
C	0.9540	0.3650
D	0.3940	0.1750
E	0.9150	0.3000
F	0.9420	0.3810
G	0.9570	0.3900
H	0.6440	0.2330
I	0.3090	0.1700
J	0.9390	0.3760
K	0.8850	0.4640
L	0.6680	0.3730
N	0.9700	0.4350
O	0.8640	0.3330
P	0.9430	0.5100
Q	0.2830	0.1700
R	0.9220	0.4390
S	0.8830	0.2600
T	0.9940	0.5820
U	0.7840	0.4100
V	0.7860	0.2850
W	0.5610	0.2430
X	0.9240	0.3760
Y	0.9390	0.3500
Z	0.3080	0.1640
a	0.7850	0.2140
b	0.8480	0.2330

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Chain	Atom inclusion	Q-score
c	0.7780	0.2450
d	0.7900	0.2360
e	0.7660	0.1910
f	0.7130	0.2310
g	0.8240	0.2150
h	0.5620	0.1710
i	0.5820	0.1510
j	0.5860	0.1740
k	0.5490	0.1770
l	0.4940	0.1640
m	0.5280	0.1770
n	0.5020	0.1600
o	0.4150	0.1780
p	0.4570	0.2020
q	0.1870	0.1670
r	0.2950	0.1550
s	0.1850	0.1630
t	0.1960	0.1830
u	0.3570	0.1770
v	0.7080	0.3850
w	0.5410	0.2370
y	0.3260	0.1650