Full wwPDB EM Validation Report ⓘ

Jul 31, 2024 – 11:06 AM JST

PDB ID	:	8I0U
EMDB ID	:	EMD-35110
Title	:	The cryo-EM structure of human Bact-IV complex
Authors	:	Zhan, X.; Lu, Y.; Shi, Y.
Deposited on	:	2023-01-11
Resolution	:	3.30 Å(reported)

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

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

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

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

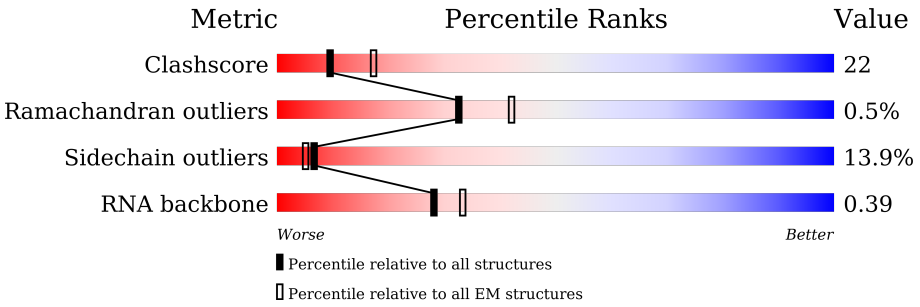
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 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	10% 53% 26% 5% 16%
2	B	117	6% 32% 34% 15% • 16%
3	C	972	45% 38% 5% 12%
4	E	357	33% 44% 7% 16%
5	F	107	• 23% 37% 25% 5% 9%
6	G	220	8% 5% 18% 10% • 64%
7	H	188	69% 20% 50% 16% • 11%

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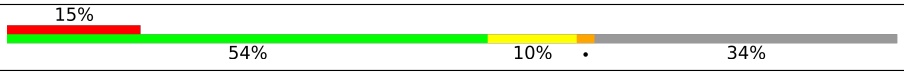
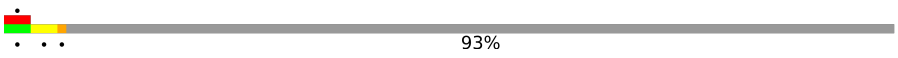
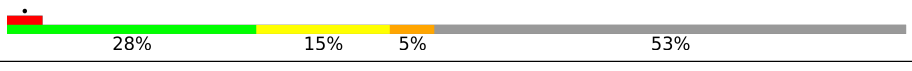
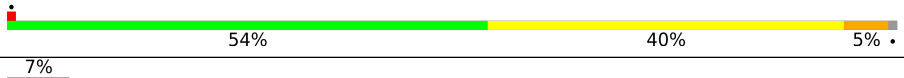
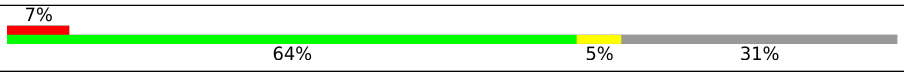
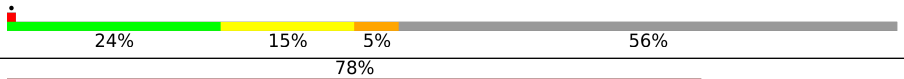
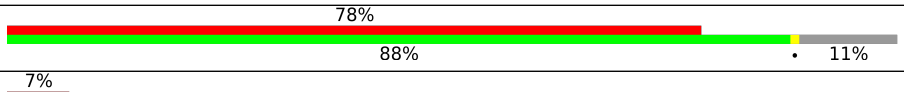
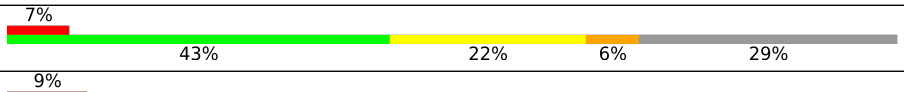
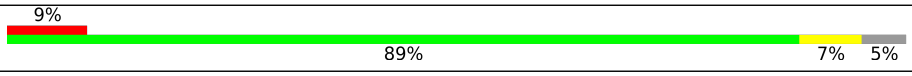
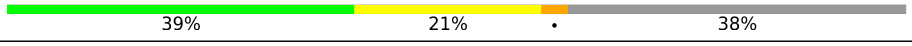
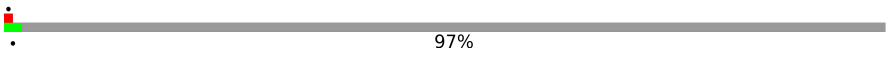
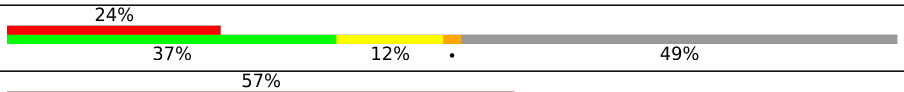
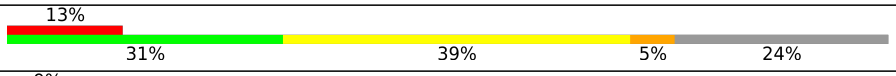
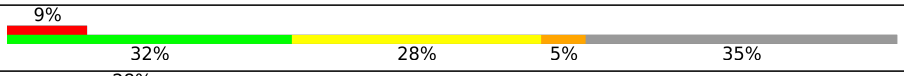
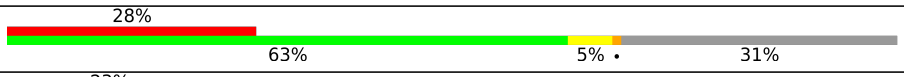
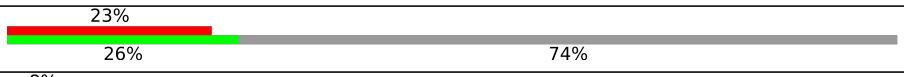
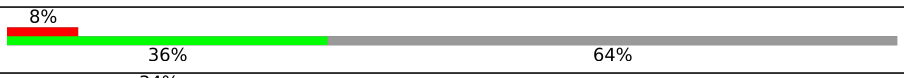
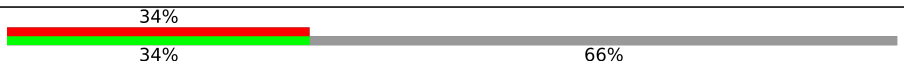
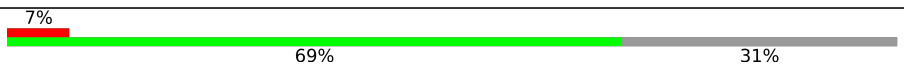
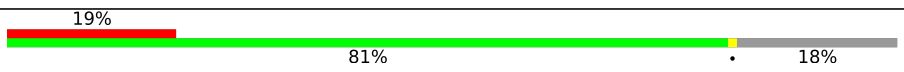
Mol	Chain	Length	Quality of chain
8	I	855	
9	J	848	
10	K	343	
11	L	802	
12	M	243	
13	N	144	
14	O	420	
15	P	229	
16	Q	1485	
17	R	536	
18	S	166	
19	T	514	
20	U	2752	
21	V	908	
22	W	579	
23	X	1041	
24	Y	492	
25	Z	225	
26	y	301	
27	a	240	
27	m	240	
28	b	119	
28	n	119	
29	c	118	
29	h	118	

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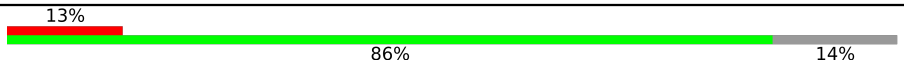
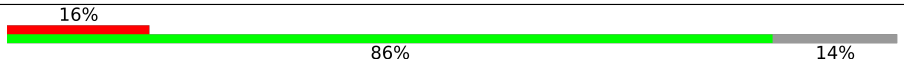
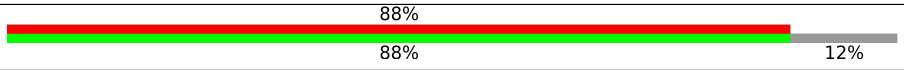
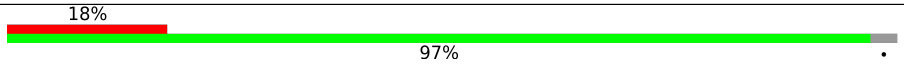
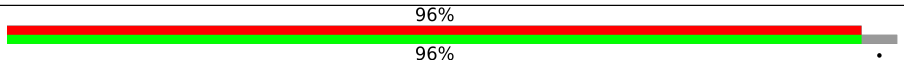
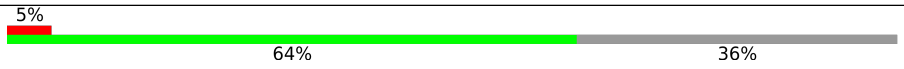
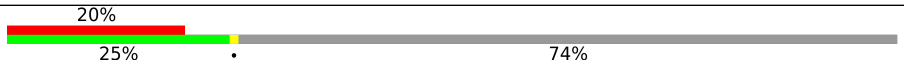
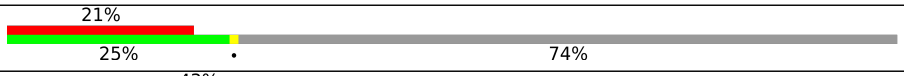
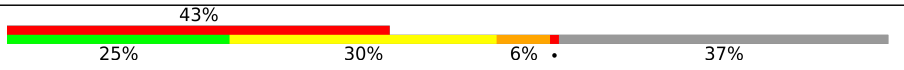
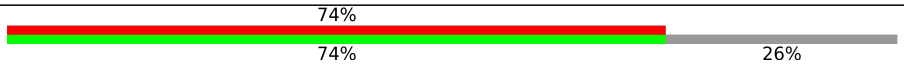
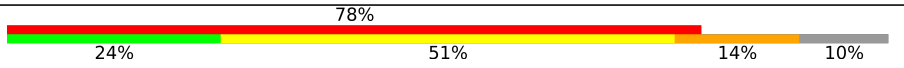
Mol	Chain	Length	Quality of chain
30	d	86	
30	i	86	
31	e	92	
31	j	92	
32	f	76	
32	k	76	
33	g	126	
33	l	126	
34	q	504	
34	r	504	
34	s	504	
34	t	504	
35	1	1304	
36	3	1217	
37	p	225	
38	w	501	
39	2	895	
40	4	424	
41	7	110	
42	5	86	
43	o	255	

2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 106396 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	1969	16331	10528	2863	2872	68	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 40 kDa protein.

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

- Molecule 5 is a RNA chain called U6 snRNA.

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

- Molecule 6 is a RNA chain called Pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	G	79	1587	708	248	552	79	0	0

- Molecule 7 is a RNA chain called U2 snRNA.

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

- Molecule 8 is a protein called Pre-mRNA-splicing factor SYF1.

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

- Molecule 9 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	561	Total	C	N	O	S	0	0
			3773	2350	709	708	6		

- Molecule 10 is a protein called RING finger protein 113A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	24	Total	C	N	O	S	0	0
			185	114	32	36	3		

- Molecule 11 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	387	Total	C	N	O	S	0	0
			2584	1596	494	489	5		

- Molecule 12 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	114	Total	C	N	O	S	0	0
			971	605	181	183	2		

- 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	1322	Total 5288	C 2644	N 1322	O 1322	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
17	R	380	Total 2915	C 1791	N 552	O 558	P 2	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 Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	y	79	Total 316	C 158	N 79	O 79	0	0

- Molecule 27 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

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

- Molecule 28 is a protein called Small nuclear ribonucleoprotein Sm D1.

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

- Molecule 29 is a protein called Small nuclear ribonucleoprotein Sm D2.

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

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

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

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

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

- Molecule 32 is a protein called Small nuclear ribonucleoprotein G.

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

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

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

- Molecule 34 is a protein called Pre-mRNA-processing factor 19.

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

- Molecule 35 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	1	816	Total 6486	C 4163	N 1119	O 1165	S 39	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	3	1177	Total 9220	C 5854	N 1566	O 1755	S 45	0	0

- Molecule 37 is a protein called U2 small nuclear ribonucleoprotein B".

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

- Molecule 38 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	w	121	Total 999	C 637	N 178	O 180	S 4	0	0

- Molecule 39 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	2	250	Total	C	N	O	S	0	0
			1803	1131	339	326	7		

- Molecule 40 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	4	151	Total	C	N	O	0	0
			743	441	151	151		

- Molecule 41 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	7	81	Total	C	N	O	S	0	0
			613	376	109	115	13		

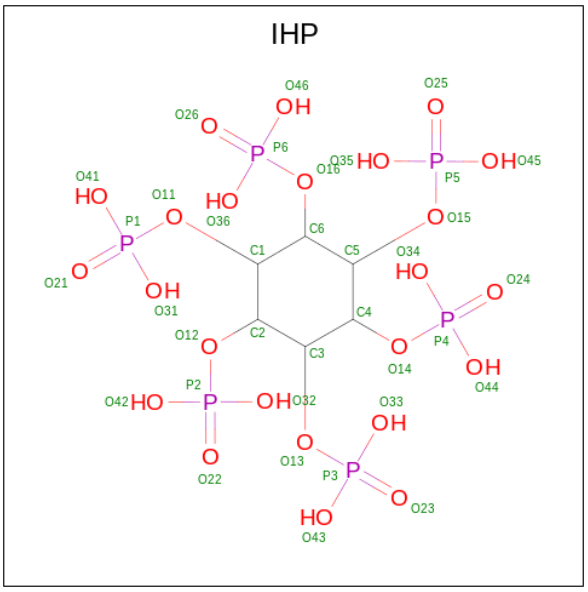
- Molecule 42 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	5	77	Total	C	N	O	S	0	0
			635	403	110	117	5		

- Molecule 43 is a protein called U2 small nuclear ribonucleoprotein A'.

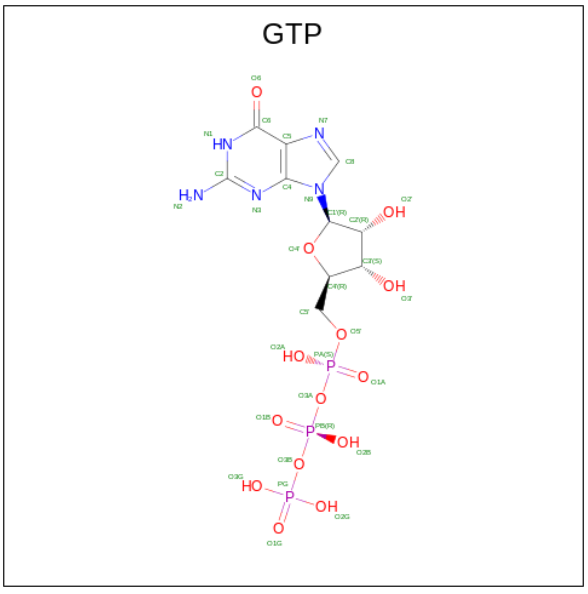
Mol	Chain	Residues	Atoms				AltConf	Trace
43	o	162	Total	C	N	O	0	0
			816	492	162	162		

- Molecule 44 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

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



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

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

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

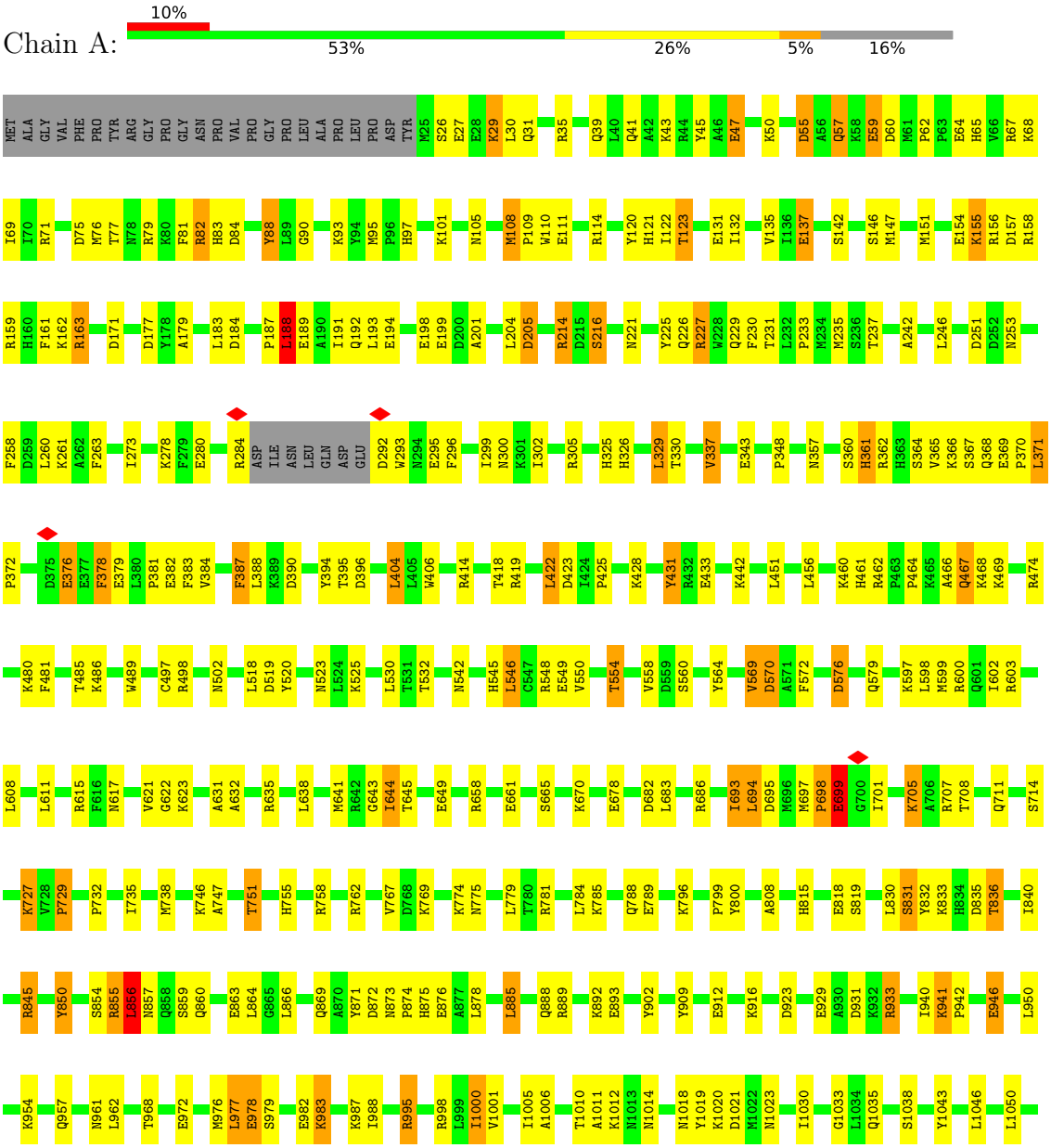
- Molecule 47 is ZINC ION (three-letter code: ZN) (formula: Zn).

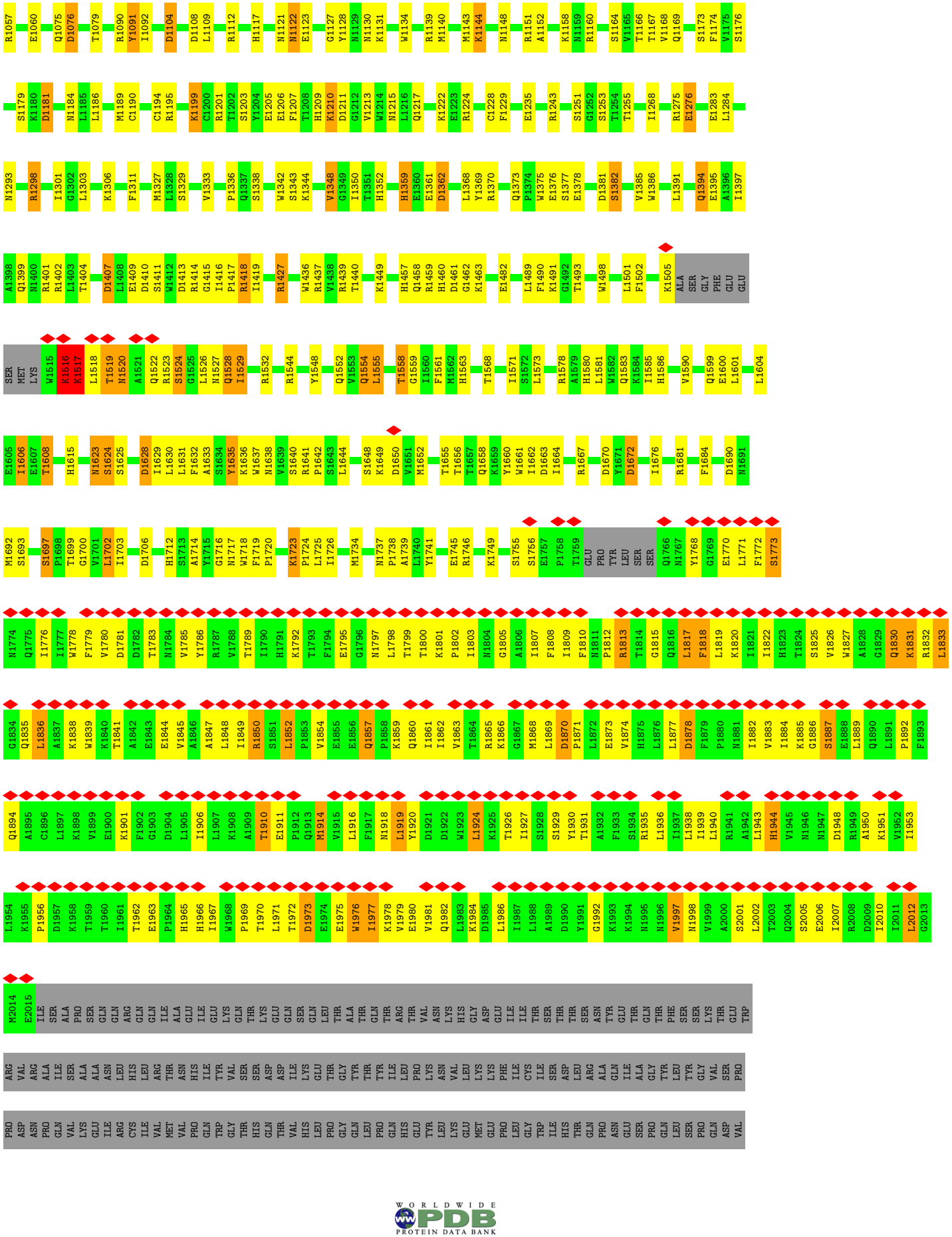
Mol	Chain	Residues	Atoms	AltConf
47	K	1	Total Zn 1 1	0
47	N	3	Total Zn 3 3	0
47	7	3	Total Zn 3 3	0

3 Residue-property plots (i)

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

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

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S1179 K1180 D1181 N1184 L1185 L1186 M1189 C1190 C1194 R1195 K1199 C1200 R1201 T1202 S1203 Y1204 E1205 E1206 F1207 T1208 H1209 K1210 D1211 G1212 V1213 W1214 N1215 L1216 Q1217 K1222 E1223 R1224 C1228 F1229 E1235 R1243 S1251 G1252 S1253 T1254 T1255 I1268 R1275 E1276 E1283 L1284
N1293 R1298 I1301 G1302 L1303 K1306 F1311 M1327 L1328 S1329 V1333 P1336 Q1337 S1338 W1342 S1343 K1344 V1348 G1349 I1350 T1351 H1352 H1359 E1360 E1361 D1362 L1368 Y1369 R1370 Q1373 P1374 W1375 E1376 S1377 E1378 D1381 S1382 V1385 W1386 L1391 Q1394 E1395 A1396 I1397
A1398 Q1399 N1400 R1401 R1402 L1403 T1404 D1407 L1408 E1409 D1410 S1411 W1412 D1413 R1414 G1415 I1416 P1417 R1418 I1419 R1427 W1436 R1437 V1438 R1439 T1440 K1449 H1457 Q1458 R1459 H1460 D1461 G1462 K1463 E1482 L1489 F1490 K1491 G1492 T1493 W1498 L1501 F1502 K1505 ALA SER GLY PHE GLU GLU
SER MET LYS W1515 K1516 K1517 L1518 T1519 N1520 A1521 Q1522 R1523 S1524 G1525 L1526 N1527 Q1528 I1529 R1532 R1544 Y1548 Q1552 V1553 Q1554 L1555 T1558 G1559 I1560 F1561 M1562 H1563 T1568 I1571 S1572 L1573 R1578 A1579 H1580 L1581 W1582 Q1583 K1584 I1585 H1586 V1590 Q1599 E1600 L1601 L1604
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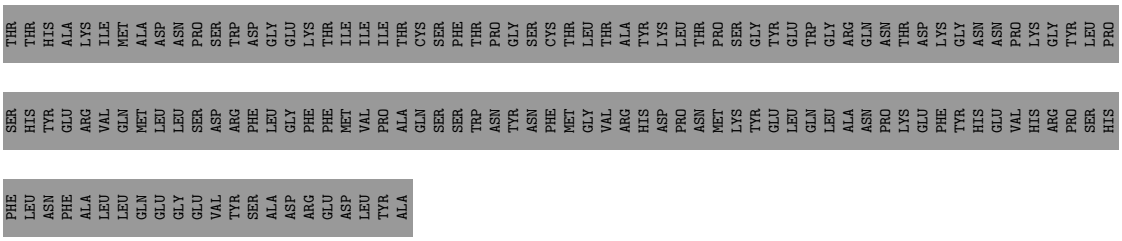
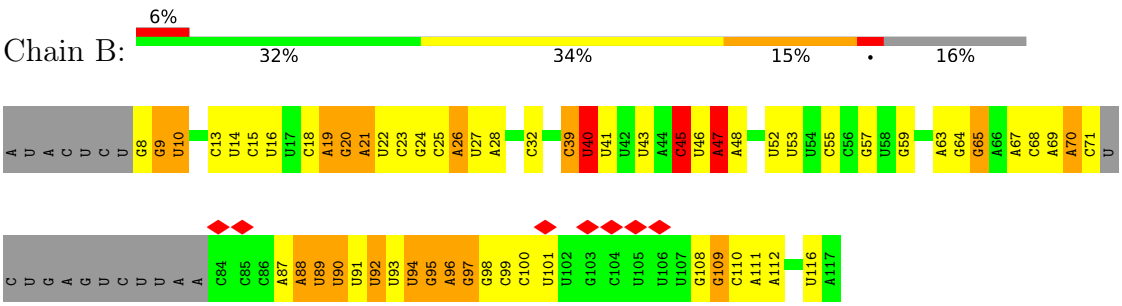
N1774 Q1775 I1776 I1777 W1778 F1779 V1780 D1781 D1782 T1783 N1784 V1785 Y1786 R1787 V1788 T1789 I1790 H1791 K1792 T1793 F1794 E1795 G1796 N1797 L1798 T1799 T1800 K1801 P1802 I1803 N1804 G1805 A1806 I1807 F1808 I1809 F1810 N1811 P1812 R1813 T1814 G1815 Q1816 L1817 F1818 L1819 K1820 I1821 I1822 H1823 T1824 S1825 V1826 W1827 A1828 G1829 Q1830 K1831 R1832 L1833
G1834 Q1835 L1836 A1837 K1838 W1839 K1840 T1841 A1842 E1843 E1844 V1845 A1846 A1847 L1848 I1849 R1850 S1851 L1852 P1853 V1854 E1855 E1856 Q1857 P1858 K1859 Q1860 I1861 I1862 V1863 T1864 R1865 K1866 G1867 M1868 L1869 D1870 P1871 L1872 E1873 V1874 H1875 L1876 L1877 D1878 F1879 P1880 N1881 I1882 V1883 I1884 K1885 G1886 S1887 E1888 L1889 Q1890 L1891 P1892 F1893
Q1894 A1895 C1896 L1897 K1898 V1899 E1900 K1901 F1902 G1903 D1904 L1905 I1906 L1907 K1908 A1909 T1910 E1911 P1912 Q1913 M1914 V1915 L1916 F1917 N1918 L1919 Y1920 D1921 D1922 W1923 L1924 K1925 T1926 I1927 S1928 S1929 Y1930 T1931 A1932 F1933 S1934 R1935 L1936 I1937 L1938 I1939 L1940 R1941 A1942 A1943 H1944 V1945 N1946 N1947 D1948 R1949 A1950 K1951 V1952 I1953
L1954 K1955 P1956 D1957 K1958 T1959 T1960 I1961 T1962 E1963 P1964 H1965 H1966 I1967 W1968 P1969 T1970 L1971 T1972 D1973 E1974 E1975 W1976 I1977 K1978 V1979 E1980 V1981 Q1982 L1983 K1984 D1985 L1986 I1987 L1988 A1989 D1990 Y1991 G1992 K1993 K1994 N1995 N1996 V1997 N1998 V1999 A2000 S2001 L2002 T2003 Q2004 S2005 E2006 I2007 R2008 D2009 I2010 I2011 L2012 G2013
M2014 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 THR ARG THR VAL ASN LYS HIS GLY ASP GLU ILE ILE THR SER THR THR THR SER ASN TYR GLU THR GLN THR PHE SER SER LYS THR GLU TRP
ARG VAL ARG ALA ILE SER ALA ALA ASN LEU HIS LEU ARG THR ASN HIS ILE TYR VAL SER SER ASP ASP ILE LYS GLU THR THR VAL HIS LEU PRO GLY GLN LEU PRO GLN HIS GLU TYR LEU LYS GLU MET GLU PRO LEU GLY TRP ILE HIS THR GLN PRO ASN GLU SER PRO GLN LEU SER PRO GLN ASP VAL
PRO ASP ASN PRO GLN VAL LYS GLU ILE ARG CYS ILE VAL MET VAL PRO GLN TRP GLY THR HIS GLN THR VAL HIS LEU PRO GLY GLN LEU PRO GLN HIS GLU TYR LEU LYS GLU MET GLU PRO LEU GLY TRP ILE HIS THR GLN PRO ASN GLU SER PRO GLN LEU SER PRO GLN ASP VAL



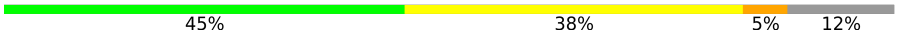


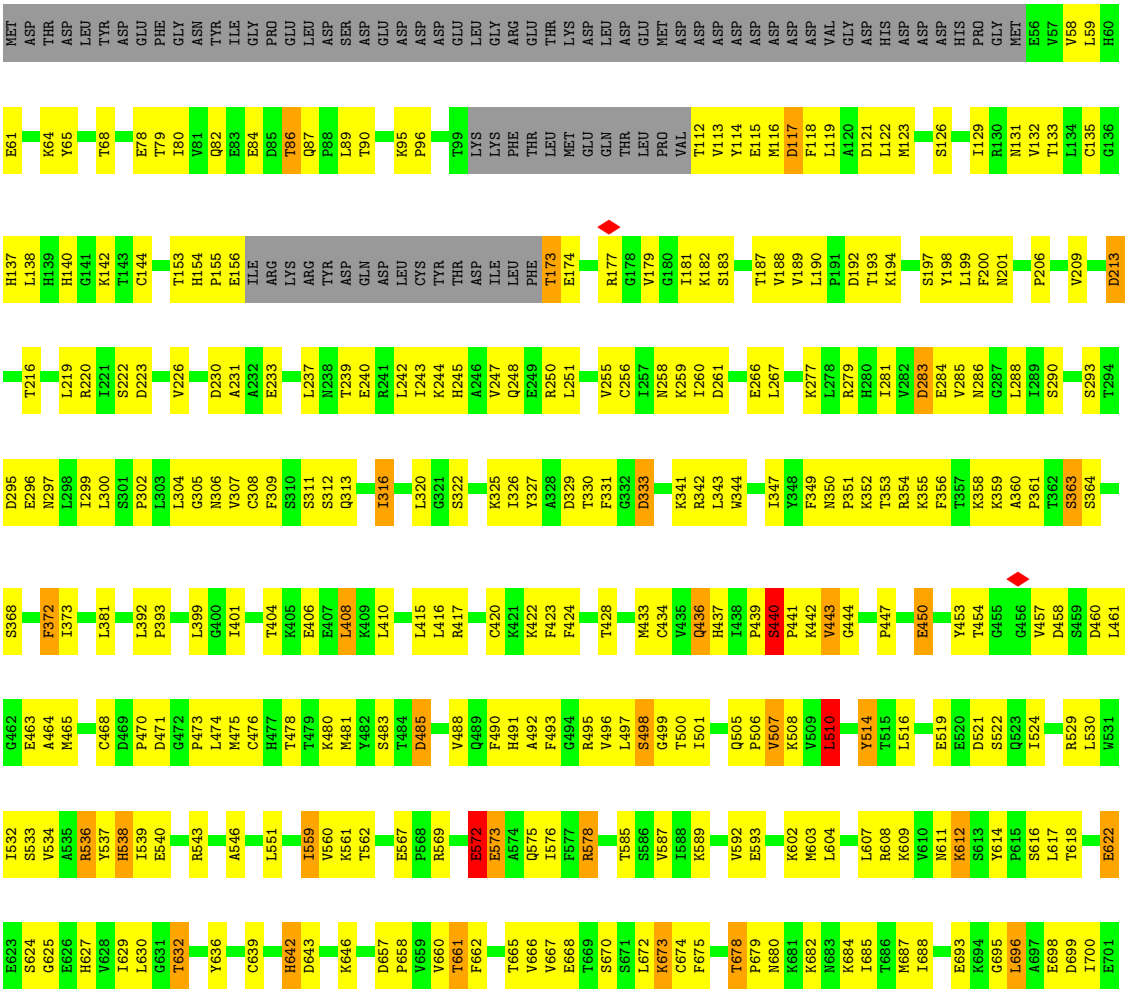
• Molecule 2: U5 snRNA

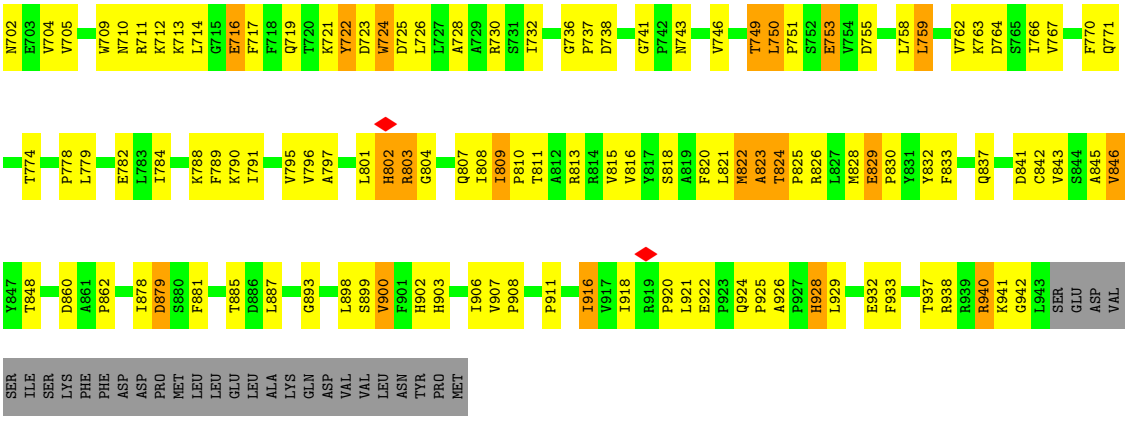
Chain B:

• Molecule 3: 116 kDa U5 small nuclear ribonucleoprotein component

Chain C:

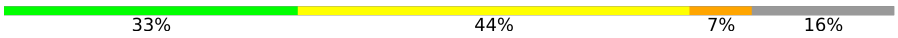


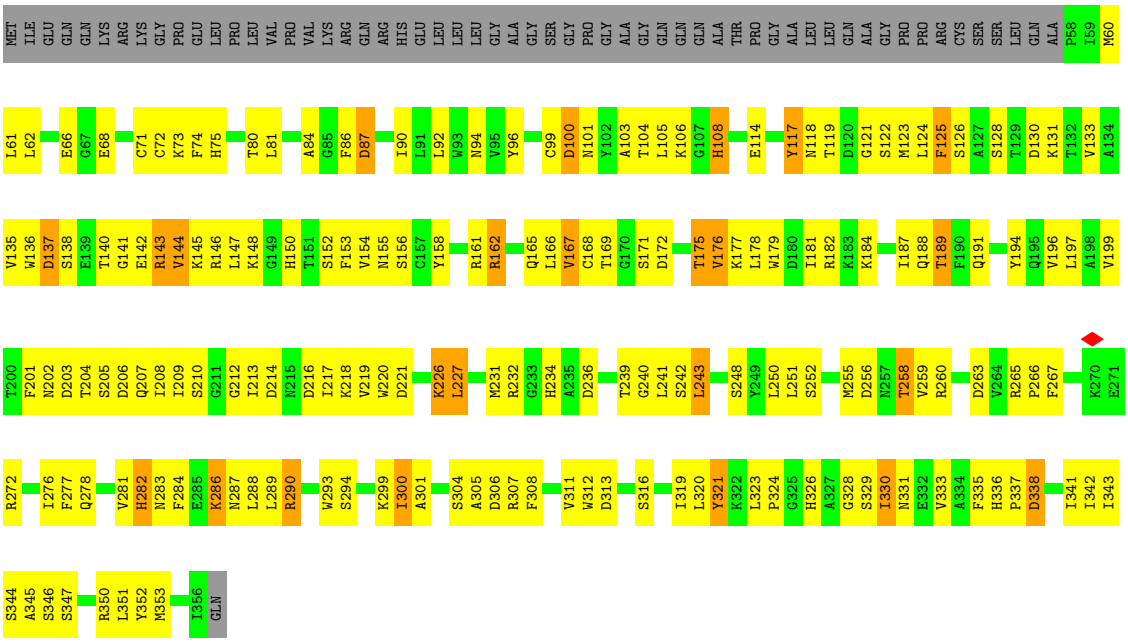




• Molecule 4: U5 small nuclear ribonucleoprotein 40 kDa protein

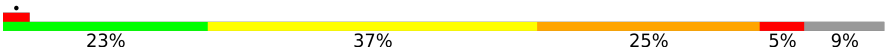
Chain E:

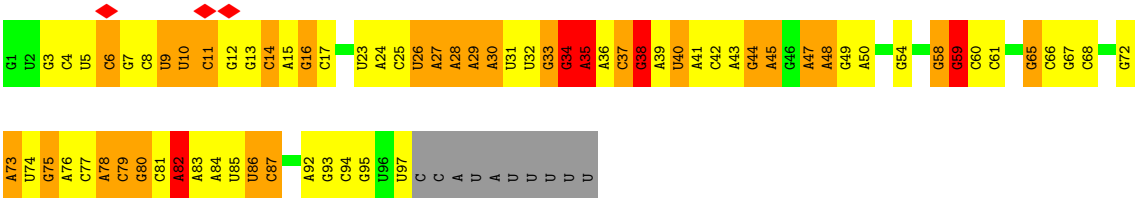




• Molecule 5: U6 snRNA

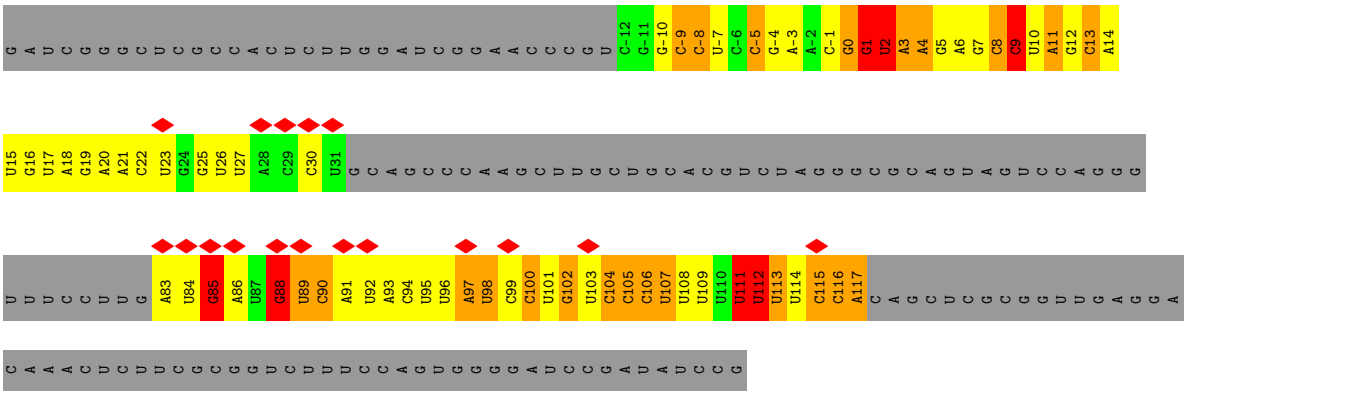
Chain F:





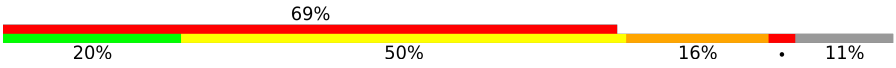
• Molecule 6: Pre-mRNA

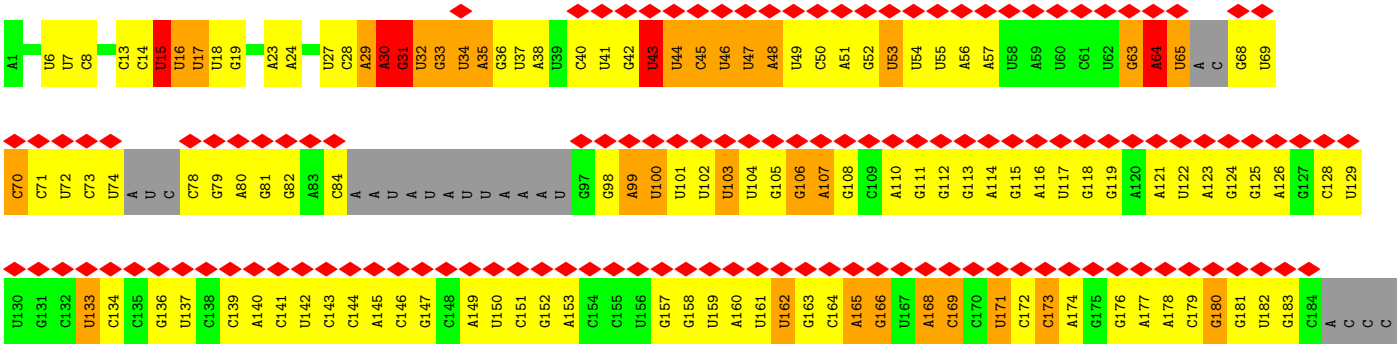
Chain G:



• Molecule 7: U2 snRNA

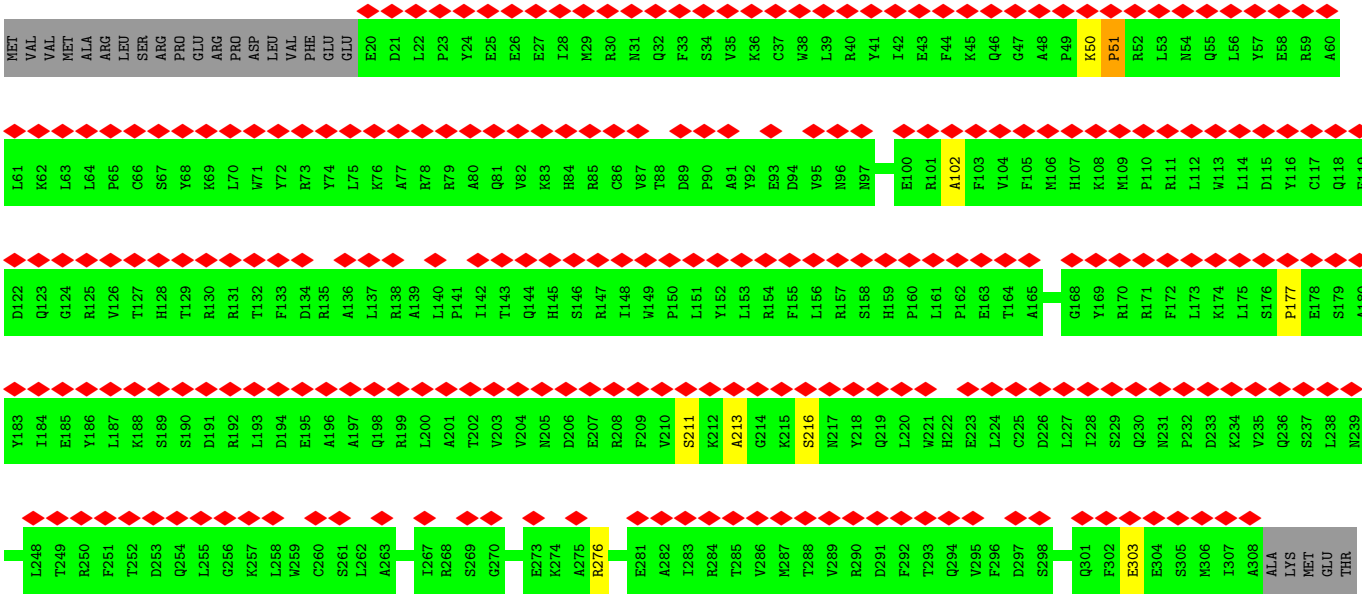
Chain H:

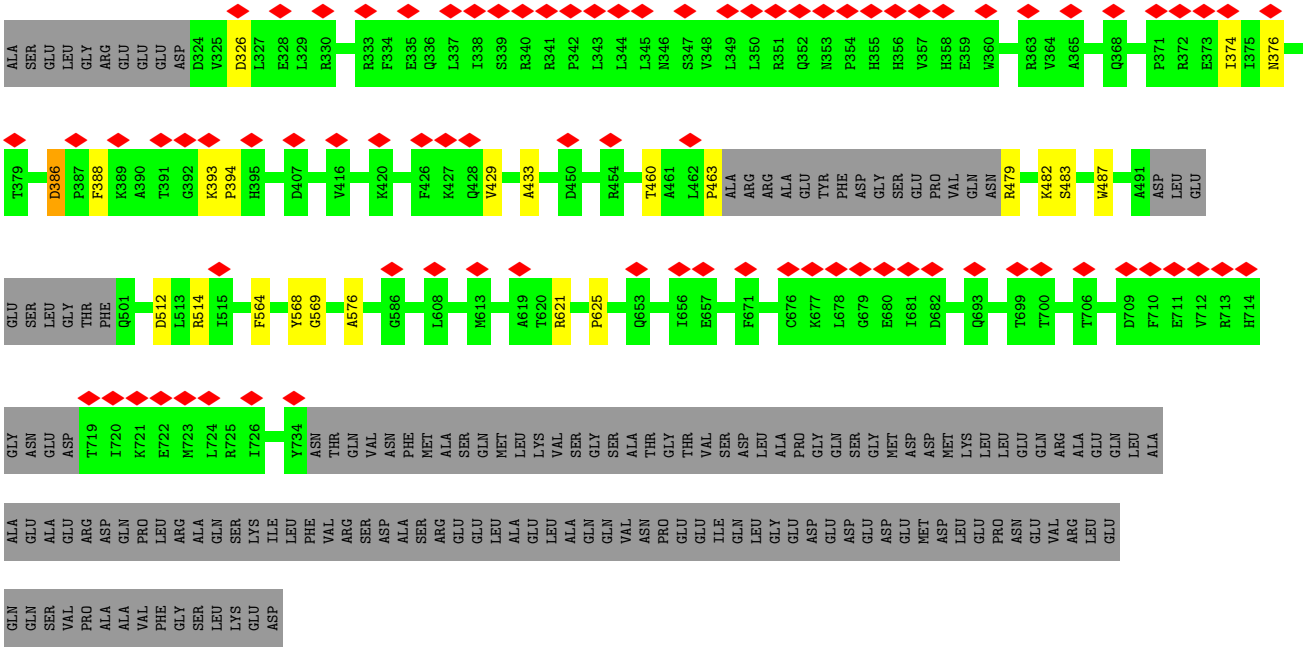




• Molecule 8: Pre-mRNA-splicing factor SYF1

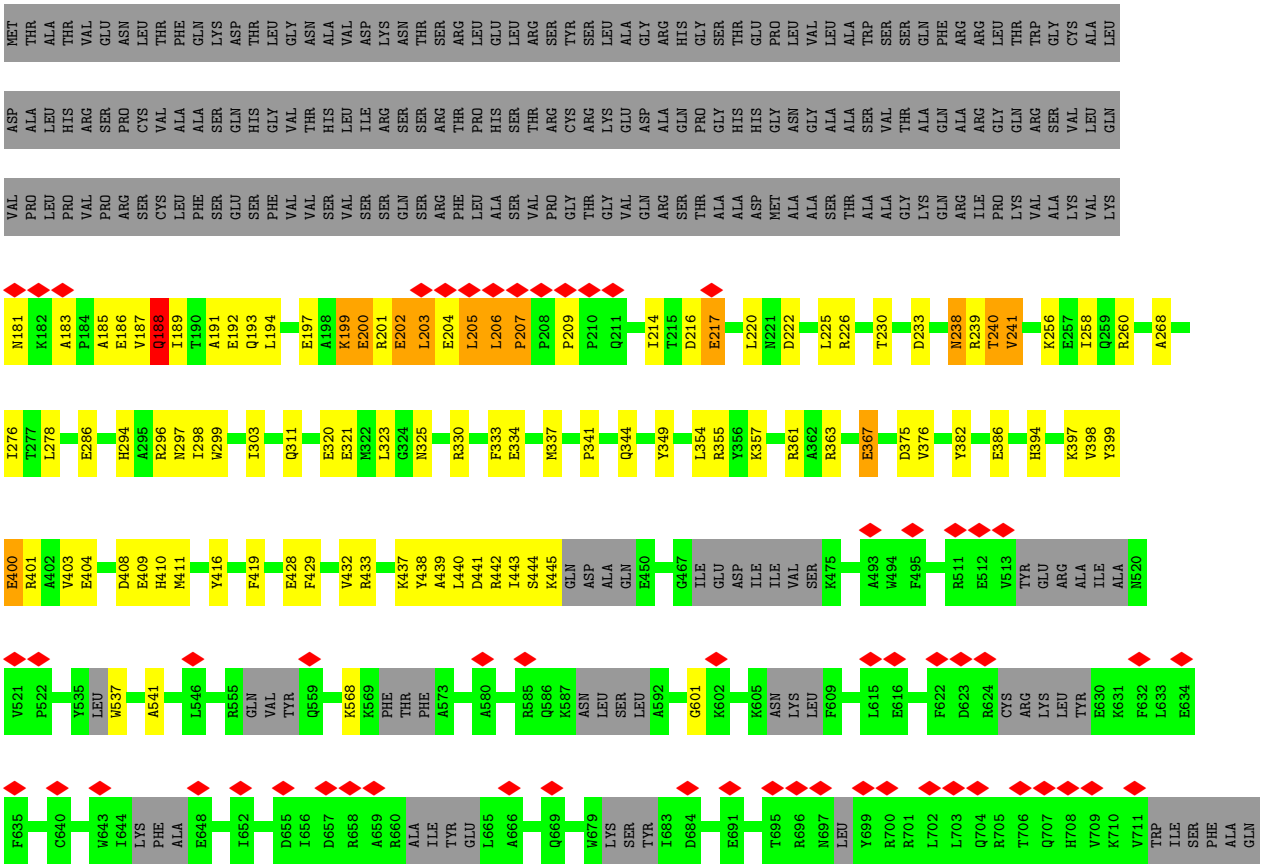
Chain I:

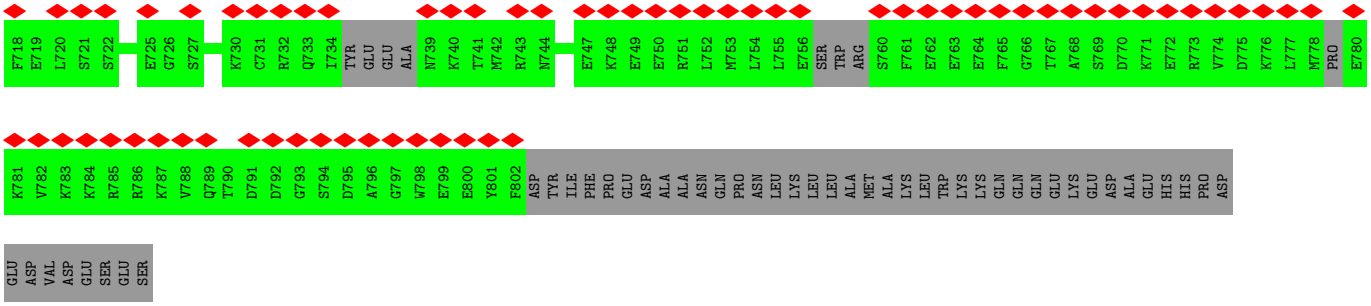




• Molecule 9: Crooked neck-like protein 1

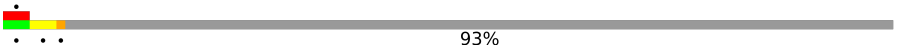
Chain J:

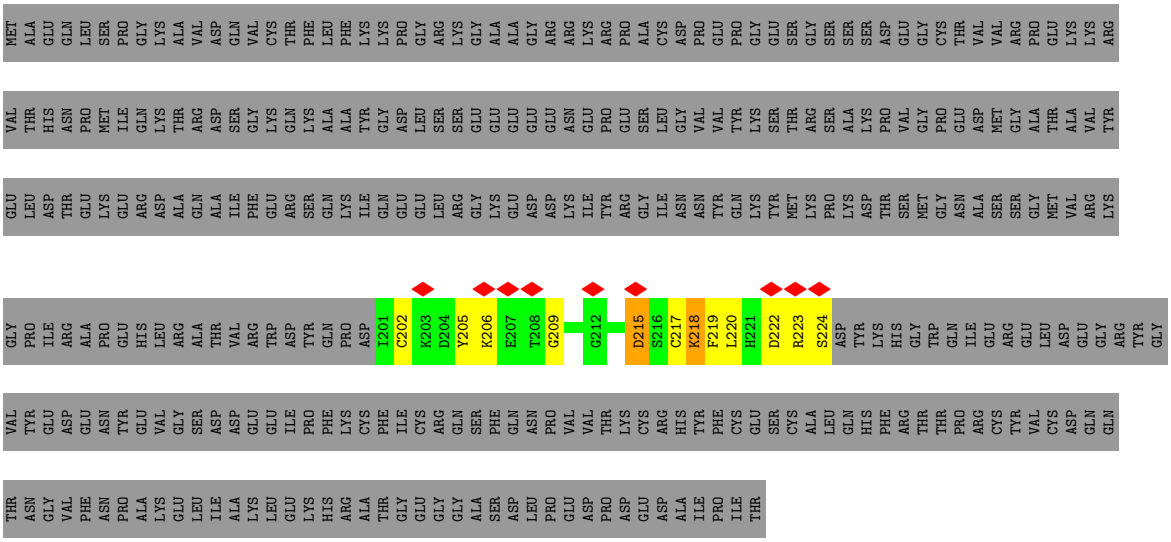




• Molecule 10: RING finger protein 113A

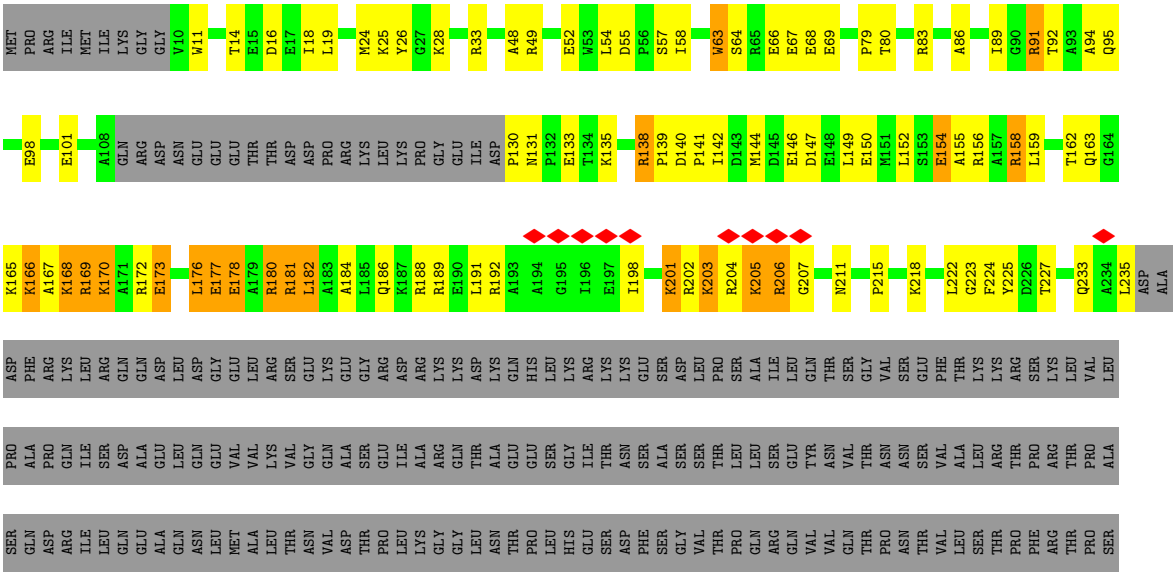
Chain K:

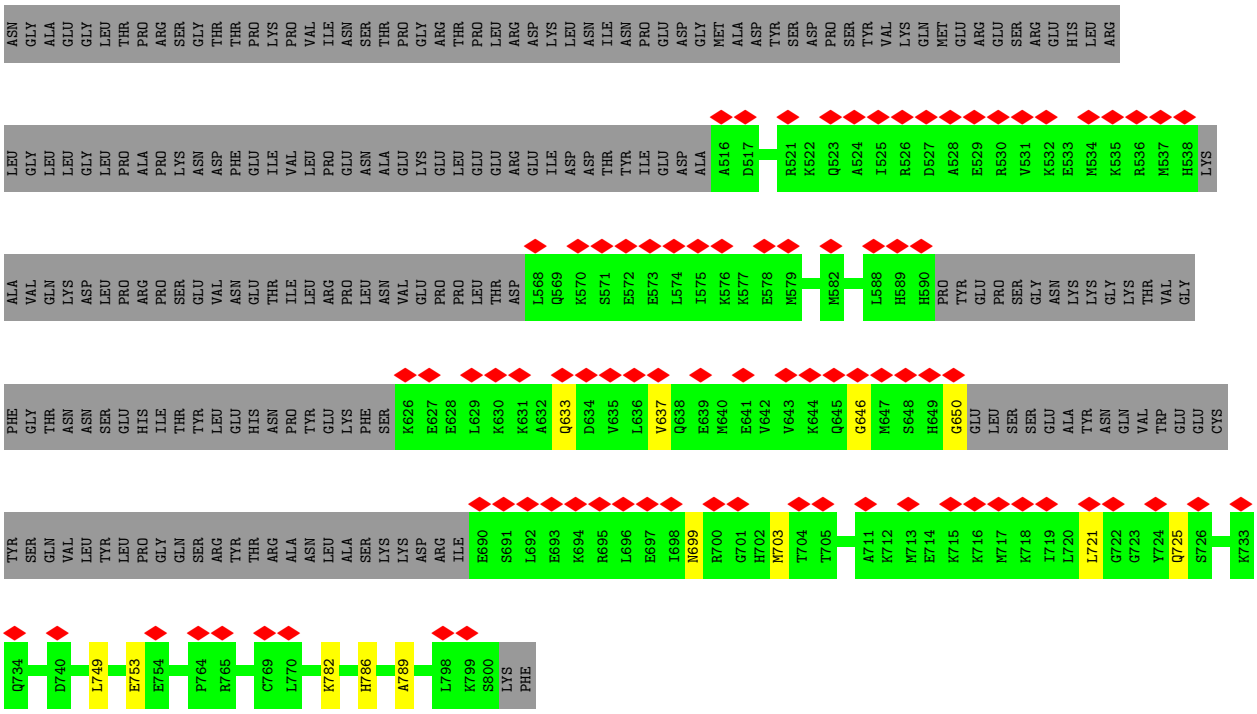




• Molecule 11: Cell division cycle 5-like protein

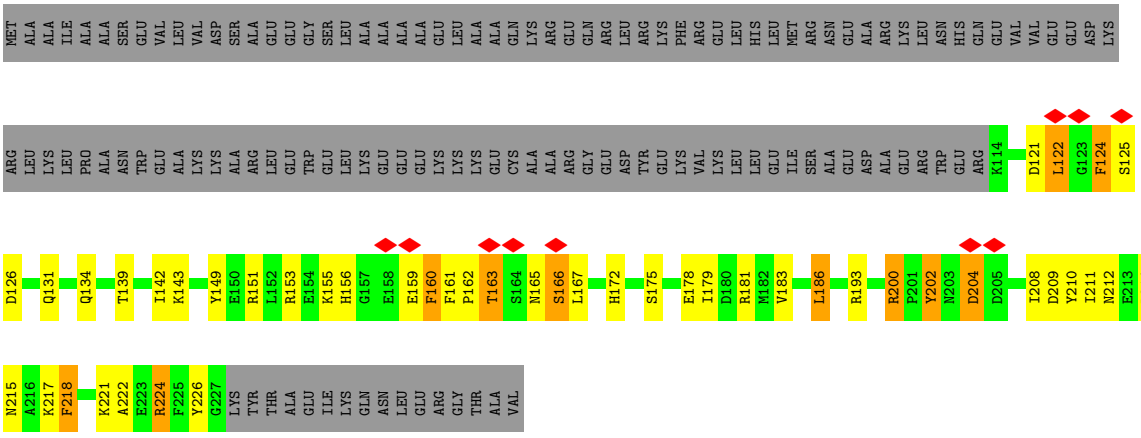
Chain L:





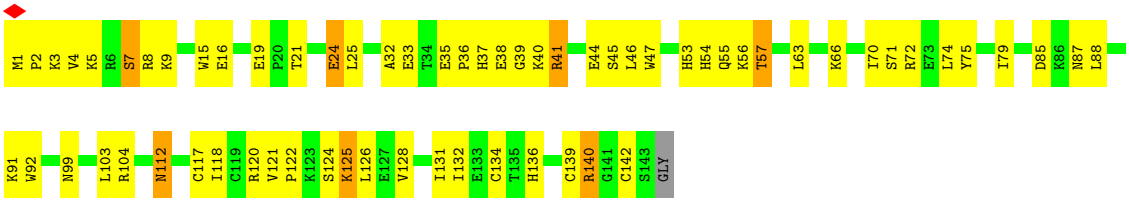
• Molecule 12: Pre-mRNA-splicing factor SYF2

Chain M:



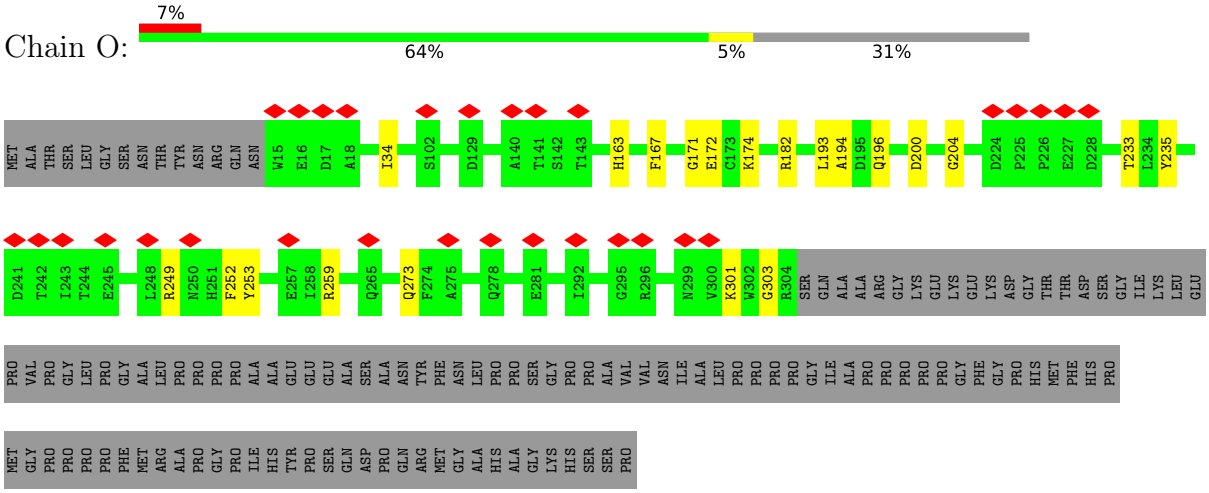
• Molecule 13: Protein BUD31 homolog

Chain N:



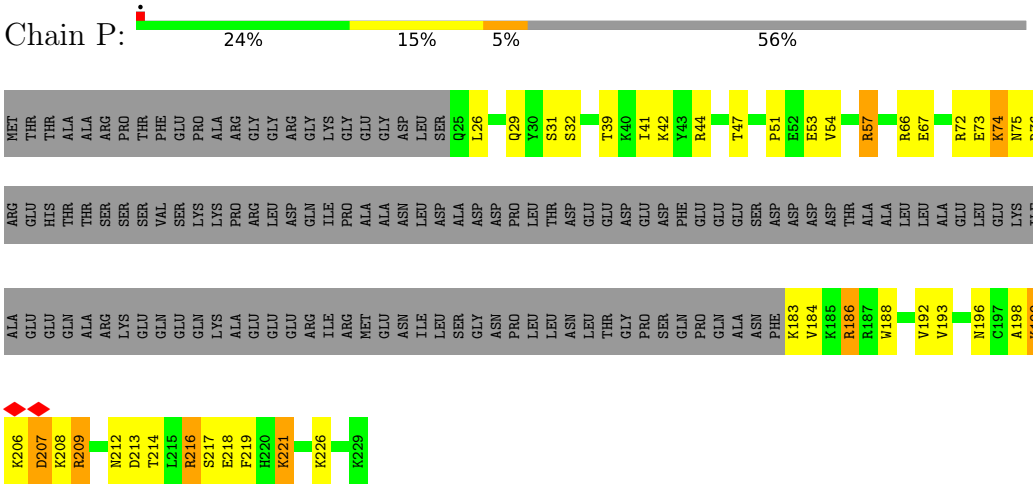
• Molecule 14: Pre-mRNA-splicing factor RBM22

Chain O:



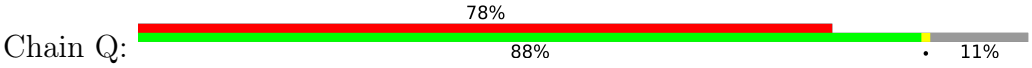
• Molecule 15: Spliceosome-associated protein CWC15 homolog

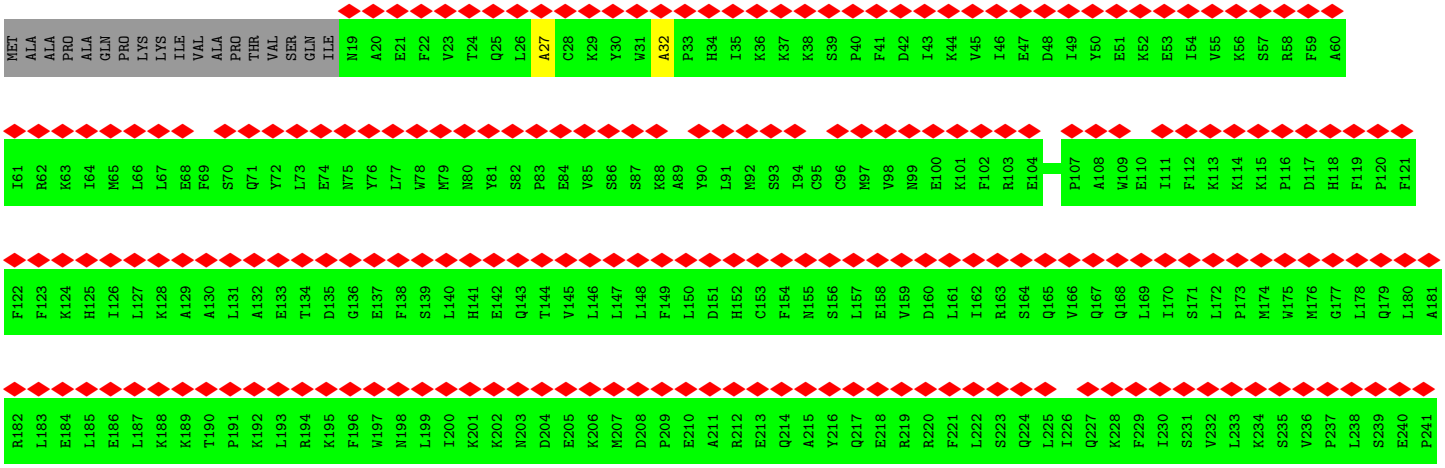
Chain P:

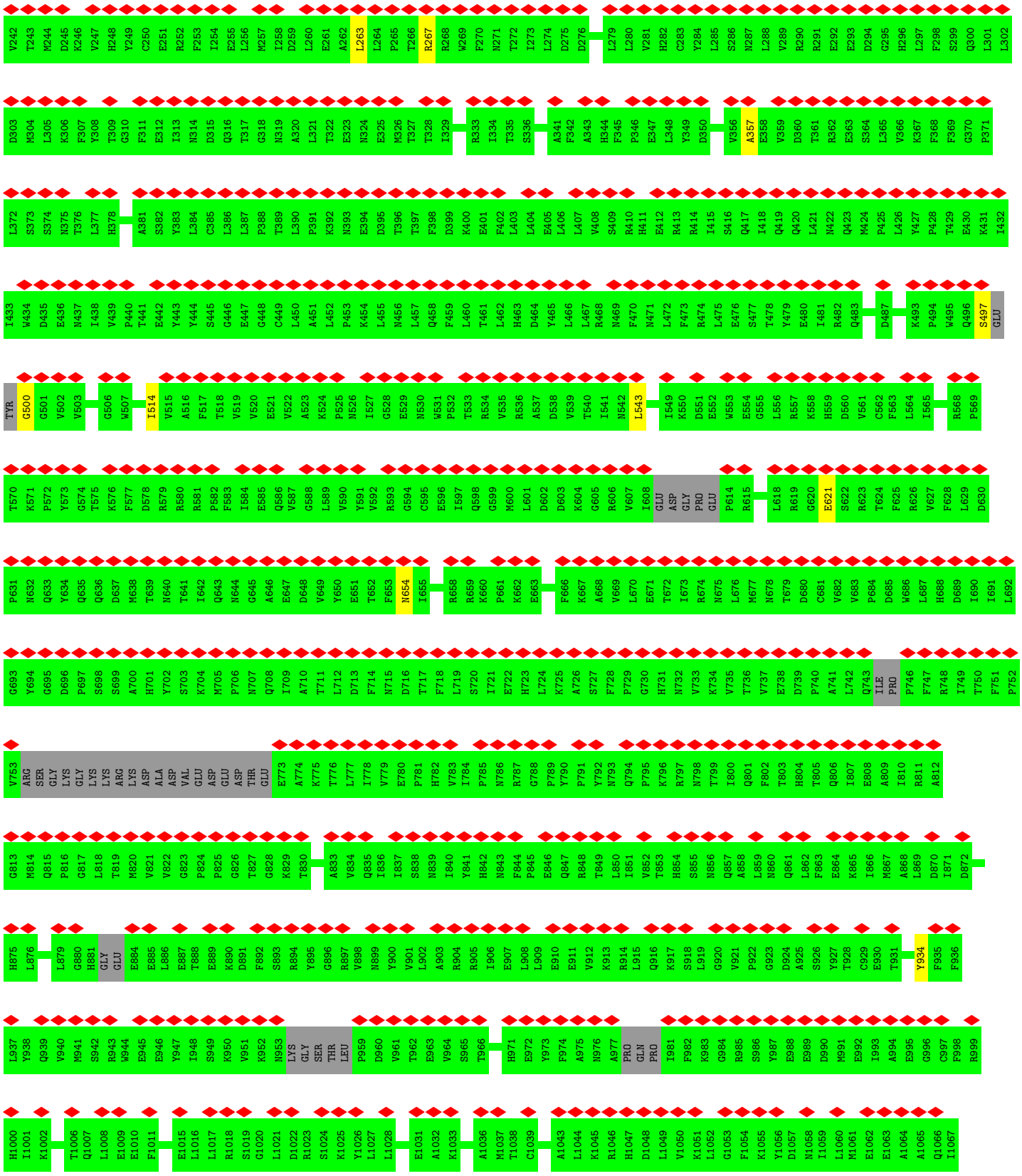


• Molecule 16: RNA helicase aquarius

Chain Q:



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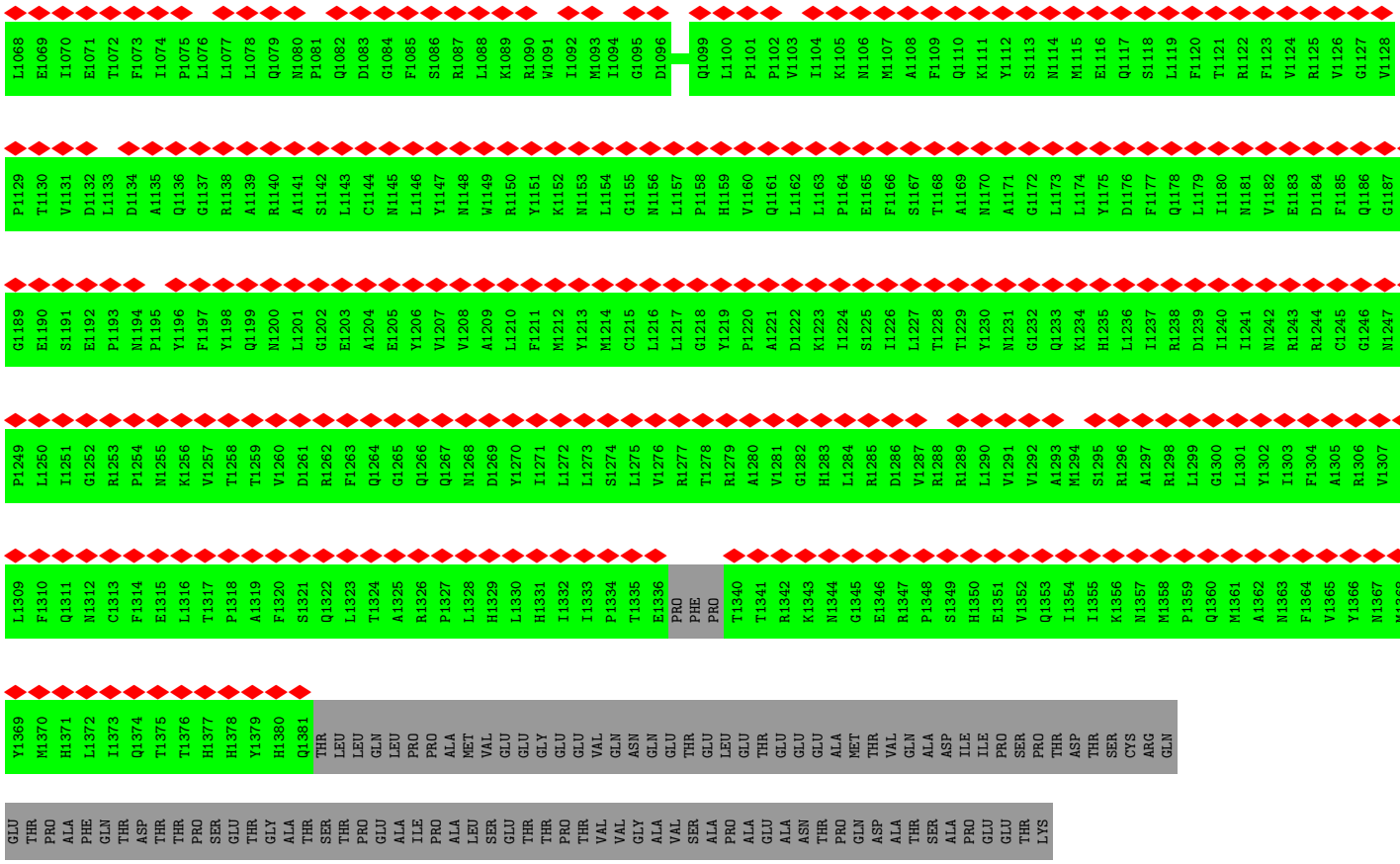
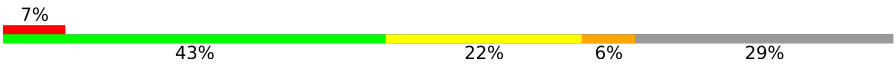
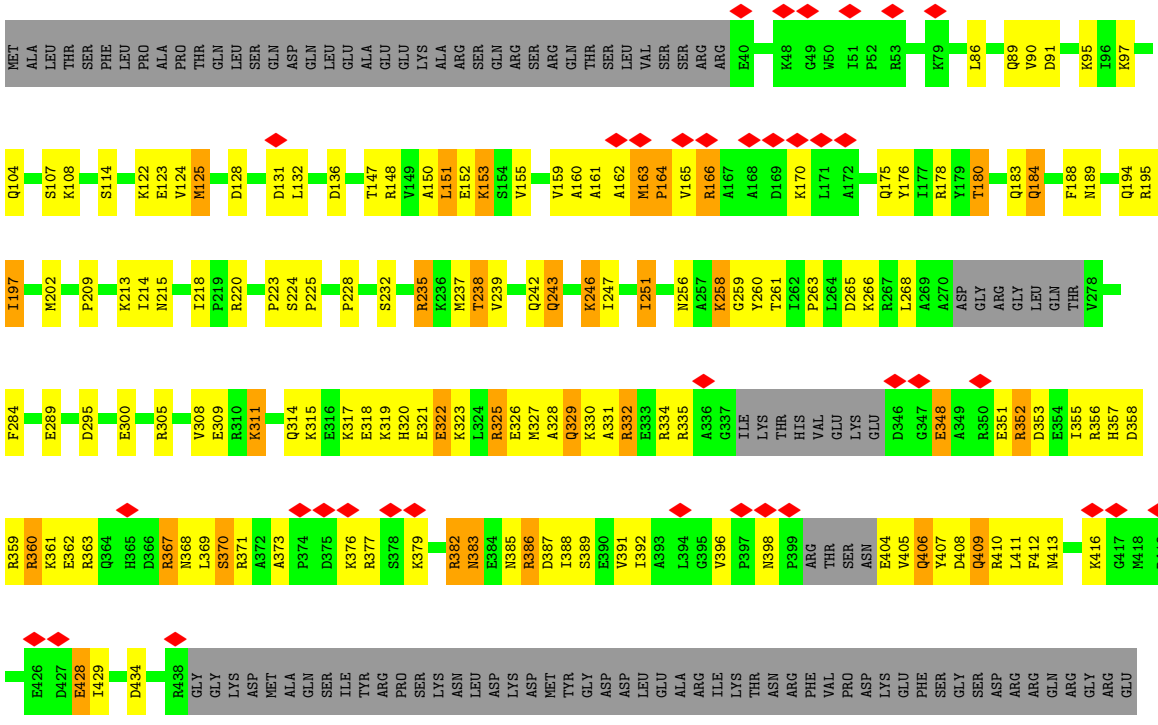
D303 M304 L305 K306 F307 Y308 T309 G310 F311 E312 I313 N314 D315 Q316 T317 G318 N319 A320 L321 T322 E323 N324 E325 M326 T327 T328 I329 R333 I334 T335 S336 A341 F342 A343 H344 F345 P346 E347 L348 Y349 D350 V356 A357 E358 V359 D360 T361 R362 E363 S364 L365 V366 K367 F368 F369 G370 P371
L372 S373 S374 N375 T376 L377 H378 A381 S382 Y383 L384 C385 L386 L387 P388 T389 L390 P391 K392 N393 E394 D395 T396 T397 F398 D399 K400 E401 F402 L403 L404 E405 L406 L407 V408 S409 R410 H411 E412 R413 R414 I415 S416 Q417 I418 Q419 Q420 L421 N422 Q423 M424 P425 L426 Y427 P428 T429 E430 K431 I432
I433 W434 D435 E436 N437 I438 V439 P440 T441 E442 Y443 Y444 S445 G446 E447 G448 C449 L450 A451 L452 P453 K454 L455 N456 L457 Q458 F459 L460 T461 L462 H463 D464 Y465 L466 L467 R468 N469 F470 N471 L472 F473 R474 L475 E476 S477 T478 Y479 E480 I481 R482 Q483 D487 K493 P494 W495 Q496 S497 GLU
TYR G500 G501 V502 V503 G506 W507 I514 V515 A516 F517 T518 V519 V520 E521 V522 A523 K524 P525 N526 I527 G528 E529 N530 W531 P532 T533 R534 V535 R536 A537 D538 V539 T540 I541 N542 L543 I549 K550 D551 E552 W553 E554 G555 L556 R557 K558 H559 D560 V561 C562 F563 L564 I565 R568 P569
T570 K571 P572 Y573 G574 T575 K576 F577 D578 R579 R580 R581 P582 F583 I584 E585 Q586 V587 G588 L589 V590 Y591 V592 R593 G594 C595 E596 I597 Q598 G599 M600 L601 D602 D603 K604 G605 R606 V607 I608 GLU ASP GLY PRO GLU P614 R615 L618 R619 G620 E621 S622 R623 T624 F625 R626 V627 F628 L629 D630
P631 N632 Q633 Y634 Q635 Q636 D637 M638 T639 N640 T641 I642 Q643 N644 G645 A646 E647 D648 V649 Y650 E651 T652 F653 N654 I655 R658 R659 K660 P661 K662 E663 F666 K667 A668 V669 L670 E671 T672 I673 R674 N675 L676 M677 N678 T679 D680 C681 V682 V683 P684 D685 W686 L687 H688 D689 I690 I691 L692
G693 Y694 G695 D696 P697 S698 S699 A700 H701 Y702 S703 K704 M705 P706 N707 Q708 I709 A710 T711 L712 D713 F714 N715 D716 T717 F718 L719 S720 I721 E722 H723 L724 K725 A726 S727 F728 P729 G730 H731 N732 V733 K734 V735 T736 V737 E738 D739 P740 A741 L742 Q743 ILE PRO P746 F747 R748 I749 T750 F751 P752
V753 ARG SER GLY LYS GLY LYS LYS ARG LYS ASP ALA ASP VAL GLU ASP GLU ASP THR GLU E773 A774 K775 T776 L777 I778 V779 E780 P781 H782 V783 I784 P785 N786 R787 G788 P789 Y790 P791 Y792 N793 Q794 P795 K796 R797 N798 T799 I800 Q801 F802 T803 H804 T805 Q806 I807 E808 A809 I810 R811 A812
G813 M814 Q815 P816 G817 L818 T819 M820 V821 V822 G823 P824 P825 G826 T827 G828 K829 T830 A833 V834 Q835 I836 I837 S838 N839 I840 Y841 H842 N843 F844 P845 E846 Q847 R848 T849 L850 I851 V852 T853 H854 S855 N856 Q857 A858 L859 N860 Q861 L862 F863 E864 K865 I866 M867 A868 L869 D870 I871 D872
H875 L876 L879 G880 H881 GLY GLU E884 E885 L886 E887 T888 E889 K890 D891 F892 S893 R894 Y895 G896 R897 V898 N899 Y900 V901 L902 A903 R904 R905 I906 E907 L908 L909 E910 E911 V912 K913 R914 L915 Q916 K917 S918 L919 G920 V921 P922 G923 D924 A925 S926 Y927 T928 G929 E930 T931 Y934 F935 F936
L937 Y938 Q939 V940 M941 S942 R943 W944 E945 E946 Y947 I948 S949 K950 V951 K952 N953 LYS GLY SER THR LEU P959 D960 V961 T962 E963 V964 S965 T966 H971 E972 Y973 F974 A975 N976 A977 PRO GLN PRO I981 F982 K983 G984 R985 S986 Y987 E988 E989 D990 M991 E992 I993 A994 E995 G996 C997 F998 R999
H1000 I1001 K1002 T1006 Q1007 L1008 E1009 E1010 F1011 E1015 L1016 L1017 R1018 S1019 G1020 L1021 D1022 R1023 S1024 K1025 Y1026 L1027 L1028 E1031 A1032 K1033 A1036 M1037 T1038 C1039 A1043 L1044 K1045 R1046 H1047 D1048 L1049 V1050 K1051 L1052 G1053 F1054 K1055 Y1056 D1057 N1058 I1059 L1060 M1061 E1062 E1063 A1064 A1065 Q1066 I1067

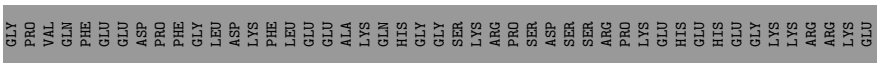


• Molecule 17: SNW domain-containing protein 1

Chain R:





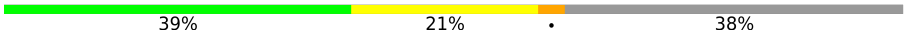


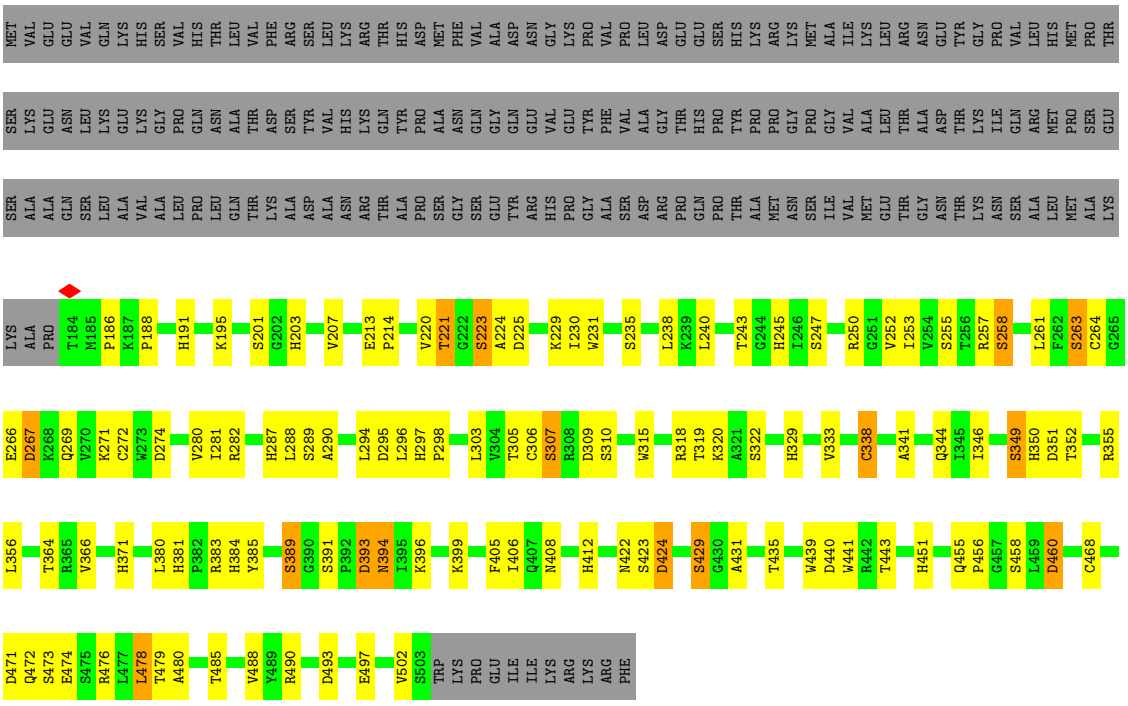
• Molecule 18: Peptidyl-prolyl cis-trans isomerase-like 1

Chain S:

• Molecule 19: Pleiotropic regulator 1

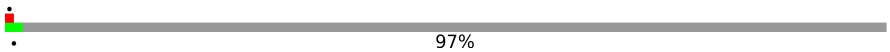
Chain T:

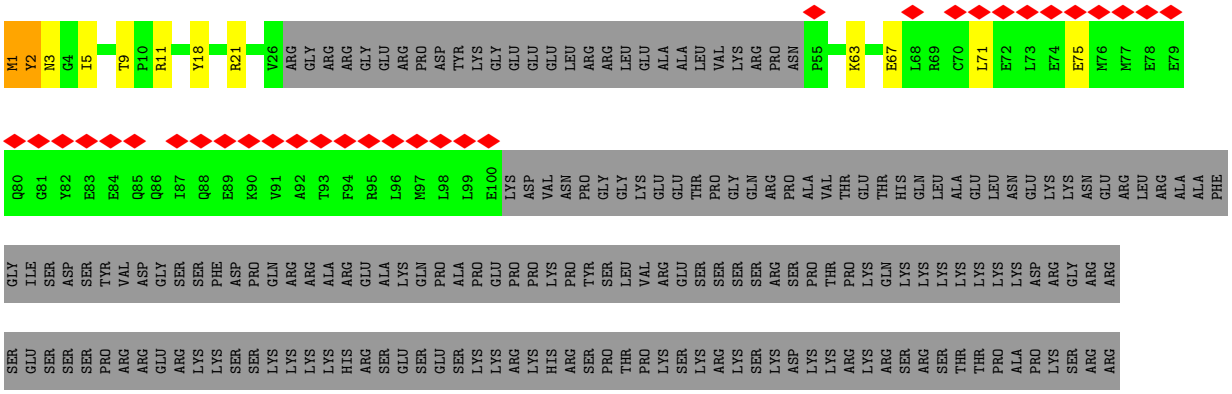


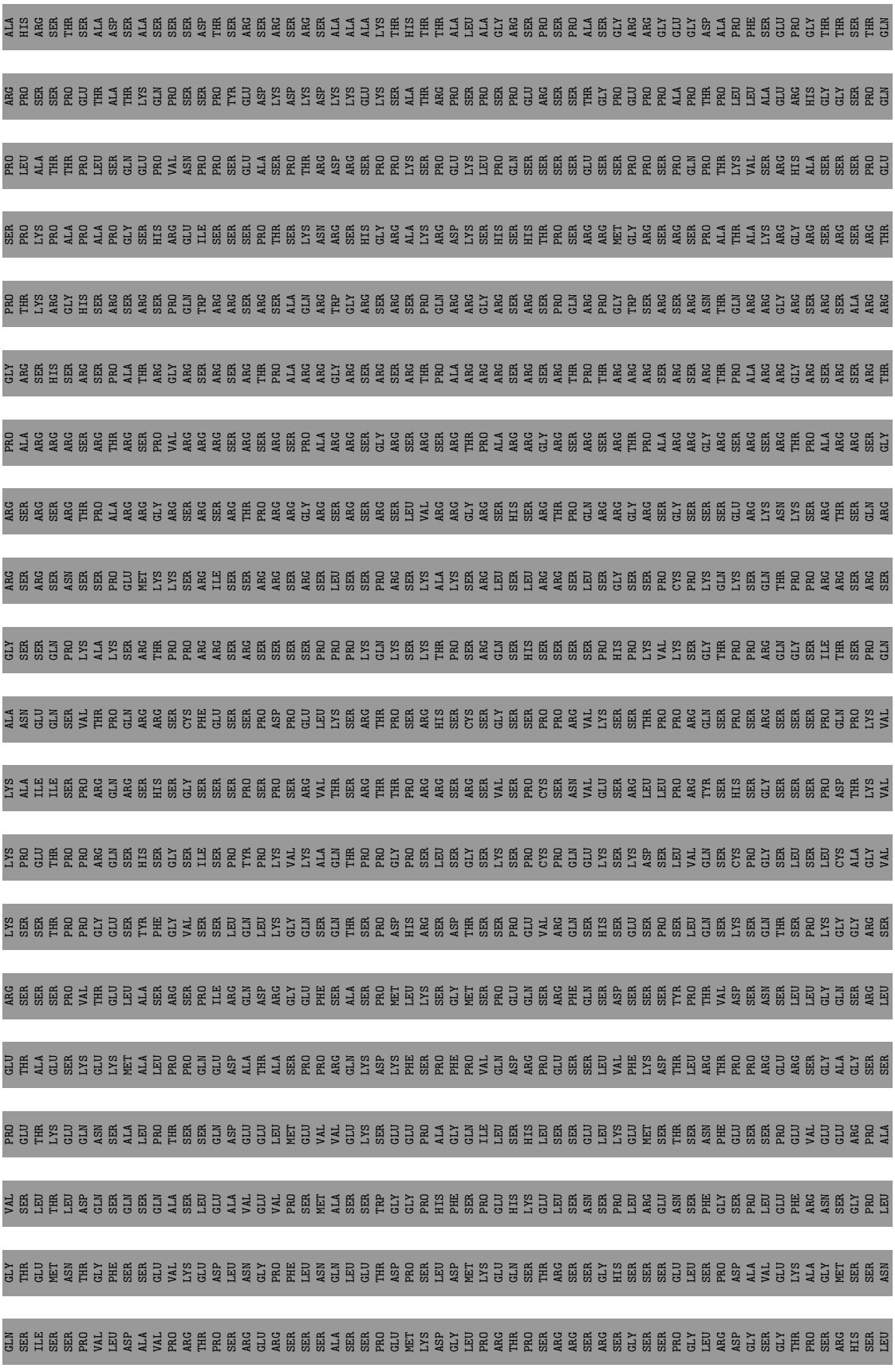


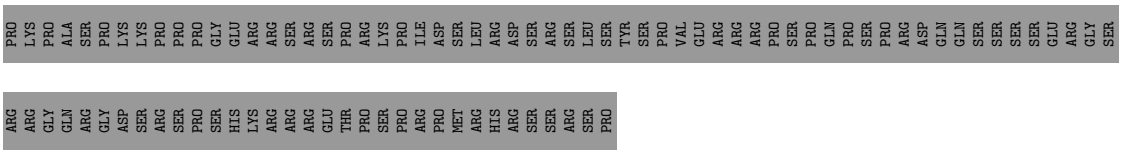
• Molecule 20: Serine/arginine repetitive matrix protein 2

Chain U:

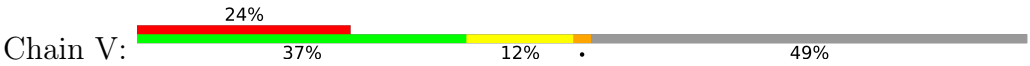


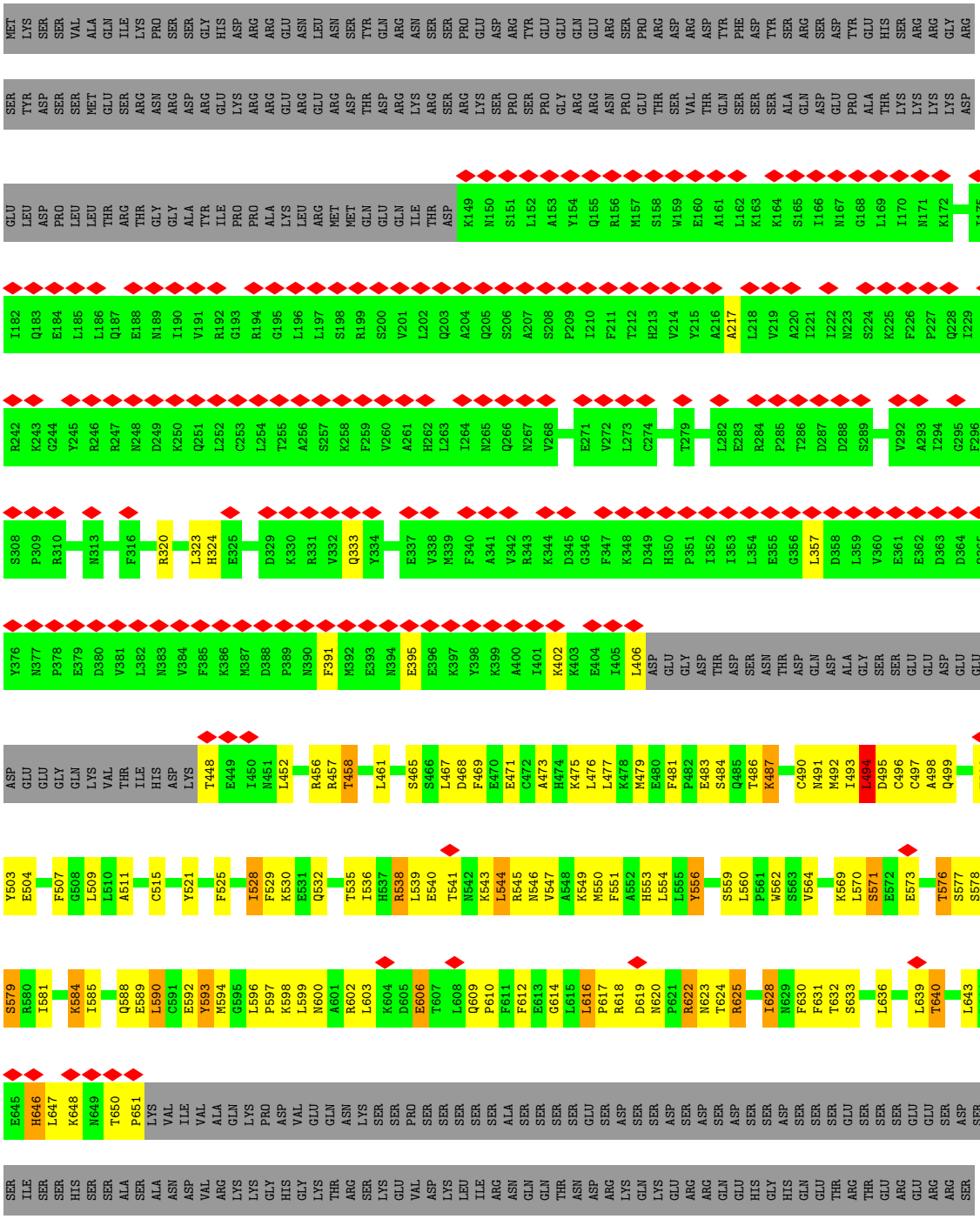


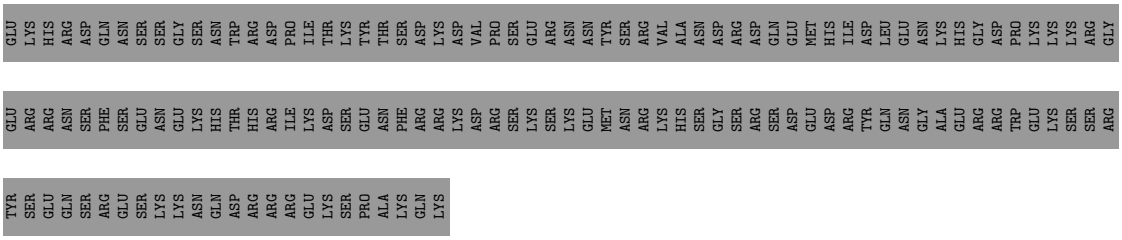




• Molecule 21: Pre-mRNA-splicing factor CWC22 homolog

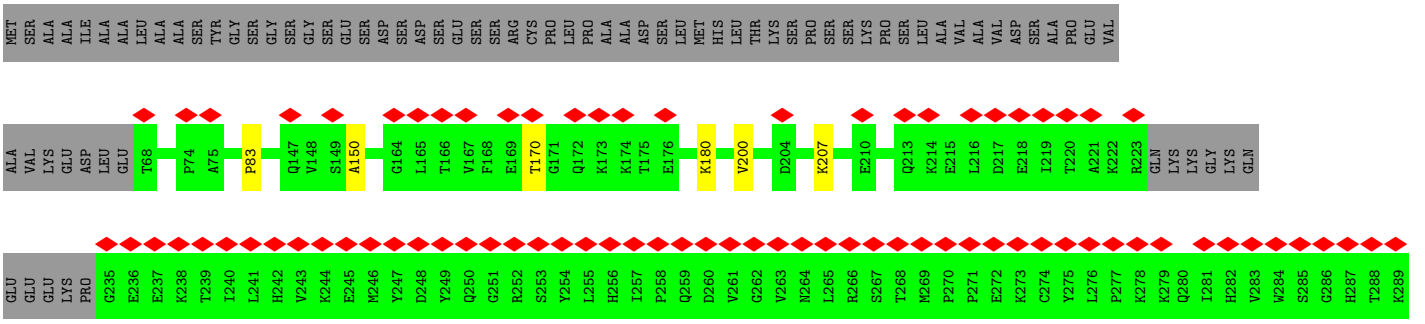






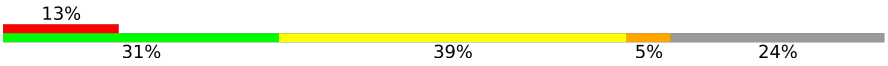
• Molecule 22: Pre-mRNA-processing factor 17

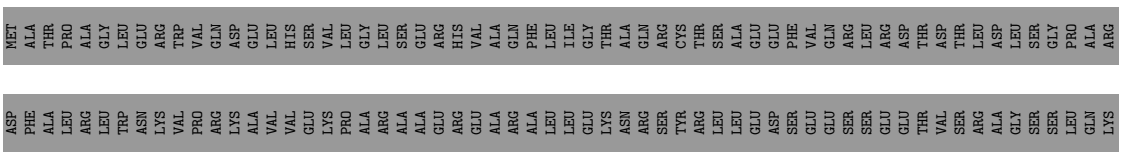
Chain W:

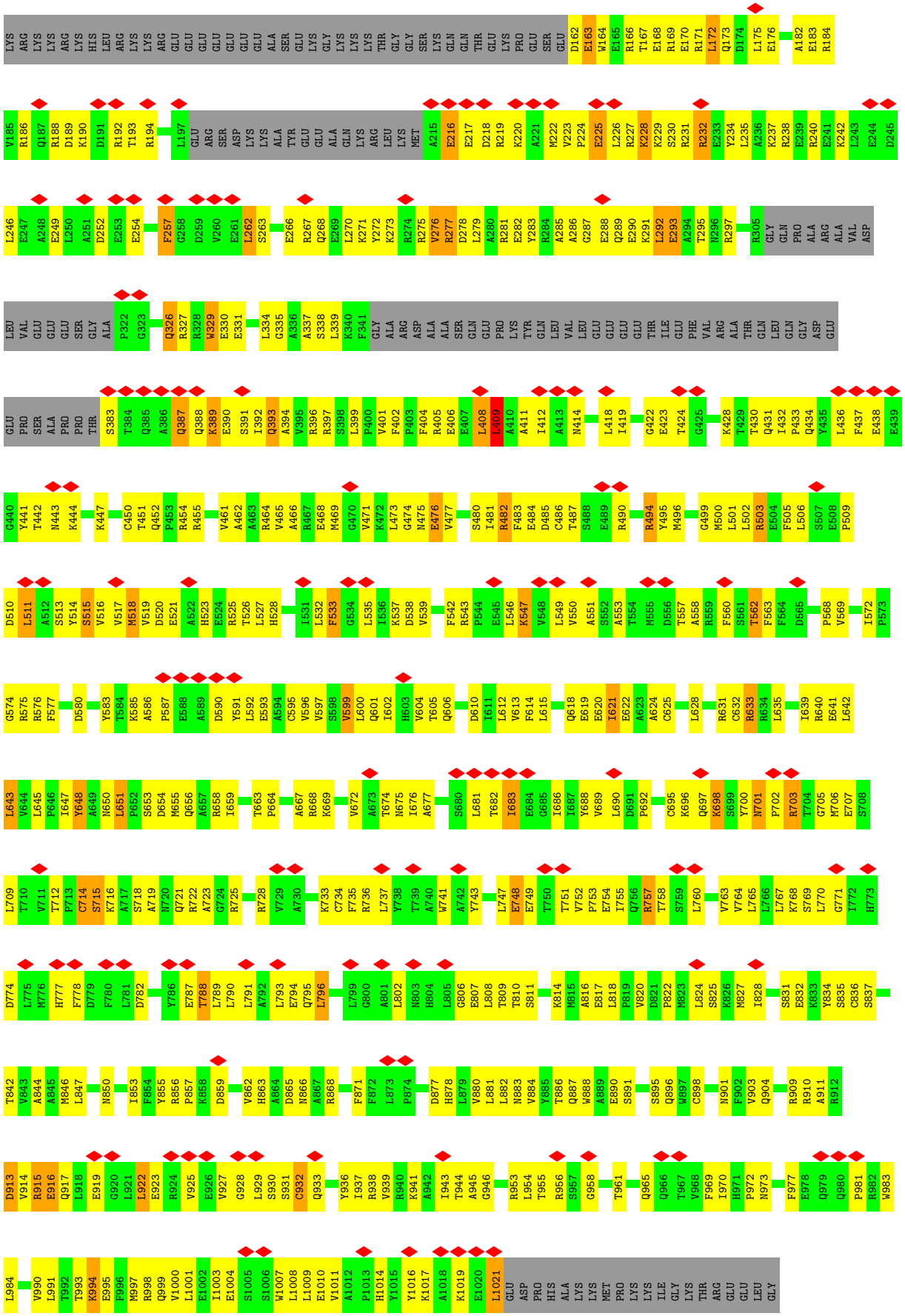


• Molecule 23: Pre-mRNA-splicing factor ATP-dependent RNA helicase DHX16

Chain X:

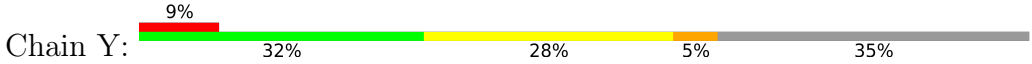


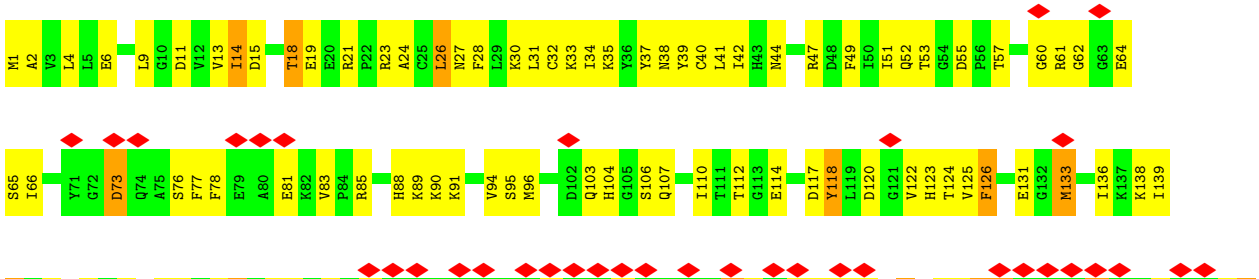




• Molecule 24: Peptidyl-prolyl cis-trans isomerase-like 4

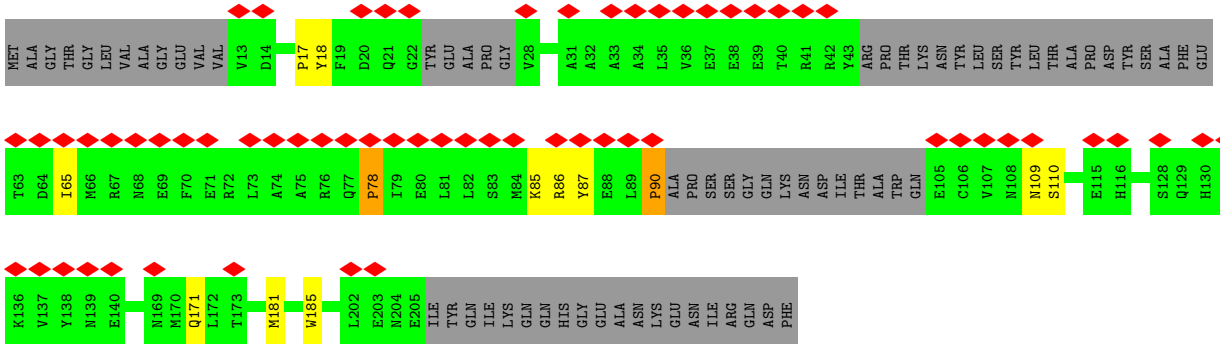
Chain Y:





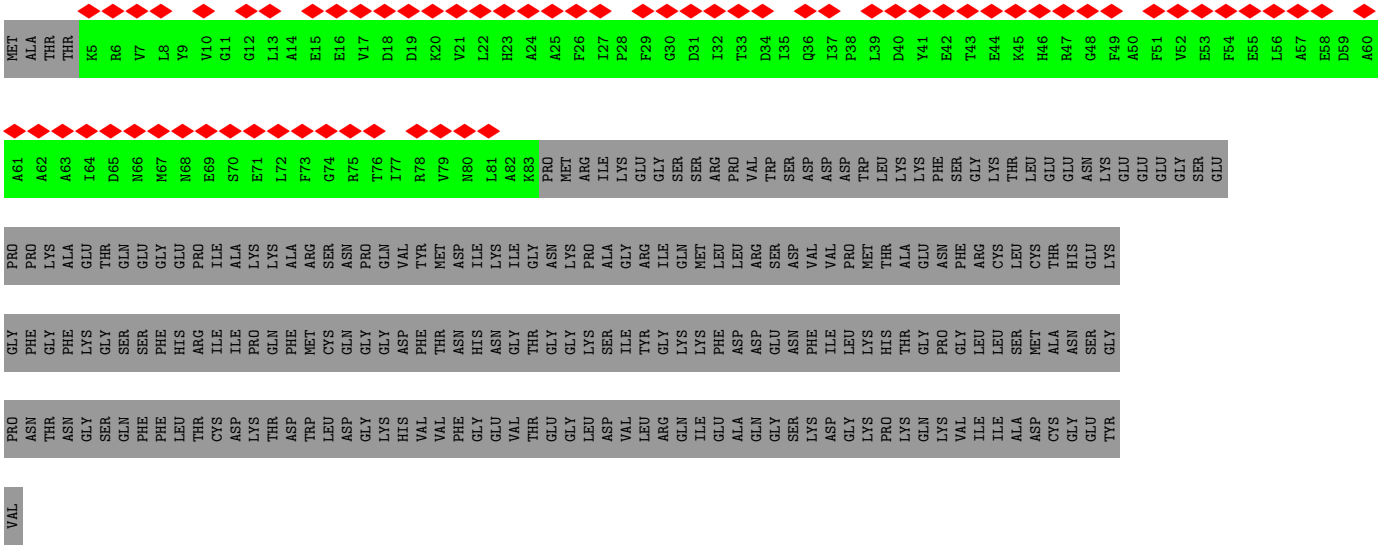
• Molecule 25: Pre-mRNA-splicing factor SPF27

Chain Z:

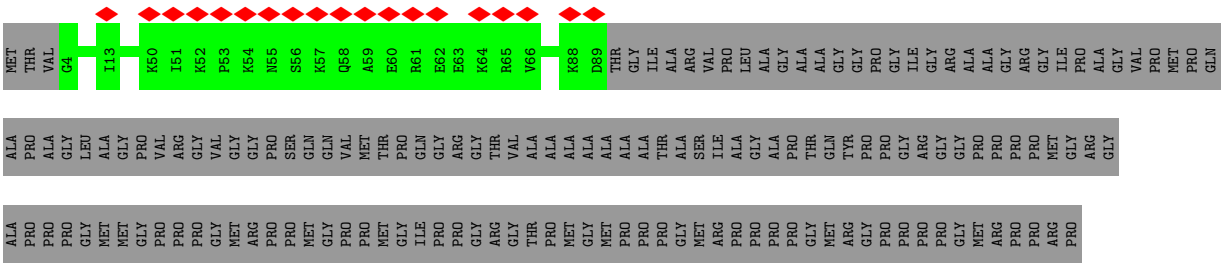


• Molecule 26: Peptidyl-prolyl cis-trans isomerase E

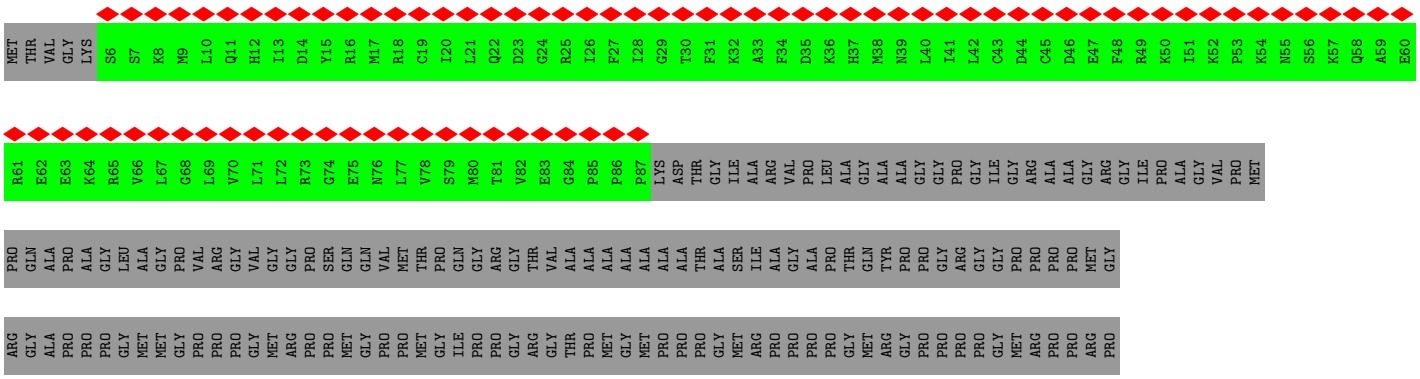
Chain y:



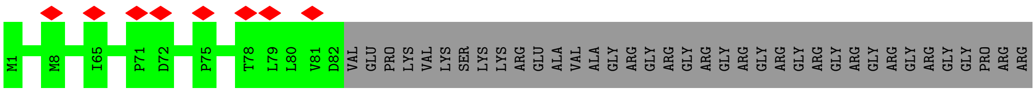
• Molecule 27: Small nuclear ribonucleoprotein-associated proteins B and B'



• Molecule 27: Small nuclear ribonucleoprotein-associated proteins B and B'

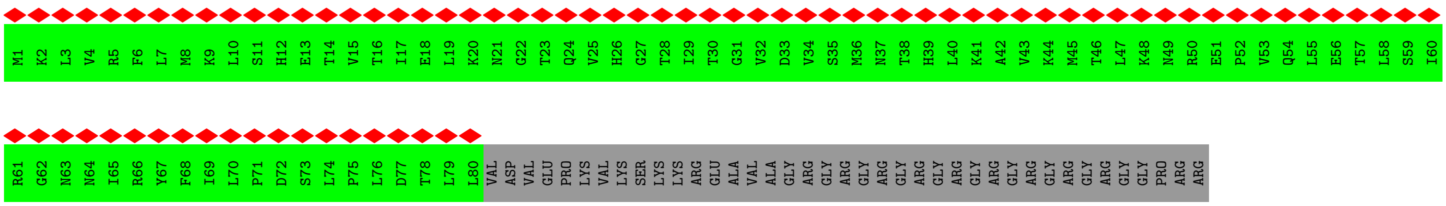


• Molecule 28: Small nuclear ribonucleoprotein Sm D1



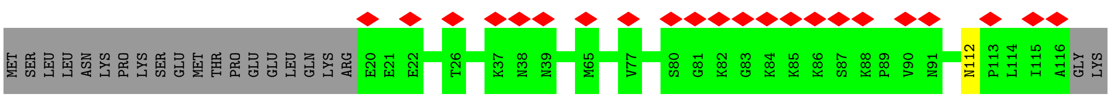
- Molecule 28: Small nuclear ribonucleoprotein Sm D1

Chain n:



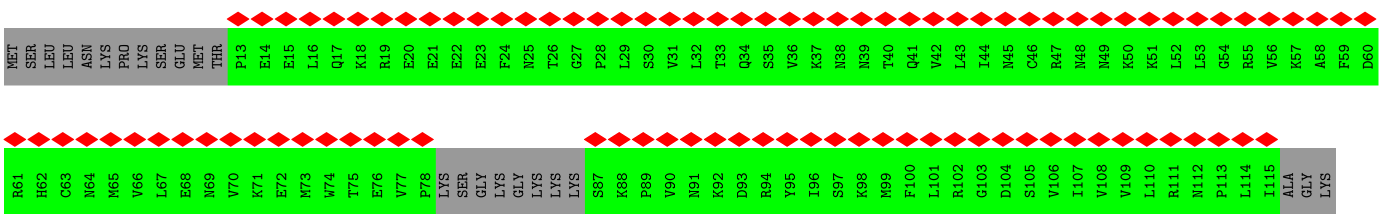
- Molecule 29: Small nuclear ribonucleoprotein Sm D2

Chain c:



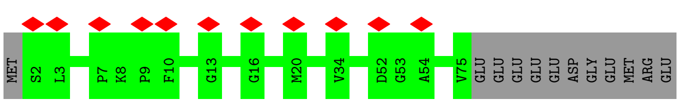
- Molecule 29: Small nuclear ribonucleoprotein Sm D2

Chain h:



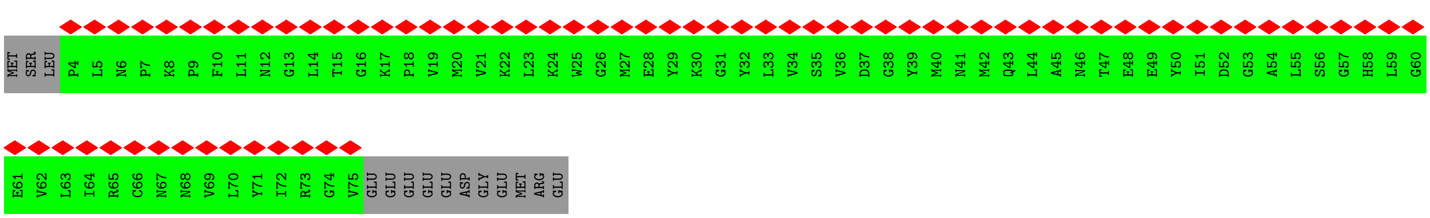
- Molecule 30: Small nuclear ribonucleoprotein F

Chain d:



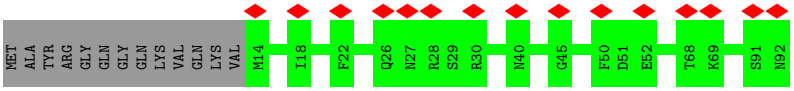
- Molecule 30: Small nuclear ribonucleoprotein F

Chain i:



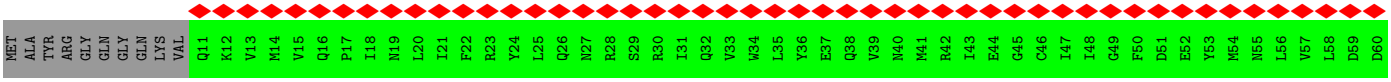
• Molecule 31: Small nuclear ribonucleoprotein E

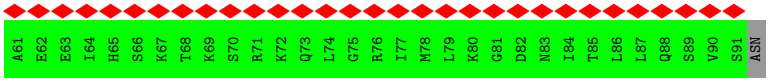
Chain e:



• Molecule 31: Small nuclear ribonucleoprotein E

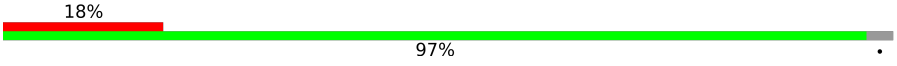
Chain j:

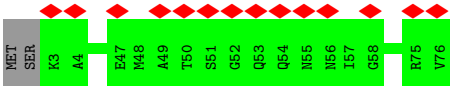




• Molecule 32: Small nuclear ribonucleoprotein G

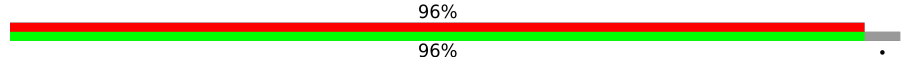
Chain f:





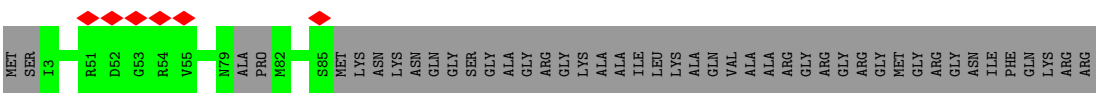
• Molecule 32: Small nuclear ribonucleoprotein G

Chain k:



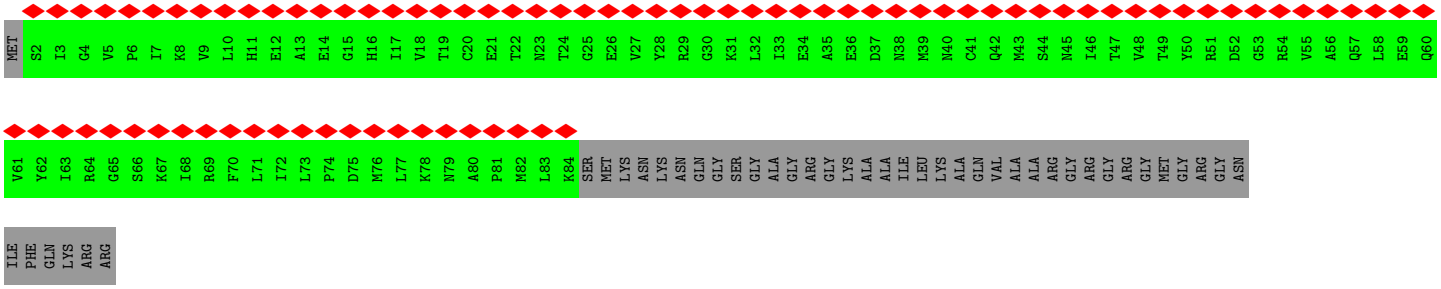
• Molecule 33: Small nuclear ribonucleoprotein Sm D3

Chain g:



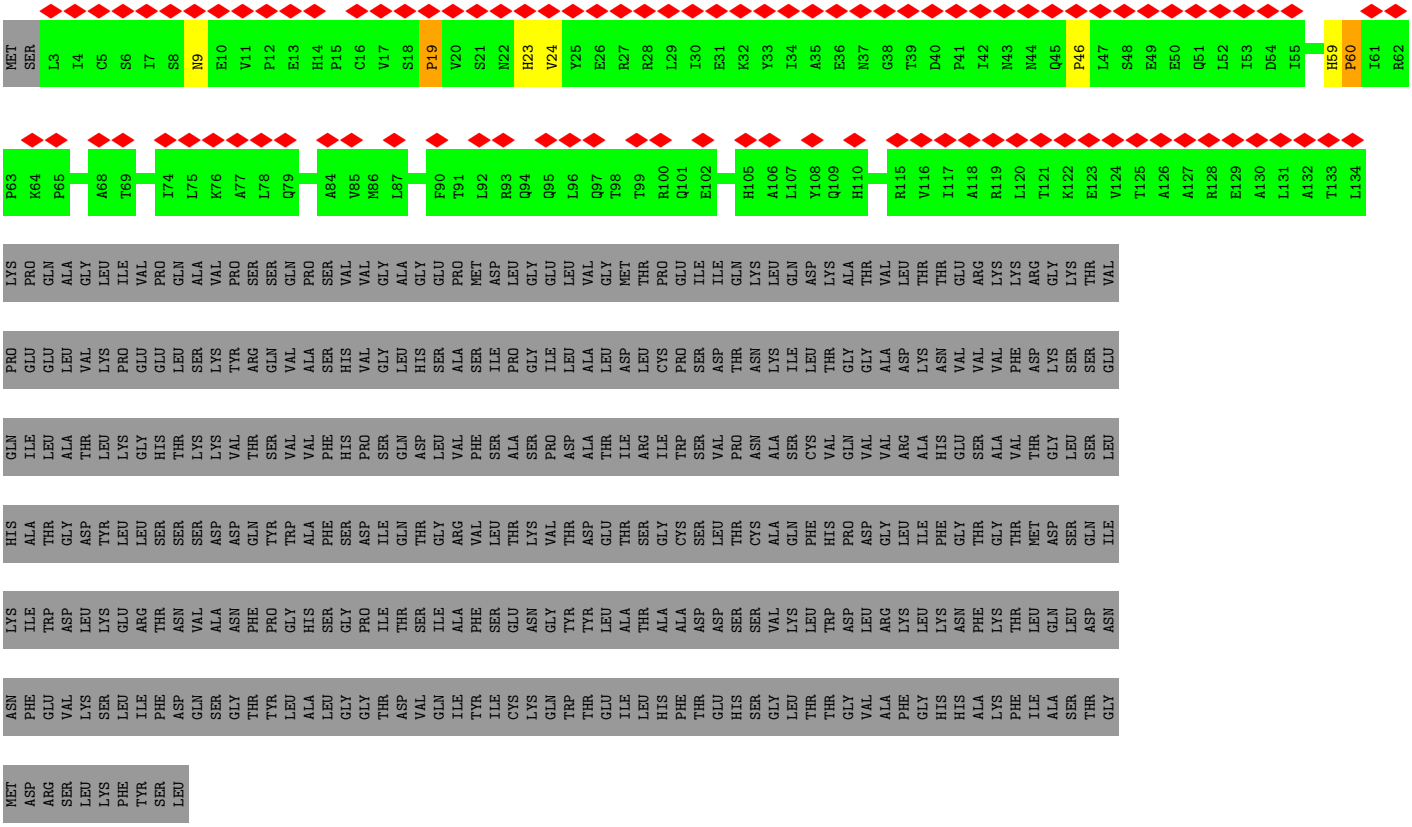
• Molecule 33: Small nuclear ribonucleoprotein Sm D3

Chain l:



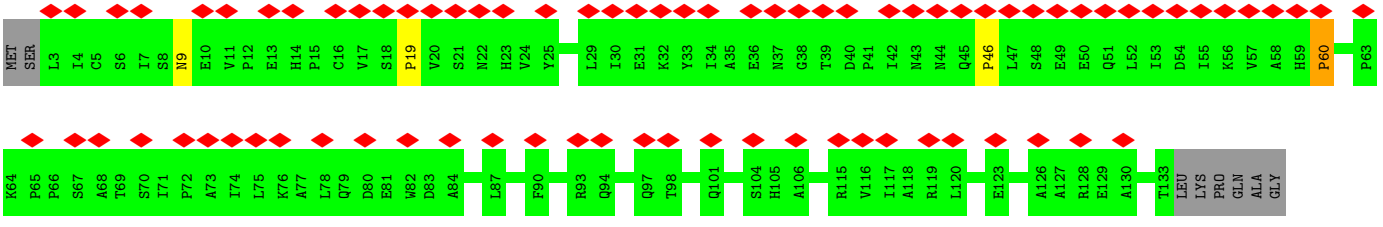
• Molecule 34: Pre-mRNA-processing factor 19

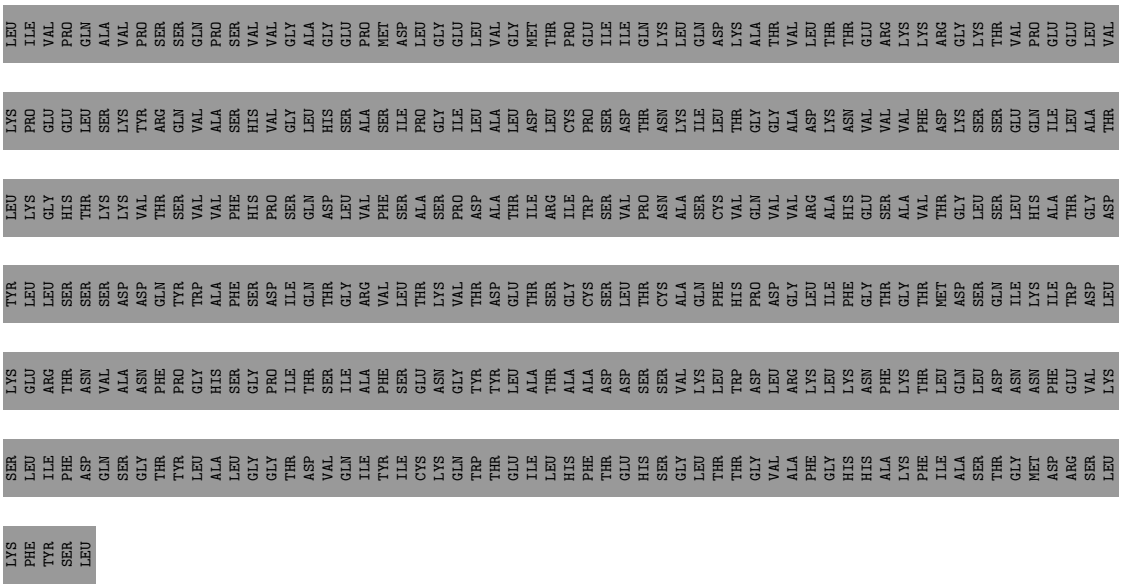
Chain q:



• Molecule 34: Pre-mRNA-processing factor 19

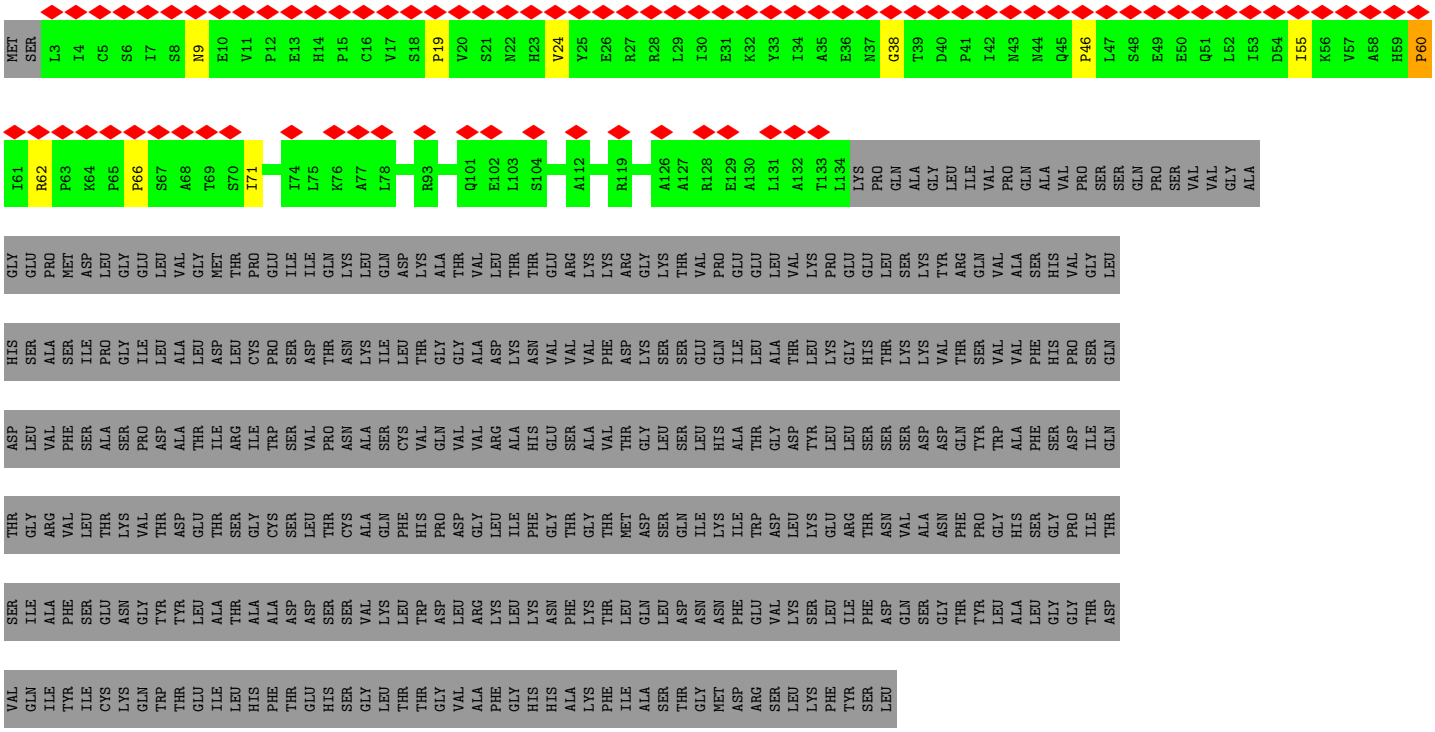
Chain r:





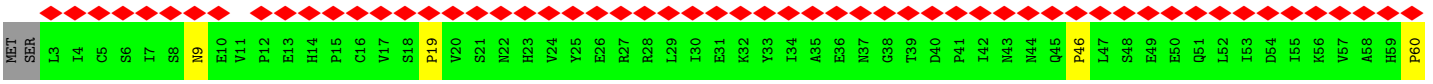
• Molecule 34: Pre-mRNA-processing factor 19

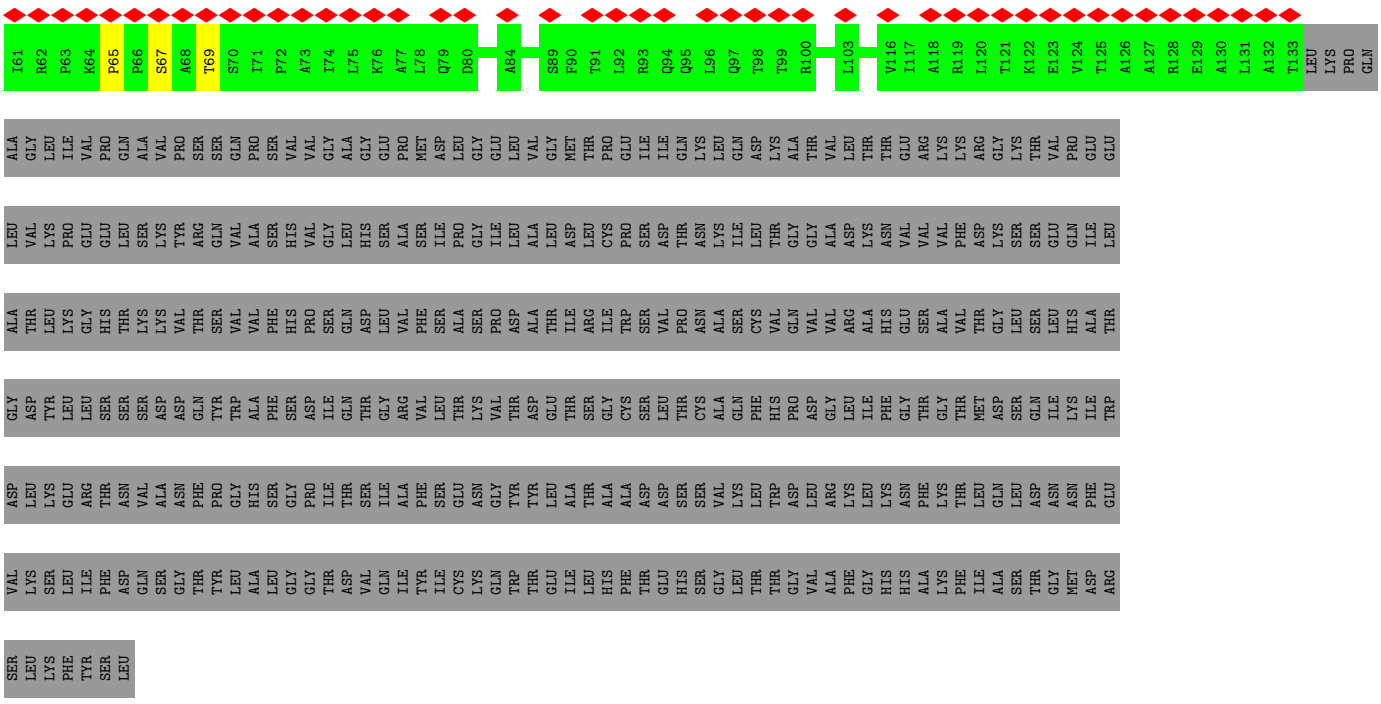
Chain s:



• Molecule 34: Pre-mRNA-processing factor 19

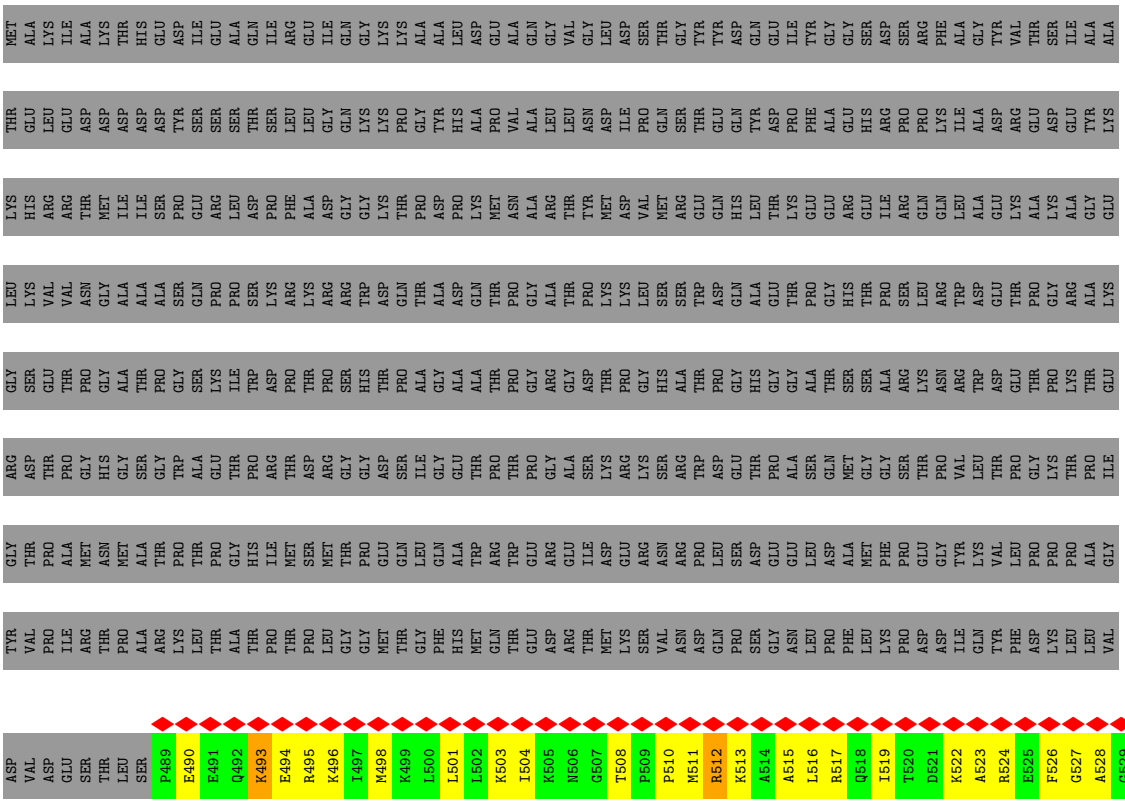
Chain t:

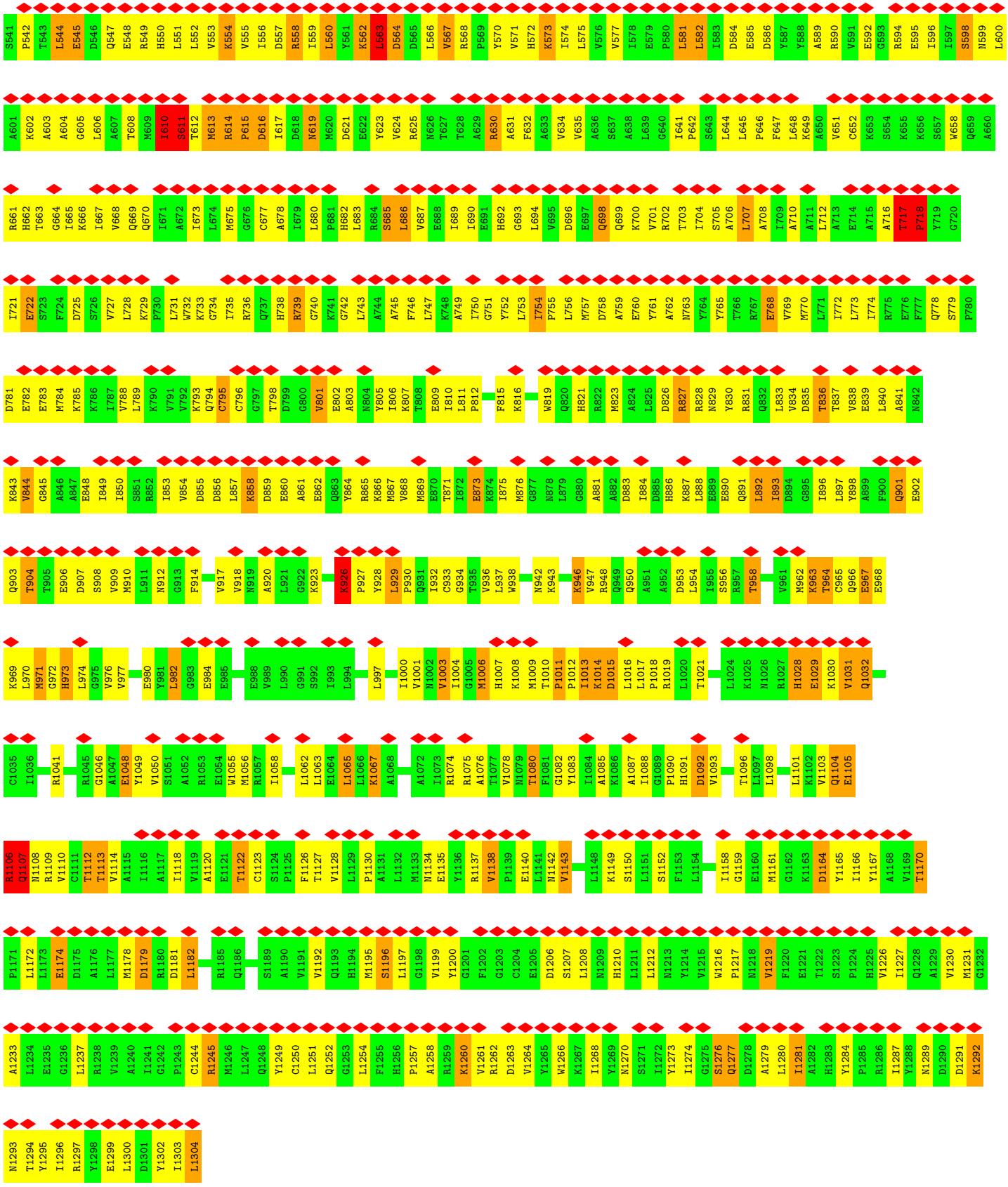




• Molecule 35: Splicing factor 3B subunit 1

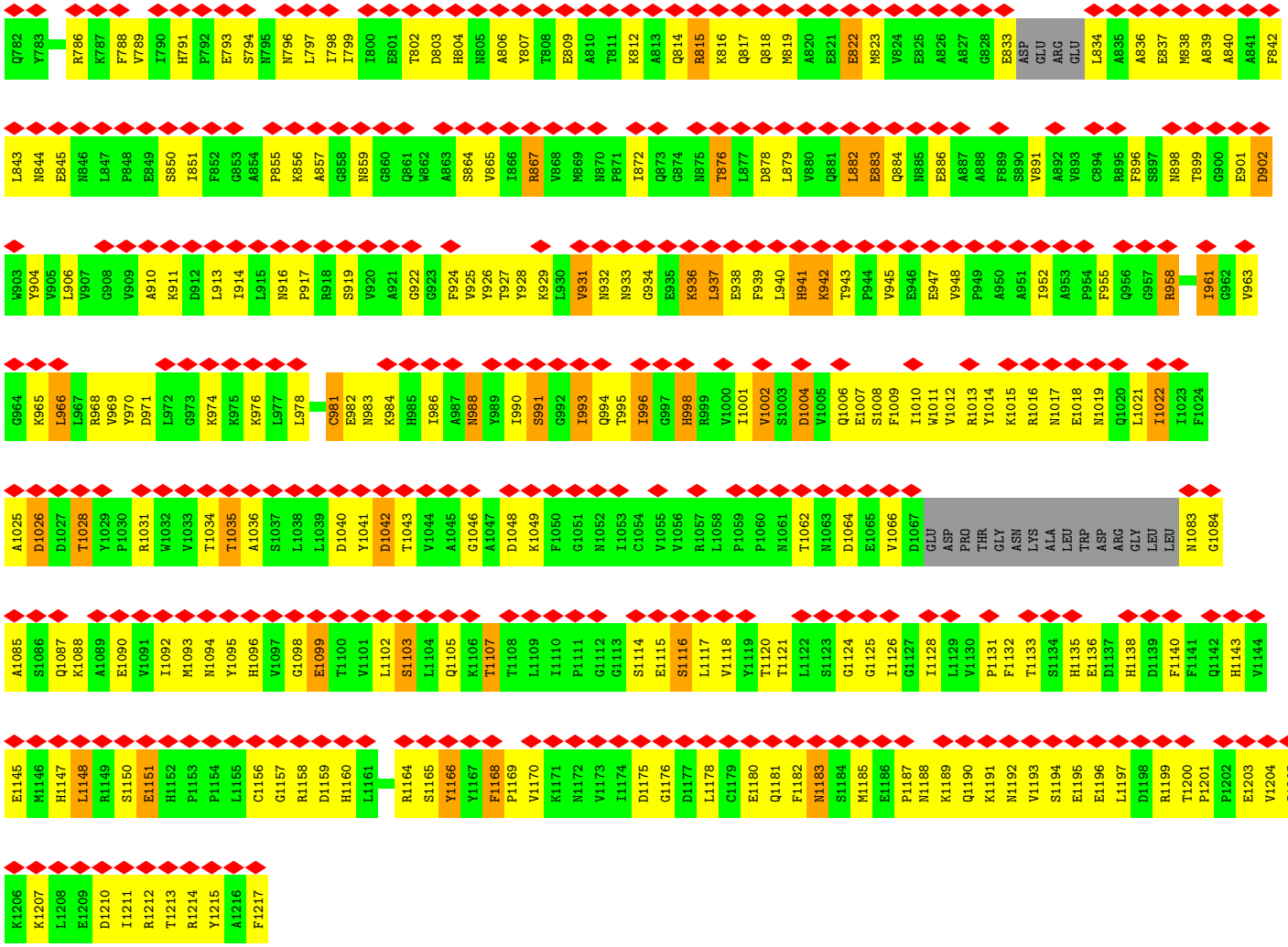
Chain 1:





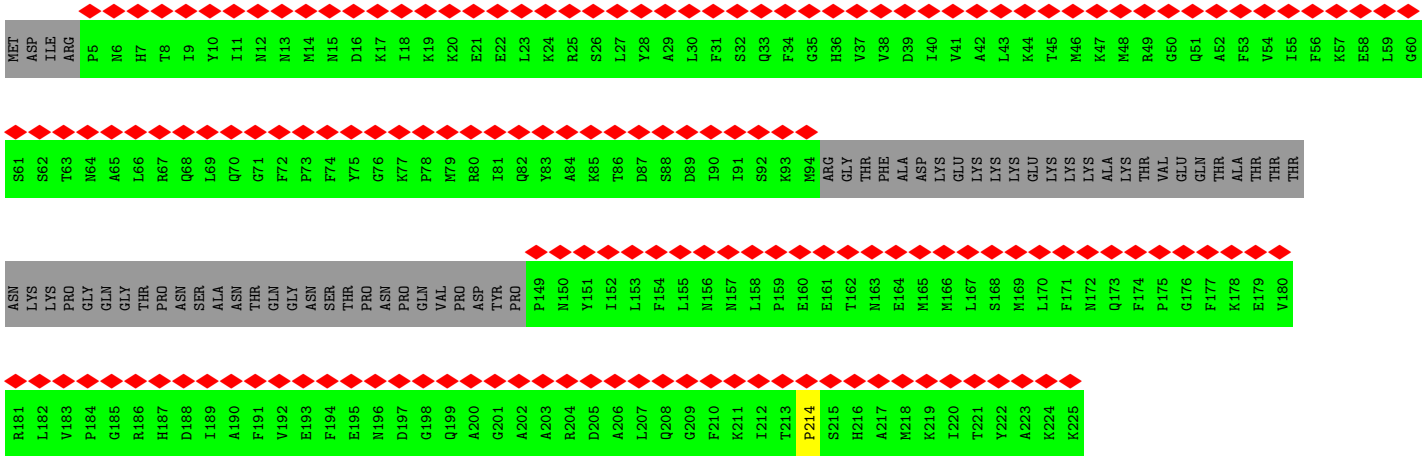
- Molecule 36: Splicing factor 3B subunit 3

Chain 3:



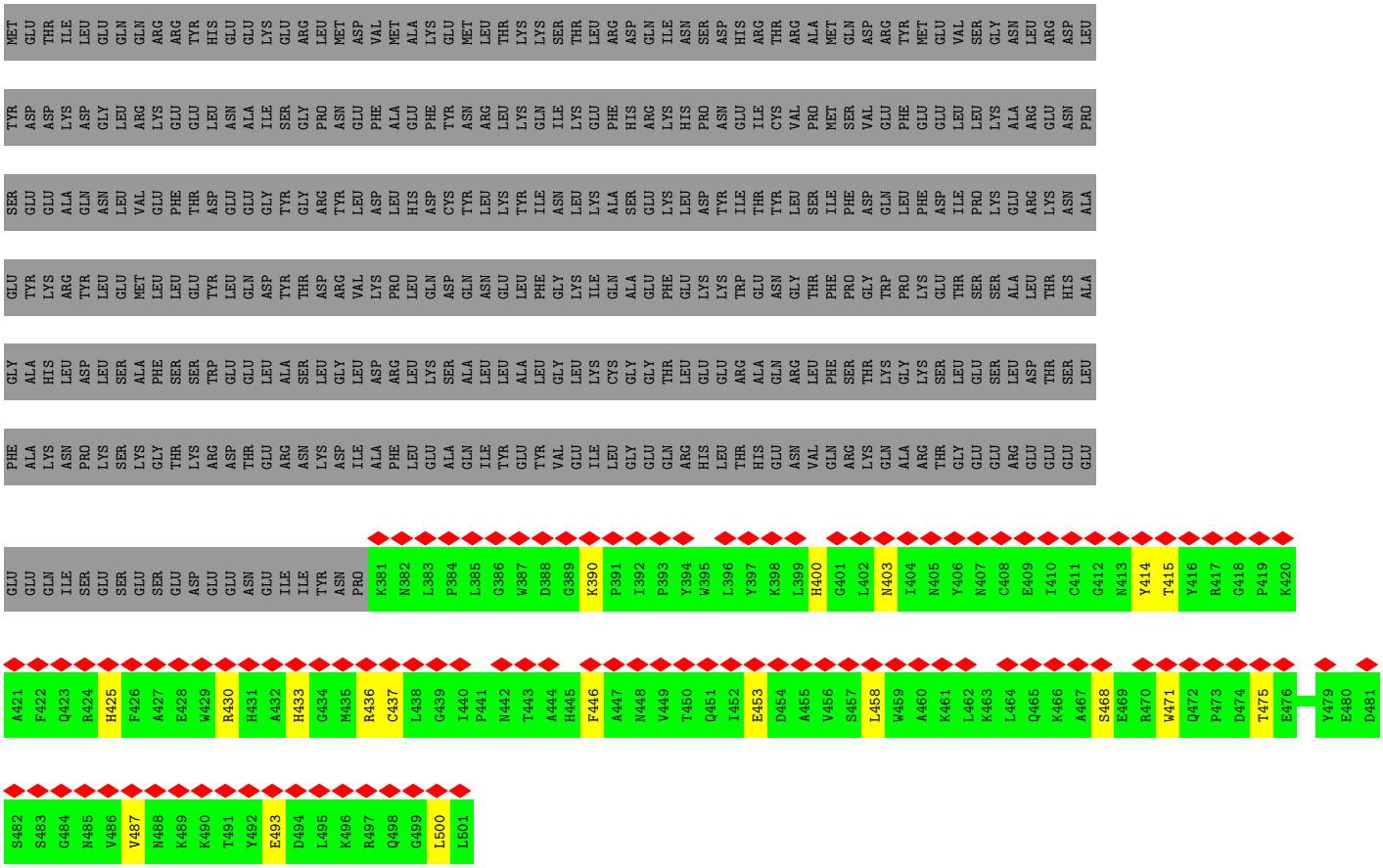
• Molecule 37: U2 small nuclear ribonucleoprotein B”

Chain p:



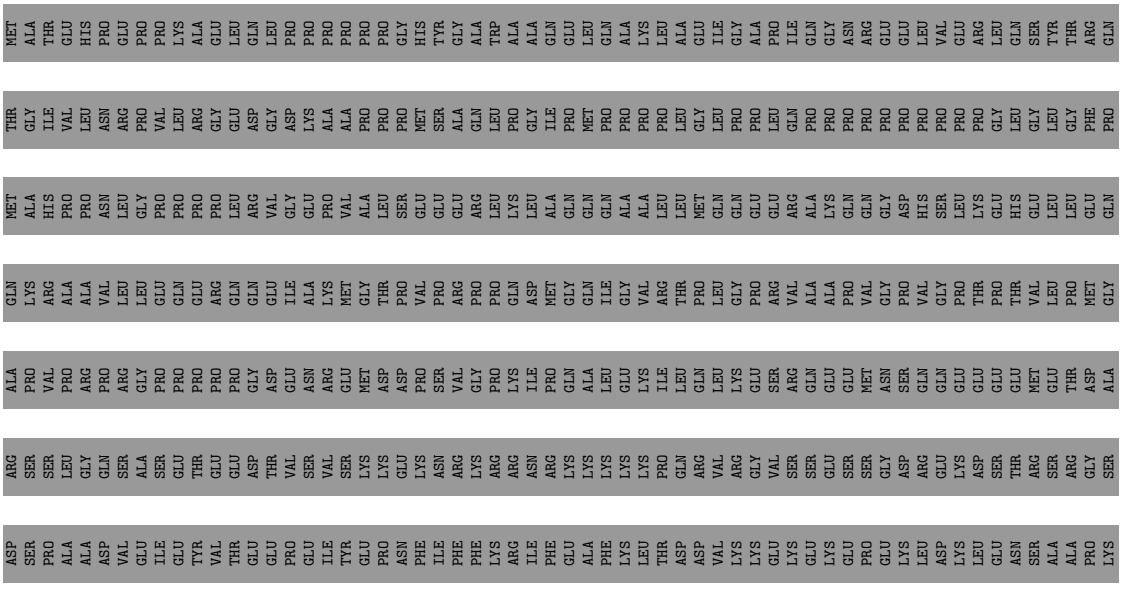
• Molecule 38: Splicing factor 3A subunit 3

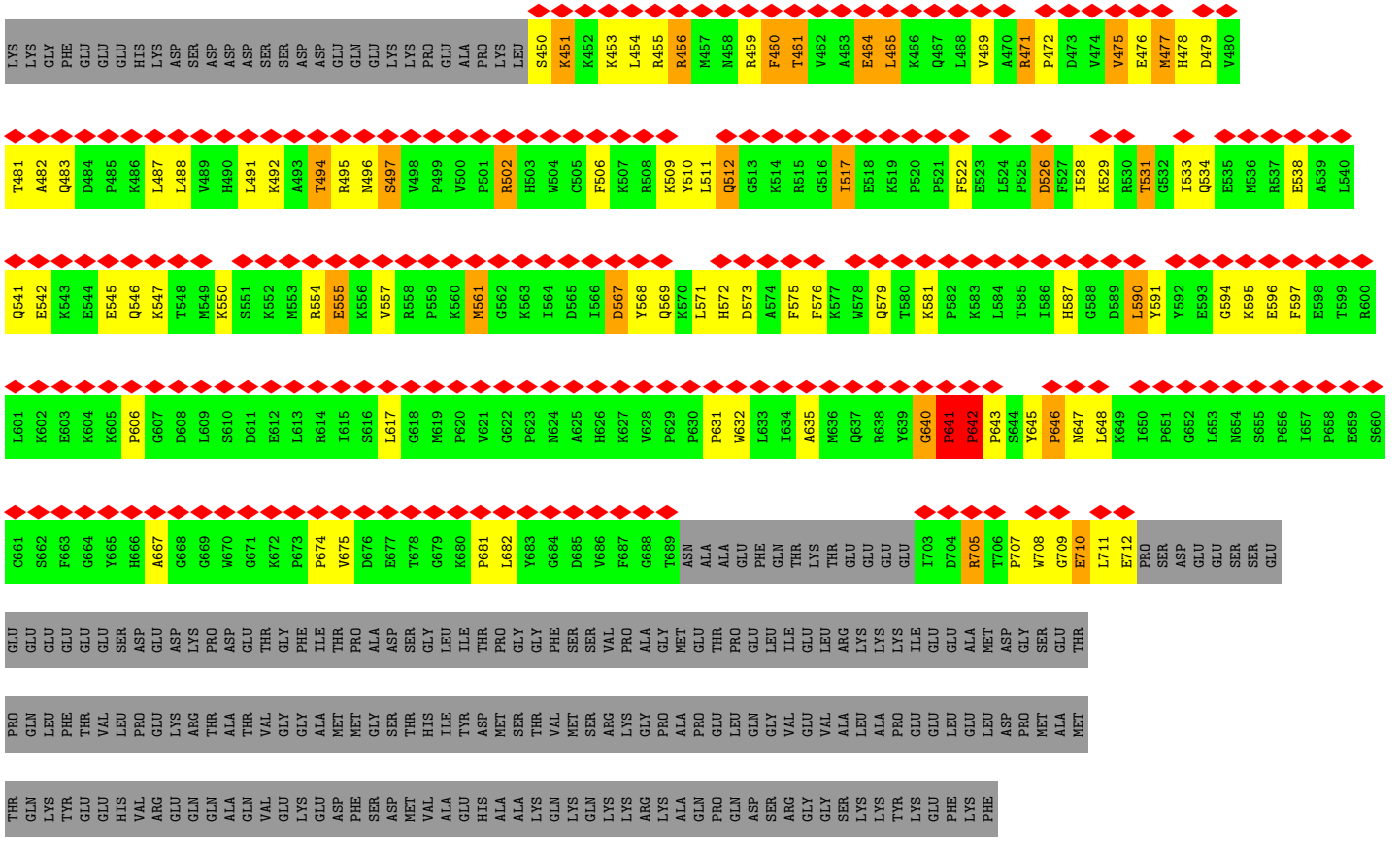
Chain w:



• Molecule 39: Splicing factor 3B subunit 2

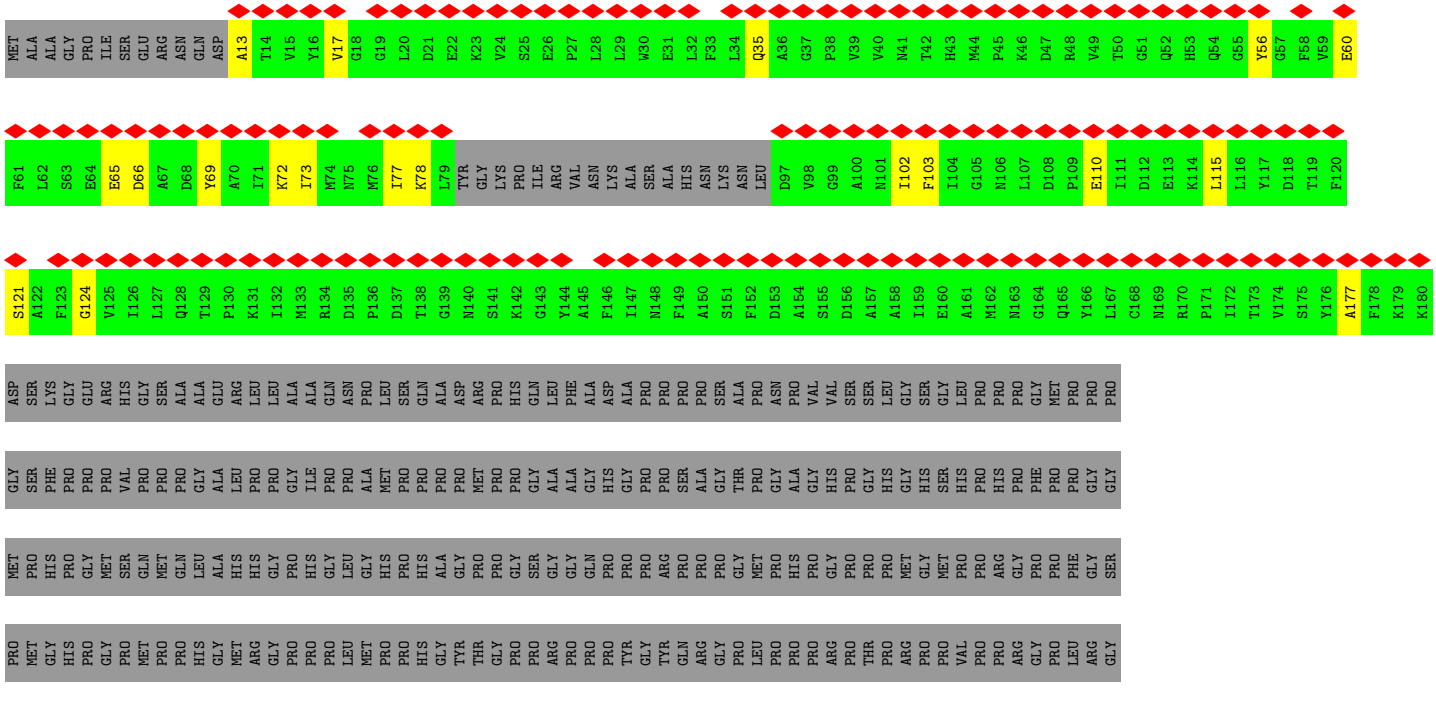
Chain 2:





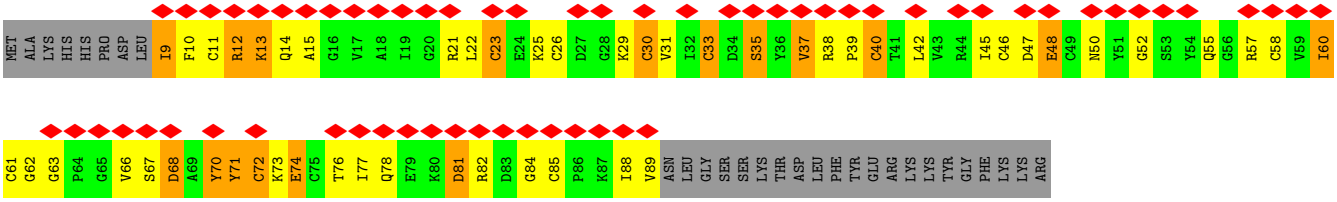
• Molecule 40: Splicing factor 3B subunit 4

Chain 4:



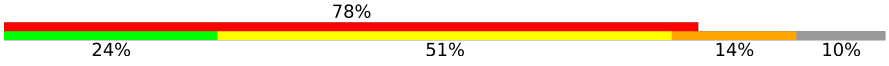
• Molecule 41: PHD finger-like domain-containing protein 5A

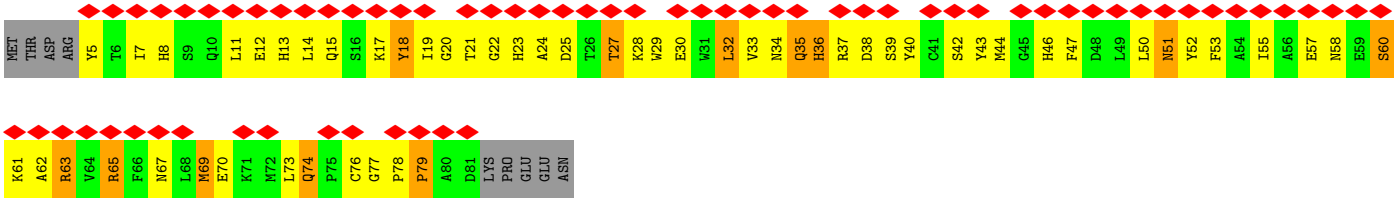
Chain 7:



• Molecule 42: Splicing factor 3B subunit 5

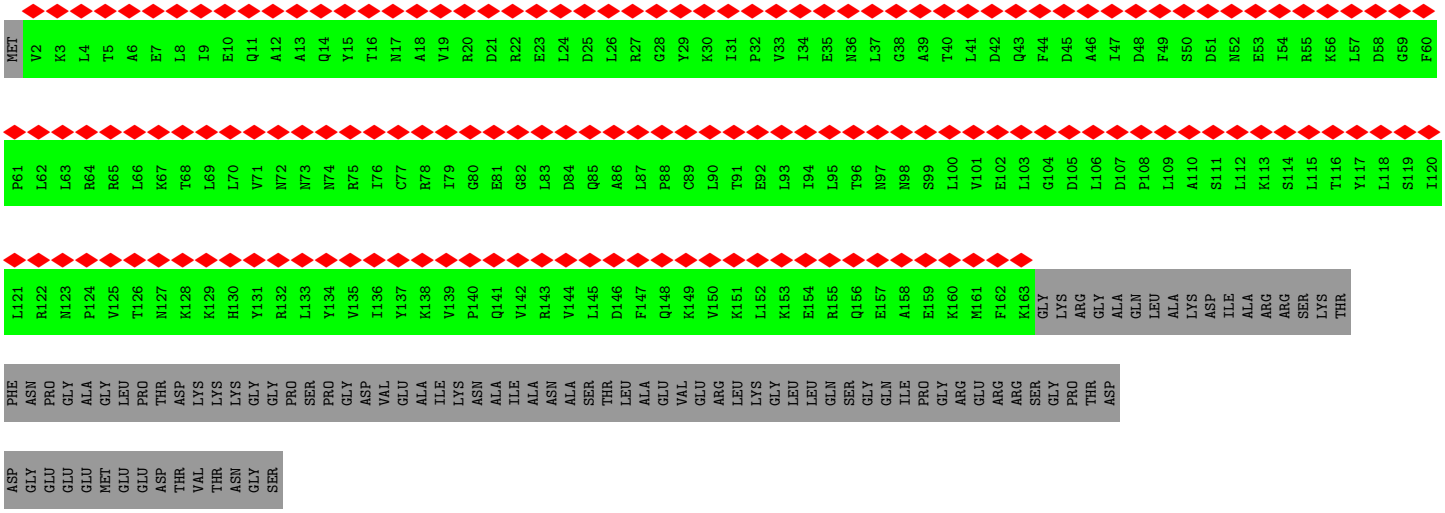
Chain 5:





• Molecule 43: U2 small nuclear ribonucleoprotein A'

Chain o:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47352	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.422	Depositor
Minimum map value	-1.073	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.24	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: IHP, ZN, GTP, SEP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.78	1/16774 (0.0%)	0.67	5/22749 (0.0%)
2	B	1.08	2/2303 (0.1%)	1.01	6/3579 (0.2%)
3	C	0.55	0/6873	0.62	2/9346 (0.0%)
4	E	0.42	0/2392	0.63	1/3242 (0.0%)
5	F	1.21	3/2323 (0.1%)	1.17	11/3619 (0.3%)
6	G	0.81	5/1764 (0.3%)	1.34	25/2737 (0.9%)
7	H	0.70	4/3947 (0.1%)	1.11	17/6138 (0.3%)
8	I	0.26	0/3406	0.43	0/4767
9	J	0.60	1/3817 (0.0%)	0.54	0/5184
10	K	0.72	0/188	0.60	0/248
11	L	0.50	0/2612	0.57	0/3548
12	M	0.48	0/991	0.75	0/1325
13	N	0.64	0/1210	0.60	0/1622
14	O	0.34	0/1447	0.48	0/2013
15	P	0.73	0/888	0.79	1/1177 (0.1%)
16	Q	0.24	0/5279	0.45	0/6583
17	R	0.53	0/2937	0.62	0/3945
18	S	0.27	0/769	0.50	0/1063
19	T	1.01	0/2574	0.72	2/3511 (0.1%)
20	U	0.43	0/424	0.48	0/582
21	V	0.32	0/2993	0.50	1/4088 (0.0%)
22	W	0.34	0/2471	0.71	0/3437
23	X	0.36	1/6479 (0.0%)	0.60	4/8747 (0.0%)
24	Y	0.33	0/2605	0.58	0/3522
25	Z	0.39	0/768	0.52	2/1067 (0.2%)
26	y	0.26	0/315	0.51	0/392
27	a	0.51	0/343	0.69	0/427
27	m	0.26	0/416	0.54	0/581
28	b	0.57	0/327	0.67	0/407
28	n	0.24	0/404	0.50	0/564
29	c	0.69	0/387	0.72	0/482
29	h	0.24	0/485	0.48	0/677

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
30	d	0.77	0/295	0.76	0/367
30	i	0.27	0/362	0.53	0/502
31	e	0.65	0/315	0.75	0/392
31	j	0.25	0/403	0.46	0/561
32	f	0.55	0/295	0.61	0/367
32	k	0.26	0/366	0.53	0/509
33	g	0.47	0/322	0.55	0/399
33	l	0.26	0/417	0.51	0/581
34	q	0.35	0/658	0.63	3/919 (0.3%)
34	r	0.32	0/653	0.59	3/912 (0.3%)
34	s	0.34	0/658	0.66	3/919 (0.3%)
34	t	0.35	0/653	0.59	3/912 (0.3%)
35	1	0.69	4/6609 (0.1%)	0.71	9/8947 (0.1%)
36	3	0.53	0/9408	0.66	1/12767 (0.0%)
37	p	0.26	0/847	0.48	0/1181
38	w	0.38	0/1029	0.54	0/1393
39	2	0.72	5/1833 (0.3%)	0.70	3/2469 (0.1%)
40	4	0.33	0/741	0.51	0/1027
41	7	0.56	0/621	0.61	0/833
42	5	0.72	0/654	0.64	0/885
43	o	0.24	0/821	0.48	0/1149
All	All	0.61	26/108871 (0.0%)	0.69	102/149360 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11
3	C	0	4
4	E	0	1
6	G	0	1
8	I	0	1
9	J	0	2
12	M	0	1
13	N	0	1
15	P	0	1
17	R	0	1
23	X	0	1
24	Y	0	1
29	c	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
35	1	0	5
36	3	0	5
39	2	0	1
41	7	0	1
42	5	0	1
All	All	0	40

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	2	642	PRO	N-CA	13.71	1.70	1.47
35	1	718	PRO	N-CA	13.30	1.69	1.47
39	2	641	PRO	N-CA	13.02	1.69	1.47
23	X	701	ASN	C-N	9.25	1.51	1.34
35	1	926	LYS	C-N	8.50	1.50	1.34
9	J	207	PRO	C-N	8.45	1.50	1.34
7	H	32	U	O3'-P	8.28	1.71	1.61
39	2	645	TYR	C-N	7.86	1.49	1.34
6	G	1	G	O3'-P	6.82	1.69	1.61
6	G	1	G	N1-C2	-6.14	1.32	1.37
35	1	717	THR	C-N	6.08	1.45	1.34
6	G	-1	C	O3'-P	-5.99	1.53	1.61
39	2	640	GLY	C-N	5.98	1.45	1.34
35	1	611	SER	C-O	5.94	1.34	1.23
7	H	30	A	O3'-P	5.92	1.68	1.61
1	A	705	LYS	CD-CE	5.89	1.66	1.51
39	2	641	PRO	C-N	5.89	1.45	1.34
2	B	32	C	N3-C4	-5.72	1.29	1.33
7	H	15	U	C4-O4	-5.63	1.19	1.23
5	F	65	G	N9-C8	-5.39	1.34	1.37
7	H	15	U	C2-O2	-5.39	1.17	1.22
6	G	1	G	C2-N2	5.35	1.40	1.34
2	B	55	C	N1-C6	-5.22	1.34	1.37
5	F	72	G	C5-C4	-5.12	1.34	1.38
6	G	-3	A	N3-C4	-5.06	1.31	1.34
5	F	65	G	C5-C4	-5.06	1.34	1.38

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	2	U	C4'-C3'-O3'	14.57	142.14	113.00
39	2	567	ASP	CB-CA-C	12.96	136.32	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	H	15	U	N3-C4-O4	-12.80	110.44	119.40
35	1	615	PRO	CA-N-CD	-11.72	95.08	111.50
6	G	0	G	N9-C1'-C2'	-11.71	98.77	114.00
6	G	1	G	O4'-C1'-N9	11.57	117.46	108.20
7	H	15	U	N3-C2-O2	-11.42	114.21	122.20
35	1	718	PRO	CA-N-CD	-11.29	95.69	111.50
7	H	32	U	N1-C1'-C2'	-9.35	101.72	112.00
7	H	15	U	N3-C4-C5	9.08	120.05	114.60
19	T	186	PRO	C-N-CA	-8.99	99.22	121.70
35	1	610	ILE	O-C-N	-8.75	108.70	122.70
7	H	32	U	C4'-C3'-O3'	8.50	130.00	113.00
7	H	15	U	C2-N3-C4	-8.28	122.03	127.00
5	F	38	G	O5'-P-OP2	-7.66	98.81	105.70
5	F	78	A	C8-N9-C4	7.32	108.73	105.80
6	G	1	G	C3'-C2'-O2'	7.25	134.34	113.30
7	H	32	U	C1'-C2'-O2'	-7.25	88.84	110.60
34	s	60	PRO	N-CA-CB	7.10	111.81	103.30
5	F	82	A	C2-N3-C4	-7.00	107.10	110.60
2	B	40	U	C2-N1-C1'	6.98	126.07	117.70
7	H	31	G	C4'-C3'-O3'	6.93	126.86	113.00
6	G	9	C	N3-C2-O2	-6.85	117.11	121.90
2	B	19	A	N9-C4-C5	-6.79	103.08	105.80
34	t	60	PRO	N-CA-CB	6.70	111.34	103.30
6	G	1	G	C4'-C3'-O3'	-6.67	95.39	109.40
34	s	46	PRO	N-CA-CB	6.58	111.20	103.30
34	q	46	PRO	N-CA-CB	6.58	111.20	103.30
34	r	46	PRO	N-CA-CB	6.55	111.16	103.30
7	H	15	U	N1-C2-N3	6.48	118.79	114.90
25	Z	90	PRO	N-CA-CB	6.42	111.01	103.30
34	q	60	PRO	N-CA-CB	6.41	111.00	103.30
21	V	494	LEU	CA-CB-CG	6.34	129.88	115.30
35	1	1107	GLN	C-N-CA	-6.33	105.88	121.70
6	G	2	U	O4'-C1'-N1	6.33	113.26	108.20
6	G	0	G	C4'-C3'-O3'	6.31	125.61	113.00
6	G	112	U	N1-C2-O2	6.29	127.21	122.80
25	Z	78	PRO	N-CA-CB	6.27	110.82	103.30
35	1	619	ASN	C-N-CA	6.25	137.31	121.70
6	G	1	G	C1'-O4'-C4'	-6.18	104.95	109.90
6	G	2	U	P-O3'-C3'	-6.12	112.36	119.70
6	G	-5	C	C2-N1-C1'	6.12	125.53	118.80
7	H	173	C	N1-C2-O2	6.07	122.54	118.90
5	F	59	G	C4-C5-N7	6.01	113.21	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	t	46	PRO	N-CA-CB	5.98	110.48	103.30
6	G	112	U	C2-N1-C1'	5.91	124.79	117.70
5	F	34	G	C4-N9-C1'	5.89	134.15	126.50
34	q	19	PRO	N-CA-CB	5.82	110.28	103.30
4	E	227	LEU	CA-CB-CG	5.79	128.63	115.30
1	A	1518	LEU	CB-CG-CD2	5.79	120.84	111.00
7	H	64	A	C5-C6-N6	-5.79	119.07	123.70
6	G	1	G	P-O3'-C3'	5.79	126.64	119.70
6	G	112	U	O5'-P-OP2	-5.76	100.52	105.70
5	F	82	A	C5-C6-N1	-5.74	114.83	117.70
7	H	31	G	N9-C1'-C2'	-5.73	105.70	112.00
34	r	19	PRO	N-CA-CB	5.72	110.17	103.30
6	G	2	U	C5'-C4'-O4'	-5.69	102.27	109.10
6	G	2	U	O5'-P-OP1	-5.68	100.59	105.70
34	t	19	PRO	N-CA-CB	5.66	110.09	103.30
5	F	59	G	C5-N7-C8	-5.61	101.50	104.30
5	F	38	G	C8-N9-C4	-5.59	104.17	106.40
6	G	111	U	OP2-P-O3'	5.58	117.47	105.20
39	2	645	TYR	C-N-CA	5.55	145.31	122.00
7	H	15	U	OP2-P-O3'	5.54	117.39	105.20
35	1	592	GLU	CB-CA-C	5.53	121.47	110.40
34	s	19	PRO	N-CA-CB	5.53	109.93	103.30
2	B	40	U	C6-N1-C1'	-5.48	113.53	121.20
34	r	60	PRO	N-CA-CB	5.48	109.88	103.30
5	F	38	G	N7-C8-N9	5.44	115.82	113.10
36	3	235	LEU	CA-CB-CG	5.41	127.74	115.30
1	A	598	LEU	CB-CG-CD2	-5.41	101.81	111.00
23	X	651	LEU	CA-CB-CG	5.41	127.73	115.30
15	P	216	ARG	NE-CZ-NH1	-5.39	117.60	120.30
7	H	15	U	N1-C2-O2	5.39	126.57	122.80
1	A	1517	LYS	CA-CB-CG	5.38	125.22	113.40
6	G	9	C	N1-C2-O2	5.36	122.12	118.90
23	X	262	LEU	CA-CB-CG	5.35	127.61	115.30
5	F	34	G	C8-N9-C1'	-5.34	120.06	127.00
6	G	85	G	C4-N9-C1'	-5.32	119.59	126.50
7	H	15	U	C5-C4-O4	5.32	129.09	125.90
2	B	19	A	N3-C4-N9	5.28	131.63	127.40
7	H	43	U	N1-C2-O2	-5.25	119.12	122.80
6	G	88	G	OP1-P-O3'	5.25	116.76	105.20
2	B	45	C	N3-C2-O2	-5.24	118.23	121.90
3	C	251	LEU	CA-CB-CG	5.24	127.35	115.30
3	C	510	LEU	CA-CB-CG	5.24	127.35	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	T	303	LEU	CA-CB-CG	5.23	127.33	115.30
35	1	929	LEU	CA-CB-CG	-5.23	103.28	115.30
35	1	563	LEU	CA-CB-CG	5.20	127.25	115.30
6	G	113	U	P-O3'-C3'	5.17	125.90	119.70
7	H	43	U	C2-N3-C4	-5.16	123.90	127.00
23	X	172	LEU	CA-CB-CG	5.16	127.17	115.30
5	F	35	A	N1-C2-N3	5.15	131.88	129.30
35	1	1280	LEU	CB-CG-CD2	-5.10	102.33	111.00
1	A	1516	LYS	C-N-CA	5.09	134.42	121.70
1	A	1817	LEU	CA-CB-CG	5.07	126.95	115.30
6	G	112	U	N3-C2-O2	-5.07	118.65	122.20
6	G	115	C	N1-C2-O2	5.06	121.94	118.90
39	2	640	GLY	C-N-CA	5.05	143.22	122.00
23	X	409	LEU	CA-CB-CG	5.04	126.89	115.30
6	G	-5	C	C5-C6-N1	5.03	123.52	121.00
2	B	47	A	O4'-C1'-N9	5.02	112.22	108.20

There are no chirality outliers.

All (40) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
35	1	1105	GLU	Peptide
35	1	1107	GLN	Peptide
35	1	1179	ASP	Peptide
35	1	567	VAL	Peptide
35	1	610	ILE	Mainchain
39	2	502	ARG	Peptide
36	3	268	ARG	Peptide
36	3	342	LEU	Peptide
36	3	490	THR	Peptide
36	3	916	ASN	Peptide
36	3	971	ASP	Peptide
42	5	79	PRO	Peptide
41	7	13	LYS	Peptide
1	A	1338	SER	Peptide
1	A	1416	ILE	Peptide
1	A	1516	LYS	Peptide
1	A	187	PRO	Peptide
1	A	365	VAL	Peptide
1	A	433	GLU	Peptide
1	A	699	GLU	Peptide
1	A	855	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	A	940	ILE	Peptide
1	A	941	LYS	Peptide
1	A	982	GLU	Peptide
3	C	443	VAL	Peptide
3	C	533	SER	Peptide
3	C	572	GLU	Peptide
3	C	823	ALA	Peptide
4	E	321	TYR	Peptide
6	G	1	G	Sidechain
8	I	386	ASP	Peptide
9	J	201	ARG	Mainchain
9	J	240	THR	Peptide
12	M	124	PHE	Peptide
13	N	36	PRO	Peptide
15	P	29	GLN	Peptide
17	R	163	MET	Peptide
23	X	326	GLN	Peptide
24	Y	204	SER	Peptide
29	c	112	ASN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	16331	0	16276	625	0
2	B	2066	0	1047	61	0
3	C	6724	0	6696	318	0
4	E	2338	0	2275	153	0
5	F	2075	0	1048	85	0
6	G	1587	0	808	127	0
7	H	3539	0	1791	118	0
8	I	3387	0	1651	22	0
9	J	3773	0	2869	90	0
10	K	185	0	165	21	0
11	L	2584	0	2096	103	0
12	M	971	0	950	70	0
13	N	1184	0	1190	45	0
14	O	1447	0	638	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	P	876	0	875	52	0
16	Q	5288	0	1361	7	0
17	R	2915	0	2794	192	0
18	S	770	0	356	6	0
19	T	2507	0	2451	83	0
20	U	422	0	291	13	0
21	V	2959	0	2237	106	0
22	W	2473	0	1096	8	0
23	X	6357	0	6349	417	0
24	Y	2556	0	2492	145	0
25	Z	772	0	342	8	0
26	y	316	0	86	0	0
27	a	344	0	93	0	0
27	m	413	0	194	0	0
28	b	328	0	89	0	0
28	n	402	0	184	0	0
29	c	388	0	102	0	0
29	h	482	0	220	0	0
30	d	296	0	87	0	0
30	i	359	0	179	0	0
31	e	316	0	85	0	0
31	j	403	0	173	0	0
32	f	296	0	84	0	0
32	k	364	0	176	0	0
33	g	324	0	89	0	0
33	l	415	0	198	0	0
34	q	659	0	296	0	0
34	r	654	0	294	0	0
34	s	659	0	296	0	0
34	t	654	0	294	0	0
35	1	6486	0	6690	660	0
36	3	9220	0	9139	672	0
37	p	841	0	420	0	0
38	w	999	0	961	0	0
39	2	1803	0	1611	189	0
40	4	743	0	344	31	0
41	7	613	0	597	46	0
42	5	635	0	595	103	0
43	o	816	0	386	0	0
44	A	36	0	6	5	0
45	C	32	0	12	0	0
46	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	F	6	0	0	0	0
47	7	3	0	0	0	0
47	K	1	0	0	0	0
47	N	3	0	0	0	0
All	All	106396	0	84124	3982	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 22.

All (3982) 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)
39:2:594:GLY:HA2	39:2:597:PHE:CE2	1.21	1.65
35:1:1056:MET:HG2	39:2:561:MET:SD	1.37	1.64
39:2:635:ALA:CB	40:4:73:ILE:HA	1.32	1.59
39:2:635:ALA:HB3	40:4:73:ILE:CA	1.10	1.55
39:2:641:PRO:N	39:2:641:PRO:CA	1.69	1.55
14:O:34:ILE:CB	17:R:197:ILE:HD11	1.36	1.54
39:2:594:GLY:HA2	39:2:597:PHE:CD2	1.39	1.54
39:2:642:PRO:N	39:2:642:PRO:CA	1.70	1.51
35:1:564:ASP:HB3	35:1:603:ALA:CB	1.39	1.50
39:2:594:GLY:CA	39:2:597:PHE:CD2	1.90	1.50
35:1:718:PRO:N	35:1:718:PRO:CA	1.69	1.39
39:2:594:GLY:CA	39:2:597:PHE:CE2	1.95	1.38
14:O:34:ILE:CB	17:R:197:ILE:CD1	2.02	1.34
23:X:787:GLU:CG	35:1:542:PRO:HG2	1.58	1.33
35:1:557:ASP:CB	35:1:596:ILE:HG22	1.59	1.32
35:1:1056:MET:SD	39:2:561:MET:CE	2.17	1.32
35:1:557:ASP:HB2	35:1:596:ILE:CG2	1.59	1.30
6:G:1:G:N2	10:K:218:LYS:HG3	1.49	1.28
23:X:170:GLU:OE2	23:X:771:GLY:HA3	1.26	1.27
35:1:540:MET:CE	35:1:577:VAL:HG12	1.64	1.26
35:1:564:ASP:CB	35:1:603:ALA:HB1	1.66	1.24
11:L:162:THR:CG2	17:R:258:LYS:O	1.85	1.23
1:A:1741:TYR:OH	35:1:937:LEU:CD2	1.86	1.22
36:3:114:ARG:NH1	42:5:37:ARG:HB2	1.52	1.22
23:X:741:TRP:CE2	35:1:782:GLU:OE2	1.92	1.20
39:2:594:GLY:C	39:2:597:PHE:HD2	1.43	1.20
11:L:163:GLN:HB3	11:L:168:LYS:NZ	1.55	1.19
35:1:1056:MET:CG	39:2:561:MET:SD	2.30	1.18
8:I:433:ALA:HA	8:I:482:LYS:CB	1.72	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:2:635:ALA:CB	40:4:73:ILE:CA	2.01	1.18
35:1:819:TRP:HB3	35:1:864:TYR:OH	1.03	1.17
11:L:162:THR:HG23	17:R:258:LYS:O	1.40	1.15
1:A:1741:TYR:OH	35:1:937:LEU:HD23	0.98	1.15
35:1:1056:MET:SD	39:2:561:MET:HE1	1.80	1.15
23:X:164:TRP:CZ2	23:X:539:VAL:HG22	1.83	1.13
35:1:819:TRP:CB	35:1:864:TYR:OH	1.97	1.13
35:1:1056:MET:CG	39:2:561:MET:CE	2.27	1.12
35:1:567:VAL:HG11	35:1:600:LEU:HD12	1.30	1.11
35:1:803:ALA:HA	35:1:843:LYS:NZ	1.67	1.10
35:1:1056:MET:SD	39:2:561:MET:HE2	1.88	1.10
1:A:1578:ARG:HD2	10:K:224:SER:HB3	1.34	1.09
6:G:19:G:N2	14:O:194:ALA:O	1.84	1.08
1:A:1741:TYR:CZ	35:1:937:LEU:HD23	1.89	1.08
17:R:325:ARG:HD3	24:Y:222:ILE:HG23	1.10	1.08
23:X:171:ARG:NH1	23:X:509:PRO:HB3	1.69	1.08
6:G:99:C:N4	7:H:32:U:H3	1.50	1.07
23:X:787:GLU:HG3	35:1:542:PRO:CG	1.84	1.07
35:1:540:MET:CE	35:1:577:VAL:CG1	2.31	1.07
35:1:1078:VAL:HG12	35:1:1118:ILE:HD12	1.09	1.07
35:1:528:ALA:H	35:1:566:LEU:HD23	1.14	1.07
35:1:540:MET:HE3	35:1:577:VAL:CG1	1.83	1.07
36:3:616:ILE:HB	36:3:629:SER:O	1.54	1.07
35:1:1001:VAL:HG22	35:1:1009:MET:HE3	1.31	1.07
35:1:1056:MET:CG	39:2:561:MET:HE2	1.82	1.05
6:G:1:G:H21	10:K:218:LYS:HG3	0.93	1.05
35:1:926:LYS:HB3	35:1:927:PRO:HD3	1.32	1.05
1:A:855:ARG:HG3	1:A:1520:ASN:HB3	1.09	1.05
1:A:1741:TYR:HE2	35:1:977:VAL:HG21	1.18	1.05
17:R:328:ALA:HB2	24:Y:226:MET:SD	1.95	1.05
35:1:625:ARG:HB3	35:1:666:LYS:NZ	1.71	1.04
35:1:721:ILE:HG22	35:1:756:LEU:HD23	1.36	1.04
35:1:721:ILE:CG2	35:1:756:LEU:HB3	1.87	1.04
39:2:606:PRO:HA	40:4:35:GLN:HA	1.35	1.04
39:2:635:ALA:HB3	40:4:73:ILE:N	1.73	1.04
39:2:594:GLY:O	39:2:597:PHE:HD2	1.37	1.03
23:X:787:GLU:CB	35:1:542:PRO:HG2	1.88	1.03
1:A:1756:SER:OG	35:1:943:LYS:CD	2.07	1.03
9:J:206:LEU:HB3	9:J:207:PRO:HD2	1.38	1.02
17:R:335:ARG:CB	23:X:272:TYR:HB2	1.88	1.02
35:1:803:ALA:CA	35:1:843:LYS:NZ	2.22	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:163:GLN:HB3	11:L:168:LYS:HZ1	0.88	1.02
23:X:787:GLU:HG3	35:1:542:PRO:HG2	1.05	1.01
11:L:163:GLN:CB	11:L:168:LYS:HZ1	1.73	1.01
39:2:635:ALA:CB	40:4:72:LYS:C	2.29	1.01
35:1:1078:VAL:CG1	35:1:1118:ILE:HD12	1.91	1.00
35:1:1262:ARG:HD2	42:5:24:ALA:O	1.61	1.00
39:2:635:ALA:CB	40:4:73:ILE:N	2.22	1.00
35:1:564:ASP:CB	35:1:603:ALA:CB	2.33	1.00
1:A:1741:TYR:CZ	35:1:937:LEU:CD2	2.44	1.00
6:G:1:G:H21	10:K:218:LYS:CG	1.75	0.99
35:1:897:LEU:HD21	35:1:932:ILE:HG13	1.41	0.99
6:G:96:U:OP1	35:1:1149:LYS:HE2	1.61	0.99
35:1:1257:PRO:HD3	39:2:482:ALA:HB2	1.45	0.99
35:1:1010:THR:OG1	35:1:1011:PRO:HD3	1.60	0.99
36:3:1116:SER:N	39:2:708:TRP:HZ2	1.61	0.99
36:3:106:THR:OG1	41:7:82:ARG:HD2	1.61	0.99
17:R:334:ARG:O	23:X:268:GLN:NE2	1.95	0.99
35:1:721:ILE:HG21	35:1:756:LEU:HB3	1.44	0.98
35:1:1137:ARG:NH1	39:2:522:PHE:O	1.95	0.98
39:2:594:GLY:HA3	39:2:597:PHE:CD2	1.95	0.98
39:2:635:ALA:HB3	40:4:73:ILE:CB	1.92	0.98
35:1:1001:VAL:CG2	35:1:1009:MET:HE3	1.93	0.98
35:1:1056:MET:HG2	39:2:561:MET:CE	1.90	0.98
39:2:635:ALA:HB2	40:4:72:LYS:O	1.62	0.98
35:1:560:LEU:HD21	35:1:600:LEU:HA	1.46	0.98
5:F:38:G:H2'	5:F:39:A:H8	1.25	0.97
35:1:540:MET:HE3	35:1:577:VAL:HG12	0.99	0.97
35:1:841:ALA:CB	35:1:875:ILE:HD13	1.94	0.97
1:A:1738:PRO:HG3	35:1:969:LYS:HB3	1.46	0.96
35:1:1295:TYR:OH	42:5:29:TRP:HD1	1.47	0.96
25:Z:85:LYS:O	25:Z:87:TYR:N	1.98	0.96
1:A:1745:GLU:OE1	35:1:980:GLU:HG2	1.66	0.96
36:3:477:SER:HB2	36:3:505:THR:H	1.28	0.96
36:3:189:TYR:HA	42:5:73:LEU:CD1	1.96	0.96
39:2:594:GLY:O	39:2:597:PHE:CD2	2.19	0.96
17:R:335:ARG:O	23:X:268:GLN:HB3	1.66	0.95
12:M:215:ASN:ND2	17:R:260:TYR:HA	1.81	0.95
23:X:741:TRP:CD2	35:1:782:GLU:OE2	2.20	0.95
11:L:16:ASP:HB2	11:L:54:LEU:HD21	1.47	0.94
23:X:741:TRP:CZ2	35:1:782:GLU:OE2	2.20	0.94
8:I:433:ALA:CA	8:I:482:LYS:CB	2.45	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:83:GLU:HA	18:S:106:ASP:HA	1.46	0.94
11:L:163:GLN:CB	11:L:168:LYS:NZ	2.31	0.94
35:1:1167:TYR:CE2	39:2:581:LYS:HG2	2.03	0.94
39:2:594:GLY:CA	39:2:597:PHE:HD2	1.47	0.94
39:2:594:GLY:HA3	39:2:597:PHE:CE2	1.99	0.94
1:A:39:GLN:HE22	22:W:170:THR:N	1.66	0.94
35:1:528:ALA:H	35:1:566:LEU:CD2	1.80	0.94
1:A:372:PRO:O	3:C:342:ARG:NH2	2.01	0.93
36:3:189:TYR:CD1	42:5:37:ARG:NH2	2.36	0.93
35:1:1295:TYR:HH	42:5:29:TRP:HD1	1.01	0.93
5:F:59:G:H1	5:F:76:A:H61	1.09	0.93
17:R:325:ARG:HD3	24:Y:222:ILE:CG2	1.99	0.93
35:1:1164:ASP:O	39:2:579:GLN:NE2	2.01	0.93
6:G:99:C:H42	7:H:32:U:H3	0.95	0.92
42:5:36:HIS:HD1	42:5:76:CYS:HG	1.05	0.92
2:B:20:G:O6	2:B:57:G:N1	2.02	0.92
36:3:459:VAL:HG21	36:3:757:ILE:HG21	1.51	0.92
35:1:1252:GLN:NE2	39:2:492:LYS:HA	1.84	0.92
17:R:325:ARG:CD	24:Y:222:ILE:HG23	2.00	0.92
39:2:635:ALA:CB	40:4:72:LYS:O	2.18	0.91
1:A:361:HIS:CE1	21:V:324:HIS:CB	2.53	0.91
1:A:467:GLN:OE1	2:B:20:G:N2	2.04	0.91
36:3:516:LEU:O	36:3:527:ILE:HB	1.70	0.91
23:X:170:GLU:OE2	23:X:771:GLY:CA	2.19	0.91
35:1:819:TRP:CB	35:1:864:TYR:HH	1.77	0.91
15:P:207:ASP:HB2	15:P:218:GLU:HB2	1.50	0.91
9:J:206:LEU:HB3	9:J:207:PRO:CD	2.01	0.91
35:1:833:LEU:HD23	35:1:867:MET:SD	2.11	0.91
35:1:840:LEU:O	35:1:844:VAL:HG22	1.69	0.91
1:A:1741:TYR:CE2	35:1:977:VAL:HG21	2.04	0.90
2:B:95:G:H21	2:B:96:A:H5"	1.35	0.90
35:1:803:ALA:CA	35:1:843:LYS:HZ2	1.81	0.90
1:A:705:LYS:NZ	17:R:247:ILE:O	2.03	0.90
2:B:46:U:O2	20:U:11:ARG:NH2	2.03	0.90
36:3:114:ARG:CZ	42:5:37:ARG:HB2	2.01	0.90
3:C:350:ASN:HD22	3:C:353:THR:HG22	1.36	0.90
35:1:703:THR:HG22	35:1:745:ALA:HB3	1.51	0.90
1:A:39:GLN:HE22	22:W:170:THR:H	0.97	0.90
23:X:164:TRP:CE2	23:X:539:VAL:HG22	2.07	0.90
39:2:635:ALA:HB2	40:4:73:ILE:HA	1.53	0.90
35:1:803:ALA:HA	35:1:843:LYS:HZ2	1.24	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:564:ASP:HB3	35:1:603:ALA:HB1	0.92	0.90
14:O:34:ILE:CA	17:R:197:ILE:CD1	2.50	0.89
8:I:463:PRO:HG2	8:I:483:SER:CB	2.00	0.89
6:G:116:C:O4'	17:R:371:ARG:HA	1.73	0.89
39:2:594:GLY:HA2	39:2:597:PHE:HE2	1.07	0.89
8:I:394:PRO:HG2	8:I:429:VAL:HA	1.53	0.89
36:3:463:ARG:H	36:3:510:LEU:HD22	1.35	0.89
12:M:215:ASN:HD21	17:R:261:THR:N	1.70	0.88
3:C:614:TYR:OH	3:C:643:ASP:OD2	1.89	0.88
25:Z:85:LYS:C	25:Z:87:TYR:H	1.72	0.88
35:1:567:VAL:CG1	35:1:600:LEU:HD12	2.02	0.88
4:E:150:HIS:HE2	4:E:169:THR:HG1	1.17	0.88
39:2:635:ALA:HB1	40:4:72:LYS:C	1.94	0.88
1:A:31:GLN:OE1	4:E:194:TYR:OH	1.92	0.88
1:A:707:ARG:HH12	7:H:18:U:H5'	1.37	0.87
1:A:1756:SER:OG	35:1:943:LYS:HD3	1.74	0.87
35:1:1217:PRO:HD3	39:2:590:LEU:HD13	1.57	0.87
36:3:193:ASP:C	42:5:79:PRO:HG2	1.94	0.87
1:A:1526:LEU:HD13	1:A:1528:GLN:H	1.40	0.87
19:T:307:SER:OG	19:T:309:ASP:OD1	1.92	0.87
24:Y:246:LYS:HE3	24:Y:312:HIS:HB2	1.57	0.87
35:1:1179:ASP:HB2	39:2:511:LEU:HB2	1.56	0.87
9:J:199:LYS:O	9:J:199:LYS:NZ	2.06	0.87
35:1:1006:MET:SD	35:1:1006:MET:N	2.48	0.87
23:X:690:LEU:HD22	23:X:735:PHE:HB2	1.57	0.87
36:3:1115:GLU:CG	39:2:708:TRP:HE1	1.88	0.87
36:3:139:LYS:HG3	36:3:160:ALA:HB3	1.57	0.86
1:A:39:GLN:NE2	22:W:170:THR:H	1.73	0.86
17:R:360:ARG:HD2	24:Y:274:ASP:OD1	1.75	0.86
3:C:478:THR:HG21	3:C:492:ALA:HB1	1.56	0.86
5:F:36:A:H3'	5:F:37:C:H5"	1.55	0.86
35:1:821:HIS:HD2	35:1:861:ALA:CB	1.87	0.86
35:1:564:ASP:HB3	35:1:603:ALA:HB2	1.56	0.86
36:3:189:TYR:CB	42:5:73:LEU:HD12	2.06	0.86
6:G:1:G:OP2	6:G:1:G:H4'	1.76	0.86
1:A:1755:SER:O	35:1:942:ASN:HA	1.75	0.85
19:T:349:SER:OG	19:T:351:ASP:OD1	1.92	0.85
35:1:803:ALA:N	35:1:843:LYS:NZ	2.24	0.85
35:1:1266:TRP:CZ3	42:5:22:GLY:HA3	2.11	0.85
35:1:528:ALA:N	35:1:566:LEU:HD23	1.91	0.85
5:F:38:G:H2'	5:F:39:A:C8	2.10	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1018:ASN:ND2	1:A:1023:ASN:OD1	2.09	0.85
17:R:325:ARG:NH1	17:R:325:ARG:O	2.10	0.85
1:A:1578:ARG:HD2	10:K:224:SER:CB	2.05	0.85
36:3:668:GLY:HA3	36:3:699:VAL:HG11	1.57	0.85
36:3:806:ALA:HA	36:3:856:LYS:HB3	1.58	0.85
36:3:585:ALA:HB1	36:3:610:VAL:HG12	1.59	0.85
9:J:187:VAL:HG13	9:J:188:GLN:H	1.42	0.84
35:1:819:TRP:HB3	35:1:864:TYR:HH	1.03	0.84
11:L:162:THR:HG21	17:R:258:LYS:O	1.75	0.84
35:1:625:ARG:HB3	35:1:666:LYS:HZ1	1.39	0.84
3:C:117:ASP:N	3:C:117:ASP:OD1	2.11	0.84
23:X:991:LEU:HA	23:X:995:GLU:HA	1.60	0.84
35:1:821:HIS:CD2	35:1:861:ALA:HB2	2.13	0.84
3:C:488:VAL:HG13	3:C:609:LYS:HD3	1.59	0.84
39:2:643:PRO:CB	40:4:65:GLU:CB	2.56	0.83
23:X:171:ARG:HH22	23:X:509:PRO:HD3	1.43	0.83
35:1:556:ILE:HG23	35:1:596:ILE:HG21	1.58	0.83
36:3:1008:SER:OG	36:3:1009:PHE:N	2.07	0.83
23:X:787:GLU:HB2	35:1:542:PRO:HG2	1.60	0.83
1:A:1738:PRO:HA	35:1:973:HIS:NE2	1.92	0.83
4:E:92:LEU:HD12	4:E:103:ALA:HB3	1.61	0.83
39:2:606:PRO:HA	40:4:35:GLN:CA	2.07	0.83
42:5:36:HIS:ND1	42:5:76:CYS:SG	2.49	0.83
1:A:184:ASP:HB2	13:N:1:MET:HA	1.61	0.83
1:A:1636:LYS:HD3	1:A:1658:GLN:HE21	1.44	0.83
35:1:1292:LYS:O	42:5:78:PRO:HD2	1.77	0.83
17:R:348:GLU:O	17:R:352:ARG:HB2	1.78	0.83
23:X:166:ARG:NH2	23:X:771:GLY:O	2.12	0.82
1:A:1741:TYR:HB3	35:1:973:HIS:NE2	1.93	0.82
12:M:215:ASN:ND2	17:R:260:TYR:CA	2.40	0.82
23:X:162:ASP:HB2	23:X:542:PHE:HZ	1.42	0.82
23:X:272:TYR:OH	24:Y:227:VAL:O	1.96	0.82
35:1:1056:MET:CB	39:2:561:MET:HE2	2.09	0.82
35:1:1179:ASP:HB2	39:2:511:LEU:CB	2.09	0.82
36:3:352:GLU:OE2	36:3:429:ARG:NH1	2.12	0.82
1:A:325:HIS:HD2	1:A:326:HIS:HD2	1.25	0.82
36:3:280:ASP:HB3	36:3:283:ARG:HG3	1.60	0.82
1:A:1756:SER:OG	35:1:943:LYS:HB3	1.79	0.82
12:M:215:ASN:HD21	17:R:261:THR:H	1.24	0.82
35:1:560:LEU:CD2	35:1:600:LEU:HA	2.09	0.82
35:1:725:ASP:HA	35:1:728:LEU:HG	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:734:GLY:O	35:1:738:HIS:HB2	1.77	0.82
3:C:670:SER:HA	3:C:823:ALA:HB3	1.61	0.82
35:1:1266:TRP:CE3	42:5:22:GLY:HA3	2.14	0.82
7:H:30:A:H2'	7:H:30:A:N3	1.94	0.82
35:1:540:MET:HE2	35:1:577:VAL:CG1	2.09	0.82
39:2:606:PRO:CA	40:4:35:GLN:HA	2.10	0.82
23:X:510:ASP:OD1	23:X:543:ARG:HD3	1.78	0.82
35:1:557:ASP:OD2	35:1:595:GLU:HB3	1.79	0.82
36:3:568:MET:HB3	36:3:574:LEU:HD12	1.60	0.82
41:7:40:CYS:SG	41:7:73:LYS:NZ	2.50	0.82
1:A:414:ARG:NH1	3:C:410:LEU:O	2.13	0.81
1:A:1741:TYR:HH	35:1:937:LEU:HD23	1.01	0.81
6:G:97:A:N1	35:1:1075:ARG:HG2	1.95	0.81
6:G:116:C:OP2	17:R:371:ARG:HD3	1.80	0.81
9:J:205:LEU:HD22	9:J:205:LEU:O	1.80	0.81
23:X:163:GLU:OE2	23:X:778:PHE:CD2	2.32	0.81
35:1:665:ILE:HD13	35:1:705:SER:HB2	1.61	0.81
36:3:29:GLU:HG3	36:3:42:ARG:HG3	1.63	0.81
39:2:594:GLY:CA	39:2:597:PHE:HE2	1.59	0.81
5:F:59:G:H1	5:F:76:A:N6	1.76	0.81
1:A:1838:LYS:HB3	1:A:1868:MET:HG3	1.60	0.81
35:1:652:CYS:HB2	35:1:692:HIS:HE1	1.46	0.81
12:M:215:ASN:HD22	17:R:260:TYR:HA	1.45	0.81
35:1:1287:ILE:HB	42:5:32:LEU:HD11	1.63	0.81
35:1:819:TRP:CZ3	35:1:867:MET:HE3	2.15	0.81
4:E:87:ASP:OD1	4:E:87:ASP:N	2.13	0.81
17:R:367:ARG:NH1	24:Y:282:CYS:SG	2.54	0.81
35:1:1090:PRO:HA	35:1:1093:VAL:HG12	1.61	0.81
4:E:92:LEU:O	4:E:101:ASN:ND2	2.14	0.80
41:7:33:CYS:SG	41:7:35:SER:OG	2.31	0.80
1:A:701:ILE:HD11	17:R:237:MET:HG3	1.63	0.80
36:3:162:LYS:HE3	36:3:165:THR:HG21	1.62	0.80
1:A:1738:PRO:CG	35:1:969:LYS:HB3	2.11	0.80
4:E:197:LEU:HG	4:E:212:GLY:HA2	1.62	0.80
1:A:1402:ARG:NH2	23:X:641:GLU:OE2	2.14	0.80
1:A:1835:GLN:HA	1:A:1838:LYS:HG3	1.63	0.80
4:E:126:SER:HG	4:E:136:TRP:HE1	1.28	0.80
35:1:532:PHE:CZ	35:1:574:ILE:HD11	2.16	0.80
35:1:757:MET:HB3	35:1:762:ALA:HB2	1.64	0.80
1:A:1807:ILE:HB	1:A:1820:LYS:HB3	1.64	0.80
36:3:170:VAL:HG23	36:3:184:CYS:HB3	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:ARG:CG	1:A:1520:ASN:HB3	2.02	0.80
15:P:186:ARG:HH11	15:P:186:ARG:HG2	1.45	0.80
23:X:604:VAL:HG13	23:X:605:THR:HG23	1.64	0.80
35:1:805:TYR:O	35:1:809:GLU:HB2	1.82	0.80
1:A:474:ARG:NH1	2:B:15:C:OP2	2.15	0.79
9:J:204:GLU:OE1	9:J:204:GLU:HA	1.82	0.79
35:1:544:LEU:HD21	35:1:549:ARG:HG3	1.64	0.79
1:A:1854:VAL:HG11	21:V:448:THR:HA	1.64	0.79
3:C:534:VAL:HG22	3:C:537:TYR:HB2	1.65	0.79
35:1:540:MET:HE2	35:1:577:VAL:HG11	1.63	0.79
35:1:963:LYS:O	35:1:966:GLN:N	2.14	0.79
3:C:343:LEU:HD13	3:C:373:ILE:HD11	1.63	0.79
11:L:169:ARG:CZ	11:L:169:ARG:HB2	2.12	0.79
36:3:412:ILE:HG12	36:3:423:LEU:HD22	1.63	0.79
6:G:1:G:N3	6:G:1:G:O2'	2.15	0.79
6:G:95:U:OP2	35:1:1106:ARG:CG	2.31	0.79
1:A:1738:PRO:HG3	35:1:969:LYS:CB	2.13	0.79
17:R:376:LYS:HA	17:R:379:LYS:HB2	1.65	0.79
36:3:114:ARG:NH1	42:5:37:ARG:CB	2.41	0.79
36:3:412:ILE:HD12	36:3:1107:THR:HG21	1.64	0.79
2:B:41:U:O4	6:G:0:G:N2	2.15	0.78
35:1:617:ILE:CD1	35:1:651:VAL:HB	2.13	0.78
35:1:926:LYS:CB	35:1:927:PRO:HD3	2.05	0.78
10:K:206:LYS:O	10:K:223:ARG:NH1	2.17	0.78
17:R:331:ALA:HA	23:X:275:ARG:NH1	1.98	0.78
35:1:598:SER:O	35:1:602:LYS:HB2	1.83	0.78
36:3:592:LEU:HD22	36:3:605:LEU:HD13	1.65	0.78
17:R:163:MET:O	17:R:165:VAL:N	2.14	0.78
19:T:191:HIS:NE2	19:T:440:ASP:OD1	2.16	0.78
1:A:55:ASP:OD1	1:A:55:ASP:N	2.17	0.78
36:3:929:LYS:HE3	36:3:938:GLU:HB2	1.65	0.78
1:A:1756:SER:OG	35:1:943:LYS:CB	2.32	0.78
35:1:1001:VAL:CG2	35:1:1009:MET:CE	2.61	0.78
10:K:223:ARG:HH21	35:1:1018:PRO:HB3	1.49	0.78
1:A:221:ASN:HB2	1:A:227:ARG:HB2	1.64	0.78
35:1:572:HIS:ND1	35:1:612:THR:HG21	1.99	0.78
2:B:94:U:H1'	2:B:95:G:OP1	1.82	0.78
1:A:1826:VAL:O	1:A:1830:GLN:NE2	2.17	0.77
17:R:308:VAL:HA	24:Y:197:ILE:HG21	1.65	0.77
23:X:171:ARG:NH1	23:X:509:PRO:CB	2.47	0.77
1:A:1756:SER:OG	35:1:943:LYS:HD2	1.81	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:3:463:ARG:HB2	36:3:510:LEU:HD13	1.66	0.77
22:W:180:LYS:HA	22:W:200:VAL:H	1.49	0.77
1:A:1878:ASP:OD1	1:A:1878:ASP:N	2.13	0.77
17:R:314:GLN:HA	23:X:290:GLU:OE1	1.85	0.77
36:3:136:GLU:OE2	36:3:189:TYR:OH	2.00	0.77
24:Y:245:CYS:SG	24:Y:246:LYS:N	2.58	0.77
36:3:464:ARG:HG2	36:3:516:LEU:HD11	1.67	0.77
1:A:1402:ARG:HH22	23:X:641:GLU:CD	1.87	0.77
6:G:95:U:OP2	35:1:1106:ARG:HG3	1.83	0.77
14:O:34:ILE:C	17:R:197:ILE:CD1	2.53	0.77
35:1:1300:LEU:HG	42:5:43:TYR:OH	1.84	0.77
35:1:625:ARG:CB	35:1:666:LYS:HZ1	1.97	0.77
1:A:923:ASP:OD2	1:A:1439:ARG:NH1	2.18	0.77
15:P:186:ARG:HB2	24:Y:49:PHE:CD1	2.19	0.77
36:3:525:ARG:HG3	36:3:533:VAL:HG13	1.67	0.77
9:J:206:LEU:CD2	9:J:207:PRO:HD3	2.14	0.77
1:A:1578:ARG:HB2	10:K:224:SER:OG	1.84	0.76
3:C:144:CYS:SG	3:C:313:GLN:NE2	2.58	0.76
35:1:821:HIS:CD2	35:1:861:ALA:CB	2.67	0.76
36:3:228:LEU:HD21	36:3:250:ILE:HG21	1.66	0.76
11:L:163:GLN:HA	11:L:163:GLN:NE2	2.00	0.76
23:X:480:SER:OG	23:X:485:ASP:OD1	2.04	0.76
3:C:684:LYS:HB3	3:C:795:VAL:HB	1.67	0.76
23:X:242:LYS:O	23:X:246:LEU:HB2	1.86	0.76
36:3:115:ILE:HG21	42:5:19:ILE:HB	1.67	0.76
36:3:351:SER:H	36:3:356:HIS:HB3	1.50	0.76
4:E:135:VAL:HG13	4:E:144:VAL:HG23	1.68	0.76
8:I:621:ARG:O	8:I:625:PRO:HD2	1.85	0.76
4:E:216:ASP:OD2	4:E:218:LYS:NZ	2.18	0.76
23:X:961:THR:O	23:X:965:GLN:NE2	2.19	0.76
35:1:524:ARG:NH1	35:1:562:LYS:O	2.18	0.76
2:B:41:U:C4	6:G:0:G:N2	2.53	0.76
35:1:554:LYS:HA	35:1:558:ARG:HH21	1.50	0.76
35:1:703:THR:CG2	35:1:745:ALA:HB3	2.15	0.76
36:3:1115:GLU:HG2	39:2:708:TRP:HE1	1.49	0.76
39:2:646:PRO:O	39:2:648:LEU:N	2.18	0.76
8:I:303:GLU:CB	8:I:326:ASP:O	2.34	0.76
36:3:89:ILE:HD12	36:3:103:HIS:HB2	1.67	0.76
1:A:57:GLN:N	1:A:57:GLN:HE21	1.84	0.76
35:1:793:LYS:HE2	35:1:839:GLU:HG3	1.67	0.76
36:3:459:VAL:HG22	36:3:476:VAL:HA	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:576:THR:HB	21:V:579:SER:H	1.49	0.75
35:1:819:TRP:CZ3	35:1:867:MET:CE	2.68	0.75
36:3:325:ILE:N	36:3:375:SER:OG	2.20	0.75
6:G:96:U:OP1	35:1:1149:LYS:CE	2.33	0.75
35:1:1001:VAL:HG22	35:1:1009:MET:CE	2.15	0.75
2:B:18:C:O2	2:B:59:G:N2	2.19	0.75
7:H:28:C:O2'	7:H:29:A:N3	2.18	0.75
1:A:1830:GLN:HB3	1:A:1836:LEU:HD22	1.68	0.75
17:R:359:ARG:HB3	17:R:363:ARG:HH21	1.52	0.75
25:Z:90:PRO:CB	25:Z:109:ASN:CB	2.64	0.75
35:1:1056:MET:HB2	39:2:561:MET:HE2	1.69	0.75
36:3:878:ASP:OD1	36:3:879:LEU:N	2.18	0.75
41:7:22:LEU:N	41:7:67:SER:O	2.18	0.75
1:A:1104:ASP:OD1	1:A:1104:ASP:N	2.19	0.75
4:E:312:TRP:HE1	4:E:319:ILE:HG12	1.50	0.75
35:1:710:ALA:HB1	35:1:752:TYR:CD1	2.20	0.75
36:3:412:ILE:H	36:3:1105:GLN:HE22	1.34	0.75
35:1:1130:PRO:HB3	39:2:528:ILE:HG23	1.68	0.75
24:Y:246:LYS:HB2	24:Y:311:ILE:HA	1.67	0.75
36:3:189:TYR:HA	42:5:73:LEU:HD12	1.68	0.75
36:3:1013:ARG:NH2	36:3:1064:ASP:OD1	2.19	0.75
1:A:1255:THR:HG22	1:A:1526:LEU:HD21	1.69	0.75
21:V:539:LEU:HD13	21:V:543:LYS:HB3	1.68	0.75
35:1:614:ARG:C	35:1:614:ARG:HD3	2.08	0.75
36:3:487:ILE:HA	36:3:491:VAL:HG13	1.69	0.75
18:S:18:THR:HA	18:S:159:ILE:HA	1.69	0.74
36:3:114:ARG:CZ	42:5:37:ARG:CB	2.65	0.74
35:1:694:LEU:HD13	35:1:727:VAL:HG21	1.68	0.74
36:3:228:LEU:HD12	36:3:229:GLU:H	1.52	0.74
36:3:1040:ASP:OD2	36:3:1043:THR:N	2.20	0.74
19:T:267:ASP:OD1	19:T:267:ASP:N	2.21	0.74
39:2:641:PRO:N	39:2:641:PRO:CB	2.51	0.74
11:L:167:ALA:HA	11:L:170:LYS:HE3	1.68	0.74
13:N:53:HIS:NE2	13:N:85:ASP:OD2	2.19	0.74
15:P:206:LYS:HB3	15:P:218:GLU:HG2	1.69	0.74
23:X:219:ARG:NH2	24:Y:292:GLU:OE2	2.20	0.74
23:X:787:GLU:HB2	35:1:542:PRO:CG	2.18	0.74
1:A:850:TYR:OH	1:A:863:GLU:OE1	2.05	0.74
35:1:625:ARG:HB3	35:1:666:LYS:HZ2	1.51	0.74
36:3:932:ASN:HB2	36:3:936:LYS:HE3	1.69	0.74
36:3:969:VAL:HB	36:3:981:CYS:HB2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:ARG:NH1	5:F:67:G:OP2	2.20	0.74
23:X:919:GLU:HA	23:X:922:LEU:HB2	1.69	0.74
36:3:206:GLN:HG3	36:3:231:HIS:HD2	1.52	0.74
1:A:875:HIS:CE1	23:X:866:ASN:HB3	2.22	0.74
35:1:840:LEU:O	35:1:844:VAL:CG2	2.35	0.74
36:3:511:LEU:HD23	36:3:512:GLY:H	1.53	0.74
1:A:1870:ASP:N	1:A:1870:ASP:OD1	2.20	0.74
6:G:1:G:C2	10:K:218:LYS:HG3	2.22	0.74
35:1:722:GLU:OE1	35:1:722:GLU:N	2.21	0.74
4:E:166:LEU:HD11	4:E:178:LEU:HG	1.70	0.73
9:J:438:TYR:O	9:J:442:ARG:HB2	1.88	0.73
17:R:125:MET:N	17:R:125:MET:SD	2.61	0.73
23:X:428:LYS:HD2	23:X:551:ALA:HB1	1.70	0.73
35:1:610:ILE:HG22	35:1:647:PHE:CE1	2.23	0.73
39:2:642:PRO:HA	40:4:66:ASP:HA	1.70	0.73
1:A:1382:SER:HB2	1:A:1415:GLY:HA2	1.69	0.73
4:E:255:MET:HB2	4:E:282:HIS:HB3	1.71	0.73
14:O:34:ILE:O	17:R:197:ILE:HA	1.87	0.73
21:V:581:ILE:HA	21:V:584:LYS:HG2	1.71	0.73
23:X:242:LYS:NZ	24:Y:220:GLN:O	2.21	0.73
35:1:861:ALA:O	35:1:864:TYR:N	2.17	0.73
36:3:193:ASP:HA	42:5:79:PRO:CG	2.18	0.73
4:E:189:THR:OG1	4:E:191:GLN:OE1	2.06	0.73
35:1:821:HIS:HD2	35:1:861:ALA:HB3	1.50	0.73
12:M:165:ASN:HB2	17:R:95:LYS:HB3	1.70	0.73
17:R:328:ALA:CB	24:Y:226:MET:SD	2.76	0.73
41:7:21:ARG:NH1	41:7:68:ASP:OD1	2.21	0.73
1:A:875:HIS:HE1	23:X:866:ASN:HB3	1.51	0.73
6:G:99:C:N4	7:H:32:U:N3	2.25	0.73
35:1:841:ALA:HA	35:1:849:ILE:HG13	1.70	0.73
35:1:897:LEU:CD2	35:1:932:ILE:HG13	2.18	0.73
41:7:73:LYS:O	41:7:77:ILE:HG13	1.88	0.73
1:A:729:PRO:HG2	12:M:226:TYR:CE1	2.24	0.73
1:A:1011:ALA:HB2	11:L:80:THR:HB	1.71	0.73
17:R:360:ARG:HD2	24:Y:274:ASP:CG	2.08	0.73
23:X:752:VAL:O	23:X:757:ARG:NH2	2.21	0.73
7:H:43:U:O2'	7:H:44:U:O5'	2.05	0.73
14:O:34:ILE:CA	17:R:197:ILE:HD13	2.18	0.73
17:R:335:ARG:CB	23:X:272:TYR:CB	2.67	0.73
12:M:224:ARG:HH11	12:M:224:ARG:CG	2.02	0.72
35:1:717:THR:HB	35:1:718:PRO:HD2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:3:565:TYR:HE1	36:3:619:LEU:HB2	1.54	0.72
39:2:491:LEU:O	39:2:494:THR:OG1	2.06	0.72
14:O:34:ILE:O	17:R:197:ILE:HD13	1.89	0.72
35:1:1167:TYR:HE2	39:2:581:LYS:HG2	1.51	0.72
36:3:1026:ASP:OD1	36:3:1026:ASP:N	2.18	0.72
36:3:1160:HIS:NE2	36:3:1175:ASP:OD2	2.20	0.72
1:A:987:LYS:NZ	3:C:61:GLU:OE1	2.19	0.72
23:X:741:TRP:CD1	35:1:782:GLU:HB3	2.24	0.72
36:3:902:ASP:OD1	36:3:902:ASP:N	2.20	0.72
36:3:1133:THR:O	39:2:712:GLU:CB	2.37	0.72
1:A:1652:MET:HG2	1:A:1719:PHE:HA	1.72	0.72
6:G:105:C:H4'	6:G:106:C:OP2	1.88	0.72
23:X:171:ARG:HH12	23:X:509:PRO:CG	2.01	0.72
1:A:888:GLN:O	1:A:889:ARG:NH1	2.22	0.72
17:R:321:GLU:HB2	23:X:283:TYR:CE2	2.25	0.72
19:T:188:PRO:HG2	19:T:502:VAL:HG11	1.70	0.72
23:X:689:VAL:O	23:X:734:CYS:HA	1.89	0.72
35:1:600:LEU:O	35:1:604:ALA:HB2	1.90	0.72
3:C:778:PRO:HB2	3:C:821:LEU:HD21	1.71	0.72
4:E:128:SER:OG	4:E:130:ASP:OD1	2.03	0.72
35:1:819:TRP:HZ3	35:1:868:VAL:HG12	1.54	0.72
35:1:1276:SER:N	36:3:113:ARG:HH22	1.87	0.72
36:3:114:ARG:NH2	42:5:37:ARG:HD2	2.03	0.72
36:3:189:TYR:CA	42:5:73:LEU:HD12	2.19	0.72
36:3:581:LYS:HD2	36:3:625:LEU:HD22	1.71	0.72
1:A:1838:LYS:O	1:A:1841:THR:OG1	2.07	0.72
19:T:223:SER:OG	19:T:225:ASP:OD2	2.03	0.72
35:1:528:ALA:HA	35:1:531:LEU:HB2	1.72	0.72
35:1:553:VAL:HA	35:1:556:ILE:HG22	1.72	0.72
35:1:613:MET:HB3	35:1:632:PHE:CE2	2.24	0.72
1:A:159:ARG:NH1	1:A:159:ARG:HA	2.05	0.72
4:E:137:ASP:O	4:E:141:GLY:N	2.19	0.72
15:P:183:LYS:O	15:P:183:LYS:HD3	1.90	0.72
23:X:945:ALA:HA	23:X:1011:VAL:HG11	1.71	0.72
1:A:27:GLU:OE1	1:A:31:GLN:NE2	2.22	0.72
2:B:18:C:N3	2:B:59:G:N1	2.34	0.72
9:J:205:LEU:HD22	9:J:205:LEU:C	2.10	0.72
17:R:327:MET:HB2	23:X:279:LEU:HD11	1.71	0.72
24:Y:51:ILE:HD11	24:Y:112:THR:HG23	1.72	0.72
35:1:549:ARG:HH22	35:1:586:ASP:CG	1.93	0.72
1:A:1637:TRP:O	1:A:1656:THR:HA	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:62:GLY:O	24:Y:107:GLN:NE2	2.23	0.72
35:1:617:ILE:HA	35:1:663:THR:HG21	1.72	0.72
1:A:855:ARG:HG3	1:A:1520:ASN:CB	2.03	0.71
7:H:43:U:H2'	7:H:44:U:C6	2.25	0.71
17:R:331:ALA:HA	23:X:275:ARG:HH12	1.55	0.71
24:Y:122:VAL:HB	24:Y:123:HIS:HD2	1.53	0.71
1:A:419:ARG:NH2	1:A:423:ASP:O	2.23	0.71
9:J:363:ARG:NH1	9:J:386:GLU:OE2	2.23	0.71
35:1:582:LEU:HG	35:1:634:VAL:HG21	1.72	0.71
36:3:1116:SER:CA	39:2:708:TRP:HZ2	2.03	0.71
1:A:1992:GLY:HA2	1:A:1997:VAL:HG23	1.73	0.71
15:P:186:ARG:HG2	15:P:186:ARG:NH1	2.03	0.71
16:Q:497:SER:O	16:Q:500:GLY:N	2.23	0.71
35:1:802:GLU:HB2	35:1:805:TYR:H	1.55	0.71
41:7:71:TYR:CE2	41:7:81:ASP:HB2	2.25	0.71
2:B:96:A:H4'	2:B:97:G:H5"	1.72	0.71
36:3:22:PHE:O	36:3:75:LYS:NZ	2.19	0.71
14:O:34:ILE:CB	17:R:197:ILE:HD12	2.18	0.71
23:X:164:TRP:CE2	23:X:539:VAL:CG2	2.72	0.71
23:X:405:ARG:NH2	23:X:438:GLU:OE1	2.24	0.71
1:A:1571:ILE:HG23	10:K:220:LEU:HD22	1.72	0.71
3:C:258:ASN:OD1	3:C:259:LYS:N	2.24	0.71
5:F:5:U:H5'	5:F:6:C:H4'	1.73	0.71
6:G:111:U:H4'	6:G:112:U:OP2	1.90	0.71
12:M:215:ASN:ND2	17:R:261:THR:H	1.88	0.71
14:O:163:HIS:O	14:O:182:ARG:N	2.23	0.71
1:A:325:HIS:CD2	1:A:326:HIS:HD2	2.09	0.71
3:C:750:LEU:HD22	20:U:63:LYS:O	1.91	0.71
12:M:224:ARG:HH11	12:M:224:ARG:CB	2.04	0.71
35:1:498:MET:HE1	35:1:530:PRO:HB2	1.72	0.71
35:1:1276:SER:H	36:3:113:ARG:HH22	1.39	0.71
36:3:1048:ASP:OD1	36:3:1049:LYS:N	2.24	0.71
1:A:1399:GLN:OE1	1:A:1401:ARG:NH1	2.24	0.71
7:H:18:U:OP2	12:M:221:LYS:NZ	2.22	0.71
35:1:841:ALA:HB2	35:1:875:ILE:HD13	1.72	0.71
36:3:487:ILE:HG13	36:3:491:VAL:HG22	1.73	0.71
35:1:1294:THR:O	42:5:76:CYS:HA	1.90	0.70
42:5:62:ALA:HA	42:5:65:ARG:HH12	1.56	0.70
35:1:1090:PRO:HA	35:1:1093:VAL:CG1	2.21	0.70
35:1:1108:ASN:O	35:1:1112:THR:HG22	1.91	0.70
39:2:646:PRO:C	39:2:648:LEU:H	1.94	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:GLN:HE22	1:A:45:TYR:HD2	1.38	0.70
1:A:857:ASN:ND2	1:A:860:GLN:OE1	2.23	0.70
1:A:1889:LEU:HD11	1:A:2012:LEU:HD21	1.73	0.70
2:B:87:A:N6	2:B:92:U:P	2.64	0.70
39:2:675:VAL:HA	39:2:681:PRO:HA	1.73	0.70
4:E:277:PHE:HE2	4:E:300:ILE:HG21	1.56	0.70
36:3:208:LEU:HD13	36:3:250:ILE:HD11	1.71	0.70
15:P:41:ILE:HG13	19:T:318:ARG:HG3	1.72	0.70
23:X:231:ARG:O	23:X:235:LEU:HG	1.92	0.70
36:3:642:ILE:O	36:3:703:ARG:NE	2.24	0.70
17:R:328:ALA:HB1	24:Y:226:MET:HA	1.73	0.70
1:A:362:ARG:NH1	21:V:323:LEU:C	2.46	0.70
1:A:1935:ARG:NE	1:A:1980:GLU:OE2	2.24	0.70
2:B:94:U:C1’	2:B:95:G:OP1	2.39	0.70
9:J:225:LEU:HG	11:L:211:ASN:HB2	1.74	0.70
17:R:328:ALA:CB	24:Y:226:MET:HA	2.21	0.70
19:T:195:LYS:HZ3	19:T:490:ARG:HD2	1.57	0.70
36:3:1116:SER:CA	39:2:708:TRP:CZ2	2.75	0.70
36:3:1194:SER:OG	36:3:1199:ARG:O	2.10	0.70
15:P:67:GLU:OE2	19:T:476:ARG:NH2	2.23	0.70
23:X:501:LEU:HB3	23:X:532:LEU:HD21	1.73	0.70
35:1:532:PHE:CE2	35:1:574:ILE:HD11	2.26	0.70
1:A:1057:ARG:NH1	1:A:1060:GLU:OE1	2.25	0.69
35:1:1181:ASP:OD1	35:1:1182:LEU:N	2.24	0.69
35:1:1276:SER:H	36:3:113:ARG:NH2	1.90	0.69
36:3:189:TYR:HA	42:5:73:LEU:HD11	1.74	0.69
1:A:1831:LYS:HG3	1:A:1832:ARG:N	2.07	0.69
6:G:1:G:N2	10:K:219:PHE:CD2	2.59	0.69
6:G:95:U:OP2	35:1:1106:ARG:CD	2.40	0.69
35:1:734:GLY:O	35:1:738:HIS:CB	2.40	0.69
35:1:1299:GLU:HA	35:1:1302:TYR:HE2	1.56	0.69
11:L:55:ASP:HB3	11:L:58:ILE:HD12	1.74	0.69
36:3:565:TYR:HB3	36:3:577:TYR:HB3	1.72	0.69
36:3:833:GLU:O	36:3:836:ALA:N	2.23	0.69
36:3:1182:PHE:O	36:3:1190:GLN:NE2	2.24	0.69
23:X:592:LEU:HD23	23:X:593:GLU:H	1.57	0.69
35:1:1179:ASP:H	39:2:511:LEU:HD13	1.55	0.69
36:3:812:LYS:HD2	36:3:856:LYS:HE3	1.74	0.69
1:A:705:LYS:HD3	17:R:247:ILE:HB	1.75	0.69
4:E:277:PHE:CE2	4:E:300:ILE:HG21	2.28	0.69
13:N:120:ARG:NH1	13:N:142:CYS:SG	2.66	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:510:ASP:OD2	23:X:543:ARG:HG3	1.93	0.69
35:1:827:ARG:HB2	35:1:827:ARG:NH2	2.08	0.69
35:1:948:ARG:NH2	35:1:984:GLU:OE2	2.25	0.69
36:3:189:TYR:HB3	42:5:73:LEU:HD12	1.73	0.69
42:5:62:ALA:HA	42:5:65:ARG:NH1	2.07	0.69
3:C:137:HIS:CD2	3:C:138:LEU:H	2.11	0.69
3:C:682:LYS:HB3	3:C:797:ALA:HB2	1.74	0.69
23:X:835:SER:OG	23:X:938:ARG:NH1	2.26	0.69
35:1:586:ASP:OD1	35:1:589:ALA:N	2.24	0.69
35:1:803:ALA:HA	35:1:843:LYS:HZ3	1.53	0.69
35:1:841:ALA:HB1	35:1:875:ILE:HD13	1.75	0.69
35:1:1178:MET:HG2	39:2:591:TYR:CZ	2.27	0.69
1:A:1179:SER:O	1:A:1201:ARG:NH1	2.23	0.69
36:3:384:THR:OG1	36:3:385:PHE:O	2.08	0.69
5:F:82:A:H4'	5:F:82:A:OP2	1.92	0.69
5:F:86:U:OP2	12:M:193:ARG:NH1	2.25	0.69
8:I:433:ALA:CB	8:I:482:LYS:CB	2.71	0.69
23:X:164:TRP:CZ2	23:X:539:VAL:CG2	2.72	0.69
36:3:968:ARG:HB2	36:3:970:TYR:HE2	1.57	0.69
1:A:372:PRO:HG3	3:C:341:LYS:HB3	1.74	0.68
4:E:68:GLU:HG2	4:E:347:SER:HB2	1.75	0.68
35:1:613:MET:HB3	35:1:632:PHE:CZ	2.28	0.68
35:1:1293:ASN:HA	42:5:77:GLY:HA3	1.74	0.68
36:3:434:SER:OG	36:3:436:ARG:NE	2.25	0.68
1:A:1807:ILE:HD11	1:A:1841:THR:HG22	1.75	0.68
3:C:131:ASN:HA	3:C:201:ASN:HB2	1.75	0.68
3:C:759:LEU:HA	3:C:762:VAL:HG12	1.74	0.68
4:E:146:ARG:HD2	4:E:148:LYS:HE2	1.75	0.68
12:M:217:LYS:HD2	12:M:217:LYS:O	1.93	0.68
21:V:484:SER:O	21:V:487:LYS:NZ	2.20	0.68
23:X:167:THR:HG23	23:X:770:LEU:HB3	1.75	0.68
1:A:1134:TRP:O	1:A:1139:ARG:NH1	2.25	0.68
6:G:116:C:C1'	17:R:371:ARG:HA	2.23	0.68
9:J:330:ARG:NH2	12:M:149:TYR:OH	2.24	0.68
35:1:1012:PRO:HG2	35:1:1015:ASP:OD1	1.93	0.68
1:A:1741:TYR:CB	35:1:973:HIS:NE2	2.56	0.68
11:L:67:GLU:OE1	11:L:91:ARG:NH2	2.26	0.68
35:1:503:LYS:HE2	35:1:511:MET:HG2	1.72	0.68
36:3:981:CYS:SG	36:3:1019:ASN:ND2	2.66	0.68
1:A:682:ASP:OD1	1:A:746:LYS:NZ	2.25	0.68
1:A:1544:ARG:NE	1:A:1672:ASP:OD2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:173:C:H2'	7:H:174:A:C8	2.28	0.68
9:J:206:LEU:CB	9:J:207:PRO:CD	2.72	0.68
19:T:471:ASP:OD1	19:T:473:SER:OG	2.07	0.68
6:G:19:G:H22	14:O:194:ALA:C	1.96	0.68
12:M:215:ASN:HD21	17:R:260:TYR:CA	2.07	0.68
13:N:25:LEU:HD13	13:N:56:LYS:HG2	1.76	0.68
23:X:281:ARG:NH1	23:X:281:ARG:HA	2.09	0.68
35:1:1010:THR:HG1	35:1:1011:PRO:HD3	1.57	0.68
35:1:1292:LYS:NZ	42:5:79:PRO:O	2.23	0.68
36:3:745:PHE:HB2	36:3:755:VAL:HG23	1.75	0.68
1:A:1936:LEU:O	1:A:1940:LEU:HG	1.93	0.68
17:R:180:THR:HG23	17:R:194:GLN:HG2	1.76	0.68
35:1:803:ALA:N	35:1:843:LYS:HZ2	1.88	0.68
36:3:193:ASP:HA	42:5:79:PRO:HG3	1.74	0.68
36:3:215:LEU:H	36:3:215:LEU:HD12	1.59	0.68
17:R:327:MET:CB	23:X:279:LEU:HD11	2.23	0.68
36:3:705:ARG:HA	36:3:710:GLU:HA	1.76	0.68
1:A:1578:ARG:HE	1:A:1746:ARG:NH2	1.91	0.68
2:B:8:G:H22	2:B:70:A:H1'	1.57	0.68
2:B:95:G:H21	2:B:96:A:C5'	2.06	0.68
35:1:694:LEU:HD12	35:1:694:LEU:H	1.59	0.68
35:1:997:LEU:HD13	35:1:1016:LEU:HD21	1.75	0.68
36:3:328:LYS:NZ	36:3:370:GLU:OE2	2.26	0.68
1:A:532:THR:OG1	6:G:3:A:OP1	2.11	0.67
1:A:1723:LYS:HB3	1:A:1724:PRO:HD3	1.75	0.67
1:A:1962:THR:HG23	1:A:1966:HIS:HB2	1.75	0.67
35:1:621:ASP:HB3	35:1:624:VAL:HG22	1.75	0.67
35:1:926:LYS:HB3	35:1:927:PRO:CD	2.16	0.67
36:3:499:PHE:HZ	36:3:516:LEU:HD22	1.57	0.67
4:E:251:LEU:HD21	4:E:300:ILE:HG13	1.76	0.67
6:G:117:A:H2'	24:Y:246:LYS:HE2	1.76	0.67
21:V:543:LYS:HA	21:V:546:ASN:ND2	2.08	0.67
35:1:1257:PRO:CD	39:2:482:ALA:HB2	2.20	0.67
36:3:185:LEU:HG	36:3:235:LEU:HD11	1.77	0.67
39:2:635:ALA:HB3	40:4:73:ILE:HA	0.68	0.67
3:C:193:THR:HG23	3:C:194:LYS:HD2	1.75	0.67
9:J:311:GLN:OE1	9:J:311:GLN:N	2.24	0.67
35:1:617:ILE:HD13	35:1:651:VAL:HB	1.75	0.67
35:1:625:ARG:CB	35:1:666:LYS:NZ	2.51	0.67
35:1:680:LEU:HA	35:1:683:LEU:HB2	1.75	0.67
36:3:427:CYS:SG	36:3:428:GLY:N	2.66	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:GLU:OE1	13:N:87:ASN:HB2	1.93	0.67
17:R:332:ARG:HA	23:X:272:TYR:CD1	2.28	0.67
35:1:641:ILE:N	35:1:642:PRO:HD2	2.10	0.67
36:3:193:ASP:C	42:5:79:PRO:CG	2.63	0.67
36:3:485:LEU:HD23	36:3:491:VAL:HG12	1.76	0.67
36:3:586:ASP:HB3	36:3:610:VAL:HB	1.77	0.67
1:A:1333:VAL:HG11	21:V:467:LEU:HD13	1.76	0.67
2:B:87:A:N6	2:B:92:U:OP2	2.26	0.67
2:B:97:G:H1	2:B:116:U:H3	1.41	0.67
4:E:217:ILE:HB	4:E:231:MET:HG3	1.74	0.67
17:R:389:SER:HA	17:R:392:ILE:HD12	1.75	0.67
4:E:294:SER:OG	4:E:299:LYS:O	2.11	0.67
6:G:102:G:H2'	6:G:102:G:N3	2.08	0.67
36:3:39:GLU:OE2	36:3:55:THR:OG1	2.12	0.67
41:7:46:CYS:H	41:7:85:CYS:HB2	1.58	0.67
1:A:873:ASN:ND2	1:A:876:GLU:OE1	2.28	0.67
1:A:946:GLU:HB3	1:A:950:LEU:HD23	1.76	0.67
15:P:212:ASN:ND2	19:T:458:SER:OG	2.27	0.67
35:1:827:ARG:HH21	35:1:827:ARG:H	1.43	0.67
36:3:697:ARG:NH2	36:3:717:SER:OG	2.28	0.67
36:3:983:ASN:ND2	36:3:1021:LEU:O	2.25	0.67
5:F:43:A:H1'	6:G:5:G:N2	2.10	0.67
17:R:367:ARG:O	17:R:371:ARG:HG3	1.93	0.67
35:1:732:TRP:NE1	35:1:768:GLU:OE2	2.27	0.67
41:7:37:VAL:HB	41:7:38:ARG:HG3	1.75	0.67
1:A:747:ALA:O	1:A:751:THR:HG22	1.94	0.67
3:C:137:HIS:HB2	3:C:239:THR:HG23	1.77	0.67
23:X:430:THR:HG23	23:X:465:VAL:HG22	1.77	0.67
36:3:603:ARG:HG3	36:3:604:PHE:CE1	2.29	0.67
36:3:620:ASP:N	36:3:620:ASP:OD1	2.27	0.67
36:3:775:ASN:HD22	36:3:775:ASN:H	1.40	0.67
36:3:840:ALA:O	36:3:844:ASN:ND2	2.27	0.67
9:J:411:MET:SD	9:J:416:TYR:HE2	2.18	0.67
35:1:1299:GLU:HA	35:1:1302:TYR:CE2	2.30	0.67
3:C:508:LYS:HG3	3:C:524:ILE:HG13	1.77	0.66
21:V:547:VAL:O	21:V:550:MET:HB2	1.95	0.66
35:1:1276:SER:O	35:1:1276:SER:OG	2.07	0.66
36:3:191:GLU:HA	36:3:194:ASN:HD22	1.59	0.66
3:C:213:ASP:OD1	3:C:616:SER:HB2	1.96	0.66
7:H:125:G:H2'	7:H:126:A:C8	2.30	0.66
11:L:201:LYS:HD2	11:L:202:ARG:H	1.58	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:34:ILE:O	17:R:197:ILE:CD1	2.43	0.66
3:C:758:LEU:HB3	3:C:796:VAL:HG11	1.78	0.66
21:V:628:ILE:O	21:V:632:THR:OG1	2.12	0.66
23:X:583:TYR:O	23:X:585:LYS:NZ	2.22	0.66
35:1:803:ALA:N	35:1:843:LYS:HZ1	1.92	0.66
1:A:1860:GLN:HG2	1:A:1883:VAL:HB	1.78	0.66
23:X:234:TYR:O	23:X:238:ARG:HB2	1.96	0.66
35:1:1277:GLN:H	36:3:113:ARG:NH2	1.94	0.66
36:3:147:ASP:OD1	36:3:151:ARG:N	2.28	0.66
5:F:41:A:N1	6:G:6:A:N6	2.41	0.66
21:V:456:ARG:NE	21:V:492:MET:SD	2.68	0.66
36:3:521:PRO:O	36:3:543:THR:OG1	2.12	0.66
39:2:476:GLU:HG2	39:2:477:MET:H	1.61	0.66
6:G:105:C:OP1	23:X:993:THR:OG1	2.13	0.66
19:T:245:HIS:HE2	19:T:263:SER:HG	1.44	0.66
23:X:827:MET:HB3	23:X:946:GLY:HA3	1.78	0.66
35:1:758:ASP:O	35:1:762:ALA:N	2.15	0.66
36:3:121:LEU:HB2	36:3:132:ILE:HD12	1.78	0.66
36:3:1132:PHE:O	39:2:711:LEU:HD23	1.96	0.66
35:1:702:ARG:HD2	35:1:746:PHE:CZ	2.30	0.66
36:3:449:VAL:HG13	36:3:763:ARG:HG2	1.76	0.66
41:7:26:CYS:SG	41:7:61:CYS:HB2	2.36	0.66
1:A:1457:HIS:ND1	1:A:1460:HIS:HD2	1.94	0.66
7:H:53:U:OP1	39:2:450:SER:OG	2.09	0.66
9:J:409:GLU:HG2	9:J:410:HIS:CD2	2.31	0.66
17:R:330:LYS:HZ2	23:X:275:ARG:HH22	1.44	0.66
36:3:189:TYR:CA	42:5:73:LEU:CD1	2.71	0.66
36:3:288:VAL:HG23	36:3:289:CYS:H	1.59	0.66
39:2:526:ASP:OD1	39:2:526:ASP:N	2.18	0.66
1:A:75:ASP:O	1:A:77:THR:N	2.29	0.66
1:A:1664:ILE:HG22	1:A:1703:ILE:HB	1.77	0.66
3:C:255:VAL:HB	3:C:307:VAL:HG12	1.77	0.66
14:O:34:ILE:C	17:R:197:ILE:HD12	2.15	0.66
36:3:511:LEU:HD21	36:3:517:VAL:HG23	1.78	0.66
36:3:635:ALA:HB3	36:3:669:LEU:HD13	1.78	0.66
36:3:700:LYS:HB3	36:3:702:PHE:CZ	2.30	0.66
39:2:642:PRO:N	39:2:642:PRO:CB	2.57	0.66
6:G:108:U:H5”	23:X:676:ILE:HB	1.78	0.66
11:L:173:GLU:OE1	11:L:173:GLU:HA	1.94	0.66
23:X:698:LYS:HD3	23:X:707:GLU:HG3	1.78	0.66
36:3:926:TYR:HB3	36:3:928:TYR:HE2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:3:1116:SER:N	39:2:708:TRP:CZ2	2.54	0.66
1:A:1631:LEU:HB2	1:A:1660:TYR:HB3	1.76	0.65
23:X:769:SER:OG	23:X:816:ALA:HB1	1.96	0.65
35:1:1001:VAL:HG23	35:1:1009:MET:CE	2.26	0.65
1:A:163:ARG:NH2	1:A:576:ASP:OD1	2.30	0.65
15:P:186:ARG:HH11	15:P:186:ARG:CG	2.09	0.65
17:R:315:LYS:O	17:R:318:GLU:HG3	1.96	0.65
35:1:862:GLU:OE1	35:1:904:THR:OG1	2.14	0.65
36:3:169:HIS:ND1	36:3:234:PHE:HB2	2.10	0.65
36:3:665:LEU:HD11	36:3:667:ILE:HG13	1.78	0.65
1:A:678:GLU:OE1	1:A:774:LYS:NZ	2.27	0.65
4:E:236:ASP:HB2	4:E:256:ASP:HB3	1.78	0.65
6:G:98:U:O4	7:H:33:G:N1	2.25	0.65
12:M:209:ASP:OD2	17:R:263:PRO:HG3	1.96	0.65
1:A:1629:ILE:HB	1:A:1662:ILE:HB	1.76	0.65
24:Y:94:VAL:HG13	24:Y:110:ILE:HG13	1.77	0.65
35:1:699:GLN:HE22	35:1:738:HIS:CE1	2.12	0.65
35:1:1126:PHE:HB2	39:2:575:PHE:CD2	2.31	0.65
36:3:1133:THR:O	39:2:712:GLU:HB3	1.96	0.65
1:A:1703:ILE:HD13	1:A:1714:ALA:HB2	1.76	0.65
1:A:1809:ILE:HB	1:A:1818:PHE:HD2	1.62	0.65
3:C:925:PRO:HG2	3:C:928:HIS:CE1	2.31	0.65
35:1:712:LEU:O	35:1:716:ALA:HB3	1.97	0.65
36:3:1117:LEU:O	36:3:1128:ILE:HA	1.96	0.65
7:H:119:G:H8	7:H:119:G:O5'	1.80	0.65
36:3:568:MET:HA	36:3:574:LEU:HA	1.79	0.65
39:2:594:GLY:C	39:2:597:PHE:CD2	2.34	0.65
1:A:1778:TRP:HB2	1:A:1861:ILE:HD12	1.79	0.65
35:1:806:ILE:CD1	35:1:843:LYS:HE3	2.26	0.65
36:3:777:VAL:HG22	36:3:779:PHE:HE1	1.61	0.65
5:F:43:A:H2	6:G:4:A:H61	1.44	0.65
21:V:622:ARG:HA	21:V:625:ARG:HE	1.61	0.65
23:X:527:LEU:HD22	23:X:763:VAL:HG11	1.77	0.65
23:X:910:ARG:O	23:X:914:VAL:HG13	1.96	0.65
24:Y:253:ASP:OD1	24:Y:253:ASP:N	2.29	0.65
35:1:549:ARG:NH2	35:1:589:ALA:HB2	2.12	0.65
36:3:206:GLN:HG3	36:3:231:HIS:CD2	2.31	0.65
23:X:824:LEU:HD21	23:X:844:ALA:HB1	1.77	0.65
35:1:662:HIS:CE1	35:1:700:LYS:HB3	2.32	0.65
35:1:897:LEU:HD21	35:1:932:ILE:CG1	2.21	0.65
4:E:118:ASN:HD21	4:E:122:SER:H	1.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:164:TRP:NE1	23:X:539:VAL:HG23	2.12	0.65
24:Y:267:ARG:N	24:Y:287:GLU:O	2.29	0.65
35:1:1276:SER:N	36:3:113:ARG:NH2	2.44	0.65
36:3:911:LYS:HB3	36:3:922:GLY:O	1.96	0.65
1:A:154:GLU:OE2	1:A:158:ARG:NE	2.29	0.64
6:G:88:G:O2'	6:G:89:U:H5'	1.98	0.64
23:X:618:GLN:HG2	23:X:648:TYR:CD2	2.32	0.64
24:Y:39:TYR:N	24:Y:156:ILE:O	2.28	0.64
35:1:1262:ARG:HB3	42:5:24:ALA:HB1	1.79	0.64
36:3:434:SER:HG	36:3:436:ARG:HE	1.45	0.64
36:3:1009:PHE:HE1	36:3:1036:ALA:HB2	1.61	0.64
1:A:1201:ARG:O	1:A:1203:SER:N	2.30	0.64
35:1:662:HIS:CD2	35:1:704:ILE:HG21	2.32	0.64
35:1:696:ASP:O	35:1:702:ARG:NH1	2.29	0.64
1:A:382:GLU:HG3	3:C:354:ARG:HG3	1.77	0.64
3:C:926:ALA:HA	3:C:929:LEU:HG	1.80	0.64
11:L:149:LEU:HA	11:L:152:LEU:HD12	1.79	0.64
1:A:90:GLY:HA3	17:R:209:PRO:HD3	1.79	0.64
21:V:525:PHE:HB3	21:V:560:LEU:HD21	1.80	0.64
39:2:469:VAL:HG12	39:2:471:ARG:H	1.62	0.64
41:7:10:PHE:HB3	41:7:12:ARG:HG2	1.79	0.64
24:Y:32:CYS:SG	24:Y:159:THR:OG1	2.49	0.64
36:3:260:ASN:OD1	36:3:261:PHE:N	2.30	0.64
15:P:206:LYS:CB	15:P:218:GLU:HG2	2.27	0.64
35:1:1006:MET:HA	35:1:1009:MET:HG3	1.80	0.64
1:A:57:GLN:HE21	1:A:57:GLN:H	1.45	0.64
1:A:1789:THR:HG22	1:A:1803:ILE:HD11	1.78	0.64
11:L:163:GLN:CB	11:L:168:LYS:CE	2.76	0.64
11:L:188:ARG:O	11:L:192:ARG:HG2	1.98	0.64
23:X:234:TYR:CE1	24:Y:317:GLN:HB3	2.33	0.64
25:Z:85:LYS:C	25:Z:87:TYR:N	2.42	0.64
35:1:490:GLU:O	35:1:494:GLU:HG2	1.98	0.64
36:3:384:THR:OG1	36:3:385:PHE:N	2.31	0.64
36:3:747:SER:N	36:3:750:CYS:O	2.31	0.64
1:A:201:ALA:HA	1:A:204:LEU:HD23	1.78	0.64
1:A:1948:ASP:HA	1:A:1951:LYS:HD3	1.80	0.64
4:E:153:PHE:HB2	4:E:172:ASP:HB2	1.79	0.64
5:F:82:A:H2'	7:H:17:U:OP1	1.97	0.64
23:X:171:ARG:HD2	23:X:770:LEU:HD22	1.80	0.64
36:3:114:ARG:NH1	42:5:38:ASP:OD1	2.30	0.64
36:3:1017:ASN:OD1	36:3:1018:GLU:N	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1778:TRP:O	1:A:1862:ILE:HG13	1.98	0.64
3:C:737:PRO:HD2	3:C:741:GLY:HA3	1.78	0.64
17:R:357:HIS:CD2	17:R:361:LYS:HE2	2.33	0.64
23:X:232:ARG:HA	23:X:235:LEU:HD12	1.80	0.64
3:C:381:LEU:HD22	3:C:416:LEU:HD21	1.78	0.64
5:F:37:C:H4'	5:F:38:G:OP2	1.97	0.64
9:J:185:ALA:HA	11:L:142:ILE:HD13	1.79	0.64
13:N:112:ASN:N	13:N:112:ASN:OD1	2.28	0.64
15:P:186:ARG:HA	24:Y:49:PHE:CE1	2.34	0.64
23:X:937:ILE:HG22	23:X:941:LYS:HD2	1.78	0.64
35:1:796:CYS:HA	35:1:801:VAL:HG11	1.77	0.64
36:3:794:SER:O	36:3:796:ASN:ND2	2.31	0.64
36:3:1031:ARG:HG2	36:3:1031:ARG:HH11	1.63	0.64
36:3:1188:ASN:OD1	36:3:1189:LYS:N	2.28	0.64
3:C:493:PHE:HD2	3:C:551:LEU:HG	1.62	0.63
4:E:175:THR:HG22	4:E:191:GLN:HG3	1.80	0.63
21:V:609:GLN:HE22	21:V:616:LEU:HD21	1.63	0.63
23:X:619:GLU:HA	23:X:622:GLU:OE1	1.97	0.63
35:1:1206:ASP:OD2	39:2:581:LYS:NZ	2.32	0.63
1:A:1528:GLN:O	1:A:1532:ARG:HB2	1.99	0.63
6:G:116:C:C4	17:R:370:SER:HB3	2.33	0.63
9:J:206:LEU:HD22	9:J:207:PRO:HD3	1.78	0.63
9:J:296:ARG:NH1	9:J:320:GLU:OE2	2.29	0.63
1:A:357:ASN:HD22	3:C:862:PRO:HB3	1.62	0.63
4:E:312:TRP:HD1	4:E:319:ILE:HA	1.63	0.63
4:E:313:ASP:OD1	4:E:316:SER:N	2.28	0.63
24:Y:303:ASN:O	24:Y:310:ARG:NH1	2.30	0.63
36:3:452:LEU:HD12	36:3:453:PRO:HD2	1.79	0.63
1:A:1741:TYR:CZ	35:1:937:LEU:HD22	2.29	0.63
35:1:859:ASP:O	35:1:865:ARG:NE	2.27	0.63
36:3:734:LEU:HD12	36:3:767:LEU:HD22	1.79	0.63
36:3:884:GLN:NE2	36:3:884:GLN:O	2.32	0.63
36:3:1201:PRO:HA	36:3:1204:VAL:HG22	1.80	0.63
1:A:1854:VAL:CG1	21:V:448:THR:HA	2.28	0.63
35:1:1165:TYR:CD1	39:2:575:PHE:CD1	2.86	0.63
36:3:169:HIS:HD2	36:3:170:VAL:H	1.44	0.63
36:3:1136:GLU:OE1	36:3:1136:GLU:N	2.27	0.63
5:F:79:C:H1'	5:F:82:A:H2	1.62	0.63
23:X:621:ILE:HG12	23:X:672:VAL:HG12	1.80	0.63
36:3:25:THR:OG1	36:3:27:GLN:N	2.31	0.63
36:3:114:ARG:HD3	42:5:38:ASP:OD1	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:3:545:VAL:HG12	36:3:546:LYS:HG2	1.79	0.63
36:3:958:ARG:NH2	36:3:1014:TYR:OH	2.31	0.63
36:3:1049:LYS:HE3	42:5:52:TYR:CZ	2.34	0.63
1:A:1222:LYS:O	21:V:592:GLU:HG3	1.99	0.63
3:C:64:LYS:HA	15:P:206:LYS:NZ	2.13	0.63
3:C:709:TRP:HB3	3:C:713:LYS:HB2	1.81	0.63
11:L:166:LYS:HG3	11:L:170:LYS:HE2	1.80	0.63
15:P:77:ASP:O	15:P:78:ARG:NE	2.32	0.63
35:1:1179:ASP:CB	39:2:511:LEU:CB	2.76	0.63
1:A:1014:ASN:ND2	1:A:1014:ASN:O	2.32	0.63
2:B:89:U:H2'	2:B:90:U:H5"	1.79	0.63
3:C:464:ALA:HB1	3:C:473:PRO:HG3	1.80	0.63
11:L:79:PRO:O	11:L:80:THR:OG1	2.16	0.63
11:L:188:ARG:HE	11:L:191:LEU:HD12	1.64	0.63
24:Y:14:ILE:HD12	24:Y:94:VAL:HG21	1.80	0.63
35:1:710:ALA:HB1	35:1:752:TYR:HD1	1.61	0.63
36:3:512:GLY:HA3	36:3:515:ALA:HB3	1.79	0.63
36:3:928:TYR:HB3	36:3:937:LEU:HB3	1.81	0.63
5:F:79:C:H1'	5:F:82:A:C2	2.33	0.63
1:A:485:THR:HG22	1:A:486:LYS:H	1.63	0.62
1:A:762:ARG:HH12	15:P:226:LYS:HZ1	1.47	0.62
11:L:163:GLN:HB2	11:L:168:LYS:CE	2.29	0.62
35:1:1174:GLU:OE2	35:1:1210:HIS:NE2	2.26	0.62
35:1:1212:LEU:HD13	35:1:1237:LEU:HD13	1.81	0.62
36:3:966:LEU:HB2	36:3:968:ARG:HD2	1.81	0.62
1:A:1014:ASN:HD21	11:L:83:ARG:HB2	1.64	0.62
1:A:1768:TYR:HA	1:A:1771:LEU:HB2	1.79	0.62
2:B:88:A:H2'	2:B:88:A:N3	2.14	0.62
3:C:560:VAL:HG22	3:C:561:LYS:H	1.64	0.62
5:F:49:G:H2'	5:F:50:A:H8	1.64	0.62
9:J:311:GLN:HG3	12:M:131:GLN:HG2	1.80	0.62
14:O:235:TYR:N	14:O:301:LYS:O	2.32	0.62
21:V:620:ASN:ND2	21:V:623:ASN:OD1	2.31	0.62
24:Y:27:ASN:O	24:Y:31:LEU:HD12	1.99	0.62
1:A:707:ARG:HH22	7:H:17:U:H4'	1.64	0.62
1:A:1578:ARG:HB2	10:K:224:SER:CB	2.29	0.62
14:O:171:GLY:O	22:W:207:LYS:HA	1.99	0.62
24:Y:39:TYR:O	24:Y:185:GLN:NE2	2.32	0.62
35:1:1013:ILE:HD11	35:1:1049:TYR:CD2	2.34	0.62
35:1:1277:GLN:HG2	36:3:113:ARG:HD3	1.81	0.62
36:3:1010:ILE:HG12	36:3:1026:ASP:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:2:674:PRO:O	39:2:682:LEU:N	2.24	0.62
41:7:46:CYS:O	41:7:50:ASN:HB2	1.99	0.62
3:C:750:LEU:HD23	3:C:751:PRO:HD3	1.82	0.62
36:3:70:LEU:HD11	36:3:152:LEU:HD13	1.80	0.62
36:3:565:TYR:CE1	36:3:619:LEU:HB2	2.33	0.62
41:7:39:PRO:HB2	41:7:70:TYR:HD1	1.63	0.62
1:A:155:LYS:NZ	1:A:622:GLY:O	2.32	0.62
1:A:1251:SER:O	1:A:1251:SER:OG	2.17	0.62
3:C:561:LYS:NZ	3:C:611:ASN:O	2.32	0.62
21:V:609:GLN:HA	21:V:612:PHE:HB2	1.80	0.62
23:X:163:GLU:OE2	23:X:778:PHE:CE2	2.53	0.62
23:X:580:ASP:OD2	23:X:733:LYS:NZ	2.31	0.62
9:J:330:ARG:HD3	9:J:361:ARG:HH22	1.64	0.62
36:3:387:PHE:HE1	36:3:389:PRO:HG3	1.64	0.62
1:A:957:GLN:O	1:A:961:ASN:ND2	2.26	0.62
6:G:95:U:P	35:1:1109:ARG:HH12	2.22	0.62
12:M:224:ARG:HH11	12:M:224:ARG:HG3	1.64	0.62
23:X:396:ARG:NH1	23:X:468:GLU:OE1	2.32	0.62
23:X:632:CYS:SG	23:X:642:LEU:HD13	2.39	0.62
35:1:742:GLY:O	35:1:746:PHE:HB2	1.99	0.62
35:1:1120:ALA:HB2	35:1:1128:VAL:HG21	1.80	0.62
36:3:293:HIS:NE2	36:3:295:THR:HB	2.15	0.62
36:3:1009:PHE:HZ	36:3:1046:GLY:HA3	1.65	0.62
41:7:30:CYS:SG	41:7:31:VAL:N	2.72	0.62
41:7:33:CYS:HB3	41:7:72:CYS:SG	2.39	0.62
1:A:758:ARG:HH21	1:A:775:ASN:HD22	1.45	0.62
2:B:63:A:H2'	2:B:64:G:H8	1.65	0.62
2:B:64:G:H2'	2:B:65:G:C8	2.34	0.62
2:B:95:G:H2'	2:B:95:G:N3	2.15	0.62
21:V:540:GLU:HG3	21:V:541:THR:H	1.65	0.62
23:X:249:GLU:HB3	23:X:273:LYS:HE2	1.82	0.62
24:Y:219:THR:O	24:Y:223:LEU:HB2	2.00	0.62
36:3:214:ASP:O	36:3:218:ASN:N	2.33	0.62
17:R:178:ARG:HD3	17:R:194:GLN:OE1	1.99	0.62
24:Y:40:CYS:O	24:Y:156:ILE:N	2.28	0.62
35:1:595:GLU:O	35:1:599:ASN:ND2	2.33	0.62
36:3:207:THR:O	36:3:209:THR:HG22	1.99	0.62
23:X:787:GLU:CG	35:1:542:PRO:CG	2.53	0.61
23:X:824:LEU:HD11	23:X:844:ALA:HA	1.82	0.61
24:Y:147:ASP:HB2	24:Y:149:VAL:HG12	1.80	0.61
36:3:325:ILE:O	36:3:374:SER:HA	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:344:GLN:N	9:J:344:GLN:OE1	2.33	0.61
17:R:320:HIS:O	17:R:323:LYS:HG2	1.99	0.61
23:X:167:THR:CG2	23:X:770:LEU:HB3	2.30	0.61
23:X:558:ALA:O	23:X:562:THR:OG1	2.17	0.61
35:1:1056:MET:HG2	39:2:561:MET:CG	2.29	0.61
36:3:233:ASN:ND2	36:3:233:ASN:H	1.95	0.61
1:A:231:THR:HG22	1:A:233:PRO:HD2	1.83	0.61
1:A:1181:ASP:OD1	1:A:1181:ASP:N	2.32	0.61
21:V:532:GLN:HE21	21:V:547:VAL:HG11	1.64	0.61
35:1:967:GLU:HG3	35:1:970:LEU:HB3	1.81	0.61
39:2:606:PRO:HA	40:4:35:GLN:CB	2.30	0.61
1:A:1276:GLU:OE1	1:A:1375:TRP:N	2.31	0.61
35:1:527:GLY:HA2	35:1:566:LEU:CD2	2.31	0.61
35:1:1055:TRP:CD1	35:1:1088:ILE:HD11	2.34	0.61
1:A:732:PRO:HG2	1:A:735:ILE:HD13	1.83	0.61
1:A:784:LEU:O	1:A:788:GLN:HG3	2.00	0.61
1:A:1608:THR:HB	1:A:1632:PHE:HB2	1.83	0.61
1:A:1870:ASP:O	1:A:1874:VAL:HG23	2.01	0.61
5:F:50:A:OP1	11:L:165:LYS:NZ	2.23	0.61
35:1:550:HIS:HD2	35:1:551:LEU:HD22	1.64	0.61
35:1:613:MET:N	35:1:613:MET:HE3	2.15	0.61
36:3:330:PHE:O	36:3:390:ARG:NH2	2.32	0.61
36:3:1049:LYS:HE3	42:5:52:TYR:OH	2.00	0.61
1:A:81:PHE:O	1:A:83:HIS:N	2.34	0.61
1:A:1869:LEU:HD22	1:A:1884:ILE:HG22	1.83	0.61
36:3:1115:GLU:HB3	39:2:708:TRP:NE1	2.16	0.61
36:3:1193:VAL:HA	36:3:1196:GLU:HG2	1.81	0.61
1:A:988:ILE:HD12	1:A:1030:ILE:HG13	1.81	0.61
1:A:1336:PRO:HB2	1:A:1350:ILE:HG12	1.83	0.61
3:C:209:VAL:HG21	3:C:237:LEU:HD23	1.82	0.61
9:J:441:ASP:OD1	9:J:445:LYS:NZ	2.34	0.61
15:P:39:THR:O	19:T:318:ARG:HD3	2.00	0.61
21:V:511:ALA:HB1	21:V:525:PHE:HZ	1.64	0.61
23:X:651:LEU:HG	23:X:656:GLN:NE2	2.16	0.61
35:1:1028:HIS:O	35:1:1032:GLN:HB2	2.01	0.61
36:3:680:ASP:CG	36:3:681:PRO:HD2	2.21	0.61
41:7:52:GLY:H	41:7:55:GLN:HE21	1.47	0.61
14:O:172:GLU:O	14:O:174:LYS:N	2.32	0.61
36:3:207:THR:O	36:3:207:THR:OG1	2.15	0.61
39:2:594:GLY:O	39:2:597:PHE:HB2	2.00	0.61
1:A:1969:PRO:HB2	1:A:1971:LEU:HD23	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:724:TRP:HH2	3:C:788:LYS:HZ2	1.48	0.61
11:L:63:TRP:CD1	11:L:67:GLU:HB3	2.36	0.61
12:M:163:THR:HG23	12:M:166:SER:HB2	1.82	0.61
17:R:122:LYS:HG2	17:R:124:VAL:HG23	1.83	0.61
35:1:625:ARG:NE	35:1:666:LYS:HZ1	1.99	0.61
36:3:12:THR:O	36:3:34:ARG:NH1	2.34	0.61
2:B:63:A:H2'	2:B:64:G:C8	2.36	0.61
4:E:108:HIS:CD2	4:E:128:SER:HB2	2.36	0.61
35:1:815:PHE:CE1	35:1:853:ILE:CG2	2.84	0.61
35:1:834:VAL:O	35:1:838:VAL:HG23	2.01	0.61
35:1:1166:ILE:O	35:1:1170:THR:HG22	2.01	0.61
35:1:1258:ALA:HB3	35:1:1261:VAL:HG13	1.83	0.61
35:1:1274:ILE:HG22	36:3:109:LYS:CE	2.30	0.61
36:3:318:ASP:OD1	36:3:319:GLU:N	2.33	0.61
36:3:462:VAL:O	36:3:472:ALA:N	2.30	0.61
36:3:807:TYR:H	36:3:856:LYS:HD2	1.65	0.61
5:F:15:A:H2'	5:F:16:G:C8	2.35	0.60
5:F:35:A:C8	6:G:12:G:C6	2.89	0.60
23:X:171:ARG:HH12	23:X:509:PRO:HG3	1.65	0.60
23:X:257:PHE:CZ	23:X:270:LEU:HB2	2.36	0.60
36:3:71:THR:O	36:3:146:ARG:NH2	2.33	0.60
36:3:138:GLN:HG2	36:3:161:HIS:CE1	2.36	0.60
36:3:139:LYS:NZ	36:3:160:ALA:O	2.34	0.60
36:3:1004:ASP:OD1	36:3:1006:GLN:N	2.28	0.60
1:A:1780:VAL:HB	1:A:1863:VAL:HG23	1.81	0.60
1:A:1862:ILE:HA	1:A:1885:LYS:O	2.01	0.60
3:C:64:LYS:HD3	15:P:209:ARG:HH12	1.66	0.60
23:X:677:ALA:O	23:X:725:ARG:NE	2.34	0.60
35:1:677:CYS:O	35:1:680:LEU:HD12	2.01	0.60
35:1:743:LEU:O	35:1:747:LEU:HB2	2.01	0.60
36:3:706:MET:HG3	36:3:707:GLN:HG2	1.83	0.60
39:2:487:LEU:HD22	42:5:28:LYS:HB2	1.82	0.60
41:7:13:LYS:NZ	41:7:48:GLU:OE1	2.26	0.60
1:A:641:MET:O	1:A:645:THR:HG23	1.99	0.60
4:E:203:ASP:N	4:E:203:ASP:OD1	2.32	0.60
5:F:36:A:H2'	5:F:38:G:OP2	2.02	0.60
35:1:590:ARG:O	35:1:594:ARG:HB2	2.02	0.60
36:3:947:GLU:HB3	36:3:963:VAL:HG13	1.82	0.60
40:4:17:VAL:O	40:4:56:TYR:HA	2.01	0.60
1:A:1892:PRO:HB3	1:A:1944:HIS:CD2	2.36	0.60
4:E:209:ILE:HG13	4:E:219:VAL:HG13	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:361:ARG:HD3	12:M:161:PHE:CE2	2.36	0.60
35:1:664:GLY:HA2	35:1:667:ILE:HD12	1.83	0.60
35:1:721:ILE:C	35:1:721:ILE:HD12	2.21	0.60
2:B:95:G:N2	2:B:96:A:H5"	2.12	0.60
36:3:910:ALA:HB1	36:3:913:LEU:HD11	1.83	0.60
1:A:278:LYS:NZ	6:G:-8:C:OP1	2.35	0.60
1:A:755:HIS:CD2	15:P:219:PHE:HE2	2.20	0.60
1:A:892:LYS:HD2	1:A:912:GLU:OE1	2.00	0.60
1:A:1490:PHE:O	1:A:1493:THR:OG1	2.19	0.60
4:E:135:VAL:HG12	4:E:145:LYS:HB2	1.82	0.60
12:M:215:ASN:ND2	17:R:260:TYR:CB	2.65	0.60
23:X:765:LEU:HD22	23:X:822:PRO:HG3	1.82	0.60
24:Y:96:MET:HB2	24:Y:124:THR:HB	1.84	0.60
39:2:477:MET:SD	39:2:478:HIS:ND1	2.75	0.60
15:P:44:ARG:NH2	19:T:255:SER:O	2.32	0.60
35:1:669:GLN:HB2	35:1:708:ALA:HA	1.83	0.60
35:1:1167:TYR:OH	39:2:581:LYS:HE2	2.02	0.60
40:4:78:LYS:CB	40:4:115:LEU:CB	2.79	0.60
1:A:972:GLU:OE1	1:A:972:GLU:N	2.30	0.60
1:A:1578:ARG:HE	1:A:1746:ARG:HH21	1.48	0.60
1:A:1663:ASP:O	1:A:1703:ILE:N	2.34	0.60
7:H:48:A:C2	7:H:65:U:H2'	2.37	0.60
15:P:42:LYS:O	19:T:258:SER:HB3	2.02	0.60
23:X:510:ASP:CG	23:X:543:ARG:HD3	2.21	0.60
23:X:802:LEU:HB3	23:X:806:GLY:HA2	1.84	0.60
1:A:47:GLU:H	1:A:47:GLU:CD	2.03	0.60
15:P:72:ARG:HA	15:P:75:ASN:ND2	2.17	0.60
18:S:99:ALA:HB2	18:S:128:ILE:HA	1.83	0.60
36:3:528:ARG:HG2	36:3:532:ARG:HH21	1.67	0.60
36:3:680:ASP:OD2	36:3:681:PRO:HD2	2.02	0.60
1:A:857:ASN:OD1	1:A:860:GLN:N	2.26	0.60
3:C:192:ASP:CG	3:C:193:THR:H	2.04	0.60
3:C:811:THR:O	3:C:815:VAL:HG23	2.00	0.60
15:P:186:ARG:O	15:P:186:ARG:HG3	2.01	0.60
19:T:271:LYS:HG2	19:T:280:VAL:HG11	1.84	0.60
23:X:406:GLU:HA	23:X:409:LEU:HD23	1.84	0.60
35:1:953:ASP:O	35:1:956:SER:OG	2.18	0.60
36:3:982:GLU:HG2	36:3:984:LYS:HE3	1.84	0.60
1:A:371:LEU:HD21	3:C:347:ILE:HD11	1.82	0.59
5:F:79:C:H4'	5:F:80:G:OP1	2.03	0.59
23:X:164:TRP:NE1	23:X:539:VAL:CG2	2.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:802:LEU:HA	23:X:807:GLU:O	2.02	0.59
24:Y:88:HIS:ND1	24:Y:120:ASP:OD1	2.35	0.59
35:1:675:MET:HB3	35:1:678:ALA:HB3	1.84	0.59
35:1:698:GLN:HB3	35:1:701:VAL:HG12	1.84	0.59
35:1:850:ILE:O	35:1:854:VAL:HG13	2.01	0.59
35:1:1192:VAL:O	35:1:1196:SER:OG	2.20	0.59
36:3:329:TYR:CE2	36:3:389:PRO:HA	2.37	0.59
1:A:390:ASP:OD1	1:A:390:ASP:N	2.35	0.59
1:A:693:ILE:HG22	1:A:694:LEU:HD23	1.82	0.59
1:A:1527:ASN:O	1:A:1529:ILE:N	2.36	0.59
23:X:272:TYR:O	23:X:276:VAL:HB	2.02	0.59
35:1:1292:LYS:CD	42:5:78:PRO:HG2	2.32	0.59
36:3:193:ASP:O	42:5:79:PRO:CG	2.49	0.59
36:3:700:LYS:HE2	36:3:715:MET:HB3	1.84	0.59
1:A:280:GLU:HG3	20:U:9:THR:HG21	1.84	0.59
44:A:3000:IHP:H1	44:A:3000:IHP:O46	2.01	0.59
3:C:64:LYS:HA	15:P:206:LYS:HZ3	1.66	0.59
3:C:724:TRP:HE1	3:C:732:ILE:HD11	1.67	0.59
4:E:114:GLU:OE2	4:E:290:ARG:NH2	2.36	0.59
9:J:206:LEU:HD23	9:J:207:PRO:HD3	1.84	0.59
9:J:439:ALA:HA	9:J:442:ARG:HB3	1.84	0.59
23:X:225:GLU:O	23:X:229:LYS:HD3	2.03	0.59
24:Y:42:ILE:HA	24:Y:53:THR:HG22	1.82	0.59
24:Y:77:PHE:HB3	24:Y:103:GLN:HB3	1.83	0.59
24:Y:91:LYS:HG3	24:Y:114:GLU:HG3	1.84	0.59
36:3:212:GLU:HB2	36:3:223:LYS:HG3	1.84	0.59
36:3:435:LEU:HD13	36:3:799:ILE:HD11	1.84	0.59
36:3:1115:GLU:CB	39:2:708:TRP:HE1	2.14	0.59
42:5:65:ARG:HB3	42:5:65:ARG:CZ	2.32	0.59
1:A:384:VAL:HG12	3:C:331:PHE:HB3	1.83	0.59
4:E:300:ILE:HG23	4:E:312:TRP:HB2	1.83	0.59
5:F:28:A:O2'	13:N:39:GLY:O	2.19	0.59
13:N:121:VAL:HG11	13:N:126:LEU:HD21	1.83	0.59
35:1:508:THR:HB	35:1:510:PRO:HD2	1.84	0.59
2:B:87:A:N6	2:B:91:U:O3'	2.35	0.59
4:E:202:ASN:ND2	4:E:204:THR:OG1	2.36	0.59
6:G:85:G:H2'	6:G:86:A:C8	2.38	0.59
13:N:70:ILE:HB	13:N:74:LEU:HD23	1.83	0.59
35:1:854:VAL:HG23	35:1:855:ASP:H	1.68	0.59
36:3:615:ARG:NH2	36:3:630:MET:HB3	2.17	0.59
1:A:1841:THR:O	1:A:1845:VAL:HG23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1919:LEU:HD12	1:A:1936:LEU:HD11	1.83	0.59
3:C:137:HIS:O	3:C:142:LYS:NZ	2.26	0.59
14:O:34:ILE:C	17:R:197:ILE:HD13	2.20	0.59
24:Y:161:ILE:HG21	24:Y:164:ASP:HB2	1.84	0.59
36:3:607:VAL:HB	36:3:615:ARG:HB2	1.85	0.59
23:X:612:LEU:O	23:X:689:VAL:HA	2.03	0.59
23:X:698:LYS:NZ	23:X:758:THR:HA	2.17	0.59
36:3:1133:THR:O	39:2:712:GLU:HB2	2.01	0.59
4:E:105:LEU:HD11	4:E:136:TRP:CD2	2.37	0.59
4:E:150:HIS:NE2	4:E:169:THR:OG1	2.19	0.59
4:E:312:TRP:CD1	4:E:319:ILE:HA	2.37	0.59
36:3:246:SER:OG	36:3:247:GLY:N	2.35	0.59
1:A:729:PRO:HG2	12:M:226:TYR:HE1	1.65	0.59
4:E:218:LYS:HD2	4:E:220:TRP:CZ2	2.38	0.59
5:F:59:G:N2	5:F:76:A:N1	2.42	0.59
7:H:46:U:O2'	7:H:47:U:OP2	2.16	0.59
7:H:180:G:H2'	7:H:181:G:C8	2.38	0.59
19:T:455:GLN:HG2	19:T:456:PRO:HD2	1.85	0.59
21:V:545:ARG:HG3	21:V:585:ILE:HG21	1.85	0.59
23:X:557:THR:HA	23:X:560:PHE:HB2	1.85	0.59
1:A:47:GLU:HA	1:A:50:LYS:HG3	1.83	0.59
3:C:453:TYR:CZ	3:C:575:GLN:HB2	2.38	0.59
4:E:251:LEU:HB2	4:E:293:TRP:CE2	2.38	0.59
35:1:495:ARG:HH21	35:1:530:PRO:HB3	1.66	0.59
35:1:610:ILE:CG2	35:1:647:PHE:CD1	2.86	0.59
1:A:425:PRO:HB2	1:A:428:LYS:HG3	1.85	0.58
1:A:1558:THR:OG1	1:A:1559:GLY:N	2.33	0.58
3:C:617:LEU:HD11	3:C:629:ILE:HG23	1.85	0.58
9:J:443:ILE:HG13	9:J:444:SER:N	2.18	0.58
12:M:224:ARG:NH1	12:M:224:ARG:O	2.36	0.58
17:R:373:ALA:HB3	17:R:376:LYS:HB3	1.84	0.58
23:X:526:THR:HG22	23:X:528:HIS:H	1.68	0.58
35:1:1270:ASN:OD1	42:5:21:THR:HB	2.03	0.58
1:A:263:PHE:HE1	1:A:273:ILE:HD11	1.68	0.58
1:A:498:ARG:O	1:A:502:ASN:ND2	2.35	0.58
1:A:758:ARG:HD3	1:A:779:LEU:HD11	1.85	0.58
17:R:332:ARG:HA	23:X:272:TYR:HD1	1.65	0.58
21:V:497:CYS:HB3	21:V:507:PHE:CG	2.37	0.58
35:1:1074:ARG:O	35:1:1078:VAL:HG23	2.03	0.58
35:1:1110:VAL:O	35:1:1113:THR:HG22	2.02	0.58
1:A:41:GLN:NE2	4:E:153:PHE:HE2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1298:ARG:HH11	1:A:1298:ARG:HB2	1.68	0.58
1:A:1407:ASP:OD1	1:A:1407:ASP:N	2.32	0.58
1:A:1519:THR:OG1	1:A:1522:GLN:HB2	2.04	0.58
7:H:50:C:H2'	7:H:51:A:C8	2.38	0.58
9:J:433:ARG:O	9:J:437:LYS:HG2	2.03	0.58
17:R:330:LYS:NZ	23:X:275:ARG:NH2	2.51	0.58
21:V:606:GLU:HA	21:V:609:GLN:CG	2.33	0.58
36:3:525:ARG:HD3	36:3:533:VAL:HG22	1.85	0.58
36:3:695:GLY:O	36:3:697:ARG:NE	2.30	0.58
4:E:140:THR:HB	4:E:142:GLU:HG2	1.85	0.58
35:1:652:CYS:HB2	35:1:692:HIS:CE1	2.35	0.58
35:1:747:LEU:HA	35:1:750:ILE:HG12	1.85	0.58
1:A:909:TYR:HB2	1:A:1033:GLY:HA3	1.85	0.58
1:A:1571:ILE:HG23	10:K:220:LEU:HD13	1.84	0.58
2:B:14:U:H2'	2:B:15:C:H6	1.69	0.58
35:1:641:ILE:HB	35:1:682:HIS:CE1	2.38	0.58
35:1:898:TYR:OH	35:1:902:GLU:HG2	2.03	0.58
36:3:326:ARG:NE	36:3:372:GLU:OE2	2.19	0.58
36:3:387:PHE:CE1	36:3:389:PRO:HG3	2.38	0.58
36:3:883:GLU:OE2	36:3:884:GLN:N	2.33	0.58
36:3:1147:HIS:O	36:3:1151:GLU:HG3	2.03	0.58
7:H:99:A:O2'	7:H:100:U:OP2	2.18	0.58
23:X:546:LEU:HD22	23:X:547:LYS:H	1.69	0.58
24:Y:13:VAL:HB	24:Y:131:GLU:HB3	1.85	0.58
35:1:512:ARG:O	35:1:516:LEU:HB2	2.04	0.58
36:3:106:THR:HG1	41:7:82:ARG:HD2	1.66	0.58
1:A:1768:TYR:HA	1:A:1771:LEU:CB	2.34	0.58
3:C:879:ASP:OD1	3:C:879:ASP:N	2.36	0.58
7:H:70:C:H2'	7:H:71:C:C6	2.39	0.58
13:N:32:ALA:HA	13:N:35:GLU:HG2	1.85	0.58
1:A:707:ARG:NH1	7:H:18:U:H5'	2.13	0.58
5:F:35:A:C2	5:F:36:A:C6	2.91	0.58
11:L:49:ARG:NH1	11:L:133:GLU:O	2.37	0.58
17:R:328:ALA:HB1	24:Y:226:MET:CA	2.34	0.58
35:1:1110:VAL:O	35:1:1114:VAL:HG23	2.03	0.58
36:3:310:ILE:O	36:3:311:PHE:HD2	1.87	0.58
1:A:1779:PHE:HB2	1:A:1810:PHE:HB3	1.85	0.58
21:V:491:ASN:HA	21:V:528:ILE:HD11	1.85	0.58
23:X:653:SER:HA	23:X:656:GLN:HG3	1.85	0.58
25:Z:181:MET:O	25:Z:185:TRP:N	2.36	0.58
36:3:195:ASP:OD2	36:3:198:GLY:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1749:LYS:HG3	35:1:980:GLU:HG2	1.85	0.58
3:C:250:ARG:NH1	3:C:447:PRO:O	2.36	0.58
4:E:158:TYR:HB3	4:E:168:CYS:SG	2.44	0.58
6:G:88:G:H4'	6:G:89:U:OP1	2.04	0.58
12:M:179:ILE:O	12:M:183:VAL:HG23	2.04	0.58
23:X:664:PRO:HG2	23:X:667:ALA:HB3	1.85	0.58
23:X:850:ASN:O	23:X:853:ILE:HG12	2.03	0.58
35:1:1179:ASP:H	39:2:511:LEU:CD1	2.15	0.58
36:3:642:ILE:H	36:3:703:ARG:HE	1.52	0.58
1:A:194:GLU:HA	1:A:194:GLU:OE2	2.03	0.57
3:C:444:GLY:O	3:C:447:PRO:HD2	2.04	0.57
13:N:57:THR:HG21	13:N:88:LEU:HD23	1.86	0.57
18:S:14:VAL:O	18:S:24:VAL:HA	2.04	0.57
21:V:543:LYS:HA	21:V:546:ASN:HD21	1.69	0.57
23:X:283:TYR:OH	24:Y:219:THR:HA	2.04	0.57
23:X:650:ASN:O	23:X:904:GLN:NE2	2.37	0.57
23:X:714:CYS:SG	23:X:718:SER:OG	2.61	0.57
36:3:25:THR:OG1	36:3:26:LYS:N	2.35	0.57
36:3:1115:GLU:HB3	39:2:708:TRP:HE1	1.69	0.57
42:5:7:ILE:HG13	42:5:8:HIS:N	2.18	0.57
42:5:14:LEU:HA	42:5:17:LYS:HB2	1.86	0.57
1:A:1436:TRP:O	1:A:1440:THR:HG23	2.04	0.57
12:M:165:ASN:HD22	17:R:95:LYS:HE2	1.69	0.57
23:X:192:ARG:HG2	23:X:192:ARG:HH11	1.68	0.57
35:1:759:ALA:O	35:1:763:ASN:N	2.35	0.57
35:1:826:ASP:HB3	35:1:829:ASN:HB2	1.86	0.57
36:3:115:ILE:HD13	42:5:19:ILE:H	1.69	0.57
36:3:169:HIS:CD2	36:3:170:VAL:H	2.22	0.57
36:3:449:VAL:HG22	36:3:763:ARG:HB3	1.86	0.57
36:3:538:THR:OG1	36:3:542:LYS:O	2.22	0.57
36:3:791:HIS:HD2	36:3:794:SER:OG	1.87	0.57
36:3:1008:SER:HG	36:3:1009:PHE:N	2.02	0.57
39:2:542:GLU:O	39:2:546:GLN:HG2	2.03	0.57
3:C:113:VAL:HG23	3:C:114:TYR:H	1.68	0.57
3:C:711:ARG:NH2	3:C:732:ILE:O	2.38	0.57
9:J:206:LEU:HD22	9:J:207:PRO:CD	2.34	0.57
11:L:11:TRP:CE2	11:L:49:ARG:HD3	2.39	0.57
17:R:161:ALA:HA	17:R:166:ARG:HH12	1.69	0.57
19:T:195:LYS:NZ	19:T:490:ARG:HD2	2.19	0.57
35:1:717:THR:CB	35:1:718:PRO:HD2	2.35	0.57
35:1:819:TRP:HE3	35:1:864:TYR:HH	1.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:3:365:GLY:HA2	36:3:394:ASN:ND2	2.19	0.57
36:3:638:GLU:OE2	36:3:698:PRO:HB3	2.04	0.57
41:7:33:CYS:HB2	41:7:74:GLU:OE1	2.04	0.57
1:A:665:SER:O	1:A:665:SER:OG	2.18	0.57
1:A:1676:ILE:HD12	1:A:1706:ASP:HB2	1.86	0.57
3:C:779:LEU:O	3:C:938:ARG:HD2	2.04	0.57
7:H:41:U:H2'	7:H:42:G:C8	2.39	0.57
23:X:707:GLU:O	23:X:990:VAL:HA	2.03	0.57
24:Y:2:ALA:HA	24:Y:15:ASP:HA	1.86	0.57
36:3:69:ARG:NH1	36:3:74:THR:HA	2.18	0.57
36:3:329:TYR:HE2	36:3:389:PRO:HA	1.69	0.57
36:3:552:ARG:HH21	36:3:567:GLU:HB3	1.69	0.57
36:3:758:SER:N	36:3:761:THR:O	2.25	0.57
36:3:1148:LEU:HA	36:3:1151:GLU:OE2	2.05	0.57
36:3:1200:THR:O	36:3:1203:GLU:N	2.38	0.57
7:H:68:G:H2'	7:H:69:U:C6	2.39	0.57
11:L:699:ASN:CB	25:Z:110:SER:CB	2.81	0.57
14:O:34:ILE:H	17:R:197:ILE:HD13	1.69	0.57
23:X:394:ALA:HA	23:X:397:ARG:HD2	1.86	0.57
23:X:1009:LEU:HD21	23:X:1021:LEU:HD11	1.85	0.57
24:Y:55:ASP:OD2	24:Y:60:GLY:N	2.37	0.57
35:1:1098:LEU:HD12	35:1:1135:GLU:HG2	1.87	0.57
35:1:1165:TYR:CE1	39:2:575:PHE:CD1	2.92	0.57
36:3:510:LEU:HD23	36:3:510:LEU:H	1.70	0.57
1:A:1275:ARG:NH1	1:A:1373:GLN:O	2.36	0.57
1:A:1604:LEU:HD21	1:A:1725:LEU:HD22	1.85	0.57
3:C:461:LEU:HB3	3:C:465:MET:HE1	1.85	0.57
7:H:125:G:H2'	7:H:126:A:H8	1.67	0.57
23:X:593:GLU:O	23:X:597:VAL:HG22	2.04	0.57
35:1:1299:GLU:OE2	42:5:40:TYR:OH	2.14	0.57
39:2:635:ALA:HB1	40:4:73:ILE:N	2.12	0.57
41:7:68:ASP:OD1	41:7:68:ASP:N	2.38	0.57
1:A:1160:ARG:HD3	15:P:192:VAL:HG11	1.87	0.57
4:E:282:HIS:NE2	22:W:150:ALA:HB2	2.18	0.57
23:X:760:LEU:O	23:X:764:VAL:HG23	2.05	0.57
24:Y:24:ALA:HA	24:Y:78:PHE:HZ	1.69	0.57
24:Y:139:ILE:HA	24:Y:142:THR:HG23	1.86	0.57
36:3:1140:PHE:HE1	36:3:1197:LEU:HD13	1.68	0.57
1:A:1776:ILE:HG22	1:A:1859:LYS:HZ3	1.69	0.57
3:C:261:ASP:OD2	3:C:261:ASP:N	2.35	0.57
12:M:163:THR:OG1	12:M:165:ASN:OD1	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:175:GLN:OE1	17:R:176:TYR:N	2.33	0.57
17:R:335:ARG:O	23:X:268:GLN:CB	2.49	0.57
21:V:491:ASN:O	21:V:494:LEU:HB3	2.05	0.57
21:V:636:LEU:O	21:V:640:THR:OG1	2.18	0.57
23:X:587:PRO:HB2	35:1:827:ARG:HH12	1.69	0.57
23:X:640:ARG:HH22	23:X:668:ARG:HB2	1.70	0.57
24:Y:33:LYS:HG3	24:Y:174:ILE:HD13	1.85	0.57
1:A:1815:GLY:O	1:A:1918:ASN:HA	2.04	0.57
1:A:1927:ILE:HD12	1:A:1931:THR:HG22	1.87	0.57
6:G:1:G:N1	10:K:217:CYS:SG	2.74	0.57
6:G:85:G:N2	7:H:45:C:N3	2.51	0.57
9:J:334:GLU:OE2	9:J:349:TYR:OH	2.10	0.57
21:V:551:PHE:HD1	21:V:554:LEU:HD12	1.69	0.57
23:X:462:ALA:HB1	23:X:473:LEU:HD11	1.87	0.57
24:Y:23:ARG:O	24:Y:26:LEU:HD23	2.05	0.57
35:1:631:ALA:O	35:1:635:VAL:HG13	2.05	0.57
35:1:1001:VAL:HG23	35:1:1009:MET:HE1	1.85	0.57
1:A:171:ASP:O	1:A:520:TYR:HB2	2.04	0.57
3:C:461:LEU:HB3	3:C:465:MET:CE	2.35	0.57
4:E:260:ARG:HD3	4:E:276:ILE:HG12	1.87	0.57
10:K:205:TYR:O	10:K:209:GLY:N	2.36	0.57
18:S:14:VAL:HA	18:S:164:PRO:HA	1.87	0.57
35:1:1104:GLN:O	35:1:1105:GLU:HB3	2.03	0.57
39:2:632:TRP:O	40:4:73:ILE:CB	2.53	0.57
1:A:30:LEU:HD22	4:E:214:ASP:OD2	2.04	0.56
1:A:1635:TYR:CZ	1:A:1636:LYS:HB2	2.40	0.56
1:A:1839:TRP:CZ3	1:A:1871:PRO:HA	2.40	0.56
2:B:87:A:C6	2:B:92:U:OP2	2.59	0.56
14:O:34:ILE:N	17:R:197:ILE:HD13	2.20	0.56
23:X:171:ARG:HH12	23:X:509:PRO:CB	2.18	0.56
23:X:234:TYR:CZ	24:Y:317:GLN:HB3	2.40	0.56
36:3:616:ILE:HG22	36:3:628:LEU:HB3	1.86	0.56
1:A:1167:THR:OG1	1:A:1168:VAL:N	2.38	0.56
1:A:1978:LYS:O	1:A:1981:VAL:HG12	2.05	0.56
15:P:209:ARG:O	15:P:209:ARG:HG2	2.05	0.56
23:X:511:LEU:HG	23:X:514:TYR:HB2	1.86	0.56
35:1:556:ILE:CG2	35:1:596:ILE:HG21	2.32	0.56
35:1:850:ILE:HG22	35:1:888:LEU:HD11	1.85	0.56
36:3:92:TYR:OH	36:3:97:ASN:OD1	2.18	0.56
36:3:876:THR:O	36:3:876:THR:OG1	2.12	0.56
1:A:1817:LEU:HD23	1:A:1919:LEU:HD21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:490:PHE:O	3:C:491:HIS:ND1	2.33	0.56
6:G:85:G:H1	7:H:45:C:H42	1.53	0.56
13:N:16:GLU:N	13:N:16:GLU:OE1	2.33	0.56
16:Q:27:ALA:O	16:Q:32:ALA:N	2.32	0.56
23:X:217:GLU:HA	23:X:220:LYS:HB2	1.87	0.56
23:X:519:VAL:HB	23:X:550:VAL:HG13	1.87	0.56
24:Y:224:LEU:HD11	24:Y:230:LEU:HD23	1.86	0.56
35:1:549:ARG:NH2	35:1:586:ASP:OD1	2.38	0.56
36:3:1180:GLU:CD	36:3:1212:ARG:HH21	2.08	0.56
1:A:711:GLN:HE22	7:H:18:U:H5"	1.71	0.56
3:C:463:GLU:H	3:C:463:GLU:CD	2.08	0.56
3:C:829:GLU:HG2	3:C:907:VAL:HB	1.86	0.56
6:G:90:C:O5'	6:G:90:C:H6	1.89	0.56
8:I:463:PRO:CG	8:I:483:SER:CB	2.80	0.56
35:1:833:LEU:CD2	35:1:867:MET:SD	2.91	0.56
36:3:141:VAL:HB	36:3:158:LEU:HD12	1.86	0.56
36:3:345:GLY:O	36:3:360:GLN:HG3	2.04	0.56
36:3:527:ILE:HG12	36:3:532:ARG:O	2.06	0.56
1:A:378:PHE:O	3:C:355:LYS:HG3	2.05	0.56
1:A:381:PRO:O	1:A:383:PHE:N	2.32	0.56
1:A:1410:ASP:OD2	1:A:1411:SER:N	2.38	0.56
2:B:110:C:H2'	2:B:111:A:H8	1.70	0.56
23:X:246:LEU:HG	23:X:277:ARG:NE	2.20	0.56
23:X:716:LYS:HG3	23:X:747:LEU:HB3	1.87	0.56
24:Y:216:GLU:HA	24:Y:219:THR:HG23	1.86	0.56
35:1:815:PHE:HE1	35:1:853:ILE:CG2	2.18	0.56
35:1:1165:TYR:HD1	39:2:575:PHE:CD1	2.24	0.56
1:A:1006:ALA:O	1:A:1010:THR:HG22	2.05	0.56
3:C:833:PHE:HB3	3:C:900:VAL:HG23	1.88	0.56
4:E:243:LEU:HG	4:E:250:LEU:HB2	1.87	0.56
11:L:28:LYS:HE2	17:R:268:LEU:HD23	1.88	0.56
23:X:430:THR:O	23:X:434:GLN:HG3	2.06	0.56
24:Y:247:LEU:HD11	24:Y:256:LEU:HD11	1.86	0.56
36:3:86:ARG:NH1	36:3:1157:GLY:O	2.38	0.56
36:3:193:ASP:CA	42:5:79:PRO:CG	2.83	0.56
36:3:342:LEU:HB3	36:3:343:LYS:O	2.06	0.56
36:3:373:PHE:HE1	36:3:385:PHE:HB3	1.70	0.56
36:3:1143:HIS:O	36:3:1147:HIS:ND1	2.39	0.56
39:2:594:GLY:N	39:2:597:PHE:HE2	2.02	0.56
1:A:431:TYR:HB3	1:A:611:LEU:HD21	1.88	0.56
1:A:854:SER:OG	1:A:855:ARG:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:197:LEU:HD11	4:E:213:ILE:HD13	1.87	0.56
7:H:72:U:H2'	7:H:73:C:C6	2.41	0.56
11:L:147:ASP:HA	11:L:150:GLU:HG3	1.88	0.56
17:R:162:ALA:C	17:R:164:PRO:HD3	2.26	0.56
17:R:317:LYS:HG3	23:X:286:ALA:HB1	1.88	0.56
24:Y:246:LYS:HD2	24:Y:310:ARG:O	2.06	0.56
35:1:970:LEU:O	35:1:973:HIS:HB2	2.06	0.56
35:1:1299:GLU:CB	42:5:43:TYR:HE2	2.18	0.56
36:3:68:PHE:CE2	36:3:77:TYR:HB2	2.41	0.56
2:B:15:C:H2'	2:B:16:U:H6	1.71	0.56
3:C:401:ILE:HD11	3:C:423:PHE:HB2	1.88	0.56
6:G:95:U:P	35:1:1106:ARG:HD2	2.46	0.56
9:J:321:GLU:OE1	9:J:355:ARG:NH1	2.39	0.56
35:1:954:LEU:O	35:1:958:THR:HG22	2.05	0.56
35:1:1178:MET:HG2	39:2:591:TYR:CE2	2.39	0.56
35:1:1179:ASP:CB	39:2:511:LEU:HB2	2.32	0.56
1:A:1980:GLU:O	1:A:1984:LYS:HG2	2.06	0.56
3:C:529:ARG:NH2	3:C:540:GLU:HB2	2.20	0.56
17:R:357:HIS:O	17:R:361:LYS:HD2	2.06	0.56
23:X:430:THR:HG22	23:X:434:GLN:NE2	2.20	0.56
35:1:1293:ASN:OD1	42:5:77:GLY:HA3	2.06	0.56
11:L:66:GLU:O	11:L:69:GLU:HG3	2.05	0.56
11:L:223:GLY:HA2	17:R:86:LEU:CD2	2.36	0.56
23:X:171:ARG:NH2	23:X:505:PHE:O	2.39	0.56
23:X:331:GLU:O	23:X:335:GLY:N	2.39	0.56
23:X:476:GLU:HG3	23:X:477:VAL:H	1.70	0.56
23:X:580:ASP:HB2	23:X:733:LYS:HG3	1.88	0.56
23:X:698:LYS:O	23:X:757:ARG:HD3	2.06	0.56
35:1:605:GLY:O	35:1:608:THR:OG1	2.16	0.56
36:3:418:GLU:OE1	36:3:419:ASP:N	2.28	0.56
42:5:14:LEU:HD23	42:5:17:LYS:HD2	1.88	0.56
1:A:35:ARG:O	1:A:39:GLN:HG3	2.06	0.55
1:A:1636:LYS:HD3	1:A:1658:GLN:NE2	2.18	0.55
3:C:678:THR:HG22	3:C:679:PRO:HD2	1.88	0.55
23:X:518:MET:HA	23:X:549:LEU:O	2.06	0.55
24:Y:257:GLU:OE2	24:Y:266:ILE:HG21	2.06	0.55
35:1:735:ILE:HD12	35:1:747:LEU:HD12	1.88	0.55
35:1:739:ARG:HA	35:1:743:LEU:HD22	1.88	0.55
36:3:477:SER:HB2	36:3:505:THR:N	2.11	0.55
36:3:479:VAL:HG23	36:3:480:ASN:ND2	2.20	0.55
36:3:703:ARG:HH11	36:3:703:ARG:HB2	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:4:13:ALA:O	40:4:60:GLU:HA	2.06	0.55
1:A:729:PRO:HG2	12:M:226:TYR:CD1	2.41	0.55
1:A:1382:SER:CB	1:A:1415:GLY:HA2	2.36	0.55
6:G:94:C:OP1	35:1:1142:ASN:OD1	2.24	0.55
6:G:111:U:O2'	23:X:482:ARG:HD2	2.06	0.55
7:H:27:U:O2'	7:H:28:C:H5'	2.06	0.55
7:H:57:A:H5'	39:2:481:THR:HG21	1.88	0.55
7:H:78:C:H2'	7:H:79:G:H8	1.71	0.55
15:P:198:ALA:O	15:P:201:VAL:HG23	2.06	0.55
23:X:164:TRP:HB2	23:X:538:ASP:HB3	1.88	0.55
23:X:602:ILE:O	23:X:606:GLN:HB2	2.06	0.55
23:X:700:TYR:HA	23:X:706:MET:O	2.07	0.55
23:X:811:SER:HA	23:X:814:LYS:NZ	2.21	0.55
35:1:703:THR:HG22	35:1:745:ALA:CB	2.30	0.55
35:1:1295:TYR:CE1	42:5:76:CYS:HB3	2.42	0.55
1:A:758:ARG:HH21	1:A:775:ASN:ND2	2.03	0.55
7:H:6:U:H2'	7:H:7:U:H6	1.70	0.55
7:H:50:C:H2'	7:H:51:A:H8	1.71	0.55
11:L:176:LEU:HD13	11:L:176:LEU:O	2.07	0.55
16:Q:543:LEU:N	16:Q:621:GLU:O	2.35	0.55
17:R:160:ALA:O	17:R:166:ARG:NH1	2.40	0.55
35:1:754:ILE:HG22	35:1:755:PRO:HD3	1.88	0.55
35:1:784:MET:O	35:1:788:VAL:HG12	2.05	0.55
35:1:926:LYS:O	35:1:929:LEU:HG	2.06	0.55
36:3:542:LYS:HB2	36:3:558:LEU:HD11	1.89	0.55
36:3:718:ARG:HB2	36:3:720:TRP:NE1	2.21	0.55
36:3:1015:LYS:O	36:3:1019:ASN:N	2.40	0.55
1:A:406:TRP:CZ2	3:C:266:GLU:HG3	2.41	0.55
1:A:762:ARG:HH22	15:P:226:LYS:HZ3	1.54	0.55
1:A:1303:LEU:HD12	1:A:1311:PHE:CE1	2.41	0.55
4:E:165:GLN:HG3	4:E:181:ILE:HD13	1.89	0.55
35:1:819:TRP:HZ2	35:1:837:THR:HG21	1.71	0.55
36:3:69:ARG:HH12	36:3:74:THR:HA	1.71	0.55
36:3:1083:ASN:OD1	36:3:1084:GLY:N	2.39	0.55
1:A:548:ARG:HG2	1:A:548:ARG:HH21	1.72	0.55
1:A:831:SER:O	1:A:831:SER:OG	2.18	0.55
1:A:1795:GLU:HG2	1:A:1797:ASN:H	1.71	0.55
3:C:441:PRO:HB3	3:C:495:ARG:HH21	1.72	0.55
9:J:199:LYS:HD3	9:J:199:LYS:C	2.27	0.55
23:X:443:ASN:O	23:X:444:LYS:HB2	2.05	0.55
23:X:647:ILE:HA	23:X:651:LEU:HD21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:495:ARG:HA	35:1:498:MET:HE3	1.88	0.55
1:A:1756:SER:HG	35:1:943:LYS:HD2	1.70	0.55
3:C:86:THR:OG1	3:C:87:GLN:N	2.38	0.55
3:C:360:ALA:H	3:C:361:PRO:HD3	1.71	0.55
3:C:711:ARG:HB3	3:C:730:ARG:HH22	1.72	0.55
4:E:105:LEU:HD11	4:E:136:TRP:CG	2.42	0.55
4:E:201:PHE:CD1	4:E:208:ILE:HD13	2.42	0.55
5:F:35:A:H8	6:G:12:G:C6	2.23	0.55
6:G:1:G:N3	6:G:1:G:C2'	2.70	0.55
13:N:38:GLU:C	13:N:40:LYS:H	2.10	0.55
23:X:275:ARG:O	23:X:279:LEU:HD23	2.07	0.55
24:Y:122:VAL:HB	24:Y:123:HIS:CD2	2.39	0.55
39:2:451:LYS:HB2	39:2:455:ARG:NH1	2.22	0.55
1:A:214:ARG:HH12	1:A:225:TYR:HB2	1.72	0.55
1:A:227:ARG:HH22	1:A:229:GLN:HE21	1.54	0.55
1:A:1502:PHE:HZ	1:A:1505:LYS:HG3	1.72	0.55
3:C:529:ARG:HH22	3:C:540:GLU:HB2	1.71	0.55
5:F:42:C:H2'	5:F:43:A:O4'	2.06	0.55
7:H:36:G:H2'	7:H:37:U:C6	2.42	0.55
19:T:349:SER:OG	19:T:350:HIS:N	2.39	0.55
24:Y:104:HIS:CD2	24:Y:124:THR:HG1	2.24	0.55
35:1:1062:LEU:HA	35:1:1065:LEU:HD12	1.88	0.55
36:3:233:ASN:HD21	36:3:286:ILE:CG2	2.19	0.55
36:3:791:HIS:NE2	36:3:934:GLY:HA3	2.22	0.55
36:3:1041:TYR:HB3	39:2:705:ARG:HG3	1.87	0.55
36:3:1145:GLU:HA	36:3:1148:LEU:HB2	1.87	0.55
3:C:506:PRO:HB2	3:C:569:ARG:NH2	2.22	0.55
3:C:632:THR:H	3:C:636:TYR:HD2	1.55	0.55
13:N:131:ILE:H	13:N:131:ILE:HD12	1.72	0.55
23:X:640:ARG:HG3	23:X:640:ARG:HH11	1.71	0.55
35:1:807:LYS:HG3	35:1:844:VAL:HG12	1.88	0.55
35:1:1130:PRO:HB2	39:2:533:ILE:HG21	1.89	0.55
35:1:1167:TYR:OH	39:2:581:LYS:CE	2.54	0.55
36:3:206:GLN:NE2	36:3:231:HIS:HA	2.21	0.55
36:3:1191:LYS:O	36:3:1195:GLU:HG3	2.06	0.55
42:5:27:THR:HG23	42:5:30:GLU:HG3	1.88	0.55
1:A:348:PRO:HB3	1:A:394:TYR:CZ	2.42	0.55
6:G:85:G:N1	7:H:44:U:N3	2.55	0.55
7:H:107:A:H2'	7:H:108:G:C8	2.42	0.55
7:H:165:A:O2'	7:H:166:G:O5'	2.24	0.55
23:X:537:LYS:HD2	23:X:563:PHE:CZ	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:1008:LEU:HB3	23:X:1016:TYR:HD2	1.71	0.55
35:1:1274:ILE:HG22	36:3:109:LYS:HE2	1.89	0.55
1:A:121:HIS:ND1	1:A:123:THR:HG23	2.21	0.55
1:A:1975:GLU:O	1:A:1979:VAL:HG22	2.07	0.55
6:G:107:U:O2	23:X:709:LEU:HD22	2.05	0.55
11:L:159:LEU:O	12:M:211:ILE:CD1	2.54	0.55
17:R:196:VAL:HG13	17:R:196:VAL:O	2.07	0.55
21:V:606:GLU:OE2	21:V:609:GLN:HG3	2.06	0.55
23:X:412:ILE:HB	23:X:418:LEU:HD22	1.88	0.55
35:1:769:VAL:HA	35:1:772:ILE:HD13	1.89	0.55
36:3:911:LYS:CB	36:3:922:GLY:O	2.55	0.55
36:3:926:TYR:HB3	36:3:928:TYR:CE2	2.41	0.55
42:5:8:HIS:NE2	42:5:12:GLU:OE2	2.37	0.55
1:A:135:VAL:O	1:A:418:THR:OG1	2.22	0.54
1:A:1206:GLU:HG2	1:A:1207:PHE:N	2.20	0.54
9:J:438:TYR:O	9:J:442:ARG:CB	2.55	0.54
11:L:782:LYS:O	11:L:786:HIS:N	2.39	0.54
17:R:408:ASP:OD1	17:R:410:ARG:N	2.28	0.54
19:T:371:HIS:CE1	19:T:396:LYS:HG3	2.42	0.54
23:X:515:SER:O	23:X:547:LYS:HB2	2.07	0.54
23:X:631:ARG:HG3	23:X:635:LEU:HD23	1.88	0.54
35:1:1297:ARG:NH1	42:5:39:SER:OG	2.40	0.54
36:3:592:LEU:HD11	36:3:619:LEU:HD21	1.88	0.54
1:A:1108:ASP:O	1:A:1112:ARG:HG3	2.06	0.54
3:C:514:TYR:HE2	3:C:522:SER:HB3	1.72	0.54
4:E:188:GLN:NE2	4:E:189:THR:H	2.05	0.54
5:F:38:G:P	5:F:38:G:H8	2.29	0.54
19:T:429:SER:HB3	19:T:439:TRP:HE1	1.72	0.54
35:1:728:LEU:HB3	35:1:765:TYR:OH	2.08	0.54
35:1:1277:GLN:CG	36:3:113:ARG:HD3	2.37	0.54
36:3:189:TYR:CG	42:5:37:ARG:NH2	2.75	0.54
36:3:406:PRO:HG2	36:3:408:LEU:HD11	1.89	0.54
36:3:642:ILE:N	36:3:703:ARG:HE	2.06	0.54
3:C:112:THR:OG1	3:C:116:MET:N	2.41	0.54
4:E:90:ILE:HD12	4:E:105:LEU:HD22	1.90	0.54
5:F:41:A:H2'	5:F:42:C:C6	2.43	0.54
11:L:224:PHE:H	17:R:86:LEU:HD23	1.72	0.54
12:M:204:ASP:OD2	12:M:204:ASP:N	2.40	0.54
23:X:695:CYS:HB3	23:X:722:ARG:HH22	1.73	0.54
36:3:191:GLU:O	36:3:194:ASN:N	2.26	0.54
36:3:567:GLU:OE2	36:3:601:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:GLN:NE2	1:A:41:GLN:O	2.41	0.54
1:A:1519:THR:HG23	1:A:1519:THR:O	2.08	0.54
2:B:8:G:H1	2:B:70:A:H1'	1.71	0.54
3:C:216:THR:HG22	3:C:245:HIS:CE1	2.42	0.54
3:C:713:LYS:HA	3:C:716:GLU:OE2	2.07	0.54
5:F:16:G:H2'	5:F:17:C:C6	2.42	0.54
19:T:371:HIS:NE2	19:T:389:SER:OG	2.37	0.54
36:3:168:TYR:OH	42:5:70:GLU:OE2	2.26	0.54
36:3:226:GLU:OE1	36:3:259:LYS:HD3	2.06	0.54
36:3:526:HIS:CG	36:3:573:GLN:HE21	2.25	0.54
1:A:1642:PRO:HA	1:A:1716:GLY:O	2.08	0.54
1:A:1861:ILE:HG22	1:A:1882:ILE:HG12	1.89	0.54
3:C:297:ASN:N	3:C:297:ASN:OD1	2.37	0.54
3:C:465:MET:HE3	3:C:475:MET:HG3	1.90	0.54
4:E:166:LEU:HD12	4:E:167:VAL:H	1.73	0.54
7:H:7:U:H2'	7:H:8:C:C6	2.42	0.54
21:V:584:LYS:HG3	21:V:585:ILE:N	2.21	0.54
36:3:193:ASP:CA	42:5:79:PRO:HG3	2.37	0.54
39:2:640:GLY:O	40:4:69:TYR:CB	2.56	0.54
40:4:121:SER:HA	40:4:124:GLY:O	2.07	0.54
41:7:57:ARG:NH1	41:7:62:GLY:O	2.39	0.54
1:A:701:ILE:H	1:A:701:ILE:HD12	1.72	0.54
9:J:216:ASP:HB3	9:J:217:GLU:OE1	2.08	0.54
11:L:205:LYS:H	11:L:205:LYS:HD3	1.71	0.54
20:U:71:LEU:O	20:U:75:GLU:N	2.38	0.54
23:X:937:ILE:HD12	23:X:937:ILE:H	1.72	0.54
24:Y:4:LEU:HD11	24:Y:11:ASP:HB3	1.90	0.54
24:Y:104:HIS:NE2	24:Y:124:THR:OG1	2.38	0.54
24:Y:255:ASP:HA	24:Y:258:ILE:HD12	1.89	0.54
35:1:785:LYS:O	35:1:789:LEU:HD12	2.07	0.54
35:1:933:CYS:SG	35:1:970:LEU:HD21	2.48	0.54
36:3:269:CYS:SG	36:3:327:LEU:HD11	2.48	0.54
36:3:717:SER:HB2	36:3:718:ARG:NH1	2.20	0.54
1:A:1130:ASN:OD1	1:A:1139:ARG:HB3	2.07	0.54
1:A:1164:SER:HB3	3:C:59:LEU:HD21	1.90	0.54
2:B:110:C:H2'	2:B:111:A:C8	2.41	0.54
3:C:674:CYS:HB3	3:C:818:SER:HB2	1.90	0.54
5:F:15:A:H2'	5:F:16:G:H8	1.73	0.54
35:1:652:CYS:SG	35:1:689:ILE:HG23	2.48	0.54
35:1:815:PHE:HE1	35:1:853:ILE:HG21	1.72	0.54
35:1:819:TRP:CZ3	35:1:868:VAL:HG12	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:933:CYS:O	35:1:936:VAL:N	2.41	0.54
36:3:312:LYS:HB2	36:3:330:PHE:HD1	1.72	0.54
1:A:122:ILE:HD12	1:A:123:THR:HG22	1.90	0.54
1:A:362:ARG:HH11	21:V:323:LEU:C	2.11	0.54
1:A:1427:ARG:HE	23:X:326:GLN:CD	2.09	0.54
4:E:202:ASN:ND2	4:E:207:GLN:OE1	2.41	0.54
9:J:568:LYS:HA	9:J:601:GLY:HA3	1.89	0.54
12:M:178:GLU:HA	12:M:181:ARG:HD3	1.90	0.54
15:P:208:LYS:O	15:P:208:LYS:NZ	2.29	0.54
21:V:609:GLN:NE2	21:V:616:LEU:HD21	2.23	0.54
23:X:648:TYR:O	23:X:656:GLN:NE2	2.40	0.54
23:X:837:SER:HB2	23:X:930:SER:O	2.08	0.54
35:1:1103:VAL:O	35:1:1109:ARG:HD3	2.07	0.54
36:3:18:ILE:HG21	36:3:67:ALA:H	1.72	0.54
1:A:1681:ARG:NH1	1:A:1681:ARG:HB3	2.23	0.54
1:A:1979:VAL:HA	1:A:1982:GLN:HB2	1.88	0.54
3:C:119:LEU:O	3:C:123:MET:HG3	2.08	0.54
3:C:699:ASP:OD1	3:C:722:TYR:OH	2.24	0.54
4:E:62:LEU:O	4:E:350:ARG:HB2	2.07	0.54
6:G:19:G:N2	14:O:194:ALA:C	2.59	0.54
21:V:589:GLU:O	21:V:593:TYR:HB2	2.07	0.54
23:X:635:LEU:HB2	23:X:639:ILE:HD11	1.89	0.54
23:X:793:LEU:HA	23:X:796:LEU:HD12	1.90	0.54
35:1:614:ARG:O	35:1:614:ARG:NH1	2.34	0.54
35:1:849:ILE:O	35:1:853:ILE:HG12	2.08	0.54
39:2:495:ARG:O	39:2:497:SER:N	2.41	0.54
3:C:126:SER:O	3:C:126:SER:OG	2.22	0.54
3:C:129:ILE:HG22	3:C:199:LEU:HB3	1.90	0.54
3:C:928:HIS:ND1	3:C:928:HIS:N	2.55	0.54
6:G:88:G:O6	7:H:40:C:N4	2.41	0.54
19:T:346:ILE:HD13	19:T:380:LEU:HD21	1.89	0.54
23:X:639:ILE:HG22	23:X:640:ARG:H	1.73	0.54
35:1:896:ILE:HD12	35:1:917:VAL:HG11	1.90	0.54
35:1:1206:ASP:OD1	35:1:1207:SER:N	2.41	0.54
35:1:1257:PRO:HD3	39:2:482:ALA:CB	2.27	0.54
36:3:234:PHE:CE1	36:3:236:ILE:HG12	2.42	0.54
36:3:943:THR:HG23	36:3:976:LYS:HB3	1.89	0.54
1:A:57:GLN:HE21	1:A:57:GLN:CA	2.20	0.53
1:A:395:THR:HG22	1:A:396:ASP:H	1.73	0.53
3:C:216:THR:HG22	3:C:245:HIS:HE1	1.73	0.53
3:C:349:PHE:HB2	3:C:356:PHE:CD1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:151:C:H2'	7:H:152:G:C8	2.43	0.53
23:X:696:LYS:HB3	23:X:709:LEU:HD11	1.90	0.53
35:1:806:ILE:HG23	35:1:810:ILE:HB	1.91	0.53
35:1:1092:ASP:O	35:1:1096:THR:HG23	2.08	0.53
35:1:1274:ILE:HG22	36:3:109:LYS:HE3	1.90	0.53
36:3:289:CYS:SG	36:3:338:ALA:HA	2.48	0.53
36:3:747:SER:OG	36:3:748:GLU:N	2.40	0.53
3:C:220:ARG:NH1	3:C:578:ARG:O	2.38	0.53
3:C:818:SER:O	3:C:822:MET:HB2	2.09	0.53
4:E:260:ARG:CD	4:E:276:ILE:HG12	2.39	0.53
12:M:224:ARG:CB	12:M:224:ARG:NH1	2.72	0.53
23:X:527:LEU:HD23	23:X:755:ILE:HD13	1.90	0.53
35:1:693:GLY:HA2	35:1:696:ASP:HB2	1.90	0.53
35:1:778:GLN:N	35:1:778:GLN:OE1	2.41	0.53
36:3:164:ASN:HA	36:3:189:TYR:CZ	2.43	0.53
36:3:994:GLN:HE22	36:3:1036:ALA:C	2.10	0.53
1:A:263:PHE:CE1	1:A:273:ILE:HD11	2.43	0.53
1:A:1189:MET:HG2	1:A:1190:CYS:H	1.72	0.53
1:A:1910:THR:OG1	1:A:1911:GLU:OE1	2.26	0.53
3:C:187:THR:HA	3:C:200:PHE:O	2.08	0.53
7:H:118:G:H2'	7:H:119:G:C8	2.44	0.53
9:J:443:ILE:HG13	9:J:444:SER:H	1.72	0.53
17:R:328:ALA:HB1	24:Y:226:MET:O	2.07	0.53
19:T:351:ASP:O	19:T:352:THR:OG1	2.25	0.53
21:V:628:ILE:HD11	21:V:643:LEU:HB2	1.90	0.53
23:X:164:TRP:CZ3	23:X:168:GLU:OE2	2.62	0.53
23:X:455:ARG:NE	23:X:481:ILE:HD13	2.23	0.53
24:Y:118:TYR:N	24:Y:118:TYR:CD1	2.77	0.53
35:1:731:LEU:O	35:1:735:ILE:HG12	2.08	0.53
35:1:883:ASP:OD2	35:1:883:ASP:N	2.35	0.53
36:3:803:ASP:OD1	36:3:804:HIS:N	2.41	0.53
1:A:214:ARG:NH1	1:A:225:TYR:HB2	2.24	0.53
1:A:836:THR:O	1:A:840:ILE:HG12	2.07	0.53
2:B:108:G:H3'	2:B:109:G:H8	1.73	0.53
3:C:825:PRO:O	3:C:826:ARG:HG2	2.08	0.53
11:L:184:ALA:O	11:L:188:ARG:N	2.31	0.53
17:R:386:ARG:NH1	17:R:391:VAL:HG21	2.24	0.53
19:T:250:ARG:HD2	19:T:266:GLU:HG3	1.90	0.53
23:X:700:TYR:HE2	23:X:705:GLY:HA2	1.73	0.53
23:X:842:THR:HB	23:X:882:LEU:HD23	1.91	0.53
24:Y:21:ARG:HH12	24:Y:83:VAL:N	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:815:PHE:HA	35:1:819:TRP:CD1	2.43	0.53
35:1:843:LYS:C	35:1:843:LYS:HD3	2.29	0.53
36:3:623:ASP:OD2	36:3:626:GLN:NE2	2.41	0.53
41:7:46:CYS:N	41:7:85:CYS:HB2	2.22	0.53
1:A:1817:LEU:CD2	1:A:1919:LEU:HD21	2.39	0.53
1:A:1920:TYR:HE1	1:A:1936:LEU:HD22	1.72	0.53
3:C:725:ASP:HB3	3:C:728:ALA:H	1.74	0.53
6:G:12:G:H3'	6:G:13:C:C6	2.44	0.53
7:H:36:G:H2'	7:H:37:U:H6	1.73	0.53
9:J:397:LYS:O	9:J:400:GLU:HG3	2.09	0.53
23:X:643:LEU:HG	23:X:669:LYS:HA	1.89	0.53
35:1:572:HIS:CE1	35:1:612:THR:HB	2.44	0.53
36:3:34:ARG:HB2	36:3:37:ILE:HB	1.91	0.53
1:A:1352:HIS:CD2	20:U:5:ILE:HG21	2.43	0.53
1:A:1771:LEU:HD21	1:A:1779:PHE:HE2	1.74	0.53
2:B:87:A:H61	2:B:92:U:P	2.32	0.53
3:C:441:PRO:O	3:C:444:GLY:HA3	2.09	0.53
6:G:83:A:P	6:G:83:A:H8	2.31	0.53
11:L:201:LYS:NZ	11:L:203:LYS:HG2	2.23	0.53
12:M:125:SER:O	17:R:242:GLN:NE2	2.42	0.53
17:R:150:ALA:O	17:R:153:LYS:HG3	2.09	0.53
17:R:351:GLU:O	17:R:355:ILE:HG13	2.08	0.53
17:R:413:ASN:O	23:X:633:ARG:HD3	2.09	0.53
19:T:287:HIS:NE2	19:T:305:THR:OG1	2.33	0.53
23:X:640:ARG:HH12	23:X:668:ARG:HB2	1.74	0.53
23:X:787:GLU:HG3	35:1:542:PRO:CD	2.39	0.53
24:Y:306:ILE:HG12	24:Y:311:ILE:HD13	1.89	0.53
36:3:193:ASP:O	42:5:79:PRO:HG2	2.08	0.53
36:3:530:ASP:O	36:3:532:ARG:N	2.40	0.53
1:A:142:SER:HA	1:A:242:ALA:HB2	1.91	0.53
1:A:1831:LYS:NZ	1:A:1832:ARG:HB2	2.24	0.53
2:B:99:C:H2'	2:B:100:C:C6	2.43	0.53
3:C:279:ARG:NH1	21:V:324:HIS:O	2.41	0.53
4:E:240:GLY:O	4:E:252:SER:HA	2.09	0.53
11:L:159:LEU:O	12:M:211:ILE:HD13	2.08	0.53
12:M:215:ASN:HD21	17:R:260:TYR:C	2.11	0.53
13:N:63:LEU:O	13:N:70:ILE:HG12	2.09	0.53
36:3:442:LEU:HD13	36:3:770:LEU:HD23	1.91	0.53
36:3:607:VAL:N	36:3:615:ARG:O	2.29	0.53
36:3:632:ALA:O	36:3:633:LEU:HD23	2.09	0.53
1:A:41:GLN:HE22	1:A:45:TYR:HB2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:HIS:NE2	6:G:16:G:O6	2.42	0.53
1:A:1143:MET:SD	1:A:1143:MET:N	2.81	0.53
3:C:439:PRO:O	3:C:443:VAL:HB	2.09	0.53
3:C:460:ASP:OD2	3:C:461:LEU:N	2.41	0.53
3:C:481:MET:SD	3:C:612:LYS:HG3	2.48	0.53
3:C:938:ARG:HG2	3:C:942:GLY:HA3	1.91	0.53
10:K:209:GLY:HA2	10:K:223:ARG:HD3	1.90	0.53
36:3:940:LEU:HB3	36:3:941:HIS:CE1	2.43	0.53
1:A:225:TYR:O	1:A:418:THR:HG21	2.09	0.53
1:A:325:HIS:HD2	1:A:326:HIS:CD2	2.16	0.53
3:C:514:TYR:CE2	3:C:522:SER:HB3	2.44	0.53
4:E:208:ILE:HG23	4:E:220:TRP:HD1	1.74	0.53
4:E:311:VAL:HB	4:E:321:TYR:HB2	1.90	0.53
6:G:1:G:C2	6:G:2:U:H1'	2.43	0.53
19:T:203:HIS:CE1	19:T:229:LYS:HG3	2.44	0.53
23:X:725:ARG:HD3	23:X:728:ARG:NH1	2.23	0.53
23:X:787:GLU:CB	35:1:542:PRO:CG	2.72	0.53
35:1:557:ASP:HB2	35:1:596:ILE:HG22	0.70	0.53
35:1:1006:MET:HB3	35:1:1013:ILE:HG12	1.90	0.53
42:5:63:ARG:O	42:5:67:ASN:ND2	2.42	0.53
23:X:741:TRP:CH2	35:1:782:GLU:OE2	2.61	0.53
35:1:557:ASP:CA	35:1:596:ILE:HG22	2.36	0.53
35:1:1274:ILE:O	36:3:113:ARG:NH1	2.26	0.53
36:3:229:GLU:HB2	36:3:230:GLU:OE1	2.09	0.53
36:3:883:GLU:HB3	36:3:886:GLU:HG3	1.89	0.53
36:3:939:PHE:CZ	36:3:942:LYS:HG2	2.44	0.53
39:2:460:PHE:HB3	39:2:464:GLU:HG2	1.91	0.53
1:A:65:HIS:O	1:A:69:ILE:HG13	2.10	0.52
1:A:1737:ASN:OD1	1:A:1739:ALA:N	2.39	0.52
4:E:258:THR:HG23	4:E:278:GLN:HE22	1.73	0.52
4:E:283:ASN:N	4:E:283:ASN:OD1	2.41	0.52
6:G:8:C:H2'	6:G:9:C:C2	2.45	0.52
19:T:468:CYS:HB3	19:T:479:THR:HG22	1.89	0.52
23:X:167:THR:O	23:X:171:ARG:HG3	2.08	0.52
23:X:390:GLU:O	23:X:393:GLN:HG3	2.09	0.52
35:1:515:ALA:O	35:1:519:ILE:HG22	2.09	0.52
35:1:1058:ILE:O	35:1:1062:LEU:HG	2.08	0.52
36:3:769:LYS:HD3	36:3:769:LYS:N	2.24	0.52
1:A:1381:ASP:OD1	1:A:1414:ARG:HG2	2.09	0.52
3:C:750:LEU:HA	3:C:753:GLU:HB2	1.91	0.52
6:G:85:G:H2'	6:G:86:A:N9	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:375:ASP:OD1	9:J:376:VAL:N	2.42	0.52
21:V:490:CYS:SG	21:V:521:TYR:HB3	2.49	0.52
23:X:936:TYR:HA	23:X:939:VAL:HG22	1.91	0.52
24:Y:6:GLU:HG3	24:Y:158:HIS:HB3	1.91	0.52
35:1:1260:LYS:O	35:1:1264:VAL:HG22	2.09	0.52
41:7:21:ARG:NH1	41:7:66:VAL:O	2.27	0.52
1:A:233:PRO:O	1:A:237:THR:HG23	2.10	0.52
1:A:885:LEU:HD23	1:A:1005:ILE:HG12	1.91	0.52
1:A:1844:GLU:O	1:A:1848:LEU:HD23	2.10	0.52
4:E:100:ASP:N	4:E:100:ASP:OD1	2.42	0.52
6:G:102:G:N3	6:G:102:G:C2'	2.71	0.52
9:J:443:ILE:HG23	9:J:444:SER:O	2.10	0.52
17:R:325:ARG:NH1	17:R:328:ALA:HB3	2.24	0.52
35:1:740:GLY:H	35:1:743:LEU:HD22	1.74	0.52
35:1:1127:THR:HA	39:2:571:LEU:HD13	1.92	0.52
1:A:1819:LEU:HD21	1:A:1906:ILE:HD11	1.91	0.52
2:B:64:G:H2'	2:B:65:G:H8	1.74	0.52
3:C:559:ILE:HD12	3:C:560:VAL:O	2.09	0.52
8:I:433:ALA:HB1	8:I:482:LYS:CB	2.38	0.52
14:O:249:ARG:O	14:O:252:PHE:N	2.43	0.52
23:X:162:ASP:HB2	23:X:542:PHE:CZ	2.33	0.52
36:3:1025:ALA:HA	36:3:1087:GLN:O	2.09	0.52
1:A:845:ARG:HH11	1:A:1440:THR:HG22	1.74	0.52
1:A:1283:GLU:OE1	1:A:1283:GLU:N	2.42	0.52
4:E:145:LYS:NZ	4:E:184:LYS:HG3	2.24	0.52
12:M:224:ARG:NH1	12:M:224:ARG:HB2	2.25	0.52
35:1:1080:THR:HA	35:1:1083:TYR:HD2	1.74	0.52
36:3:477:SER:CB	36:3:505:THR:H	2.11	0.52
41:7:39:PRO:HB2	41:7:70:TYR:CD1	2.44	0.52
1:A:832:TYR:OH	1:A:929:GLU:OE2	2.25	0.52
1:A:1894:GLN:HE21	1:A:1944:HIS:CE1	2.26	0.52
4:E:108:HIS:NE2	4:E:128:SER:HB2	2.24	0.52
4:E:281:VAL:HG21	4:E:306:ASP:HB2	1.91	0.52
6:G:85:G:O6	7:H:44:U:O4	2.28	0.52
7:H:172:C:N4	7:H:173:C:H41	2.07	0.52
23:X:164:TRP:HB2	23:X:538:ASP:CB	2.39	0.52
23:X:276:VAL:CG2	24:Y:227:VAL:HA	2.40	0.52
35:1:560:LEU:HD11	35:1:600:LEU:HD13	1.92	0.52
35:1:1274:ILE:CG2	36:3:109:LYS:HE2	2.40	0.52
36:3:120:PHE:HB2	36:3:133:SER:OG	2.09	0.52
36:3:206:GLN:NE2	36:3:232:GLY:H	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1972:THR:O	1:A:1976:TRP:HB2	2.09	0.52
2:B:95:G:N3	2:B:95:G:C2'	2.73	0.52
3:C:497:LEU:O	3:C:546:ALA:HB1	2.10	0.52
4:E:135:VAL:CG1	4:E:145:LYS:HB2	2.40	0.52
35:1:547:GLN:HA	35:1:550:HIS:HB3	1.92	0.52
35:1:1007:HIS:CD2	35:1:1008:LYS:HG3	2.45	0.52
36:3:147:ASP:OD1	36:3:150:ALA:N	2.43	0.52
36:3:233:ASN:HD21	36:3:286:ILE:HG22	1.75	0.52
36:3:819:MET:HA	36:3:822:GLU:OE1	2.10	0.52
1:A:75:ASP:O	1:A:77:THR:HG22	2.10	0.52
1:A:1650:ASP:OD1	1:A:1718:TRP:HB2	2.10	0.52
23:X:223:VAL:HA	23:X:226:LEU:HG	1.92	0.52
36:3:642:ILE:HB	36:3:703:ARG:HH21	1.73	0.52
36:3:777:VAL:HG22	36:3:779:PHE:CE1	2.43	0.52
1:A:872:ASP:O	1:A:874:PRO:HD3	2.10	0.52
1:A:1786:TYR:CD1	1:A:1833:LEU:HB2	2.45	0.52
3:C:750:LEU:CD2	20:U:63:LYS:O	2.56	0.52
7:H:103:U:H4'	7:H:104:U:H5'	1.92	0.52
17:R:91:ASP:OD1	17:R:95:LYS:N	2.27	0.52
35:1:545:GLU:HG2	35:1:548:GLU:HG3	1.91	0.52
35:1:1167:TYR:OH	39:2:581:LYS:CD	2.57	0.52
35:1:1291:ASP:OD1	35:1:1292:LYS:N	2.43	0.52
35:1:1297:ARG:HG2	42:5:36:HIS:NE2	2.25	0.52
36:3:390:ARG:HD3	36:3:393:LYS:HE3	1.91	0.52
36:3:519:VAL:HB	36:3:524:ILE:HG23	1.91	0.52
39:2:531:THR:O	39:2:531:THR:OG1	2.25	0.52
1:A:1785:VAL:O	1:A:1805:GLY:HA3	2.10	0.52
3:C:320:LEU:HD13	3:C:343:LEU:HB2	1.92	0.52
3:C:333:ASP:OD1	3:C:333:ASP:N	2.43	0.52
4:E:145:LYS:HE2	4:E:184:LYS:HE2	1.92	0.52
4:E:208:ILE:O	4:E:219:VAL:HA	2.10	0.52
11:L:63:TRP:HB3	11:L:68:GLU:HG3	1.91	0.52
23:X:287:GLY:O	23:X:291:LYS:HG2	2.10	0.52
23:X:432:ILE:HB	23:X:433:PRO:HD3	1.91	0.52
24:Y:27:ASN:HD21	24:Y:65:SER:HA	1.75	0.52
36:3:317:THR:HB	36:3:322:VAL:HA	1.92	0.52
36:3:413:ALA:HB1	36:3:415:LEU:HD13	1.92	0.52
1:A:1973:ASP:OD1	1:A:1973:ASP:N	2.42	0.51
3:C:131:ASN:OD1	3:C:201:ASN:ND2	2.43	0.51
3:C:209:VAL:HG23	3:C:898:LEU:HD13	1.92	0.51
5:F:41:A:C2	6:G:7:G:N1	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:116:C:H2'	6:G:117:A:H5'	1.91	0.51
15:P:213:ASP:OD2	15:P:216:ARG:HB2	2.10	0.51
17:R:319:LYS:O	17:R:322:GLU:HG3	2.10	0.51
21:V:511:ALA:HB1	21:V:525:PHE:CZ	2.43	0.51
23:X:401:VAL:HG12	23:X:572:ILE:HD12	1.91	0.51
23:X:700:TYR:HB3	23:X:757:ARG:O	2.09	0.51
35:1:1289:ASN:HB3	35:1:1295:TYR:H	1.75	0.51
36:3:515:ALA:HB2	36:3:528:ARG:CZ	2.40	0.51
36:3:872:ILE:HD12	36:3:872:ILE:H	1.75	0.51
39:2:451:LYS:O	39:2:455:ARG:HD2	2.11	0.51
1:A:1427:ARG:HB3	23:X:329:TRP:CE3	2.45	0.51
1:A:1718:TRP:CZ3	1:A:1726:ILE:HD11	2.45	0.51
2:B:69:A:H3'	2:B:70:A:C8	2.45	0.51
17:R:243:GLN:O	17:R:246:LYS:HG2	2.09	0.51
23:X:683:ILE:HD13	23:X:686:ILE:HG13	1.91	0.51
35:1:886:HIS:HD2	35:1:887:LYS:HD3	1.74	0.51
36:3:91:GLU:HG2	36:3:92:TYR:N	2.25	0.51
36:3:266:ASP:OD1	36:3:266:ASP:N	2.40	0.51
36:3:424:TYR:CD1	36:3:437:VAL:HG22	2.46	0.51
3:C:713:LYS:HA	3:C:716:GLU:CD	2.30	0.51
23:X:424:THR:HG21	23:X:728:ARG:NH2	2.25	0.51
23:X:441:TYR:OH	23:X:547:LYS:NZ	2.39	0.51
23:X:586:ALA:HB1	35:1:826:ASP:HA	1.92	0.51
23:X:877:ASP:O	23:X:881:LEU:HG	2.10	0.51
35:1:648:LEU:HA	35:1:651:VAL:HG22	1.92	0.51
35:1:972:GLY:O	35:1:976:VAL:HG12	2.10	0.51
36:3:991:SER:O	36:3:991:SER:OG	2.28	0.51
1:A:59:GLU:HB3	13:N:103:LEU:HD21	1.92	0.51
3:C:112:THR:OG1	3:C:112:THR:O	2.25	0.51
3:C:213:ASP:OD2	3:C:213:ASP:N	2.42	0.51
3:C:750:LEU:HD13	20:U:67:GLU:HA	1.92	0.51
5:F:40:U:H2'	5:F:41:A:C8	2.45	0.51
6:G:116:C:C5	17:R:370:SER:HB2	2.45	0.51
19:T:381:HIS:HD2	19:T:441:TRP:CE2	2.29	0.51
23:X:289:GLN:HG2	23:X:293:GLU:OE1	2.11	0.51
23:X:882:LEU:O	23:X:886:THR:OG1	2.20	0.51
24:Y:213:ALA:HA	24:Y:216:GLU:HG3	1.92	0.51
36:3:356:HIS:CD2	36:3:403:SER:HG	2.28	0.51
36:3:1168:PHE:N	36:3:1168:PHE:CD2	2.77	0.51
39:2:646:PRO:C	39:2:648:LEU:N	2.59	0.51
1:A:357:ASN:ND2	3:C:862:PRO:HB3	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:VAL:HA	3:C:331:PHE:HD2	1.75	0.51
15:P:74:LYS:O	15:P:77:ASP:HB3	2.11	0.51
17:R:148:ARG:O	17:R:152:GLU:HG3	2.11	0.51
17:R:367:ARG:HH11	17:R:371:ARG:NH1	2.09	0.51
23:X:412:ILE:HD13	23:X:418:LEU:HB2	1.91	0.51
24:Y:95:SER:OG	24:Y:125:VAL:HA	2.11	0.51
35:1:661:ARG:HG2	35:1:692:HIS:NE2	2.25	0.51
35:1:1122:THR:OG1	35:1:1123:CYS:N	2.41	0.51
35:1:1179:ASP:HB2	39:2:511:LEU:CD1	2.40	0.51
35:1:1179:ASP:HB2	39:2:511:LEU:HD12	1.93	0.51
36:3:187:MET:HE1	42:5:73:LEU:HD22	1.92	0.51
36:3:605:LEU:O	36:3:617:ILE:N	2.42	0.51
36:3:695:GLY:HA3	36:3:717:SER:OG	2.10	0.51
41:7:58:CYS:HB3	41:7:62:GLY:N	2.25	0.51
1:A:71:ARG:NH1	1:A:177:ASP:OD1	2.43	0.51
1:A:1502:PHE:CZ	1:A:1505:LYS:HG3	2.46	0.51
1:A:1516:LYS:O	1:A:1517:LYS:HD2	2.10	0.51
7:H:181:G:H2'	7:H:182:U:C6	2.46	0.51
10:K:223:ARG:HH21	35:1:1018:PRO:CB	2.22	0.51
12:M:165:ASN:HB2	17:R:95:LYS:CB	2.38	0.51
17:R:321:GLU:HB2	23:X:283:TYR:CD2	2.46	0.51
19:T:272:CYS:HB3	19:T:282:ARG:HB3	1.92	0.51
24:Y:244:VAL:HG13	24:Y:312:HIS:O	2.11	0.51
35:1:712:LEU:O	35:1:716:ALA:CB	2.58	0.51
36:3:43:PRO:HB3	36:3:50:VAL:HG22	1.93	0.51
36:3:614:VAL:HG23	36:3:633:LEU:HD11	1.93	0.51
36:3:628:LEU:HD21	36:3:681:PRO:HA	1.92	0.51
39:2:534:GLN:O	39:2:538:GLU:HG3	2.11	0.51
1:A:1121:ASN:HB2	1:A:1123:GLU:OE2	2.11	0.51
20:U:1:MET:O	20:U:3:ASN:N	2.44	0.51
24:Y:215:LYS:O	24:Y:218:LYS:N	2.44	0.51
36:3:1:MET:CG	39:2:709:GLY:O	2.59	0.51
36:3:379:LEU:HD12	36:3:380:GLU:H	1.76	0.51
36:3:451:GLU:HA	36:3:761:THR:HG22	1.92	0.51
36:3:663:LEU:HD23	36:3:679:LEU:HB3	1.92	0.51
1:A:26:SER:HB3	1:A:29:LYS:HB2	1.93	0.51
1:A:93:LYS:O	1:A:649:GLU:HG2	2.10	0.51
1:A:661:GLU:HB3	17:R:214:ILE:HG12	1.93	0.51
1:A:693:ILE:O	1:A:695:ASP:N	2.43	0.51
1:A:1554:GLN:HG3	1:A:1561:PHE:CE1	2.46	0.51
1:A:1935:ARG:O	1:A:1938:LEU:HG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:72:CYS:SG	4:E:81:LEU:HD11	2.51	0.51
4:E:84:ALA:HB2	4:E:90:ILE:HG12	1.93	0.51
5:F:40:U:H3	6:G:7:G:H1	1.59	0.51
6:G:95:U:OP2	35:1:1106:ARG:HD2	2.10	0.51
13:N:54:HIS:CE1	13:N:92:TRP:HZ2	2.28	0.51
19:T:274:ASP:HB2	19:T:281:ILE:HD13	1.92	0.51
23:X:418:LEU:HD12	23:X:568:PRO:HG2	1.92	0.51
35:1:663:THR:HA	35:1:666:LYS:HE3	1.93	0.51
35:1:687:VAL:O	35:1:690:ILE:HG13	2.11	0.51
35:1:848:GLU:OE2	35:1:848:GLU:HA	2.10	0.51
35:1:906:GLU:N	35:1:906:GLU:OE1	2.44	0.51
36:3:606:ALA:HA	36:3:616:ILE:HA	1.92	0.51
36:3:644:GLU:HG2	36:3:645:MET:N	2.25	0.51
39:2:453:LYS:HB3	39:2:456:ARG:HH21	1.74	0.51
1:A:1375:TRP:O	1:A:1378:GLU:N	2.44	0.51
3:C:782:GLU:OE2	3:C:941:LYS:NZ	2.44	0.51
7:H:133:U:H2'	7:H:134:C:C6	2.46	0.51
7:H:173:C:H2'	7:H:174:A:H8	1.76	0.51
9:J:200:GLU:C	9:J:202:GLU:H	2.13	0.51
11:L:166:LYS:HA	11:L:166:LYS:HE3	1.93	0.51
23:X:330:GLU:O	23:X:334:LEU:HD12	2.11	0.51
23:X:451:THR:HA	23:X:496:MET:O	2.10	0.51
36:3:146:ARG:HB3	36:3:150:ALA:HA	1.93	0.51
36:3:233:ASN:ND2	36:3:233:ASN:N	2.59	0.51
36:3:288:VAL:HG12	42:5:62:ALA:HB3	1.93	0.51
36:3:458:ALA:HB1	36:3:460:TRP:HZ3	1.76	0.51
36:3:720:TRP:CE3	36:3:731:LEU:HG	2.45	0.51
36:3:819:MET:HA	36:3:822:GLU:CD	2.31	0.51
1:A:422:LEU:HD22	1:A:638:LEU:HD13	1.93	0.51
1:A:1590:VAL:HG21	1:A:1628:ASP:OD1	2.11	0.51
5:F:45:A:C6	6:G:3:A:C5	2.99	0.51
7:H:165:A:O2'	7:H:166:G:O4'	2.29	0.51
8:I:393:LYS:N	8:I:394:PRO:HD3	2.26	0.51
12:M:159:GLU:OE2	12:M:167:LEU:HB3	2.11	0.51
13:N:104:ARG:HD3	13:N:136:HIS:HB3	1.92	0.51
17:R:189:ASN:HA	17:R:195:ARG:NH2	2.25	0.51
23:X:257:PHE:CE1	23:X:270:LEU:HB2	2.47	0.51
23:X:483:PHE:HE1	23:X:917:GLN:HB2	1.76	0.51
36:3:168:TYR:CE1	42:5:70:GLU:OE2	2.64	0.51
36:3:169:HIS:HD2	36:3:170:VAL:N	2.09	0.51
36:3:700:LYS:O	36:3:714:ALA:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:3:932:ASN:O	36:3:933:ASN:ND2	2.44	0.51
36:3:1131:PRO:HD3	39:2:708:TRP:CH2	2.46	0.51
1:A:362:ARG:HG2	21:V:333:GLN:HA	1.93	0.50
1:A:1599:GLN:HB2	1:A:1600:GLU:OE1	2.10	0.50
11:L:192:ARG:NH1	11:L:198:ILE:HB	2.26	0.50
21:V:550:MET:O	21:V:554:LEU:HG	2.11	0.50
23:X:171:ARG:NH2	23:X:509:PRO:HD3	2.21	0.50
23:X:596:VAL:O	23:X:600:LEU:HG	2.12	0.50
23:X:721:GLN:O	23:X:725:ARG:N	2.43	0.50
23:X:880:VAL:O	23:X:884:VAL:HG23	2.11	0.50
35:1:731:LEU:HD23	35:1:746:PHE:CD1	2.46	0.50
36:3:185:LEU:HD13	36:3:206:GLN:OE1	2.11	0.50
36:3:550:ASN:HD22	36:3:553:GLN:HB2	1.75	0.50
36:3:776:GLN:HG2	36:3:777:VAL:N	2.26	0.50
1:A:1770:GLU:O	1:A:1773:SER:OG	2.29	0.50
3:C:343:LEU:HA	3:C:368:SER:OG	2.11	0.50
3:C:534:VAL:CG2	3:C:537:TYR:HB2	2.38	0.50
4:E:152:SER:OG	4:E:153:PHE:N	2.43	0.50
4:E:308:PHE:HE1	4:E:324:PRO:HB3	1.76	0.50
6:G:85:G:H2'	6:G:86:A:C4	2.46	0.50
11:L:26:TYR:OH	11:L:158:ARG:NH1	2.36	0.50
21:V:536:ILE:HG21	21:V:579:SER:OG	2.11	0.50
23:X:430:THR:HG22	23:X:434:GLN:HE21	1.77	0.50
23:X:697:GLN:NE2	23:X:751:THR:OG1	2.42	0.50
23:X:810:THR:O	23:X:814:LYS:HG3	2.11	0.50
35:1:1134:ASN:ND2	39:2:534:GLN:HG3	2.26	0.50
36:3:259:LYS:HE2	36:3:266:ASP:HB3	1.94	0.50
36:3:677:THR:HA	36:3:685:ASP:O	2.12	0.50
1:A:467:GLN:HG3	2:B:19:A:N7	2.26	0.50
1:A:1845:VAL:O	1:A:1849:ILE:HG12	2.11	0.50
5:F:30:A:H61	6:G:16:G:H1'	1.76	0.50
8:I:386:ASP:O	8:I:388:PHE:N	2.44	0.50
9:J:429:PHE:O	9:J:432:VAL:HG22	2.11	0.50
13:N:139:CYS:SG	13:N:140:ARG:N	2.84	0.50
19:T:309:ASP:OD1	19:T:309:ASP:N	2.43	0.50
23:X:944:THR:HG23	23:X:1003:ILE:HD11	1.93	0.50
35:1:830:TYR:O	35:1:834:VAL:HG23	2.11	0.50
35:1:908:SER:OG	35:1:912:ASN:OD1	2.28	0.50
36:3:929:LYS:HG3	36:3:931:VAL:HG22	1.93	0.50
36:3:940:LEU:HB3	36:3:941:HIS:ND1	2.26	0.50
1:A:916:LYS:HD2	1:A:1035:GLN:NE2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1712:HIS:ND1	1:A:1734:MET:HG3	2.26	0.50
1:A:1866:LYS:HG3	1:A:1886:GLY:HA3	1.94	0.50
2:B:98:G:H2'	2:B:99:C:C6	2.47	0.50
3:C:300:LEU:HD23	3:C:306:ASN:HB3	1.92	0.50
3:C:687:MET:HE2	3:C:791:ILE:HG12	1.93	0.50
4:E:243:LEU:HA	4:E:250:LEU:HA	1.93	0.50
7:H:41:U:H2'	7:H:42:G:H8	1.75	0.50
7:H:152:G:H2'	7:H:153:A:C8	2.47	0.50
12:M:218:PHE:CD1	12:M:218:PHE:C	2.85	0.50
23:X:230:SER:O	23:X:234:TYR:HB2	2.11	0.50
23:X:601:GLN:HA	23:X:604:VAL:HG12	1.93	0.50
23:X:856:ARG:NH2	23:X:865:ASP:OD1	2.44	0.50
24:Y:217:ALA:O	24:Y:220:GLN:HG3	2.12	0.50
35:1:573:LYS:H	35:1:573:LYS:HD2	1.75	0.50
35:1:862:GLU:HA	35:1:865:ARG:NH1	2.27	0.50
36:3:642:ILE:H	36:3:703:ARG:NE	2.09	0.50
41:7:71:TYR:CD2	41:7:81:ASP:HB2	2.46	0.50
1:A:1397:ILE:HD11	17:R:405:VAL:HA	1.94	0.50
4:E:60:MET:CB	4:E:353:MET:HB3	2.41	0.50
11:L:176:LEU:HD13	11:L:176:LEU:C	2.32	0.50
23:X:741:TRP:CE3	35:1:782:GLU:OE2	2.65	0.50
36:3:275:ARG:HB3	36:3:275:ARG:HH21	1.75	0.50
1:A:79:ARG:HB3	1:A:79:ARG:NH1	2.26	0.50
1:A:216:SER:O	1:A:216:SER:OG	2.27	0.50
1:A:1207:PHE:HB2	1:A:1209:HIS:CD2	2.47	0.50
1:A:1745:GLU:OE1	35:1:980:GLU:CG	2.51	0.50
19:T:231:TRP:CZ3	19:T:238:LEU:HB2	2.46	0.50
23:X:184:ARG:O	23:X:188:ARG:HG3	2.12	0.50
35:1:831:ARG:O	35:1:834:VAL:HB	2.11	0.50
36:3:209:THR:OG1	36:3:210:PHE:N	2.45	0.50
36:3:469:GLU:HG2	36:3:470:PHE:CD1	2.47	0.50
36:3:823:MET:SD	36:3:838:MET:HG3	2.52	0.50
36:3:1031:ARG:HG2	36:3:1031:ARG:NH1	2.27	0.50
36:3:1114:SER:HB2	36:3:1215:TYR:CE1	2.46	0.50
1:A:1785:VAL:O	1:A:1822:ILE:HD11	2.11	0.50
3:C:115:GLU:OE1	3:C:115:GLU:N	2.45	0.50
3:C:406:GLU:OE1	3:C:406:GLU:N	2.39	0.50
3:C:726:LEU:O	3:C:730:ARG:HG2	2.11	0.50
5:F:35:A:H8	6:G:12:G:O6	1.93	0.50
7:H:151:C:H2'	7:H:152:G:H8	1.76	0.50
9:J:222:ASP:OD1	9:J:226:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:235:ARG:NE	17:R:235:ARG:H	2.10	0.50
17:R:246:LYS:NZ	17:R:246:LYS:HB3	2.26	0.50
19:T:422:ASN:OD1	19:T:474:GLU:HB3	2.11	0.50
22:W:459:PRO:CB	39:2:567:ASP:HB3	2.42	0.50
23:X:834:TYR:CZ	23:X:941:LYS:HB3	2.47	0.50
24:Y:274:ASP:HB3	24:Y:277:THR:OG1	2.12	0.50
35:1:819:TRP:HE3	35:1:864:TYR:CZ	2.30	0.50
35:1:1292:LYS:HD3	42:5:78:PRO:HG2	1.93	0.50
36:3:181:MET:HB3	36:3:212:GLU:HA	1.92	0.50
36:3:463:ARG:HD3	36:3:468:ASP:HB3	1.94	0.50
36:3:700:LYS:HB3	36:3:702:PHE:HZ	1.74	0.50
3:C:300:LEU:HA	3:C:306:ASN:ND2	2.27	0.50
3:C:710:ASN:OD1	3:C:712:LYS:HB3	2.12	0.50
11:L:19:LEU:HD23	11:L:54:LEU:HD22	1.92	0.50
11:L:63:TRP:HD1	11:L:67:GLU:HB3	1.77	0.50
11:L:178:GLU:O	11:L:182:LEU:HB2	2.12	0.50
19:T:497:GLU:OE1	19:T:497:GLU:N	2.33	0.50
21:V:217:ALA:HB2	21:V:357:LEU:HA	1.94	0.50
21:V:540:GLU:O	21:V:544:LEU:HB2	2.12	0.50
21:V:553:HIS:CD2	21:V:556:TYR:HE1	2.30	0.50
21:V:571:SER:OG	21:V:573:GLU:OE2	2.29	0.50
23:X:171:ARG:NE	23:X:505:PHE:O	2.43	0.50
23:X:612:LEU:HB2	23:X:686:ILE:HD12	1.93	0.50
23:X:715:SER:O	23:X:718:SER:OG	2.29	0.50
24:Y:37:TYR:O	24:Y:40:CYS:HB2	2.10	0.50
25:Z:18:TYR:CB	25:Z:171:GLN:CB	2.90	0.50
36:3:945:VAL:HG21	36:3:963:VAL:HG21	1.93	0.50
36:3:1207:LYS:O	36:3:1211:ILE:HG12	2.12	0.50
3:C:687:MET:HA	3:C:790:LYS:O	2.12	0.50
6:G:90:C:H42	7:H:40:C:H42	1.60	0.50
8:I:460:THR:CB	8:I:487:TRP:CB	2.90	0.50
19:T:213:GLU:HG2	19:T:214:PRO:N	2.26	0.50
23:X:480:SER:HB3	23:X:500:MET:CE	2.42	0.50
24:Y:298:PHE:HE2	24:Y:314:ASP:HA	1.77	0.50
35:1:1076:ALA:O	35:1:1080:THR:HG23	2.12	0.50
35:1:1287:ILE:HB	42:5:32:LEU:CD1	2.38	0.50
36:3:616:ILE:O	36:3:628:LEU:N	2.45	0.50
1:A:550:VAL:O	1:A:554:THR:HG23	2.12	0.49
2:B:39:C:H4'	2:B:40:U:OP1	2.12	0.49
4:E:66:GLU:N	4:E:87:ASP:OD2	2.45	0.49
8:I:102:ALA:HB1	16:Q:934:TYR:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:471:VAL:HG21	23:X:476:GLU:CD	2.33	0.49
24:Y:183:ARG:HA	24:Y:183:ARG:NE	2.26	0.49
24:Y:305:LEU:HD23	24:Y:305:LEU:H	1.77	0.49
35:1:1010:THR:N	35:1:1011:PRO:CD	2.74	0.49
36:3:713:LEU:HD13	36:3:714:ALA:N	2.27	0.49
36:3:1040:ASP:OD2	36:3:1042:ASP:N	2.45	0.49
1:A:1014:ASN:ND2	11:L:83:ARG:HB2	2.28	0.49
1:A:1418:ARG:HB2	1:A:1462:GLY:HA3	1.94	0.49
1:A:1571:ILE:CG2	10:K:220:LEU:HD13	2.42	0.49
2:B:98:G:H2'	2:B:99:C:H6	1.77	0.49
3:C:536:ARG:O	3:C:536:ARG:HD3	2.12	0.49
4:E:105:LEU:HD21	4:E:136:TRP:CE2	2.48	0.49
4:E:181:ILE:H	4:E:181:ILE:HD12	1.77	0.49
4:E:248:SER:HB2	4:E:263:ASP:OD2	2.12	0.49
9:J:238:ASN:C	9:J:240:THR:H	2.15	0.49
19:T:243:THR:O	19:T:243:THR:OG1	2.23	0.49
35:1:581:LEU:O	35:1:584:ASP:HB3	2.12	0.49
35:1:1003:VAL:HG22	35:1:1004:ILE:N	2.27	0.49
35:1:1126:PHE:HD2	39:2:571:LEU:HB3	1.76	0.49
41:7:15:ALA:HB2	41:7:84:GLY:HA2	1.94	0.49
1:A:525:LYS:HB2	1:A:525:LYS:HZ3	1.76	0.49
1:A:597:LYS:N	2:B:45:C:OP1	2.45	0.49
1:A:800:TYR:HB3	3:C:59:LEU:HD23	1.93	0.49
1:A:1771:LEU:HD21	1:A:1779:PHE:CE2	2.47	0.49
1:A:1785:VAL:HG23	1:A:1786:TYR:CD2	2.47	0.49
2:B:100:C:H2'	2:B:101:U:C6	2.46	0.49
6:G:111:U:H5'	23:X:499:GLY:HA3	1.94	0.49
7:H:33:G:C6	7:H:34:U:C4	3.01	0.49
17:R:263:PRO:HB2	17:R:265:ASP:OD1	2.12	0.49
21:V:503:TYR:CD1	21:V:549:LYS:HD2	2.47	0.49
24:Y:211:ILE:O	24:Y:215:LYS:HG2	2.13	0.49
35:1:702:ARG:HD2	35:1:746:PHE:CE2	2.48	0.49
35:1:1012:PRO:O	35:1:1015:ASP:OD1	2.30	0.49
35:1:1159:GLY:O	35:1:1161:MET:N	2.46	0.49
36:3:234:PHE:C	36:3:235:LEU:HD12	2.33	0.49
36:3:639:SER:OG	36:3:699:VAL:O	2.14	0.49
2:B:13:C:H2'	2:B:14:U:C6	2.48	0.49
3:C:404:THR:O	3:C:408:LEU:HD12	2.12	0.49
3:C:474:LEU:HA	3:C:498:SER:O	2.11	0.49
3:C:832:TYR:CD2	3:C:899:SER:HB2	2.46	0.49
5:F:49:G:N2	7:H:29:A:N7	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:86:U:H5”	12:M:134:GLN:HE22	1.77	0.49
9:J:320:GLU:OE1	9:J:325:ASN:HB3	2.13	0.49
9:J:330:ARG:CZ	9:J:361:ARG:HH12	2.26	0.49
11:L:86:ALA:HB1	11:L:91:ARG:O	2.12	0.49
11:L:169:ARG:CZ	11:L:169:ARG:CB	2.88	0.49
19:T:201:SER:HB3	19:T:485:THR:HG22	1.95	0.49
19:T:297:HIS:HA	19:T:338:CYS:SG	2.53	0.49
23:X:163:GLU:OE2	23:X:778:PHE:HD2	1.89	0.49
23:X:164:TRP:CB	23:X:538:ASP:HB3	2.43	0.49
23:X:856:ARG:HD2	23:X:868:ARG:HH12	1.77	0.49
23:X:1007:TRP:HA	23:X:1010:GLU:HB2	1.94	0.49
24:Y:182:THR:OG1	24:Y:183:ARG:N	2.45	0.49
35:1:517:ARG:HB3	35:1:517:ARG:CZ	2.43	0.49
35:1:933:CYS:SG	35:1:970:LEU:HD11	2.52	0.49
36:3:1187:PRO:O	36:3:1191:LYS:HG3	2.12	0.49
3:C:132:VAL:HG11	3:C:226:VAL:HG23	1.93	0.49
4:E:75:HIS:CE1	4:E:121:GLY:HA3	2.47	0.49
4:E:75:HIS:HB2	4:E:80:THR:H	1.78	0.49
7:H:57:A:OP1	39:2:459:ARG:NH1	2.37	0.49
9:J:185:ALA:HB2	11:L:141:PRO:O	2.13	0.49
11:L:166:LYS:HE3	11:L:166:LYS:CA	2.42	0.49
17:R:89:GLN:OE1	17:R:90:VAL:N	2.39	0.49
17:R:104:GLN:HE21	17:R:225:PRO:HB3	1.77	0.49
21:V:596:LEU:N	21:V:597:PRO:HD2	2.27	0.49
23:X:419:ILE:HD11	23:X:560:PHE:HB3	1.95	0.49
23:X:496:MET:HB2	23:X:500:MET:HB3	1.95	0.49
24:Y:290:LYS:HB3	24:Y:293:ASP:H	1.78	0.49
36:3:388:GLN:NE2	36:3:845:GLU:OE1	2.46	0.49
36:3:1011:TRP:HB2	36:3:1025:ALA:O	2.11	0.49
1:A:162:LYS:HE2	1:A:163:ARG:O	2.13	0.49
1:A:1953:ILE:O	1:A:1956:PRO:HD3	2.13	0.49
2:B:92:U:H3’	2:B:92:U:H6	1.77	0.49
3:C:447:PRO:HA	3:C:450:GLU:OE1	2.13	0.49
3:C:767:VAL:O	3:C:771:GLN:HG3	2.12	0.49
3:C:770:PHE:HE1	3:C:789:PHE:CD1	2.30	0.49
4:E:182:ARG:NE	4:E:182:ARG:HA	2.28	0.49
4:E:337:PRO:HG2	4:E:338:ASP:OD2	2.12	0.49
5:F:80:G:H22	9:J:209:PRO:HD3	1.78	0.49
7:H:54:U:H2’	7:H:55:U:C6	2.48	0.49
9:J:189:ILE:HG22	9:J:189:ILE:O	2.12	0.49
12:M:155:LYS:HD2	12:M:156:HIS:NE2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:460:ASP:OD2	19:T:460:ASP:N	2.45	0.49
23:X:743:TYR:O	23:X:747:LEU:HB2	2.12	0.49
23:X:972:PRO:HA	23:X:977:PHE:CD2	2.47	0.49
35:1:528:ALA:N	35:1:566:LEU:CD2	2.59	0.49
35:1:610:ILE:HG22	35:1:647:PHE:CD1	2.46	0.49
35:1:841:ALA:CA	35:1:849:ILE:HG13	2.39	0.49
35:1:898:TYR:CZ	35:1:902:GLU:HG2	2.47	0.49
36:3:2:PHE:C	36:3:3:LEU:HD23	2.32	0.49
36:3:22:PHE:HA	36:3:76:ASP:HB2	1.95	0.49
36:3:22:PHE:N	36:3:29:GLU:OE1	2.45	0.49
36:3:581:LYS:HB2	36:3:625:LEU:HD22	1.94	0.49
36:3:968:ARG:HG2	36:3:982:GLU:OE1	2.12	0.49
1:A:485:THR:HG22	1:A:486:LYS:N	2.27	0.49
2:B:14:U:H2'	2:B:15:C:C6	2.46	0.49
3:C:480:LYS:HB2	3:C:493:PHE:HB3	1.93	0.49
3:C:514:TYR:OH	3:C:519:GLU:HG2	2.13	0.49
23:X:227:ARG:NE	24:Y:239:GLU:OE2	2.44	0.49
23:X:828:ILE:O	23:X:831:SER:OG	2.29	0.49
24:Y:89:LYS:HB3	24:Y:90:LYS:HD3	1.95	0.49
24:Y:104:HIS:CE1	24:Y:124:THR:HG1	2.29	0.49
24:Y:246:LYS:CE	24:Y:312:HIS:HB2	2.38	0.49
35:1:970:LEU:O	35:1:974:LEU:HG	2.13	0.49
35:1:1273:TYR:OH	42:5:38:ASP:OD2	2.28	0.49
36:3:757:ILE:HG22	36:3:762:LEU:HG	1.94	0.49
1:A:226:GLN:HA	1:A:418:THR:HG22	1.94	0.49
1:A:278:LYS:NZ	6:G:-9:C:O3'	2.46	0.49
1:A:1661:TRP:NE1	1:A:1697:SER:O	2.41	0.49
1:A:1738:PRO:CA	35:1:973:HIS:NE2	2.70	0.49
3:C:114:TYR:N	3:C:115:GLU:OE1	2.46	0.49
9:J:286:GLU:HG3	9:J:298:ILE:HD12	1.94	0.49
19:T:220:VAL:HG13	19:T:252:VAL:HG21	1.95	0.49
19:T:396:LYS:HD3	19:T:405:PHE:HE1	1.78	0.49
21:V:391:PHE:O	21:V:395:GLU:CB	2.61	0.49
23:X:855:TYR:CE2	23:X:857:PRO:HG3	2.46	0.49
24:Y:77:PHE:O	24:Y:103:GLN:NE2	2.46	0.49
36:3:181:MET:HB2	36:3:211:TYR:O	2.13	0.49
36:3:503:THR:HG22	36:3:504:PRO:HD2	1.95	0.49
41:7:52:GLY:N	41:7:55:GLN:HE21	2.10	0.49
1:A:1786:TYR:HD1	1:A:1833:LEU:HB2	1.78	0.49
3:C:538:HIS:CE1	3:C:551:LEU:HD13	2.47	0.49
5:F:31:U:H3'	5:F:32:U:H6	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:16:U:H6	7:H:16:U:OP1	1.96	0.49
12:M:142:ILE:HD12	12:M:143:LYS:H	1.78	0.49
21:V:473:ALA:O	21:V:477:LEU:HG	2.12	0.49
36:3:42:ARG:HB2	36:3:53:LEU:HD11	1.93	0.49
36:3:112:CYS:SG	42:5:46:HIS:CD2	3.06	0.49
36:3:612:ASN:HA	36:3:636:GLN:HA	1.95	0.49
42:5:60:SER:O	42:5:63:ARG:N	2.46	0.49
1:A:983:LYS:HE3	1:A:983:LYS:HB3	1.52	0.49
1:A:1524:SER:HB3	10:K:215:ASP:HB2	1.95	0.49
3:C:302:PRO:HB2	3:C:320:LEU:HG	1.94	0.49
4:E:94:ASN:O	4:E:99:CYS:HA	2.13	0.49
6:G:11:A:H2'	6:G:12:G:O4'	2.12	0.49
9:J:286:GLU:HG3	9:J:298:ILE:CD1	2.43	0.49
9:J:399:TYR:O	9:J:403:VAL:HG23	2.13	0.49
17:R:123:GLU:HB3	17:R:125:MET:CE	2.43	0.49
19:T:424:ASP:OD1	19:T:424:ASP:N	2.46	0.49
23:X:618:GLN:HG2	23:X:648:TYR:CG	2.48	0.49
35:1:796:CYS:HB3	35:1:806:ILE:HG12	1.95	0.49
36:3:249:LEU:HA	36:3:257:THR:O	2.12	0.49
36:3:914:ILE:HD12	36:3:919:SER:HB3	1.95	0.49
41:7:42:LEU:HG	41:7:70:TYR:CE2	2.48	0.49
1:A:156:ARG:NH2	1:A:157:ASP:OD2	2.46	0.48
1:A:1301:ILE:HD11	1:A:1306:LYS:HD3	1.95	0.48
3:C:133:THR:OG1	3:C:222:SER:OG	2.30	0.48
3:C:476:CYS:SG	3:C:496:VAL:HG12	2.53	0.48
3:C:843:VAL:O	3:C:846:VAL:HG13	2.13	0.48
4:E:156:SER:HB2	4:E:199:VAL:HG12	1.95	0.48
7:H:106:G:N3	7:H:107:A:C6	2.81	0.48
9:J:206:LEU:CD2	9:J:207:PRO:CD	2.86	0.48
11:L:48:ALA:O	11:L:52:GLU:HG2	2.12	0.48
23:X:281:ARG:HA	23:X:281:ARG:CZ	2.42	0.48
23:X:447:LYS:HB2	23:X:514:TYR:CD1	2.47	0.48
23:X:533:PHE:CE1	23:X:550:VAL:HG11	2.48	0.48
23:X:888:TRP:O	23:X:891:SER:OG	2.24	0.48
24:Y:241:VAL:HG22	24:Y:287:GLU:HA	1.95	0.48
35:1:522:LYS:HD3	35:1:526:PHE:CE2	2.48	0.48
35:1:610:ILE:CG2	35:1:647:PHE:CE1	2.95	0.48
35:1:632:PHE:O	35:1:635:VAL:HG22	2.13	0.48
35:1:1082:GLY:O	35:1:1085:ALA:HB3	2.13	0.48
36:3:294:LYS:HZ2	36:3:294:LYS:C	2.15	0.48
39:2:594:GLY:O	39:2:597:PHE:CB	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ASP:N	1:A:251:ASP:OD2	2.45	0.48
1:A:1749:LYS:HG3	35:1:980:GLU:CG	2.43	0.48
1:A:1812:PRO:O	1:A:1920:TYR:OH	2.22	0.48
1:A:1866:LYS:HE2	1:A:1886:GLY:H	1.79	0.48
3:C:325:LYS:HG2	3:C:329:ASP:OD2	2.14	0.48
3:C:363:SER:O	3:C:364:SER:OG	2.28	0.48
3:C:471:ASP:H	3:C:499:GLY:HA2	1.78	0.48
3:C:724:TRP:HA	3:C:724:TRP:CE3	2.48	0.48
7:H:64:A:H2'	7:H:65:U:C6	2.48	0.48
12:M:165:ASN:HB2	17:R:95:LYS:HA	1.95	0.48
17:R:256:ASN:ND2	17:R:259:GLY:HA2	2.28	0.48
17:R:408:ASP:OD1	17:R:409:GLN:N	2.46	0.48
19:T:220:VAL:HG23	19:T:230:ILE:HG12	1.95	0.48
23:X:648:TYR:CE2	23:X:651:LEU:HB3	2.48	0.48
23:X:768:LYS:HE3	23:X:802:LEU:HD21	1.94	0.48
35:1:770:MET:HA	35:1:773:LEU:HG	1.95	0.48
35:1:1010:THR:OG1	35:1:1011:PRO:CD	2.48	0.48
35:1:1252:GLN:CD	39:2:492:LYS:HA	2.33	0.48
36:3:407:ILE:HD11	36:3:1124:GLY:CA	2.43	0.48
36:3:594:ASN:OD1	36:3:594:ASN:N	2.46	0.48
36:3:1165:SER:HB2	36:3:1169:PRO:HA	1.94	0.48
42:5:51:ASN:OD1	42:5:51:ASN:N	2.46	0.48
1:A:111:GLU:OE2	1:A:114:ARG:NH2	2.41	0.48
1:A:147:MET:O	1:A:151:MET:HG2	2.13	0.48
1:A:643:GLY:HA3	2:B:28:A:O2'	2.13	0.48
1:A:1738:PRO:HA	35:1:973:HIS:CE1	2.48	0.48
4:E:242:SER:O	4:E:293:TRP:NE1	2.45	0.48
19:T:355:ARG:HH11	19:T:364:THR:HG21	1.78	0.48
23:X:701:ASN:ND2	23:X:703:ARG:HD3	2.28	0.48
35:1:702:ARG:HG2	35:1:746:PHE:HZ	1.78	0.48
36:3:346:PHE:HA	36:3:360:GLN:HA	1.95	0.48
36:3:357:TYR:HE1	36:3:400:GLU:HG3	1.77	0.48
36:3:804:HIS:NE2	36:3:859:ASN:O	2.46	0.48
1:A:82:ARG:NH2	6:G:16:G:H1	2.11	0.48
3:C:764:ASP:OD2	3:C:764:ASP:N	2.46	0.48
3:C:820:PHE:HD1	3:C:821:LEU:HD23	1.77	0.48
5:F:77:C:H2'	5:F:78:A:O4'	2.13	0.48
15:P:26:LEU:HD13	15:P:26:LEU:HA	1.68	0.48
21:V:471:GLU:OE1	21:V:475:LYS:NZ	2.33	0.48
35:1:556:ILE:HG23	35:1:596:ILE:CG2	2.39	0.48
35:1:717:THR:HB	35:1:718:PRO:CD	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:796:CYS:HA	35:1:801:VAL:HG21	1.94	0.48
35:1:1006:MET:HB2	35:1:1049:TYR:CZ	2.49	0.48
35:1:1126:PHE:CB	39:2:575:PHE:CD2	2.96	0.48
36:3:49:LYS:HD3	36:3:49:LYS:HA	1.59	0.48
36:3:238:VAL:HB	36:3:247:GLY:O	2.12	0.48
36:3:745:PHE:CB	36:3:755:VAL:HG23	2.43	0.48
36:3:1095:TYR:CE1	36:3:1164:ARG:HD2	2.48	0.48
1:A:1874:VAL:O	1:A:1877:LEU:HG	2.13	0.48
3:C:719:GLN:NE2	3:C:726:LEU:HA	2.28	0.48
3:C:746:VAL:O	3:C:791:ILE:HG13	2.13	0.48
4:E:255:MET:HB2	4:E:282:HIS:CB	2.43	0.48
14:O:259:ARG:N	14:O:273:GLN:O	2.39	0.48
17:R:358:ASP:O	17:R:362:GLU:HB2	2.13	0.48
17:R:369:LEU:HG	17:R:376:LYS:HG3	1.95	0.48
23:X:818:LEU:HD21	23:X:925:VAL:HG21	1.95	0.48
35:1:495:ARG:HA	35:1:498:MET:HB3	1.95	0.48
35:1:523:ALA:C	35:1:563:LEU:HD11	2.33	0.48
36:3:636:GLN:HG2	36:3:637:PRO:HD2	1.96	0.48
36:3:665:LEU:HD21	36:3:667:ILE:HD11	1.94	0.48
36:3:674:LEU:C	36:3:675:LEU:HD12	2.34	0.48
36:3:706:MET:HG2	36:3:770:LEU:HD12	1.94	0.48
1:A:205:ASP:OD2	1:A:205:ASP:N	2.43	0.48
1:A:1635:TYR:CE1	1:A:1636:LYS:HB2	2.48	0.48
3:C:230:ASP:OD2	3:C:259:LYS:HD2	2.13	0.48
3:C:589:LYS:HD2	3:C:661:THR:HG22	1.96	0.48
4:E:328:GLY:O	4:E:346:SER:OG	2.31	0.48
6:G:95:U:O5’	35:1:1106:ARG:HD2	2.12	0.48
7:H:182:U:H2’	7:H:183:G:C8	2.48	0.48
9:J:230:THR:HA	9:J:233:ASP:OD2	2.14	0.48
13:N:21:THR:O	13:N:24:GLU:HG3	2.13	0.48
17:R:124:VAL:O	17:R:124:VAL:HG12	2.13	0.48
21:V:535:THR:HB	21:V:538:ARG:HG3	1.95	0.48
23:X:190:LYS:HG2	24:Y:310:ARG:HH21	1.79	0.48
23:X:461:VAL:O	23:X:465:VAL:HG23	2.14	0.48
23:X:461:VAL:HA	23:X:464:ARG:HE	1.78	0.48
23:X:527:LEU:HG	23:X:754:GLU:OE1	2.13	0.48
23:X:618:GLN:HG2	23:X:648:TYR:CE2	2.48	0.48
23:X:820:VAL:HG21	23:X:824:LEU:HD22	1.94	0.48
35:1:1140:GLU:HB2	35:1:1143:VAL:CG1	2.44	0.48
36:3:24:GLY:HA2	36:3:74:THR:O	2.14	0.48
39:2:617:LEU:HA	40:4:78:LYS:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:2:705:ARG:N	39:2:705:ARG:HD2	2.28	0.48
1:A:384:VAL:HA	3:C:331:PHE:CD2	2.48	0.48
1:A:835:ASP:HB3	1:A:878:LEU:HD13	1.95	0.48
1:A:1019:TYR:O	1:A:1020:LYS:C	2.52	0.48
1:A:1831:LYS:HG3	1:A:1832:ARG:H	1.75	0.48
2:B:111:A:H2'	2:B:112:A:C8	2.49	0.48
7:H:139:C:H2'	7:H:140:A:H8	1.78	0.48
11:L:19:LEU:HD23	11:L:54:LEU:CD2	2.44	0.48
11:L:163:GLN:HB3	11:L:168:LYS:HZ3	1.69	0.48
24:Y:241:VAL:HA	24:Y:286:ILE:O	2.12	0.48
35:1:815:PHE:O	35:1:819:TRP:HB2	2.13	0.48
36:3:19:HIS:ND1	36:3:19:HIS:O	2.46	0.48
36:3:302:LEU:HA	36:3:311:PHE:O	2.14	0.48
36:3:617:ILE:HG12	36:3:627:PRO:HA	1.95	0.48
41:7:58:CYS:HB3	41:7:62:GLY:H	1.79	0.48
1:A:1303:LEU:HD12	1:A:1311:PHE:HE1	1.78	0.48
4:E:308:PHE:CE1	4:E:324:PRO:HB3	2.49	0.48
11:L:176:LEU:HD12	11:L:180:ARG:HD2	1.95	0.48
11:L:201:LYS:HD2	11:L:202:ARG:N	2.28	0.48
17:R:235:ARG:HB3	17:R:235:ARG:CZ	2.43	0.48
23:X:878:HIS:CE1	23:X:1001:LEU:HB2	2.48	0.48
24:Y:133:MET:HA	24:Y:136:ILE:HB	1.96	0.48
36:3:143:ILE:H	36:3:143:ILE:HD12	1.79	0.48
36:3:436:ARG:HD3	36:3:776:GLN:OE1	2.14	0.48
36:3:740:GLU:HB2	36:3:758:SER:HA	1.95	0.48
36:3:926:TYR:CZ	36:3:942:LYS:HD2	2.48	0.48
40:4:102:ILE:C	40:4:177:ALA:HB2	2.33	0.48
41:7:30:CYS:SG	41:7:33:CYS:HB3	2.53	0.48
1:A:1210:LYS:HD3	1:A:1210:LYS:N	2.29	0.48
3:C:118:PHE:HA	3:C:121:ASP:OD2	2.14	0.48
3:C:918:ILE:HG23	3:C:924:GLN:NE2	2.29	0.48
4:E:105:LEU:HD21	4:E:136:TRP:CZ2	2.49	0.48
5:F:13:G:H8	5:F:13:G:O5'	1.97	0.48
13:N:132:ILE:O	13:N:140:ARG:HG3	2.13	0.48
19:T:493:ASP:OD1	19:T:493:ASP:N	2.34	0.48
23:X:224:PRO:O	23:X:228:LYS:HD2	2.14	0.48
23:X:285:ALA:HA	23:X:288:GLU:OE2	2.13	0.48
36:3:664:TYR:CG	36:3:729:PHE:HZ	2.32	0.48
36:3:757:ILE:HA	36:3:762:LEU:HA	1.94	0.48
1:A:41:GLN:NE2	1:A:45:TYR:HB2	2.28	0.48
1:A:845:ARG:NH1	1:A:1440:THR:HG22	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1352:HIS:HD2	20:U:5:ILE:HG21	1.79	0.48
1:A:1664:ILE:HG13	1:A:1664:ILE:O	2.13	0.48
3:C:181:ILE:O	3:C:206:PRO:HG3	2.14	0.48
3:C:592:VAL:O	3:C:593:GLU:HG2	2.14	0.48
3:C:826:ARG:NH1	3:C:911:PRO:HD2	2.29	0.48
7:H:34:U:H2'	7:H:35:A:C8	2.49	0.48
7:H:106:G:H1'	7:H:107:A:N7	2.29	0.48
11:L:206:ARG:HD2	11:L:206:ARG:O	2.13	0.48
12:M:200:ARG:HD2	12:M:200:ARG:N	2.28	0.48
12:M:222:ALA:HB1	17:R:266:LYS:HE3	1.96	0.48
23:X:503:ARG:NH2	23:X:817:GLU:O	2.47	0.48
23:X:835:SER:OG	23:X:835:SER:O	2.31	0.48
35:1:524:ARG:HD3	35:1:563:LEU:HD12	1.96	0.48
36:3:1:MET:HG2	39:2:709:GLY:O	2.14	0.48
36:3:18:ILE:HD12	36:3:67:ALA:HB2	1.95	0.48
36:3:347:LEU:CD2	36:3:359:TYR:HB2	2.44	0.48
36:3:373:PHE:CE1	36:3:385:PHE:HB3	2.48	0.48
36:3:642:ILE:H	36:3:703:ARG:HH21	1.61	0.48
1:A:105:ASN:O	1:A:489:TRP:NE1	2.47	0.47
1:A:235:MET:HB3	1:A:404:LEU:HD11	1.95	0.47
2:B:15:C:H2'	2:B:16:U:C6	2.49	0.47
3:C:192:ASP:CG	3:C:193:THR:N	2.67	0.47
8:I:564:PHE:O	8:I:568:TYR:N	2.44	0.47
21:V:606:GLU:HA	21:V:609:GLN:HG2	1.96	0.47
23:X:503:ARG:O	23:X:506:LEU:HB3	2.14	0.47
35:1:841:ALA:HB2	35:1:875:ILE:CD1	2.40	0.47
35:1:1299:GLU:O	35:1:1302:TYR:HD2	1.97	0.47
36:3:316:GLU:O	36:3:323:THR:OG1	2.29	0.47
36:3:457:ASN:ND2	36:3:479:VAL:HG12	2.29	0.47
36:3:477:SER:HA	36:3:482:THR:HG23	1.95	0.47
36:3:603:ARG:HD2	36:3:603:ARG:O	2.13	0.47
39:2:461:THR:OG1	39:2:464:GLU:N	2.26	0.47
1:A:123:THR:O	1:A:123:THR:OG1	2.30	0.47
1:A:1352:HIS:HD1	20:U:21:ARG:HA	1.79	0.47
1:A:1792:LYS:HE2	1:A:1798:LEU:HG	1.95	0.47
1:A:1836:LEU:HA	1:A:1839:TRP:HD1	1.79	0.47
1:A:1838:LYS:HE2	1:A:1868:MET:CE	2.44	0.47
4:E:145:LYS:HZ3	4:E:184:LYS:HG3	1.79	0.47
11:L:204:ARG:HE	11:L:207:GLY:HA3	1.78	0.47
35:1:663:THR:HA	35:1:666:LYS:CE	2.43	0.47
35:1:789:LEU:HB3	35:1:836:THR:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:819:TRP:CE3	35:1:867:MET:CE	2.96	0.47
35:1:854:VAL:HG11	35:1:891:GLN:HE21	1.79	0.47
35:1:967:GLU:CG	35:1:970:LEU:HB3	2.43	0.47
35:1:1006:MET:CB	35:1:1013:ILE:HG12	2.44	0.47
35:1:1197:LEU:CD2	41:7:78:GLN:HE21	2.26	0.47
36:3:415:LEU:HB2	36:3:424:TYR:CE2	2.49	0.47
36:3:484:VAL:O	36:3:485:LEU:HD12	2.13	0.47
1:A:41:GLN:NE2	4:E:153:PHE:CE2	2.81	0.47
1:A:767:VAL:HG21	2:B:39:C:O2'	2.15	0.47
1:A:1391:LEU:O	1:A:1394:GLN:HG3	2.13	0.47
1:A:1684:PHE:HD1	1:A:1702:LEU:HG	1.78	0.47
3:C:153:THR:O	3:C:155:PRO:HD3	2.14	0.47
3:C:441:PRO:HA	3:C:444:GLY:HA3	1.96	0.47
6:G:85:G:N2	7:H:45:C:C2	2.80	0.47
7:H:6:U:H2'	7:H:7:U:C6	2.48	0.47
7:H:70:C:H2'	7:H:71:C:H6	1.80	0.47
12:M:222:ALA:CB	17:R:266:LYS:HE3	2.44	0.47
21:V:497:CYS:HB3	21:V:507:PHE:CB	2.44	0.47
21:V:549:LYS:O	21:V:549:LYS:HD3	2.13	0.47
35:1:647:PHE:O	35:1:651:VAL:HG13	2.15	0.47
35:1:770:MET:O	35:1:774:ILE:HG12	2.14	0.47
35:1:795:CYS:O	35:1:798:THR:HG23	2.13	0.47
35:1:819:TRP:CH2	35:1:867:MET:HE3	2.49	0.47
35:1:893:ILE:HD13	35:1:893:ILE:HA	1.67	0.47
35:1:914:PHE:O	35:1:918:VAL:HG23	2.14	0.47
40:4:103:PHE:N	40:4:177:ALA:HB2	2.29	0.47
1:A:253:ASN:O	3:C:893:GLY:HA3	2.15	0.47
1:A:1211:ASP:C	1:A:1213:VAL:H	2.18	0.47
1:A:1491:LYS:HE3	1:A:1491:LYS:HB2	1.49	0.47
3:C:116:MET:HA	3:C:119:LEU:HD12	1.95	0.47
3:C:737:PRO:HD3	3:C:743:ASN:HD22	1.80	0.47
4:E:60:MET:HB3	4:E:353:MET:HB3	1.96	0.47
6:G:116:C:OP2	17:R:371:ARG:HB3	2.15	0.47
17:R:328:ALA:HB2	24:Y:226:MET:CG	2.44	0.47
17:R:348:GLU:HB2	23:X:263:SER:H	1.79	0.47
17:R:360:ARG:CD	24:Y:274:ASP:OD1	2.55	0.47
19:T:213:GLU:HG2	19:T:214:PRO:HD2	1.97	0.47
19:T:295:ASP:OD1	19:T:296:LEU:N	2.40	0.47
23:X:698:LYS:HZ1	23:X:758:THR:HA	1.79	0.47
24:Y:44:ASN:OD1	24:Y:52:GLN:HB3	2.13	0.47
35:1:864:TYR:O	35:1:868:VAL:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:3:169:HIS:CD2	36:3:170:VAL:N	2.82	0.47
36:3:558:LEU:HG	36:3:559:THR:N	2.30	0.47
41:7:33:CYS:HB3	41:7:72:CYS:HG	1.79	0.47
41:7:73:LYS:HA	41:7:76:THR:HG22	1.95	0.47
1:A:762:ARG:HA	1:A:902:TYR:O	2.15	0.47
1:A:1776:ILE:HD11	1:A:1778:TRP:NE1	2.29	0.47
3:C:352:LYS:HE2	3:C:352:LYS:H	1.80	0.47
3:C:667:VAL:HG13	3:C:826:ARG:HG3	1.97	0.47
4:E:124:LEU:O	4:E:135:VAL:HA	2.14	0.47
4:E:131:LYS:HA	4:E:152:SER:O	2.15	0.47
4:E:150:HIS:HA	4:E:177:LYS:NZ	2.29	0.47
5:F:49:G:H2'	5:F:50:A:C8	2.47	0.47
13:N:44:GLU:HB2	13:N:47:TRP:CE3	2.49	0.47
17:R:235:ARG:H	17:R:235:ARG:HE	1.62	0.47
21:V:556:TYR:HB2	21:V:594:MET:SD	2.54	0.47
23:X:597:VAL:HA	23:X:600:LEU:HD12	1.96	0.47
35:1:616:ASP:HA	35:1:619:ASN:ND2	2.30	0.47
35:1:699:GLN:NE2	35:1:738:HIS:CE1	2.82	0.47
36:3:75:LYS:HE3	36:3:76:ASP:H	1.79	0.47
36:3:839:ALA:O	36:3:843:LEU:HD12	2.14	0.47
41:7:13:LYS:HD2	41:7:48:GLU:OE2	2.15	0.47
1:A:179:ALA:HA	1:A:183:LEU:HB2	1.96	0.47
1:A:608:LEU:HD13	1:A:632:ALA:HB1	1.96	0.47
1:A:818:GLU:OE2	17:R:305:ARG:HD2	2.14	0.47
1:A:1624:SER:OG	1:A:1625:SER:N	2.47	0.47
1:A:1630:LEU:HA	1:A:1660:TYR:O	2.14	0.47
7:H:171:U:N3	7:H:172:C:C4	2.83	0.47
9:J:189:ILE:HD12	11:L:140:ASP:OD2	2.13	0.47
23:X:183:GLU:HA	23:X:186:ARG:HD2	1.96	0.47
23:X:291:LYS:O	23:X:295:THR:HG22	2.15	0.47
23:X:618:GLN:HA	23:X:648:TYR:CE1	2.50	0.47
23:X:811:SER:HA	23:X:814:LYS:HZ2	1.80	0.47
23:X:970:ILE:HD12	23:X:977:PHE:O	2.14	0.47
24:Y:27:ASN:OD1	24:Y:66:ILE:N	2.36	0.47
36:3:70:LEU:HD13	36:3:146:ARG:HG2	1.96	0.47
36:3:698:PRO:O	36:3:700:LYS:NZ	2.34	0.47
39:2:631:PRO:CB	40:4:77:ILE:HA	2.44	0.47
1:A:137:GLU:HG2	1:A:419:ARG:HD3	1.97	0.47
1:A:376:GLU:H	1:A:376:GLU:HG3	1.49	0.47
1:A:464:PRO:O	1:A:466:ALA:N	2.47	0.47
1:A:697:MET:N	1:A:698:PRO:HD3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:833:LYS:O	1:A:833:LYS:HD3	2.14	0.47
1:A:1779:PHE:CG	1:A:1862:ILE:HD11	2.49	0.47
1:A:1862:ILE:HG22	1:A:1885:LYS:HB3	1.95	0.47
1:A:1935:ARG:O	1:A:1939:ILE:HG13	2.14	0.47
1:A:1943:LEU:HD12	1:A:1950:ALA:HB1	1.97	0.47
3:C:311:SER:HB2	3:C:316:ILE:HG23	1.96	0.47
3:C:496:VAL:HG23	3:C:546:ALA:HA	1.97	0.47
4:E:161:ARG:HH12	4:E:203:ASP:HB3	1.79	0.47
4:E:241:LEU:HA	4:E:251:LEU:O	2.14	0.47
4:E:343:ILE:HA	4:E:352:TYR:O	2.14	0.47
7:H:51:A:H2'	7:H:52:G:O4'	2.15	0.47
7:H:107:A:C6	7:H:108:G:C6	3.02	0.47
7:H:176:G:H8	7:H:176:G:O5'	1.97	0.47
12:M:165:ASN:ND2	17:R:95:LYS:HE2	2.28	0.47
14:O:233:THR:O	14:O:303:GLY:N	2.41	0.47
15:P:67:GLU:CD	19:T:476:ARG:HH21	2.15	0.47
21:V:577:SER:O	21:V:581:ILE:HG12	2.14	0.47
23:X:189:ASP:O	23:X:193:THR:HG22	2.15	0.47
23:X:718:SER:OG	23:X:719:ALA:N	2.47	0.47
23:X:824:LEU:O	23:X:828:ILE:HG13	2.15	0.47
23:X:911:ALA:HA	23:X:914:VAL:HG22	1.97	0.47
24:Y:212:LYS:O	24:Y:216:GLU:HG3	2.15	0.47
35:1:796:CYS:C	35:1:801:VAL:HG21	2.34	0.47
35:1:854:VAL:HG12	35:1:892:LEU:CD2	2.45	0.47
35:1:860:GLU:O	35:1:865:ARG:NH2	2.48	0.47
35:1:1165:TYR:HD1	39:2:575:PHE:CE1	2.33	0.47
35:1:1197:LEU:HD21	41:7:78:GLN:HE21	1.79	0.47
35:1:1249:TYR:CE2	39:2:587:HIS:CE1	3.03	0.47
36:3:181:MET:HE3	36:3:212:GLU:HB2	1.96	0.47
36:3:484:VAL:C	36:3:485:LEU:HD12	2.34	0.47
36:3:524:ILE:O	36:3:535:GLU:HA	2.15	0.47
36:3:605:LEU:HD23	36:3:617:ILE:HG22	1.95	0.47
36:3:945:VAL:HG23	36:3:968:ARG:HH12	1.79	0.47
36:3:1158:ARG:HG3	36:3:1159:ASP:H	1.79	0.47
3:C:320:LEU:HD11	3:C:344:TRP:HB2	1.96	0.47
3:C:350:ASN:HD22	3:C:353:THR:H	1.63	0.47
4:E:259:VAL:HG22	4:E:277:PHE:HB2	1.97	0.47
11:L:98:GLU:O	11:L:101:GLU:HG3	2.15	0.47
13:N:1:MET:N	13:N:2:PRO:HD2	2.30	0.47
17:R:434:ASP:OD2	17:R:434:ASP:N	2.48	0.47
21:V:562:TRP:CE2	21:V:602:ARG:HD3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:702:PRO:HG2	23:X:788:THR:HB	1.96	0.47
23:X:842:THR:O	23:X:846:MET:HG2	2.15	0.47
25:Z:90:PRO:CB	25:Z:109:ASN:C	2.83	0.47
35:1:746:PHE:O	35:1:750:ILE:HG23	2.15	0.47
35:1:982:LEU:HD21	35:1:1016:LEU:HD11	1.95	0.47
35:1:1277:GLN:NE2	35:1:1277:GLN:O	2.48	0.47
36:3:232:GLY:HA3	36:3:252:SER:HA	1.97	0.47
36:3:334:PRO:HB3	36:3:432:ARG:NH1	2.30	0.47
36:3:867:ARG:NH1	36:3:879:LEU:HD13	2.30	0.47
36:3:1116:SER:HA	39:2:708:TRP:CH2	2.50	0.47
36:3:1199:ARG:HH21	36:3:1207:LYS:HD3	1.80	0.47
1:A:693:ILE:HB	1:A:738:MET:SD	2.55	0.47
1:A:1413:ASP:O	1:A:1414:ARG:HG3	2.14	0.47
1:A:1901:LYS:NZ	1:A:1967:ILE:HA	2.30	0.47
3:C:200:PHE:HE1	3:C:434:CYS:SG	2.37	0.47
3:C:243:ILE:O	3:C:247:VAL:HG13	2.14	0.47
3:C:284:GLU:O	3:C:288:LEU:HG	2.14	0.47
3:C:702:ASN:HB2	3:C:704:VAL:HG23	1.95	0.47
3:C:801:LEU:HD13	3:C:802:HIS:NE2	2.30	0.47
3:C:804:GLY:O	3:C:808:ILE:HG12	2.15	0.47
7:H:166:G:N3	7:H:166:G:H2'	2.29	0.47
9:J:325:ASN:HB2	12:M:172:HIS:HD2	1.80	0.47
12:M:121:ASP:OD2	12:M:122:LEU:N	2.47	0.47
15:P:186:ARG:CA	24:Y:49:PHE:CE1	2.97	0.47
23:X:606:GLN:HG3	23:X:688:TYR:CE1	2.50	0.47
35:1:573:LYS:O	35:1:577:VAL:HG23	2.15	0.47
35:1:1299:GLU:HB3	42:5:43:TYR:HE2	1.78	0.47
36:3:193:ASP:HB3	42:5:29:TRP:HH2	1.79	0.47
36:3:563:LEU:O	36:3:580:ARG:HB3	2.14	0.47
36:3:604:PHE:HA	36:3:618:SER:HA	1.96	0.47
36:3:665:LEU:CB	36:3:679:LEU:HD23	2.45	0.47
36:3:952:ILE:HG12	36:3:961:ILE:HG12	1.95	0.47
1:A:59:GLU:CD	13:N:87:ASN:HB2	2.35	0.47
1:A:682:ASP:O	1:A:686:ARG:HG2	2.14	0.47
1:A:762:ARG:NH1	15:P:226:LYS:HZ1	2.13	0.47
1:A:1090:ARG:HG2	1:A:1091:TYR:O	2.15	0.47
3:C:239:THR:O	3:C:243:ILE:HG23	2.14	0.47
4:E:124:LEU:HD21	4:E:138:SER:HB3	1.97	0.47
4:E:137:ASP:HB2	4:E:140:THR:OG1	2.14	0.47
5:F:3:G:H2'	5:F:4:C:C6	2.50	0.47
19:T:221:THR:OG1	19:T:231:TRP:NE1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:267:ARG:O	23:X:271:LYS:HD3	2.14	0.47
23:X:591:TYR:HB2	23:X:737:LEU:HD23	1.97	0.47
23:X:871:PHE:HZ	23:X:901:ASN:HB3	1.80	0.47
35:1:560:LEU:CD2	35:1:600:LEU:CA	2.87	0.47
36:3:193:ASP:CA	42:5:79:PRO:HG2	2.44	0.47
36:3:565:TYR:HE1	36:3:619:LEU:HD12	1.80	0.47
36:3:592:LEU:HD11	36:3:619:LEU:HD11	1.97	0.47
36:3:633:LEU:HD12	36:3:637:PRO:HG3	1.97	0.47
1:A:296:PHE:O	1:A:302:ILE:HD11	2.14	0.46
1:A:1852:LEU:HD23	1:A:1857:GLN:HA	1.97	0.46
3:C:514:TYR:HD1	3:C:514:TYR:C	2.19	0.46
3:C:693:GLU:OE1	3:C:695:GLY:N	2.38	0.46
13:N:117:CYS:SG	13:N:136:HIS:ND1	2.87	0.46
14:O:167:PHE:O	14:O:171:GLY:N	2.48	0.46
15:P:53:GLU:HB3	15:P:57:ARG:HH12	1.80	0.46
16:Q:263:LEU:O	16:Q:267:ARG:N	2.47	0.46
19:T:315:TRP:CZ3	19:T:322:SER:HB2	2.51	0.46
24:Y:65:SER:N	24:Y:76:SER:O	2.27	0.46
35:1:527:GLY:CA	35:1:566:LEU:CD2	2.93	0.46
35:1:570:TYR:HA	35:1:573:LYS:HD3	1.96	0.46
35:1:823:MET:O	35:1:829:ASN:HB2	2.14	0.46
35:1:871:THR:O	35:1:875:ILE:HG13	2.15	0.46
35:1:1179:ASP:CB	39:2:511:LEU:HB3	2.45	0.46
35:1:1233:ALA:O	35:1:1237:LEU:HB2	2.15	0.46
36:3:272:PRO:HD3	36:3:327:LEU:HD13	1.97	0.46
36:3:449:VAL:HG11	36:3:763:ARG:NH1	2.29	0.46
36:3:511:LEU:HD21	36:3:517:VAL:CG2	2.44	0.46
39:2:529:LYS:HB2	39:2:529:LYS:HE2	1.61	0.46
1:A:362:ARG:HD3	1:A:362:ARG:HA	1.69	0.46
1:A:497:CYS:SG	1:A:558:VAL:HG11	2.55	0.46
1:A:781:ARG:O	1:A:785:LYS:HG3	2.14	0.46
2:B:21:A:H2'	2:B:21:A:N3	2.31	0.46
3:C:137:HIS:CG	3:C:138:LEU:H	2.33	0.46
3:C:219:LEU:HD23	3:C:219:LEU:HA	1.68	0.46
3:C:514:TYR:C	3:C:514:TYR:CD1	2.89	0.46
3:C:668:GLU:HG3	3:C:824:THR:HG21	1.97	0.46
5:F:29:A:H2'	5:F:30:A:O4'	2.14	0.46
7:H:18:U:C5	12:M:218:PHE:CE2	3.02	0.46
12:M:125:SER:HA	17:R:242:GLN:OE1	2.14	0.46
24:Y:21:ARG:NH1	24:Y:83:VAL:O	2.48	0.46
35:1:898:TYR:HA	35:1:901:GLN:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:5:8:HIS:HA	42:5:11:LEU:HB2	1.97	0.46
1:A:1629:ILE:O	1:A:1661:TRP:HA	2.14	0.46
2:B:99:C:H2'	2:B:100:C:H6	1.80	0.46
3:C:749:THR:O	3:C:753:GLU:HB2	2.16	0.46
3:C:916:ILE:HG21	3:C:928:HIS:HB3	1.97	0.46
4:E:126:SER:OG	4:E:136:TRP:NE1	2.26	0.46
5:F:86:U:H5"	12:M:134:GLN:NE2	2.30	0.46
6:G:1:G:H21	10:K:218:LYS:CD	2.27	0.46
6:G:90:C:H42	7:H:40:C:N4	2.14	0.46
9:J:297:ASN:OD1	11:L:225:TYR:HB2	2.15	0.46
21:V:594:MET:O	21:V:598:LYS:HE3	2.15	0.46
23:X:172:LEU:HD12	23:X:173:GLN:N	2.31	0.46
23:X:941:LYS:HE2	23:X:1007:TRP:NE1	2.31	0.46
23:X:998:ARG:O	23:X:999:GLN:HG2	2.16	0.46
35:1:1279:ALA:O	35:1:1281:ILE:N	2.48	0.46
36:3:451:GLU:HG3	36:3:760:ASN:O	2.16	0.46
36:3:1117:LEU:HD12	36:3:1117:LEU:HA	1.60	0.46
1:A:120:TYR:HE1	1:A:485:THR:HG1	1.61	0.46
1:A:371:LEU:HD22	1:A:371:LEU:HA	1.74	0.46
1:A:468:LYS:HA	1:A:468:LYS:HZ2	1.80	0.46
1:A:1019:TYR:CG	1:A:1020:LYS:N	2.83	0.46
1:A:1919:LEU:N	1:A:1919:LEU:HD23	2.29	0.46
1:A:1998:ASN:OD1	1:A:2001:SER:N	2.48	0.46
6:G:95:U:P	35:1:1106:ARG:HG3	2.54	0.46
12:M:175:SER:N	12:M:178:GLU:OE2	2.49	0.46
13:N:38:GLU:CD	13:N:38:GLU:H	2.18	0.46
17:R:377:ARG:HE	23:X:240:ARG:HH22	1.61	0.46
19:T:393:ASP:OD2	19:T:393:ASP:N	2.40	0.46
23:X:474:GLY:HA2	23:X:486:CYS:O	2.15	0.46
35:1:554:LYS:HD2	35:1:558:ARG:HE	1.80	0.46
35:1:666:LYS:HB3	35:1:704:ILE:HD13	1.96	0.46
35:1:923:LYS:O	35:1:923:LYS:HG2	2.15	0.46
35:1:967:GLU:HB3	35:1:970:LEU:HB3	1.98	0.46
35:1:1000:ILE:O	35:1:1003:VAL:HG13	2.16	0.46
36:3:115:ILE:CD1	42:5:19:ILE:H	2.28	0.46
36:3:910:ALA:CB	36:3:913:LEU:HD11	2.45	0.46
36:3:1041:TYR:CD2	39:2:705:ARG:HG3	2.51	0.46
36:3:1181:GLN:O	36:3:1185:MET:HG3	2.14	0.46
1:A:81:PHE:C	1:A:83:HIS:H	2.19	0.46
1:A:1091:TYR:O	1:A:1092:ILE:C	2.52	0.46
1:A:1382:SER:HA	1:A:1415:GLY:HA2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1892:PRO:HG2	1:A:1940:LEU:CB	2.45	0.46
3:C:281:ILE:O	3:C:285:VAL:HG12	2.15	0.46
3:C:622:GLU:O	3:C:625:GLY:N	2.41	0.46
4:E:345:ALA:HA	4:E:351:LEU:HD23	1.97	0.46
5:F:41:A:H2	6:G:6:A:N1	2.14	0.46
6:G:116:C:C2	17:R:370:SER:O	2.68	0.46
21:V:540:GLU:HG3	21:V:541:THR:N	2.28	0.46
21:V:618:ARG:HB3	21:V:646:HIS:CE1	2.50	0.46
23:X:249:GLU:CB	23:X:273:LYS:HE2	2.45	0.46
24:Y:236:LYS:HA	24:Y:236:LYS:HD3	1.69	0.46
35:1:641:ILE:N	35:1:642:PRO:CD	2.78	0.46
35:1:662:HIS:HE1	35:1:700:LYS:HB3	1.81	0.46
35:1:1006:MET:HA	35:1:1009:MET:CG	2.44	0.46
36:3:69:ARG:HG3	36:3:75:LYS:O	2.15	0.46
36:3:809:GLU:O	36:3:812:LYS:HB2	2.15	0.46
1:A:1000:ILE:HD12	1:A:1000:ILE:HA	1.59	0.46
3:C:532:ILE:HB	3:C:539:ILE:HD11	1.97	0.46
3:C:841:ASP:OD1	3:C:842:CYS:N	2.49	0.46
4:E:147:LEU:HA	4:E:147:LEU:HD23	1.72	0.46
6:G:9:C:O2'	6:G:10:U:O4'	2.25	0.46
17:R:251:ILE:O	17:R:251:ILE:HG12	2.15	0.46
21:V:609:GLN:HE21	21:V:612:PHE:HD2	1.64	0.46
23:X:257:PHE:CZ	23:X:266:GLU:HG3	2.50	0.46
23:X:663:THR:HG23	23:X:669:LYS:HB2	1.98	0.46
23:X:818:LEU:HD12	23:X:825:SER:OG	2.15	0.46
35:1:567:VAL:CG1	35:1:600:LEU:CD1	2.85	0.46
35:1:614:ARG:HB3	35:1:615:PRO:HD2	1.98	0.46
35:1:644:LEU:HB3	35:1:648:LEU:CD1	2.46	0.46
35:1:907:ASP:OD2	35:1:909:VAL:HB	2.16	0.46
35:1:1195:MET:O	35:1:1199:VAL:HG23	2.16	0.46
36:3:226:GLU:HB3	36:3:261:PHE:CE2	2.51	0.46
36:3:1102:LEU:HD12	36:3:1102:LEU:HA	1.66	0.46
36:3:1204:VAL:HG23	36:3:1205:SER:N	2.30	0.46
41:7:12:ARG:NH1	41:7:84:GLY:O	2.48	0.46
42:5:13:HIS:ND1	42:5:17:LYS:HE3	2.30	0.46
1:A:260:LEU:HD23	1:A:260:LEU:HA	1.70	0.46
1:A:464:PRO:HG2	2:B:20:G:C5	2.51	0.46
1:A:1638:ASN:O	1:A:1652:MET:HB3	2.15	0.46
1:A:1660:TYR:CE1	1:A:1699:THR:HG22	2.51	0.46
1:A:1865:ARG:HD2	1:A:1865:ARG:HA	1.76	0.46
3:C:283:ASP:OD2	3:C:284:GLU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:62:LEU:HD21	4:E:99:CYS:HB2	1.98	0.46
9:J:325:ASN:HB2	12:M:172:HIS:CD2	2.51	0.46
12:M:214:ARG:HB3	17:R:260:TYR:OH	2.14	0.46
15:P:205:LYS:CB	15:P:208:LYS:HB3	2.45	0.46
35:1:586:ASP:O	35:1:590:ARG:HG3	2.16	0.46
35:1:1135:GLU:O	35:1:1138:VAL:HG12	2.15	0.46
35:1:1263:ASP:HA	42:5:24:ALA:HB2	1.97	0.46
35:1:1304:LEU:HD12	42:5:52:TYR:CD2	2.50	0.46
36:3:2:PHE:CD2	39:2:711:LEU:HG	2.51	0.46
36:3:184:CYS:HG	36:3:211:TYR:HE1	1.63	0.46
36:3:864:SER:O	36:3:865:VAL:HG23	2.15	0.46
36:3:1125:GLY:C	36:3:1126:ILE:HG13	2.35	0.46
1:A:845:ARG:HA	1:A:845:ARG:HD2	1.61	0.46
1:A:1199:LYS:HE2	1:A:1206:GLU:HG3	1.97	0.46
1:A:1275:ARG:O	1:A:1369:TYR:HE1	1.99	0.46
2:B:8:G:N2	2:B:70:A:H1'	2.26	0.46
3:C:465:MET:O	3:C:468:CYS:N	2.46	0.46
3:C:604:LEU:HD21	3:C:627:HIS:HE1	1.80	0.46
3:C:710:ASN:O	3:C:714:LEU:HD13	2.16	0.46
5:F:23:U:H2'	5:F:24:A:O4'	2.15	0.46
6:G:99:C:C2'	6:G:100:C:H5'	2.46	0.46
13:N:25:LEU:HD23	13:N:25:LEU:HA	1.70	0.46
17:R:91:ASP:HA	17:R:97:LYS:NZ	2.31	0.46
17:R:382:ARG:NH2	17:R:385:ASN:HB2	2.31	0.46
19:T:412:HIS:ND1	19:T:429:SER:OG	2.47	0.46
23:X:487:THR:HG21	23:X:494:ARG:HD2	1.98	0.46
23:X:520:ASP:HB3	23:X:521:GLU:OE1	2.15	0.46
23:X:953:ARG:HB3	23:X:983:TRP:CZ3	2.51	0.46
35:1:582:LEU:HA	35:1:590:ARG:HA	1.97	0.46
35:1:826:ASP:OD1	35:1:828:ARG:N	2.42	0.46
35:1:929:LEU:N	35:1:930:PRO:HD2	2.30	0.46
36:3:1034:THR:HG22	36:3:1049:LYS:HG3	1.96	0.46
39:2:635:ALA:CA	40:4:73:ILE:HA	2.31	0.46
41:7:47:ASP:HA	41:7:50:ASN:HB3	1.97	0.46
1:A:67:ARG:HE	1:A:67:ARG:HB2	1.47	0.46
1:A:191:ILE:O	1:A:191:ILE:HG22	2.16	0.46
1:A:361:HIS:HD1	1:A:361:HIS:N	2.14	0.46
1:A:1868:MET:O	1:A:1871:PRO:HD2	2.15	0.46
3:C:921:LEU:HD23	3:C:921:LEU:HA	1.78	0.46
4:E:143:ARG:CZ	4:E:146:ARG:HE	2.28	0.46
5:F:31:U:H3'	5:F:32:U:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:38:G:OP2	5:F:38:G:H8	1.99	0.46
9:J:191:ALA:O	9:J:194:LEU:N	2.49	0.46
13:N:15:TRP:NE1	13:N:19:GLU:OE1	2.49	0.46
13:N:122:PRO:HB2	13:N:125:LYS:HD3	1.98	0.46
17:R:377:ARG:HH21	17:R:377:ARG:HG2	1.81	0.46
23:X:640:ARG:HG3	23:X:640:ARG:NH1	2.30	0.46
24:Y:198:ASP:CG	24:Y:199:ASP:H	2.19	0.46
35:1:567:VAL:HG23	35:1:568:ARG:HA	1.98	0.46
36:3:164:ASN:HA	36:3:189:TYR:OH	2.15	0.46
36:3:676:ARG:HD2	36:3:729:PHE:CD2	2.51	0.46
39:2:542:GLU:HA	39:2:545:GLU:HG2	1.98	0.46
41:7:23:CYS:N	41:7:58:CYS:SG	2.73	0.46
1:A:1552:GLN:OE1	1:A:1563:HIS:NE2	2.48	0.46
1:A:1914:MET:HE3	1:A:1916:LEU:HD23	1.97	0.46
3:C:351:PRO:O	3:C:354:ARG:HD3	2.16	0.46
4:E:117:TYR:CD1	4:E:121:GLY:HA2	2.52	0.46
7:H:158:G:H2'	7:H:159:U:O4'	2.17	0.46
8:I:569:GLY:HA3	8:I:576:ALA:HB2	1.97	0.46
9:J:537:TRP:O	9:J:541:ALA:N	2.48	0.46
11:L:223:GLY:HA2	17:R:86:LEU:HD21	1.98	0.46
23:X:576:ARG:HB3	23:X:577:PHE:CD2	2.51	0.46
23:X:624:ALA:O	23:X:628:LEU:HG	2.16	0.46
35:1:881:ALA:HB1	35:1:884:ILE:HG12	1.97	0.46
35:1:903:GLN:HG2	35:1:910:MET:HG3	1.98	0.46
35:1:1284:TYR:CE2	42:5:35:GLN:HB2	2.51	0.46
36:3:112:CYS:HG	42:5:46:HIS:CD2	2.34	0.46
36:3:159:GLU:CD	36:3:161:HIS:H	2.19	0.46
36:3:185:LEU:O	36:3:186:GLU:HG3	2.16	0.46
36:3:304:GLN:HE21	36:3:308:GLY:HA2	1.80	0.46
36:3:569:ASP:O	36:3:572:GLY:N	2.45	0.46
36:3:817:GLN:HG3	36:3:818:GLN:OE1	2.15	0.46
36:3:1210:ASP:HA	36:3:1213:THR:OG1	2.15	0.46
1:A:84:ASP:O	1:A:88:TYR:HB2	2.16	0.45
1:A:198:GLU:HG2	1:A:199:GLU:H	1.82	0.45
1:A:468:LYS:NZ	1:A:469:LYS:H	2.14	0.45
1:A:1144:LYS:O	1:A:1148:ASN:HB2	2.16	0.45
1:A:1359:HIS:HD2	1:A:1361:GLU:O	1.99	0.45
1:A:1391:LEU:O	1:A:1395:GLU:HG2	2.16	0.45
1:A:1870:ASP:HA	1:A:1873:GLU:OE1	2.16	0.45
3:C:350:ASN:HD21	3:C:352:LYS:HB2	1.80	0.45
3:C:510:LEU:HB3	3:C:576:ILE:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:711:ARG:HB3	3:C:730:ARG:NH2	2.31	0.45
4:E:171:SER:H	4:E:196:VAL:HG13	1.81	0.45
4:E:207:GLN:HB3	4:E:219:VAL:HG12	1.98	0.45
6:G:99:C:N3	7:H:33:G:C4	2.84	0.45
11:L:94:ALA:O	11:L:98:GLU:HG3	2.16	0.45
12:M:210:TYR:CG	12:M:210:TYR:O	2.69	0.45
23:X:228:LYS:HA	23:X:231:ARG:HD3	1.99	0.45
23:X:741:TRP:CG	35:1:782:GLU:HB3	2.50	0.45
23:X:1008:LEU:HB3	23:X:1016:TYR:CD2	2.50	0.45
35:1:581:LEU:HD13	35:1:589:ALA:HB1	1.98	0.45
35:1:706:ALA:O	35:1:749:ALA:HB2	2.16	0.45
35:1:1012:PRO:C	35:1:1014:LYS:N	2.68	0.45
35:1:1090:PRO:CA	35:1:1093:VAL:CG1	2.92	0.45
35:1:1165:TYR:CD1	39:2:575:PHE:CE1	3.04	0.45
36:3:288:VAL:HG23	36:3:289:CYS:N	2.30	0.45
36:3:515:ALA:HA	36:3:528:ARG:HA	1.97	0.45
1:A:101:LYS:HD3	1:A:101:LYS:HA	1.76	0.45
1:A:1275:ARG:C	1:A:1276:GLU:HG3	2.35	0.45
1:A:1361:GLU:HG3	1:A:1362:ASP:OD2	2.17	0.45
1:A:1670:ASP:N	1:A:1670:ASP:OD1	2.48	0.45
1:A:1977:ILE:HG22	1:A:1978:LYS:HD2	1.98	0.45
4:E:118:ASN:ND2	4:E:122:SER:H	2.10	0.45
6:G:13:C:C2	6:G:14:A:C8	3.04	0.45
7:H:56:A:O2'	39:2:481:THR:OG1	2.20	0.45
21:V:562:TRP:CD2	21:V:602:ARG:HD3	2.51	0.45
21:V:569:LYS:HD2	21:V:614:GLY:HA3	1.98	0.45
23:X:171:ARG:CZ	23:X:509:PRO:HB3	2.42	0.45
23:X:715:SER:HB3	23:X:718:SER:HB3	1.98	0.45
23:X:787:GLU:HB2	35:1:542:PRO:HG3	1.98	0.45
35:1:833:LEU:O	35:1:837:THR:OG1	2.23	0.45
36:3:184:CYS:SG	36:3:211:TYR:HE1	2.40	0.45
36:3:259:LYS:HB2	36:3:259:LYS:HE3	1.69	0.45
36:3:503:THR:OG1	36:3:522:ASP:OD2	2.21	0.45
36:3:528:ARG:NH1	36:3:572:GLY:O	2.49	0.45
36:3:565:TYR:CE1	36:3:619:LEU:HD12	2.51	0.45
36:3:745:PHE:CG	36:3:755:VAL:HG23	2.51	0.45
36:3:788:PHE:HB2	36:3:799:ILE:HA	1.98	0.45
36:3:833:GLU:C	36:3:836:ALA:H	2.13	0.45
36:3:910:ALA:HB2	36:3:948:VAL:HG23	1.98	0.45
36:3:1159:ASP:OD1	36:3:1160:HIS:N	2.50	0.45
1:A:362:ARG:NH1	21:V:324:HIS:N	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:977:LEU:HG	1:A:978:GLU:N	2.31	0.45
1:A:1831:LYS:HZ3	1:A:1832:ARG:HB2	1.79	0.45
3:C:845:ALA:O	3:C:848:THR:OG1	2.31	0.45
5:F:36:A:N1	6:G:10:U:C4	2.84	0.45
6:G:97:A:C2	35:1:1075:ARG:HG2	2.51	0.45
12:M:160:PHE:HB3	12:M:161:PHE:CD1	2.51	0.45
19:T:341:ALA:O	19:T:344:GLN:HG3	2.16	0.45
23:X:790:LEU:O	23:X:794:GLU:HG2	2.16	0.45
35:1:662:HIS:HB2	35:1:701:VAL:HB	1.98	0.45
35:1:997:LEU:HA	35:1:997:LEU:HD23	1.84	0.45
35:1:1226:VAL:O	35:1:1230:VAL:HG23	2.17	0.45
36:3:185:LEU:HD23	36:3:185:LEU:HA	1.69	0.45
36:3:234:PHE:HE1	36:3:236:ILE:HG12	1.81	0.45
36:3:604:PHE:CE1	36:3:681:PRO:HD3	2.51	0.45
1:A:1127:GLY:HA3	1:A:1151:ARG:HH22	1.81	0.45
1:A:1526:LEU:HD22	1:A:1527:ASN:H	1.81	0.45
3:C:860:ASP:N	3:C:860:ASP:OD1	2.49	0.45
5:F:33:G:C2	5:F:34:G:C8	3.05	0.45
6:G:99:C:N4	7:H:32:U:C4	2.84	0.45
7:H:150:U:H3	7:H:181:G:H22	1.64	0.45
12:M:139:THR:O	12:M:142:ILE:HG22	2.17	0.45
12:M:210:TYR:O	12:M:210:TYR:CD2	2.69	0.45
15:P:186:ARG:HB2	24:Y:49:PHE:CE1	2.50	0.45
19:T:203:HIS:CE1	19:T:223:SER:HB3	2.51	0.45
19:T:329:HIS:CE1	19:T:349:SER:HB3	2.51	0.45
23:X:235:LEU:HD22	24:Y:217:ALA:HA	1.97	0.45
23:X:807:GLU:HA	23:X:807:GLU:OE2	2.17	0.45
23:X:997:MET:HE2	23:X:997:MET:HB3	1.65	0.45
24:Y:73:ASP:OD1	24:Y:73:ASP:N	2.48	0.45
35:1:1017:LEU:HD22	35:1:1050:VAL:HG11	1.98	0.45
35:1:1135:GLU:O	35:1:1135:GLU:HG3	2.15	0.45
35:1:1216:TRP:O	35:1:1219:VAL:HB	2.16	0.45
36:3:5:ASN:O	36:3:1176:GLY:HA3	2.16	0.45
36:3:193:ASP:HB3	42:5:29:TRP:CH2	2.51	0.45
36:3:404:LEU:HD12	36:3:404:LEU:HA	1.77	0.45
36:3:477:SER:O	36:3:477:SER:OG	2.32	0.45
36:3:1116:SER:C	39:2:708:TRP:CZ2	2.90	0.45
1:A:1571:ILE:HG23	10:K:220:LEU:CD2	2.41	0.45
1:A:1817:LEU:O	1:A:1916:LEU:HA	2.17	0.45
3:C:137:HIS:HB3	3:C:140:HIS:CE1	2.51	0.45
3:C:662:PHE:CE1	3:C:829:GLU:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:918:ILE:HG21	3:C:932:GLU:OE2	2.16	0.45
6:G:15:U:C2	6:G:16:G:C8	3.05	0.45
6:G:107:U:O2	23:X:709:LEU:CD2	2.65	0.45
11:L:749:LEU:O	11:L:753:GLU:N	2.45	0.45
12:M:224:ARG:HH11	12:M:224:ARG:C	2.20	0.45
17:R:309:GLU:OE1	17:R:309:GLU:HA	2.17	0.45
19:T:391:SER:OG	19:T:393:ASP:OD2	2.26	0.45
21:V:560:LEU:HD23	21:V:560:LEU:HA	1.80	0.45
23:X:592:LEU:O	23:X:596:VAL:HG23	2.16	0.45
23:X:774:ASP:CG	23:X:777:HIS:HD1	2.18	0.45
35:1:869:MET:O	35:1:873:GLU:HB3	2.15	0.45
36:3:14:ILE:HD11	36:3:356:HIS:CD2	2.51	0.45
36:3:93:GLN:O	36:3:97:ASN:N	2.50	0.45
36:3:249:LEU:HD23	36:3:256:ILE:HD11	1.98	0.45
36:3:333:VAL:HG21	36:3:349:VAL:HG21	1.97	0.45
36:3:458:ALA:O	36:3:459:VAL:HG23	2.16	0.45
36:3:642:ILE:H	36:3:703:ARG:NH2	2.13	0.45
36:3:704:VAL:C	36:3:710:GLU:HG3	2.37	0.45
36:3:986:ILE:HG21	36:3:990:ILE:HG12	1.99	0.45
1:A:292:ASP:CG	1:A:293:TRP:H	2.20	0.45
1:A:699:GLU:OE1	1:A:699:GLU:HA	2.14	0.45
1:A:727:LYS:HE2	1:A:727:LYS:HB3	1.70	0.45
2:B:53:U:OP1	15:P:39:THR:OG1	2.34	0.45
3:C:530:LEU:HD23	3:C:530:LEU:HA	1.70	0.45
3:C:755:ASP:O	3:C:758:LEU:N	2.48	0.45
4:E:209:ILE:HG23	4:E:219:VAL:HG22	1.99	0.45
5:F:10:U:H2'	5:F:11:C:H4'	1.99	0.45
7:H:43:U:H2'	7:H:44:U:C5	2.51	0.45
7:H:105:G:N2	7:H:107:A:H5'	2.32	0.45
35:1:508:THR:HB	35:1:510:PRO:CD	2.46	0.45
35:1:761:TYR:O	35:1:765:TYR:HB2	2.17	0.45
36:3:147:ASP:OD2	36:3:151:ARG:HG2	2.16	0.45
36:3:601:ARG:HD3	36:3:620:ASP:HB3	1.98	0.45
36:3:725:TYR:O	36:3:728:ARG:HB2	2.16	0.45
36:3:741:PHE:HB3	36:3:757:ILE:HG13	1.99	0.45
36:3:996:ILE:HG21	36:3:1041:TYR:CD1	2.52	0.45
39:2:526:ASP:O	39:2:528:ILE:N	2.50	0.45
39:2:569:GLN:O	39:2:573:ASP:HB2	2.17	0.45
1:A:188:LEU:HD23	1:A:188:LEU:HA	1.80	0.45
1:A:542:ASN:O	1:A:546:LEU:HB2	2.17	0.45
1:A:832:TYR:HB3	1:A:835:ASP:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1785:VAL:HG11	1:A:1807:ILE:HD13	1.99	0.45
11:L:176:LEU:C	11:L:176:LEU:CD1	2.85	0.45
15:P:51:PRO:HA	15:P:54:VAL:HG22	1.99	0.45
21:V:490:CYS:HA	21:V:493:ILE:HD12	1.99	0.45
23:X:172:LEU:HA	23:X:175:LEU:HD23	1.99	0.45
23:X:725:ARG:HD3	23:X:728:ARG:HH12	1.82	0.45
23:X:871:PHE:HB3	23:X:883:ASN:HD22	1.82	0.45
24:Y:117:ASP:N	24:Y:117:ASP:OD1	2.48	0.45
35:1:1015:ASP:OD1	35:1:1015:ASP:N	2.49	0.45
35:1:1167:TYR:CZ	39:2:581:LYS:HG2	2.49	0.45
36:3:528:ARG:HG3	36:3:529:ALA:N	2.31	0.45
36:3:1085:ALA:HB3	36:3:1088:LYS:HE2	1.97	0.45
42:5:33:VAL:CG2	42:5:76:CYS:HB2	2.47	0.45
1:A:1458:GLN:NE2	1:A:1463:LYS:HD3	2.32	0.45
3:C:177:ARG:C	3:C:179:VAL:H	2.20	0.45
3:C:188:VAL:HG23	3:C:190:LEU:HD11	1.98	0.45
3:C:678:THR:HB	3:C:680:ASN:O	2.17	0.45
9:J:357:LYS:N	9:J:357:LYS:HD2	2.31	0.45
14:O:167:PHE:O	14:O:172:GLU:N	2.48	0.45
14:O:249:ARG:O	14:O:253:TYR:N	2.50	0.45
15:P:73:GLU:HG2	15:P:76:ARG:HH21	1.81	0.45
17:R:184:GLN:HE21	17:R:184:GLN:HB3	1.46	0.45
19:T:399:LYS:HB2	19:T:406:ILE:HD11	1.98	0.45
19:T:478:LEU:HD23	19:T:488:VAL:HG22	1.98	0.45
21:V:503:TYR:CE2	21:V:550:MET:HG2	2.52	0.45
21:V:647:LEU:O	21:V:651:PRO:HD3	2.17	0.45
23:X:475:ASN:ND2	23:X:490:ARG:HD3	2.32	0.45
23:X:502:LEU:O	23:X:505:PHE:HB2	2.17	0.45
35:1:625:ARG:HH21	35:1:662:HIS:CG	2.35	0.45
35:1:694:LEU:HD22	35:1:727:VAL:CG2	2.47	0.45
35:1:826:ASP:OD1	35:1:827:ARG:N	2.50	0.45
36:3:27:GLN:OE1	36:3:42:ARG:NH1	2.50	0.45
36:3:164:ASN:HD22	36:3:190:GLU:HG2	1.82	0.45
36:3:1116:SER:HA	39:2:708:TRP:CZ2	2.50	0.45
1:A:108:MET:O	1:A:110:TRP:N	2.50	0.45
1:A:362:ARG:HH22	21:V:320:ARG:HA	1.82	0.45
1:A:1359:HIS:CD2	1:A:1361:GLU:O	2.70	0.45
1:A:1661:TRP:HH2	1:A:1684:PHE:CE1	2.35	0.45
3:C:685:ILE:HB	3:C:815:VAL:HG21	1.99	0.45
3:C:803:ARG:O	3:C:807:GLN:HG3	2.17	0.45
4:E:108:HIS:CE1	4:E:128:SER:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:176:VAL:O	4:E:189:THR:HA	2.17	0.45
11:L:14:THR:HG23	11:L:152:LEU:HD21	1.99	0.45
11:L:699:ASN:O	11:L:703:MET:N	2.50	0.45
17:R:147:THR:O	17:R:151:LEU:HB2	2.17	0.45
17:R:360:ARG:HD2	24:Y:274:ASP:OD2	2.16	0.45
23:X:674:THR:HG22	23:X:675:ASN:N	2.32	0.45
23:X:984:LEU:HD21	23:X:1000:VAL:HG21	1.97	0.45
35:1:550:HIS:CD2	35:1:551:LEU:HD22	2.49	0.45
35:1:854:VAL:HG11	35:1:891:GLN:HG3	1.97	0.45
35:1:1017:LEU:HD21	35:1:1058:ILE:HD11	1.99	0.45
35:1:1080:THR:HA	35:1:1083:TYR:CD2	2.52	0.45
36:3:243:ASP:OD1	36:3:244:GLY:N	2.50	0.45
36:3:407:ILE:HD11	36:3:1124:GLY:HA2	1.99	0.45
36:3:442:LEU:HD23	36:3:442:LEU:HA	1.71	0.45
36:3:611:ASP:O	36:3:612:ASN:HB2	2.17	0.45
41:7:9:ILE:O	41:7:88:ILE:HG22	2.17	0.45
1:A:995:ARG:HH11	1:A:998:ARG:HH11	1.64	0.45
1:A:1799:THR:O	1:A:1801:LYS:NZ	2.42	0.45
1:A:1820:LYS:NZ	1:A:1914:MET:HB2	2.32	0.45
2:B:26:A:H2'	2:B:27:U:O4'	2.17	0.45
3:C:774:THR:HG22	3:C:784:ILE:HD11	1.99	0.45
9:J:187:VAL:CG1	9:J:188:GLN:H	2.23	0.45
9:J:367:GLU:OE1	9:J:382:TYR:CZ	2.70	0.45
13:N:9:LYS:HE2	13:N:9:LYS:HB3	1.57	0.45
15:P:184:VAL:HG13	15:P:184:VAL:O	2.16	0.45
17:R:386:ARG:NE	17:R:386:ARG:HA	2.29	0.45
21:V:539:LEU:HB3	21:V:543:LYS:HB2	1.99	0.45
21:V:551:PHE:HA	21:V:554:LEU:HD12	1.98	0.45
35:1:685:SER:O	35:1:689:ILE:HG12	2.17	0.45
35:1:721:ILE:C	35:1:721:ILE:CD1	2.85	0.45
35:1:856:ASP:HB3	35:1:864:TYR:CE2	2.51	0.45
35:1:963:LYS:O	35:1:965:CYS:N	2.50	0.45
35:1:1063:LEU:HA	35:1:1063:LEU:HD23	1.64	0.45
36:3:292:THR:HG1	36:3:301:PHE:HD1	1.64	0.45
36:3:312:LYS:HB2	36:3:330:PHE:CD1	2.50	0.45
36:3:485:LEU:HA	36:3:494:VAL:HB	1.98	0.45
36:3:558:LEU:HD23	36:3:562:GLU:HB3	1.99	0.45
36:3:717:SER:HB2	36:3:718:ARG:HH12	1.81	0.45
36:3:1021:LEU:HD23	36:3:1021:LEU:HA	1.77	0.45
36:3:1041:TYR:HD2	39:2:705:ARG:HG3	1.81	0.45
39:2:541:GLN:O	39:2:545:GLU:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:GLU:OE1	1:A:64:GLU:N	2.35	0.44
1:A:367:SER:OG	1:A:368:GLN:N	2.50	0.44
1:A:1189:MET:CG	1:A:1190:CYS:H	2.30	0.44
1:A:1606:ILE:HD11	1:A:1631:LEU:HD13	1.98	0.44
1:A:2007:ILE:HA	1:A:2010:ILE:HG22	1.99	0.44
2:B:67:A:H2'	2:B:68:C:O4'	2.17	0.44
6:G:1:G:C6	6:G:2:U:H1'	2.52	0.44
6:G:99:C:N3	7:H:33:G:C5	2.86	0.44
7:H:106:G:N3	7:H:107:A:N6	2.65	0.44
9:J:205:LEU:C	9:J:205:LEU:CD2	2.84	0.44
17:R:411:LEU:HD13	17:R:411:LEU:HA	1.74	0.44
35:1:536:LEU:O	35:1:540:MET:HG2	2.16	0.44
35:1:721:ILE:CG2	35:1:756:LEU:HD23	2.26	0.44
35:1:1046:GLY:O	35:1:1048:GLU:N	2.50	0.44
35:1:1304:LEU:HD21	42:5:55:ILE:HG22	1.99	0.44
36:3:38:LEU:HD12	36:3:38:LEU:HA	1.79	0.44
36:3:965:LYS:HB3	36:3:965:LYS:HE2	1.69	0.44
36:3:1156:CYS:O	36:3:1158:ARG:N	2.50	0.44
39:2:596:GLU:N	39:2:596:GLU:OE2	2.50	0.44
1:A:67:ARG:HD2	13:N:33:GLU:OE2	2.17	0.44
3:C:260:ILE:CD1	3:C:309:PHE:HB3	2.47	0.44
3:C:719:GLN:HG3	3:C:724:TRP:O	2.17	0.44
4:E:266:PRO:CG	11:L:789:ALA:HA	2.47	0.44
7:H:114:A:H2'	7:H:115:G:C8	2.53	0.44
15:P:188:TRP:O	15:P:188:TRP:CD1	2.70	0.44
15:P:205:LYS:HG2	15:P:208:LYS:HB3	1.98	0.44
17:R:404:GLU:OE1	23:X:327:ARG:NE	2.42	0.44
23:X:182:ALA:HB1	23:X:186:ARG:HH21	1.82	0.44
23:X:388:GLN:O	23:X:392:ILE:HG13	2.17	0.44
23:X:719:ALA:HB1	23:X:736:ARG:HE	1.82	0.44
24:Y:221:ALA:O	24:Y:225:GLU:HG2	2.17	0.44
35:1:645:LEU:HD13	35:1:682:HIS:CD2	2.53	0.44
35:1:1277:GLN:H	36:3:113:ARG:CZ	2.30	0.44
35:1:1299:GLU:HB3	42:5:43:TYR:CE2	2.52	0.44
36:3:101:LYS:HB2	36:3:101:LYS:HE3	1.65	0.44
36:3:275:ARG:HH21	36:3:275:ARG:CB	2.31	0.44
36:3:925:VAL:O	36:3:942:LYS:HA	2.18	0.44
36:3:988:ASN:ND2	36:3:1004:ASP:OD1	2.50	0.44
36:3:1211:ILE:HD12	36:3:1214:ARG:HE	1.82	0.44
1:A:122:ILE:HG13	1:A:481:PHE:O	2.17	0.44
1:A:305:ARG:HG3	3:C:878:ILE:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:LEU:HD23	1:A:329:LEU:H	1.83	0.44
1:A:644:ILE:HD12	1:A:644:ILE:HA	1.80	0.44
1:A:1117:HIS:CE1	15:P:199:LYS:HG3	2.53	0.44
1:A:1498:TRP:O	1:A:1501:LEU:HG	2.16	0.44
3:C:304:LEU:H	3:C:304:LEU:HD12	1.82	0.44
3:C:585:THR:O	3:C:587:VAL:HG23	2.17	0.44
3:C:687:MET:HB3	3:C:815:VAL:CG1	2.47	0.44
4:E:263:ASP:O	4:E:272:ARG:HD2	2.16	0.44
5:F:30:A:H2'	5:F:31:U:O4'	2.17	0.44
5:F:58:G:HO2'	5:F:59:G:P	2.38	0.44
5:F:93:G:H2'	5:F:94:C:C6	2.52	0.44
7:H:18:U:O2	17:R:258:LYS:HB2	2.17	0.44
11:L:233:GLN:H	11:L:233:GLN:CD	2.19	0.44
17:R:184:GLN:H	17:R:184:GLN:HG2	1.50	0.44
17:R:383:ASN:N	17:R:383:ASN:OD1	2.51	0.44
19:T:435:THR:HB	19:T:451:HIS:CE1	2.53	0.44
21:V:503:TYR:HE2	21:V:550:MET:HG2	1.82	0.44
21:V:532:GLN:HE22	21:V:539:LEU:HD11	1.82	0.44
23:X:698:LYS:HZ2	23:X:758:THR:HA	1.82	0.44
23:X:1017:LYS:HE2	23:X:1017:LYS:HB2	1.76	0.44
24:Y:246:LYS:HE3	24:Y:312:HIS:CB	2.40	0.44
35:1:658:TRP:CZ3	35:1:698:GLN:HG2	2.52	0.44
35:1:750:ILE:HG13	35:1:751:GLY:N	2.32	0.44
35:1:946:LYS:O	35:1:950:GLN:HG3	2.17	0.44
35:1:1158:ILE:HG13	35:1:1159:GLY:N	2.32	0.44
36:3:341:VAL:HG12	36:3:347:LEU:HB2	2.00	0.44
36:3:488:GLY:C	36:3:490:THR:H	2.20	0.44
39:2:477:MET:SD	39:2:478:HIS:CE1	3.10	0.44
1:A:159:ARG:HA	1:A:159:ARG:CZ	2.48	0.44
1:A:1554:GLN:HG3	1:A:1561:PHE:HE1	1.82	0.44
3:C:461:LEU:HD21	3:C:572:GLU:OE2	2.18	0.44
3:C:642:HIS:O	3:C:646:LYS:HB2	2.18	0.44
3:C:711:ARG:HA	3:C:714:LEU:HD22	1.99	0.44
4:E:181:ILE:HG22	4:E:182:ARG:NH1	2.32	0.44
7:H:160:A:C2	7:H:171:U:C2	3.05	0.44
12:M:160:PHE:C	12:M:161:PHE:HD1	2.20	0.44
12:M:215:ASN:ND2	17:R:261:THR:N	2.49	0.44
23:X:289:GLN:HA	23:X:292:LEU:HD23	2.00	0.44
24:Y:126:PHE:C	24:Y:126:PHE:CD2	2.91	0.44
35:1:781:ASP:O	35:1:785:LYS:HG3	2.17	0.44
35:1:857:LEU:HA	35:1:865:ARG:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:1142:ASN:H	35:1:1142:ASN:HD22	1.64	0.44
36:3:124:ASP:OD2	36:3:128:ARG:HG3	2.17	0.44
36:3:125:PRO:HG2	36:3:174:ASP:HA	1.99	0.44
36:3:278:LEU:HD21	36:3:816:LYS:NZ	2.32	0.44
36:3:543:THR:C	36:3:558:LEU:HD12	2.38	0.44
36:3:924:PHE:HA	36:3:943:THR:O	2.18	0.44
36:3:993:ILE:HG23	36:3:1002:VAL:HG23	1.99	0.44
36:3:1151:GLU:OE2	36:3:1193:VAL:HG21	2.18	0.44
1:A:120:TYR:HE1	1:A:485:THR:OG1	2.01	0.44
1:A:758:ARG:HD2	1:A:775:ASN:HD21	1.83	0.44
1:A:1284:LEU:HA	1:A:1284:LEU:HD23	1.72	0.44
3:C:118:PHE:O	3:C:122:LEU:HD12	2.17	0.44
3:C:514:TYR:HB2	3:C:521:ASP:HB2	1.99	0.44
5:F:44:G:H8	5:F:44:G:OP2	2.00	0.44
5:F:79:C:O2'	5:F:80:G:O5'	2.32	0.44
12:M:125:SER:HB2	17:R:237:MET:O	2.18	0.44
15:P:78:ARG:HD3	15:P:78:ARG:HA	1.72	0.44
17:R:86:LEU:HD23	17:R:86:LEU:H	1.81	0.44
21:V:468:ASP:OD1	21:V:468:ASP:N	2.49	0.44
21:V:497:CYS:HB3	21:V:507:PHE:HB2	1.99	0.44
21:V:622:ARG:NH2	21:V:623:ASN:HB3	2.32	0.44
23:X:461:VAL:HA	23:X:464:ARG:NE	2.33	0.44
23:X:461:VAL:HG22	23:X:464:ARG:HH21	1.83	0.44
24:Y:33:LYS:HD3	24:Y:33:LYS:HA	1.67	0.44
24:Y:186:LEU:HD23	24:Y:186:LEU:HA	1.71	0.44
35:1:1167:TYR:OH	39:2:581:LYS:HD3	2.18	0.44
36:3:1:MET:SD	39:2:709:GLY:O	2.76	0.44
36:3:331:ASP:CG	36:3:390:ARG:HH21	2.20	0.44
36:3:404:LEU:HB3	36:3:407:ILE:HG12	1.99	0.44
36:3:485:LEU:CD2	36:3:491:VAL:HG12	2.46	0.44
36:3:753:GLY:O	36:3:754:ILE:HD13	2.17	0.44
36:3:1098:GLY:C	36:3:1099:GLU:HG3	2.38	0.44
1:A:369:GLU:OE1	1:A:370:PRO:HD2	2.18	0.44
1:A:564:TYR:HA	1:A:569:VAL:HG23	1.99	0.44
1:A:1043:TYR:O	1:A:1046:LEU:HB3	2.18	0.44
4:E:181:ILE:HD12	4:E:181:ILE:N	2.32	0.44
5:F:26:U:H3'	5:F:27:A:H5"	2.00	0.44
9:J:333:PHE:O	9:J:337:MET:HG2	2.18	0.44
11:L:223:GLY:O	11:L:225:TYR:N	2.51	0.44
15:P:218:GLU:HA	15:P:221:LYS:HG3	2.00	0.44
17:R:330:LYS:NZ	23:X:275:ARG:HH22	2.07	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:191:HIS:CD2	19:T:440:ASP:OD1	2.70	0.44
21:V:617:PRO:HB3	21:V:623:ASN:ND2	2.32	0.44
24:Y:194:ASP:N	24:Y:194:ASP:OD1	2.50	0.44
35:1:566:LEU:HD12	35:1:566:LEU:HA	1.89	0.44
35:1:668:VAL:HG22	35:1:686:LEU:HD23	1.99	0.44
36:3:114:ARG:NH1	42:5:34:ASN:O	2.51	0.44
36:3:590:MET:HB2	36:3:606:ALA:O	2.18	0.44
42:5:50:LEU:HA	42:5:50:LEU:HD12	1.54	0.44
1:A:946:GLU:HG2	1:A:954:LYS:NZ	2.33	0.44
3:C:349:PHE:HE1	3:C:354:ARG:HA	1.83	0.44
3:C:485:ASP:OD2	3:C:485:ASP:N	2.47	0.44
4:E:304:SER:O	4:E:330:ILE:HD12	2.17	0.44
9:J:428:GLU:O	9:J:432:VAL:HG13	2.18	0.44
17:R:348:GLU:OE1	23:X:263:SER:HB3	2.17	0.44
21:V:554:LEU:HA	21:V:559:SER:OG	2.18	0.44
23:X:659:ILE:O	23:X:669:LYS:NZ	2.50	0.44
35:1:769:VAL:HG13	35:1:773:LEU:HD21	1.98	0.44
36:3:595:VAL:HG22	36:3:596:PRO:O	2.17	0.44
1:A:1635:TYR:CE2	1:A:1636:LYS:HB2	2.52	0.44
1:A:1813:ARG:HA	1:A:1929:SER:HB2	1.99	0.44
1:A:1963:GLU:O	1:A:1965:HIS:N	2.51	0.44
3:C:587:VAL:HG11	3:C:830:PRO:HG3	1.99	0.44
3:C:789:PHE:CE2	3:C:816:VAL:HG13	2.53	0.44
3:C:902:HIS:ND1	3:C:903:HIS:HD2	2.16	0.44
5:F:32:U:H2'	5:F:33:G:C8	2.53	0.44
17:R:325:ARG:HA	17:R:325:ARG:HD2	1.50	0.44
21:V:570:LEU:HD23	21:V:570:LEU:HA	1.86	0.44
23:X:620:GLU:CD	23:X:620:GLU:H	2.15	0.44
23:X:824:LEU:HA	23:X:827:MET:HG2	1.99	0.44
24:Y:39:TYR:HB3	24:Y:185:GLN:HE22	1.82	0.44
35:1:575:LEU:HD11	35:1:613:MET:SD	2.58	0.44
35:1:666:LYS:HB3	35:1:704:ILE:CD1	2.48	0.44
36:3:528:ARG:HG3	36:3:529:ALA:H	1.83	0.44
36:3:554:VAL:HG12	36:3:556:ILE:HG23	2.00	0.44
1:A:929:GLU:OE1	1:A:933:ARG:NH2	2.51	0.44
1:A:1527:ASN:O	1:A:1529:ILE:HD12	2.17	0.44
1:A:1854:VAL:HA	1:A:1857:GLN:OE1	2.17	0.44
1:A:1865:ARG:HA	1:A:1865:ARG:NH2	2.33	0.44
3:C:78:GLU:HG3	3:C:79:THR:N	2.33	0.44
3:C:267:LEU:HD23	3:C:267:LEU:HA	1.80	0.44
3:C:305:GLY:O	3:C:433:MET:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:470:PRO:HA	3:C:499:GLY:O	2.18	0.44
4:E:287:ASN:OD1	4:E:288:LEU:N	2.51	0.44
6:G:99:C:C4	7:H:33:G:C5	3.05	0.44
6:G:99:C:C4	7:H:33:G:C6	3.05	0.44
9:J:199:LYS:C	9:J:199:LYS:CD	2.84	0.44
13:N:124:SER:OG	13:N:125:LYS:HD2	2.18	0.44
17:R:311:LYS:HG3	24:Y:200:PHE:HZ	1.83	0.44
35:1:807:LYS:CG	35:1:844:VAL:HG12	2.47	0.44
35:1:819:TRP:CE3	35:1:867:MET:HE1	2.52	0.44
35:1:1212:LEU:HD12	35:1:1212:LEU:HA	1.76	0.44
35:1:1281:ILE:HD11	42:5:38:ASP:HB3	2.00	0.44
36:3:325:ILE:HB	36:3:375:SER:HB3	1.99	0.44
36:3:565:TYR:HB3	36:3:577:TYR:CB	2.46	0.44
36:3:770:LEU:HD23	36:3:770:LEU:HA	1.82	0.44
39:2:534:GLN:HG2	39:2:538:GLU:OE1	2.18	0.44
1:A:599:MET:O	1:A:603:ARG:HG3	2.17	0.43
5:F:13:G:H2'	5:F:14:C:C6	2.53	0.43
5:F:36:A:C3'	5:F:37:C:H5"	2.37	0.43
5:F:58:G:O2'	5:F:59:G:H5'	2.17	0.43
5:F:87:C:OP2	12:M:193:ARG:HA	2.18	0.43
8:I:50:LYS:CB	8:I:51:PRO:HD3	2.47	0.43
9:J:440:LEU:O	9:J:445:LYS:HD2	2.17	0.43
19:T:266:GLU:HG2	19:T:290:ALA:HB1	2.00	0.43
23:X:681:LEU:O	23:X:725:ARG:NH2	2.50	0.43
23:X:1003:ILE:HG13	23:X:1004:GLU:N	2.33	0.43
24:Y:28:PHE:O	24:Y:32:CYS:HB2	2.18	0.43
35:1:827:ARG:HB2	35:1:827:ARG:CZ	2.47	0.43
35:1:967:GLU:HB3	35:1:971:MET:H	1.83	0.43
36:3:234:PHE:CD1	36:3:235:LEU:N	2.86	0.43
36:3:543:THR:O	36:3:558:LEU:HD12	2.17	0.43
36:3:595:VAL:HG21	36:3:600:GLN:C	2.39	0.43
1:A:1963:GLU:O	1:A:1966:HIS:N	2.50	0.43
3:C:436:GLN:HB3	3:C:437:HIS:HD2	1.82	0.43
5:F:34:G:H2'	5:F:35:A:C8	2.54	0.43
6:G:88:G:H2'	6:G:88:G:N3	2.33	0.43
7:H:161:U:H2'	7:H:163:G:N2	2.32	0.43
13:N:120:ARG:HA	13:N:120:ARG:HD2	1.66	0.43
17:R:320:HIS:HA	17:R:323:LYS:CE	2.48	0.43
19:T:333:VAL:HA	19:T:349:SER:HB2	1.99	0.43
21:V:496:CYS:HA	21:V:499:GLN:OE1	2.17	0.43
23:X:871:PHE:HB3	23:X:883:ASN:ND2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:892:LEU:HD22	35:1:892:LEU:HA	1.70	0.43
35:1:1108:ASN:N	35:1:1108:ASN:OD1	2.51	0.43
36:3:696:SER:O	36:3:696:SER:OG	2.32	0.43
39:2:451:LYS:O	39:2:454:LEU:HG	2.18	0.43
39:2:469:VAL:HG12	39:2:471:ARG:N	2.31	0.43
42:5:44:MET:HE2	42:5:44:MET:HB2	1.80	0.43
1:A:1401:ARG:HG2	1:A:1401:ARG:HH11	1.82	0.43
1:A:1690:ASP:OD1	1:A:1693:SER:OG	2.29	0.43
1:A:1779:PHE:CD2	1:A:1862:ILE:HD11	2.53	0.43
3:C:660:VAL:HG22	3:C:878:ILE:HD11	2.01	0.43
3:C:682:LYS:HB3	3:C:797:ALA:CB	2.45	0.43
4:E:283:ASN:O	4:E:286:LYS:HD2	2.19	0.43
18:S:96:GLY:O	18:S:131:ARG:HA	2.19	0.43
23:X:915:ARG:O	23:X:919:GLU:HG3	2.18	0.43
35:1:617:ILE:CA	35:1:663:THR:HG21	2.46	0.43
35:1:1254:LEU:O	35:1:1262:ARG:HG2	2.19	0.43
36:3:549:VAL:HG12	36:3:550:ASN:O	2.18	0.43
36:3:604:PHE:CZ	36:3:681:PRO:HD3	2.53	0.43
36:3:779:PHE:N	36:3:779:PHE:CD1	2.86	0.43
1:A:41:GLN:NE2	1:A:45:TYR:HD2	2.09	0.43
3:C:173:THR:O	3:C:177:ARG:HB2	2.18	0.43
4:E:96:TYR:OH	4:E:336:HIS:NE2	2.49	0.43
6:G:116:C:C5	17:R:370:SER:CB	3.01	0.43
7:H:56:A:HO2'	39:2:481:THR:HG1	1.50	0.43
19:T:288:LEU:O	19:T:289:SER:OG	2.34	0.43
21:V:515:CYS:HA	21:V:521:TYR:HB2	2.00	0.43
21:V:546:ASN:OD1	21:V:547:VAL:N	2.51	0.43
23:X:297:ARG:HE	23:X:297:ARG:HB3	1.60	0.43
23:X:743:TYR:HA	23:X:747:LEU:HD23	2.00	0.43
35:1:721:ILE:HG22	35:1:756:LEU:CD2	2.26	0.43
35:1:969:LYS:HD2	35:1:969:LYS:H	1.83	0.43
35:1:1252:GLN:NE2	39:2:497:SER:OG	2.51	0.43
36:3:249:LEU:HD12	36:3:249:LEU:N	2.33	0.43
36:3:424:TYR:HD1	36:3:437:VAL:HG22	1.82	0.43
36:3:955:PHE:HZ	36:3:1014:TYR:CD2	2.36	0.43
39:2:528:ILE:O	39:2:531:THR:HG23	2.18	0.43
41:7:74:GLU:O	41:7:78:GLN:HG3	2.18	0.43
1:A:1580:HIS:HB3	1:A:1583:GLN:NE2	2.33	0.43
1:A:1660:TYR:OH	1:A:1717:ASN:O	2.23	0.43
3:C:392:LEU:HB3	3:C:393:PRO:HD3	2.01	0.43
4:E:301:ALA:HB2	4:E:335:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:326:HIS:CE1	4:E:346:SER:HB2	2.52	0.43
6:G:90:C:H2'	6:G:91:A:C8	2.53	0.43
7:H:35:A:H3'	7:H:36:G:H8	1.83	0.43
12:M:153:ARG:HB2	12:M:160:PHE:HE2	1.83	0.43
13:N:7:SER:O	13:N:8:ARG:HB2	2.18	0.43
17:R:353:ASP:O	17:R:357:HIS:HB2	2.19	0.43
35:1:806:ILE:HA	35:1:810:ILE:HD12	2.00	0.43
36:3:705:ARG:NH2	36:3:746:ALA:HB2	2.34	0.43
39:2:512:GLN:N	39:2:512:GLN:OE1	2.51	0.43
42:5:63:ARG:HD3	42:5:63:ARG:HA	1.77	0.43
1:A:1109:LEU:HG	1:A:1152:ALA:HB1	2.00	0.43
1:A:1586:HIS:NE2	1:A:1664:ILE:HG13	2.34	0.43
3:C:154:HIS:C	3:C:156:GLU:H	2.22	0.43
3:C:231:ALA:O	3:C:277:LYS:HE3	2.18	0.43
4:E:133:VAL:HG22	4:E:154:VAL:HG21	2.00	0.43
4:E:239:THR:OG1	4:E:289:LEU:O	2.22	0.43
8:I:276:ARG:CB	16:Q:357:ALA:CA	2.97	0.43
9:J:240:THR:HG22	9:J:241:VAL:N	2.33	0.43
9:J:400:GLU:O	9:J:404:GLU:HG2	2.19	0.43
19:T:213:GLU:HG2	19:T:214:PRO:CD	2.48	0.43
19:T:269:GLN:HE21	19:T:269:GLN:HB3	1.60	0.43
23:X:523:HIS:O	23:X:525:ARG:HG2	2.18	0.43
23:X:586:ALA:CB	35:1:826:ASP:HA	2.49	0.43
23:X:654:ASP:OD1	23:X:655:MET:N	2.52	0.43
24:Y:147:ASP:OD2	24:Y:147:ASP:N	2.51	0.43
24:Y:225:GLU:OE1	24:Y:233:ALA:HA	2.18	0.43
35:1:503:LYS:HE2	35:1:511:MET:CG	2.44	0.43
35:1:781:ASP:HB3	35:1:784:MET:HB2	2.00	0.43
35:1:1106:ARG:H	35:1:1109:ARG:HG3	1.84	0.43
36:3:35:GLY:HA3	42:5:47:PHE:CZ	2.54	0.43
36:3:131:MET:HB2	36:3:141:VAL:HG22	2.01	0.43
36:3:412:ILE:H	36:3:1105:GLN:NE2	2.09	0.43
36:3:526:HIS:HB2	36:3:574:LEU:CD2	2.48	0.43
36:3:715:MET:HE3	36:3:739:LEU:H	1.84	0.43
36:3:791:HIS:NE2	36:3:793:GLU:HB2	2.34	0.43
36:3:1114:SER:HB2	36:3:1215:TYR:HE1	1.83	0.43
39:2:511:LEU:HA	39:2:511:LEU:HD23	1.73	0.43
39:2:707:PRO:HG2	39:2:710:GLU:HG2	2.00	0.43
1:A:82:ARG:HE	1:A:82:ARG:HB3	1.70	0.43
1:A:785:LYS:HB3	1:A:785:LYS:HE3	1.67	0.43
1:A:1661:TRP:HH2	1:A:1684:PHE:HE1	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1799:THR:O	1:A:1801:LYS:HG3	2.19	0.43
1:A:1969:PRO:HB2	1:A:1971:LEU:CD2	2.47	0.43
3:C:177:ARG:HG3	3:C:179:VAL:HB	2.01	0.43
3:C:665:THR:HG21	3:C:828:MET:HG3	2.01	0.43
4:E:335:PHE:CE1	4:E:342:ILE:HD12	2.54	0.43
6:G:90:C:H2'	6:G:91:A:C4	2.54	0.43
6:G:107:U:C2	23:X:709:LEU:HD13	2.54	0.43
7:H:118:G:C6	7:H:140:A:N6	2.87	0.43
9:J:429:PHE:HA	9:J:432:VAL:HG22	1.99	0.43
11:L:92:THR:OG1	11:L:95:GLN:HG3	2.19	0.43
17:R:428:GLU:O	17:R:429:ILE:HD13	2.19	0.43
21:V:609:GLN:N	21:V:610:PRO:HD2	2.33	0.43
23:X:268:GLN:HA	23:X:271:LYS:HE2	2.00	0.43
23:X:289:GLN:NE2	23:X:293:GLU:OE2	2.51	0.43
24:Y:183:ARG:HA	24:Y:183:ARG:CZ	2.48	0.43
35:1:551:LEU:O	35:1:555:VAL:HG23	2.19	0.43
35:1:641:ILE:CG2	35:1:682:HIS:NE2	2.82	0.43
35:1:962:MET:O	35:1:967:GLU:HB2	2.18	0.43
36:3:16:PHE:HE2	36:3:63:ARG:C	2.22	0.43
36:3:169:HIS:HD2	36:3:170:VAL:O	2.02	0.43
36:3:373:PHE:HD1	36:3:385:PHE:CD2	2.36	0.43
36:3:641:CYS:H	36:3:701:LEU:HD23	1.83	0.43
36:3:769:LYS:HD3	36:3:769:LYS:H	1.81	0.43
39:2:472:PRO:O	39:2:475:VAL:HG23	2.19	0.43
39:2:483:GLN:OE1	39:2:483:GLN:N	2.51	0.43
1:A:191:ILE:HD13	1:A:191:ILE:HG21	1.69	0.43
1:A:305:ARG:HG3	3:C:878:ILE:CG2	2.48	0.43
1:A:1213:VAL:HG22	1:A:1229:PHE:CD1	2.54	0.43
1:A:1623:ASN:H	1:A:1623:ASN:ND2	2.17	0.43
1:A:1718:TRP:HZ3	1:A:1726:ILE:HD11	1.84	0.43
1:A:1781:ASP:HB2	1:A:1808:PHE:HB3	2.01	0.43
6:G:88:G:H1'	7:H:42:G:N2	2.33	0.43
6:G:112:U:OP1	23:X:503:ARG:HG2	2.19	0.43
7:H:162:U:H4'	7:H:163:G:O4'	2.18	0.43
9:J:354:LEU:HA	9:J:354:LEU:HD23	1.81	0.43
19:T:356:LEU:HD13	19:T:366:VAL:HB	2.00	0.43
19:T:394:ASN:OD1	19:T:394:ASN:N	2.51	0.43
21:V:547:VAL:HA	21:V:550:MET:HG3	2.00	0.43
23:X:399:LEU:HD23	23:X:399:LEU:HA	1.84	0.43
23:X:868:ARG:NH2	23:X:973:ASN:HD21	2.16	0.43
35:1:963:LYS:HG3	35:1:964:THR:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:3:331:ASP:OD2	36:3:393:LYS:N	2.39	0.43
36:3:1035:THR:HG21	36:3:1103:SER:HA	2.01	0.43
36:3:1183:ASN:OD1	36:3:1183:ASN:N	2.51	0.43
1:A:64:GLU:H	1:A:64:GLU:CD	2.21	0.43
1:A:1050:LEU:HD23	1:A:1050:LEU:HA	1.83	0.43
1:A:1224:ARG:HG2	21:V:592:GLU:O	2.19	0.43
1:A:1975:GLU:HG2	1:A:1979:VAL:HG13	2.00	0.43
3:C:112:THR:HG1	3:C:116:MET:HB3	1.84	0.43
3:C:193:THR:HB	3:C:428:THR:CG2	2.49	0.43
3:C:242:LEU:HD23	3:C:242:LEU:HA	1.68	0.43
3:C:300:LEU:HA	3:C:306:ASN:HD22	1.84	0.43
4:E:305:ALA:HA	4:E:329:SER:HB2	1.99	0.43
5:F:80:G:N2	9:J:209:PRO:HD3	2.34	0.43
13:N:7:SER:C	13:N:9:LYS:H	2.22	0.43
17:R:391:VAL:HG13	17:R:396:VAL:HB	2.01	0.43
21:V:502:THR:HG22	21:V:503:TYR:H	1.84	0.43
23:X:419:ILE:HG21	23:X:557:THR:OG1	2.19	0.43
23:X:535:LEU:O	23:X:539:VAL:HG23	2.19	0.43
23:X:587:PRO:HB2	35:1:827:ARG:NH1	2.32	0.43
35:1:493:LYS:O	35:1:496:LYS:N	2.52	0.43
35:1:1167:TYR:CE2	39:2:581:LYS:HA	2.53	0.43
35:1:1273:TYR:O	35:1:1277:GLN:HB3	2.19	0.43
36:3:192:ALA:HA	36:3:200:ALA:HB3	2.01	0.43
36:3:638:GLU:O	36:3:638:GLU:HG3	2.19	0.43
39:2:517:ILE:H	39:2:517:ILE:HG13	1.27	0.43
41:7:30:CYS:CB	41:7:72:CYS:HG	2.32	0.43
42:5:20:GLY:HA2	42:5:34:ASN:ND2	2.33	0.43
1:A:976:MET:HB2	1:A:976:MET:HE2	1.71	0.43
1:A:1581:LEU:HD22	1:A:1746:ARG:HH11	1.84	0.43
3:C:200:PHE:CE1	3:C:434:CYS:SG	3.12	0.43
3:C:478:THR:CG2	3:C:492:ALA:HB1	2.37	0.43
3:C:624:SER:OG	3:C:941:LYS:HA	2.19	0.43
3:C:658:PRO:HB2	3:C:881:PHE:CZ	2.54	0.43
3:C:673:LYS:HB3	3:C:688:ILE:CG2	2.49	0.43
5:F:37:C:H6	5:F:37:C:H2'	1.48	0.43
5:F:97:U:O5'	5:F:97:U:H6	2.01	0.43
6:G:20:A:H1'	14:O:193:LEU:O	2.19	0.43
9:J:260:ARG:NH1	11:L:215:PRO:HD3	2.33	0.43
11:L:178:GLU:HA	11:L:181:ARG:CG	2.49	0.43
11:L:646:GLY:O	11:L:650:GLY:N	2.52	0.43
12:M:165:ASN:O	17:R:95:LYS:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:72:ARG:HA	15:P:75:ASN:HD21	1.83	0.43
17:R:327:MET:HB3	23:X:279:LEU:HD11	1.99	0.43
21:V:545:ARG:HG3	21:V:585:ILE:HD13	2.00	0.43
23:X:516:VAL:HG13	23:X:549:LEU:HD13	2.01	0.43
23:X:913:ASP:O	23:X:916:GLU:HG3	2.19	0.43
35:1:548:GLU:O	35:1:552:LEU:HG	2.19	0.43
35:1:606:LEU:HD12	35:1:606:LEU:HA	1.75	0.43
35:1:1172:LEU:HD12	39:2:522:PHE:CE1	2.54	0.43
36:3:123:VAL:HG22	36:3:124:ASP:H	1.84	0.43
36:3:595:VAL:HG21	36:3:601:ARG:N	2.34	0.43
36:3:665:LEU:HB2	36:3:679:LEU:HD23	2.00	0.43
36:3:882:LEU:HD13	36:3:882:LEU:HA	1.73	0.43
1:A:75:ASP:OD1	1:A:75:ASP:N	2.47	0.42
1:A:387:PHE:HZ	3:C:330:THR:HG21	1.83	0.42
1:A:1397:ILE:HA	1:A:1397:ILE:HD13	1.72	0.42
1:A:1719:PHE:HB2	1:A:1720:PRO:HD2	2.01	0.42
3:C:189:VAL:HA	3:C:198:TYR:O	2.19	0.42
3:C:506:PRO:HB2	3:C:569:ARG:HH22	1.84	0.42
3:C:938:ARG:O	3:C:942:GLY:N	2.50	0.42
7:H:152:G:C6	7:H:153:A:N6	2.87	0.42
9:J:197:GLU:OE2	11:L:156:ARG:HD3	2.19	0.42
11:L:57:SER:O	11:L:57:SER:OG	2.36	0.42
17:R:155:VAL:O	17:R:159:VAL:HG12	2.18	0.42
19:T:253:ILE:O	19:T:261:LEU:HD12	2.19	0.42
19:T:471:ASP:OD2	19:T:472:GLN:N	2.48	0.42
23:X:257:PHE:CE2	23:X:262:LEU:HD21	2.54	0.42
23:X:396:ARG:NE	23:X:431:GLN:HE22	2.17	0.42
23:X:397:ARG:HA	23:X:402:PHE:CD1	2.54	0.42
23:X:991:LEU:HB2	23:X:995:GLU:OE1	2.19	0.42
35:1:666:LYS:O	35:1:670:GLN:HG2	2.19	0.42
35:1:1149:LYS:O	35:1:1152:SER:HB3	2.17	0.42
35:1:1294:THR:O	42:5:76:CYS:CA	2.65	0.42
36:3:804:HIS:O	42:5:58:ASN:ND2	2.52	0.42
1:A:382:GLU:N	1:A:382:GLU:OE1	2.52	0.42
1:A:1076:ASP:N	1:A:1076:ASP:OD1	2.52	0.42
1:A:1555:LEU:HD22	1:A:1555:LEU:HA	1.71	0.42
1:A:1756:SER:HA	35:1:943:LYS:HB3	2.01	0.42
3:C:89:LEU:HD12	19:T:240:LEU:HD11	2.01	0.42
3:C:193:THR:HB	3:C:428:THR:HG21	2.01	0.42
3:C:255:VAL:O	3:C:307:VAL:HA	2.18	0.42
3:C:933:PHE:O	3:C:937:THR:HG22	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:35:A:H2	5:F:36:A:N6	2.16	0.42
5:F:42:C:H3'	5:F:43:A:C8	2.54	0.42
6:G:90:C:N4	7:H:40:C:H42	2.16	0.42
17:R:367:ARG:HD2	17:R:368:ASN:N	2.35	0.42
19:T:394:ASN:ND2	19:T:408:ASN:HD22	2.17	0.42
23:X:419:ILE:HG21	23:X:569:VAL:HG22	2.01	0.42
24:Y:183:ARG:HH21	24:Y:187:ASP:CG	2.21	0.42
24:Y:207:GLU:HA	24:Y:210:GLU:HB3	2.01	0.42
35:1:815:PHE:HA	35:1:819:TRP:HD1	1.83	0.42
35:1:903:GLN:OE1	35:1:910:MET:HB2	2.19	0.42
35:1:1199:VAL:HG12	35:1:1199:VAL:O	2.19	0.42
35:1:1227:ILE:O	35:1:1231:MET:HG2	2.19	0.42
36:3:77:TYR:HE2	36:3:152:LEU:HD22	1.84	0.42
36:3:115:ILE:HD11	42:5:18:TYR:HA	2.02	0.42
36:3:483:LEU:HD11	36:3:493:GLU:OE2	2.19	0.42
36:3:499:PHE:CZ	36:3:516:LEU:HD22	2.46	0.42
36:3:514:ASP:OD1	36:3:514:ASP:N	2.52	0.42
36:3:1028:THR:O	39:2:496:ASN:ND2	2.52	0.42
36:3:1158:ARG:HG3	36:3:1159:ASP:N	2.34	0.42
36:3:1175:ASP:OD1	36:3:1178:LEU:N	2.52	0.42
42:5:12:GLU:HA	42:5:15:GLN:HB3	2.01	0.42
1:A:57:GLN:O	1:A:57:GLN:NE2	2.52	0.42
1:A:758:ARG:NH2	1:A:775:ASN:HD22	2.15	0.42
3:C:505:GLN:HG3	3:C:507:VAL:HG13	2.00	0.42
3:C:665:THR:OG1	3:C:666:VAL:N	2.52	0.42
4:E:218:LYS:HE2	4:E:218:LYS:HB2	1.81	0.42
4:E:341:ILE:C	4:E:342:ILE:HD13	2.39	0.42
5:F:35:A:C5	6:G:11:A:N1	2.87	0.42
5:F:73:A:OP1	5:F:75:G:O2'	2.32	0.42
9:J:183:ALA:O	11:L:142:ILE:HG12	2.19	0.42
11:L:131:ASN:O	11:L:135:LYS:NZ	2.53	0.42
13:N:75:TYR:CZ	13:N:79:ILE:HD11	2.54	0.42
17:R:328:ALA:HB1	24:Y:226:MET:C	2.40	0.42
19:T:351:ASP:OD1	19:T:351:ASP:N	2.37	0.42
21:V:590:LEU:HB3	21:V:599:LEU:HD22	2.00	0.42
23:X:277:ARG:O	23:X:281:ARG:HG2	2.20	0.42
23:X:431:GLN:HA	23:X:434:GLN:NE2	2.35	0.42
23:X:658:ARG:HE	23:X:658:ARG:HB3	1.73	0.42
35:1:501:LEU:HD23	35:1:501:LEU:HA	1.72	0.42
35:1:823:MET:SD	35:1:829:ASN:ND2	2.92	0.42
35:1:974:LEU:HG	35:1:974:LEU:H	1.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:1101:LEU:HD23	35:1:1101:LEU:HA	1.92	0.42
35:1:1165:TYR:CD1	39:2:575:PHE:HD1	2.34	0.42
36:3:182:PHE:O	36:3:210:PHE:HA	2.19	0.42
36:3:212:GLU:HG2	36:3:213:LEU:N	2.35	0.42
36:3:329:TYR:HB3	36:3:370:GLU:CD	2.39	0.42
36:3:484:VAL:O	36:3:494:VAL:HB	2.20	0.42
39:2:456:ARG:HE	39:2:456:ARG:HB3	1.79	0.42
1:A:299:ILE:HD12	3:C:920:PRO:HB2	2.01	0.42
1:A:364:SER:O	1:A:366:LYS:HD3	2.19	0.42
2:B:46:U:C2'	2:B:47:A:H5'	2.49	0.42
3:C:80:ILE:HG22	3:C:82:GLN:HG2	2.01	0.42
3:C:603:MET:O	3:C:607:LEU:HD12	2.18	0.42
3:C:668:GLU:O	3:C:824:THR:OG1	2.37	0.42
3:C:763:LYS:O	3:C:767:VAL:HG22	2.20	0.42
4:E:299:LYS:HE2	4:E:299:LYS:HB2	1.79	0.42
5:F:36:A:H5"	5:F:37:C:OP2	2.20	0.42
5:F:92:A:H2'	5:F:93:G:C8	2.54	0.42
7:H:44:U:OP2	7:H:44:U:H6	2.02	0.42
8:I:177:PRO:HB3	8:I:211:SER:HA	2.01	0.42
23:X:192:ARG:HG2	23:X:192:ARG:NH1	2.30	0.42
23:X:218:ASP:O	23:X:222:MET:HG2	2.19	0.42
23:X:862:VAL:HG13	23:X:863:HIS:CD2	2.54	0.42
24:Y:267:ARG:HB3	24:Y:287:GLU:HG2	2.02	0.42
35:1:933:CYS:O	35:1:934:GLY:C	2.58	0.42
35:1:936:VAL:HG12	35:1:937:LEU:HD12	2.01	0.42
35:1:1087:ALA:HB3	35:1:1088:ILE:HD12	2.01	0.42
36:3:206:GLN:HE22	36:3:232:GLY:H	1.66	0.42
36:3:423:LEU:HB2	36:3:438:LEU:HB2	2.02	0.42
36:3:462:VAL:HG11	36:3:516:LEU:HD23	2.00	0.42
36:3:576:GLU:OE1	36:3:580:ARG:NH2	2.52	0.42
36:3:947:GLU:HG3	36:3:948:VAL:H	1.84	0.42
36:3:1015:LYS:HD2	36:3:1015:LYS:HA	1.79	0.42
1:A:76:MET:HE2	1:A:84:ASP:HB2	2.02	0.42
1:A:251:ASP:HB3	1:A:337:VAL:HG13	2.01	0.42
1:A:808:ALA:HB1	15:P:193:VAL:HG11	2.01	0.42
1:A:856:LEU:H	1:A:856:LEU:HG	1.36	0.42
1:A:1000:ILE:HG22	1:A:1001:VAL:HG13	2.00	0.42
1:A:1436:TRP:CZ3	1:A:1457:HIS:HB2	2.54	0.42
1:A:1826:VAL:HB	1:A:1830:GLN:HE22	1.85	0.42
3:C:602:LYS:HE2	3:C:602:LYS:HB3	1.84	0.42
3:C:762:VAL:HG23	3:C:808:ILE:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:74:PHE:CZ	4:E:343:ILE:HG13	2.55	0.42
4:E:287:ASN:ND2	4:E:331:ASN:OD1	2.52	0.42
6:G:1:G:C8	6:G:2:U:H4'	2.55	0.42
11:L:205:LYS:H	11:L:205:LYS:CD	2.33	0.42
12:M:186:LEU:HA	12:M:186:LEU:HD22	1.82	0.42
13:N:37:HIS:O	13:N:37:HIS:CG	2.72	0.42
19:T:309:ASP:O	19:T:310:SER:OG	2.26	0.42
21:V:584:LYS:HE2	21:V:584:LYS:HB2	1.92	0.42
23:X:787:GLU:O	23:X:790:LEU:HB3	2.19	0.42
23:X:814:LYS:NZ	23:X:814:LYS:HB2	2.34	0.42
23:X:898:CYS:HB3	23:X:903:VAL:O	2.19	0.42
24:Y:35:LYS:NZ	24:Y:159:THR:O	2.50	0.42
24:Y:224:LEU:CD1	24:Y:230:LEU:HD23	2.50	0.42
35:1:1090:PRO:CA	35:1:1093:VAL:HG12	2.43	0.42
36:3:577:TYR:HE2	36:3:579:GLU:HB3	1.85	0.42
36:3:675:LEU:HB3	36:3:686:LEU:HD12	2.02	0.42
36:3:996:ILE:O	36:3:998:HIS:N	2.53	0.42
1:A:110:TRP:O	1:A:192:GLN:NE2	2.53	0.42
1:A:278:LYS:NZ	6:G:-8:C:P	2.93	0.42
1:A:1169:GLN:O	1:A:1173:SER:OG	2.24	0.42
1:A:1352:HIS:CD2	20:U:5:ILE:HG12	2.55	0.42
1:A:1397:ILE:CG1	17:R:405:VAL:HG22	2.50	0.42
3:C:299:ILE:HD13	3:C:299:ILE:HA	1.79	0.42
3:C:522:SER:O	3:C:522:SER:OG	2.36	0.42
3:C:809:ILE:CG1	3:C:810:PRO:HD3	2.49	0.42
3:C:809:ILE:H	3:C:809:ILE:HG12	1.46	0.42
3:C:810:PRO:HA	3:C:813:ARG:HG2	2.01	0.42
4:E:162:ARG:HE	4:E:162:ARG:HB2	1.52	0.42
4:E:208:ILE:HA	4:E:208:ILE:HD12	1.81	0.42
9:J:268:ALA:HB1	9:J:278:LEU:HD21	2.01	0.42
11:L:201:LYS:HZ2	11:L:203:LYS:HG2	1.84	0.42
11:L:721:LEU:O	11:L:725:GLN:N	2.39	0.42
17:R:330:LYS:HZ1	23:X:275:ARG:NH2	2.17	0.42
17:R:356:ARG:O	17:R:360:ARG:HB2	2.19	0.42
35:1:753:LEU:HD23	35:1:753:LEU:HA	1.81	0.42
36:3:58:VAL:HG21	36:3:62:ILE:CD1	2.49	0.42
36:3:66:MET:HE3	36:3:123:VAL:HG12	2.01	0.42
36:3:212:GLU:CB	36:3:223:LYS:HG3	2.49	0.42
39:2:526:ASP:HA	39:2:529:LYS:NZ	2.34	0.42
39:2:547:LYS:NZ	39:2:555:GLU:HG2	2.35	0.42
1:A:35:ARG:HG2	1:A:35:ARG:HH11	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1217:GLN:OE1	1:A:1224:ARG:NE	2.52	0.42
1:A:1633:ALA:HB2	1:A:1637:TRP:CZ3	2.55	0.42
1:A:1640:SER:HB3	1:A:1652:MET:HA	2.01	0.42
8:I:512:ASP:O	8:I:514:ARG:N	2.52	0.42
9:J:238:ASN:O	9:J:239:ARG:HB3	2.20	0.42
9:J:256:LYS:HG3	11:L:235:LEU:HD23	2.01	0.42
12:M:208:ILE:O	12:M:208:ILE:HG22	2.20	0.42
12:M:224:ARG:NH1	12:M:224:ARG:C	2.73	0.42
15:P:73:GLU:HG2	15:P:76:ARG:NH2	2.34	0.42
17:R:352:ARG:HG2	17:R:356:ARG:NH2	2.35	0.42
21:V:452:LEU:HD11	21:V:456:ARG:CZ	2.49	0.42
21:V:487:LYS:H	21:V:487:LYS:HD3	1.85	0.42
23:X:450:CYS:O	23:X:495:TYR:HA	2.20	0.42
23:X:595:CYS:O	23:X:599:VAL:HG22	2.20	0.42
23:X:1004:GLU:HB2	23:X:1007:TRP:CD2	2.55	0.42
24:Y:30:LYS:O	24:Y:34:ILE:HG23	2.19	0.42
24:Y:31:LEU:HD11	24:Y:66:ILE:N	2.35	0.42
35:1:1029:GLU:H	35:1:1029:GLU:HG3	1.73	0.42
36:3:724:SER:HB2	36:3:727:SER:HA	2.01	0.42
36:3:789:VAL:HG13	36:3:891:VAL:HG13	2.01	0.42
36:3:1199:ARG:HH21	36:3:1207:LYS:NZ	2.18	0.42
42:5:61:LYS:HB3	42:5:65:ARG:HH22	1.83	0.42
1:A:525:LYS:HB2	1:A:525:LYS:NZ	2.34	0.42
3:C:243:ILE:HG13	3:C:244:LYS:N	2.33	0.42
3:C:440:SER:O	3:C:442:LYS:N	2.52	0.42
3:C:736:GLY:HA2	3:C:771:GLN:HG2	2.02	0.42
3:C:907:VAL:HA	3:C:908:PRO:HD3	1.84	0.42
9:J:189:ILE:HA	9:J:193:GLN:OE1	2.20	0.42
9:J:278:LEU:HD12	9:J:278:LEU:HA	1.69	0.42
9:J:299:TRP:O	9:J:303:ILE:HG23	2.19	0.42
23:X:480:SER:HB3	23:X:500:MET:HE1	2.02	0.42
24:Y:24:ALA:HA	24:Y:78:PHE:CZ	2.53	0.42
35:1:549:ARG:NH2	35:1:586:ASP:CG	2.69	0.42
36:3:311:PHE:HZ	36:3:387:PHE:CE2	2.38	0.42
36:3:690:ARG:HH12	36:3:696:SER:H	1.67	0.42
36:3:791:HIS:CB	36:3:796:ASN:O	2.68	0.42
39:2:465:LEU:HB3	39:2:475:VAL:HG11	2.01	0.42
39:2:550:LYS:HG2	39:2:554:ARG:HH21	1.84	0.42
1:A:68:LYS:NZ	13:N:45:SER:O	2.53	0.42
1:A:1489:LEU:HD12	1:A:1489:LEU:HA	1.77	0.42
1:A:1857:GLN:HE21	1:A:1857:GLN:HB2	1.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:381:LEU:CD2	3:C:416:LEU:HD21	2.49	0.42
4:E:179:TRP:HA	4:E:187:ILE:HG12	2.02	0.42
5:F:45:A:N6	6:G:3:A:C8	2.88	0.42
7:H:63:G:N1	7:H:64:A:N6	2.67	0.42
7:H:182:U:H2'	7:H:183:G:H8	1.85	0.42
8:I:213:ALA:HA	8:I:216:SER:O	2.20	0.42
11:L:633:GLN:O	11:L:637:VAL:N	2.50	0.42
13:N:2:PRO:O	13:N:4:VAL:N	2.53	0.42
17:R:314:GLN:HA	23:X:290:GLU:CD	2.39	0.42
17:R:352:ARG:HG2	17:R:356:ARG:HH21	1.85	0.42
19:T:423:SER:HB3	19:T:474:GLU:OE1	2.20	0.42
21:V:600:ASN:OD1	21:V:639:LEU:HB2	2.20	0.42
21:V:617:PRO:HB2	21:V:624:THR:OG1	2.19	0.42
23:X:406:GLU:HA	23:X:409:LEU:CD2	2.48	0.42
23:X:692:PRO:HA	23:X:737:LEU:HB2	2.02	0.42
23:X:832:GLU:HG2	23:X:927:VAL:HG22	2.02	0.42
23:X:887:GLN:O	23:X:890:GLU:HB3	2.19	0.42
35:1:664:GLY:O	35:1:668:VAL:HG23	2.20	0.42
36:3:43:PRO:HA	36:3:50:VAL:HA	2.01	0.42
36:3:275:ARG:HB3	36:3:386:PHE:HB3	2.02	0.42
39:2:461:THR:HG1	39:2:464:GLU:H	1.60	0.42
41:7:58:CYS:N	41:7:63:GLY:O	2.52	0.42
42:5:11:LEU:O	42:5:14:LEU:HB2	2.19	0.42
1:A:47:GLU:OE1	1:A:47:GLU:N	2.52	0.42
1:A:1661:TRP:CD2	1:A:1700:GLY:HA3	2.55	0.42
1:A:1755:SER:OG	35:1:938:TRP:CZ2	2.67	0.42
44:A:3000:IHP:O12	44:A:3000:IHP:P1	2.78	0.42
4:E:308:PHE:N	4:E:330:ILE:HD11	2.35	0.42
5:F:86:U:O2'	5:F:87:C:O5'	2.36	0.42
5:F:92:A:H2'	5:F:93:G:H8	1.85	0.42
6:G:86:A:H2	7:H:44:U:O2	2.02	0.42
11:L:177:GLU:HA	11:L:180:ARG:CD	2.50	0.42
12:M:160:PHE:O	12:M:162:PRO:HD3	2.19	0.42
17:R:352:ARG:HA	17:R:355:ILE:HD12	2.02	0.42
24:Y:41:LEU:HD23	24:Y:155:ARG:HH12	1.85	0.42
24:Y:204:SER:OG	24:Y:207:GLU:HG2	2.20	0.42
35:1:630:ARG:O	35:1:634:VAL:HG23	2.19	0.42
35:1:807:LYS:HD3	35:1:848:GLU:HG3	2.02	0.42
35:1:1249:TYR:HE2	39:2:587:HIS:CE1	2.38	0.42
36:3:1:MET:HG3	36:3:1092:ILE:HD12	2.02	0.42
36:3:70:LEU:HA	36:3:70:LEU:HD23	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:3:896:PHE:H	36:3:896:PHE:HD2	1.68	0.42
36:3:1200:THR:N	36:3:1203:GLU:OE1	2.38	0.42
39:2:456:ARG:HA	39:2:459:ARG:HB2	2.02	0.42
1:A:246:LEU:HD23	1:A:246:LEU:HA	1.82	0.41
1:A:296:PHE:HZ	3:C:593:GLU:HB2	1.85	0.41
1:A:569:VAL:O	1:A:570:ASP:HB2	2.19	0.41
1:A:599:MET:HA	1:A:602:ILE:HB	2.01	0.41
1:A:1604:LEU:HB3	1:A:1606:ILE:CD1	2.50	0.41
1:A:1885:LYS:HG2	1:A:1886:GLY:N	2.35	0.41
3:C:121:ASP:OD1	3:C:122:LEU:N	2.53	0.41
3:C:420:CYS:O	3:C:424:PHE:HB2	2.20	0.41
3:C:662:PHE:HE1	3:C:829:GLU:HB3	1.84	0.41
5:F:10:U:H2'	5:F:11:C:C4'	2.50	0.41
6:G:117:A:C2'	24:Y:246:LYS:HE2	2.49	0.41
7:H:41:U:C2	7:H:42:G:C8	3.08	0.41
8:I:374:ILE:O	8:I:376:ASN:N	2.52	0.41
24:Y:317:GLN:NE2	24:Y:317:GLN:HA	2.35	0.41
35:1:608:THR:O	35:1:611:SER:HB3	2.20	0.41
36:3:436:ARG:HG2	36:3:778:ALA:CB	2.49	0.41
36:3:610:VAL:HA	36:3:636:GLN:HE21	1.85	0.41
36:3:1191:LYS:O	36:3:1192:ASN:C	2.57	0.41
39:2:572:HIS:O	39:2:576:PHE:HB2	2.20	0.41
1:A:79:ARG:HG2	1:A:82:ARG:HG3	2.02	0.41
1:A:857:ASN:OD1	1:A:859:SER:N	2.53	0.41
1:A:1385:VAL:HG12	1:A:1419:ILE:HD11	2.01	0.41
1:A:1633:ALA:HB3	1:A:1658:GLN:HA	2.02	0.41
3:C:174:GLU:OE1	3:C:182:LYS:NZ	2.52	0.41
3:C:529:ARG:HH12	3:C:540:GLU:HG3	1.86	0.41
3:C:801:LEU:HD13	3:C:802:HIS:CE1	2.56	0.41
3:C:940:ARG:H	3:C:940:ARG:HG2	1.71	0.41
4:E:290:ARG:HG3	4:E:331:ASN:O	2.20	0.41
4:E:313:ASP:OD1	4:E:316:SER:OG	2.32	0.41
12:M:153:ARG:HA	12:M:160:PHE:CE2	2.55	0.41
13:N:41:ARG:HB3	13:N:44:GLU:HG2	2.02	0.41
14:O:34:ILE:O	17:R:197:ILE:HD12	2.18	0.41
17:R:387:ASP:OD1	17:R:388:ILE:N	2.53	0.41
21:V:612:PHE:O	21:V:616:LEU:HG	2.20	0.41
21:V:630:PHE:HD1	21:V:631:PHE:HD2	1.68	0.41
23:X:587:PRO:HB2	35:1:827:ARG:HH22	1.85	0.41
23:X:832:GLU:CD	23:X:928:GLY:H	2.23	0.41
23:X:932:CYS:HB2	23:X:938:ARG:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:551:LEU:O	35:1:554:LYS:HB3	2.19	0.41
35:1:556:ILE:O	35:1:560:LEU:HB2	2.21	0.41
35:1:564:ASP:HB2	35:1:603:ALA:HB1	1.80	0.41
35:1:613:MET:HB3	35:1:632:PHE:HE2	1.80	0.41
35:1:632:PHE:HA	35:1:635:VAL:HG22	2.01	0.41
35:1:769:VAL:O	35:1:772:ILE:HB	2.21	0.41
35:1:858:LYS:HB3	35:1:858:LYS:HE2	1.67	0.41
35:1:1028:HIS:HB3	35:1:1031:VAL:HG13	2.02	0.41
35:1:1130:PRO:HB3	39:2:528:ILE:CG2	2.46	0.41
36:3:91:GLU:OE1	36:3:102:ILE:HD11	2.20	0.41
1:A:1019:TYR:O	1:A:1021:ASP:N	2.53	0.41
1:A:1122:ASN:OD1	1:A:1122:ASN:N	2.53	0.41
1:A:1684:PHE:HB2	1:A:1702:LEU:HD11	2.03	0.41
1:A:1802:PRO:HB3	1:A:1827:TRP:CZ3	2.55	0.41
44:A:3000:IHP:P3	44:A:3000:IHP:O24	2.79	0.41
2:B:9:G:H2'	2:B:10:U:C6	2.55	0.41
3:C:493:PHE:CD2	3:C:551:LEU:HG	2.50	0.41
3:C:696:LEU:O	3:C:700:ILE:HG12	2.20	0.41
3:C:833:PHE:O	3:C:899:SER:HA	2.20	0.41
3:C:846:VAL:HB	3:C:887:LEU:HD11	2.02	0.41
4:E:145:LYS:NZ	4:E:181:ILE:O	2.44	0.41
4:E:266:PRO:HG3	11:L:789:ALA:HA	2.01	0.41
6:G:18:A:C2	14:O:196:GLN:O	2.73	0.41
9:J:400:GLU:OE2	9:J:401:ARG:HG3	2.20	0.41
11:L:138:ARG:HA	11:L:139:PRO:HD3	1.96	0.41
11:L:169:ARG:HH21	11:L:169:ARG:HG3	1.85	0.41
23:X:535:LEU:HA	23:X:535:LEU:HD23	1.78	0.41
23:X:610:ASP:HB2	23:X:686:ILE:HA	2.01	0.41
24:Y:41:LEU:HD23	24:Y:155:ARG:NH1	2.34	0.41
24:Y:241:VAL:O	24:Y:316:SER:HB3	2.20	0.41
35:1:527:GLY:HA2	35:1:566:LEU:HD23	2.02	0.41
35:1:729:LYS:O	35:1:733:LYS:HG2	2.21	0.41
35:1:1055:TRP:HA	35:1:1055:TRP:CE3	2.55	0.41
35:1:1109:ARG:O	35:1:1112:THR:HG23	2.20	0.41
36:3:898:ASN:OD1	36:3:899:THR:N	2.52	0.41
36:3:914:ILE:HG22	36:3:917:PRO:HD2	2.02	0.41
1:A:796:LYS:HB3	1:A:796:LYS:HE3	1.80	0.41
1:A:1638:ASN:HA	1:A:1655:THR:O	2.20	0.41
1:A:1776:ILE:HG23	1:A:1859:LYS:HG3	2.02	0.41
1:A:1778:TRP:C	1:A:1779:PHE:HD2	2.24	0.41
4:E:251:LEU:HB2	4:E:293:TRP:NE1	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:313:ASP:HB3	4:E:320:LEU:HD11	2.02	0.41
4:E:321:TYR:HB3	4:E:323:LEU:HG	2.02	0.41
5:F:23:U:C4	13:N:118:ILE:HD13	2.55	0.41
7:H:55:U:H2'	7:H:57:A:OP2	2.21	0.41
9:J:189:ILE:HG21	11:L:152:LEU:HD22	2.02	0.41
11:L:169:ARG:HH21	11:L:169:ARG:CG	2.34	0.41
23:X:169:ARG:O	23:X:173:GLN:HG3	2.20	0.41
24:Y:18:THR:HB	24:Y:166:PHE:CE2	2.55	0.41
35:1:646:PRO:O	35:1:649:LYS:HB2	2.20	0.41
35:1:802:GLU:HG2	35:1:805:TYR:HB2	2.02	0.41
36:3:199:GLU:OE2	36:3:199:GLU:HA	2.19	0.41
36:3:289:CYS:SG	36:3:290:SER:N	2.93	0.41
36:3:1015:LYS:NZ	36:3:1016:ARG:H	2.18	0.41
36:3:1022:ILE:HA	36:3:1022:ILE:HD13	1.77	0.41
39:2:451:LYS:HA	39:2:454:LEU:HD23	2.02	0.41
39:2:459:ARG:HD2	39:2:481:THR:HA	2.03	0.41
1:A:300:ASN:OD1	1:A:300:ASN:N	2.45	0.41
1:A:379:GLU:HA	3:C:354:ARG:O	2.21	0.41
1:A:623:LYS:O	44:A:3000:IHP:O44	2.39	0.41
1:A:1386:TRP:CD1	23:X:337:ALA:HB1	2.55	0.41
1:A:1847:ALA:O	1:A:1850:ARG:HB3	2.21	0.41
1:A:1978:LYS:HA	1:A:1978:LYS:HE3	2.03	0.41
3:C:286:ASN:ND2	3:C:299:ILE:HG23	2.35	0.41
3:C:759:LEU:HA	3:C:759:LEU:HD12	1.83	0.41
6:G:97:A:C6	35:1:1075:ARG:HG2	2.54	0.41
6:G:104:C:O2	6:G:104:C:C2'	2.68	0.41
7:H:34:U:H2'	7:H:35:A:C1'	2.51	0.41
17:R:265:ASP:OD1	17:R:265:ASP:N	2.52	0.41
17:R:377:ARG:HG2	17:R:377:ARG:NH2	2.35	0.41
19:T:423:SER:N	19:T:474:GLU:OE2	2.52	0.41
23:X:411:ALA:HA	23:X:414:ASN:ND2	2.36	0.41
23:X:969:PHE:CD2	23:X:994:LYS:HG2	2.55	0.41
35:1:694:LEU:CD1	35:1:727:VAL:HG21	2.44	0.41
35:1:699:GLN:HE22	35:1:738:HIS:HE1	1.60	0.41
35:1:862:GLU:O	35:1:866:LYS:HB2	2.21	0.41
35:1:912:ASN:OD1	35:1:912:ASN:N	2.53	0.41
36:3:497:SER:OG	36:3:499:PHE:HB2	2.21	0.41
36:3:1004:ASP:OD2	36:3:1007:GLU:HB2	2.21	0.41
1:A:329:LEU:HB2	3:C:177:ARG:NH2	2.36	0.41
1:A:456:LEU:HD22	1:A:460:LYS:NZ	2.35	0.41
1:A:1636:LYS:HE3	1:A:1656:THR:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:480:LYS:C	3:C:481:MET:HG3	2.40	0.41
3:C:828:MET:HG2	3:C:906:ILE:HD13	2.03	0.41
7:H:31:G:N3	7:H:31:G:C2'	2.83	0.41
9:J:200:GLU:C	9:J:202:GLU:N	2.74	0.41
9:J:323:LEU:HA	9:J:323:LEU:HD23	1.77	0.41
11:L:130:PRO:HB2	11:L:131:ASN:H	1.62	0.41
21:V:469:PHE:CZ	21:V:509:LEU:HD22	2.55	0.41
21:V:476:LEU:O	21:V:479:MET:HB2	2.21	0.41
23:X:234:TYR:CD1	24:Y:317:GLN:HB3	2.55	0.41
23:X:910:ARG:HA	23:X:913:ASP:OD2	2.20	0.41
35:1:504:ILE:HG13	35:1:515:ALA:HB3	2.03	0.41
35:1:806:ILE:HD12	35:1:843:LYS:HE3	1.99	0.41
36:3:164:ASN:N	36:3:164:ASN:OD1	2.53	0.41
39:2:510:TYR:O	39:2:511:LEU:HD23	2.20	0.41
39:2:667:ALA:HB2	40:4:110:GLU:CB	2.50	0.41
1:A:611:LEU:HD12	1:A:611:LEU:HA	1.90	0.41
1:A:699:GLU:HB3	17:R:237:MET:HE2	2.02	0.41
1:A:1130:ASN:HD21	1:A:1140:MET:CB	2.33	0.41
1:A:1457:HIS:O	1:A:1461:ASP:HB2	2.20	0.41
1:A:1482:GLU:N	1:A:1482:GLU:OE2	2.54	0.41
3:C:95:LYS:HA	3:C:96:PRO:HD3	1.90	0.41
3:C:353:THR:HG23	3:C:355:LYS:H	1.84	0.41
3:C:406:GLU:H	3:C:406:GLU:CD	2.22	0.41
3:C:736:GLY:O	3:C:738:ASP:N	2.53	0.41
4:E:81:LEU:O	4:E:92:LEU:HA	2.21	0.41
7:H:28:C:O2'	7:H:29:A:C4	2.69	0.41
13:N:55:GLN:HE21	13:N:55:GLN:HB2	1.75	0.41
17:R:159:VAL:O	17:R:162:ALA:N	2.54	0.41
21:V:603:LEU:HA	21:V:603:LEU:HD12	1.78	0.41
21:V:650:THR:HB	21:V:651:PRO:HD3	2.03	0.41
23:X:483:PHE:HB2	23:X:484:GLU:OE1	2.20	0.41
23:X:955:THR:OG1	23:X:958:GLY:O	2.24	0.41
23:X:981:PRO:HD2	23:X:984:LEU:HD13	2.02	0.41
35:1:625:ARG:HB3	35:1:666:LYS:CE	2.49	0.41
36:3:438:LEU:HD23	36:3:438:LEU:HA	1.72	0.41
36:3:610:VAL:HG23	36:3:636:GLN:NE2	2.36	0.41
36:3:855:PRO:O	36:3:856:LYS:HD3	2.20	0.41
42:5:74:GLN:NE2	42:5:78:PRO:HA	2.36	0.41
1:A:57:GLN:HE21	1:A:57:GLN:C	2.23	0.41
1:A:615:ARG:HE	1:A:615:ARG:HB2	1.69	0.41
1:A:888:GLN:C	1:A:889:ARG:HG2	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1184:ASN:OD1	1:A:1195:ARG:NH1	2.51	0.41
1:A:2002:LEU:HD22	1:A:2006:GLU:OE1	2.21	0.41
6:G:90:C:H4'	9:J:181:ASN:N	2.36	0.41
7:H:7:U:H2'	7:H:8:C:H6	1.82	0.41
11:L:26:TYR:CE1	11:L:33:ARG:HB3	2.56	0.41
15:P:188:TRP:O	15:P:188:TRP:CG	2.70	0.41
17:R:114:SER:HB3	17:R:228:PRO:HG2	2.02	0.41
17:R:213:LYS:NZ	17:R:215:ASN:OD1	2.48	0.41
17:R:325:ARG:HH12	17:R:329:GLN:N	2.18	0.41
19:T:223:SER:OG	19:T:224:ALA:N	2.52	0.41
19:T:306:CYS:HB2	19:T:333:VAL:HG12	2.02	0.41
21:V:617:PRO:HB3	21:V:623:ASN:HD22	1.86	0.41
23:X:173:GLN:HA	23:X:176:GLU:OE2	2.21	0.41
23:X:246:LEU:HG	23:X:277:ARG:CZ	2.51	0.41
23:X:533:PHE:HE1	23:X:550:VAL:HG11	1.86	0.41
23:X:614:PHE:O	23:X:615:LEU:HD12	2.21	0.41
23:X:645:LEU:HB3	23:X:659:ILE:HG22	2.02	0.41
23:X:790:LEU:HD23	23:X:791:LEU:N	2.35	0.41
24:Y:2:ALA:O	24:Y:162:LEU:HB3	2.20	0.41
24:Y:212:LYS:HA	24:Y:212:LYS:HD2	1.80	0.41
35:1:699:GLN:NE2	35:1:738:HIS:HE1	2.17	0.41
35:1:816:LYS:HB3	35:1:816:LYS:HE3	1.82	0.41
35:1:841:ALA:O	35:1:845:GLY:N	2.50	0.41
35:1:876:MET:HE3	35:1:920:ALA:HB3	2.02	0.41
35:1:1251:LEU:HA	35:1:1251:LEU:HD23	1.68	0.41
36:3:447:MET:HE1	36:3:751:PRO:HD2	2.03	0.41
36:3:615:ARG:O	36:3:616:ILE:HD12	2.21	0.41
36:3:637:PRO:HB3	36:3:640:LEU:HD21	2.03	0.41
39:2:506:PHE:N	39:2:506:PHE:CD1	2.88	0.41
1:A:62:PRO:HB2	1:A:64:GLU:OE1	2.20	0.41
1:A:65:HIS:CD2	13:N:46:LEU:HD13	2.56	0.41
1:A:131:GLU:HG2	1:A:132:ILE:N	2.35	0.41
1:A:519:ASP:OD2	1:A:523:ASN:HB2	2.20	0.41
1:A:631:ALA:O	1:A:635:ARG:HG3	2.21	0.41
1:A:799:PRO:HD3	17:R:284:PHE:CE1	2.56	0.41
1:A:1194:CYS:HB3	1:A:1228:CYS:SG	2.60	0.41
1:A:1581:LEU:O	1:A:1585:ILE:HG13	2.20	0.41
1:A:1631:LEU:HD23	1:A:1631:LEU:HA	1.79	0.41
1:A:1965:HIS:N	1:A:1965:HIS:CD2	2.87	0.41
3:C:129:ILE:HA	3:C:199:LEU:O	2.21	0.41
3:C:177:ARG:HA	3:C:177:ARG:HE	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:501:ILE:HG22	3:C:530:LEU:HD11	2.01	0.41
3:C:516:LEU:HD23	3:C:516:LEU:H	1.86	0.41
3:C:705:VAL:HB	3:C:717:PHE:CZ	2.55	0.41
4:E:125:PHE:CD2	4:E:125:PHE:N	2.89	0.41
4:E:168:CYS:SG	4:E:208:ILE:HD11	2.60	0.41
5:F:33:G:C2	5:F:34:G:H8	2.39	0.41
6:G:18:A:H2	14:O:196:GLN:O	2.03	0.41
6:G:90:C:N3	7:H:40:C:N3	2.68	0.41
6:G:93:A:C2	7:H:38:A:C2	3.08	0.41
6:G:109:U:H5"	23:X:454:ARG:HD3	2.02	0.41
6:G:112:U:H5"	23:X:500:MET:HE3	2.03	0.41
7:H:168:A:H5"	7:H:169:C:C6	2.56	0.41
9:J:203:LEU:CD2	9:J:203:LEU:O	2.69	0.41
9:J:294:HIS:CE1	11:L:227:THR:OG1	2.73	0.41
9:J:394:HIS:O	9:J:398:VAL:HG23	2.21	0.41
14:O:200:ASP:O	14:O:204:GLY:N	2.46	0.41
17:R:246:LYS:NZ	17:R:246:LYS:CB	2.84	0.41
17:R:246:LYS:HB3	17:R:246:LYS:HZ3	1.86	0.41
17:R:408:ASP:HB3	17:R:411:LEU:HD23	2.02	0.41
19:T:207:VAL:HG12	19:T:480:ALA:HB1	2.03	0.41
21:V:402:LYS:O	21:V:406:LEU:N	2.53	0.41
21:V:495:ASP:O	21:V:498:ALA:HB3	2.21	0.41
23:X:246:LEU:HG	23:X:277:ARG:HE	1.84	0.41
23:X:276:VAL:HG22	24:Y:227:VAL:HA	2.03	0.41
23:X:387:GLN:NE2	23:X:391:SER:OG	2.54	0.41
23:X:389:LYS:NZ	23:X:390:GLU:HG3	2.35	0.41
23:X:393:GLN:HA	23:X:396:ARG:HB2	2.02	0.41
23:X:422:GLY:O	23:X:553:ALA:HA	2.19	0.41
23:X:595:CYS:SG	23:X:613:VAL:HG11	2.61	0.41
23:X:716:LYS:HB2	23:X:748:GLU:O	2.21	0.41
23:X:741:TRP:HE1	35:1:783:GLU:H	1.67	0.41
23:X:931:SER:O	23:X:933:GLN:NE2	2.54	0.41
24:Y:41:LEU:HA	24:Y:155:ARG:HA	2.02	0.41
24:Y:255:ASP:OD2	24:Y:259:ILE:HD11	2.21	0.41
35:1:534:GLN:O	35:1:538:LEU:HD12	2.20	0.41
35:1:563:LEU:HB3	35:1:566:LEU:HB2	2.02	0.41
35:1:686:LEU:HA	35:1:689:ILE:HG12	2.03	0.41
35:1:1208:LEU:HB3	35:1:1237:LEU:HD21	2.03	0.41
35:1:1292:LYS:HD2	42:5:78:PRO:HG2	2.01	0.41
36:3:128:ARG:HH21	36:3:180:PRO:HG3	1.85	0.41
36:3:184:CYS:SG	36:3:211:TYR:CE1	3.14	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:3:469:GLU:OE1	36:3:469:GLU:N	2.53	0.41
36:3:515:ALA:HB2	36:3:528:ARG:NE	2.36	0.41
36:3:605:LEU:HB3	36:3:619:LEU:HD22	2.02	0.41
36:3:665:LEU:O	36:3:676:ARG:HA	2.21	0.41
36:3:671:ASN:HB3	36:3:696:SER:HA	2.01	0.41
36:3:998:HIS:HE1	36:3:1041:TYR:OH	2.04	0.41
36:3:1140:PHE:CE1	36:3:1197:LEU:HD13	2.53	0.41
1:A:27:GLU:O	1:A:31:GLN:HG2	2.21	0.41
1:A:1402:ARG:HD2	17:R:406:GLN:OE1	2.21	0.41
1:A:1868:MET:O	1:A:1868:MET:HG2	2.21	0.41
1:A:1939:ILE:HD11	1:A:1976:TRP:HH2	1.86	0.41
3:C:680:ASN:O	3:C:682:LYS:N	2.53	0.41
5:F:8:C:H3'	5:F:9:U:O4'	2.20	0.41
7:H:15:U:O3'	7:H:16:U:H2'	2.21	0.41
7:H:42:G:C6	7:H:43:U:C4	3.09	0.41
13:N:91:LYS:HA	13:N:91:LYS:HD3	1.80	0.41
15:P:66:ARG:HE	15:P:66:ARG:HB2	1.49	0.41
17:R:238:THR:OG1	17:R:239:VAL:N	2.53	0.41
19:T:297:HIS:CG	19:T:298:PRO:HD2	2.56	0.41
21:V:458:THR:HG21	21:V:479:MET:HE1	2.03	0.41
23:X:674:THR:HG22	23:X:675:ASN:H	1.86	0.41
35:1:510:PRO:HA	35:1:513:LYS:HE2	2.03	0.41
35:1:758:ASP:OD2	35:1:761:TYR:HB2	2.21	0.41
35:1:1067:LYS:HB3	35:1:1067:LYS:HE2	1.67	0.41
36:3:164:ASN:ND2	36:3:190:GLU:HG2	2.35	0.41
36:3:192:ALA:O	42:5:74:GLN:NE2	2.35	0.41
36:3:334:PRO:HG2	36:3:357:TYR:CD2	2.56	0.41
36:3:343:LYS:C	36:3:345:GLY:H	2.24	0.41
36:3:615:ARG:C	36:3:616:ILE:HD12	2.41	0.41
36:3:941:HIS:CE1	36:3:974:LYS:HA	2.56	0.41
36:3:1001:ILE:HD12	36:3:1011:TRP:NE1	2.36	0.41
41:7:26:CYS:SG	41:7:60:ILE:HG13	2.61	0.41
1:A:461:HIS:O	1:A:462:ARG:NH1	2.54	0.40
1:A:850:TYR:HD2	1:A:864:LEU:HD21	1.85	0.40
1:A:1012:LYS:O	1:A:1012:LYS:HG3	2.20	0.40
3:C:183:SER:HG	3:C:480:LYS:HZ1	1.60	0.40
3:C:717:PHE:CE1	3:C:721:LYS:HE2	2.55	0.40
5:F:94:C:H2'	5:F:95:G:C8	2.56	0.40
6:G:-8:C:O4'	20:U:18:TYR:HB2	2.21	0.40
6:G:7:G:C2	6:G:8:C:C2	3.09	0.40
6:G:8:C:H2'	6:G:9:C:C4	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:405:PHE:HZ	19:T:408:ASN:OD1	2.04	0.40
21:V:461:LEU:HA	21:V:461:LEU:HD23	1.88	0.40
21:V:529:PHE:CE1	21:V:564:VAL:HB	2.56	0.40
23:X:466:ALA:HA	23:X:469:MET:HB2	2.03	0.40
23:X:856:ARG:HB3	23:X:856:ARG:CZ	2.51	0.40
23:X:868:ARG:HH22	23:X:973:ASN:HD21	1.69	0.40
23:X:909:ARG:HG2	23:X:909:ARG:HH11	1.86	0.40
24:Y:26:LEU:HB2	24:Y:166:PHE:CG	2.56	0.40
24:Y:55:ASP:OD1	24:Y:57:THR:OG1	2.39	0.40
35:1:563:LEU:HB3	35:1:566:LEU:CB	2.51	0.40
35:1:835:ASP:O	35:1:839:GLU:HG2	2.22	0.40
35:1:897:LEU:HD21	35:1:932:ILE:CD1	2.51	0.40
35:1:914:PHE:O	35:1:917:VAL:HG12	2.21	0.40
35:1:1142:ASN:HD22	35:1:1142:ASN:N	2.19	0.40
35:1:1179:ASP:HB3	39:2:511:LEU:HB3	2.03	0.40
36:3:541:LYS:HD3	36:3:541:LYS:HA	1.87	0.40
36:3:768:GLU:HB3	36:3:769:LYS:H	1.63	0.40
36:3:926:TYR:CD1	36:3:942:LYS:HB3	2.56	0.40
36:3:1041:TYR:CB	39:2:705:ARG:HG3	2.51	0.40
41:7:12:ARG:HA	41:7:12:ARG:HD2	1.68	0.40
42:5:53:PHE:O	42:5:57:GLU:HG2	2.21	0.40
1:A:76:MET:HE3	1:A:76:MET:HB3	1.76	0.40
1:A:451:LEU:HD23	1:A:451:LEU:HA	1.86	0.40
1:A:617:ASN:HA	1:A:621:VAL:HB	2.02	0.40
1:A:962:LEU:HD23	1:A:962:LEU:HA	1.80	0.40
1:A:1268:ILE:HD13	1:A:1268:ILE:HG21	1.87	0.40
1:A:1684:PHE:N	1:A:1702:LEU:HD21	2.36	0.40
2:B:13:C:H2'	2:B:14:U:H6	1.86	0.40
3:C:415:LEU:HD12	3:C:415:LEU:HA	1.83	0.40
4:E:136:TRP:CZ3	4:E:143:ARG:HG2	2.56	0.40
4:E:323:LEU:HD21	22:W:83:PRO:O	2.22	0.40
7:H:13:C:H5"	7:H:14:C:C5	2.56	0.40
7:H:57:A:C5'	39:2:481:THR:HG21	2.51	0.40
7:H:160:A:H2'	7:H:161:U:O4'	2.21	0.40
8:I:479:ARG:O	8:I:483:SER:N	2.36	0.40
11:L:55:ASP:OD2	11:L:57:SER:HB3	2.22	0.40
11:L:141:PRO:HG2	11:L:144:MET:HA	2.03	0.40
11:L:186:GLN:HG3	11:L:189:ARG:HH12	1.87	0.40
13:N:66:LYS:HD2	13:N:66:LYS:HA	1.84	0.40
15:P:206:LYS:O	15:P:209:ARG:O	2.39	0.40
16:Q:514:ILE:N	16:Q:654:ASN:O	2.31	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:412:PHE:HE2	23:X:326:GLN:HE22	1.69	0.40
19:T:320:LYS:HE2	19:T:320:LYS:HB2	1.64	0.40
23:X:173:GLN:O	23:X:176:GLU:HG2	2.21	0.40
23:X:716:LYS:N	23:X:747:LEU:HD12	2.36	0.40
23:X:832:GLU:OE1	23:X:927:VAL:HG13	2.21	0.40
35:1:555:VAL:HG12	35:1:559:ILE:HD13	2.02	0.40
35:1:641:ILE:HG22	35:1:682:HIS:NE2	2.37	0.40
35:1:840:LEU:HD13	35:1:840:LEU:HA	1.80	0.40
35:1:841:ALA:CB	35:1:875:ILE:CD1	2.82	0.40
35:1:1277:GLN:HG3	36:3:113:ARG:CD	2.51	0.40
36:3:174:ASP:HB3	36:3:240:GLY:H	1.86	0.40
36:3:180:PRO:HD2	36:3:215:LEU:HD11	2.03	0.40
36:3:278:LEU:HD21	36:3:816:LYS:HZ3	1.86	0.40
36:3:280:ASP:H	36:3:857:ALA:CB	2.33	0.40
36:3:373:PHE:HD1	36:3:385:PHE:CG	2.40	0.40
36:3:408:LEU:HD12	36:3:427:CYS:HA	2.02	0.40
36:3:459:VAL:HA	36:3:475:ILE:O	2.21	0.40
36:3:706:MET:HG2	36:3:770:LEU:CD1	2.51	0.40
36:3:755:VAL:HG22	36:3:764:ILE:CD1	2.52	0.40
1:A:229:GLN:O	1:A:230:PHE:HD1	2.03	0.40
1:A:442:LYS:NZ	44:A:3000:IHP:O33	2.54	0.40
1:A:1130:ASN:HD21	1:A:1140:MET:HB2	1.87	0.40
1:A:1215:ASN:HB3	1:A:1224:ARG:HH11	1.85	0.40
1:A:1409:GLU:OE2	1:A:1409:GLU:HA	2.20	0.40
1:A:1776:ILE:HG22	1:A:1859:LYS:NZ	2.35	0.40
1:A:1868:MET:C	1:A:1871:PRO:HD2	2.41	0.40
1:A:1924:LEU:HD12	1:A:1924:LEU:HA	1.85	0.40
3:C:368:SER:O	3:C:372:PHE:HB2	2.21	0.40
3:C:572:GLU:HG3	3:C:573:GLU:H	1.86	0.40
3:C:618:THR:OG1	3:C:630:LEU:HB3	2.21	0.40
3:C:823:ALA:O	3:C:824:THR:OG1	2.35	0.40
4:E:197:LEU:HD21	4:E:213:ILE:HD11	2.03	0.40
6:G:5:G:N1	6:G:6:A:N6	2.69	0.40
6:G:7:G:C5	6:G:8:C:C4	3.10	0.40
6:G:96:U:H5”	6:G:97:A:OP2	2.21	0.40
7:H:99:A:HO2’	7:H:100:U:P	2.43	0.40
7:H:142:U:C2	7:H:143:C:C5	3.09	0.40
11:L:11:TRP:CD2	11:L:49:ARG:HD3	2.56	0.40
11:L:154:GLU:HG3	11:L:155:ALA:N	2.35	0.40
17:R:151:LEU:HD22	17:R:151:LEU:HA	1.87	0.40
23:X:216:GLU:HG2	23:X:217:GLU:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:423:GLU:HB2	23:X:574:GLY:O	2.22	0.40
23:X:723:ALA:HA	23:X:734:CYS:SG	2.61	0.40
23:X:929:LEU:HD23	23:X:929:LEU:HA	1.89	0.40
24:Y:47:ARG:HA	24:Y:140:ASN:HD21	1.85	0.40
24:Y:247:LEU:HG	24:Y:248:ASN:N	2.36	0.40
35:1:540:MET:SD	35:1:577:VAL:HG12	2.58	0.40
35:1:669:GLN:NE2	35:1:707:LEU:HD22	2.37	0.40
35:1:811:LEU:HB2	35:1:812:PRO:HD3	2.03	0.40
35:1:1179:ASP:CB	39:2:511:LEU:CD1	3.00	0.40
35:1:1216:TRP:CH2	35:1:1268:ILE:HD13	2.56	0.40
35:1:1304:LEU:HD12	42:5:52:TYR:CE2	2.57	0.40
36:3:327:LEU:O	36:3:373:PHE:HB2	2.22	0.40
36:3:719:SER:OG	36:3:734:LEU:HB2	2.22	0.40
36:3:739:LEU:HD23	36:3:739:LEU:HA	1.71	0.40
36:3:998:HIS:CE1	36:3:1041:TYR:OH	2.75	0.40
39:2:568:TYR:O	39:2:569:GLN:HB2	2.22	0.40
42:5:69:MET:HE2	42:5:69:MET:HB2	1.85	0.40
1:A:154:GLU:HG2	1:A:572:PHE:CD1	2.56	0.40
1:A:545:HIS:O	1:A:549:GLU:HG2	2.21	0.40
1:A:1342:TRP:HB2	1:A:1348:VAL:HG21	2.03	0.40
1:A:1636:LYS:HE3	1:A:1656:THR:CG2	2.51	0.40
1:A:1741:TYR:HH	35:1:937:LEU:CD2	1.95	0.40
3:C:672:LEU:HG	3:C:673:LYS:H	1.86	0.40
4:E:137:ASP:OD1	4:E:137:ASP:N	2.54	0.40
4:E:221:ASP:OD1	4:E:226:LYS:HE3	2.22	0.40
4:E:323:LEU:HD23	4:E:323:LEU:HA	1.92	0.40
5:F:47:A:H4'	5:F:48:A:OP1	2.21	0.40
17:R:124:VAL:O	17:R:124:VAL:CG1	2.69	0.40
19:T:412:HIS:NE2	19:T:431:ALA:HB2	2.37	0.40
23:X:480:SER:HB3	23:X:500:MET:HE2	2.03	0.40
23:X:681:LEU:H	23:X:725:ARG:NH2	2.19	0.40
23:X:753:PRO:HG2	23:X:782:ASP:OD2	2.22	0.40
35:1:614:ARG:HD3	35:1:615:PRO:CD	2.52	0.40
35:1:933:CYS:CB	35:1:970:LEU:HD11	2.51	0.40
35:1:1244:CYS:O	35:1:1245:ARG:C	2.60	0.40
36:3:2:PHE:CE2	39:2:711:LEU:HD12	2.56	0.40
36:3:151:ARG:O	36:3:151:ARG:HG3	2.21	0.40
36:3:1096:HIS:ND1	36:3:1166:TYR:HB2	2.36	0.40
1:A:1131:LYS:HE2	1:A:1174:PHE:CE2	2.55	0.40
1:A:1573:LEU:HA	1:A:1573:LEU:HD23	1.89	0.40
1:A:1885:LYS:HE2	1:A:1887:SER:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:89:U:C2'	2:B:90:U:H5"	2.47	0.40
3:C:878:ILE:HD12	3:C:878:ILE:HG23	1.90	0.40
5:F:39:A:C2'	5:F:40:U:H5'	2.51	0.40
9:J:401:ARG:HA	9:J:404:GLU:HG2	2.03	0.40
11:L:186:GLN:HG3	11:L:189:ARG:NH1	2.37	0.40
17:R:376:LYS:CA	17:R:379:LYS:HB2	2.42	0.40
20:U:5:ILE:O	20:U:5:ILE:HD12	2.22	0.40
23:X:404:PHE:O	23:X:408:LEU:HD23	2.22	0.40
23:X:859:ASP:OD2	23:X:859:ASP:N	2.52	0.40
24:Y:136:ILE:O	24:Y:140:ASN:HB2	2.22	0.40
36:3:168:TYR:OH	36:3:187:MET:SD	2.63	0.40
36:3:258:TYR:HB3	36:3:267:ILE:HB	2.04	0.40
36:3:258:TYR:CG	36:3:259:LYS:N	2.90	0.40
36:3:278:LEU:HA	36:3:815:ARG:NH1	2.37	0.40
36:3:592:LEU:HD13	36:3:592:LEU:HA	1.64	0.40
36:3:1135:HIS:HA	36:3:1138:HIS:HB3	2.03	0.40
41:7:23:CYS:HB3	41:7:58:CYS:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1961/2335 (84%)	1760 (90%)	186 (10%)	15 (1%)	19 51
3	C	854/972 (88%)	751 (88%)	100 (12%)	3 (0%)	34 66
4	E	297/357 (83%)	270 (91%)	27 (9%)	0	100 100
8	I	662/855 (77%)	575 (87%)	86 (13%)	1 (0%)	47 77
9	J	525/848 (62%)	487 (93%)	33 (6%)	5 (1%)	15 46
10	K	22/343 (6%)	18 (82%)	4 (18%)	0	100 100
11	L	375/802 (47%)	358 (96%)	16 (4%)	1 (0%)	41 71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
12	M	112/243 (46%)	105 (94%)	5 (4%)	2 (2%)	8 35
13	N	141/144 (98%)	125 (89%)	16 (11%)	0	100 100
14	O	288/420 (69%)	262 (91%)	26 (9%)	0	100 100
15	P	97/229 (42%)	89 (92%)	7 (7%)	1 (1%)	15 46
16	Q	1304/1485 (88%)	1279 (98%)	25 (2%)	0	100 100
17	R	370/536 (69%)	336 (91%)	31 (8%)	3 (1%)	19 51
18	S	156/166 (94%)	144 (92%)	12 (8%)	0	100 100
19	T	318/514 (62%)	300 (94%)	18 (6%)	0	100 100
20	U	68/2752 (2%)	63 (93%)	4 (6%)	1 (2%)	10 38
21	V	458/908 (50%)	433 (94%)	25 (6%)	0	100 100
22	W	497/579 (86%)	473 (95%)	24 (5%)	0	100 100
23	X	778/1041 (75%)	728 (94%)	49 (6%)	1 (0%)	51 81
24	Y	318/492 (65%)	296 (93%)	22 (7%)	0	100 100
25	Z	147/225 (65%)	138 (94%)	5 (3%)	4 (3%)	5 26
26	y	77/301 (26%)	76 (99%)	1 (1%)	0	100 100
27	a	84/240 (35%)	82 (98%)	2 (2%)	0	100 100
27	m	80/240 (33%)	72 (90%)	8 (10%)	0	100 100
28	b	80/119 (67%)	77 (96%)	3 (4%)	0	100 100
28	n	78/119 (66%)	67 (86%)	11 (14%)	0	100 100
29	c	95/118 (80%)	91 (96%)	4 (4%)	0	100 100
29	h	91/118 (77%)	82 (90%)	9 (10%)	0	100 100
30	d	72/86 (84%)	69 (96%)	3 (4%)	0	100 100
30	i	70/86 (81%)	64 (91%)	6 (9%)	0	100 100
31	e	77/92 (84%)	76 (99%)	1 (1%)	0	100 100
31	j	79/92 (86%)	73 (92%)	6 (8%)	0	100 100
32	f	72/76 (95%)	70 (97%)	2 (3%)	0	100 100
32	k	71/76 (93%)	63 (89%)	8 (11%)	0	100 100
33	g	77/126 (61%)	76 (99%)	1 (1%)	0	100 100
33	l	81/126 (64%)	70 (86%)	11 (14%)	0	100 100
34	q	130/504 (26%)	117 (90%)	7 (5%)	6 (5%)	2 15
34	r	129/504 (26%)	118 (92%)	9 (7%)	2 (2%)	9 36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
34	s	130/504 (26%)	114 (88%)	8 (6%)	8 (6%)	1 10
34	t	129/504 (26%)	116 (90%)	9 (7%)	4 (3%)	4 23
35	1	814/1304 (62%)	703 (86%)	101 (12%)	10 (1%)	13 42
36	3	1165/1217 (96%)	992 (85%)	172 (15%)	1 (0%)	51 81
37	p	163/225 (72%)	147 (90%)	15 (9%)	1 (1%)	25 57
38	w	119/501 (24%)	107 (90%)	12 (10%)	0	100 100
39	2	246/895 (28%)	208 (85%)	34 (14%)	4 (2%)	9 36
40	4	147/424 (35%)	129 (88%)	18 (12%)	0	100 100
41	7	79/110 (72%)	65 (82%)	14 (18%)	0	100 100
42	5	75/86 (87%)	64 (85%)	11 (15%)	0	100 100
43	o	160/255 (63%)	136 (85%)	24 (15%)	0	100 100
All	All	14418/25294 (57%)	13114 (91%)	1231 (8%)	73 (0%)	32 61

All (73) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1417	PRO
9	J	202	GLU
17	R	164	PRO
25	Z	78	PRO
25	Z	86	ARG
34	q	24	VAL
34	q	59	HIS
34	q	60	PRO
34	s	9	ASN
34	s	55	ILE
34	s	60	PRO
34	s	66	PRO
34	s	71	ILE
34	t	9	ASN
34	t	69	THR
35	1	718	PRO
39	2	642	PRO
39	2	646	PRO
39	2	647	ASN
1	A	699	GLU
1	A	856	LEU
1	A	1517	LYS

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Mol	Chain	Res	Type
3	C	84	GLU
9	J	241	VAL
12	M	202	TYR
15	P	199	LYS
23	X	703	ARG
34	q	9	ASN
34	s	24	VAL
35	1	1013	ILE
35	1	1107	GLN
39	2	641	PRO
1	A	1418	ARG
1	A	1528	GLN
9	J	206	LEU
12	M	124	PHE
34	q	19	PRO
34	q	23	HIS
34	r	9	ASN
34	t	67	SER
35	1	722	GLU
35	1	926	LYS
35	1	1106	ARG
1	A	378	PHE
1	A	570	ASP
1	A	698	PRO
3	C	358	LYS
9	J	188	GLN
11	L	146	GLU
17	R	428	GLU
20	U	2	TYR
25	Z	65	ILE
34	t	65	PRO
35	1	611	SER
35	1	717	THR
1	A	188	LEU
9	J	341	PRO
34	s	62	ARG
35	1	1011	PRO
35	1	1091	HIS
1	A	108	MET
1	A	227	ARG
17	R	223	PRO
37	p	214	PRO

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Mol	Chain	Res	Type
1	A	942	PRO
3	C	440	SER
25	Z	17	PRO
1	A	109	PRO
8	I	51	PRO
34	s	38	GLY
36	3	672	GLY
1	A	729	PRO
34	r	60	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	1768/2108 (84%)	1579 (89%)	189 (11%)	6 25
3	C	747/866 (86%)	654 (88%)	93 (12%)	4 19
4	E	256/300 (85%)	213 (83%)	43 (17%)	2 9
8	I	24/749 (3%)	24 (100%)	0	100 100
9	J	239/751 (32%)	222 (93%)	17 (7%)	14 42
10	K	20/294 (7%)	16 (80%)	4 (20%)	1 5
11	L	171/709 (24%)	143 (84%)	28 (16%)	2 10
12	M	104/209 (50%)	91 (88%)	13 (12%)	4 19
13	N	130/130 (100%)	116 (89%)	14 (11%)	6 24
14	O	3/361 (1%)	3 (100%)	0	100 100
15	P	95/203 (47%)	80 (84%)	15 (16%)	2 11
17	R	282/457 (62%)	235 (83%)	47 (17%)	2 10
19	T	273/441 (62%)	248 (91%)	25 (9%)	9 31
20	U	21/2432 (1%)	19 (90%)	2 (10%)	8 29
21	V	188/838 (22%)	156 (83%)	32 (17%)	2 9
23	X	682/897 (76%)	600 (88%)	82 (12%)	5 20
24	Y	286/451 (63%)	246 (86%)	40 (14%)	3 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
27	m	4/177 (2%)	4 (100%)	0	100 100
28	n	3/101 (3%)	3 (100%)	0	100 100
29	h	5/110 (4%)	5 (100%)	0	100 100
30	i	4/74 (5%)	4 (100%)	0	100 100
31	j	1/84 (1%)	1 (100%)	0	100 100
32	k	3/66 (4%)	3 (100%)	0	100 100
33	l	3/101 (3%)	3 (100%)	0	100 100
35	1	700/1104 (63%)	601 (86%)	99 (14%)	3 16
36	3	1018/1051 (97%)	810 (80%)	208 (20%)	1 4
37	p	8/195 (4%)	8 (100%)	0	100 100
38	w	104/446 (23%)	85 (82%)	19 (18%)	1 7
39	2	151/776 (20%)	125 (83%)	26 (17%)	2 9
41	7	69/95 (73%)	47 (68%)	22 (32%)	0 1
42	5	68/77 (88%)	53 (78%)	15 (22%)	1 3
43	o	6/218 (3%)	6 (100%)	0	100 100
All	All	7436/16871 (44%)	6403 (86%)	1033 (14%)	7 16

All (1033) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	43	LYS
1	A	47	GLU
1	A	55	ASP
1	A	57	GLN
1	A	59	GLU
1	A	60	ASP
1	A	82	ARG
1	A	88	TYR
1	A	95	MET
1	A	97	HIS
1	A	123	THR
1	A	137	GLU
1	A	146	SER
1	A	155	LYS
1	A	161	PHE
1	A	163	ARG

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Mol	Chain	Res	Type
1	A	188	LEU
1	A	189	GLU
1	A	193	LEU
1	A	205	ASP
1	A	214	ARG
1	A	216	SER
1	A	258	PHE
1	A	261	LYS
1	A	284	ARG
1	A	295	GLU
1	A	329	LEU
1	A	330	THR
1	A	337	VAL
1	A	343	GLU
1	A	360	SER
1	A	361	HIS
1	A	371	LEU
1	A	376	GLU
1	A	387	PHE
1	A	388	LEU
1	A	404	LEU
1	A	422	LEU
1	A	431	TYR
1	A	467	GLN
1	A	480	LYS
1	A	518	LEU
1	A	530	LEU
1	A	546	LEU
1	A	554	THR
1	A	560	SER
1	A	569	VAL
1	A	576	ASP
1	A	579	GLN
1	A	600	ARG
1	A	644	ILE
1	A	670	LYS
1	A	683	LEU
1	A	693	ILE
1	A	694	LEU
1	A	708	THR
1	A	714	SER
1	A	727	LYS

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Mol	Chain	Res	Type
1	A	751	THR
1	A	769	LYS
1	A	789	GLU
1	A	815	HIS
1	A	819	SER
1	A	830	LEU
1	A	831	SER
1	A	836	THR
1	A	845	ARG
1	A	850	TYR
1	A	856	LEU
1	A	866	LEU
1	A	869	GLN
1	A	871	TYR
1	A	885	LEU
1	A	893	GLU
1	A	931	ASP
1	A	933	ARG
1	A	941	LYS
1	A	946	GLU
1	A	968	THR
1	A	977	LEU
1	A	978	GLU
1	A	979	SER
1	A	983	LYS
1	A	995	ARG
1	A	1000	ILE
1	A	1038	SER
1	A	1075	GLN
1	A	1076	ASP
1	A	1079	THR
1	A	1091	TYR
1	A	1104	ASP
1	A	1122	ASN
1	A	1128	TYR
1	A	1144	LYS
1	A	1158	LYS
1	A	1166	THR
1	A	1176	SER
1	A	1181	ASP
1	A	1186	LEU
1	A	1199	LYS

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Mol	Chain	Res	Type
1	A	1205	GLU
1	A	1210	LYS
1	A	1235	GLU
1	A	1243	ARG
1	A	1253	SER
1	A	1276	GLU
1	A	1293	ASN
1	A	1298	ARG
1	A	1327	MET
1	A	1329	SER
1	A	1343	SER
1	A	1344	LYS
1	A	1348	VAL
1	A	1359	HIS
1	A	1362	ASP
1	A	1368	LEU
1	A	1370	ARG
1	A	1376	GLU
1	A	1377	SER
1	A	1382	SER
1	A	1394	GLN
1	A	1404	THR
1	A	1407	ASP
1	A	1427	ARG
1	A	1437	ARG
1	A	1449	LYS
1	A	1459	ARG
1	A	1517	LYS
1	A	1519	THR
1	A	1520	ASN
1	A	1523	ARG
1	A	1524	SER
1	A	1529	ILE
1	A	1548	TYR
1	A	1554	GLN
1	A	1555	LEU
1	A	1558	THR
1	A	1568	THR
1	A	1601	LEU
1	A	1606	ILE
1	A	1608	THR
1	A	1615	HIS

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Mol	Chain	Res	Type
1	A	1623	ASN
1	A	1624	SER
1	A	1628	ASP
1	A	1635	TYR
1	A	1641	ARG
1	A	1644	LEU
1	A	1648	SER
1	A	1649	LYS
1	A	1667	ARG
1	A	1672	ASP
1	A	1692	MET
1	A	1697	SER
1	A	1702	LEU
1	A	1723	LYS
1	A	1772	PHE
1	A	1773	SER
1	A	1783	THR
1	A	1800	THR
1	A	1813	ARG
1	A	1818	PHE
1	A	1825	SER
1	A	1830	GLN
1	A	1831	LYS
1	A	1833	LEU
1	A	1836	LEU
1	A	1850	ARG
1	A	1852	LEU
1	A	1857	GLN
1	A	1870	ASP
1	A	1878	ASP
1	A	1887	SER
1	A	1910	THR
1	A	1914	MET
1	A	1919	LEU
1	A	1924	LEU
1	A	1926	THR
1	A	1930	TYR
1	A	1944	HIS
1	A	1970	THR
1	A	1973	ASP
1	A	1976	TRP
1	A	1977	ILE

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Mol	Chain	Res	Type
1	A	1986	LEU
1	A	1997	VAL
1	A	2005	SER
1	A	2012	LEU
3	C	58	VAL
3	C	65	TYR
3	C	68	THR
3	C	86	THR
3	C	90	THR
3	C	117	ASP
3	C	135	CYS
3	C	173	THR
3	C	197	SER
3	C	213	ASP
3	C	223	ASP
3	C	233	GLU
3	C	240	GLU
3	C	248	GLN
3	C	256	CYS
3	C	283	ASP
3	C	290	SER
3	C	293	SER
3	C	295	ASP
3	C	296	GLU
3	C	308	CYS
3	C	312	SER
3	C	316	ILE
3	C	322	SER
3	C	326	ILE
3	C	327	TYR
3	C	333	ASP
3	C	359	LYS
3	C	363	SER
3	C	372	PHE
3	C	399	LEU
3	C	408	LEU
3	C	417	ARG
3	C	422	LYS
3	C	436	GLN
3	C	440	SER
3	C	450	GLU
3	C	454	THR

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Mol	Chain	Res	Type
3	C	457	VAL
3	C	458	ASP
3	C	483	SER
3	C	485	ASP
3	C	498	SER
3	C	500	THR
3	C	507	VAL
3	C	510	LEU
3	C	514	TYR
3	C	536	ARG
3	C	538	HIS
3	C	543	ARG
3	C	559	ILE
3	C	562	THR
3	C	567	GLU
3	C	572	GLU
3	C	573	GLU
3	C	578	ARG
3	C	608	ARG
3	C	612	LYS
3	C	622	GLU
3	C	632	THR
3	C	639	CYS
3	C	642	HIS
3	C	657	ASP
3	C	661	THR
3	C	673	LYS
3	C	675	PHE
3	C	678	THR
3	C	696	LEU
3	C	698	GLU
3	C	716	GLU
3	C	722	TYR
3	C	723	ASP
3	C	724	TRP
3	C	749	THR
3	C	750	LEU
3	C	753	GLU
3	C	759	LEU
3	C	766	ILE
3	C	802	HIS
3	C	803	ARG

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Mol	Chain	Res	Type
3	C	809	ILE
3	C	822	MET
3	C	824	THR
3	C	829	GLU
3	C	837	GLN
3	C	846	VAL
3	C	879	ASP
3	C	885	THR
3	C	900	VAL
3	C	916	ILE
3	C	922	GLU
3	C	928	HIS
3	C	940	ARG
4	E	61	LEU
4	E	71	CYS
4	E	73	LYS
4	E	86	PHE
4	E	87	ASP
4	E	100	ASP
4	E	104	THR
4	E	106	LYS
4	E	108	HIS
4	E	117	TYR
4	E	119	THR
4	E	123	MET
4	E	125	PHE
4	E	137	ASP
4	E	143	ARG
4	E	144	VAL
4	E	155	ASN
4	E	162	ARG
4	E	167	VAL
4	E	175	THR
4	E	176	VAL
4	E	189	THR
4	E	205	SER
4	E	206	ASP
4	E	210	SER
4	E	226	LYS
4	E	227	LEU
4	E	232	ARG
4	E	234	HIS

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Mol	Chain	Res	Type
4	E	243	LEU
4	E	258	THR
4	E	265	ARG
4	E	267	PHE
4	E	282	HIS
4	E	284	PHE
4	E	286	LYS
4	E	290	ARG
4	E	300	ILE
4	E	307	ARG
4	E	330	ILE
4	E	333	VAL
4	E	338	ASP
4	E	344	SER
9	J	186	GLU
9	J	188	GLN
9	J	192	GLU
9	J	199	LYS
9	J	200	GLU
9	J	203	LEU
9	J	205	LEU
9	J	214	ILE
9	J	217	GLU
9	J	220	LEU
9	J	238	ASN
9	J	258	ILE
9	J	276	ILE
9	J	367	GLU
9	J	400	GLU
9	J	408	ASP
9	J	419	PHE
10	K	202	CYS
10	K	215	ASP
10	K	218	LYS
10	K	222	ASP
11	L	18	ILE
11	L	24	MET
11	L	25	LYS
11	L	63	TRP
11	L	64	SER
11	L	89	ILE
11	L	91	ARG

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Mol	Chain	Res	Type
11	L	138	ARG
11	L	154	GLU
11	L	158	ARG
11	L	166	LYS
11	L	168	LYS
11	L	169	ARG
11	L	170	LYS
11	L	172	ARG
11	L	173	GLU
11	L	176	LEU
11	L	177	GLU
11	L	178	GLU
11	L	180	ARG
11	L	181	ARG
11	L	182	LEU
11	L	201	LYS
11	L	203	LYS
11	L	205	LYS
11	L	206	ARG
11	L	218	LYS
11	L	222	LEU
12	M	122	LEU
12	M	126	ASP
12	M	151	ARG
12	M	160	PHE
12	M	163	THR
12	M	166	SER
12	M	186	LEU
12	M	200	ARG
12	M	202	TYR
12	M	204	ASP
12	M	212	ASN
12	M	218	PHE
12	M	224	ARG
13	N	3	LYS
13	N	5	LYS
13	N	7	SER
13	N	24	GLU
13	N	41	ARG
13	N	57	THR
13	N	71	SER
13	N	72	ARG

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Mol	Chain	Res	Type
13	N	99	ASN
13	N	112	ASN
13	N	125	LYS
13	N	128	VAL
13	N	134	CYS
13	N	140	ARG
15	P	31	SER
15	P	32	SER
15	P	47	THR
15	P	57	ARG
15	P	74	LYS
15	P	78	ARG
15	P	186	ARG
15	P	196	ASN
15	P	201	VAL
15	P	205	LYS
15	P	207	ASP
15	P	209	ARG
15	P	214	THR
15	P	217	SER
15	P	221	LYS
17	R	107	SER
17	R	108	LYS
17	R	125	MET
17	R	128	ASP
17	R	131	ASP
17	R	132	LEU
17	R	136	ASP
17	R	151	LEU
17	R	153	LYS
17	R	166	ARG
17	R	170	LYS
17	R	180	THR
17	R	183	GLN
17	R	184	GLN
17	R	188	PHE
17	R	197	ILE
17	R	202	MET
17	R	218	ILE
17	R	220	ARG
17	R	235	ARG
17	R	238	THR

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Mol	Chain	Res	Type
17	R	243	GLN
17	R	246	LYS
17	R	251	ILE
17	R	258	LYS
17	R	289	GLU
17	R	295	ASP
17	R	300	GLU
17	R	311	LYS
17	R	322	GLU
17	R	325	ARG
17	R	326	GLU
17	R	329	GLN
17	R	332	ARG
17	R	348	GLU
17	R	352	ARG
17	R	360	ARG
17	R	367	ARG
17	R	370	SER
17	R	382	ARG
17	R	383	ASN
17	R	386	ARG
17	R	398	ASN
17	R	406	GLN
17	R	407	TYR
17	R	409	GLN
17	R	416	LYS
19	T	221	THR
19	T	223	SER
19	T	235	SER
19	T	247	SER
19	T	257	ARG
19	T	258	SER
19	T	263	SER
19	T	264	CYS
19	T	267	ASP
19	T	294	LEU
19	T	307	SER
19	T	319	THR
19	T	338	CYS
19	T	349	SER
19	T	383	ARG
19	T	384	HIS

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Mol	Chain	Res	Type
19	T	385	TYR
19	T	389	SER
19	T	393	ASP
19	T	394	ASN
19	T	424	ASP
19	T	429	SER
19	T	443	THR
19	T	460	ASP
19	T	478	LEU
20	U	1	MET
20	U	2	TYR
21	V	457	ARG
21	V	458	THR
21	V	465	SER
21	V	481	PHE
21	V	483	GLU
21	V	486	THR
21	V	487	LYS
21	V	494	LEU
21	V	504	GLU
21	V	528	ILE
21	V	530	LYS
21	V	538	ARG
21	V	544	LEU
21	V	556	TYR
21	V	571	SER
21	V	576	THR
21	V	578	SER
21	V	579	SER
21	V	584	LYS
21	V	588	GLN
21	V	590	LEU
21	V	593	TYR
21	V	606	GLU
21	V	616	LEU
21	V	619	ASP
21	V	622	ARG
21	V	625	ARG
21	V	628	ILE
21	V	633	SER
21	V	640	THR
21	V	646	HIS

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Mol	Chain	Res	Type
21	V	648	LYS
23	X	163	GLU
23	X	194	ARG
23	X	216	GLU
23	X	225	GLU
23	X	228	LYS
23	X	232	ARG
23	X	237	LYS
23	X	252	ASP
23	X	254	GLU
23	X	257	PHE
23	X	276	VAL
23	X	277	ARG
23	X	278	ASP
23	X	282	GLU
23	X	292	LEU
23	X	293	GLU
23	X	329	TRP
23	X	338	SER
23	X	339	LEU
23	X	383	SER
23	X	387	GLN
23	X	389	LYS
23	X	393	GLN
23	X	408	LEU
23	X	409	LEU
23	X	436	LEU
23	X	437	PHE
23	X	442	THR
23	X	452	GLN
23	X	476	GLU
23	X	482	ARG
23	X	494	ARG
23	X	503	ARG
23	X	511	LEU
23	X	513	SER
23	X	515	SER
23	X	517	VAL
23	X	518	MET
23	X	533	PHE
23	X	547	LYS
23	X	562	THR

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Mol	Chain	Res	Type
23	X	575	ARG
23	X	590	ASP
23	X	599	VAL
23	X	621	ILE
23	X	625	CYS
23	X	633	ARG
23	X	643	LEU
23	X	648	TYR
23	X	682	THR
23	X	683	ILE
23	X	698	LYS
23	X	712	THR
23	X	714	CYS
23	X	715	SER
23	X	748	GLU
23	X	749	GLU
23	X	757	ARG
23	X	767	LEU
23	X	788	THR
23	X	789	LEU
23	X	795	GLN
23	X	796	LEU
23	X	808	LEU
23	X	809	THR
23	X	836	CYS
23	X	847	LEU
23	X	895	SER
23	X	896	GLN
23	X	913	ASP
23	X	915	ARG
23	X	916	GLU
23	X	922	LEU
23	X	923	GLU
23	X	932	CYS
23	X	943	ILE
23	X	954	LEU
23	X	956	ARG
23	X	994	LYS
23	X	1014	HIS
23	X	1019	LYS
23	X	1021	LEU
24	Y	1	MET

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Mol	Chain	Res	Type
24	Y	9	LEU
24	Y	14	ILE
24	Y	18	THR
24	Y	19	GLU
24	Y	26	LEU
24	Y	38	ASN
24	Y	61	ARG
24	Y	64	GLU
24	Y	73	ASP
24	Y	81	GLU
24	Y	85	ARG
24	Y	106	SER
24	Y	118	TYR
24	Y	126	PHE
24	Y	133	MET
24	Y	138	LYS
24	Y	140	ASN
24	Y	159	THR
24	Y	177	ARG
24	Y	182	THR
24	Y	188	SER
24	Y	194	ASP
24	Y	199	ASP
24	Y	200	PHE
24	Y	211	ILE
24	Y	219	THR
24	Y	232	ASP
24	Y	245	CYS
24	Y	251	THR
24	Y	253	ASP
24	Y	255	ASP
24	Y	257	GLU
24	Y	274	ASP
24	Y	276	LYS
24	Y	279	GLU
24	Y	280	SER
24	Y	305	LEU
24	Y	312	HIS
24	Y	319	VAL
35	1	493	LYS
35	1	512	ARG
35	1	544	LEU

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Mol	Chain	Res	Type
35	1	545	GLU
35	1	554	LYS
35	1	558	ARG
35	1	560	LEU
35	1	562	LYS
35	1	563	LEU
35	1	564	ASP
35	1	571	VAL
35	1	573	LYS
35	1	581	LEU
35	1	582	LEU
35	1	585	GLU
35	1	598	SER
35	1	610	ILE
35	1	613	MET
35	1	614	ARG
35	1	616	ASP
35	1	623	TYR
35	1	630	ARG
35	1	673	ILE
35	1	685	SER
35	1	686	LEU
35	1	698	GLN
35	1	707	LEU
35	1	736	ARG
35	1	739	ARG
35	1	754	ILE
35	1	760	GLU
35	1	768	GLU
35	1	779	SER
35	1	794	GLN
35	1	795	CYS
35	1	801	VAL
35	1	827	ARG
35	1	836	THR
35	1	844	VAL
35	1	858	LYS
35	1	873	GLU
35	1	890	GLU
35	1	892	LEU
35	1	893	ILE
35	1	901	GLN

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Mol	Chain	Res	Type
35	1	904	THR
35	1	928	TYR
35	1	946	LYS
35	1	947	VAL
35	1	958	THR
35	1	963	LYS
35	1	964	THR
35	1	967	GLU
35	1	968	GLU
35	1	971	MET
35	1	973	HIS
35	1	982	LEU
35	1	1003	VAL
35	1	1006	MET
35	1	1014	LYS
35	1	1015	ASP
35	1	1019	ARG
35	1	1021	THR
35	1	1028	HIS
35	1	1029	GLU
35	1	1030	LYS
35	1	1031	VAL
35	1	1032	GLN
35	1	1041	ARG
35	1	1048	GLU
35	1	1065	LEU
35	1	1067	LYS
35	1	1080	THR
35	1	1092	ASP
35	1	1104	GLN
35	1	1106	ARG
35	1	1112	THR
35	1	1113	THR
35	1	1122	THR
35	1	1138	VAL
35	1	1143	VAL
35	1	1150	SER
35	1	1164	ASP
35	1	1170	THR
35	1	1174	GLU
35	1	1182	LEU
35	1	1196	SER

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Mol	Chain	Res	Type
35	1	1200	TYR
35	1	1219	VAL
35	1	1245	ARG
35	1	1250	CYS
35	1	1260	LYS
35	1	1276	SER
35	1	1277	GLN
35	1	1281	ILE
35	1	1292	LYS
35	1	1296	ILE
35	1	1303	ILE
35	1	1304	LEU
36	3	1	MET
36	3	9	GLN
36	3	18	ILE
36	3	25	THR
36	3	33	SER
36	3	36	LYS
36	3	41	LEU
36	3	44	ASP
36	3	52	THR
36	3	56	VAL
36	3	66	MET
36	3	68	PHE
36	3	74	THR
36	3	76	ASP
36	3	78	ILE
36	3	90	LEU
36	3	92	TYR
36	3	98	MET
36	3	106	THR
36	3	110	SER
36	3	116	VAL
36	3	121	LEU
36	3	124	ASP
36	3	126	LYS
36	3	130	VAL
36	3	131	MET
36	3	133	SER
36	3	139	LYS
36	3	143	ILE
36	3	153	THR

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Mol	Chain	Res	Type
36	3	164	ASN
36	3	170	VAL
36	3	173	VAL
36	3	184	CYS
36	3	188	ASP
36	3	195	ASP
36	3	203	ASN
36	3	204	THR
36	3	207	THR
36	3	209	THR
36	3	221	VAL
36	3	222	ARG
36	3	225	SER
36	3	226	GLU
36	3	230	GLU
36	3	233	ASN
36	3	242	SER
36	3	256	ILE
36	3	261	PHE
36	3	263	ASP
36	3	264	GLN
36	3	266	ASP
36	3	271	ILE
36	3	273	ARG
36	3	275	ARG
36	3	282	GLU
36	3	286	ILE
36	3	287	PHE
36	3	294	LYS
36	3	315	LEU
36	3	317	THR
36	3	318	ASP
36	3	320	ASP
36	3	327	LEU
36	3	330	PHE
36	3	331	ASP
36	3	332	THR
36	3	340	CYS
36	3	343	LYS
36	3	344	THR
36	3	347	LEU
36	3	355	ASN

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Mol	Chain	Res	Type
36	3	356	HIS
36	3	364	LEU
36	3	384	THR
36	3	390	ARG
36	3	392	LEU
36	3	403	SER
36	3	404	LEU
36	3	408	LEU
36	3	411	GLN
36	3	417	ASN
36	3	419	ASP
36	3	427	CYS
36	3	433	SER
36	3	435	LEU
36	3	439	ARG
36	3	443	GLU
36	3	455	ASN
36	3	461	THR
36	3	464	ARG
36	3	465	HIS
36	3	469	GLU
36	3	471	ASP
36	3	475	ILE
36	3	477	SER
36	3	482	THR
36	3	492	GLU
36	3	510	LEU
36	3	511	LEU
36	3	514	ASP
36	3	526	HIS
36	3	527	ILE
36	3	537	LYS
36	3	541	LYS
36	3	543	THR
36	3	544	ILE
36	3	547	CYS
36	3	568	MET
36	3	573	GLN
36	3	574	LEU
36	3	580	ARG
36	3	584	SER
36	3	592	LEU

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Mol	Chain	Res	Type
36	3	594	ASN
36	3	595	VAL
36	3	603	ARG
36	3	604	PHE
36	3	605	LEU
36	3	612	ASN
36	3	617	ILE
36	3	620	ASP
36	3	630	MET
36	3	638	GLU
36	3	665	LEU
36	3	669	LEU
36	3	676	ARG
36	3	677	THR
36	3	679	LEU
36	3	685	ASP
36	3	689	THR
36	3	697	ARG
36	3	703	ARG
36	3	704	VAL
36	3	715	MET
36	3	727	SER
36	3	732	THR
36	3	738	THR
36	3	743	SER
36	3	758	SER
36	3	768	GLU
36	3	775	ASN
36	3	776	GLN
36	3	786	ARG
36	3	797	LEU
36	3	798	ILE
36	3	802	THR
36	3	814	GLN
36	3	815	ARG
36	3	822	GLU
36	3	834	LEU
36	3	837	GLU
36	3	842	PHE
36	3	850	SER
36	3	851	ILE
36	3	867	ARG

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Mol	Chain	Res	Type
36	3	876	THR
36	3	882	LEU
36	3	883	GLU
36	3	901	GLU
36	3	902	ASP
36	3	904	TYR
36	3	906	LEU
36	3	927	THR
36	3	931	VAL
36	3	936	LYS
36	3	937	LEU
36	3	941	HIS
36	3	942	LYS
36	3	958	ARG
36	3	961	ILE
36	3	966	LEU
36	3	978	LEU
36	3	981	CYS
36	3	988	ASN
36	3	991	SER
36	3	993	ILE
36	3	995	THR
36	3	996	ILE
36	3	998	HIS
36	3	1002	VAL
36	3	1004	ASP
36	3	1012	VAL
36	3	1022	ILE
36	3	1026	ASP
36	3	1028	THR
36	3	1035	THR
36	3	1042	ASP
36	3	1062	THR
36	3	1066	VAL
36	3	1090	GLU
36	3	1093	MET
36	3	1094	ASN
36	3	1099	GLU
36	3	1103	SER
36	3	1107	THR
36	3	1116	SER
36	3	1118	VAL

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Mol	Chain	Res	Type
36	3	1120	THR
36	3	1121	THR
36	3	1148	LEU
36	3	1150	SER
36	3	1151	GLU
36	3	1166	TYR
36	3	1168	PHE
36	3	1170	VAL
36	3	1183	ASN
36	3	1217	PHE
38	w	390	LYS
38	w	400	HIS
38	w	403	ASN
38	w	414	TYR
38	w	415	THR
38	w	425	HIS
38	w	430	ARG
38	w	433	HIS
38	w	436	ARG
38	w	437	CYS
38	w	446	PHE
38	w	453	GLU
38	w	458	LEU
38	w	468	SER
38	w	471	TRP
38	w	475	THR
38	w	487	VAL
38	w	493	GLU
38	w	500	LEU
39	2	451	LYS
39	2	456	ARG
39	2	460	PHE
39	2	461	THR
39	2	464	GLU
39	2	465	LEU
39	2	471	ARG
39	2	475	VAL
39	2	477	MET
39	2	479	ASP
39	2	488	LEU
39	2	494	THR
39	2	497	SER

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Mol	Chain	Res	Type
39	2	502	ARG
39	2	509	LYS
39	2	512	GLN
39	2	517	ILE
39	2	526	ASP
39	2	531	THR
39	2	555	GLU
39	2	557	VAL
39	2	561	MET
39	2	590	LEU
39	2	595	LYS
39	2	705	ARG
39	2	710	GLU
41	7	9	ILE
41	7	11	CYS
41	7	12	ARG
41	7	14	GLN
41	7	23	CYS
41	7	25	LYS
41	7	29	LYS
41	7	30	CYS
41	7	33	CYS
41	7	35	SER
41	7	37	VAL
41	7	40	CYS
41	7	45	ILE
41	7	48	GLU
41	7	60	ILE
41	7	68	ASP
41	7	70	TYR
41	7	71	TYR
41	7	72	CYS
41	7	74	GLU
41	7	81	ASP
41	7	89	VAL
42	5	5	TYR
42	5	18	TYR
42	5	23	HIS
42	5	25	ASP
42	5	27	THR
42	5	32	LEU
42	5	35	GLN

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Mol	Chain	Res	Type
42	5	36	HIS
42	5	42	SER
42	5	51	ASN
42	5	60	SER
42	5	63	ARG
42	5	65	ARG
42	5	69	MET
42	5	74	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (153) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	41	GLN
1	A	57	GLN
1	A	73	HIS
1	A	78	ASN
1	A	105	ASN
1	A	112	GLN
1	A	229	GLN
1	A	321	ASN
1	A	322	ASN
1	A	325	HIS
1	A	326	HIS
1	A	357	ASN
1	A	495	GLN
1	A	502	ASN
1	A	654	ASN
1	A	659	GLN
1	A	664	HIS
1	A	711	GLN
1	A	755	HIS
1	A	775	ASN
1	A	788	GLN
1	A	834	HIS
1	A	1014	ASN
1	A	1117	HIS
1	A	1121	ASN
1	A	1400	ASN
1	A	1424	GLN
1	A	1460	HIS
1	A	1546	ASN

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Mol	Chain	Res	Type
1	A	1552	GLN
1	A	1554	GLN
1	A	1583	GLN
1	A	1623	ASN
1	A	1658	GLN
1	A	1774	ASN
1	A	1804	ASN
1	A	1823	HIS
1	A	1830	GLN
1	A	1857	GLN
1	A	1944	HIS
1	A	1965	HIS
3	C	82	GLN
3	C	139	HIS
3	C	245	HIS
3	C	306	ASN
3	C	313	GLN
3	C	350	ASN
3	C	402	HIS
3	C	437	HIS
3	C	505	GLN
3	C	538	HIS
3	C	627	HIS
3	C	903	HIS
3	C	924	GLN
4	E	188	GLN
4	E	225	ASN
4	E	257	ASN
4	E	280	ASN
9	J	238	ASN
9	J	410	HIS
11	L	45	GLN
11	L	81	GLN
11	L	163	GLN
11	L	233	GLN
12	M	134	GLN
12	M	172	HIS
12	M	189	GLN
12	M	215	ASN
12	M	219	ASN
13	N	54	HIS
13	N	95	GLN

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Mol	Chain	Res	Type
15	P	45	GLN
15	P	212	ASN
17	R	104	GLN
17	R	184	GLN
17	R	243	GLN
17	R	279	HIS
17	R	357	HIS
17	R	381	GLN
17	R	398	ASN
19	T	203	HIS
19	T	269	GLN
19	T	407	GLN
19	T	408	ASN
19	T	446	ASN
21	V	451	ASN
21	V	532	GLN
21	V	553	HIS
21	V	609	GLN
23	X	387	GLN
23	X	414	ASN
23	X	475	ASN
23	X	523	HIS
23	X	697	GLN
23	X	745	HIS
23	X	803	ASN
23	X	863	HIS
23	X	904	GLN
24	Y	115	ASN
24	Y	123	HIS
24	Y	140	ASN
24	Y	312	HIS
35	1	534	GLN
35	1	550	HIS
35	1	599	ASN
35	1	619	ASN
35	1	692	HIS
35	1	763	ASN
35	1	817	HIS
35	1	821	HIS
35	1	829	ASN
35	1	886	HIS
35	1	1028	HIS

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Mol	Chain	Res	Type
35	1	1032	GLN
35	1	1134	ASN
35	1	1277	GLN
36	3	5	ASN
36	3	19	HIS
36	3	46	ASN
36	3	145	ASN
36	3	169	HIS
36	3	179	ASN
36	3	194	ASN
36	3	205	GLN
36	3	206	GLN
36	3	231	HIS
36	3	233	ASN
36	3	264	GLN
36	3	411	GLN
36	3	480	ASN
36	3	550	ASN
36	3	573	GLN
36	3	612	ASN
36	3	636	GLN
36	3	709	GLN
36	3	730	HIS
36	3	775	ASN
36	3	791	HIS
36	3	796	ASN
36	3	817	GLN
36	3	844	ASN
36	3	861	GLN
36	3	933	ASN
36	3	994	GLN
36	3	1052	ASN
36	3	1105	GLN
36	3	1172	ASN
38	w	413	ASN
38	w	445	HIS
39	2	546	GLN
41	7	55	GLN
41	7	78	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	96/117 (82%)	28 (29%)	3 (3%)
5	F	96/107 (89%)	42 (43%)	6 (6%)
6	G	77/220 (35%)	44 (57%)	12 (15%)
7	H	163/188 (86%)	69 (42%)	9 (5%)
All	All	432/632 (68%)	183 (42%)	30 (6%)

All (183) 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	26	A
2	B	40	U
2	B	43	U
2	B	45	C
2	B	47	A
2	B	48	A
2	B	52	U
2	B	65	G
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	109	G
5	F	6	C
5	F	7	G
5	F	9	U
5	F	10	U
5	F	11	C
5	F	12	G

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Mol	Chain	Res	Type
5	F	14	C
5	F	16	G
5	F	25	C
5	F	26	U
5	F	27	A
5	F	28	A
5	F	29	A
5	F	30	A
5	F	33	G
5	F	34	G
5	F	35	A
5	F	37	C
5	F	38	G
5	F	40	U
5	F	44	G
5	F	45	A
5	F	48	A
5	F	54	G
5	F	59	G
5	F	60	C
5	F	61	C
5	F	65	G
5	F	66	C
5	F	68	C
5	F	73	A
5	F	74	U
5	F	75	G
5	F	79	C
5	F	80	G
5	F	81	C
5	F	82	A
5	F	83	A
5	F	84	A
5	F	85	U
5	F	86	U
5	F	87	C
6	G	-10	G
6	G	-9	C
6	G	-8	C
6	G	-7	U
6	G	-5	C
6	G	-4	G

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Mol	Chain	Res	Type
6	G	1	G
6	G	2	U
6	G	3	A
6	G	4	A
6	G	8	C
6	G	9	C
6	G	11	A
6	G	13	C
6	G	17	U
6	G	21	A
6	G	22	C
6	G	23	U
6	G	25	G
6	G	26	U
6	G	27	U
6	G	30	C
6	G	84	U
6	G	85	G
6	G	88	G
6	G	89	U
6	G	90	C
6	G	92	U
6	G	97	A
6	G	98	U
6	G	100	C
6	G	101	U
6	G	102	G
6	G	103	U
6	G	104	C
6	G	106	C
6	G	107	U
6	G	111	U
6	G	112	U
6	G	113	U
6	G	114	U
6	G	115	C
6	G	116	C
6	G	117	A
7	H	15	U
7	H	16	U
7	H	17	U
7	H	19	G

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Mol	Chain	Res	Type
7	H	23	A
7	H	24	A
7	H	29	A
7	H	30	A
7	H	31	G
7	H	33	G
7	H	34	U
7	H	35	A
7	H	44	U
7	H	45	C
7	H	46	U
7	H	47	U
7	H	48	A
7	H	49	U
7	H	53	U
7	H	63	G
7	H	64	A
7	H	65	U
7	H	70	C
7	H	74	U
7	H	80	A
7	H	81	G
7	H	82	G
7	H	84	C
7	H	98	G
7	H	99	A
7	H	100	U
7	H	101	U
7	H	102	U
7	H	103	U
7	H	106	G
7	H	107	A
7	H	110	A
7	H	111	G
7	H	112	G
7	H	113	G
7	H	116	A
7	H	117	U
7	H	121	A
7	H	122	U
7	H	123	A
7	H	124	G

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Mol	Chain	Res	Type
7	H	128	C
7	H	129	U
7	H	133	U
7	H	136	G
7	H	137	U
7	H	141	C
7	H	144	C
7	H	145	A
7	H	146	C
7	H	147	G
7	H	149	A
7	H	157	G
7	H	162	U
7	H	164	C
7	H	165	A
7	H	166	G
7	H	168	A
7	H	169	C
7	H	171	U
7	H	177	A
7	H	178	A
7	H	179	C
7	H	180	G

All (30) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	39	C
2	B	94	U
2	B	96	A
5	F	37	C
5	F	47	A
5	F	58	G
5	F	79	C
5	F	84	A
5	F	86	U
6	G	1	G
6	G	21	A
6	G	84	U
6	G	88	G
6	G	89	U
6	G	100	C

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Mol	Chain	Res	Type
6	G	101	U
6	G	102	G
6	G	103	U
6	G	105	C
6	G	111	U
6	G	113	U
7	H	15	U
7	H	16	U
7	H	29	A
7	H	30	A
7	H	31	G
7	H	43	U
7	H	45	C
7	H	47	U
7	H	165	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	SEP	R	224	17	8,9,10	1.42	1 (12%)	8,12,14	1.63	2 (25%)
17	SEP	R	232	17	8,9,10	1.51	1 (12%)	8,12,14	1.31	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	SEP	R	224	17	-	1/5/8/10	-
17	SEP	R	232	17	-	2/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	R	232	SEP	P-O1P	3.21	1.60	1.50
17	R	224	SEP	P-O1P	3.12	1.60	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	R	224	SEP	P-OG-CB	-3.28	109.27	118.30
17	R	224	SEP	OG-CB-CA	2.44	110.52	108.14
17	R	232	SEP	P-OG-CB	-2.25	112.09	118.30

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

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	$\#\|Z\| > 2$
44	IHP	A	3000	-	36,36,36	1.00	1 (2%)	54,60,60	1.84	12 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
45	GTP	C	1500	46	26,34,34	1.59	4 (15%)	32,54,54	2.02	9 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	IHP	A	3000	-	-	5/30/54/54	0/1/1/1
45	GTP	C	1500	46	-	4/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	C	1500	GTP	C5-C6	-5.09	1.37	1.47
45	C	1500	GTP	C2'-C1'	-2.95	1.49	1.53
45	C	1500	GTP	C5-C4	-2.34	1.37	1.43
44	A	3000	IHP	P5-O15	2.13	1.63	1.59
45	C	1500	GTP	O4'-C4'	-2.00	1.40	1.45

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	C	1500	GTP	PB-O3B-PG	-5.18	115.04	132.83
44	A	3000	IHP	O41-P1-O31	4.71	125.65	107.64
44	A	3000	IHP	C5-C4-C3	4.59	120.46	110.41
44	A	3000	IHP	C5-C6-C1	4.39	120.02	110.41
44	A	3000	IHP	O15-C5-C4	4.29	118.81	108.69
45	C	1500	GTP	C5-C6-N1	4.01	121.03	113.95
45	C	1500	GTP	PA-O3A-PB	-3.93	119.33	132.83
44	A	3000	IHP	O41-P1-O11	-3.91	88.48	105.99
45	C	1500	GTP	C2-N1-C6	-3.73	118.23	125.10
44	A	3000	IHP	C4-C3-C2	3.15	117.31	110.41
45	C	1500	GTP	C8-N7-C5	3.15	108.98	102.99
45	C	1500	GTP	O2G-PG-O3B	2.89	114.31	104.64
44	A	3000	IHP	O16-C6-C5	2.77	115.22	108.69
44	A	3000	IHP	C6-C1-C2	2.69	116.29	110.41
44	A	3000	IHP	O15-C5-C6	2.68	114.99	108.69
44	A	3000	IHP	O36-P6-O26	2.52	120.54	110.68
45	C	1500	GTP	O6-C6-C5	-2.41	119.66	124.37
44	A	3000	IHP	O12-P2-O22	-2.28	100.61	109.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	C	1500	GTP	O5'-C5'-C4'	2.26	116.76	108.99
45	C	1500	GTP	O2'-C2'-C1'	-2.08	103.17	110.85
44	A	3000	IHP	O34-P4-O24	2.01	118.57	110.68

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
44	A	3000	IHP	C3-C4-O14-P4
44	A	3000	IHP	C3-O13-P3-O23
44	A	3000	IHP	C5-O15-P5-O25
45	C	1500	GTP	C4'-C5'-O5'-PA
45	C	1500	GTP	C3'-C4'-C5'-O5'
45	C	1500	GTP	O4'-C4'-C5'-O5'
44	A	3000	IHP	C1-C6-O16-P6
44	A	3000	IHP	C3-O13-P3-O43
45	C	1500	GTP	C5'-O5'-PA-O1A

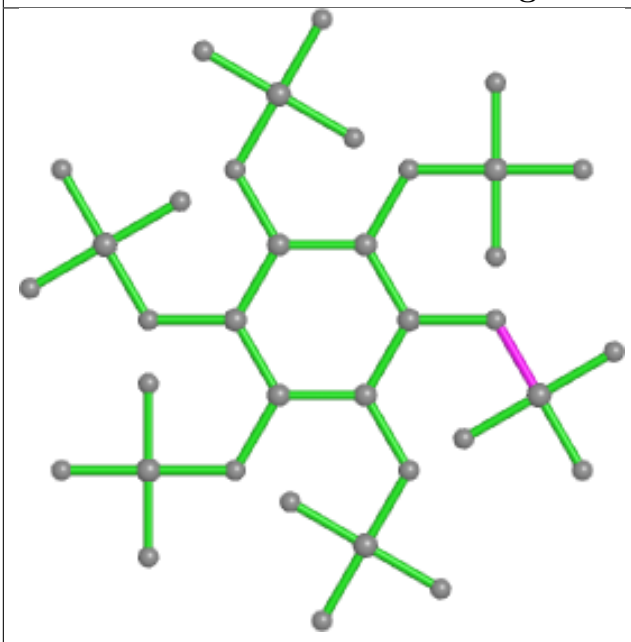
There are no ring outliers.

1 monomer is involved in 5 short contacts:

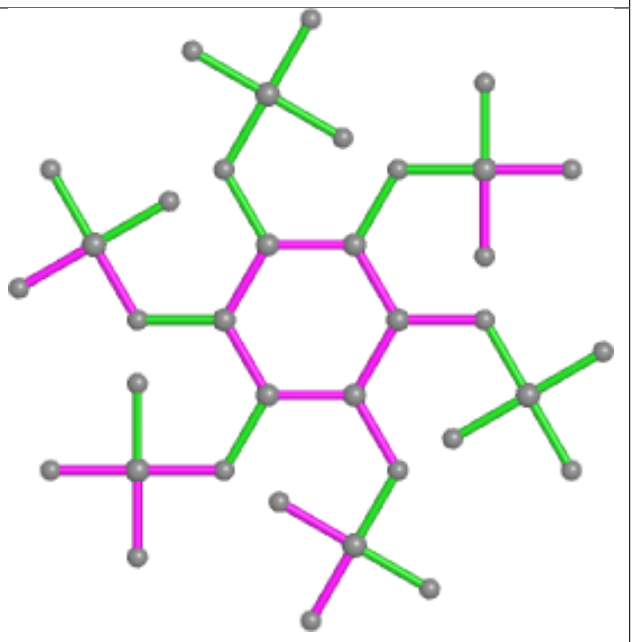
Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	A	3000	IHP	5	0

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.

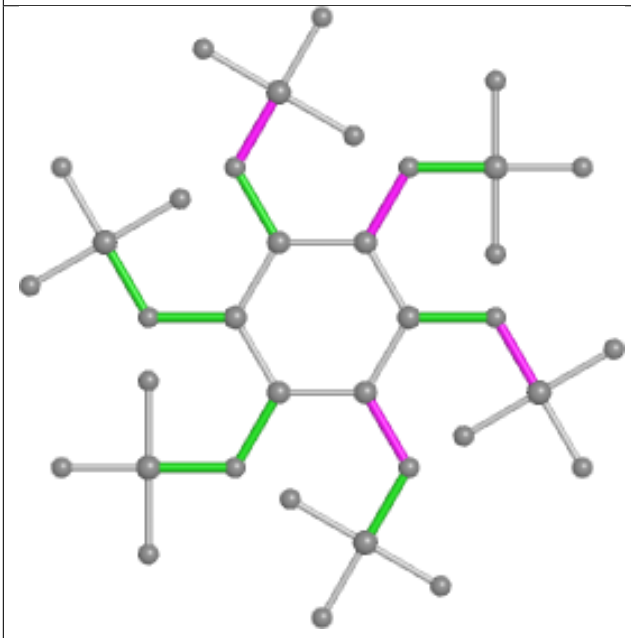
Ligand IHP A 3000



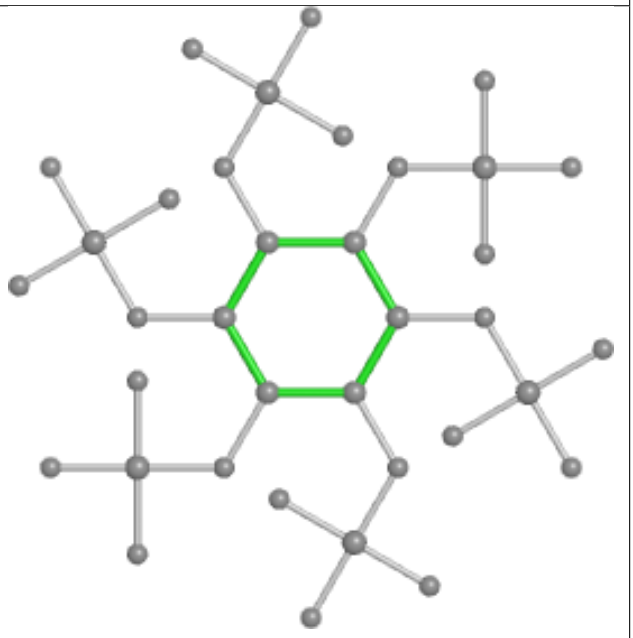
Bond lengths



Bond angles

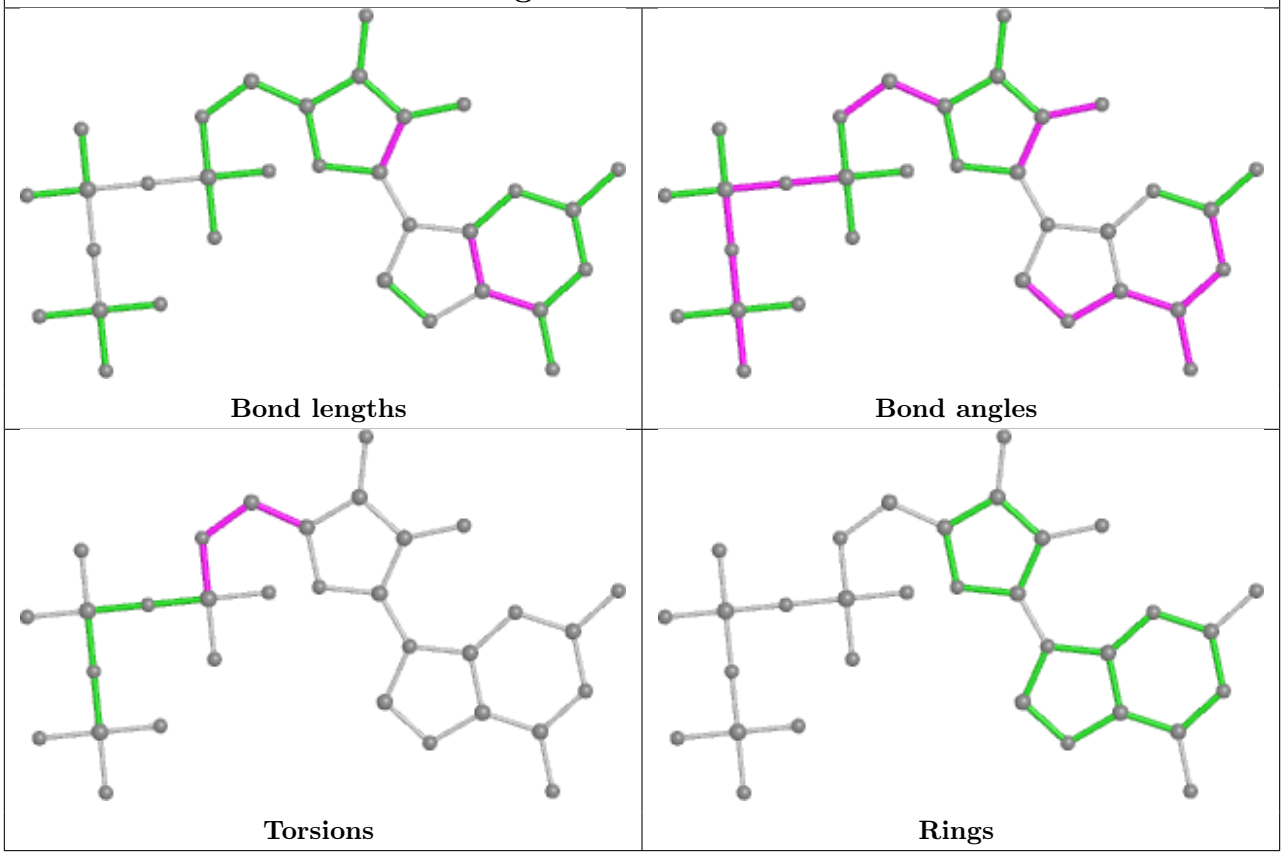


Torsions



Rings

Ligand GTP C 1500



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

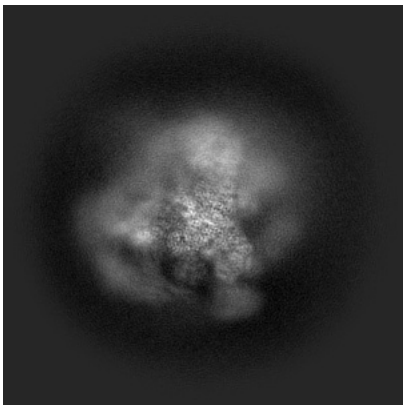
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35110. These allow visual inspection of the internal detail of the map and identification of artifacts.

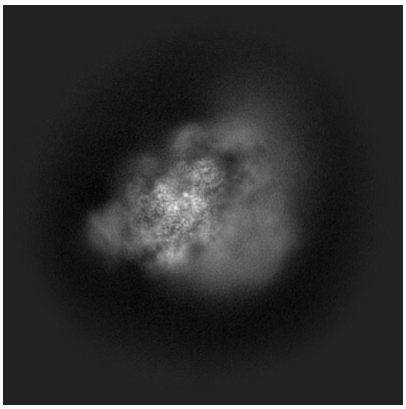
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

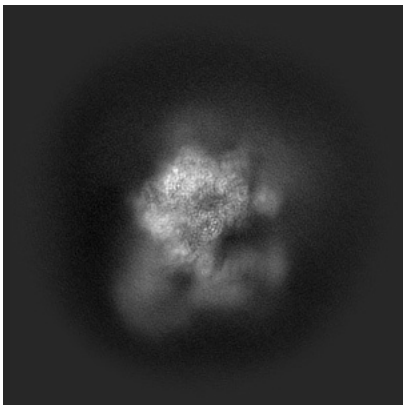
6.1.1 Primary map



X

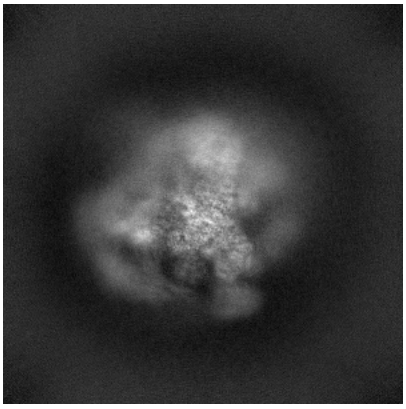


Y

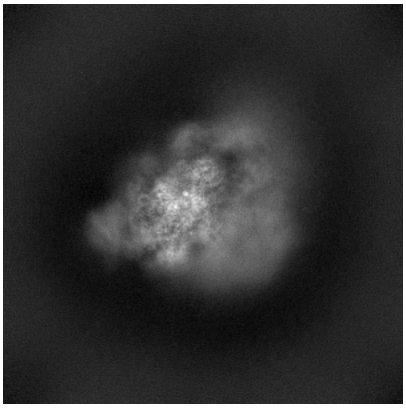


Z

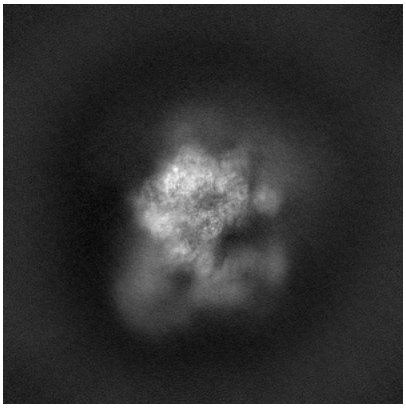
6.1.2 Raw map



X



Y

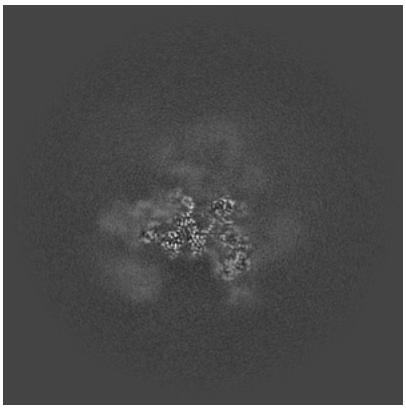


Z

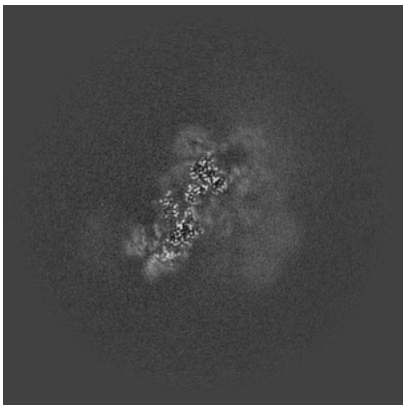
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

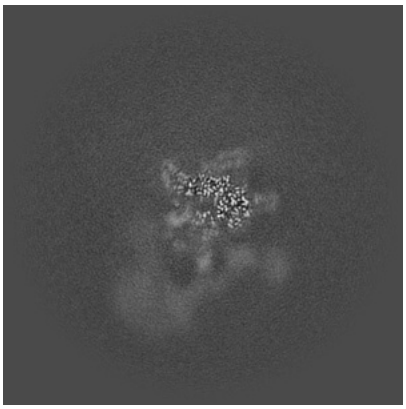
6.2.1 Primary map



X Index: 240

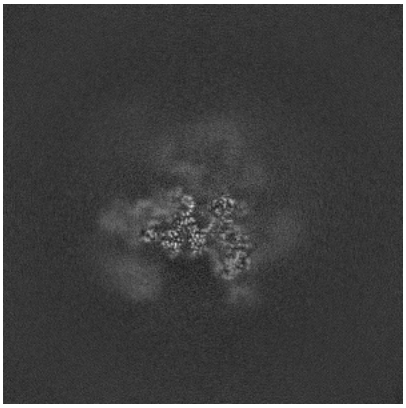


Y Index: 240

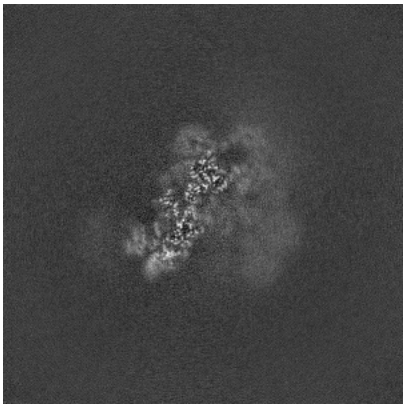


Z Index: 240

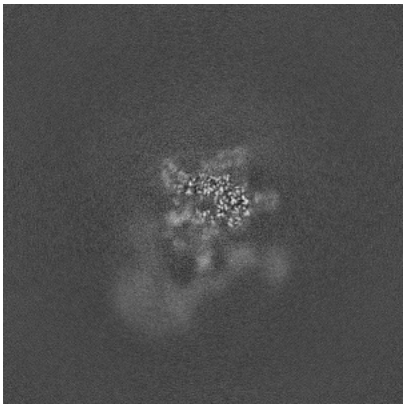
6.2.2 Raw map



X Index: 240



Y Index: 240

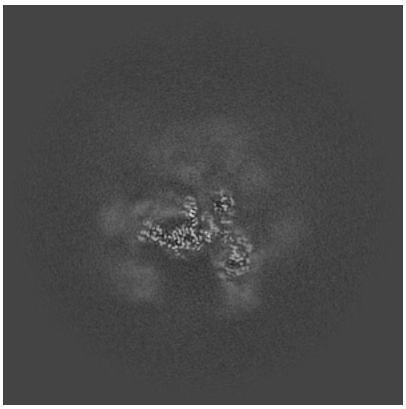


Z Index: 240

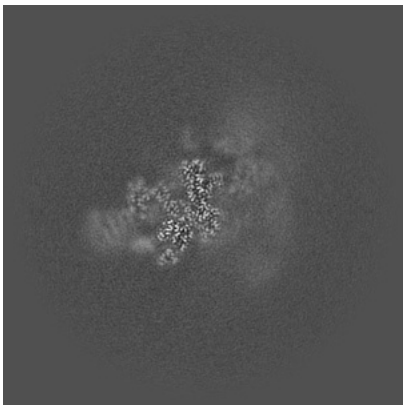
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

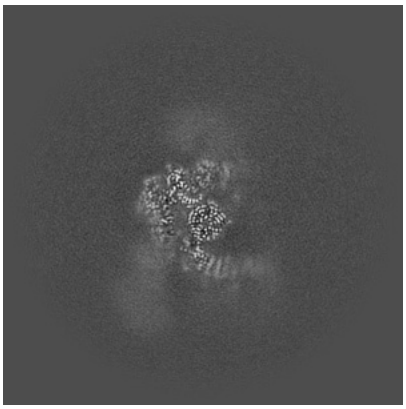
6.3.1 Primary map



X Index: 235

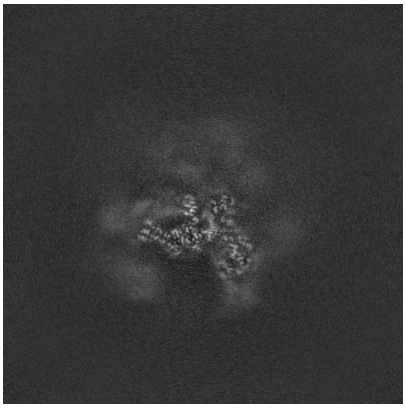


Y Index: 262

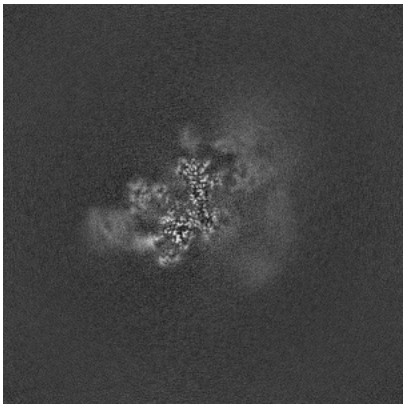


Z Index: 200

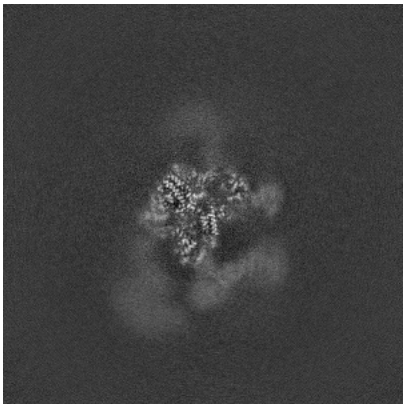
6.3.2 Raw map



X Index: 236



Y Index: 259

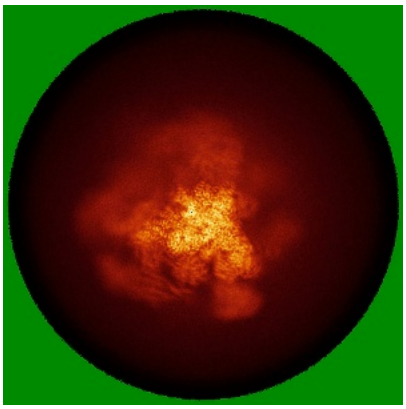


Z Index: 218

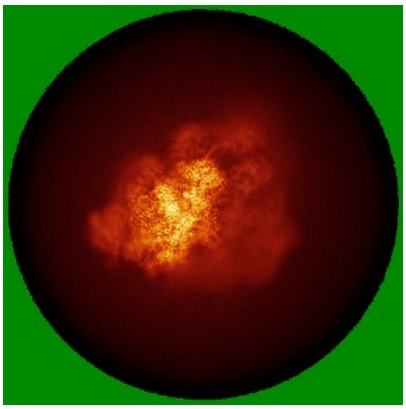
The images above show the largest variance slices of the map in three orthogonal directions.

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

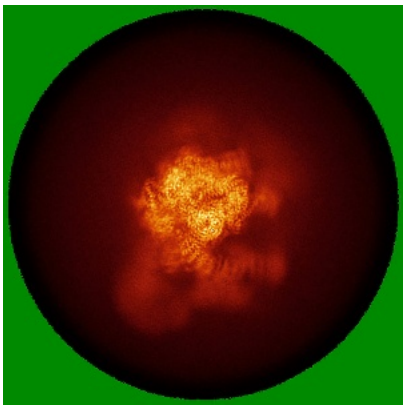
6.4.1 Primary map



X

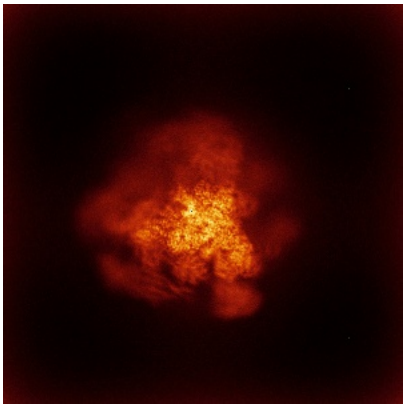


Y

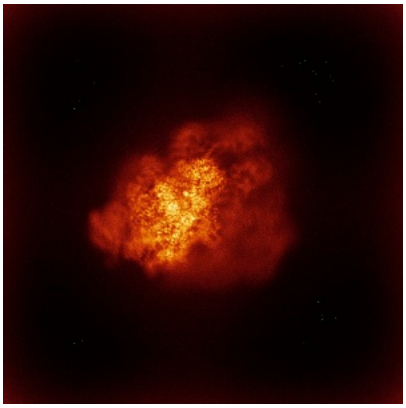


Z

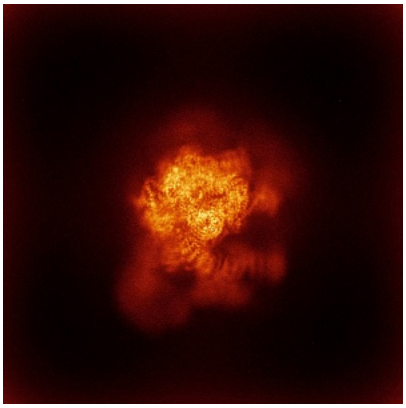
6.4.2 Raw map



X



Y



Z

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

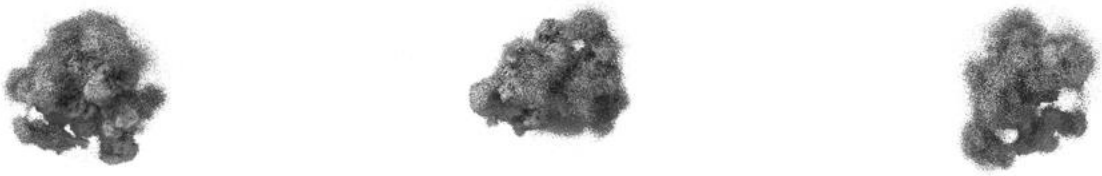
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.24. 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.

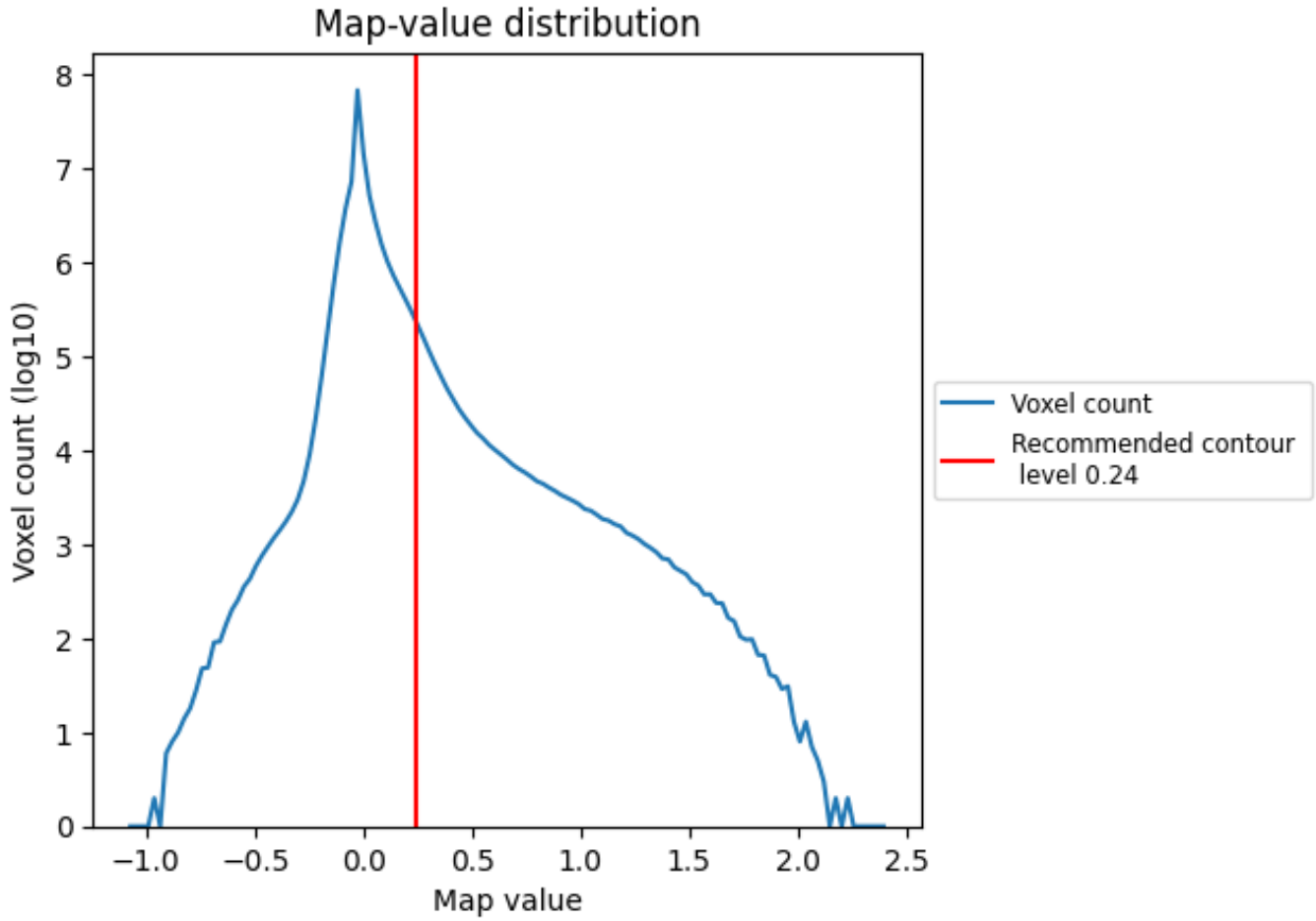
6.6 Mask visualisation (i)

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

7 Map analysis

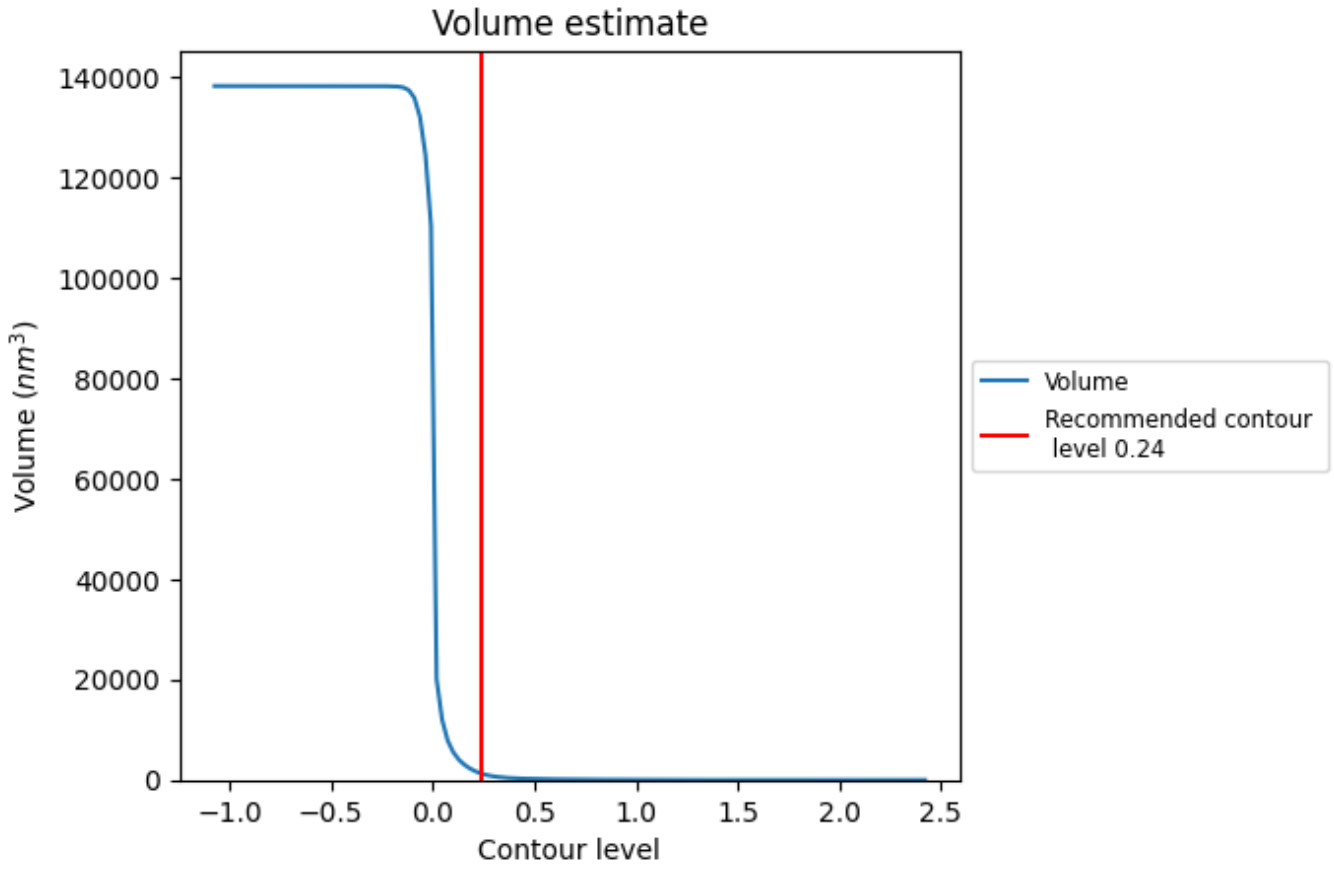
This section contains the results of statistical analysis of the map.

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.

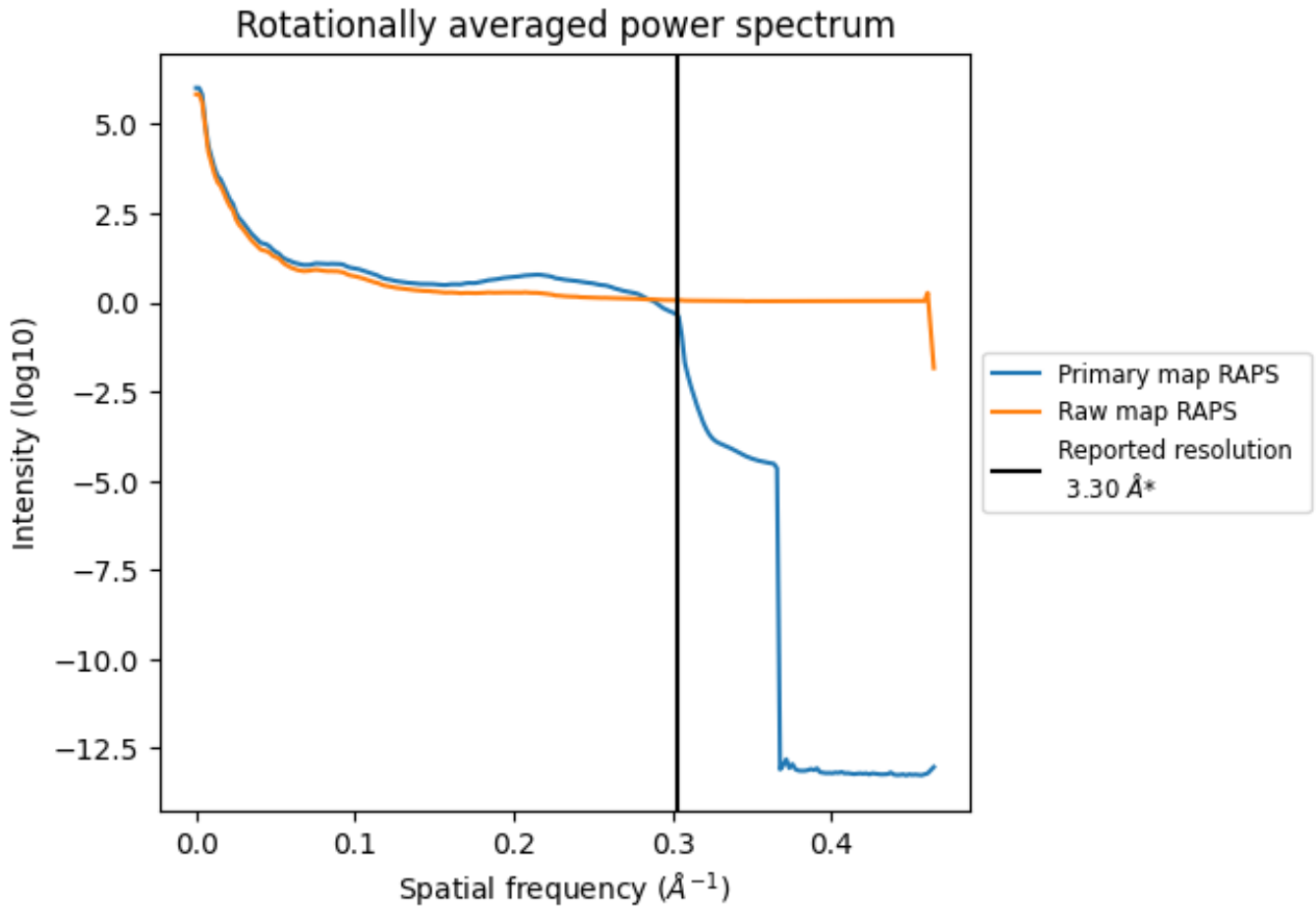
7.2 Volume estimate



The volume at the recommended contour level is 1270 nm^3; this corresponds to an approximate mass of 1147 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)

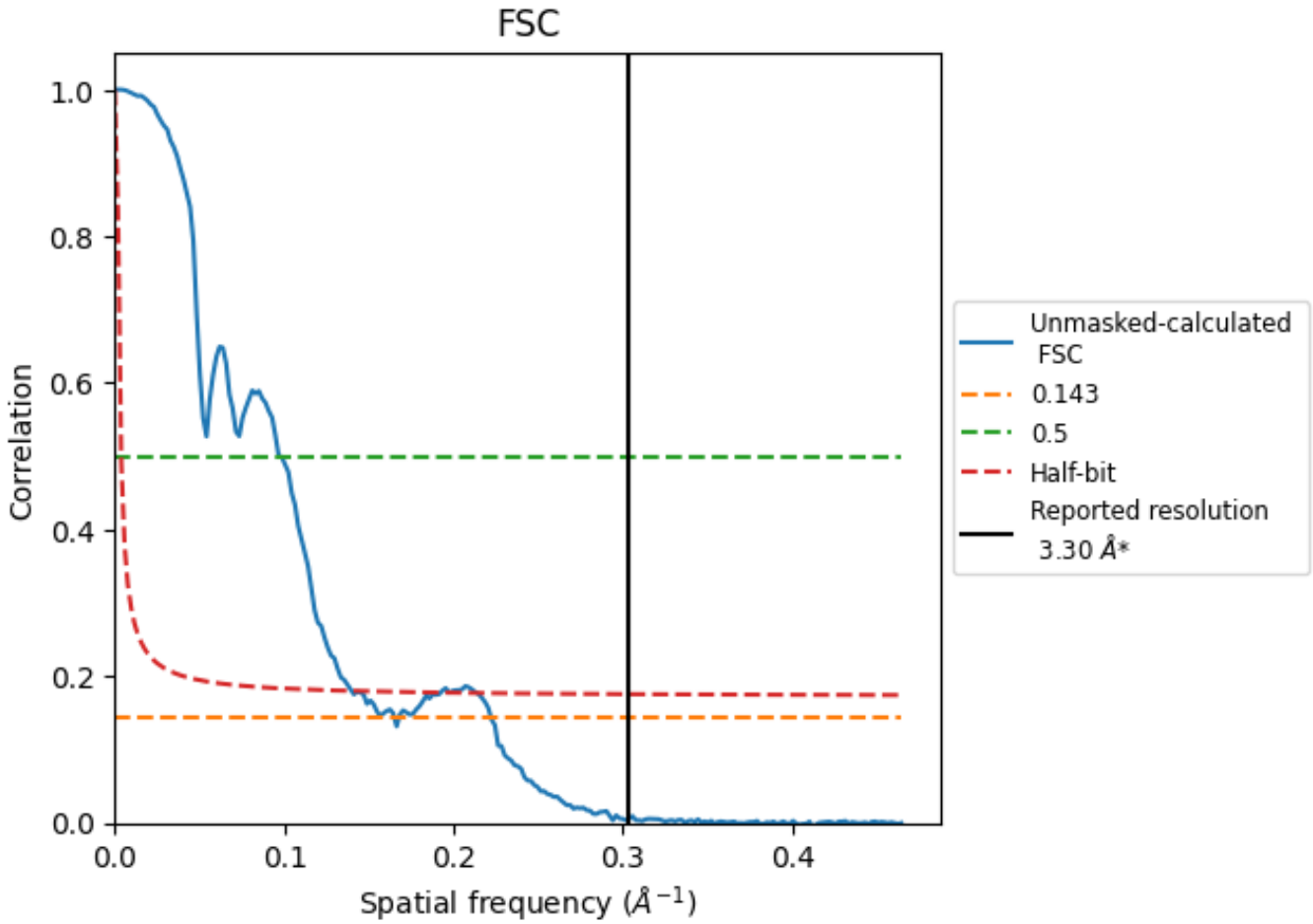


*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

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 0.303 Å^{-1}

8.2 Resolution estimates (i)

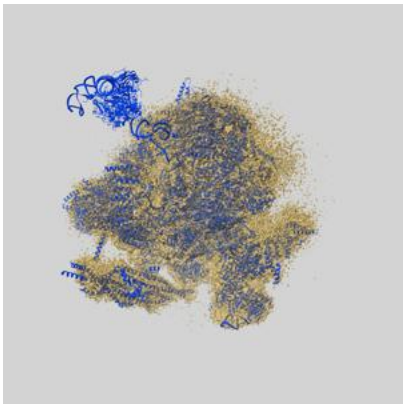
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.06	10.25	7.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.06 differs from the reported value 3.3 by more than 10 %

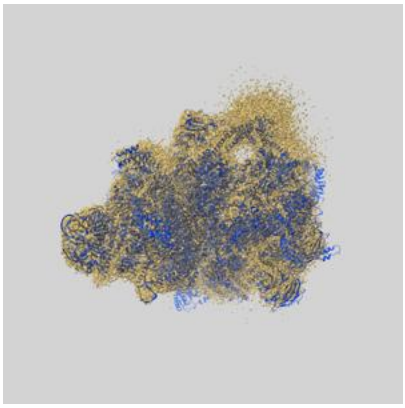
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35110 and PDB model 8I0U. Per-residue inclusion information can be found in section 3 on page 14.

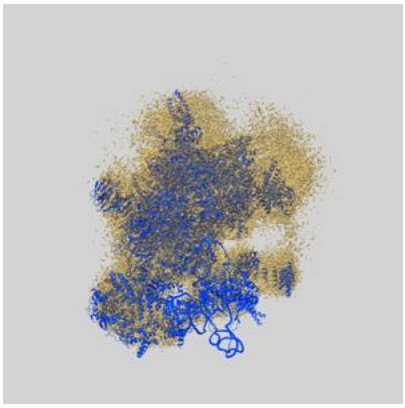
9.1 Map-model overlay



X



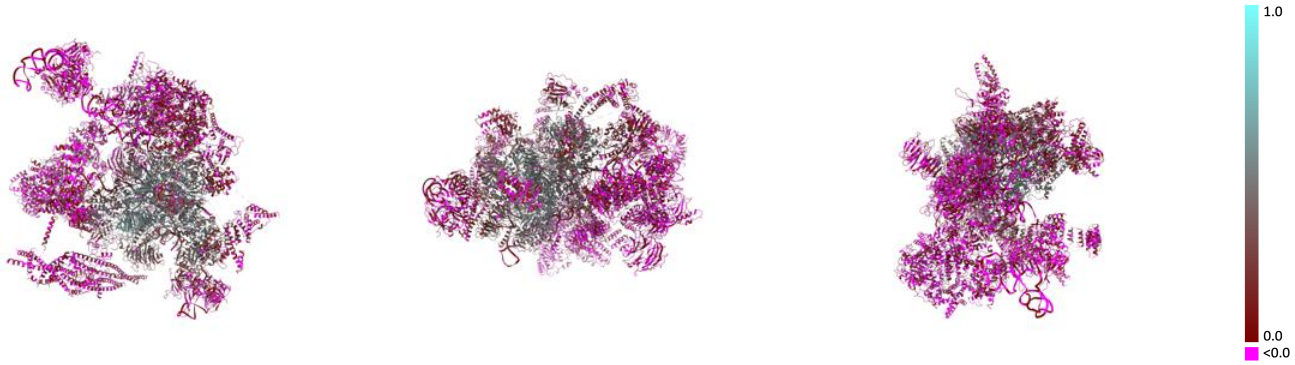
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.24 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.

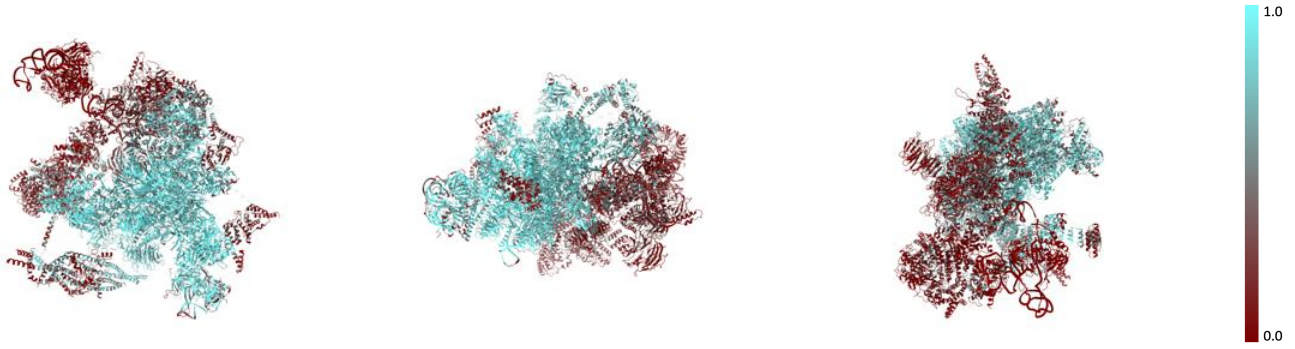
9.2 Q-score mapped to coordinate model (i)



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.

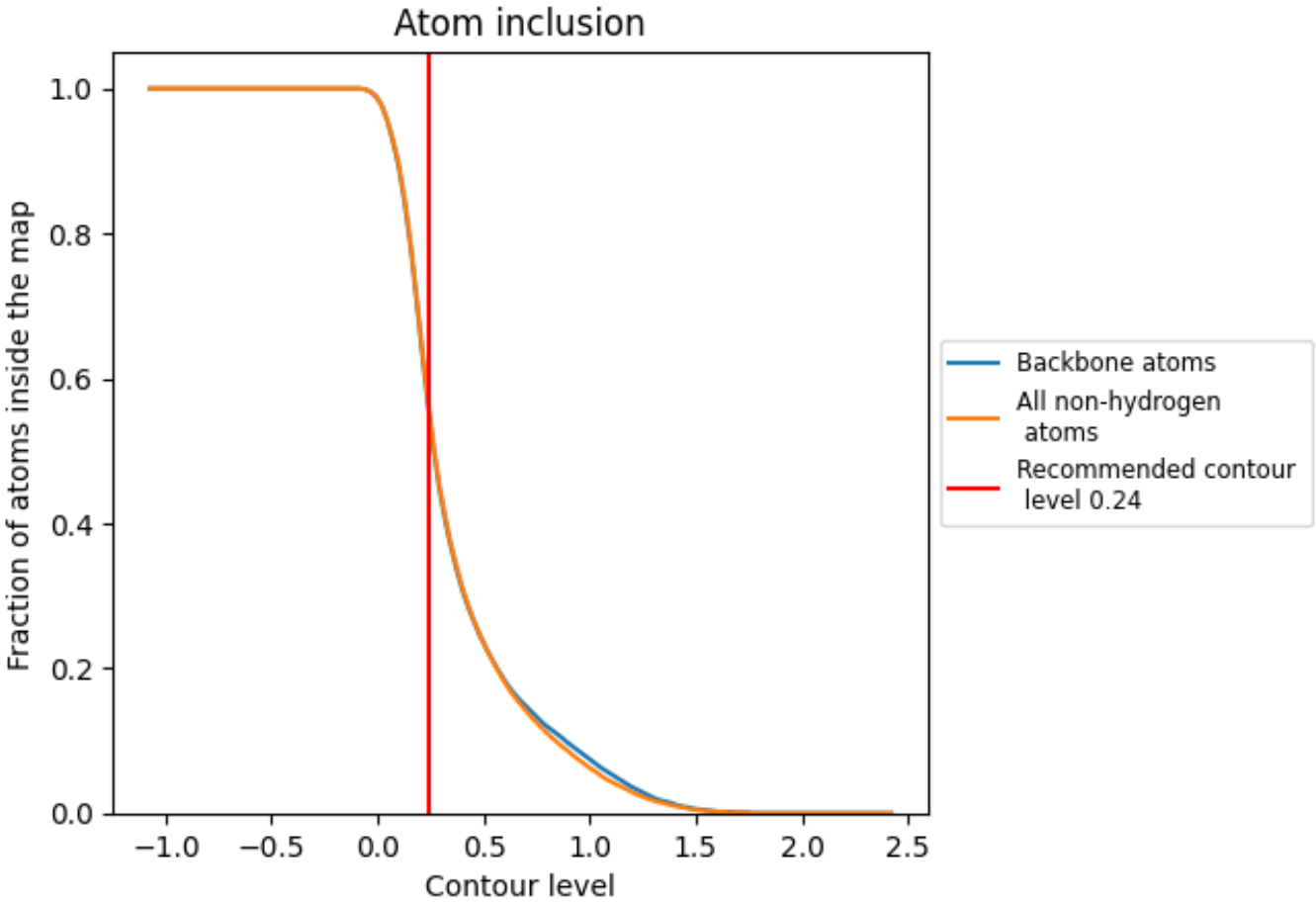
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.24).

9.4 Atom inclusion (i)



At the recommended contour level, 56% of all backbone atoms, 56% 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 (0.24) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5640	0.1950
1	0.3010	0.0610
2	0.1370	0.0270
3	0.1540	0.0140
4	0.0820	0.0730
5	0.1900	0.0420
7	0.2500	0.0280
A	0.8410	0.4130
B	0.8840	0.2950
C	0.9260	0.3690
E	0.9220	0.3010
F	0.8990	0.3120
G	0.7160	0.1670
H	0.2260	0.0480
I	0.4770	0.0620
J	0.7680	0.2640
K	0.5190	0.1250
L	0.7490	0.2670
M	0.7880	0.2730
N	0.9310	0.4230
O	0.8600	0.3210
P	0.8790	0.4120
Q	0.1160	0.0130
R	0.8110	0.3270
S	0.8680	0.1710
T	0.9810	0.5470
U	0.6150	0.2860
V	0.5210	0.1380
W	0.3650	0.0840
X	0.6580	0.1520
Y	0.7070	0.1480
Z	0.5870	0.0830
a	0.7410	0.1220
b	0.8170	0.0700
c	0.6830	0.0420

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
d	0.7370	0.0720
e	0.7220	0.0200
f	0.7030	0.0640
g	0.8890	0.1830
h	0.0000	-0.0280
i	0.0000	0.0130
j	0.0000	0.0080
k	0.0000	-0.0330
l	0.0020	0.0010
m	0.0000	0.0040
n	0.0000	0.0480
o	0.0000	-0.0050
p	0.0020	0.0130
q	0.2560	0.0050
r	0.4110	0.0430
s	0.3380	0.0280
t	0.2160	0.0160
w	0.1590	0.0060
y	0.1270	0.0130