Full wwPDB EM Validation Report ⓘ

Jan 31, 2024 – 03:33 PM EST

PDB ID	:	8VK4
EMDB ID	:	EMD-43304
Title	:	Structure of mouse RyR1 in complex with S100A1 (high-Ca2+/CFF/ATP dataset)
Authors	:	Weninger, G.; Marks, A.R.
Deposited on	:	2024-01-08
Resolution	:	3.56 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:

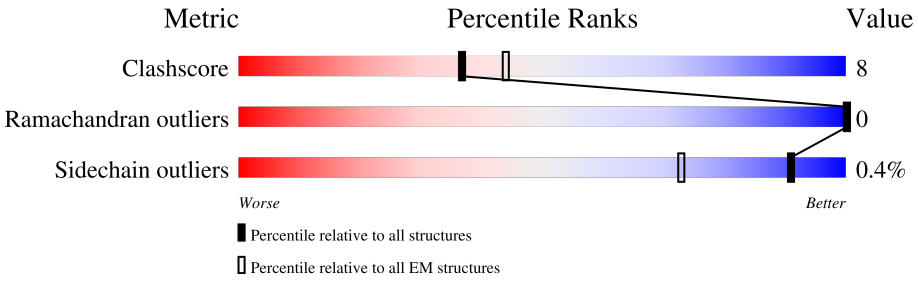
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.56 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

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	E	108	86% 13%
1	F	108	88% 11%
1	G	108	84% 15%
1	H	108	85% 14%
2	I	94	35% 50% 49%
2	J	94	26% 50% 49%
2	K	94	36% 50% 49%
2	L	94	24% 51% 48%

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Mol	Chain	Length	Quality of chain
2	M	94	36% 50% 49%
2	N	94	24% 52% 47%
2	O	94	36% 51% 48%
2	P	94	24% 51% 48%
3	A	5035	10% 71% 16% 13%
3	B	5035	10% 71% 16% 13%
3	C	5035	10% 71% 15% 13%
3	D	5035	10% 72% 15% 13%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 149304 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 Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	107	Total	C	N	O	S	0	0
			829	526	145	155	3		
1	F	107	Total	C	N	O	S	0	0
			829	526	145	155	3		
1	G	107	Total	C	N	O	S	0	0
			829	526	145	155	3		
1	H	107	Total	C	N	O	S	0	0
			829	526	145	155	3		

- Molecule 2 is a protein called Protein S100A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	93	Total	C	N	O	S	0	0
			729	460	114	152	3		
2	J	93	Total	C	N	O	S	0	0
			729	460	114	152	3		
2	K	93	Total	C	N	O	S	0	0
			729	460	114	152	3		
2	L	93	Total	C	N	O	S	0	0
			729	460	114	152	3		
2	N	93	Total	C	N	O	S	0	0
			729	460	114	152	3		
2	M	93	Total	C	N	O	S	0	0
			729	460	114	152	3		
2	O	93	Total	C	N	O	S	0	0
			729	460	114	152	3		
2	P	93	Total	C	N	O	S	0	0
			729	460	114	152	3		

- Molecule 3 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	4379	Total	C	N	O	S	0	0
			34849	22163	5998	6451	237		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	4379	Total 34849	C 22163	N 5998	O 6451	S 237	0	0
3	B	4379	Total 34849	C 22163	N 5998	O 6451	S 237	0	0
3	C	4379	Total 34849	C 22163	N 5998	O 6451	S 237	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	I	2	Total 2	Ca 2	0
4	J	2	Total 2	Ca 2	0
4	D	1	Total 1	Ca 1	0
4	A	1	Total 1	Ca 1	0
4	B	1	Total 1	Ca 1	0
4	C	1	Total 1	Ca 1	0
4	K	2	Total 2	Ca 2	0
4	L	2	Total 2	Ca 2	0
4	N	2	Total 2	Ca 2	0
4	M	2	Total 2	Ca 2	0
4	O	2	Total 2	Ca 2	0
4	P	2	Total 2	Ca 2	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	D	1	Total 1	Zn 1	0

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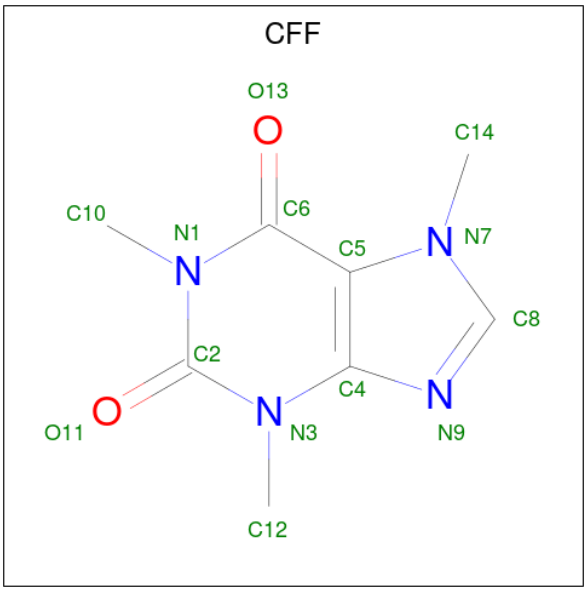
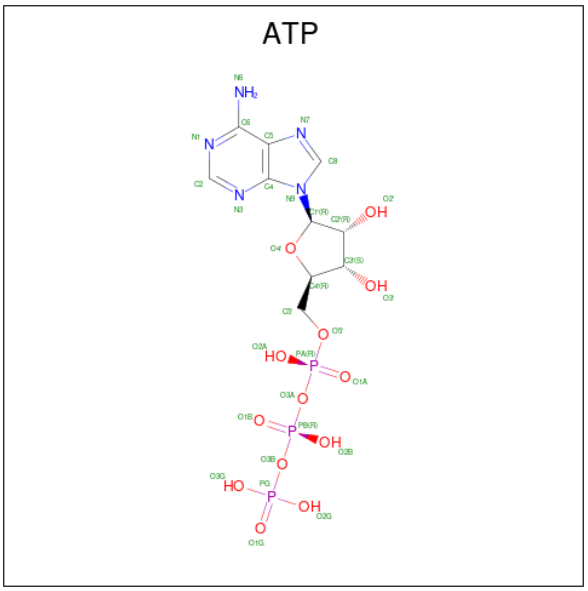
Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total Zn 1 1	0
5	B	1	Total Zn 1 1	0
5	C	1	Total Zn 1 1	0

- Molecule 6 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



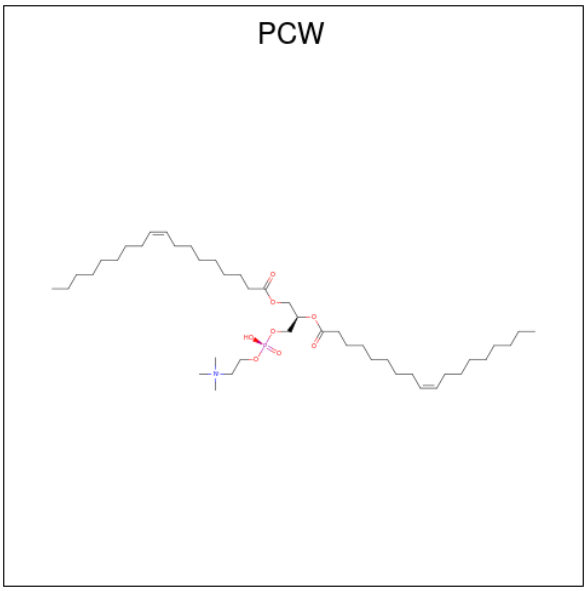
Mol	Chain	Residues	Atoms	AltConf
6	D	1	Total C N O 14 8 4 2	0
6	A	1	Total C N O 14 8 4 2	0
6	B	1	Total C N O 14 8 4 2	0
6	C	1	Total C N O 14 8 4 2	0

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
7	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 8 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
8	D	1	Total	C	N	O	P	0
			54	44	1	8	1	
8	D	1	Total	C	N	O	P	0
			54	44	1	8	1	
8	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
8	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
8	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
8	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
8	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
8	C	1	Total	C	N	O	P	0
			54	44	1	8	1	

3 Residue-property plots (i)

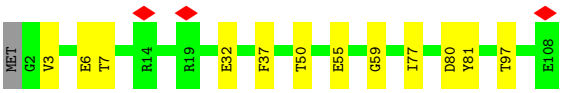
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain E:

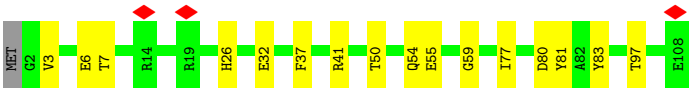
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain F:



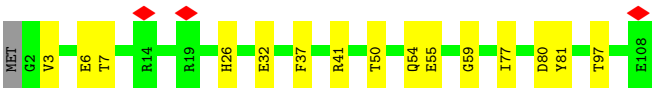
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain G:



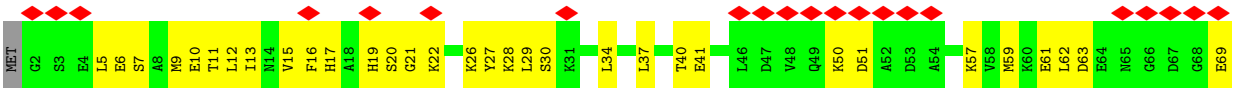
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A

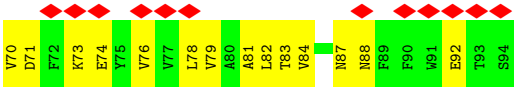
Chain H:



• Molecule 2: Protein S100A1

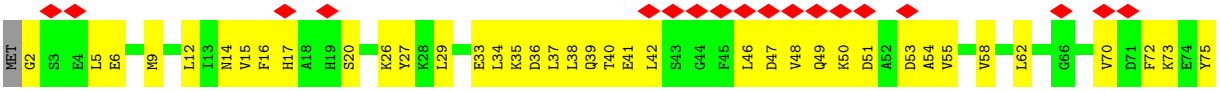
Chain I:

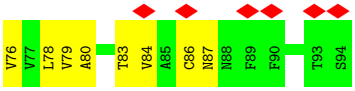




• Molecule 2: Protein S100A1

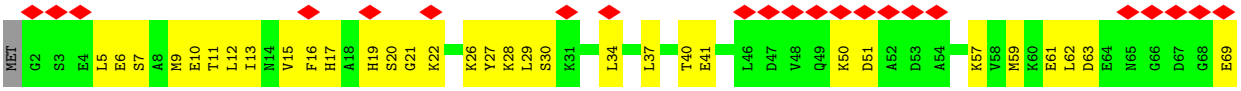
Chain J:

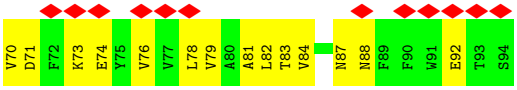




• Molecule 2: Protein S100A1

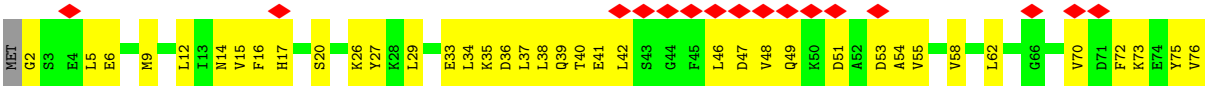
Chain K:

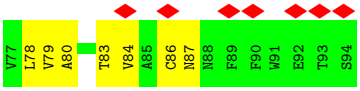




• Molecule 2: Protein S100A1

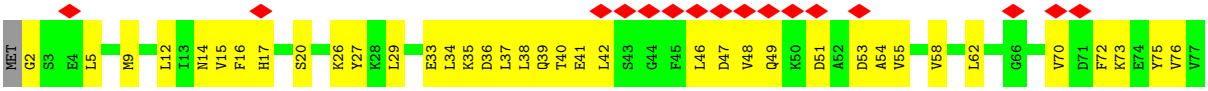
Chain L:

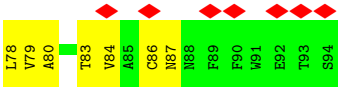




• Molecule 2: Protein S100A1

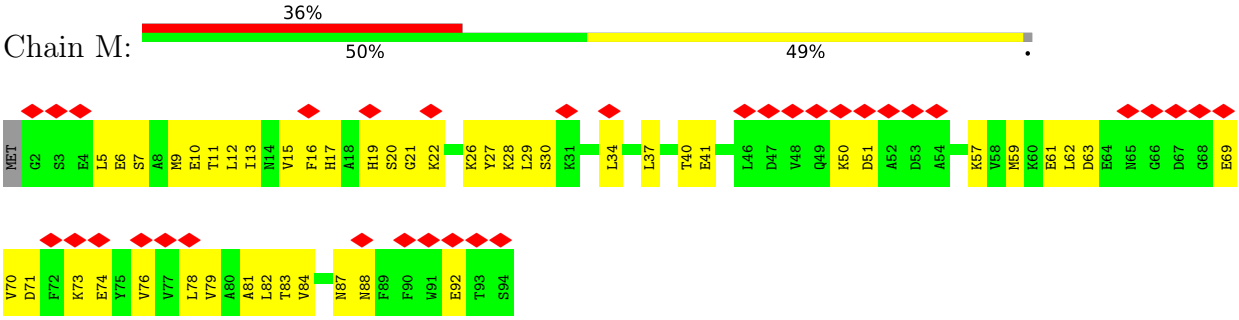
Chain N:





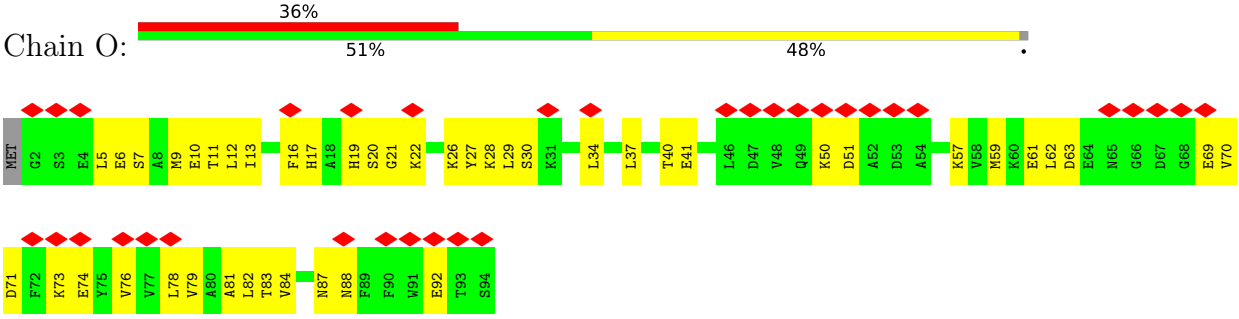
• Molecule 2: Protein S100A1

Chain M:



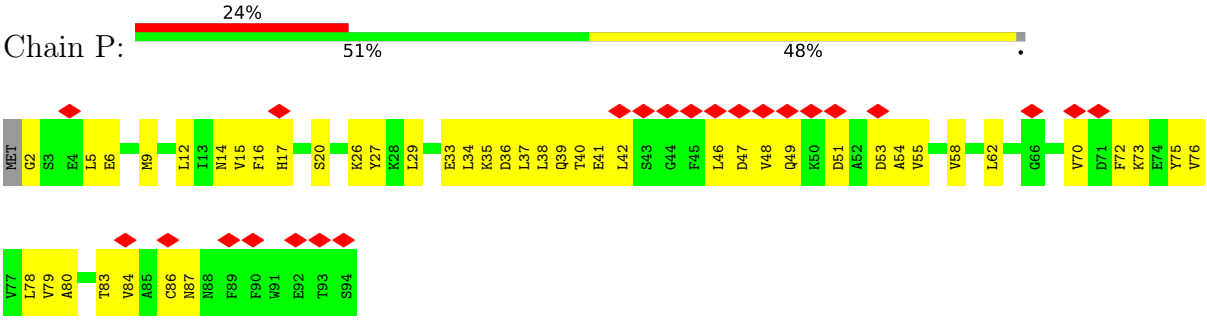
• Molecule 2: Protein S100A1

Chain O:



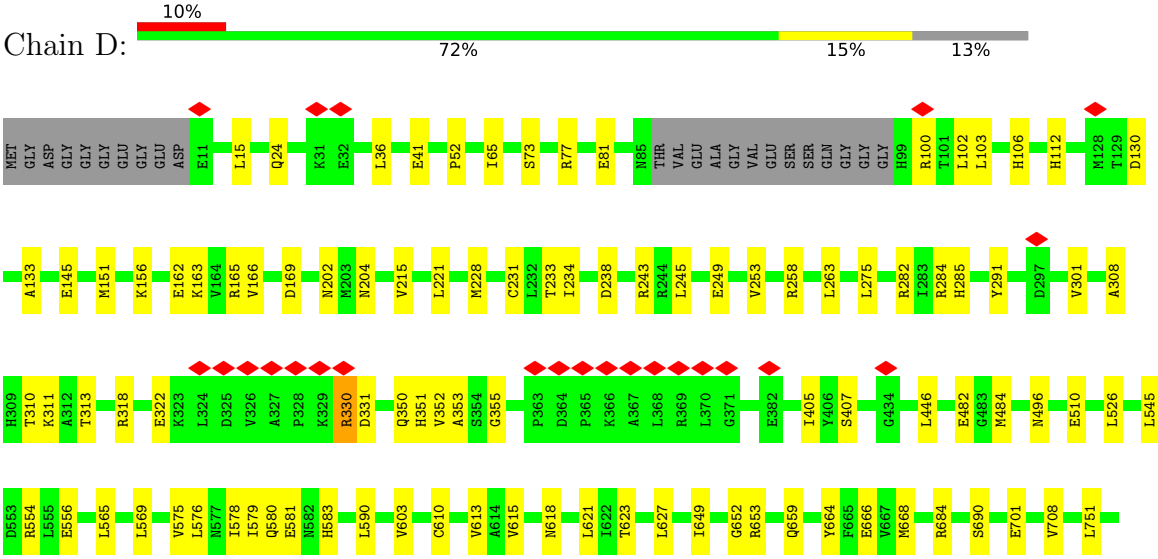
• Molecule 2: Protein S100A1

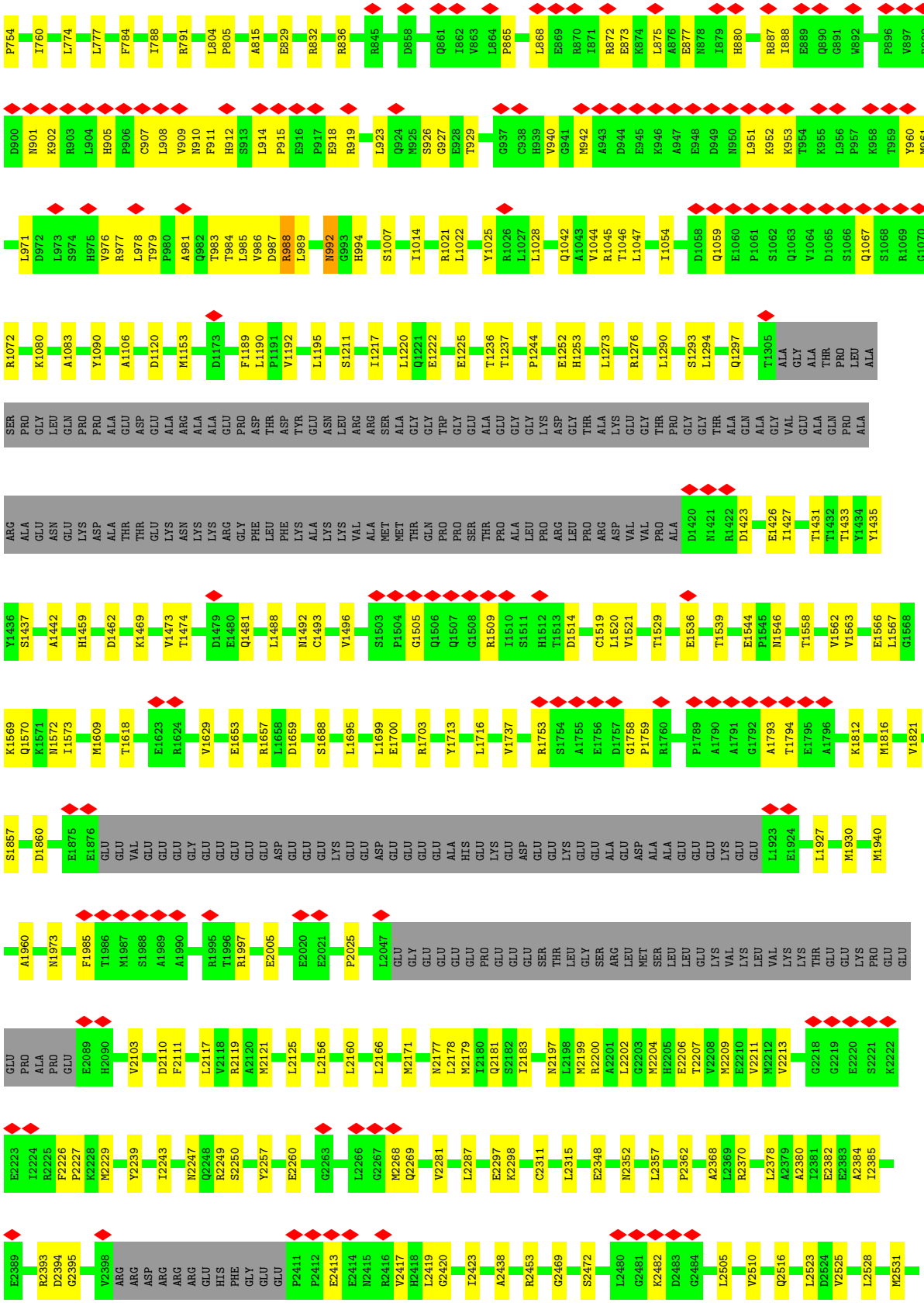
Chain P:

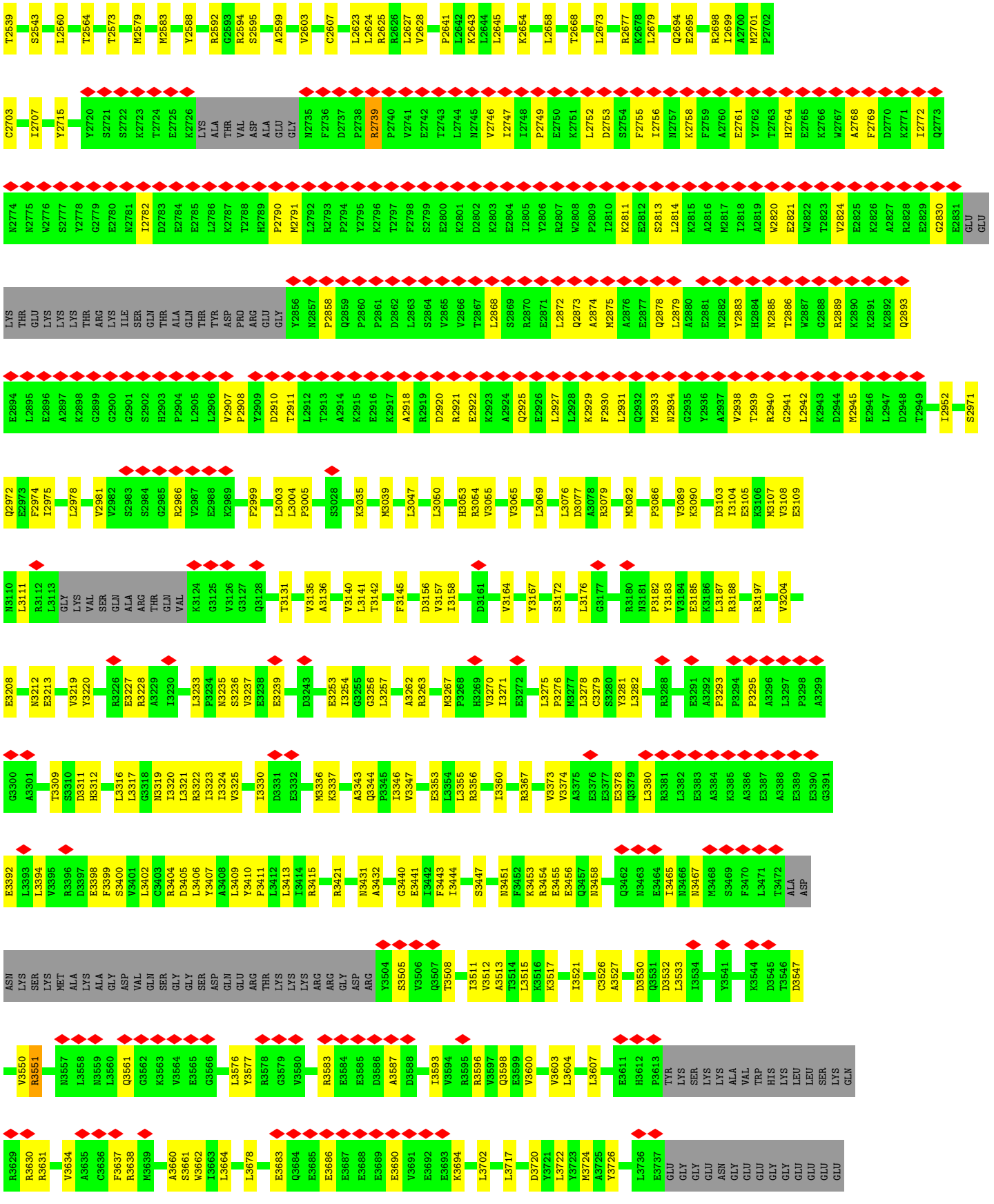


• Molecule 3: Ryanodine receptor 1

Chain D:




P754 I760 L774 L777 F784 I788 R791 L804 P805 A815 E829 R832 R836 R845 D858 Q861 I862 V863 L864 P865 L868 E869 R870 I871 R872 E873 K874 L875 A876 E877 N878 I879 H880 R887 I888 E889 Q890 G891 W892 P896 V897 R898 D899
D900 N901 K902 R903 L904 H905 P906 C907 L908 V909 N910 F911 H912 S913 L914 P915 E916 P917 E918 R919 L923 Q924 M925 S926 G927 E928 T929 G937 C938 H939 V940 G941 N942 A943 D944 E945 K946 A947 E948 D949 N950 L951 K952 K953 T954 K955 L956 P957 K958 T959 Y960 M961 M962 S963 N964 G965 P968
L971 D972 L973 S974 H975 V976 R977 L978 T979 P980 A981 Q982 T983 T984 L985 V986 D987 R988 L989 N992 G993 H994 S1007 I1014 R1021 L1022 Y1025 R1026 L1027 L1028 Q1042 A1043 V1044 R1045 T1046 L1047 I1054 D1058 Q1059 E1060 P1061 S1062 Q1063 V1064 D1065 S1066 Q1067 S1068 R1069 G1070 D1071
R1072 K1080 A1083 Y1090 A1106 D1120 M1153 D1173 F1189 L1190 P1191 V1192 L1195 S1211 I1217 L1220 Q1221 E1222 E1225 T1236 T1237 P1244 E1252 H1253 L1273 R1276 L1290 S1293 L1294 Q1297 T1305 ALA GLY ALA THR PRO LEU ALA
SER PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP THR ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS ASP GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR ALA GLN ALA GLY VAL GLU ALA GLN PRO ALA
ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS VAL ALA MET MET THR GLN PRO PRO SER THR PRO ALA LEU PRO ARG LEU PRO ARG ASP VAL VAL PRO ALA D1420 N1421 R1422 D1423 E1426 I1427 T1431 T1432 T1433 Y1434 Y1435
Y1436 S1437 A1442 H1459 D1462 K1469 V1473 T1474 D1479 E1480 Q1481 L1488 N1492 C1493 V1496 S1503 P1504 G1505 Q1506 Q1507 G1508 R1509 I1510 S1511 H1512 T1513 D1514 C1519 L1520 V1521 T1529 E1536 T1539 E1544 P1545 N1546 T1558 V1562 V1563 E1566 L1567 G1568
K1569 Q1570 K1571 N1572 I1573 M1609 T1618 E1623 R1624 V1629 E1653 R1657 L1658 D1659 S1688 L1695 L1699 E1700 R1703 Y1713 L1716 V1737 R1753 S1754 A1755 E1756 D1757 G1758 P1759 R1760 P1789 A1790 A1791 G1792 A1793 T1794 E1795 A1796 K1812 M1816 V1821
S1857 D1860 E1875 E1876 GLU GLU VAL GLU GLU GLU GLU GLY GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU GLU ALA HIS GLU LYS GLU ASP GLU GLU LYS GLU GLU ALA GLU ASP ALA ALA GLU GLU GLU LYS GLU L1923 E1924 L1927 M1930 M1940
A1960 N1973 F1985 T1986 M1987 S1988 A1989 A1990 R1995 T1996 R1997 E2005 E2020 E2021 P2025 L2047 GLU GLY GLU GLU GLU GLU PRO GLU GLU GLU SER THR LEU GLY SER ARG LEU MET SER LEU LEU GLU LYS VAL LYS LEU VAL LYS LYS THR GLU GLU LYS PRO GLU GLU
GLU PRO ALA PRO GLU E2089 H2090 V2103 D2110 F2111 L2117 V2118 R2119 A2120 M2121 L2125 L2156 L2160 L2166 M2171 N2177 L2178 M2179 I2180 Q2181 S2182 I2183 N2197 L2198 M2199 R2200 A2201 L2202 G2203 M2204 H2205 E2206 T2207 V2208 M2209 E2210 V2211 M2212 V2213 G2218 G2219 E2220 S2221 K2222
E2223 I2224 R2225 F2226 P2227 K2228 M2229 Y2239 I2243 N2247 Q2248 R2249 S2250 V2257 E2260 G2263 L2266 G2267 M2268 Q2269 V2281 L2287 E2297 K2298 C2311 L2315 E2348 N2352 L2357 P2362 A2368 L2369 R2370 L2378 A2379 A2380 I2381 E2382 E2383 A2384 I2385
E2389 R2393 D2394 G2395 V2398 ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU P2411 P2412 E2413 E2414 N2415 R2416 V2417 H2418 L2419 G2420 I2423 A2438 R2453 G2469 S2472 L2480 G2481 K2482 D2483 G2484 L2505 V2510 Q2516 L2523 D2524 V2525 L2528 M2531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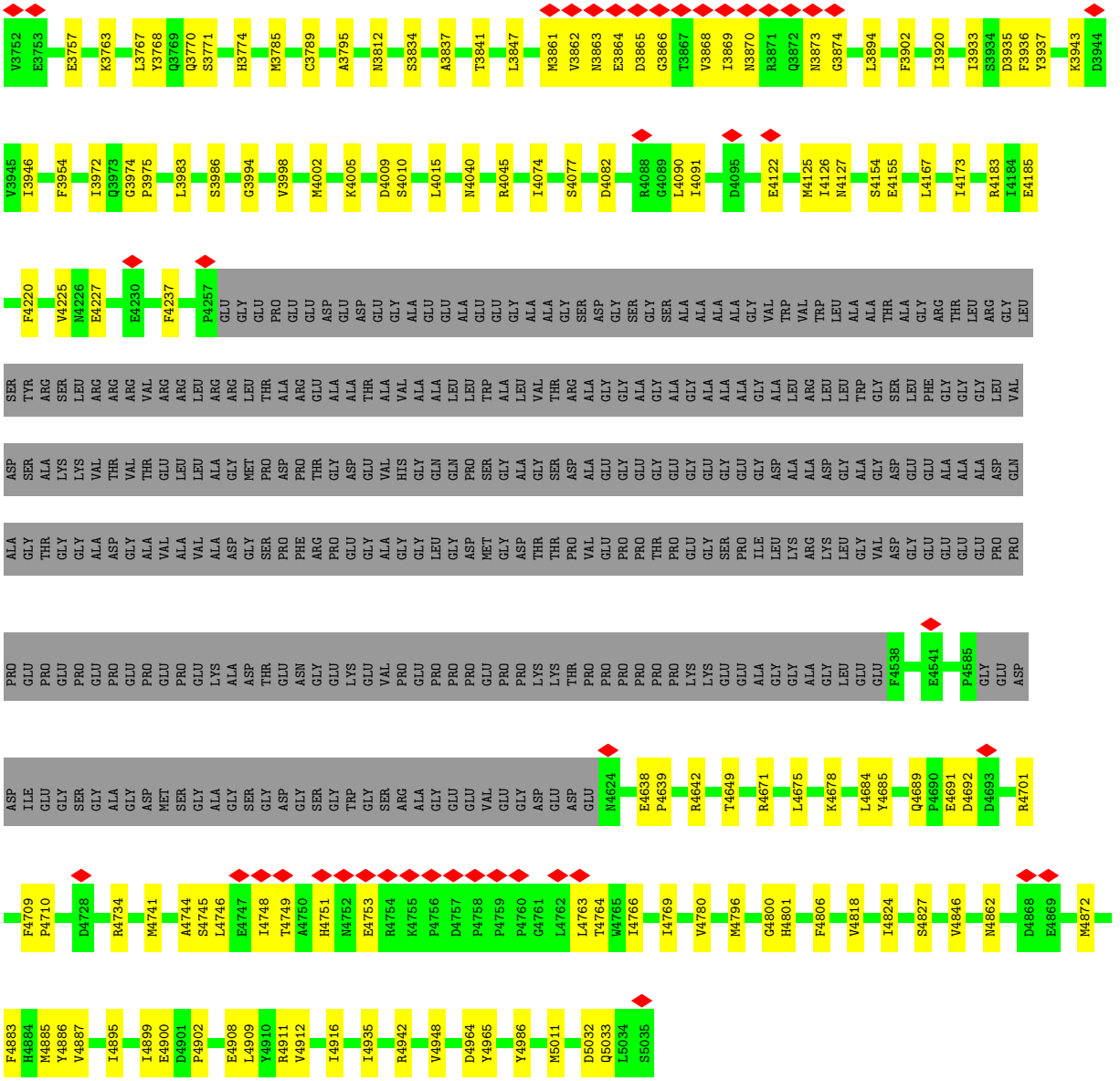
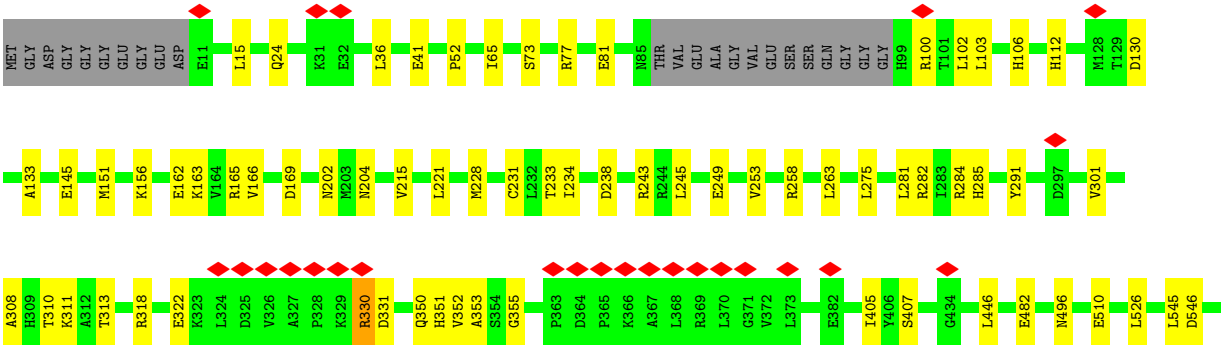
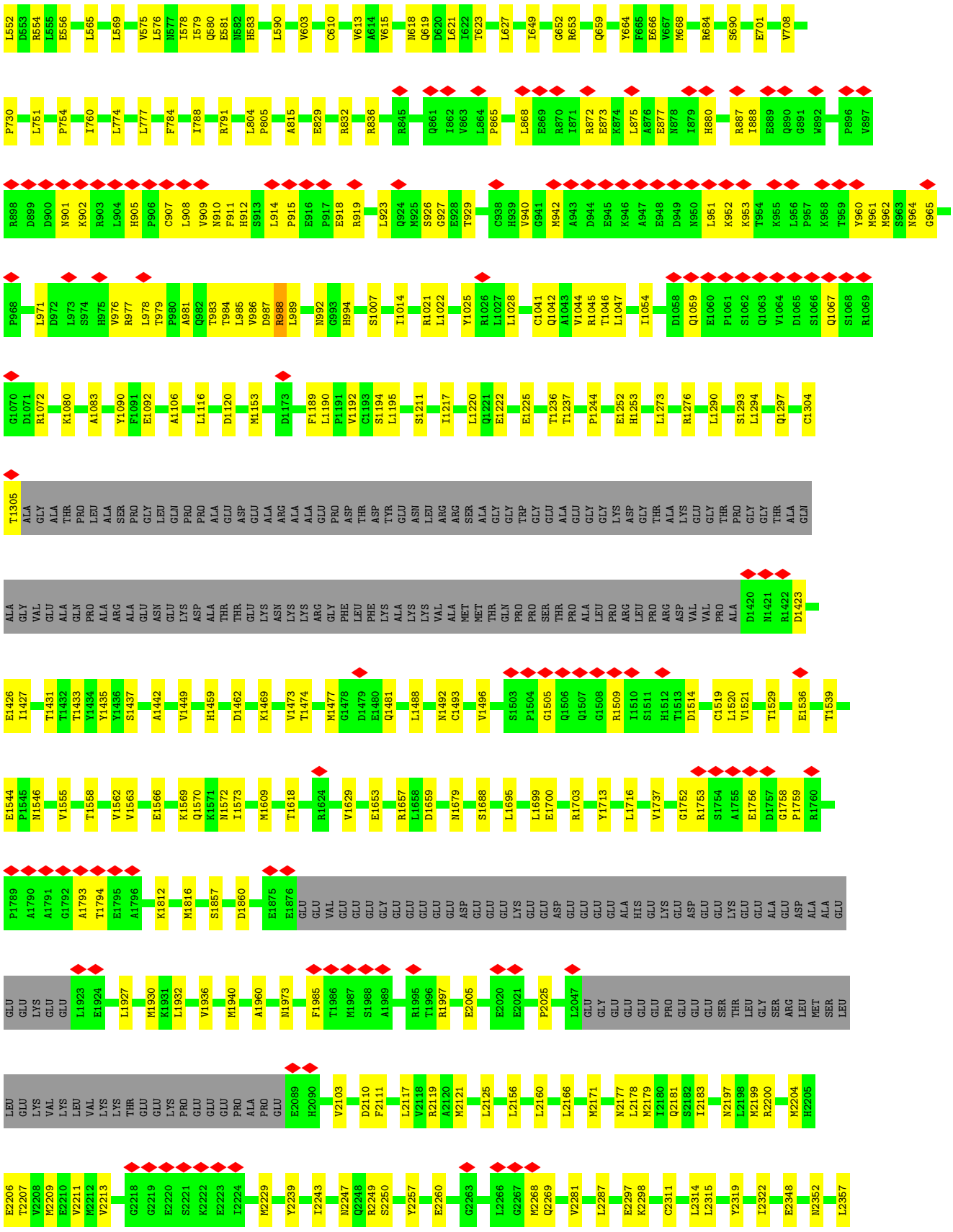


• Molecule 3: Ryanodine receptor 1

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ALA GLY VAL GLU ALA GLN PRO ALA ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS VAL ALA MET MET THR GLN PRO PRO SER THR PRO ALA LEU PRO ARG LEU PRO ARG ASP VAL VAL PRO ALA D1420 N1421 R1422 D1423
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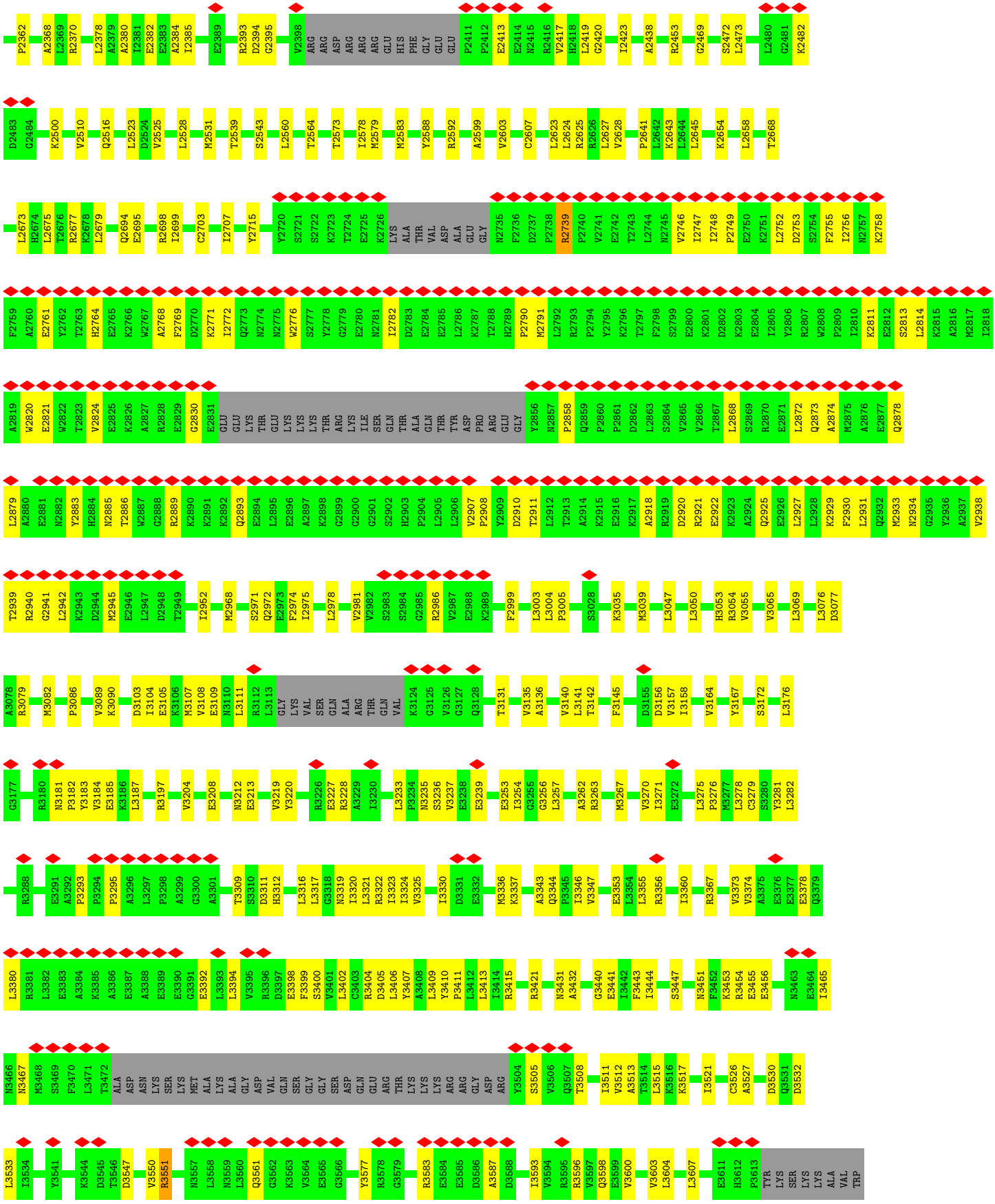
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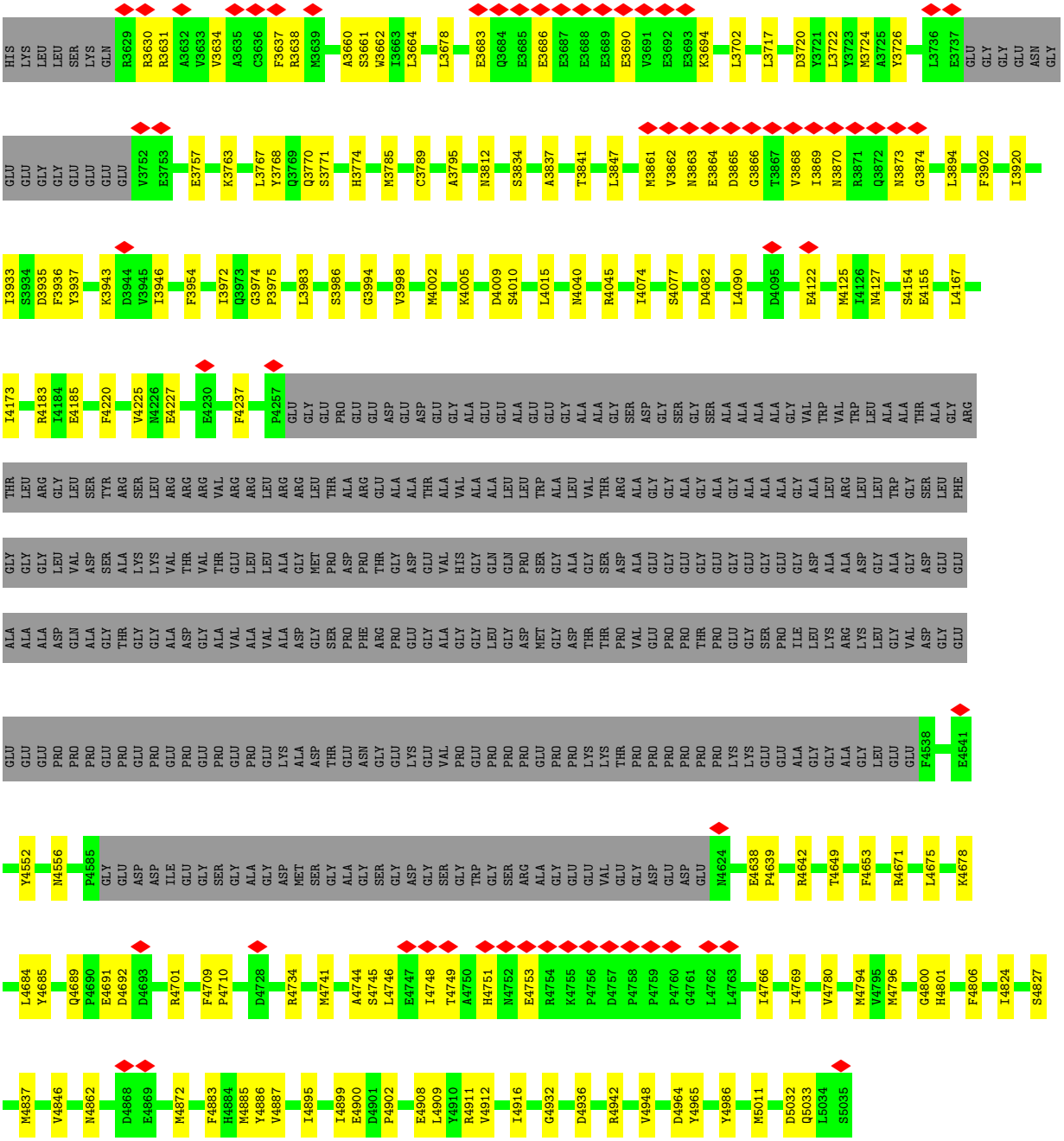
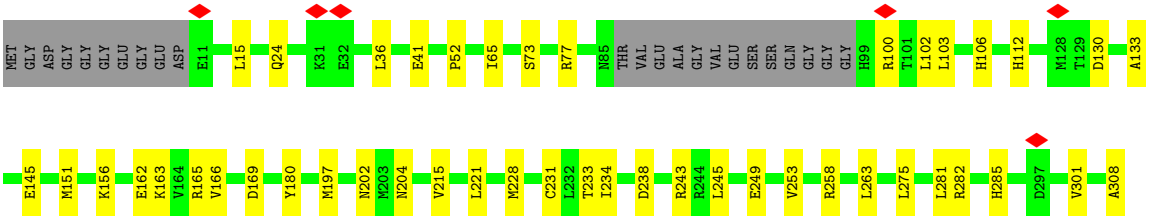
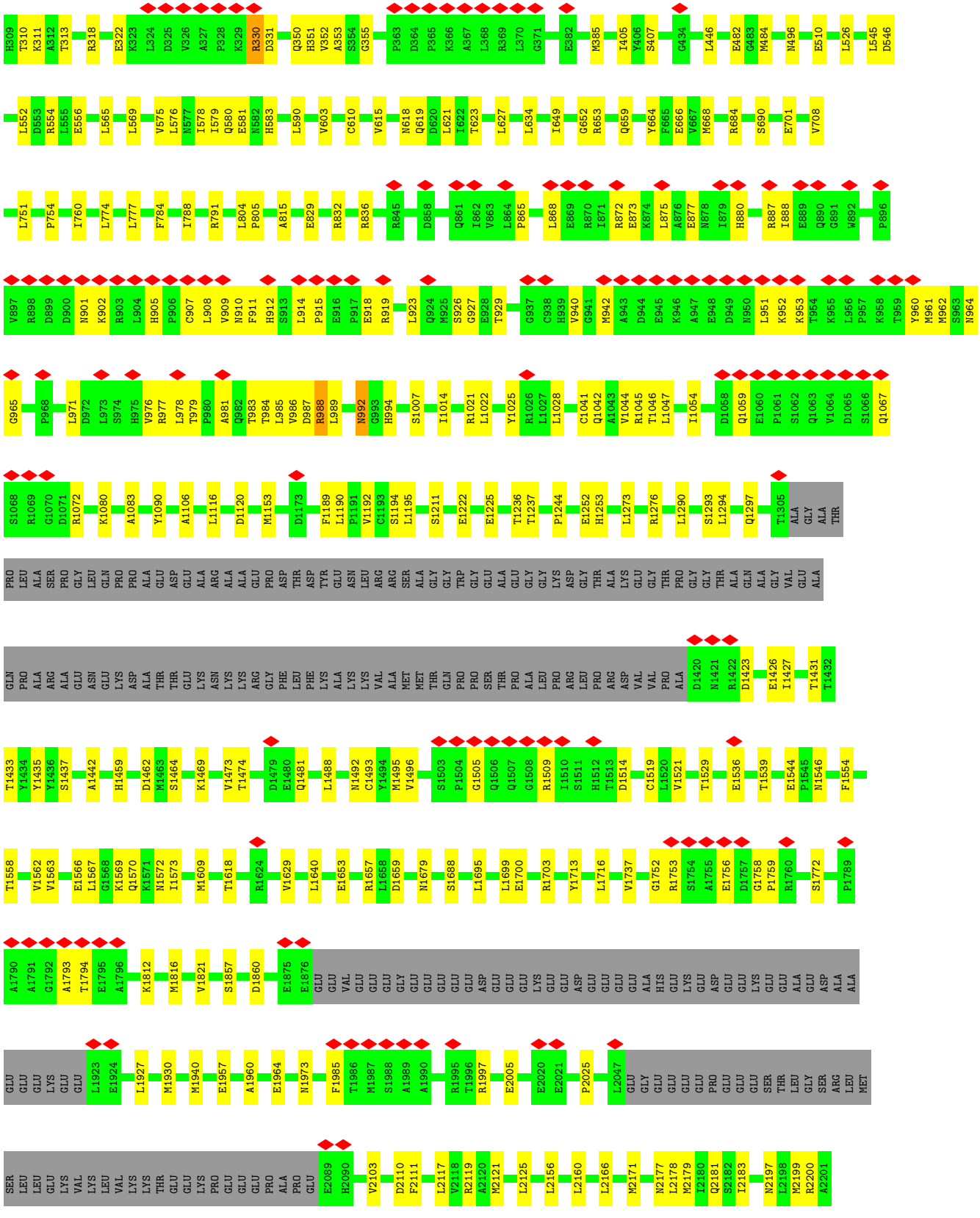


• Molecule 3: Ryanodine receptor 1

Chain B:

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GLN PRO ALA ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS VAL ALA MET MET THR THR GLN PRO PRO PRO SER THR PRO ALA LEU PRO PRO ARG LEU PRO ARG ASP VAL VAL PRO ALA D1420 N1421 R1422 D1423 E1426 I1427 T1431 T1432
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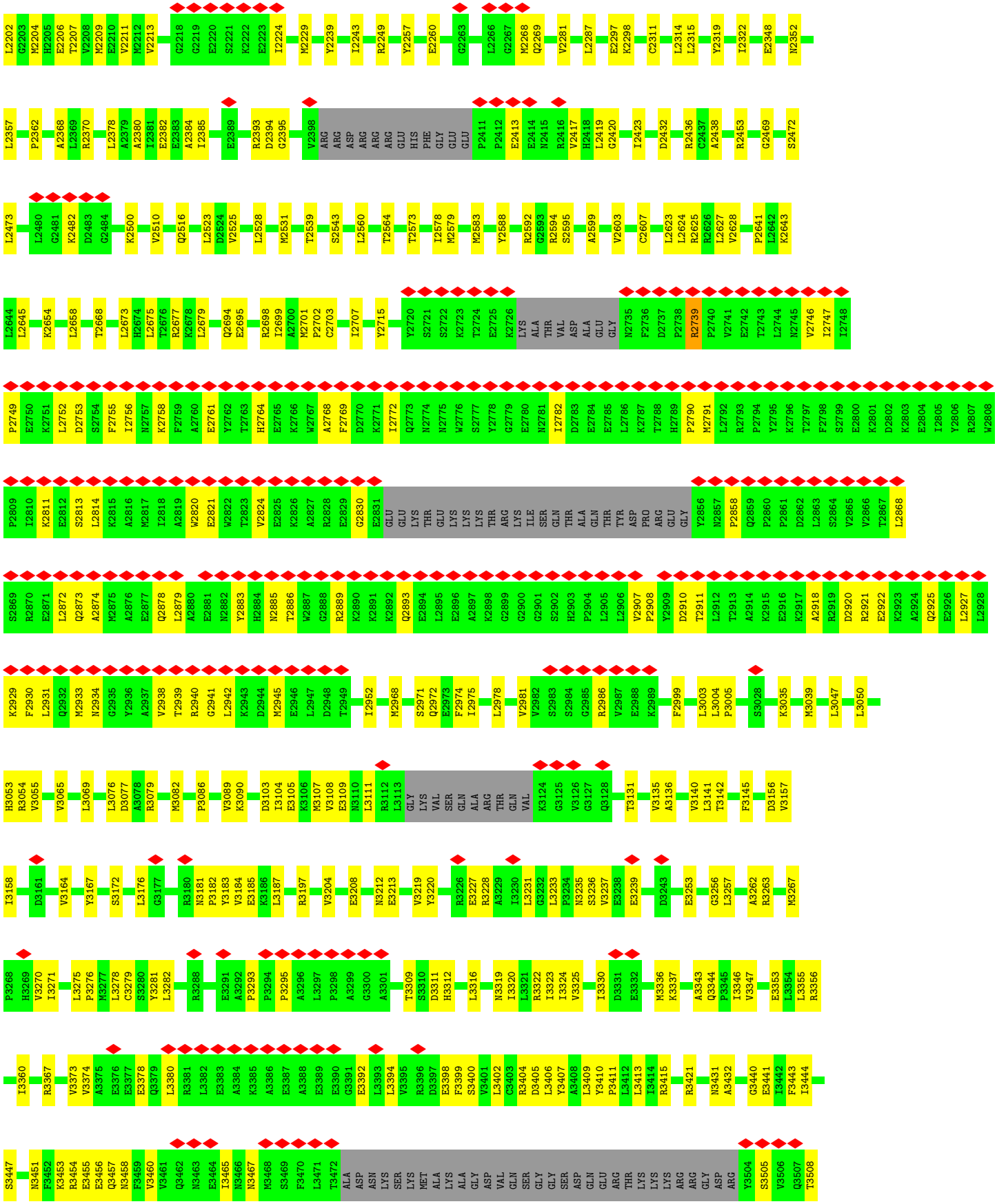
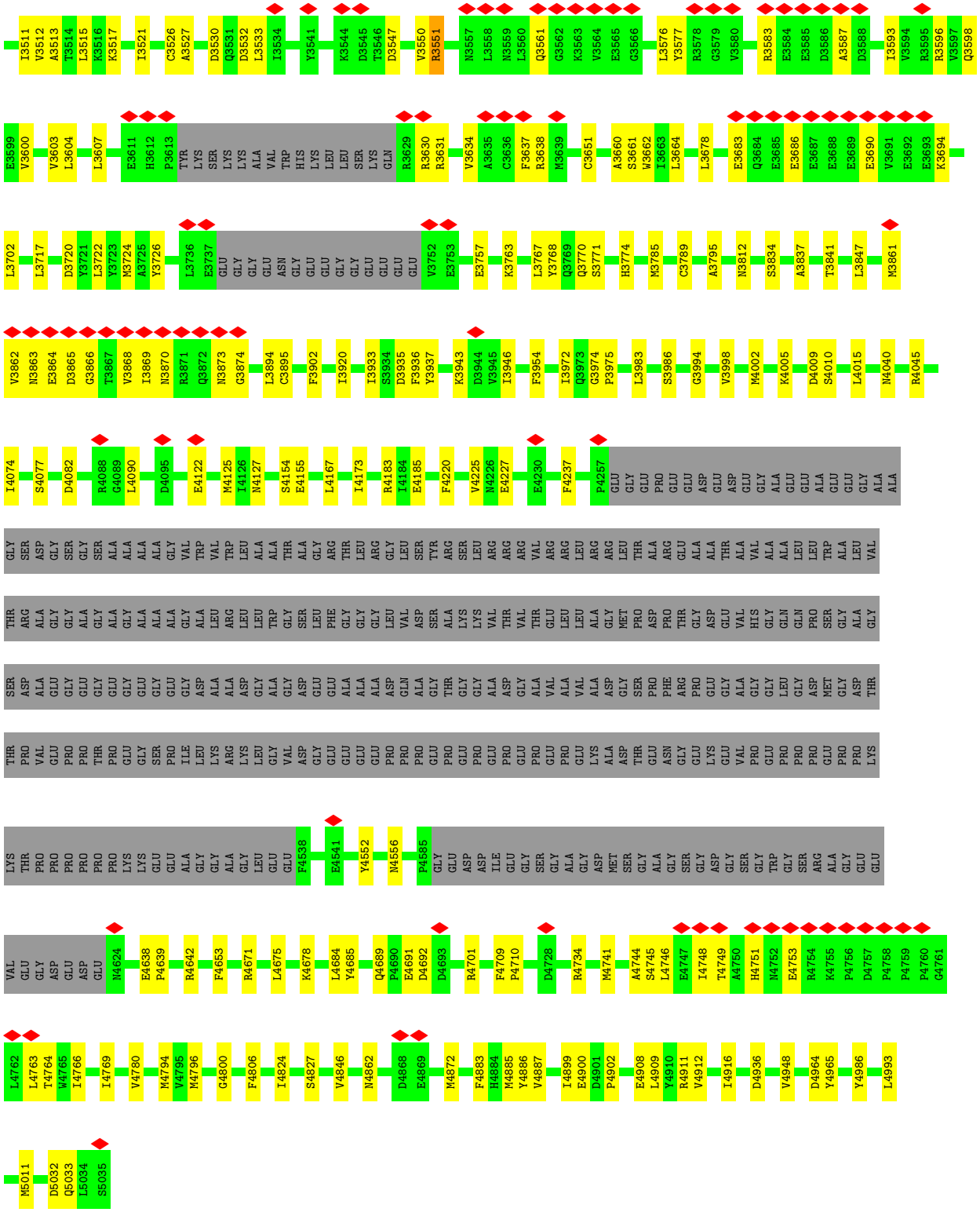
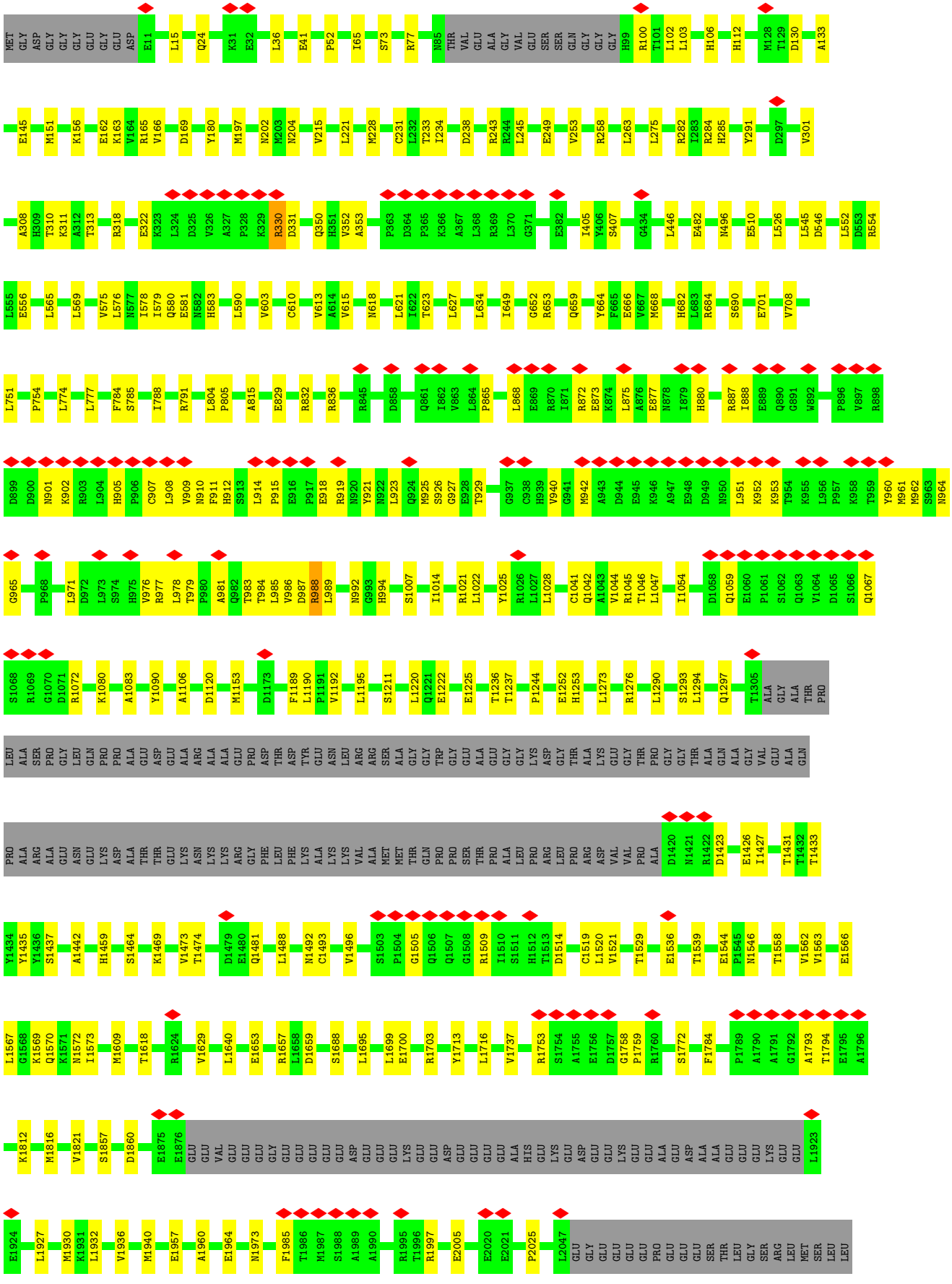
SER LEU LEU GLU LYS VAL LYS LEU VAL LYS LYS THR GLU GLU LYS PRO GLU GLU GLU PRO ALA PRO GLU E2089 H2090 V2103 D2110 F2111 L2117 V2118 R2119 A2120 M2121 L2125 L2156 L2160 L2166 M2171 N2177 L2178 M2179 I2180 Q2181 S2182 I2183 N2197 L2198 M2199 R2200 A2201





• Molecule 3: Ryanodine receptor 1

Chain C: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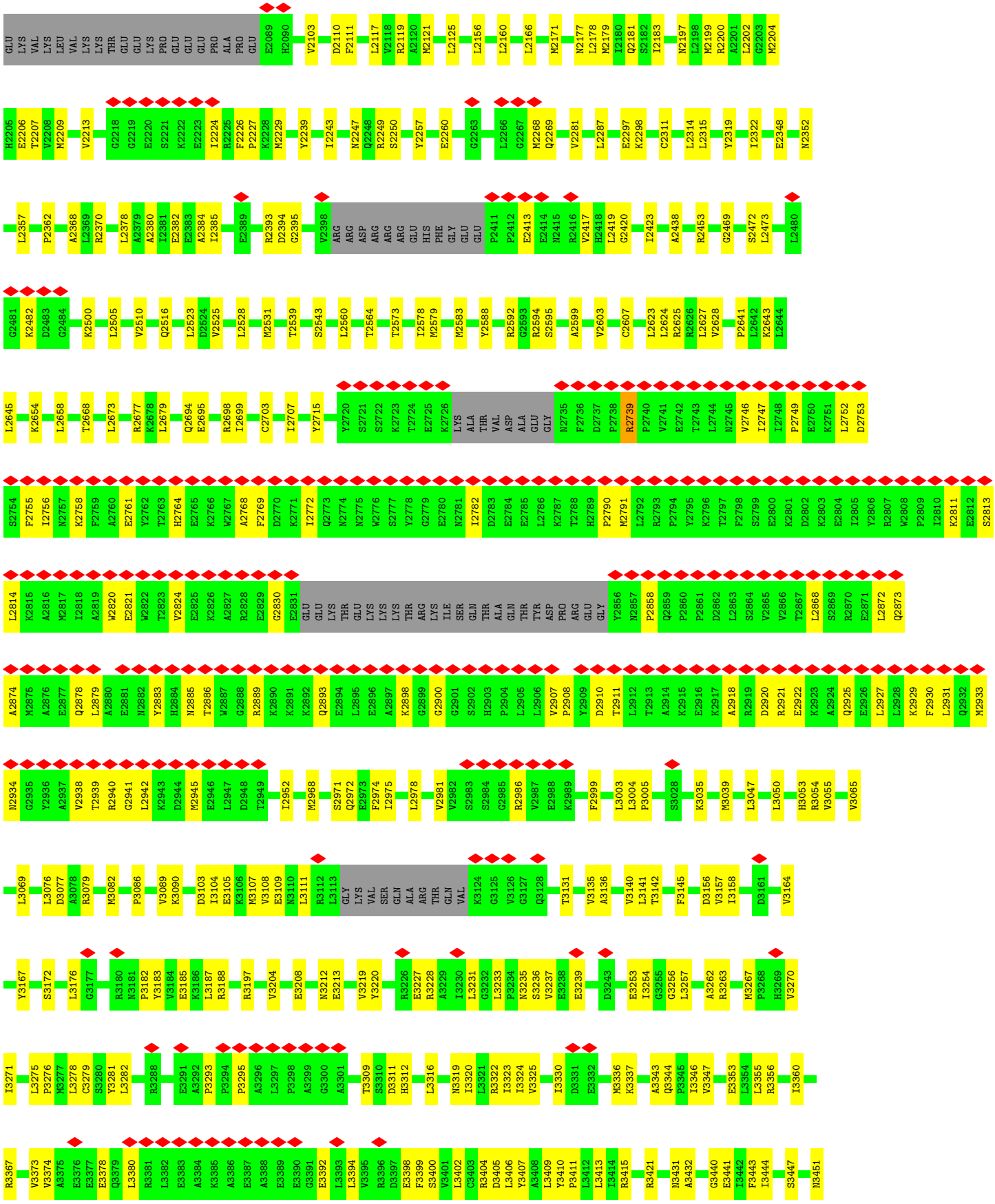
E145 M151 K156 E162 K163 V164 R165 V166 D169 Y180 M197 N202 M203 N204 V215 L221 M228 C231 L232 T233 I234 D238 R243 R244 L245 E249 V253 R258 L263 L275 R282 I283 R284 H285 Y291 D297 V301
A308 H309 T310 K311 A312 T313 R318 E322 K323 L324 D325 V326 A327 P328 K329 R330 D331 Q350 H351 V352 A353 P363 D364 P365 K366 A367 L368 R369 L370 G371 E382 I405 Y406 S407 G434 L446 E482 N496 E510 L526 L545 D546 L552 D553 R554
L555 E556 L565 L569 V575 L576 N577 I578 I579 Q580 E581 N582 H583 L590 V603 C610 V613 A614 V615 N618 L621 I622 T623 L627 L634 I649 G652 R653 Q659 Y664 F665 E666 V667 M668 H682 L683 R684 S690 E701 V708
L751 P754 L774 L777 F784 S785 I788 R791 L804 P805 A815 E829 R832 R836 R845 D858 Q861 I862 V863 L864 P865 L868 E869 R870 I871 R872 E873 K874 L875 A876 E877 N878 I879 H880 R887 I888 E889 Q890 G891 W892 P896 V897 R898
D899 D900 N901 K902 R903 L904 H905 P906 C907 L908 V909 N910 F911 H912 S913 L914 P915 E916 P917 E918 R919 N920 Y921 N922 L923 Q924 M925 S926 G927 E928 T929 G937 C938 H939 V940 G941 M942 A943 D944 E945 K946 A947 E948 D949 N950 L951 K952 K953 T954 K955 L956 P957 K958 T959 Y960 M961 M962 S963 N964
G965 P968 L971 D972 L973 S974 H975 V976 R977 L978 T979 P980 A981 Q982 T983 T984 L985 V986 D987 R988 L989 N992 G993 H994 S1007 I1014 R1021 L1022 Y1025 R1026 L1027 L1028 C1041 Q1042 A1043 V1044 R1045 T1046 L1047 I1054 D1058 Q1059 E1060 P1061 S1062 Q1063 V1064 D1065 S1066 Q1067
S1068 R1069 G1070 D1071 R1072 K1080 A1083 Y1090 A1106 D1120 M1153 D1173 F1189 L1190 P1191 V1192 L1195 S1211 L1220 Q1221 E1222 E1225 T1236 T1237 P1244 E1252 H1253 L1273 R1276 L1290 S1293 L1294 Q1297 T1305 ALA GLY ALA THR PRO
LEU ALA SER PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP THR ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS ASP GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR ALA GLN ALA GLY VAL GLU ALA GLN
PRO ALA ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS VAL ALA MET MET THR GLN PRO PRO SER THR PRO ALA LEU PRO ARG LEU PRO ARG ASP VAL VAL PRO ALA D1420 N1421 R1422 D1423 E1426 I1427 T1431 T1432 T1433
Y1434 Y1435 Y1436 S1437 A1442 H1459 S1464 K1469 V1473 T1474 D1479 E1480 Q1481 L1488 N1492 C1493 V1496 S1503 P1504 G1505 Q1506 Q1507 G1508 R1509 I1510 S1511 H1512 T1513 D1514 C1519 L1520 V1521 T1529 E1536 T1539 E1544 P1545 N1546 T1558 V1562 V1563 E1566
L1567 G1568 K1569 Q1570 K1571 N1572 I1573 M1609 T1618 R1624 V1629 L1640 E1653 R1657 L1658 D1659 S1688 L1695 L1699 E1700 R1703 Y1713 L1716 V1737 R1753 S1754 A1755 E1756 D1757 G1758 P1759 R1760 S1772 F1784 P1789 A1790 A1791 G1792 A1793 T1794 E1795 A1796
K1812 M1816 V1821 S1857 D1860 E1875 E1876 GLU GLU VAL GLU GLU GLU GLY GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU ASP GLU GLU GLU GLU GLU GLU ALA HIS GLU LYS GLU ASP GLU GLU LYS GLU GLU ALA GLU ASP ALA ALA GLU GLU GLU GLU LYS GLU GLU L1923
E1924 L1927 M1930 K1931 L1932 V1936 M1940 E1957 A1960 E1964 N1973 F1985 T1986 M1987 S1988 A1989 A1990 R1995 T1996 R1997 E2005 E2020 E2021 P2025 L2047 GLU GLY GLU GLU GLU PRO GLU GLU GLU SER THR LEU GLY SER ARG LEU MET SER LEU LEU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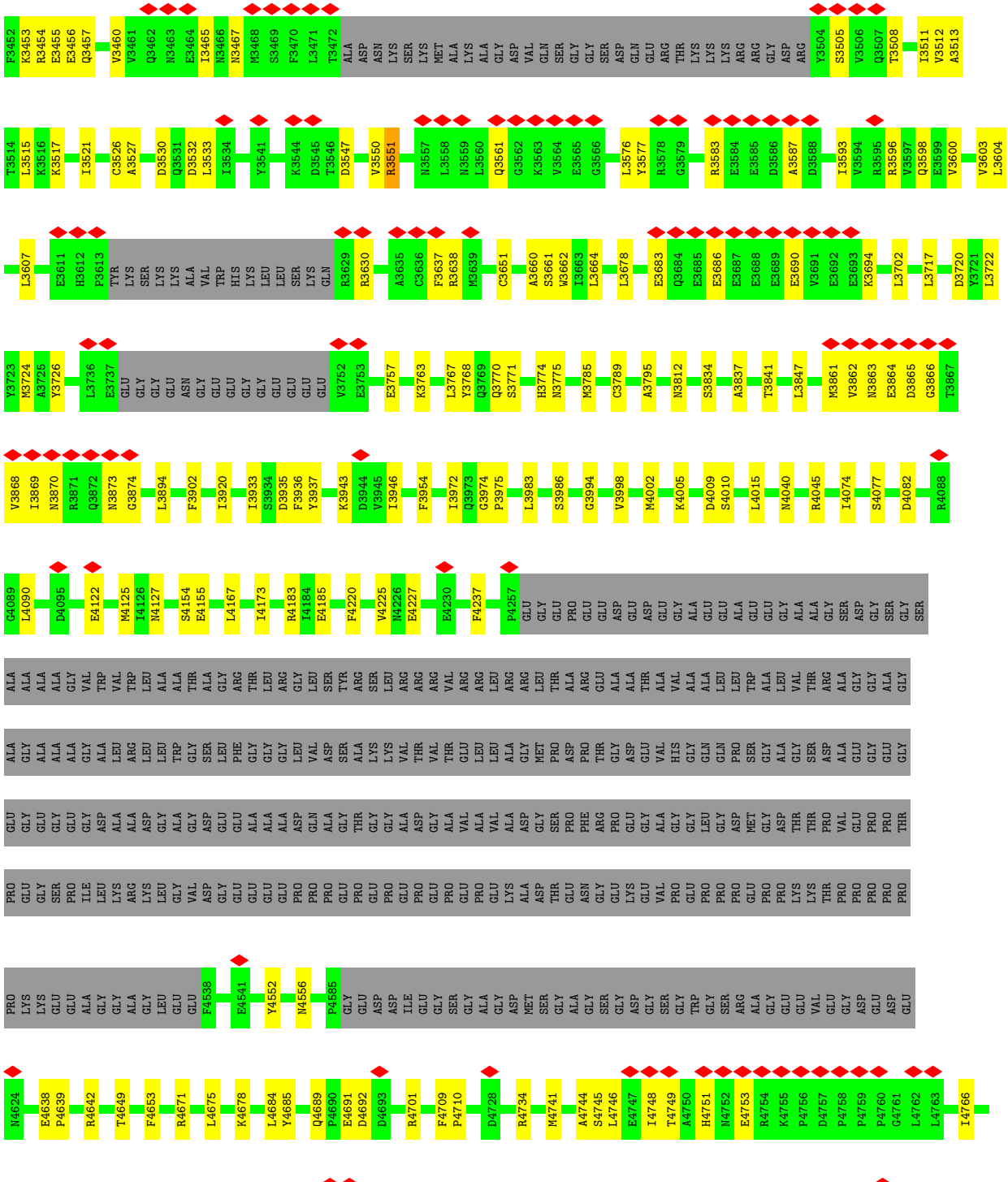
E2089 H2090 V2103 D2110 F2111 L2117 V2118 R2119 A2120 M2121 L2125 L2156 L2160 L2166 M2171 N2177 L2178 M2179 I2180 Q2181 S2182 I2183 N2197 L2198 M2199 R2200 A2201 L2202 G2203 M2204
H2205 E2206 T2207 V2208 M2209 V2213 G2218 G2219 E2220 S2221 K2222 E2223 I2224 R2225 F2226 P2227 K2228 M2229 Y2239 I2243 N2247 Q2248 R2249 S2250 Y2257 E2260 G2263 L2266 G2267 M2268 Q2269 V2281 L2287 E2297 K2298 C2311 L2314 L2315 Y2319 I2322 E2348 N2352
L2357 P2362 A2368 L2369 R2370 L2378 A2379 A2380 I2381 E2382 E2383 A2384 I2385 E2389 R2393 D2394 G2395 V2398 ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU P2411 P2412 E2413 E2414 W2415 R2416 V2417 H2418 L2419 G2420 I2423 A2438 R2453 G2469 S2472 L2473 L2480
G2481 K2482 D2483 G2484 K2500 L2505 V2510 Q2516 L2523 D2524 V2525 L2528 M2531 T2539 S2543 L2560 T2564 T2573 I2578 M2579 M2583 Y2588 R2592 G2593 R2594 S2595 A2599 V2603 C2607 L2623 L2624 R2625 R2626 L2627 V2628 P2641 L2642 K2643 L2644
L2645 K2654 L2658 T2668 L2673 R2677 K2678 L2679 Q2694 E2695 R2698 I2699 C2703 I2707 Y2715 Y2720 S2721 S2722 K2723 T2724 E2725 K2726 LYS ALA THR VAL ASP ALA GLU GLY N2735 F2736 D2737 P2738 R2739 P2740 V2741 E2742 T2743 L2744 N2745 V2746 I2747 I2748 P2749 E2750 K2751 L2752 D2753
S2754 F2755 I2756 N2757 K2758 F2759 A2760 E2761 Y2762 T2763 H2764 E2765 K2766 W2767 A2768 F2769 D2770 K2771 I2772 Q2773 N2774 N2775 W2776 S2777 Y2778 G2779 E2780 N2781 I2782 D2783 E2784 E2785 L2786 K2787 T2788 H2789 P2790 M2791 L2792 R2793 P2794 Y2795 K2796 T2797 F2798 S2799 E2800 K2801 D2802 K2803 E2804 I2805 Y2806 R2807 W2808 P2809 I2810 K2811 E2812 S2813
L2814 K2815 A2816 M2817 I2818 A2819 W2820 E2821 W2822 T2823 V2824 E2825 K2826 A2827 R2828 E2829 G2830 E2831 GLU GLU LYS THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY Y2856 N2857 P2858 Q2859 P2860 P2861 D2862 L2863 S2864 V2865 V2866 T2867 L2868 S2869 R2870 E2871 L2872 Q2873
A2874 M2875 A2876 E2877 Q2878 L2879 A2880 E2881 N2882 Y2883 H2884 N2885 T2886 W2887 G2888 R2889 K2890 K2891 K2892 Q2893 E2894 L2895 E2896 A2897 K2898 G2899 G2900 G2901 S2902 H2903 P2904 L2905 L2906 V2907 P2908 Y2909 D2910 T2911 L2912 T2913 A2914 K2915 E2916 K2917 A2918 R2919 D2920 R2921 E2922 K2923 A2924 Q2925 E2926 L2927 L2928 K2929 F2930 L2931 Q2932 M2933
N2934 G2935 Y2936 A2937 V2938 T2939 R2940 G2941 L2942 K2943 D2944 M2945 E2946 L2947 D2948 T2949 I2952 M2968 S2971 Q2972 E2973 F2974 I2975 L2978 V2981 V2982 S2983 S2984 G2985 R2986 V2987 E2988 K2989 F2999 L3003 L3004 P3005 S3028 K3035 M3039 L3047 L3050 H3053 R3054 V3055 V3065
L3069 L3076 D3077 A3078 R3079 M3082 P3086 V3089 K3090 D3103 I3104 E3105 K3106 M3107 V3108 E3109 N3110 L3111 R3112 L3113 GLY LYS VAL SER GLN ALA ARG THR GLN VAL K3124 G3125 V3126 G3127 Q3128 T3131 V3135 A3136 V3140 L3141 T3142 F3145 D3156 V3157 I3158 D3161 V3164
Y3167 S3172 L3176 G3177 R3180 N3181 P3182 Y3183 V3184 E3185 K3186 L3187 R3188 R3197 V3204 E3208 N3212 E3213 V3219 Y3220 R3226 E3227 R3228 A3229 I3230 L3231 G3232 L3233 P3234 N3235 S3236 V3237 E3238 E3239 D3243 E3253 I3254 G3255 G3256 L3257 A3262 R3263 M3267 P3268 H3269 V3270
I3271 L3275 P3276 M3277 L3278 C3279 S3280 Y3281 L3282 R3288 E3291 A3292 P3293 P3294 P3295 A3296 L3297 P3298 A3299 G3300 A3301 T3309 S3310 D3311 H3312 L3316 N3319 I3320 L3321 R3322 I3323 I3324 V3325 I3330 D3331 E3332 M3336 K3337 A3343 Q3344 P3345 I3346 V3347 E3353 L3354 L3355 R3356 I3360
R3367 V3373 V3374 A3375 E3376 E3377 E3378 Q3379 L3380 R3381 L3382 E3383 A3384 K3385 A3386 E3387 A3388 E3389 E3390 G3391 E3392 L3393 L3394 V3395 R3396 D3397 E3398 F3399 S3400 V3401 L3402 C3403 R3404 D3405 L3406 Y3407 A3408 L3409 Y3410 P3411 L3412 L3413 I3414 R3415 R3421 N3431 A3432 G3440 E3441 I3442 F3443 I3444 S3447 N3451



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31572	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.547	Depositor
Minimum map value	0.000	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	426.496, 426.496, 426.496	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.833, 0.833, 0.833	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ZN, CFF, PCW, CA

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	E	0.30	0/847	0.50	0/1142
1	F	0.30	0/847	0.50	0/1142
1	G	0.30	0/847	0.50	0/1142
1	H	0.30	0/847	0.50	0/1142
2	I	0.26	0/739	0.43	0/992
2	J	0.31	0/739	0.53	0/992
2	K	0.26	0/739	0.43	0/992
2	L	0.31	0/739	0.52	0/992
2	M	0.26	0/739	0.43	0/992
2	N	0.31	0/739	0.53	0/992
2	O	0.27	0/739	0.43	0/992
2	P	0.31	0/739	0.53	0/992
3	A	0.29	0/35638	0.49	0/48272
3	B	0.29	0/35638	0.49	0/48272
3	C	0.29	0/35638	0.49	0/48272
3	D	0.29	0/35638	0.49	0/48272
All	All	0.29	0/151852	0.49	0/205592

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	E	829	0	826	10	0
1	F	829	0	826	9	0
1	G	829	0	826	11	0
1	H	829	0	826	10	0
2	I	729	0	705	50	0
2	J	729	0	705	53	0
2	K	729	0	705	51	0
2	L	729	0	705	52	0
2	M	729	0	705	51	0
2	N	729	0	705	51	0
2	O	729	0	705	49	0
2	P	729	0	705	52	0
3	A	34849	0	34448	540	0
3	B	34849	0	34448	543	0
3	C	34849	0	34448	538	0
3	D	34849	0	34448	532	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	I	2	0	0	0	0
4	J	2	0	0	0	0
4	K	2	0	0	0	0
4	L	2	0	0	0	0
4	M	2	0	0	0	0
4	N	2	0	0	0	0
4	O	2	0	0	0	0
4	P	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	14	0	10	0	0
6	B	14	0	10	0	0
6	C	14	0	10	0	0
6	D	14	0	10	0	0
7	A	62	0	24	2	0
7	B	62	0	24	2	0
7	C	62	0	24	3	0
7	D	62	0	24	3	0
8	A	108	0	167	6	0
8	B	108	0	167	6	0
8	C	108	0	167	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	108	0	167	5	0
All	All	149304	0	147540	2468	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 8.

All (2468) 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)
2:I:10:GLU:OE2	3:A:2694:GLN:NE2	1.72	1.23
3:C:2694:GLN:NE2	2:M:10:GLU:OE2	1.72	1.23
3:D:2694:GLN:NE2	2:O:10:GLU:OE2	1.72	1.22
3:B:2694:GLN:NE2	2:K:10:GLU:OE2	1.72	1.21
3:A:875:LEU:HD11	3:A:1047:LEU:HD21	1.41	1.02
3:D:875:LEU:HD11	3:D:1047:LEU:HD21	1.41	1.01
3:C:875:LEU:HD11	3:C:1047:LEU:HD21	1.41	0.98
3:B:875:LEU:HD11	3:B:1047:LEU:HD21	1.41	0.98
2:I:6:GLU:OE2	2:J:42:LEU:HD13	1.65	0.95
2:N:42:LEU:HD13	2:M:6:GLU:OE2	1.65	0.95
2:O:6:GLU:OE2	2:P:42:LEU:HD13	1.65	0.94
2:K:6:GLU:OE2	2:L:42:LEU:HD13	1.65	0.94
3:A:4040:ASN:O	3:A:4045:ARG:NH1	2.12	0.83
3:B:4040:ASN:O	3:B:4045:ARG:NH1	2.12	0.83
3:C:4040:ASN:O	3:C:4045:ARG:NH1	2.12	0.82
2:I:41:GLU:OE1	2:J:2:GLY:N	2.13	0.82
2:N:2:GLY:N	2:M:41:GLU:OE1	2.13	0.82
2:K:41:GLU:OE1	2:L:2:GLY:N	2.13	0.81
3:D:4040:ASN:O	3:D:4045:ARG:NH1	2.12	0.81
2:K:84:VAL:HG13	2:L:72:PHE:HE2	1.44	0.81
2:O:41:GLU:OE1	2:P:2:GLY:N	2.13	0.81
3:C:3319:ASN:O	3:C:3323:ILE:HD12	1.80	0.81
3:D:3319:ASN:O	3:D:3323:ILE:HD12	1.80	0.81
2:I:84:VAL:HG13	2:J:72:PHE:HE2	1.44	0.81
3:D:145:GLU:OE1	3:C:2453:ARG:NH2	2.14	0.80
3:A:3309:THR:OG1	3:A:3311:ASP:OD1	1.99	0.80
3:D:3309:THR:OG1	3:D:3311:ASP:OD1	2.00	0.80
2:O:84:VAL:HG13	2:P:72:PHE:HE2	1.44	0.80
3:A:3319:ASN:O	3:A:3323:ILE:HD12	1.80	0.80
3:B:3319:ASN:O	3:B:3323:ILE:HD12	1.80	0.80
2:N:72:PHE:HE2	2:M:84:VAL:HG13	1.44	0.80
3:A:3236:SER:OG	3:A:3239:GLU:OE1	2.01	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3309:THR:OG1	3:B:3311:ASP:OD1	2.00	0.79
3:D:1713:TYR:OH	3:D:1816:MET:SD	2.41	0.79
3:D:156:LYS:CG	3:C:228:MET:SD	2.71	0.79
3:B:1435:TYR:OH	3:B:1570:GLN:N	2.16	0.79
3:C:1713:TYR:OH	3:C:1816:MET:SD	2.41	0.79
3:C:3309:THR:OG1	3:C:3311:ASP:OD1	2.00	0.79
3:D:1435:TYR:OH	3:D:1570:GLN:N	2.16	0.79
3:B:2453:ARG:NH2	3:C:145:GLU:OE1	2.14	0.79
3:C:1435:TYR:OH	3:C:1570:GLN:N	2.16	0.79
3:A:4082:ASP:OD2	3:B:4734:ARG:NH1	2.16	0.78
3:B:3236:SER:OG	3:B:3239:GLU:OE1	2.01	0.78
3:B:3367:ARG:NH1	3:B:3441:GLU:OE2	2.16	0.78
3:A:2213:VAL:HG11	3:A:2257:TYR:HE2	1.48	0.78
3:B:1713:TYR:OH	3:B:1816:MET:SD	2.41	0.78
3:C:3236:SER:OG	3:C:3239:GLU:OE1	2.01	0.78
3:C:3367:ARG:NH1	3:C:3441:GLU:OE2	2.16	0.78
3:D:1653:GLU:OE1	3:D:1657:ARG:NH1	2.17	0.78
3:D:3236:SER:OG	3:D:3239:GLU:OE1	2.01	0.78
3:D:3367:ARG:NH1	3:D:3441:GLU:OE2	2.16	0.78
3:A:1653:GLU:OE1	3:A:1657:ARG:NH1	2.17	0.78
3:A:1713:TYR:OH	3:A:1816:MET:SD	2.41	0.78
3:A:3367:ARG:NH1	3:A:3441:GLU:OE2	2.17	0.78
3:B:2269:GLN:NE2	3:B:2413:GLU:OE2	2.17	0.78
3:D:2213:VAL:HG11	3:D:2257:TYR:HE2	1.48	0.78
3:A:2453:ARG:NH2	3:B:145:GLU:OE1	2.16	0.78
3:D:1423:ASP:OD2	3:D:1569:LYS:NZ	2.17	0.78
3:C:1423:ASP:OD2	3:C:1569:LYS:NZ	2.17	0.78
3:C:2269:GLN:NE2	3:C:2413:GLU:OE2	2.17	0.78
3:A:2269:GLN:NE2	3:A:2413:GLU:OE2	2.17	0.77
3:B:3316:LEU:O	3:B:3320:ILE:HD12	1.85	0.77
3:A:3316:LEU:O	3:A:3320:ILE:HD12	1.85	0.77
3:B:228:MET:SD	3:C:156:LYS:CG	2.71	0.77
3:D:2269:GLN:NE2	3:D:2413:GLU:OE2	2.17	0.77
3:D:2453:ARG:NH2	3:A:145:GLU:OE1	2.18	0.77
3:A:1435:TYR:OH	3:A:1570:GLN:N	2.16	0.77
3:B:1653:GLU:OE1	3:B:1657:ARG:NH1	2.17	0.77
3:B:2213:VAL:HG11	3:B:2257:TYR:HE2	1.48	0.77
3:C:1653:GLU:OE1	3:C:1657:ARG:NH1	2.17	0.77
3:C:2213:VAL:HG11	3:C:2257:TYR:HE2	1.48	0.77
3:B:1423:ASP:OD2	3:B:1569:LYS:NZ	2.17	0.76
3:D:3316:LEU:O	3:D:3320:ILE:HD12	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:53:ASP:OD2	2:J:54:ALA:N	2.19	0.76
2:N:53:ASP:OD2	2:N:54:ALA:N	2.19	0.76
3:C:3316:LEU:O	3:C:3320:ILE:HD12	1.85	0.76
3:D:3400:SER:OG	3:D:3455:GLU:OE1	2.04	0.76
3:A:1042:GLN:O	3:A:1046:THR:HG23	1.86	0.76
3:B:3407:TYR:OH	3:B:3456:GLU:OE2	2.04	0.76
3:C:1042:GLN:O	3:C:1046:THR:HG23	1.86	0.76
2:L:53:ASP:OD2	2:L:54:ALA:N	2.19	0.76
3:A:836:ARG:NH2	3:A:1211:SER:O	2.20	0.75
3:D:156:LYS:HG2	3:C:228:MET:SD	2.27	0.75
3:D:2873:GLN:OE1	3:D:2921:ARG:NH2	2.19	0.75
3:B:1042:GLN:O	3:B:1046:THR:HG23	1.86	0.75
3:B:4744:ALA:O	3:B:4748:ILE:HD12	1.87	0.75
3:C:2873:GLN:OE1	3:C:2921:ARG:NH2	2.19	0.75
3:D:24:GLN:OE1	3:D:204:ASN:ND2	2.20	0.75
3:C:836:ARG:NH2	3:C:1211:SER:O	2.20	0.75
3:B:2813:SER:OG	3:B:2883:TYR:OH	2.03	0.75
3:A:4744:ALA:O	3:A:4748:ILE:HD12	1.87	0.75
3:B:836:ARG:NH2	3:B:1211:SER:O	2.20	0.75
3:C:4744:ALA:O	3:C:4748:ILE:HD12	1.87	0.75
2:P:53:ASP:OD2	2:P:54:ALA:N	2.19	0.75
3:D:4744:ALA:O	3:D:4748:ILE:HD12	1.87	0.75
3:A:24:GLN:OE1	3:A:204:ASN:ND2	2.20	0.75
3:A:2873:GLN:OE1	3:A:2921:ARG:NH2	2.19	0.75
3:B:228:MET:SD	3:C:156:LYS:HG2	2.27	0.75
3:D:836:ARG:NH2	3:D:1211:SER:O	2.20	0.75
3:A:3400:SER:OG	3:A:3455:GLU:OE1	2.04	0.75
3:A:3407:TYR:OH	3:A:3456:GLU:OE2	2.04	0.75
3:C:24:GLN:OE1	3:C:204:ASN:ND2	2.20	0.75
3:D:3407:TYR:OH	3:D:3456:GLU:OE2	2.04	0.74
3:D:4900:GLU:O	3:D:4911:ARG:NH2	2.21	0.74
3:A:228:MET:SD	3:B:156:LYS:CG	2.75	0.74
3:D:330:ARG:NH1	3:D:331:ASP:OD1	2.21	0.74
3:A:330:ARG:NH1	3:A:331:ASP:OD1	2.21	0.74
3:B:2873:GLN:OE1	3:B:2921:ARG:NH2	2.19	0.74
3:C:4900:GLU:O	3:C:4911:ARG:NH2	2.21	0.74
2:J:80:ALA:O	2:J:84:VAL:HG22	1.88	0.74
3:B:24:GLN:OE1	3:B:204:ASN:ND2	2.20	0.74
2:P:80:ALA:O	2:P:84:VAL:HG22	1.88	0.74
3:C:3400:SER:OG	3:C:3455:GLU:OE1	2.04	0.74
3:C:3407:TYR:OH	3:C:3456:GLU:OE2	2.04	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:80:ALA:O	2:N:84:VAL:HG22	1.88	0.74
3:B:330:ARG:NH1	3:B:331:ASP:OD1	2.21	0.74
3:D:1042:GLN:O	3:D:1046:THR:HG23	1.86	0.74
3:B:3400:SER:OG	3:B:3455:GLU:OE1	2.04	0.73
3:C:330:ARG:NH1	3:C:331:ASP:OD1	2.21	0.73
3:A:1423:ASP:OD2	3:A:1569:LYS:NZ	2.17	0.73
3:D:908:LEU:O	3:D:964:ASN:ND2	2.22	0.73
3:B:4900:GLU:O	3:B:4911:ARG:NH2	2.21	0.73
3:B:4638:GLU:OE2	3:B:4642:ARG:NH1	2.21	0.73
3:D:4638:GLU:OE2	3:D:4642:ARG:NH1	2.21	0.73
3:A:4900:GLU:O	3:A:4911:ARG:NH2	2.20	0.73
3:B:908:LEU:O	3:B:964:ASN:ND2	2.22	0.73
3:A:951:LEU:HB3	3:A:971:LEU:HD23	1.71	0.73
3:A:908:LEU:O	3:A:964:ASN:ND2	2.22	0.73
3:C:4638:GLU:OE2	3:C:4642:ARG:NH1	2.21	0.73
3:D:2813:SER:OG	3:D:2883:TYR:OH	2.03	0.73
2:L:80:ALA:O	2:L:84:VAL:HG22	1.88	0.72
3:A:4638:GLU:OE2	3:A:4642:ARG:NH1	2.21	0.72
3:B:951:LEU:HB3	3:B:971:LEU:HD23	1.71	0.72
3:A:2813:SER:OG	3:A:2883:TYR:OH	2.03	0.72
3:C:908:LEU:O	3:C:964:ASN:ND2	2.22	0.72
3:C:914:LEU:HD21	3:C:918:GLU:OE1	1.90	0.72
3:D:951:LEU:HB3	3:D:971:LEU:HD23	1.71	0.72
3:B:1505:GLY:O	3:B:1509:ARG:NH1	2.23	0.72
3:B:914:LEU:HD21	3:B:918:GLU:OE1	1.90	0.72
3:B:2889:ARG:O	3:B:2893:GLN:NE2	2.23	0.72
3:D:3111:LEU:O	3:D:3183:TYR:OH	2.07	0.72
3:A:4883:PHE:O	3:A:4887:VAL:HG22	1.90	0.72
3:C:951:LEU:HB3	3:C:971:LEU:HD23	1.71	0.72
3:D:2889:ARG:O	3:D:2893:GLN:NE2	2.23	0.72
3:A:914:LEU:HD21	3:A:918:GLU:OE1	1.90	0.71
3:B:4883:PHE:O	3:B:4887:VAL:HG22	1.90	0.71
3:C:1505:GLY:O	3:C:1509:ARG:NH1	2.23	0.71
3:D:228:MET:SD	3:A:156:LYS:CG	2.78	0.71
3:A:2889:ARG:O	3:A:2893:GLN:NE2	2.23	0.71
3:D:914:LEU:HD21	3:D:918:GLU:OE1	1.90	0.71
3:D:1505:GLY:O	3:D:1509:ARG:NH1	2.23	0.71
3:D:4883:PHE:O	3:D:4887:VAL:HG22	1.90	0.71
3:C:2698:ARG:NH2	2:M:17:HIS:ND1	2.38	0.71
3:C:4883:PHE:O	3:C:4887:VAL:HG22	1.90	0.71
3:B:2698:ARG:NH2	2:K:17:HIS:ND1	2.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:PHE:O	3:A:1688:SER:OG	2.07	0.71
3:A:1505:GLY:O	3:A:1509:ARG:NH1	2.23	0.71
3:C:2889:ARG:O	3:C:2893:GLN:NE2	2.23	0.71
2:I:17:HIS:ND1	3:A:2698:ARG:NH2	2.38	0.70
1:G:37:PHE:O	3:C:1688:SER:OG	2.07	0.70
3:D:2564:THR:HG22	3:D:2607:CYS:HA	1.74	0.70
3:D:2539:THR:O	3:D:2543:SER:OG	2.10	0.70
3:D:2698:ARG:NH2	2:O:17:HIS:ND1	2.38	0.70
3:D:4082:ASP:OD2	3:A:4734:ARG:NH1	2.24	0.70
3:A:2564:THR:HG22	3:A:2607:CYS:HA	1.74	0.70
3:A:228:MET:SD	3:B:156:LYS:HG2	2.31	0.70
2:I:61:GLU:O	3:A:3638:ARG:NH1	2.25	0.70
3:C:3638:ARG:NH1	2:M:61:GLU:O	2.25	0.70
3:C:2564:THR:HG22	3:C:2607:CYS:HA	1.74	0.70
3:C:2813:SER:OG	3:C:2883:TYR:OH	2.03	0.69
3:D:3638:ARG:NH1	2:O:61:GLU:O	2.25	0.69
3:B:829:GLU:OE2	3:B:832:ARG:NH1	2.26	0.69
3:B:2564:THR:HG22	3:B:2607:CYS:HA	1.74	0.69
3:C:829:GLU:OE2	3:C:832:ARG:NH1	2.26	0.69
3:C:2539:THR:O	3:C:2543:SER:OG	2.10	0.69
3:D:829:GLU:OE2	3:D:832:ARG:NH1	2.26	0.69
3:D:3108:VAL:HG21	3:D:3172:SER:HB2	1.73	0.69
3:C:3111:LEU:O	3:C:3183:TYR:OH	2.07	0.69
1:H:37:PHE:O	3:D:1688:SER:OG	2.06	0.69
3:D:4734:ARG:NH1	3:C:4082:ASP:OD2	2.26	0.69
3:B:1431:THR:HG22	3:B:1433:THR:H	1.58	0.69
3:B:3111:LEU:O	3:B:3183:TYR:OH	2.07	0.69
3:B:3638:ARG:NH1	2:K:61:GLU:O	2.25	0.69
3:C:3108:VAL:HG21	3:C:3172:SER:HB2	1.74	0.69
3:C:3467:ASN:ND2	3:C:3508:THR:O	2.26	0.69
2:M:37:LEU:O	2:M:40:THR:OG1	2.10	0.69
3:D:3467:ASN:ND2	3:D:3508:THR:O	2.26	0.69
3:A:3108:VAL:HG21	3:A:3172:SER:HB2	1.74	0.69
3:B:3108:VAL:HG21	3:B:3172:SER:HB2	1.74	0.69
3:C:3530:ASP:OD1	3:C:3561:GLN:NE2	2.26	0.69
3:D:3208:GLU:OE1	3:D:3281:TYR:OH	2.11	0.68
3:A:1431:THR:HG22	3:A:1433:THR:H	1.58	0.68
3:B:3530:ASP:OD1	3:B:3561:GLN:NE2	2.26	0.68
3:C:1431:THR:HG22	3:C:1433:THR:H	1.58	0.68
3:D:3530:ASP:OD1	3:D:3561:GLN:NE2	2.26	0.68
3:B:41:GLU:OE2	3:B:407:SER:OG	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1273:LEU:HD22	3:C:1290:LEU:HD11	1.76	0.68
3:A:3111:LEU:O	3:A:3183:TYR:OH	2.07	0.68
3:B:2539:THR:O	3:B:2543:SER:OG	2.10	0.68
3:D:3053:HIS:NE2	3:D:3103:ASP:OD1	2.27	0.68
3:B:3053:HIS:NE2	3:B:3103:ASP:OD1	2.27	0.68
3:A:3053:HIS:NE2	3:A:3103:ASP:OD1	2.27	0.68
3:A:3530:ASP:OD1	3:A:3561:GLN:NE2	2.26	0.68
3:B:2560:LEU:O	3:B:2564:THR:HG23	1.94	0.68
1:E:32:GLU:OE1	1:E:97:THR:OG1	2.10	0.68
3:C:2560:LEU:O	3:C:2564:THR:HG23	1.94	0.68
3:A:1273:LEU:HD22	3:A:1290:LEU:HD11	1.76	0.68
3:B:1273:LEU:HD22	3:B:1290:LEU:HD11	1.76	0.68
3:D:1297:GLN:NE2	3:D:1546:ASN:OD1	2.27	0.68
3:D:2560:LEU:O	3:D:2564:THR:HG23	1.94	0.68
3:A:2523:LEU:HD11	3:A:2583:MET:SD	2.33	0.68
3:B:4082:ASP:OD2	3:C:4734:ARG:NH1	2.26	0.68
3:C:3053:HIS:NE2	3:C:3103:ASP:OD1	2.27	0.68
2:L:37:LEU:O	2:L:40:THR:OG1	2.11	0.68
3:D:1273:LEU:HD22	3:D:1290:LEU:HD11	1.76	0.68
3:A:829:GLU:OE2	3:A:832:ARG:NH1	2.26	0.68
3:C:1297:GLN:NE2	3:C:1546:ASN:OD1	2.27	0.68
3:A:2560:LEU:O	3:A:2564:THR:HG23	1.94	0.67
3:B:3467:ASN:ND2	3:B:3508:THR:O	2.26	0.67
3:C:2588:TYR:OH	3:C:2592:ARG:NH2	2.28	0.67
3:D:2523:LEU:HD11	3:D:2583:MET:SD	2.34	0.67
3:A:3467:ASN:ND2	3:A:3508:THR:O	2.26	0.67
3:B:2523:LEU:HD11	3:B:2583:MET:SD	2.34	0.67
3:B:2588:TYR:OH	3:B:2592:ARG:NH2	2.28	0.67
3:D:910:ASN:O	3:D:914:LEU:N	2.28	0.67
3:D:2588:TYR:OH	3:D:2592:ARG:NH2	2.28	0.67
3:A:2588:TYR:OH	3:A:2592:ARG:NH2	2.28	0.67
3:C:3530:ASP:OD2	3:C:3596:ARG:NH2	2.28	0.67
1:F:37:PHE:O	3:B:1688:SER:OG	2.07	0.67
3:A:910:ASN:O	3:A:914:LEU:N	2.28	0.67
3:B:3530:ASP:OD2	3:B:3596:ARG:NH2	2.28	0.67
3:C:2523:LEU:HD11	3:C:2583:MET:SD	2.34	0.67
3:B:1297:GLN:NE2	3:B:1546:ASN:OD1	2.27	0.67
3:D:1431:THR:HG22	3:D:1433:THR:H	1.58	0.67
3:A:1297:GLN:NE2	3:A:1546:ASN:OD1	2.26	0.67
3:B:910:ASN:O	3:B:914:LEU:N	2.28	0.67
3:D:552:LEU:HD11	3:D:565:LEU:HD22	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:552:LEU:HD11	3:A:565:LEU:HD22	1.77	0.67
3:B:3208:GLU:OE1	3:B:3281:TYR:OH	2.11	0.67
3:B:552:LEU:HD11	3:B:565:LEU:HD22	1.77	0.67
3:D:41:GLU:OE2	3:D:407:SER:OG	2.11	0.66
3:A:3530:ASP:OD2	3:A:3596:ARG:NH2	2.28	0.66
2:I:84:VAL:HG22	2:J:72:PHE:CD2	2.31	0.66
2:J:37:LEU:O	2:J:40:THR:OG1	2.11	0.66
3:C:3344:GLN:O	3:C:3347:VAL:HG22	1.95	0.66
2:N:72:PHE:CD2	2:M:84:VAL:HG22	2.30	0.66
3:D:3344:GLN:O	3:D:3347:VAL:HG22	1.95	0.66
3:D:3530:ASP:OD2	3:D:3596:ARG:NH2	2.28	0.66
3:C:910:ASN:O	3:C:914:LEU:N	2.28	0.66
3:B:3076:LEU:HD23	3:B:3077:ASP:N	2.11	0.66
2:K:37:LEU:O	2:K:40:THR:OG1	2.11	0.66
3:D:3082:MET:O	3:D:3090:LYS:NZ	2.29	0.66
3:A:2539:THR:O	3:A:2543:SER:OG	2.10	0.66
3:A:4074:ILE:O	3:A:4077:SER:OG	2.06	0.66
3:C:41:GLU:OE2	3:C:407:SER:OG	2.11	0.66
3:C:552:LEU:HD11	3:C:565:LEU:HD22	1.77	0.66
3:D:228:MET:SD	3:A:156:LYS:HG2	2.34	0.66
3:B:3320:ILE:O	3:B:3324:ILE:HD12	1.96	0.66
3:B:3344:GLN:O	3:B:3347:VAL:HG22	1.95	0.66
2:K:84:VAL:HG22	2:L:72:PHE:CD2	2.31	0.66
3:B:1021:ARG:HE	7:B:8005:ATP:HN62	1.43	0.66
3:B:2752:LEU:HB3	3:B:2814:LEU:HD13	1.77	0.66
3:A:3344:GLN:O	3:A:3347:VAL:HG22	1.95	0.66
3:C:2703:CYS:O	3:C:2707:ILE:HD12	1.96	0.66
2:O:84:VAL:HG22	2:P:72:PHE:CD2	2.30	0.66
3:A:3320:ILE:O	3:A:3324:ILE:HD12	1.96	0.66
3:B:3082:MET:O	3:B:3090:LYS:NZ	2.29	0.66
3:C:2752:LEU:HB3	3:C:2814:LEU:HD13	1.77	0.66
3:B:3505:SER:O	3:B:3508:THR:OG1	2.12	0.65
3:D:3076:LEU:HD23	3:D:3077:ASP:N	2.11	0.65
3:D:3532:ASP:OD1	3:D:3533:LEU:N	2.29	0.65
3:A:41:GLU:OE2	3:A:407:SER:OG	2.11	0.65
3:B:3532:ASP:OD1	3:B:3533:LEU:N	2.29	0.65
3:C:1021:ARG:HE	7:C:5106:ATP:HN62	1.43	0.65
3:C:3532:ASP:OD1	3:C:3533:LEU:N	2.29	0.65
3:D:701:GLU:OE2	3:D:1459:HIS:NE2	2.29	0.65
3:A:3082:MET:O	3:A:3090:LYS:NZ	2.29	0.65
3:C:3208:GLU:OE1	3:C:3281:TYR:OH	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:6:GLU:OE2	2:L:42:LEU:CD1	2.44	0.65
3:A:701:GLU:OE2	3:A:1459:HIS:NE2	2.29	0.65
3:A:3208:GLU:OE1	3:A:3281:TYR:OH	2.11	0.65
3:A:3410:TYR:O	3:A:3413:LEU:N	2.30	0.65
3:A:3505:SER:O	3:A:3508:THR:OG1	2.12	0.65
2:N:37:LEU:O	2:N:40:THR:OG1	2.11	0.65
3:D:2703:CYS:O	3:D:2707:ILE:HD12	1.96	0.65
3:C:3076:LEU:HD23	3:C:3077:ASP:N	2.11	0.65
1:E:3:VAL:HG23	1:E:77:ILE:HD13	1.78	0.65
3:C:3082:MET:O	3:C:3090:LYS:NZ	2.29	0.65
2:I:37:LEU:O	2:I:40:THR:OG1	2.11	0.65
3:D:3410:TYR:O	3:D:3413:LEU:N	2.30	0.65
3:D:3505:SER:O	3:D:3508:THR:OG1	2.12	0.65
3:A:1021:ARG:HE	7:A:8005:ATP:HN62	1.43	0.65
3:D:2752:LEU:HB3	3:D:2814:LEU:HD13	1.77	0.65
3:A:3532:ASP:OD1	3:A:3533:LEU:N	2.29	0.65
3:C:3320:ILE:O	3:C:3324:ILE:HD12	1.96	0.65
3:C:3410:TYR:O	3:C:3413:LEU:N	2.30	0.64
2:O:37:LEU:O	2:O:40:THR:OG1	2.11	0.64
3:A:2752:LEU:HB3	3:A:2814:LEU:HD13	1.77	0.64
3:A:3076:LEU:HD23	3:A:3077:ASP:N	2.11	0.64
2:N:72:PHE:CE2	2:M:84:VAL:HG13	2.31	0.64
1:F:3:VAL:HG23	1:F:77:ILE:HD13	1.80	0.64
1:H:32:GLU:OE1	1:H:97:THR:OG1	2.15	0.64
3:A:2755:PHE:HD2	3:A:2814:LEU:HD11	1.63	0.64
2:K:84:VAL:HG13	2:L:72:PHE:CE2	2.31	0.64
2:N:42:LEU:CD1	2:M:6:GLU:OE2	2.44	0.64
2:J:72:PHE:HA	2:J:75:TYR:CE1	2.33	0.64
1:G:3:VAL:HG23	1:G:77:ILE:HD13	1.79	0.64
1:H:3:VAL:HG23	1:H:77:ILE:HD13	1.79	0.64
3:D:3235:ASN:OD1	3:D:3236:SER:N	2.31	0.64
3:B:2703:CYS:O	3:B:2707:ILE:HD12	1.96	0.64
3:C:701:GLU:OE2	3:C:1459:HIS:NE2	2.29	0.64
3:D:1021:ARG:HE	7:D:8005:ATP:HN62	1.43	0.64
3:D:3320:ILE:O	3:D:3324:ILE:HD12	1.96	0.64
2:P:72:PHE:HA	2:P:75:TYR:CE1	2.33	0.64
3:A:2703:CYS:O	3:A:2707:ILE:HD12	1.96	0.64
3:B:3410:TYR:O	3:B:3413:LEU:N	2.30	0.64
1:F:32:GLU:OE2	1:F:97:THR:OG1	2.15	0.64
3:D:4796:MET:CE	8:D:8007:PCW:H222	2.27	0.64
3:B:2755:PHE:HD2	3:B:2814:LEU:HD11	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:72:PHE:HA	2:L:75:TYR:CE1	2.33	0.64
1:G:32:GLU:OE1	1:G:97:THR:OG1	2.15	0.64
3:B:3235:ASN:OD1	3:B:3236:SER:N	2.31	0.64
3:B:3443:PHE:CG	3:B:3515:LEU:HD22	2.33	0.64
3:C:3235:ASN:OD1	3:C:3236:SER:N	2.31	0.64
3:D:554:ARG:NE	3:D:556:GLU:OE2	2.31	0.64
2:N:72:PHE:HA	2:N:75:TYR:CE1	2.33	0.64
2:I:6:GLU:OE2	2:J:42:LEU:CD1	2.44	0.64
3:A:3235:ASN:OD1	3:A:3236:SER:N	2.31	0.63
3:B:3212:ASN:OD1	3:B:3213:GLU:N	2.31	0.63
3:C:3505:SER:O	3:C:3508:THR:OG1	2.12	0.63
3:A:2209:MET:O	3:A:2213:VAL:HG13	1.99	0.63
3:C:2599:ALA:O	3:C:2603:VAL:HG23	1.99	0.63
3:C:3212:ASN:OD1	3:C:3213:GLU:N	2.31	0.63
3:D:3431:ASN:OD1	3:D:3432:ALA:N	2.32	0.63
3:D:4741:MET:HE2	3:D:4746:LEU:HD11	1.81	0.63
3:A:3443:PHE:CG	3:A:3515:LEU:HD22	2.33	0.63
3:B:554:ARG:NE	3:B:556:GLU:OE2	2.31	0.63
3:B:2209:MET:O	3:B:2213:VAL:HG13	1.99	0.63
3:B:3431:ASN:OD1	3:B:3432:ALA:N	2.32	0.63
3:C:3443:PHE:CG	3:C:3515:LEU:HD22	2.33	0.63
3:D:804:LEU:HD23	3:D:805:PRO:O	1.99	0.63
3:D:3770:GLN:OE1	3:D:3812:ASN:ND2	2.32	0.63
3:A:3212:ASN:OD1	3:A:3213:GLU:N	2.31	0.63
3:C:2755:PHE:HD2	3:C:2814:LEU:HD11	1.63	0.63
3:D:2209:MET:O	3:D:2213:VAL:HG13	1.99	0.63
3:D:2933:MET:SD	3:D:2934:ASN:N	2.72	0.63
3:D:2599:ALA:O	3:D:2603:VAL:HG23	1.99	0.63
3:B:1442:ALA:N	3:B:1514:ASP:OD1	2.32	0.63
3:D:2755:PHE:HD2	3:D:2814:LEU:HD11	1.63	0.62
3:D:3443:PHE:CG	3:D:3515:LEU:HD22	2.33	0.62
3:A:901:ASN:OD1	3:A:902:LYS:N	2.32	0.62
3:B:2933:MET:SD	3:B:2934:ASN:N	2.72	0.62
3:B:3864:GLU:O	3:B:3868:VAL:HG22	1.99	0.62
3:C:901:ASN:OD1	3:C:902:LYS:N	2.32	0.62
3:C:2933:MET:SD	3:C:2934:ASN:N	2.72	0.62
3:C:3770:GLN:OE1	3:C:3812:ASN:ND2	2.32	0.62
3:D:901:ASN:OD1	3:D:902:LYS:N	2.32	0.62
3:A:804:LEU:HD23	3:A:805:PRO:O	1.99	0.62
3:A:2297:GLU:OE1	3:A:2357:LEU:HD22	2.00	0.62
3:A:2599:ALA:O	3:A:2603:VAL:HG23	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2933:MET:SD	3:A:2934:ASN:N	2.72	0.62
3:B:2297:GLU:OE1	3:B:2357:LEU:HD22	2.00	0.62
3:D:3212:ASN:OD1	3:D:3213:GLU:N	2.31	0.62
3:D:3864:GLU:O	3:D:3868:VAL:HG22	1.99	0.62
3:A:554:ARG:NE	3:A:556:GLU:OE2	2.31	0.62
3:C:3864:GLU:O	3:C:3868:VAL:HG22	1.99	0.62
2:P:37:LEU:O	2:P:40:THR:OG1	2.11	0.62
2:I:84:VAL:HG13	2:J:72:PHE:CE2	2.31	0.62
3:A:3770:GLN:OE1	3:A:3812:ASN:ND2	2.32	0.62
3:B:2599:ALA:O	3:B:2603:VAL:HG23	1.99	0.62
2:I:82:LEU:HD12	3:A:3630:ARG:HD3	1.82	0.62
3:D:865:PRO:HD2	3:D:868:LEU:HD12	1.82	0.62
3:B:249:GLU:HB2	3:B:253:VAL:HG11	1.82	0.62
3:B:701:GLU:OE2	3:B:1459:HIS:NE2	2.29	0.62
2:O:84:VAL:HG13	2:P:72:PHE:CE2	2.31	0.62
3:D:4009:ASP:OD1	3:D:4010:SER:N	2.33	0.62
3:A:3864:GLU:O	3:A:3868:VAL:HG22	1.99	0.62
3:B:901:ASN:OD1	3:B:902:LYS:N	2.32	0.62
3:C:554:ARG:NE	3:C:556:GLU:OE2	2.31	0.62
3:C:3954:PHE:CD2	3:C:4015:LEU:HD21	2.34	0.62
3:D:1442:ALA:N	3:D:1514:ASP:OD1	2.32	0.62
3:A:4009:ASP:OD1	3:A:4010:SER:N	2.33	0.62
3:B:914:LEU:HD12	3:B:915:PRO:HD2	1.82	0.62
3:A:914:LEU:HD12	3:A:915:PRO:HD2	1.82	0.62
3:A:1442:ALA:N	3:A:1514:ASP:OD1	2.32	0.62
3:A:3954:PHE:CD2	3:A:4015:LEU:HD21	2.34	0.62
3:A:4796:MET:CE	8:A:8007:PCW:H222	2.29	0.62
3:B:2749:PRO:HD2	3:B:2752:LEU:HD12	1.82	0.62
3:C:3431:ASN:OD1	3:C:3432:ALA:N	2.32	0.62
3:B:865:PRO:HD2	3:B:868:LEU:HD12	1.82	0.62
3:B:3630:ARG:HD3	2:K:82:LEU:HD12	1.82	0.62
3:B:4009:ASP:OD1	3:B:4010:SER:N	2.33	0.62
3:C:308:ALA:HB1	3:C:313:THR:HG21	1.81	0.62
3:C:914:LEU:HD12	3:C:915:PRO:HD2	1.82	0.62
2:J:42:LEU:HD23	2:J:46:LEU:HB2	1.82	0.62
3:D:2627:LEU:HD12	3:D:2641:PRO:HB3	1.81	0.62
3:A:249:GLU:HB2	3:A:253:VAL:HG11	1.82	0.62
3:A:2627:LEU:HD12	3:A:2641:PRO:HB3	1.81	0.62
3:C:1442:ALA:N	3:C:1514:ASP:OD1	2.32	0.62
3:C:2209:MET:O	3:C:2213:VAL:HG13	1.99	0.62
3:C:4009:ASP:OD1	3:C:4010:SER:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:308:ALA:HB1	3:D:313:THR:HG21	1.81	0.61
3:D:914:LEU:HD12	3:D:915:PRO:HD2	1.82	0.61
3:A:865:PRO:HD2	3:A:868:LEU:HD12	1.82	0.61
3:C:804:LEU:HD23	3:C:805:PRO:O	1.99	0.61
3:C:2297:GLU:OE1	3:C:2357:LEU:HD22	2.00	0.61
3:C:2627:LEU:HD12	3:C:2641:PRO:HB3	1.81	0.61
3:D:2749:PRO:HD2	3:D:2752:LEU:HD12	1.82	0.61
3:D:3630:ARG:HD3	2:O:82:LEU:HD12	1.82	0.61
3:D:3954:PHE:CD2	3:D:4015:LEU:HD21	2.34	0.61
3:D:4796:MET:HE1	8:D:8007:PCW:H222	1.81	0.61
3:B:2627:LEU:HD12	3:B:2641:PRO:HB3	1.81	0.61
3:B:3954:PHE:CD2	3:B:4015:LEU:HD21	2.34	0.61
3:C:2749:PRO:HD2	3:C:2752:LEU:HD12	1.82	0.61
3:A:2749:PRO:HD2	3:A:2752:LEU:HD12	1.82	0.61
3:A:4796:MET:HE1	8:A:8007:PCW:H222	1.81	0.61
2:P:42:LEU:HD23	2:P:46:LEU:HB2	1.82	0.61
3:C:4074:ILE:O	3:C:4077:SER:OG	2.06	0.61
3:D:4900:GLU:O	3:D:4911:ARG:NH1	2.32	0.61
3:A:3311:ASP:OD1	3:A:3312:HIS:N	2.34	0.61
2:L:42:LEU:HD23	2:L:46:LEU:HB2	1.82	0.61
3:D:249:GLU:HB2	3:D:253:VAL:HG11	1.82	0.61
3:D:258:ARG:O	3:D:285:HIS:NE2	2.33	0.61
3:A:258:ARG:O	3:A:285:HIS:NE2	2.33	0.61
3:A:405:ILE:HG21	3:A:482:GLU:HG2	1.83	0.61
3:A:3431:ASN:OD1	3:A:3432:ALA:N	2.32	0.61
3:B:3770:GLN:OE1	3:B:3812:ASN:ND2	2.32	0.61
3:B:4741:MET:HE2	3:B:4746:LEU:HD11	1.82	0.61
2:M:88:ASN:O	2:M:92:GLU:HG2	2.01	0.61
3:C:865:PRO:HD2	3:C:868:LEU:HD12	1.82	0.61
3:C:3630:ARG:HD3	2:M:82:LEU:HD12	1.82	0.61
3:A:914:LEU:O	3:A:919:ARG:NE	2.34	0.61
2:I:88:ASN:O	2:I:92:GLU:HG2	2.01	0.61
3:B:282:ARG:NH1	3:B:313:THR:OG1	2.34	0.61
3:B:405:ILE:HG21	3:B:482:GLU:HG2	1.83	0.61
3:C:282:ARG:NH1	3:C:313:THR:OG1	2.34	0.61
3:C:405:ILE:HG21	3:C:482:GLU:HG2	1.83	0.61
3:C:3311:ASP:OD1	3:C:3312:HIS:N	2.34	0.61
3:D:2005:GLU:N	3:D:2005:GLU:OE1	2.34	0.60
3:A:282:ARG:NH1	3:A:313:THR:OG1	2.34	0.60
3:A:318:ARG:NH1	3:A:350:GLN:OE1	2.34	0.60
3:A:926:SER:O	3:A:929:THR:OG1	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4900:GLU:O	3:A:4911:ARG:NH1	2.32	0.60
3:B:3311:ASP:OD1	3:B:3312:HIS:N	2.34	0.60
3:B:4900:GLU:O	3:B:4911:ARG:NH1	2.32	0.60
3:C:4900:GLU:O	3:C:4911:ARG:NH1	2.32	0.60
3:D:3311:ASP:OD1	3:D:3312:HIS:N	2.34	0.60
3:B:804:LEU:HD23	3:B:805:PRO:O	1.99	0.60
3:D:4074:ILE:O	3:D:4077:SER:OG	2.06	0.60
3:A:308:ALA:HB1	3:A:313:THR:HG21	1.81	0.60
3:B:258:ARG:O	3:B:285:HIS:NE2	2.33	0.60
3:B:914:LEU:O	3:B:919:ARG:NE	2.34	0.60
3:C:318:ARG:NH1	3:C:350:GLN:OE1	2.34	0.60
3:C:914:LEU:O	3:C:919:ARG:NE	2.34	0.60
3:C:2005:GLU:OE1	3:C:2005:GLU:N	2.34	0.60
3:A:2005:GLU:N	3:A:2005:GLU:OE1	2.34	0.60
3:A:2394:ASP:OD1	3:A:2395:GLY:N	2.35	0.60
3:B:2394:ASP:OD1	3:B:2395:GLY:N	2.35	0.60
3:B:3660:ALA:HA	3:B:3664:LEU:HD12	1.84	0.60
2:N:5:LEU:HD23	2:N:9:MET:HE1	1.83	0.60
3:D:282:ARG:NH1	3:D:313:THR:OG1	2.34	0.60
3:D:2297:GLU:OE1	3:D:2357:LEU:HD22	2.00	0.60
3:D:2623:LEU:O	3:D:2627:LEU:HD23	2.02	0.60
3:D:3660:ALA:HA	3:D:3664:LEU:HD12	1.84	0.60
3:B:308:ALA:HB1	3:B:313:THR:HG21	1.81	0.60
3:D:914:LEU:O	3:D:919:ARG:NE	2.34	0.60
3:A:2623:LEU:O	3:A:2627:LEU:HD23	2.02	0.60
3:C:249:GLU:HB2	3:C:253:VAL:HG11	1.82	0.60
3:C:2623:LEU:O	3:C:2627:LEU:HD23	2.02	0.60
3:C:2879:LEU:HD21	3:C:2927:LEU:HD23	1.83	0.60
3:D:405:ILE:HG21	3:D:482:GLU:HG2	1.83	0.60
3:B:2005:GLU:OE1	3:B:2005:GLU:N	2.34	0.60
3:C:258:ARG:O	3:C:285:HIS:NE2	2.33	0.60
3:A:3660:ALA:HA	3:A:3664:LEU:HD12	1.84	0.60
3:B:318:ARG:NH1	3:B:350:GLN:OE1	2.34	0.60
3:C:3660:ALA:HA	3:C:3664:LEU:HD12	1.84	0.60
3:C:4741:MET:HE2	3:C:4746:LEU:HD11	1.83	0.60
2:K:88:ASN:O	2:K:92:GLU:HG2	2.01	0.60
3:D:3035:LYS:O	3:D:3039:MET:HE3	2.02	0.60
3:B:2623:LEU:O	3:B:2627:LEU:HD23	2.02	0.60
3:C:2394:ASP:OD1	3:C:2395:GLY:N	2.35	0.60
2:N:42:LEU:HD23	2:N:46:LEU:HB2	1.82	0.60
3:D:926:SER:O	3:D:929:THR:OG1	2.19	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2879:LEU:HD21	3:D:2927:LEU:HD23	1.83	0.59
2:O:88:ASN:O	2:O:92:GLU:HG2	2.01	0.59
3:D:318:ARG:NH1	3:D:350:GLN:OE1	2.34	0.59
3:B:4796:MET:CE	8:B:8007:PCW:H222	2.32	0.59
3:C:3220:TYR:CD1	3:C:3237:VAL:HG22	2.38	0.59
1:E:12:ASP:OD1	1:E:13:GLY:N	2.36	0.59
3:D:2394:ASP:OD1	3:D:2395:GLY:N	2.35	0.59
3:D:3220:TYR:CD1	3:D:3237:VAL:HG22	2.38	0.59
3:B:3347:VAL:HG21	3:B:3415:ARG:HB2	1.84	0.59
3:C:4796:MET:CE	8:C:5101:PCW:H222	2.33	0.59
3:D:3347:VAL:HG21	3:D:3415:ARG:HB2	1.84	0.59
3:C:3105:GLU:O	3:C:3109:GLU:OE1	2.21	0.59
3:C:3347:VAL:HG21	3:C:3415:ARG:HB2	1.84	0.59
3:D:4689:GLN:OE1	3:D:4701:ARG:NH2	2.36	0.59
3:B:926:SER:O	3:B:929:THR:OG1	2.19	0.59
3:C:1253:HIS:O	3:C:1276:ARG:NH1	2.36	0.59
3:C:926:SER:O	3:C:929:THR:OG1	2.19	0.59
3:D:1427:ILE:O	3:D:1431:THR:OG1	2.17	0.59
3:A:1253:HIS:O	3:A:1276:ARG:NH1	2.36	0.59
3:B:3220:TYR:CD1	3:B:3237:VAL:HG22	2.38	0.59
3:B:4689:GLN:OE1	3:B:4701:ARG:NH2	2.36	0.59
3:B:2879:LEU:HD21	3:B:2927:LEU:HD23	1.83	0.59
3:B:3105:GLU:O	3:B:3109:GLU:OE1	2.21	0.59
2:N:84:VAL:HG21	2:M:76:VAL:HG11	1.85	0.59
2:P:5:LEU:HD23	2:P:9:MET:HE1	1.85	0.59
3:A:3220:TYR:CD1	3:A:3237:VAL:HG22	2.38	0.59
3:A:4689:GLN:OE1	3:A:4701:ARG:NH2	2.36	0.59
3:C:1618:THR:HG22	3:C:1629:VAL:HG12	1.85	0.59
3:A:3347:VAL:HG21	3:A:3415:ARG:HB2	1.84	0.58
3:B:615:VAL:HG23	3:B:618:ASN:HB2	1.85	0.58
3:A:615:VAL:HG23	3:A:618:ASN:HB2	1.85	0.58
3:B:3035:LYS:O	3:B:3039:MET:HE3	2.03	0.58
3:C:2886:THR:HG22	3:C:2889:ARG:HH21	1.68	0.58
2:O:6:GLU:OE2	2:P:42:LEU:CD1	2.44	0.58
1:F:50:THR:N	1:F:55:GLU:OE1	2.34	0.58
3:D:2886:THR:HG22	3:D:2889:ARG:HH21	1.68	0.58
3:D:3262:ALA:HB3	3:D:3267:MET:HE3	1.86	0.58
3:C:162:GLU:OE1	3:C:162:GLU:N	2.36	0.58
2:N:16:PHE:CE1	2:N:29:LEU:HD23	2.38	0.58
2:P:16:PHE:CE1	2:P:29:LEU:HD23	2.38	0.58
1:F:59:GLY:HA3	1:F:77:ILE:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1253:HIS:O	3:B:1276:ARG:NH1	2.36	0.58
3:B:3406:LEU:HD11	3:B:3410:TYR:CZ	2.39	0.58
3:C:3954:PHE:HD2	3:C:4015:LEU:HD21	1.69	0.58
1:G:59:GLY:HA3	1:G:77:ILE:HD12	1.86	0.58
3:B:162:GLU:N	3:B:162:GLU:OE1	2.36	0.58
2:I:5:LEU:HD23	2:J:41:GLU:HB2	1.86	0.58
3:A:2879:LEU:HD21	3:A:2927:LEU:HD23	1.83	0.58
3:A:3406:LEU:HD11	3:A:3410:TYR:CZ	2.39	0.58
3:B:3954:PHE:HD2	3:B:4015:LEU:HD21	1.69	0.58
3:B:4185:GLU:O	3:B:4986:TYR:OH	2.20	0.58
3:A:103:LEU:HD21	3:A:106:HIS:CE1	2.39	0.58
3:A:1618:THR:HG22	3:A:1629:VAL:HG12	1.85	0.58
3:C:615:VAL:HG23	3:C:618:ASN:HB2	1.85	0.58
3:C:1427:ILE:O	3:C:1431:THR:OG1	2.17	0.58
3:D:3105:GLU:O	3:D:3109:GLU:OE1	2.21	0.58
2:K:5:LEU:HD23	2:L:41:GLU:HB2	1.86	0.58
2:L:16:PHE:CE1	2:L:29:LEU:HD23	2.38	0.58
3:B:103:LEU:HD21	3:B:106:HIS:CE1	2.39	0.58
3:B:2886:THR:HG22	3:B:2889:ARG:HH21	1.68	0.58
3:C:2213:VAL:HG11	3:C:2257:TYR:CE2	2.35	0.58
3:C:3406:LEU:HD11	3:C:3410:TYR:CZ	2.39	0.58
3:D:103:LEU:HD23	3:D:103:LEU:H	1.69	0.58
2:O:5:LEU:HD23	2:P:41:GLU:HB2	1.86	0.58
3:D:2769:PHE:O	3:D:2772:ILE:HG22	2.04	0.57
3:A:162:GLU:OE1	3:A:162:GLU:N	2.36	0.57
3:A:1857:SER:OG	3:A:1860:ASP:OD1	2.22	0.57
3:A:3105:GLU:O	3:A:3109:GLU:OE1	2.21	0.57
3:C:4689:GLN:OE1	3:C:4701:ARG:NH2	2.36	0.57
2:I:76:VAL:HG11	2:J:84:VAL:HG21	1.85	0.57
1:H:59:GLY:HA3	1:H:77:ILE:HD12	1.86	0.57
3:D:3406:LEU:HD11	3:D:3410:TYR:CZ	2.39	0.57
3:A:2886:THR:HG22	3:A:2889:ARG:HH21	1.68	0.57
3:A:3035:LYS:O	3:A:3039:MET:HE3	2.04	0.57
3:C:3353:GLU:OE1	3:C:3353:GLU:N	2.37	0.57
2:K:76:VAL:HG11	2:L:84:VAL:HG21	1.85	0.57
2:O:76:VAL:HG11	2:P:84:VAL:HG21	1.85	0.57
2:J:29:LEU:HD13	2:J:33:GLU:HB3	1.87	0.57
3:D:162:GLU:OE1	3:D:162:GLU:N	2.36	0.57
3:D:4675:LEU:HD23	3:D:4709:PHE:CE1	2.40	0.57
3:A:3353:GLU:OE1	3:A:3353:GLU:N	2.37	0.57
3:A:4741:MET:HE2	3:A:4746:LEU:HD11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2769:PHE:O	3:B:2772:ILE:HG22	2.04	0.57
3:B:4675:LEU:HD23	3:B:4709:PHE:CE1	2.40	0.57
3:D:1253:HIS:O	3:D:1276:ARG:NH1	2.36	0.57
3:D:1618:THR:HG22	3:D:1629:VAL:HG12	1.85	0.57
3:A:2769:PHE:O	3:A:2772:ILE:HG22	2.04	0.57
3:B:2213:VAL:HG11	3:B:2257:TYR:CE2	2.35	0.57
3:B:3239:GLU:OE1	3:B:3239:GLU:N	2.38	0.57
3:B:3600:VAL:HG22	3:B:3604:LEU:HD13	1.87	0.57
3:C:3515:LEU:HD21	3:C:3603:VAL:HG13	1.87	0.57
3:D:615:VAL:HG23	3:D:618:ASN:HB2	1.85	0.57
3:A:873:GLU:O	3:A:877:GLU:OE1	2.23	0.57
3:C:4675:LEU:HD23	3:C:4709:PHE:CE1	2.40	0.57
2:J:16:PHE:CE1	2:J:29:LEU:HD23	2.38	0.57
3:D:3972:ILE:HG21	3:D:3983:LEU:HD12	1.86	0.57
3:B:1857:SER:OG	3:B:1860:ASP:OD1	2.22	0.57
3:A:4675:LEU:HD23	3:A:4709:PHE:CE1	2.40	0.57
3:C:103:LEU:HD23	3:C:103:LEU:H	1.69	0.57
3:C:103:LEU:HD21	3:C:106:HIS:CE1	2.39	0.57
3:C:3262:ALA:HB3	3:C:3267:MET:HE3	1.86	0.57
3:C:3972:ILE:HG21	3:C:3983:LEU:HD12	1.86	0.57
2:N:41:GLU:HB2	2:M:5:LEU:HD23	1.86	0.57
2:P:29:LEU:HD13	2:P:33:GLU:HB3	1.87	0.57
3:A:3954:PHE:HD2	3:A:4015:LEU:HD21	1.69	0.57
3:B:3262:ALA:HB3	3:B:3267:MET:HE3	1.85	0.57
3:C:3239:GLU:OE1	3:C:3239:GLU:N	2.38	0.57
1:E:59:GLY:HA3	1:E:77:ILE:HD12	1.87	0.57
3:D:103:LEU:HD21	3:D:106:HIS:CE1	2.39	0.57
3:D:3954:PHE:HD2	3:D:4015:LEU:HD21	1.69	0.57
3:B:1618:THR:HG22	3:B:1629:VAL:HG12	1.85	0.57
3:D:3515:LEU:HD21	3:D:3603:VAL:HG13	1.87	0.57
3:A:2110:ASP:OD1	3:A:2111:PHE:N	2.38	0.57
3:A:3600:VAL:HG22	3:A:3604:LEU:HD13	1.87	0.57
3:A:3972:ILE:HG21	3:A:3983:LEU:HD12	1.86	0.57
3:C:873:GLU:O	3:C:877:GLU:OE1	2.23	0.57
3:C:3035:LYS:O	3:C:3039:MET:HE3	2.05	0.57
2:N:29:LEU:HD13	2:N:33:GLU:HB3	1.87	0.57
3:A:103:LEU:HD23	3:A:103:LEU:H	1.69	0.56
3:D:1857:SER:OG	3:D:1860:ASP:OD1	2.22	0.56
3:D:3239:GLU:OE1	3:D:3239:GLU:N	2.38	0.56
3:A:4741:MET:CE	3:A:4746:LEU:HD11	2.35	0.56
3:B:3515:LEU:HD21	3:B:3603:VAL:HG13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2769:PHE:O	3:C:2772:ILE:HG22	2.04	0.56
3:D:3353:GLU:OE1	3:D:3353:GLU:N	2.37	0.56
3:D:4741:MET:CE	3:D:4746:LEU:HD11	2.35	0.56
3:A:3239:GLU:OE1	3:A:3239:GLU:N	2.38	0.56
3:A:3262:ALA:HB3	3:A:3267:MET:HE3	1.85	0.56
3:B:552:LEU:HD22	3:B:590:LEU:HD11	1.87	0.56
3:B:2516:GLN:OE1	3:B:2573:THR:HG22	2.06	0.56
3:B:3353:GLU:N	3:B:3353:GLU:OE1	2.37	0.56
3:B:4709:PHE:HB3	3:B:4710:PRO:HD3	1.87	0.56
3:C:552:LEU:HD22	3:C:590:LEU:HD11	1.87	0.56
3:C:2260:GLU:OE2	3:C:2298:LYS:NZ	2.22	0.56
3:C:2482:LYS:O	3:C:2482:LYS:HD2	2.06	0.56
2:L:29:LEU:HD13	2:L:33:GLU:HB3	1.87	0.56
3:A:2756:ILE:HD13	3:A:2811:LYS:HG2	1.88	0.56
3:A:2921:ARG:O	3:A:2925:GLN:HG3	2.06	0.56
3:A:4824:ILE:O	3:A:4827:SER:OG	2.14	0.56
3:B:2110:ASP:OD1	3:B:2111:PHE:N	2.38	0.56
3:B:2921:ARG:O	3:B:2925:GLN:HG3	2.06	0.56
3:C:3600:VAL:HG22	3:C:3604:LEU:HD13	1.87	0.56
3:D:3600:VAL:HG22	3:D:3604:LEU:HD13	1.87	0.56
3:A:2469:GLY:O	3:A:2472:SER:OG	2.22	0.56
3:A:2482:LYS:HD2	3:A:2482:LYS:O	2.05	0.56
3:B:2756:ILE:HD13	3:B:2811:LYS:HG2	1.88	0.56
3:D:2119:ARG:NH2	3:D:3720:ASP:OD1	2.38	0.56
2:I:62:LEU:HD13	2:I:78:LEU:HD22	1.87	0.56
3:D:552:LEU:HD22	3:D:590:LEU:HD11	1.87	0.56
3:D:873:GLU:O	3:D:877:GLU:OE1	2.23	0.56
3:D:2753:ASP:HA	3:D:2756:ILE:HD12	1.88	0.56
3:D:4709:PHE:HB3	3:D:4710:PRO:HD3	1.87	0.56
3:A:2119:ARG:NH2	3:A:3720:ASP:OD1	2.38	0.56
3:B:103:LEU:HD23	3:B:103:LEU:H	1.69	0.56
3:B:2482:LYS:HD2	3:B:2482:LYS:O	2.06	0.56
2:K:62:LEU:HD13	2:K:78:LEU:HD22	1.87	0.56
3:A:1793:ALA:O	3:A:1794:THR:OG1	2.23	0.56
3:B:1252:GLU:OE1	3:B:1252:GLU:N	2.39	0.56
3:B:4899:ILE:HG13	3:B:4911:ARG:NH2	2.20	0.56
2:L:26:LYS:HD2	2:L:27:TYR:N	2.21	0.56
2:O:13:ILE:HA	2:O:16:PHE:CE1	2.41	0.56
3:D:2213:VAL:HG11	3:D:2257:TYR:CE2	2.35	0.56
3:D:2516:GLN:OE1	3:D:2573:THR:HG22	2.06	0.56
3:A:2516:GLN:OE1	3:A:2573:THR:HG22	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4185:GLU:O	3:A:4986:TYR:OH	2.20	0.56
3:C:2756:ILE:HD13	3:C:2811:LYS:HG2	1.88	0.56
3:D:1252:GLU:N	3:D:1252:GLU:OE1	2.39	0.56
3:D:2482:LYS:HD2	3:D:2482:LYS:O	2.06	0.56
3:D:4899:ILE:HG13	3:D:4911:ARG:NH2	2.20	0.56
3:C:2119:ARG:NH2	3:C:3720:ASP:OD1	2.38	0.56
3:D:2110:ASP:OD1	3:D:2111:PHE:N	2.38	0.55
3:D:2698:ARG:NH2	2:O:17:HIS:CE1	2.74	0.55
3:B:228:MET:SD	3:C:156:LYS:HG3	2.46	0.55
3:B:873:GLU:O	3:B:877:GLU:OE1	2.23	0.55
3:B:4753:GLU:N	3:B:4753:GLU:OE1	2.39	0.55
3:C:2516:GLN:OE1	3:C:2573:THR:HG22	2.06	0.55
3:C:3050:LEU:O	3:C:3054:ARG:NH1	2.40	0.55
2:L:35:LYS:O	2:L:39:GLN:OE1	2.24	0.55
2:N:35:LYS:O	2:N:39:GLN:OE1	2.24	0.55
2:P:26:LYS:HD2	2:P:27:TYR:N	2.21	0.55
3:A:964:ASN:OD1	3:A:965:GLY:N	2.39	0.55
3:A:4899:ILE:HG13	3:A:4911:ARG:NH2	2.20	0.55
3:B:653:ARG:NH1	3:B:751:LEU:O	2.40	0.55
3:B:2119:ARG:NH2	3:B:3720:ASP:OD1	2.38	0.55
3:B:2643:LYS:HD2	3:B:2699:ILE:HD12	1.88	0.55
3:B:3690:GLU:OE1	3:B:3690:GLU:N	2.39	0.55
3:C:653:ARG:NH1	3:C:751:LEU:O	2.40	0.55
3:C:2469:GLY:O	3:C:2472:SER:OG	2.22	0.55
3:C:2643:LYS:HD2	3:C:2699:ILE:HD12	1.88	0.55
3:C:4741:MET:CE	3:C:4746:LEU:HD11	2.35	0.55
2:I:17:HIS:CE1	3:A:2698:ARG:NH2	2.74	0.55
3:A:2368:ALA:CB	3:A:2380:ALA:HB2	2.36	0.55
3:A:2753:ASP:HA	3:A:2756:ILE:HD12	1.88	0.55
3:A:3447:SER:O	3:A:3453:LYS:NZ	2.38	0.55
3:B:4741:MET:CE	3:B:4746:LEU:HD11	2.35	0.55
2:K:13:ILE:HA	2:K:16:PHE:CE1	2.41	0.55
2:K:84:VAL:HG22	2:L:72:PHE:CE2	2.42	0.55
2:J:26:LYS:HD2	2:J:27:TYR:N	2.21	0.55
3:D:653:ARG:NH1	3:D:751:LEU:O	2.40	0.55
3:A:3515:LEU:HD21	3:A:3603:VAL:HG13	1.87	0.55
3:A:4709:PHE:HB3	3:A:4710:PRO:HD3	1.87	0.55
3:A:4753:GLU:OE1	3:A:4753:GLU:N	2.39	0.55
3:B:3972:ILE:HG21	3:B:3983:LEU:HD12	1.86	0.55
3:C:964:ASN:OD1	3:C:965:GLY:N	2.39	0.55
3:C:1237:THR:OG1	3:C:1609:MET:SD	2.61	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:26:LYS:HD2	2:N:27:TYR:N	2.21	0.55
2:M:62:LEU:HD13	2:M:78:LEU:HD22	1.87	0.55
3:D:2368:ALA:CB	3:D:2380:ALA:HB2	2.37	0.55
3:A:1252:GLU:N	3:A:1252:GLU:OE1	2.39	0.55
3:A:3050:LEU:O	3:A:3054:ARG:NH1	2.40	0.55
3:C:1488:LEU:HD22	3:C:1544:GLU:OE2	2.07	0.55
3:C:2110:ASP:OD1	3:C:2111:PHE:N	2.38	0.55
3:C:2753:ASP:HA	3:C:2756:ILE:HD12	1.88	0.55
3:C:2921:ARG:O	3:C:2925:GLN:HG3	2.06	0.55
3:C:4899:ILE:HG13	3:C:4911:ARG:NH2	2.20	0.55
2:P:35:LYS:O	2:P:39:GLN:OE1	2.24	0.55
3:D:2921:ARG:O	3:D:2925:GLN:HG3	2.06	0.55
3:A:65:ILE:O	3:A:112:HIS:NE2	2.39	0.55
3:B:3167:TYR:OH	3:B:3204:VAL:HG11	2.07	0.55
3:C:163:LYS:O	3:C:165:ARG:NH1	2.38	0.55
3:C:4753:GLU:OE1	3:C:4753:GLU:N	2.39	0.55
2:K:78:LEU:O	2:K:82:LEU:HD23	2.07	0.55
2:N:12:LEU:HD21	2:N:76:VAL:HG12	1.89	0.55
3:D:2756:ILE:HD13	3:D:2811:LYS:HG2	1.88	0.55
3:B:1237:THR:OG1	3:B:1609:MET:SD	2.61	0.55
3:B:2469:GLY:O	3:B:2472:SER:OG	2.22	0.55
3:C:2378:LEU:O	3:C:2382:GLU:OE1	2.25	0.55
2:L:34:LEU:O	2:L:38:LEU:HD13	2.07	0.55
2:N:72:PHE:CE2	2:M:84:VAL:HG22	2.42	0.55
2:O:62:LEU:HD13	2:O:78:LEU:HD22	1.87	0.55
2:P:34:LEU:O	2:P:38:LEU:HD13	2.07	0.55
2:I:84:VAL:HG22	2:J:72:PHE:CE2	2.42	0.55
3:D:1488:LEU:HD22	3:D:1544:GLU:OE2	2.07	0.55
3:D:4753:GLU:OE1	3:D:4753:GLU:N	2.39	0.55
3:A:552:LEU:HD22	3:A:590:LEU:HD11	1.87	0.55
3:A:652:GLY:N	3:A:659:GLN:OE1	2.39	0.55
3:A:653:ARG:NH1	3:A:751:LEU:O	2.40	0.55
3:B:923:LEU:O	3:B:926:SER:OG	2.23	0.55
3:B:964:ASN:OD1	3:B:965:GLY:N	2.39	0.55
3:B:1488:LEU:HD22	3:B:1544:GLU:OE2	2.07	0.55
3:C:4709:PHE:HB3	3:C:4710:PRO:HD3	1.87	0.55
2:O:78:LEU:O	2:O:82:LEU:HD23	2.07	0.55
2:P:12:LEU:HD21	2:P:76:VAL:HG12	1.89	0.55
2:I:13:ILE:HA	2:I:16:PHE:CE1	2.41	0.55
2:J:12:LEU:HD21	2:J:76:VAL:HG12	1.89	0.55
2:J:35:LYS:O	2:J:39:GLN:OE1	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2378:LEU:O	3:D:2382:GLU:OE1	2.25	0.55
3:D:2643:LYS:HD2	3:D:2699:ILE:HD12	1.88	0.55
2:M:78:LEU:O	2:M:82:LEU:HD23	2.07	0.55
2:I:12:LEU:O	2:I:16:PHE:CD1	2.60	0.55
3:D:981:ALA:O	3:D:984:THR:OG1	2.25	0.55
3:D:1237:THR:OG1	3:D:1609:MET:SD	2.61	0.55
3:D:2971:SER:HA	3:D:2974:PHE:CE1	2.42	0.55
3:B:2368:ALA:CB	3:B:2380:ALA:HB2	2.37	0.55
3:B:2753:ASP:HA	3:B:2756:ILE:HD12	1.88	0.55
3:D:3167:TYR:OH	3:D:3204:VAL:HG11	2.07	0.54
3:A:3690:GLU:OE1	3:A:3690:GLU:N	2.39	0.54
3:B:2378:LEU:O	3:B:2382:GLU:OE1	2.25	0.54
3:C:2698:ARG:NH2	2:M:17:HIS:CE1	2.74	0.54
3:C:3167:TYR:OH	3:C:3204:VAL:HG11	2.07	0.54
2:M:12:LEU:O	2:M:16:PHE:CD1	2.61	0.54
2:O:84:VAL:HG22	2:P:72:PHE:CE2	2.42	0.54
3:A:2213:VAL:HG11	3:A:2257:TYR:CE2	2.35	0.54
3:C:1252:GLU:OE1	3:C:1252:GLU:N	2.39	0.54
3:C:1857:SER:OG	3:C:1860:ASP:OD1	2.22	0.54
2:N:34:LEU:O	2:N:38:LEU:HD13	2.07	0.54
2:O:19:HIS:HB2	2:O:37:LEU:HD12	1.89	0.54
3:D:964:ASN:OD1	3:D:965:GLY:N	2.39	0.54
3:D:3447:SER:O	3:D:3453:LYS:NZ	2.38	0.54
3:A:2643:LYS:HD2	3:A:2699:ILE:HD12	1.88	0.54
3:B:981:ALA:O	3:B:984:THR:OG1	2.25	0.54
3:B:3050:LEU:O	3:B:3054:ARG:NH1	2.40	0.54
2:K:12:LEU:O	2:K:16:PHE:CD1	2.61	0.54
2:L:12:LEU:HD21	2:L:76:VAL:HG12	1.89	0.54
2:M:13:ILE:HA	2:M:16:PHE:CE1	2.41	0.54
1:H:7:THR:HG23	1:H:7:THR:O	2.07	0.54
3:D:2999:PHE:HA	3:D:3003:LEU:HD12	1.89	0.54
3:D:3690:GLU:OE1	3:D:3690:GLU:N	2.39	0.54
3:D:4185:GLU:O	3:D:4986:TYR:OH	2.20	0.54
3:A:1435:TYR:HB2	3:A:1519:CYS:O	2.08	0.54
3:A:1488:LEU:HD22	3:A:1544:GLU:OE2	2.07	0.54
3:C:652:GLY:N	3:C:659:GLN:OE1	2.39	0.54
3:C:2368:ALA:CB	3:C:2380:ALA:HB2	2.37	0.54
2:I:78:LEU:O	2:I:82:LEU:HD23	2.07	0.54
2:J:34:LEU:O	2:J:38:LEU:HD13	2.07	0.54
3:D:3771:SER:HA	3:D:3774:HIS:CE1	2.43	0.54
3:A:2907:VAL:HG22	3:A:2908:PRO:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3771:SER:HA	3:A:3774:HIS:CE1	2.43	0.54
3:B:3868:VAL:HG23	3:B:3870:ASN:H	1.73	0.54
3:C:3690:GLU:OE1	3:C:3690:GLU:N	2.39	0.54
2:M:19:HIS:HB2	2:M:37:LEU:HD12	1.90	0.54
3:A:2999:PHE:HA	3:A:3003:LEU:HD12	1.89	0.54
3:A:3253:GLU:O	3:A:3257:LEU:HD12	2.08	0.54
3:B:2698:ARG:NH2	2:K:17:HIS:CE1	2.74	0.54
3:B:2999:PHE:HA	3:B:3003:LEU:HD12	1.89	0.54
3:B:3771:SER:HA	3:B:3774:HIS:CE1	2.43	0.54
3:B:5032:ASP:OD2	3:B:5033:GLN:N	2.41	0.54
3:C:3262:ALA:HB3	3:C:3267:MET:CE	2.38	0.54
3:D:5032:ASP:OD2	3:D:5033:GLN:N	2.41	0.54
3:B:65:ILE:O	3:B:112:HIS:NE2	2.39	0.54
3:C:623:THR:HG23	3:C:627:LEU:HD12	1.90	0.54
3:C:2907:VAL:HG22	3:C:2908:PRO:HD2	1.89	0.54
3:C:2971:SER:HA	3:C:2974:PHE:CE1	2.42	0.54
3:C:2999:PHE:HA	3:C:3003:LEU:HD12	1.89	0.54
3:D:623:THR:HG23	3:D:627:LEU:HD12	1.90	0.54
3:A:2378:LEU:O	3:A:2382:GLU:OE1	2.25	0.54
3:A:3167:TYR:OH	3:A:3204:VAL:HG11	2.07	0.54
2:O:12:LEU:O	2:O:16:PHE:CD1	2.60	0.54
3:D:3050:LEU:O	3:D:3054:ARG:NH1	2.40	0.54
3:B:1435:TYR:HB2	3:B:1519:CYS:O	2.08	0.54
3:C:1435:TYR:HB2	3:C:1519:CYS:O	2.08	0.54
3:C:5032:ASP:OD2	3:C:5033:GLN:N	2.41	0.54
2:I:19:HIS:HB2	2:I:37:LEU:HD12	1.89	0.54
3:A:2971:SER:HA	3:A:2974:PHE:CE1	2.42	0.54
3:B:446:LEU:HD23	3:B:526:LEU:HD22	1.90	0.54
3:B:1025:TYR:CD1	3:B:1028:LEU:HD12	2.43	0.54
3:B:2348:GLU:OE2	3:B:2352:ASN:ND2	2.41	0.54
3:C:976:VAL:O	3:C:977:ARG:NE	2.41	0.54
3:D:1435:TYR:HB2	3:D:1519:CYS:O	2.08	0.53
3:D:2907:VAL:HG22	3:D:2908:PRO:HD2	1.89	0.53
3:D:3065:VAL:O	3:D:3069:LEU:HD23	2.08	0.53
3:A:976:VAL:O	3:A:977:ARG:NE	2.41	0.53
3:A:994:HIS:CD2	3:A:1028:LEU:HD11	2.43	0.53
3:B:2907:VAL:HG22	3:B:2908:PRO:HD2	1.89	0.53
3:C:3868:VAL:HG23	3:C:3870:ASN:H	1.73	0.53
2:L:5:LEU:HD23	2:L:9:MET:HE1	1.91	0.53
2:I:28:LYS:NZ	2:I:71:ASP:OD1	2.42	0.53
3:D:156:LYS:HG3	3:C:228:MET:SD	2.46	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:5032:ASP:OD2	3:A:5033:GLN:N	2.41	0.53
3:B:976:VAL:O	3:B:977:ARG:NE	2.41	0.53
3:B:3262:ALA:HB3	3:B:3267:MET:CE	2.38	0.53
3:C:3065:VAL:O	3:C:3069:LEU:HD23	2.08	0.53
3:D:994:HIS:CD2	3:D:1028:LEU:HD11	2.43	0.53
3:A:2925:GLN:OE1	3:A:2929:LYS:HE2	2.08	0.53
3:B:2971:SER:HA	3:B:2974:PHE:CE1	2.42	0.53
3:B:3253:GLU:O	3:B:3257:LEU:HD12	2.08	0.53
3:C:4824:ILE:O	3:C:4827:SER:OG	2.14	0.53
3:D:3262:ALA:HB3	3:D:3267:MET:CE	2.38	0.53
3:A:1025:TYR:CD1	3:A:1028:LEU:HD12	2.43	0.53
3:B:994:HIS:CD2	3:B:1028:LEU:HD11	2.43	0.53
3:B:2925:GLN:OE1	3:B:2929:LYS:HE2	2.08	0.53
3:C:994:HIS:CD2	3:C:1028:LEU:HD11	2.43	0.53
3:C:3055:VAL:HG21	3:C:3135:VAL:HG11	1.90	0.53
2:J:16:PHE:HE1	2:J:29:LEU:HD23	1.74	0.53
3:D:2925:GLN:OE1	3:D:2929:LYS:HE2	2.08	0.53
3:B:4074:ILE:O	3:B:4077:SER:OG	2.06	0.53
3:C:1025:TYR:CD1	3:C:1028:LEU:HD12	2.43	0.53
2:L:16:PHE:HE1	2:L:29:LEU:HD23	1.74	0.53
3:D:3868:VAL:HG23	3:D:3870:ASN:H	1.73	0.53
3:A:3065:VAL:O	3:A:3069:LEU:HD23	2.08	0.53
3:B:163:LYS:O	3:B:165:ARG:NH1	2.38	0.53
3:D:1558:THR:HG22	3:D:1558:THR:O	2.09	0.53
3:D:3055:VAL:HG21	3:D:3135:VAL:HG11	1.90	0.53
3:D:4883:PHE:CE1	3:D:4887:VAL:HG21	2.44	0.53
3:A:4225:VAL:HG11	3:A:4948:VAL:HA	1.91	0.53
3:B:3447:SER:O	3:B:3453:LYS:NZ	2.38	0.53
2:P:16:PHE:HE1	2:P:29:LEU:HD23	1.74	0.53
2:J:5:LEU:HD23	2:J:9:MET:HE1	1.90	0.53
3:D:976:VAL:O	3:D:977:ARG:NE	2.41	0.53
3:D:1025:TYR:CD1	3:D:1028:LEU:HD12	2.43	0.53
3:A:3868:VAL:HG23	3:A:3870:ASN:H	1.73	0.53
3:B:3065:VAL:O	3:B:3069:LEU:HD23	2.08	0.53
3:C:496:ASN:OD1	3:C:554:ARG:NE	2.42	0.53
3:C:3253:GLU:O	3:C:3257:LEU:HD12	2.08	0.53
3:C:4883:PHE:CE1	3:C:4887:VAL:HG21	2.44	0.53
3:A:4883:PHE:CE1	3:A:4887:VAL:HG21	2.44	0.53
3:C:1558:THR:O	3:C:1558:THR:HG22	2.09	0.53
3:C:3661:SER:HG	3:C:3662:TRP:HD1	1.55	0.53
3:C:3771:SER:HA	3:C:3774:HIS:CE1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:4796:MET:HE1	8:C:5101:PCW:H222	1.91	0.53
2:N:16:PHE:HE1	2:N:29:LEU:HD23	1.74	0.53
3:B:3763:LYS:O	3:B:3767:LEU:HD13	2.09	0.53
3:C:1083:ALA:HB2	3:C:1190:LEU:HD11	1.91	0.53
3:A:623:THR:HG23	3:A:627:LEU:HD12	1.90	0.52
3:A:1758:GLY:N	3:A:1759:PRO:CD	2.72	0.52
3:A:3079:ARG:NE	3:A:3156:ASP:OD2	2.36	0.52
3:A:3142:THR:HG23	3:A:3197:ARG:HG3	1.92	0.52
3:A:3262:ALA:HB3	3:A:3267:MET:CE	2.38	0.52
3:B:623:THR:HG23	3:B:627:LEU:HD12	1.90	0.52
3:B:4883:PHE:CE1	3:B:4887:VAL:HG21	2.44	0.52
3:C:2925:GLN:OE1	3:C:2929:LYS:HE2	2.08	0.52
3:C:3763:LYS:O	3:C:3767:LEU:HD13	2.09	0.52
2:K:19:HIS:HB2	2:K:37:LEU:HD12	1.90	0.52
2:P:36:ASP:O	2:P:40:THR:HG23	2.09	0.52
3:D:65:ILE:O	3:D:112:HIS:NE2	2.39	0.52
3:A:446:LEU:HD23	3:A:526:LEU:HD22	1.90	0.52
3:A:3055:VAL:HG21	3:A:3135:VAL:HG11	1.90	0.52
3:B:1758:GLY:N	3:B:1759:PRO:CD	2.72	0.52
3:B:2910:ASP:OD1	3:B:2911:THR:N	2.43	0.52
3:B:3055:VAL:HG21	3:B:3135:VAL:HG11	1.90	0.52
3:C:65:ILE:O	3:C:112:HIS:NE2	2.39	0.52
3:C:546:ASP:OD1	3:C:583:HIS:NE2	2.39	0.52
2:O:28:LYS:NZ	2:O:71:ASP:OD1	2.42	0.52
3:D:1083:ALA:HB2	3:D:1190:LEU:HD11	1.91	0.52
3:D:3142:THR:HG23	3:D:3197:ARG:HG3	1.91	0.52
3:A:3763:LYS:O	3:A:3767:LEU:HD13	2.09	0.52
3:A:4745:SER:O	3:A:4749:THR:HG23	2.10	0.52
3:B:3142:THR:HG23	3:B:3197:ARG:HG3	1.91	0.52
1:E:80:ASP:OD2	1:E:81:TYR:N	2.43	0.52
3:D:2348:GLU:OE2	3:D:2352:ASN:ND2	2.41	0.52
3:D:3253:GLU:O	3:D:3257:LEU:HD12	2.08	0.52
3:C:3142:THR:HG23	3:C:3197:ARG:HG3	1.91	0.52
2:L:36:ASP:O	2:L:40:THR:HG23	2.09	0.52
1:G:7:THR:O	1:G:7:THR:HG23	2.09	0.52
3:D:1758:GLY:N	3:D:1759:PRO:CD	2.72	0.52
3:D:3763:LYS:O	3:D:3767:LEU:HD13	2.09	0.52
3:B:1558:THR:HG22	3:B:1558:THR:O	2.09	0.52
3:C:545:LEU:HD21	3:C:579:ILE:HD13	1.91	0.52
3:C:1758:GLY:N	3:C:1759:PRO:CD	2.72	0.52
3:C:2910:ASP:OD1	3:C:2911:THR:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:446:LEU:HD23	3:D:526:LEU:HD22	1.90	0.52
3:D:2910:ASP:OD1	3:D:2911:THR:N	2.43	0.52
3:A:1558:THR:O	3:A:1558:THR:HG22	2.09	0.52
3:A:2156:LEU:HD21	3:A:2199:MET:CE	2.40	0.52
3:B:4225:VAL:HG11	3:B:4948:VAL:HA	1.91	0.52
3:B:4745:SER:O	3:B:4749:THR:HG23	2.10	0.52
3:D:1793:ALA:O	3:D:1794:THR:OG1	2.23	0.52
3:D:3972:ILE:CG2	3:D:3983:LEU:HD12	2.40	0.52
3:A:1927:LEU:HD13	3:A:1940:MET:HE1	1.92	0.52
3:C:1793:ALA:O	3:C:1794:THR:OG1	2.23	0.52
2:K:28:LYS:NZ	2:K:71:ASP:OD1	2.42	0.52
3:D:2156:LEU:HD21	3:D:2199:MET:CE	2.40	0.52
3:A:875:LEU:HD11	3:A:1047:LEU:CD2	2.29	0.52
3:D:3576:LEU:HD21	3:A:1220:LEU:HD22	1.92	0.52
3:A:545:LEU:HD21	3:A:579:ILE:HD13	1.91	0.52
3:C:682:HIS:H	3:C:785:SER:HG	1.58	0.52
3:D:496:ASN:OD1	3:D:554:ARG:NE	2.42	0.52
3:D:985:LEU:O	3:D:989:LEU:HG	2.10	0.52
3:C:1985:PHE:CZ	2:M:92:GLU:OE2	2.63	0.52
2:M:28:LYS:NZ	2:M:71:ASP:OD1	2.42	0.52
3:D:228:MET:SD	3:A:156:LYS:HG3	2.50	0.51
3:D:979:THR:O	3:D:983:THR:HG23	2.11	0.51
3:D:2469:GLY:O	3:D:2472:SER:OG	2.22	0.51
3:B:496:ASN:OD1	3:B:554:ARG:NE	2.42	0.51
3:B:1083:ALA:HB2	3:B:1190:LEU:HD11	1.91	0.51
3:C:3447:SER:O	3:C:3453:LYS:NZ	2.38	0.51
3:C:3972:ILE:CG2	3:C:3983:LEU:HD12	2.40	0.51
2:N:36:ASP:O	2:N:40:THR:HG23	2.09	0.51
3:A:496:ASN:OD1	3:A:554:ARG:NE	2.42	0.51
3:B:1562:VAL:HG12	3:B:1563:VAL:HG13	1.93	0.51
3:C:981:ALA:O	3:C:984:THR:OG1	2.25	0.51
3:C:985:LEU:O	3:C:989:LEU:HG	2.10	0.51
3:C:1562:VAL:HG12	3:C:1563:VAL:HG13	1.93	0.51
3:D:545:LEU:HD21	3:D:579:ILE:HD13	1.91	0.51
3:D:1737:VAL:HG11	3:D:1960:ALA:CB	2.40	0.51
3:D:2824:VAL:HG12	3:D:2938:VAL:HB	1.92	0.51
3:D:4745:SER:O	3:D:4749:THR:HG23	2.10	0.51
3:A:979:THR:O	3:A:983:THR:HG23	2.11	0.51
3:A:985:LEU:O	3:A:989:LEU:HG	2.10	0.51
3:A:2910:ASP:OD1	3:A:2911:THR:N	2.43	0.51
3:A:3220:TYR:CE1	3:A:3237:VAL:HG22	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3837:ALA:O	3:A:3841:THR:HG23	2.11	0.51
3:B:545:LEU:HD21	3:B:579:ILE:HD13	1.91	0.51
3:B:2156:LEU:HD21	3:B:2199:MET:CE	2.40	0.51
3:C:4225:VAL:HG11	3:C:4948:VAL:HA	1.91	0.51
3:D:3079:ARG:NE	3:D:3156:ASP:OD2	2.36	0.51
3:A:1699:LEU:O	3:A:1816:MET:HE1	2.11	0.51
3:A:1737:VAL:HG11	3:A:1960:ALA:CB	2.40	0.51
3:A:3374:VAL:O	3:A:3378:GLU:OE1	2.29	0.51
3:A:4675:LEU:HD23	3:A:4709:PHE:HE1	1.76	0.51
3:B:546:ASP:OD1	3:B:583:HIS:NE2	2.39	0.51
3:B:3861:MET:HB2	3:B:3868:VAL:HG21	1.93	0.51
3:C:446:LEU:HD23	3:C:526:LEU:HD22	1.90	0.51
3:C:979:THR:O	3:C:983:THR:HG23	2.11	0.51
2:I:92:GLU:OE2	3:A:1985:PHE:CZ	2.63	0.51
3:D:4225:VAL:HG11	3:D:4948:VAL:HA	1.91	0.51
3:D:4675:LEU:HD23	3:D:4709:PHE:HE1	1.76	0.51
3:A:2177:ASN:O	3:A:2181:GLN:OE1	2.29	0.51
3:B:664:TYR:OH	3:B:666:GLU:OE2	2.27	0.51
3:B:3943:LYS:O	3:B:4005:LYS:NZ	2.34	0.51
3:C:2156:LEU:HD21	3:C:2199:MET:CE	2.40	0.51
3:C:2177:ASN:O	3:C:2181:GLN:OE1	2.29	0.51
3:D:3374:VAL:O	3:D:3378:GLU:OE1	2.29	0.51
3:D:3837:ALA:O	3:D:3841:THR:HG23	2.11	0.51
3:D:4824:ILE:O	3:D:4827:SER:OG	2.14	0.51
3:A:1083:ALA:HB2	3:A:1190:LEU:HD11	1.91	0.51
3:B:1737:VAL:HG11	3:B:1960:ALA:CB	2.40	0.51
3:B:2103:VAL:HG13	3:B:2121:MET:HB2	1.93	0.51
3:B:3227:GLU:O	3:B:3228:ARG:HG2	2.11	0.51
3:A:1562:VAL:HG12	3:A:1563:VAL:HG13	1.93	0.51
3:B:3276:PRO:HA	3:B:3279:CYS:SG	2.51	0.51
3:C:2348:GLU:OE2	3:C:2352:ASN:ND2	2.41	0.51
3:C:4745:SER:O	3:C:4749:THR:HG23	2.10	0.51
2:L:16:PHE:CG	2:L:75:TYR:OH	2.60	0.51
2:M:62:LEU:HD13	2:M:78:LEU:CD2	2.41	0.51
2:O:76:VAL:HG21	2:P:84:VAL:HG21	1.93	0.51
2:J:36:ASP:O	2:J:40:THR:HG23	2.09	0.51
3:A:3227:GLU:O	3:A:3228:ARG:HG2	2.11	0.51
3:A:3276:PRO:HA	3:A:3279:CYS:SG	2.51	0.51
3:A:3861:MET:HB2	3:A:3868:VAL:HG21	1.93	0.51
3:B:872:ARG:HE	3:B:927:GLY:HA3	1.76	0.51
3:B:985:LEU:O	3:B:989:LEU:HG	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1985:PHE:CZ	2:K:92:GLU:OE2	2.63	0.51
3:D:3227:GLU:O	3:D:3228:ARG:HG2	2.11	0.51
3:B:3972:ILE:CG2	3:B:3983:LEU:HD12	2.40	0.51
3:C:2103:VAL:HG13	3:C:2121:MET:HB2	1.93	0.51
3:C:2824:VAL:HG12	3:C:2938:VAL:HB	1.92	0.51
2:I:76:VAL:HG21	2:J:84:VAL:HG21	1.93	0.50
1:G:80:ASP:OD2	1:G:81:TYR:N	2.44	0.50
3:D:3661:SER:HG	3:D:3662:TRP:HD1	1.57	0.50
3:A:228:MET:SD	3:B:156:LYS:HG3	2.49	0.50
3:A:981:ALA:O	3:A:984:THR:OG1	2.25	0.50
3:A:2677:ARG:NH2	3:A:2715:TYR:O	2.45	0.50
3:B:652:GLY:N	3:B:659:GLN:OE1	2.39	0.50
3:B:2677:ARG:NH2	3:B:2715:TYR:O	2.45	0.50
3:B:3220:TYR:CE1	3:B:3237:VAL:HG22	2.46	0.50
3:B:3837:ALA:O	3:B:3841:THR:HG23	2.11	0.50
3:C:872:ARG:HE	3:C:927:GLY:HA3	1.76	0.50
3:C:1737:VAL:HG13	3:C:1737:VAL:O	2.12	0.50
3:C:2677:ARG:NH2	3:C:2715:TYR:O	2.45	0.50
2:K:62:LEU:HD13	2:K:78:LEU:CD2	2.41	0.50
2:O:62:LEU:HD13	2:O:78:LEU:CD2	2.41	0.50
1:G:50:THR:N	1:G:55:GLU:OE2	2.39	0.50
3:D:872:ARG:HE	3:D:927:GLY:HA3	1.76	0.50
3:D:1562:VAL:HG12	3:D:1563:VAL:HG13	1.93	0.50
3:D:2177:ASN:O	3:D:2181:GLN:OE1	2.29	0.50
3:D:3278:LEU:O	3:D:3282:LEU:HD23	2.11	0.50
3:A:2348:GLU:OE2	3:A:2352:ASN:ND2	2.41	0.50
3:A:3278:LEU:O	3:A:3282:LEU:HD23	2.11	0.50
3:B:3374:VAL:O	3:B:3378:GLU:OE1	2.29	0.50
3:C:923:LEU:O	3:C:926:SER:OG	2.23	0.50
3:C:3220:TYR:CE1	3:C:3237:VAL:HG22	2.46	0.50
1:E:7:THR:HG23	1:E:7:THR:O	2.12	0.50
3:D:652:GLY:N	3:D:659:GLN:OE1	2.39	0.50
3:A:872:ARG:HE	3:A:927:GLY:HA3	1.76	0.50
3:A:1737:VAL:O	3:A:1737:VAL:HG13	2.12	0.50
3:B:2177:ASN:O	3:B:2181:GLN:OE1	2.29	0.50
3:C:1189:PHE:C	3:C:1190:LEU:HD12	2.32	0.50
3:C:3276:PRO:HA	3:C:3279:CYS:SG	2.51	0.50
1:H:80:ASP:OD2	1:H:81:TYR:N	2.44	0.50
3:A:923:LEU:O	3:A:926:SER:OG	2.23	0.50
3:A:1572:ASN:O	3:A:1573:ILE:HD13	2.12	0.50
3:B:1427:ILE:O	3:B:1431:THR:OG1	2.17	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3227:GLU:O	3:C:3228:ARG:HG2	2.11	0.50
3:C:3278:LEU:O	3:C:3282:LEU:HD23	2.11	0.50
3:D:1927:LEU:HD13	3:D:1940:MET:HE1	1.94	0.50
3:A:1189:PHE:C	3:A:1190:LEU:HD12	2.32	0.50
3:A:3972:ILE:CG2	3:A:3983:LEU:HD12	2.40	0.50
3:C:1927:LEU:HD13	3:C:1940:MET:HE1	1.93	0.50
3:C:3374:VAL:O	3:C:3378:GLU:OE1	2.29	0.50
3:C:3837:ALA:O	3:C:3841:THR:HG23	2.10	0.50
3:D:1985:PHE:CZ	2:O:92:GLU:OE2	2.63	0.50
3:D:3220:TYR:CE1	3:D:3237:VAL:HG22	2.46	0.50
3:B:1572:ASN:O	3:B:1573:ILE:HD13	2.12	0.50
3:B:1927:LEU:HD13	3:B:1940:MET:HE1	1.94	0.50
3:B:2824:VAL:HG12	3:B:2938:VAL:HB	1.92	0.50
3:B:3104:ILE:O	3:B:3108:VAL:HG23	2.12	0.50
3:C:1737:VAL:HG11	3:C:1960:ALA:CB	2.40	0.50
3:C:3861:MET:HB2	3:C:3868:VAL:HG21	1.93	0.50
2:I:62:LEU:HD13	2:I:78:LEU:CD2	2.41	0.50
3:D:546:ASP:OD1	3:D:583:HIS:NE2	2.39	0.50
3:D:3276:PRO:HA	3:D:3279:CYS:SG	2.51	0.50
3:D:3717:LEU:HD21	3:D:3785:MET:CE	2.42	0.50
3:B:784:PHE:CB	3:B:788:ILE:HD13	2.42	0.50
3:B:979:THR:O	3:B:983:THR:HG23	2.11	0.50
3:B:3278:LEU:O	3:B:3282:LEU:HD23	2.11	0.50
3:D:1189:PHE:C	3:D:1190:LEU:HD12	2.32	0.50
3:D:1572:ASN:O	3:D:1573:ILE:HD13	2.12	0.50
3:D:1699:LEU:O	3:D:1816:MET:HE1	2.12	0.50
3:D:2103:VAL:HG13	3:D:2121:MET:HB2	1.93	0.50
3:D:2677:ARG:NH2	3:D:2715:TYR:O	2.45	0.50
3:D:3861:MET:HB2	3:D:3868:VAL:HG21	1.93	0.50
3:B:1189:PHE:C	3:B:1190:LEU:HD12	2.32	0.50
3:B:3894:LEU:HB3	3:B:3902:PHE:CE2	2.47	0.50
3:C:2249:ARG:CD	3:C:2287:LEU:HD21	2.42	0.50
3:C:3104:ILE:O	3:C:3108:VAL:HG23	2.12	0.50
2:K:76:VAL:HA	2:K:79:VAL:HG22	1.94	0.50
1:F:80:ASP:OD2	1:F:81:TYR:N	2.44	0.50
3:D:923:LEU:O	3:D:926:SER:OG	2.23	0.50
3:D:3894:LEU:HB3	3:D:3902:PHE:CE2	2.47	0.50
3:A:546:ASP:OD1	3:A:583:HIS:NE2	2.39	0.50
2:M:76:VAL:HA	2:M:79:VAL:HG22	1.94	0.50
2:O:84:VAL:HG22	2:P:72:PHE:HD2	1.77	0.50
3:A:784:PHE:CB	3:A:788:ILE:HD13	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2117:LEU:O	3:A:2121:MET:HG2	2.12	0.49
3:A:2668:THR:HG21	3:A:2673:LEU:HD21	1.94	0.49
3:B:3717:LEU:HD21	3:B:3785:MET:CE	2.42	0.49
3:C:784:PHE:CB	3:C:788:ILE:HD13	2.42	0.49
3:C:2918:ALA:O	3:C:2922:GLU:OE1	2.30	0.49
3:C:4675:LEU:HD23	3:C:4709:PHE:HE1	1.76	0.49
2:K:76:VAL:HG21	2:L:84:VAL:HG21	1.93	0.49
2:O:76:VAL:HA	2:O:79:VAL:HG22	1.94	0.49
2:J:51:ASP:O	2:J:55:VAL:HG23	2.12	0.49
3:D:2117:LEU:O	3:D:2121:MET:HG2	2.12	0.49
3:A:1427:ILE:O	3:A:1431:THR:OG1	2.17	0.49
3:A:2249:ARG:CD	3:A:2287:LEU:HD21	2.42	0.49
3:A:2824:VAL:HG12	3:A:2938:VAL:HB	1.92	0.49
3:B:2249:ARG:CD	3:B:2287:LEU:HD21	2.42	0.49
3:C:2594:ARG:O	3:C:2595:SER:OG	2.25	0.49
3:C:3183:TYR:O	3:C:3187:LEU:HD23	2.12	0.49
2:N:51:ASP:O	2:N:55:VAL:HG23	2.12	0.49
1:F:7:THR:HG23	1:F:7:THR:O	2.12	0.49
3:A:3894:LEU:HB3	3:A:3902:PHE:CE2	2.47	0.49
3:B:2199:MET:SD	3:B:2204:MET:HE1	2.52	0.49
3:A:510:GLU:N	3:A:510:GLU:OE2	2.44	0.49
3:A:2103:VAL:HG13	3:A:2121:MET:HB2	1.93	0.49
3:C:2199:MET:SD	3:C:2204:MET:HE1	2.52	0.49
2:N:84:VAL:HG21	2:M:76:VAL:HG21	1.93	0.49
3:D:784:PHE:CB	3:D:788:ILE:HD13	2.42	0.49
3:D:3847:LEU:CD2	3:D:3936:PHE:HD1	2.26	0.49
3:B:2918:ALA:O	3:B:2922:GLU:OE1	2.30	0.49
3:B:4675:LEU:HD23	3:B:4709:PHE:HE1	1.76	0.49
3:C:1572:ASN:O	3:C:1573:ILE:HD13	2.12	0.49
3:C:3847:LEU:CD2	3:C:3936:PHE:HD1	2.26	0.49
2:I:76:VAL:HA	2:I:79:VAL:HG22	1.94	0.49
2:I:84:VAL:HG22	2:J:72:PHE:HD2	1.77	0.49
3:D:3183:TYR:O	3:D:3187:LEU:HD23	2.13	0.49
3:A:664:TYR:OH	3:A:666:GLU:OE2	2.27	0.49
3:A:3183:TYR:O	3:A:3187:LEU:HD23	2.13	0.49
3:B:2166:LEU:HD21	3:B:2178:LEU:HD23	1.95	0.49
3:B:4684:LEU:HD23	3:B:4685:TYR:CE1	2.48	0.49
3:C:3394:LEU:O	3:C:3398:GLU:OE1	2.30	0.49
3:D:3141:LEU:HD11	3:D:3145:PHE:CZ	2.48	0.49
3:A:163:LYS:O	3:A:165:ARG:NH1	2.37	0.49
3:A:3394:LEU:O	3:A:3398:GLU:OE1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:318:ARG:NH2	3:B:322:GLU:O	2.46	0.49
1:E:50:THR:N	1:E:55:GLU:OE2	2.39	0.49
1:H:50:THR:N	1:H:55:GLU:OE2	2.38	0.49
3:D:1737:VAL:O	3:D:1737:VAL:HG13	2.12	0.49
3:D:2249:ARG:CD	3:D:2287:LEU:HD21	2.42	0.49
3:D:2393:ARG:O	3:D:2419:LEU:HD12	2.13	0.49
3:D:3394:LEU:O	3:D:3398:GLU:OE1	2.30	0.49
3:A:1481:GLN:OE1	3:A:1481:GLN:N	2.46	0.49
3:A:2393:ARG:O	3:A:2419:LEU:HD12	2.13	0.49
3:A:4684:LEU:HD23	3:A:4685:TYR:CE1	2.48	0.49
3:B:3394:LEU:O	3:B:3398:GLU:OE1	2.30	0.49
3:B:4886:TYR:HA	3:C:4916:ILE:HD11	1.95	0.49
3:C:3717:LEU:HD21	3:C:3785:MET:CE	2.42	0.49
3:C:3894:LEU:HB3	3:C:3902:PHE:CE2	2.47	0.49
2:P:51:ASP:O	2:P:55:VAL:HG23	2.12	0.49
3:D:102:LEU:HD23	3:D:102:LEU:H	1.78	0.49
3:A:3104:ILE:O	3:A:3108:VAL:HG23	2.12	0.49
3:B:942:MET:HG2	3:B:942:MET:O	2.13	0.49
3:B:1481:GLN:N	3:B:1481:GLN:OE1	2.46	0.49
3:B:1737:VAL:HG13	3:B:1737:VAL:O	2.12	0.49
3:C:684:ARG:NH1	3:C:708:VAL:O	2.43	0.49
3:C:1481:GLN:OE1	3:C:1481:GLN:N	2.46	0.49
3:C:3079:ARG:NE	3:C:3156:ASP:OD2	2.36	0.49
2:I:37:LEU:O	2:I:41:GLU:HG2	2.13	0.49
2:J:72:PHE:O	2:J:76:VAL:HG13	2.13	0.49
1:F:6:GLU:N	1:F:6:GLU:OE2	2.46	0.49
3:D:510:GLU:OE2	3:D:510:GLU:N	2.44	0.49
3:D:2668:THR:HG21	3:D:2673:LEU:HD21	1.95	0.49
3:D:3104:ILE:O	3:D:3108:VAL:HG23	2.12	0.49
3:A:3717:LEU:HD21	3:A:3785:MET:CE	2.42	0.49
3:A:3847:LEU:CD2	3:A:3936:PHE:HD1	2.26	0.49
3:A:4122:GLU:OE1	3:A:4122:GLU:N	2.44	0.49
3:B:3183:TYR:O	3:B:3187:LEU:HD23	2.12	0.49
3:B:3847:LEU:CD2	3:B:3936:PHE:HD1	2.26	0.49
3:B:3873:ASN:OD1	3:B:3874:GLY:N	2.46	0.49
3:C:2166:LEU:HD21	3:C:2178:LEU:HD23	1.95	0.49
2:M:37:LEU:O	2:M:41:GLU:HG2	2.13	0.49
3:D:3344:GLN:OE1	3:D:3415:ARG:NH2	2.46	0.48
3:D:3873:ASN:OD1	3:D:3874:GLY:N	2.46	0.48
3:A:1237:THR:OG1	3:A:1609:MET:SD	2.61	0.48
3:A:3344:GLN:OE1	3:A:3415:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2668:THR:HG21	3:B:2673:LEU:HD21	1.95	0.48
3:C:102:LEU:HD23	3:C:102:LEU:H	1.78	0.48
3:C:664:TYR:OH	3:C:666:GLU:OE2	2.27	0.48
3:C:3141:LEU:HD11	3:C:3145:PHE:CZ	2.48	0.48
3:C:3344:GLN:OE1	3:C:3415:ARG:NH2	2.46	0.48
3:C:3873:ASN:OD1	3:C:3874:GLY:N	2.46	0.48
2:L:51:ASP:O	2:L:55:VAL:HG23	2.12	0.48
2:N:72:PHE:HD2	2:M:84:VAL:HG22	1.77	0.48
3:A:942:MET:O	3:A:942:MET:HG2	2.13	0.48
3:A:2166:LEU:HD21	3:A:2178:LEU:HD23	1.94	0.48
3:B:510:GLU:N	3:B:510:GLU:OE2	2.44	0.48
3:D:3865:ASP:OD1	3:D:3866:GLY:N	2.46	0.48
3:A:318:ARG:NH2	3:A:322:GLU:O	2.46	0.48
3:A:3141:LEU:HD11	3:A:3145:PHE:CZ	2.48	0.48
3:B:2523:LEU:HD22	3:B:2579:MET:SD	2.54	0.48
3:B:3344:GLN:OE1	3:B:3415:ARG:NH2	2.46	0.48
3:D:1481:GLN:OE1	3:D:1481:GLN:N	2.46	0.48
3:D:2166:LEU:HD21	3:D:2178:LEU:HD23	1.95	0.48
3:A:578:ILE:O	3:A:580:GLN:NE2	2.47	0.48
3:A:4902:PRO:HB3	3:A:4911:ARG:HD3	1.96	0.48
3:B:102:LEU:HD23	3:B:102:LEU:H	1.78	0.48
3:B:3141:LEU:HD11	3:B:3145:PHE:CZ	2.48	0.48
3:C:942:MET:O	3:C:942:MET:HG2	2.13	0.48
3:C:2739:ARG:O	3:C:2885:ASN:ND2	2.47	0.48
3:C:4684:LEU:HD23	3:C:4685:TYR:CE1	2.48	0.48
2:P:72:PHE:O	2:P:76:VAL:HG13	2.13	0.48
3:A:2523:LEU:HD22	3:A:2579:MET:SD	2.54	0.48
3:B:3253:GLU:O	3:B:3256:GLY:N	2.47	0.48
3:C:2117:LEU:O	3:C:2121:MET:HG2	2.12	0.48
2:N:72:PHE:O	2:N:76:VAL:HG13	2.13	0.48
2:M:30:SER:N	2:M:69:GLU:OE2	2.47	0.48
2:P:86:CYS:SG	2:P:87:ASN:N	2.87	0.48
3:D:2739:ARG:O	3:D:2885:ASN:ND2	2.47	0.48
3:D:2918:ALA:O	3:D:2922:GLU:OE1	2.30	0.48
3:A:1067:GLN:OE1	3:A:1072:ARG:NH2	2.47	0.48
3:A:2206:GLU:OE1	3:A:2206:GLU:N	2.46	0.48
3:C:4900:GLU:O	3:C:4911:ARG:CZ	2.62	0.48
2:M:7:SER:O	2:M:11:THR:HG23	2.14	0.48
2:O:37:LEU:O	2:O:41:GLU:HG2	2.13	0.48
3:D:942:MET:HG2	3:D:942:MET:O	2.13	0.48
3:A:2918:ALA:O	3:A:2922:GLU:OE1	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1067:GLN:OE1	3:B:1072:ARG:NH2	2.47	0.48
3:B:2362:PRO:O	3:B:2370:ARG:NH1	2.47	0.48
2:I:30:SER:N	2:I:69:GLU:OE2	2.47	0.48
3:A:569:LEU:HD12	3:A:603:VAL:HG13	1.96	0.48
3:A:2362:PRO:O	3:A:2370:ARG:NH1	2.47	0.48
3:A:3865:ASP:OD1	3:A:3866:GLY:N	2.46	0.48
3:B:578:ILE:O	3:B:580:GLN:NE2	2.47	0.48
3:B:2117:LEU:O	3:B:2121:MET:HG2	2.12	0.48
3:B:2739:ARG:O	3:B:2885:ASN:ND2	2.47	0.48
3:B:3079:ARG:NE	3:B:3156:ASP:OD2	2.36	0.48
3:B:3182:PRO:O	3:B:3185:GLU:HG3	2.14	0.48
3:B:4796:MET:HE1	8:B:8007:PCW:H222	1.95	0.48
3:C:2523:LEU:HD22	3:C:2579:MET:SD	2.54	0.48
3:C:2668:THR:HG21	3:C:2673:LEU:HD21	1.95	0.48
3:C:3253:GLU:O	3:C:3256:GLY:N	2.47	0.48
2:K:7:SER:O	2:K:11:THR:HG23	2.14	0.48
2:K:37:LEU:O	2:K:41:GLU:HG2	2.13	0.48
2:J:42:LEU:CD2	2:J:46:LEU:HB2	2.44	0.48
3:D:875:LEU:HD11	3:D:1047:LEU:CD2	2.29	0.48
3:D:2362:PRO:O	3:D:2370:ARG:NH1	2.47	0.48
3:D:4684:LEU:HD23	3:D:4685:TYR:CE1	2.48	0.48
3:D:4916:ILE:HD11	3:C:4886:TYR:HA	1.95	0.48
3:A:3253:GLU:O	3:A:3256:GLY:N	2.47	0.48
3:B:1758:GLY:N	3:B:1759:PRO:HD2	2.29	0.48
3:B:3865:ASP:OD1	3:B:3866:GLY:N	2.46	0.48
3:B:4902:PRO:HB3	3:B:4911:ARG:HD3	1.96	0.48
3:C:4122:GLU:OE1	3:C:4122:GLU:N	2.44	0.48
2:K:30:SER:N	2:K:69:GLU:OE2	2.47	0.48
2:O:7:SER:O	2:O:11:THR:HG23	2.14	0.48
2:P:5:LEU:HD23	2:P:9:MET:CE	2.44	0.48
2:P:58:VAL:HG13	2:P:62:LEU:HD23	1.96	0.48
2:J:5:LEU:HD23	2:J:9:MET:CE	2.44	0.48
3:D:318:ARG:NH2	3:D:322:GLU:O	2.46	0.48
3:D:1659:ASP:N	3:D:1659:ASP:OD1	2.47	0.48
3:D:4090:LEU:HB3	3:D:4125:MET:HE3	1.96	0.48
3:D:4900:GLU:O	3:D:4911:ARG:CZ	2.62	0.48
3:A:2528:LEU:HA	3:A:2531:MET:HE2	1.96	0.48
3:B:2197:ASN:OD1	3:B:2200:ARG:NH2	2.46	0.48
3:B:2206:GLU:OE1	3:B:2206:GLU:N	2.46	0.48
3:C:2393:ARG:O	3:C:2419:LEU:HD12	2.13	0.48
2:L:86:CYS:SG	2:L:87:ASN:N	2.87	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:42:LEU:CD2	2:N:46:LEU:HB2	2.44	0.48
3:D:578:ILE:O	3:D:580:GLN:NE2	2.47	0.47
3:A:1758:GLY:N	3:A:1759:PRO:HD2	2.29	0.47
3:A:4908:GLU:O	3:A:4912:VAL:HG13	2.14	0.47
3:B:1659:ASP:OD1	3:B:1659:ASP:N	2.47	0.47
3:B:1699:LEU:O	3:B:1816:MET:HE1	2.14	0.47
3:B:2393:ARG:O	3:B:2419:LEU:HD12	2.13	0.47
3:C:510:GLU:OE2	3:C:510:GLU:N	2.44	0.47
3:C:3865:ASP:OD1	3:C:3866:GLY:N	2.46	0.47
2:K:84:VAL:HG22	2:L:72:PHE:HD2	1.77	0.47
2:J:86:CYS:SG	2:J:87:ASN:N	2.87	0.47
3:D:2197:ASN:OD1	3:D:2200:ARG:NH2	2.46	0.47
3:D:3253:GLU:O	3:D:3256:GLY:N	2.47	0.47
3:D:4902:PRO:HB3	3:D:4911:ARG:HD3	1.96	0.47
3:A:4900:GLU:O	3:A:4911:ARG:CZ	2.62	0.47
3:B:4908:GLU:O	3:B:4912:VAL:HG13	2.14	0.47
3:C:4090:LEU:HB3	3:C:4125:MET:HE3	1.96	0.47
2:O:30:SER:N	2:O:69:GLU:OE2	2.47	0.47
3:A:3182:PRO:O	3:A:3185:GLU:HG3	2.14	0.47
3:B:2368:ALA:HB2	3:B:2380:ALA:HB2	1.96	0.47
3:C:318:ARG:NH2	3:C:322:GLU:O	2.46	0.47
3:C:888:ILE:HG12	3:C:960:TYR:HA	1.97	0.47
2:L:72:PHE:O	2:L:76:VAL:HG13	2.13	0.47
3:D:888:ILE:HG12	3:D:960:TYR:HA	1.97	0.47
3:D:2368:ALA:HB2	3:D:2380:ALA:HB2	1.96	0.47
3:D:2523:LEU:HD22	3:D:2579:MET:SD	2.54	0.47
3:A:910:ASN:OD1	3:A:911:PHE:N	2.48	0.47
3:A:3873:ASN:OD1	3:A:3874:GLY:N	2.46	0.47
3:B:569:LEU:HD12	3:B:603:VAL:HG13	1.96	0.47
3:B:3164:VAL:HG22	3:B:3233:LEU:HD11	1.96	0.47
3:B:3661:SER:HG	3:B:3662:TRP:HD1	1.62	0.47
3:C:754:PRO:HG3	3:C:774:LEU:HD11	1.96	0.47
3:C:875:LEU:HD11	3:C:1047:LEU:CD2	2.29	0.47
3:C:1659:ASP:OD1	3:C:1659:ASP:N	2.47	0.47
3:C:2473:LEU:O	3:C:2500:LYS:NZ	2.45	0.47
3:C:3182:PRO:O	3:C:3185:GLU:HG3	2.14	0.47
2:N:54:ALA:O	2:N:58:VAL:HG23	2.15	0.47
2:N:86:CYS:SG	2:N:87:ASN:N	2.87	0.47
3:D:2472:SER:HB3	3:D:2525:VAL:HG12	1.97	0.47
2:I:7:SER:O	2:I:11:THR:HG23	2.14	0.47
1:H:6:GLU:N	1:H:6:GLU:OE1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3182:PRO:O	3:D:3185:GLU:HG3	2.14	0.47
8:D:8006:PCW:H62	8:C:5101:PCW:O31	2.15	0.47
3:B:754:PRO:HG3	3:B:774:LEU:HD11	1.96	0.47
3:B:1793:ALA:O	3:B:1794:THR:OG1	2.23	0.47
3:B:4900:GLU:O	3:B:4911:ARG:CZ	2.62	0.47
3:C:578:ILE:O	3:C:580:GLN:NE2	2.47	0.47
3:C:2694:GLN:NE2	2:M:10:GLU:CD	2.63	0.47
3:D:569:LEU:HD12	3:D:603:VAL:HG13	1.96	0.47
3:D:910:ASN:OD1	3:D:911:PHE:N	2.48	0.47
3:D:1067:GLN:OE1	3:D:1072:ARG:NH2	2.47	0.47
3:D:3600:VAL:O	3:D:3604:LEU:HD13	2.15	0.47
3:A:888:ILE:HG12	3:A:960:TYR:HA	1.97	0.47
3:A:2368:ALA:HB2	3:A:2380:ALA:HB2	1.95	0.47
3:A:2739:ARG:O	3:A:2885:ASN:ND2	2.47	0.47
3:A:3661:SER:HG	3:A:3662:TRP:HD1	1.62	0.47
3:A:4090:LEU:HB3	3:A:4125:MET:HE3	1.97	0.47
8:A:8007:PCW:O31	8:B:8006:PCW:H62	2.15	0.47
3:B:4122:GLU:OE1	3:B:4122:GLU:N	2.44	0.47
3:C:233:THR:HG21	3:C:253:VAL:HG21	1.97	0.47
3:C:1067:GLN:OE1	3:C:1072:ARG:NH2	2.47	0.47
3:C:1758:GLY:N	3:C:1759:PRO:HD2	2.29	0.47
3:C:2362:PRO:O	3:C:2370:ARG:NH1	2.47	0.47
3:C:3600:VAL:O	3:C:3604:LEU:HD13	2.15	0.47
2:L:5:LEU:HD23	2:L:9:MET:CE	2.44	0.47
2:N:5:LEU:HD23	2:N:9:MET:CE	2.44	0.47
2:P:42:LEU:CD2	2:P:46:LEU:HB2	2.44	0.47
3:D:233:THR:HG21	3:D:253:VAL:HG21	1.97	0.47
3:D:2370:ARG:NE	3:D:2370:ARG:HA	2.30	0.47
3:A:2370:ARG:NE	3:A:2370:ARG:HA	2.30	0.47
3:A:3547:ASP:O	3:A:3550:VAL:HG22	2.15	0.47
3:B:910:ASN:OD1	3:B:911:PHE:N	2.48	0.47
3:B:4090:LEU:HB3	3:B:4125:MET:HE3	1.97	0.47
3:C:2206:GLU:OE1	3:C:2206:GLU:N	2.46	0.47
3:C:3547:ASP:O	3:C:3550:VAL:HG22	2.15	0.47
3:C:4902:PRO:HB3	3:C:4911:ARG:HD3	1.96	0.47
2:L:42:LEU:CD2	2:L:46:LEU:HB2	2.44	0.47
2:L:54:ALA:O	2:L:58:VAL:HG23	2.15	0.47
2:L:58:VAL:HG13	2:L:62:LEU:HD23	1.96	0.47
1:E:6:GLU:N	1:E:6:GLU:OE1	2.48	0.47
3:D:664:TYR:OH	3:D:666:GLU:OE2	2.27	0.47
3:D:1758:GLY:N	3:D:1759:PRO:HD2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2625:ARG:HD2	3:D:2907:VAL:HG21	1.97	0.47
3:A:102:LEU:HD23	3:A:102:LEU:H	1.78	0.47
3:B:233:THR:HG21	3:B:253:VAL:HG21	1.97	0.47
3:C:2370:ARG:NE	3:C:2370:ARG:HA	2.30	0.47
2:N:58:VAL:HG13	2:N:62:LEU:HD23	1.96	0.47
2:P:54:ALA:O	2:P:58:VAL:HG23	2.15	0.47
3:A:2260:GLU:OE2	3:A:2298:LYS:NZ	2.22	0.47
3:A:4964:ASP:OD1	3:A:4965:TYR:N	2.47	0.47
3:C:569:LEU:HD12	3:C:603:VAL:HG13	1.96	0.47
3:C:2625:ARG:HD2	3:C:2907:VAL:HG21	1.97	0.47
2:K:83:THR:O	2:K:87:ASN:ND2	2.48	0.47
3:D:163:LYS:O	3:D:165:ARG:NH1	2.38	0.46
3:A:754:PRO:HG3	3:A:774:LEU:HD11	1.96	0.46
3:A:2874:ALA:O	3:A:2878:GLN:OE1	2.33	0.46
3:A:4691:GLU:O	3:A:4692:ASP:OD1	2.33	0.46
3:B:2625:ARG:HD2	3:B:2907:VAL:HG21	1.97	0.46
3:B:3212:ASN:ND2	3:B:3237:VAL:HG21	2.31	0.46
3:B:3600:VAL:O	3:B:3604:LEU:HD13	2.15	0.46
3:C:2472:SER:HB3	3:C:2525:VAL:HG12	1.97	0.46
3:C:3164:VAL:HG22	3:C:3233:LEU:HD11	1.96	0.46
2:J:58:VAL:HG13	2:J:62:LEU:HD23	1.96	0.46
3:D:3164:VAL:HG22	3:D:3233:LEU:HD11	1.96	0.46
3:D:3768:TYR:HH	3:D:4751:HIS:CE1	2.33	0.46
3:A:3600:VAL:O	3:A:3604:LEU:HD13	2.15	0.46
3:B:888:ILE:HG12	3:B:960:TYR:HA	1.97	0.46
3:B:4964:ASP:OD1	3:B:4965:TYR:N	2.47	0.46
3:C:3943:LYS:O	3:C:4005:LYS:NZ	2.34	0.46
3:C:4185:GLU:O	3:C:4986:TYR:OH	2.20	0.46
2:I:81:ALA:O	2:I:84:VAL:HB	2.16	0.46
3:D:2972:GLN:O	3:D:2975:ILE:HG22	2.16	0.46
3:D:4649:THR:HG1	3:D:4801:HIS:CD2	2.31	0.46
3:A:2972:GLN:O	3:A:2975:ILE:HG22	2.16	0.46
3:B:2370:ARG:NE	3:B:2370:ARG:HA	2.30	0.46
3:B:2972:GLN:O	3:B:2975:ILE:HG22	2.16	0.46
3:B:3547:ASP:O	3:B:3550:VAL:HG22	2.15	0.46
3:B:4824:ILE:O	3:B:4827:SER:OG	2.14	0.46
8:B:8007:PCW:O31	8:C:5107:PCW:H62	2.15	0.46
3:D:754:PRO:HG3	3:D:774:LEU:HD11	1.96	0.46
3:D:2179:MET:HE1	3:D:2183:ILE:HD11	1.97	0.46
3:D:4908:GLU:O	3:D:4912:VAL:HG13	2.14	0.46
3:A:233:THR:HG21	3:A:253:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2564:THR:HG22	3:A:2607:CYS:CA	2.45	0.46
3:A:3943:LYS:O	3:A:4005:LYS:NZ	2.34	0.46
3:B:231:CYS:SG	3:B:253:VAL:HG13	2.56	0.46
3:B:2472:SER:HB3	3:B:2525:VAL:HG12	1.97	0.46
3:C:910:ASN:OD1	3:C:911:PHE:N	2.48	0.46
3:C:2197:ASN:OD1	3:C:2200:ARG:NH2	2.46	0.46
3:C:2368:ALA:HB2	3:C:2380:ALA:HB2	1.96	0.46
3:C:4908:GLU:O	3:C:4912:VAL:HG13	2.14	0.46
2:M:83:THR:O	2:M:87:ASN:ND2	2.48	0.46
1:G:6:GLU:OE1	1:G:6:GLU:N	2.48	0.46
3:D:2206:GLU:N	3:D:2206:GLU:OE1	2.46	0.46
3:A:1659:ASP:N	3:A:1659:ASP:OD1	2.47	0.46
3:A:3330:ILE:O	3:A:3404:ARG:NH2	2.49	0.46
3:A:3355:LEU:HD12	3:A:3356:ARG:N	2.30	0.46
3:C:2311:CYS:O	3:C:2315:LEU:HD23	2.16	0.46
3:C:2889:ARG:HG2	3:C:2893:GLN:HE22	1.81	0.46
3:C:3212:ASN:ND2	3:C:3237:VAL:HG21	2.31	0.46
2:J:16:PHE:CG	2:J:75:TYR:OH	2.60	0.46
2:J:38:LEU:HB3	2:J:46:LEU:HD21	1.98	0.46
3:D:3212:ASN:ND2	3:D:3237:VAL:HG21	2.31	0.46
3:D:3293:PRO:O	3:D:3295:PRO:HD3	2.16	0.46
3:A:3004:LEU:HB2	3:A:3005:PRO:HD3	1.98	0.46
3:B:984:THR:HA	3:B:987:ASP:OD2	2.16	0.46
3:B:2889:ARG:HG2	3:B:2893:GLN:HE22	1.80	0.46
3:B:3686:GLU:OE1	3:B:3686:GLU:N	2.49	0.46
3:B:3768:TYR:HH	3:B:4751:HIS:CE1	2.34	0.46
3:C:231:CYS:SG	3:C:253:VAL:HG13	2.56	0.46
3:C:243:ARG:NH1	3:C:482:GLU:OE2	2.48	0.46
3:C:2179:MET:HE1	3:C:2183:ILE:HD11	1.98	0.46
3:C:2564:THR:HG22	3:C:2607:CYS:CA	2.45	0.46
3:C:3355:LEU:HD12	3:C:3356:ARG:N	2.30	0.46
3:C:3920:ILE:HD12	3:C:3986:SER:HB3	1.98	0.46
2:L:38:LEU:HB3	2:L:46:LEU:HD21	1.98	0.46
3:D:231:CYS:SG	3:D:253:VAL:HG13	2.56	0.46
3:D:1435:TYR:OH	3:D:1570:GLN:HG2	2.15	0.46
3:D:1700:GLU:OE1	3:D:1812:LYS:NZ	2.49	0.46
3:D:2311:CYS:O	3:D:2315:LEU:HD23	2.16	0.46
3:D:3547:ASP:O	3:D:3550:VAL:HG22	2.15	0.46
3:A:2625:ARG:HD2	3:A:2907:VAL:HG21	1.97	0.46
3:A:3686:GLU:OE1	3:A:3686:GLU:N	2.49	0.46
3:B:3004:LEU:HB2	3:B:3005:PRO:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1699:LEU:O	3:C:1816:MET:HE1	2.15	0.46
3:C:2820:TRP:O	3:C:2821:GLU:HB2	2.16	0.46
3:C:4691:GLU:O	3:C:4692:ASP:OD1	2.33	0.46
2:K:81:ALA:O	2:K:84:VAL:HB	2.16	0.46
2:O:81:ALA:O	2:O:84:VAL:HB	2.16	0.46
2:I:83:THR:O	2:I:87:ASN:ND2	2.48	0.46
2:J:54:ALA:O	2:J:58:VAL:HG23	2.15	0.46
3:D:234:ILE:HD12	3:D:243:ARG:HB3	1.98	0.46
3:D:1699:LEU:HD11	3:D:1716:LEU:HD13	1.98	0.46
3:D:3330:ILE:O	3:D:3404:ARG:NH2	2.49	0.46
8:D:8007:PCW:O31	8:A:8006:PCW:H62	2.15	0.46
3:A:231:CYS:SG	3:A:253:VAL:HG13	2.56	0.46
3:A:2472:SER:HB3	3:A:2525:VAL:HG12	1.97	0.46
3:A:2942:LEU:O	3:A:2945:MET:HG2	2.16	0.46
3:A:3212:ASN:ND2	3:A:3237:VAL:HG21	2.30	0.46
3:B:951:LEU:CB	3:B:971:LEU:HD23	2.45	0.46
3:B:4691:GLU:O	3:B:4692:ASP:OD1	2.33	0.46
3:C:3004:LEU:HB2	3:C:3005:PRO:HD3	1.98	0.46
2:N:72:PHE:O	2:N:76:VAL:HG22	2.16	0.46
2:J:72:PHE:O	2:J:76:VAL:HG22	2.16	0.46
3:D:1220:LEU:HD22	3:C:3576:LEU:HD21	1.98	0.46
3:D:2874:ALA:O	3:D:2878:GLN:OE1	2.33	0.46
3:D:2942:LEU:O	3:D:2945:MET:HG2	2.16	0.46
3:D:4091:ILE:O	3:D:4126:ILE:N	2.39	0.46
3:A:2311:CYS:O	3:A:2315:LEU:HD23	2.16	0.46
3:A:3920:ILE:HD12	3:A:3986:SER:HB3	1.97	0.46
3:B:668:MET:SD	3:B:791:ARG:NH2	2.87	0.46
3:B:1772:SER:OG	3:B:1957:GLU:OE2	2.23	0.46
3:B:3355:LEU:HD12	3:B:3356:ARG:N	2.30	0.46
3:C:234:ILE:HD12	3:C:243:ARG:HB3	1.98	0.46
3:C:1699:LEU:HD11	3:C:1716:LEU:HD13	1.98	0.46
3:C:2874:ALA:O	3:C:2878:GLN:OE1	2.33	0.46
3:C:2942:LEU:O	3:C:2945:MET:HG2	2.16	0.46
2:L:72:PHE:O	2:L:76:VAL:HG22	2.16	0.46
3:D:3355:LEU:HD12	3:D:3356:ARG:N	2.30	0.46
3:A:1700:GLU:OE1	3:A:1812:LYS:NZ	2.49	0.46
3:A:2179:MET:HE1	3:A:2183:ILE:HD11	1.97	0.46
3:A:3047:LEU:CD2	3:A:3069:LEU:HD22	2.46	0.46
3:A:3164:VAL:HG22	3:A:3233:LEU:HD11	1.97	0.46
3:B:2260:GLU:OE2	3:B:2298:LYS:NZ	2.22	0.46
3:B:2311:CYS:O	3:B:2315:LEU:HD23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2564:THR:HG22	3:B:2607:CYS:CA	2.45	0.46
3:C:3267:MET:HG3	3:C:3267:MET:O	2.16	0.46
2:N:16:PHE:CG	2:N:75:TYR:OH	2.60	0.46
3:D:2594:ARG:O	3:D:2595:SER:OG	2.25	0.45
3:D:3004:LEU:HB2	3:D:3005:PRO:HD3	1.98	0.45
3:D:3267:MET:HG3	3:D:3267:MET:O	2.16	0.45
3:D:3600:VAL:HG22	3:D:3604:LEU:CD1	2.46	0.45
3:D:3943:LYS:O	3:D:4005:LYS:NZ	2.34	0.45
3:D:4886:TYR:HA	3:A:4916:ILE:HD11	1.97	0.45
3:A:234:ILE:HD12	3:A:243:ARG:HB3	1.98	0.45
3:A:668:MET:SD	3:A:791:ARG:NH2	2.87	0.45
3:B:1435:TYR:OH	3:B:1570:GLN:HG2	2.15	0.45
3:B:1700:GLU:OE1	3:B:1812:LYS:NZ	2.49	0.45
3:B:2874:ALA:O	3:B:2878:GLN:OE1	2.33	0.45
3:B:3600:VAL:HG22	3:B:3604:LEU:CD1	2.46	0.45
3:C:3293:PRO:O	3:C:3295:PRO:HD3	2.16	0.45
3:C:4649:THR:HG1	3:C:4801:HIS:CD2	2.33	0.45
3:A:243:ARG:NH1	3:A:482:GLU:OE2	2.48	0.45
3:A:2889:ARG:HG2	3:A:2893:GLN:HE22	1.81	0.45
3:B:2179:MET:HE1	3:B:2183:ILE:HD11	1.98	0.45
3:B:3267:MET:O	3:B:3267:MET:HG3	2.16	0.45
3:C:887:ARG:NH2	7:C:5106:ATP:O3G	2.49	0.45
3:C:3768:TYR:HH	3:C:4751:HIS:CE1	2.34	0.45
2:O:20:SER:OG	2:O:29:LEU:HD23	2.17	0.45
2:O:83:THR:O	2:O:87:ASN:ND2	2.48	0.45
2:P:38:LEU:HB3	2:P:46:LEU:HD21	1.98	0.45
3:D:36:LEU:HD23	3:D:52:PRO:HA	1.99	0.45
3:D:668:MET:SD	3:D:791:ARG:NH2	2.87	0.45
3:D:3271:ILE:H	3:D:3271:ILE:HD12	1.81	0.45
3:D:4122:GLU:OE1	3:D:4122:GLU:N	2.44	0.45
3:B:887:ARG:NH2	7:B:8005:ATP:O3G	2.49	0.45
3:B:3330:ILE:O	3:B:3404:ARG:NH2	2.49	0.45
3:C:1435:TYR:OH	3:C:1570:GLN:HG2	2.15	0.45
3:C:1700:GLU:OE1	3:C:1812:LYS:NZ	2.49	0.45
3:C:3686:GLU:OE1	3:C:3686:GLU:N	2.49	0.45
2:N:38:LEU:HB3	2:N:46:LEU:HD21	1.98	0.45
2:P:72:PHE:O	2:P:76:VAL:HG22	2.16	0.45
3:D:2249:ARG:HD2	3:D:2287:LEU:HD21	1.98	0.45
3:D:2382:GLU:O	3:D:2385:ILE:HG22	2.17	0.45
3:D:2889:ARG:HG2	3:D:2893:GLN:HE22	1.80	0.45
3:A:984:THR:HA	3:A:987:ASP:OD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1435:TYR:OH	3:A:1570:GLN:HG2	2.16	0.45
3:A:1699:LEU:HD11	3:A:1716:LEU:HD13	1.98	0.45
3:B:1699:LEU:HD11	3:B:1716:LEU:HD13	1.98	0.45
3:B:2249:ARG:HD2	3:B:2287:LEU:HD21	1.98	0.45
3:B:2382:GLU:O	3:B:2385:ILE:HG22	2.17	0.45
3:B:2694:GLN:NE2	2:K:10:GLU:CD	2.63	0.45
3:C:668:MET:SD	3:C:791:ARG:NH2	2.87	0.45
3:C:951:LEU:CB	3:C:971:LEU:HD23	2.45	0.45
2:L:78:LEU:HD12	2:L:79:VAL:N	2.32	0.45
1:H:54:GLN:OE1	1:H:54:GLN:N	2.50	0.45
3:D:984:THR:HA	3:D:987:ASP:OD2	2.16	0.45
3:D:3443:PHE:CD2	3:D:3515:LEU:HD22	2.52	0.45
3:D:3686:GLU:N	3:D:3686:GLU:OE1	2.49	0.45
3:D:4691:GLU:O	3:D:4692:ASP:OD1	2.33	0.45
3:D:4964:ASP:OD1	3:D:4965:TYR:N	2.47	0.45
3:A:2528:LEU:HA	3:A:2531:MET:CE	2.47	0.45
8:A:8007:PCW:H232	8:A:8007:PCW:H20	1.76	0.45
3:B:234:ILE:HD12	3:B:243:ARG:HB3	1.98	0.45
3:B:2746:VAL:HG22	3:B:2747:ILE:N	2.32	0.45
3:B:3047:LEU:CD2	3:B:3069:LEU:HD22	2.46	0.45
3:B:3724:MET:CE	3:B:3795:ALA:HB1	2.47	0.45
3:C:984:THR:HA	3:C:987:ASP:OD2	2.16	0.45
3:C:2125:LEU:CD2	3:C:3678:LEU:HD21	2.47	0.45
3:C:2972:GLN:O	3:C:2975:ILE:HG22	2.16	0.45
3:C:3600:VAL:HG22	3:C:3604:LEU:CD1	2.46	0.45
3:C:3702:LEU:HD21	3:C:3726:TYR:CD1	2.52	0.45
3:C:3724:MET:CE	3:C:3795:ALA:HB1	2.47	0.45
2:P:73:LYS:O	2:P:76:VAL:HG22	2.16	0.45
2:P:79:VAL:O	2:P:83:THR:HG22	2.17	0.45
2:J:78:LEU:HD12	2:J:79:VAL:N	2.32	0.45
3:D:2528:LEU:HA	3:D:2531:MET:CE	2.47	0.45
3:D:3047:LEU:CD2	3:D:3069:LEU:HD22	2.46	0.45
3:D:3724:MET:CE	3:D:3795:ALA:HB1	2.47	0.45
3:D:3920:ILE:HD12	3:D:3986:SER:HB3	1.98	0.45
3:A:330:ARG:NH1	3:A:331:ASP:O	2.50	0.45
3:A:1222:GLU:OE1	3:A:1222:GLU:N	2.49	0.45
3:A:3293:PRO:O	3:A:3295:PRO:HD3	2.16	0.45
3:A:3443:PHE:CD2	3:A:3515:LEU:HD22	2.52	0.45
3:A:3768:TYR:HH	3:A:4751:HIS:CE1	2.34	0.45
3:B:2125:LEU:CD2	3:B:3678:LEU:HD21	2.47	0.45
3:B:2473:LEU:O	3:B:2500:LYS:NZ	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2645:LEU:HD13	3:B:2679:LEU:HD11	1.98	0.45
3:B:2820:TRP:O	3:B:2821:GLU:HB2	2.16	0.45
3:B:2942:LEU:O	3:B:2945:MET:HG2	2.16	0.45
3:B:3920:ILE:HD12	3:B:3986:SER:HB3	1.97	0.45
3:B:4800:GLY:HA2	3:B:4806:PHE:HB2	1.99	0.45
3:C:1007:SER:C	3:C:1022:LEU:HD23	2.37	0.45
3:C:3047:LEU:CD2	3:C:3069:LEU:HD22	2.46	0.45
3:C:3330:ILE:O	3:C:3404:ARG:NH2	2.49	0.45
2:L:73:LYS:O	2:L:76:VAL:HG22	2.16	0.45
3:D:2125:LEU:CD2	3:D:3678:LEU:HD21	2.47	0.45
3:D:3136:ALA:O	3:D:3140:VAL:HG12	2.17	0.45
3:D:3421:ARG:NH2	3:D:3517:LYS:O	2.50	0.45
3:D:3521:ILE:H	3:D:3521:ILE:HD12	1.82	0.45
3:D:3702:LEU:HD21	3:D:3726:TYR:CD1	2.52	0.45
3:A:36:LEU:HD23	3:A:52:PRO:HA	1.98	0.45
3:A:887:ARG:NH2	7:A:8005:ATP:O3G	2.49	0.45
3:A:2249:ARG:HD2	3:A:2287:LEU:HD21	1.98	0.45
3:A:3320:ILE:HD12	3:A:3320:ILE:H	1.82	0.45
3:A:3933:ILE:HG22	3:A:3998:VAL:HG11	1.99	0.45
3:B:330:ARG:NH1	3:B:331:ASP:O	2.50	0.45
3:C:3443:PHE:CD2	3:C:3515:LEU:HD22	2.52	0.45
2:K:20:SER:OG	2:K:29:LEU:HD23	2.17	0.45
2:N:73:LYS:O	2:N:76:VAL:HG22	2.16	0.45
3:D:887:ARG:NH2	7:D:8005:ATP:O3G	2.49	0.45
3:D:1222:GLU:OE1	3:D:1222:GLU:N	2.49	0.45
3:D:3320:ILE:HD12	3:D:3320:ILE:H	1.82	0.45
3:D:4909:LEU:HA	3:D:4912:VAL:HG22	1.99	0.45
3:A:2952:ILE:H	3:A:2952:ILE:HD12	1.82	0.45
3:B:684:ARG:NH1	3:B:708:VAL:O	2.43	0.45
3:B:1973:ASN:ND2	3:B:2025:PRO:HD3	2.32	0.45
3:B:3322:ARG:HA	3:B:3325:VAL:HG12	1.99	0.45
3:B:3394:LEU:HD23	3:B:3398:GLU:OE1	2.17	0.45
3:C:36:LEU:HD23	3:C:52:PRO:HA	1.99	0.45
3:C:330:ARG:NH1	3:C:331:ASP:O	2.50	0.45
3:C:2249:ARG:HD2	3:C:2287:LEU:HD21	1.98	0.45
3:C:3421:ARG:NH2	3:C:3517:LYS:O	2.50	0.45
2:K:84:VAL:CG1	2:L:72:PHE:HE2	2.23	0.45
2:M:50:LYS:NZ	2:M:51:ASP:OD2	2.50	0.45
2:I:9:MET:HG2	2:J:84:VAL:HG12	1.99	0.45
1:G:54:GLN:OE1	1:G:54:GLN:N	2.50	0.45
3:D:912:HIS:O	3:D:919:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2645:LEU:HD13	3:D:2679:LEU:HD11	1.98	0.45
3:D:3227:GLU:O	3:D:3228:ARG:CG	2.65	0.45
3:D:3789:CYS:SG	3:D:3834:SER:OG	2.75	0.45
3:A:1973:ASN:ND2	3:A:2025:PRO:HD3	2.32	0.45
3:A:3322:ARG:HA	3:A:3325:VAL:HG12	1.99	0.45
3:A:3521:ILE:H	3:A:3521:ILE:HD12	1.82	0.45
3:B:581:GLU:HG3	3:B:621:LEU:HD22	1.99	0.45
3:B:2908:PRO:O	3:B:2911:THR:OG1	2.30	0.45
3:B:3136:ALA:O	3:B:3140:VAL:HG12	2.17	0.45
3:B:3421:ARG:NH2	3:B:3517:LYS:O	2.50	0.45
3:C:1090:TYR:N	3:C:1225:GLU:O	2.50	0.45
3:C:3521:ILE:H	3:C:3521:ILE:HD12	1.82	0.45
3:C:4800:GLY:HA2	3:C:4806:PHE:HB2	1.99	0.45
2:M:34:LEU:CD1	2:M:70:VAL:HG21	2.47	0.45
2:O:9:MET:HG2	2:P:84:VAL:HG12	1.99	0.45
2:I:20:SER:OG	2:I:29:LEU:HD23	2.17	0.45
2:J:47:ASP:OD2	2:J:50:LYS:NZ	2.37	0.45
3:D:2746:VAL:HG22	3:D:2747:ILE:N	2.32	0.45
3:D:3394:LEU:HD23	3:D:3398:GLU:OE1	2.17	0.45
3:A:1090:TYR:N	3:A:1225:GLU:O	2.50	0.45
3:A:2125:LEU:CD2	3:A:3678:LEU:HD21	2.47	0.45
3:A:3208:GLU:OE1	3:A:3208:GLU:N	2.50	0.45
3:A:3267:MET:HG3	3:A:3267:MET:O	2.16	0.45
3:A:3724:MET:CE	3:A:3795:ALA:HB1	2.47	0.45
3:B:2528:LEU:HA	3:B:2531:MET:CE	2.47	0.45
3:B:2952:ILE:H	3:B:2952:ILE:HD12	1.82	0.45
3:B:3208:GLU:OE1	3:B:3208:GLU:N	2.50	0.45
3:B:3293:PRO:O	3:B:3295:PRO:HD3	2.16	0.45
3:B:3576:LEU:HD21	3:C:1220:LEU:HD22	1.97	0.45
3:C:1529:THR:OG1	3:C:1536:GLU:OE2	2.35	0.45
3:C:3271:ILE:H	3:C:3271:ILE:HD12	1.81	0.45
2:K:50:LYS:NZ	2:K:51:ASP:OD2	2.50	0.45
2:L:79:VAL:O	2:L:83:THR:HG22	2.17	0.45
2:N:78:LEU:HD12	2:N:79:VAL:N	2.32	0.45
2:J:79:VAL:O	2:J:83:THR:HG22	2.17	0.44
3:D:1007:SER:C	3:D:1022:LEU:HD23	2.37	0.44
3:D:3869:ILE:HG22	3:D:3869:ILE:O	2.17	0.44
3:A:130:ASP:OD1	3:A:133:ALA:N	2.50	0.44
3:A:215:VAL:CG1	3:A:275:LEU:HD12	2.47	0.44
3:A:2382:GLU:O	3:A:2385:ILE:HG22	2.17	0.44
3:A:2782:ILE:HG23	3:A:2790:PRO:CD	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3402:LEU:HD23	3:A:3402:LEU:O	2.18	0.44
3:A:3702:LEU:HD21	3:A:3726:TYR:CD1	2.52	0.44
3:B:1007:SER:C	3:B:1022:LEU:HD23	2.37	0.44
3:B:2594:ARG:O	3:B:2595:SER:OG	2.25	0.44
3:B:3227:GLU:O	3:B:3228:ARG:CG	2.65	0.44
3:B:4796:MET:HE3	8:B:8007:PCW:H222	1.99	0.44
3:C:1120:ASP:N	3:C:1120:ASP:OD1	2.50	0.44
3:C:4155:GLU:OE2	3:C:4183:ARG:NH1	2.50	0.44
2:K:9:MET:HG2	2:L:84:VAL:HG12	1.99	0.44
2:P:78:LEU:HD12	2:P:79:VAL:N	2.32	0.44
3:D:1090:TYR:N	3:D:1225:GLU:O	2.50	0.44
3:D:2820:TRP:O	3:D:2821:GLU:HB2	2.16	0.44
3:D:3270:VAL:HG12	3:D:3275:LEU:HD23	1.99	0.44
3:D:3402:LEU:HD23	3:D:3402:LEU:O	2.17	0.44
3:D:3577:TYR:CZ	3:D:3583:ARG:HD3	2.53	0.44
3:A:2645:LEU:HD13	3:A:2679:LEU:HD11	1.98	0.44
3:A:2746:VAL:HG22	3:A:2747:ILE:N	2.32	0.44
3:A:2820:TRP:O	3:A:2821:GLU:HB2	2.16	0.44
3:A:3227:GLU:O	3:A:3228:ARG:CG	2.65	0.44
3:A:3270:VAL:HG12	3:A:3275:LEU:HD23	2.00	0.44
3:B:3104:ILE:O	3:B:3107:MET:HB3	2.17	0.44
3:B:3521:ILE:HD12	3:B:3521:ILE:H	1.82	0.44
3:B:4155:GLU:OE2	3:B:4183:ARG:NH1	2.50	0.44
3:C:169:ASP:OD1	3:C:202:ASN:ND2	2.51	0.44
3:C:2782:ILE:HG23	3:C:2790:PRO:CD	2.47	0.44
3:C:3410:TYR:O	3:C:3411:PRO:C	2.56	0.44
3:C:3869:ILE:O	3:C:3869:ILE:HG22	2.17	0.44
2:K:34:LEU:CD1	2:K:70:VAL:HG21	2.47	0.44
2:N:62:LEU:HD13	2:N:78:LEU:HD21	2.00	0.44
2:M:81:ALA:O	2:M:84:VAL:HB	2.16	0.44
2:P:62:LEU:HD13	2:P:78:LEU:HD21	2.00	0.44
2:J:6:GLU:HA	2:J:9:MET:HE1	1.99	0.44
3:D:2782:ILE:HG23	3:D:2790:PRO:CD	2.47	0.44
3:D:3104:ILE:O	3:D:3107:MET:HB3	2.17	0.44
3:D:3511:ILE:HG23	3:D:3512:VAL:N	2.33	0.44
3:A:245:LEU:HD23	3:A:301:VAL:HG12	1.99	0.44
3:A:912:HIS:O	3:A:919:ARG:NH1	2.50	0.44
3:A:3600:VAL:HG22	3:A:3604:LEU:CD1	2.46	0.44
3:A:4886:TYR:HA	3:B:4916:ILE:HD11	1.99	0.44
3:B:2782:ILE:HG23	3:B:2790:PRO:CD	2.47	0.44
3:B:3271:ILE:H	3:B:3271:ILE:HD12	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:581:GLU:HG3	3:C:621:LEU:HD22	1.99	0.44
3:C:2247:ASN:O	3:C:2250:SER:OG	2.28	0.44
3:C:2382:GLU:O	3:C:2385:ILE:HG22	2.17	0.44
3:C:3104:ILE:O	3:C:3107:MET:HB3	2.17	0.44
3:C:3136:ALA:O	3:C:3140:VAL:HG12	2.17	0.44
3:C:3208:GLU:OE1	3:C:3208:GLU:N	2.50	0.44
2:L:6:GLU:HA	2:L:9:MET:HE1	1.99	0.44
2:O:34:LEU:CD1	2:O:70:VAL:HG21	2.47	0.44
3:D:130:ASP:OD1	3:D:133:ALA:N	2.50	0.44
3:D:215:VAL:CG1	3:D:275:LEU:HD12	2.47	0.44
3:D:330:ARG:NH1	3:D:331:ASP:O	2.50	0.44
3:A:169:ASP:OD1	3:A:202:ASN:ND2	2.51	0.44
3:A:951:LEU:CB	3:A:971:LEU:HD23	2.45	0.44
3:A:2156:LEU:HD21	3:A:2199:MET:HE1	1.99	0.44
3:A:3136:ALA:O	3:A:3140:VAL:HG12	2.17	0.44
3:A:3271:ILE:H	3:A:3271:ILE:HD12	1.82	0.44
3:A:3577:TYR:CZ	3:A:3583:ARG:HD3	2.53	0.44
3:A:3869:ILE:HG22	3:A:3869:ILE:O	2.17	0.44
3:B:576:LEU:HD22	3:B:610:CYS:HB2	1.99	0.44
3:B:1222:GLU:OE1	3:B:1222:GLU:N	2.49	0.44
3:B:3270:VAL:HG12	3:B:3275:LEU:HD23	1.99	0.44
3:B:4653:PHE:N	3:B:4794:MET:HE1	2.32	0.44
3:C:912:HIS:O	3:C:919:ARG:NH1	2.50	0.44
3:C:3322:ARG:HA	3:C:3325:VAL:HG12	1.99	0.44
3:C:3511:ILE:HG23	3:C:3512:VAL:N	2.33	0.44
2:L:62:LEU:HD13	2:L:78:LEU:HD21	1.99	0.44
2:N:72:PHE:HE2	2:M:84:VAL:CG1	2.23	0.44
2:N:79:VAL:O	2:N:83:THR:HG22	2.17	0.44
2:N:84:VAL:HG12	2:M:9:MET:HG2	1.99	0.44
2:I:34:LEU:CD1	2:I:70:VAL:HG21	2.47	0.44
2:J:62:LEU:HD13	2:J:78:LEU:HD21	2.00	0.44
3:D:3208:GLU:OE1	3:D:3208:GLU:N	2.50	0.44
3:A:1007:SER:C	3:A:1022:LEU:HD23	2.37	0.44
3:A:3394:LEU:HD23	3:A:3398:GLU:OE1	2.17	0.44
3:A:3410:TYR:O	3:A:3411:PRO:C	2.56	0.44
3:A:3421:ARG:NH2	3:A:3517:LYS:O	2.50	0.44
3:B:2239:TYR:O	3:B:2243:ILE:HG12	2.18	0.44
3:B:3320:ILE:HD12	3:B:3320:ILE:H	1.82	0.44
3:B:3410:TYR:O	3:B:3411:PRO:C	2.56	0.44
3:B:3577:TYR:CZ	3:B:3583:ARG:HD3	2.53	0.44
3:B:3702:LEU:HD21	3:B:3726:TYR:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1973:ASN:ND2	3:C:2025:PRO:HD3	2.32	0.44
3:C:3227:GLU:O	3:C:3228:ARG:CG	2.65	0.44
3:C:4173:ILE:H	3:C:4173:ILE:HD12	1.83	0.44
2:M:20:SER:OG	2:M:29:LEU:HD23	2.17	0.44
3:D:1473:VAL:HG22	3:D:1474:THR:N	2.33	0.44
3:D:1529:THR:OG1	3:D:1536:GLU:OE2	2.35	0.44
3:D:1973:ASN:ND2	3:D:2025:PRO:HD3	2.32	0.44
3:D:3322:ARG:HA	3:D:3325:VAL:HG12	1.99	0.44
3:B:130:ASP:OD1	3:B:133:ALA:N	2.50	0.44
3:B:2624:LEU:O	3:B:2628:VAL:HG23	2.18	0.44
3:B:3402:LEU:O	3:B:3402:LEU:HD23	2.17	0.44
3:B:3443:PHE:CD2	3:B:3515:LEU:HD22	2.52	0.44
3:C:130:ASP:OD1	3:C:133:ALA:N	2.50	0.44
3:C:576:LEU:HD22	3:C:610:CYS:HB2	1.99	0.44
3:C:3320:ILE:HD12	3:C:3320:ILE:H	1.82	0.44
3:C:3402:LEU:O	3:C:3402:LEU:HD23	2.17	0.44
3:C:4653:PHE:N	3:C:4794:MET:HE1	2.33	0.44
2:L:20:SER:HB3	2:L:27:TYR:HA	1.99	0.44
3:D:684:ARG:NH1	3:D:708:VAL:O	2.43	0.44
3:D:2268:MET:O	3:D:2269:GLN:HB3	2.18	0.44
3:D:2830:GLY:N	3:D:2934:ASN:OD1	2.51	0.44
3:D:3373:VAL:HG22	3:D:3399:PHE:CE1	2.53	0.44
3:D:3380:LEU:HD21	3:D:3392:GLU:HA	2.00	0.44
3:D:3410:TYR:O	3:D:3411:PRO:C	2.56	0.44
3:D:4227:GLU:N	3:D:4227:GLU:OE2	2.51	0.44
3:A:1492:ASN:OD1	3:A:1493:CYS:N	2.51	0.44
3:A:3373:VAL:HG22	3:A:3399:PHE:CE1	2.53	0.44
3:A:4909:LEU:HA	3:A:4912:VAL:HG22	1.99	0.44
3:B:912:HIS:O	3:B:919:ARG:NH1	2.50	0.44
3:B:1495:MET:HE3	3:B:1554:PHE:CE2	2.53	0.44
3:B:3406:LEU:HD11	3:B:3410:TYR:OH	2.18	0.44
3:B:3451:ASN:O	3:B:3454:ARG:HG2	2.18	0.44
3:C:215:VAL:CG1	3:C:275:LEU:HD12	2.47	0.44
3:C:2199:MET:HE1	3:C:2202:LEU:HD12	1.99	0.44
3:C:2528:LEU:HA	3:C:2531:MET:CE	2.47	0.44
3:C:2624:LEU:O	3:C:2628:VAL:HG23	2.18	0.44
3:C:4227:GLU:N	3:C:4227:GLU:OE2	2.51	0.44
2:N:20:SER:HB3	2:N:27:TYR:HA	1.99	0.44
2:J:73:LYS:O	2:J:76:VAL:HG22	2.16	0.44
3:D:245:LEU:HD23	3:D:301:VAL:HG12	1.99	0.44
3:D:1426:GLU:HG2	3:D:1427:ILE:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3933:ILE:HG22	3:D:3998:VAL:HG11	1.99	0.44
3:D:4155:GLU:OE2	3:D:4183:ARG:NH1	2.50	0.44
3:D:4766:ILE:HA	3:D:4769:ILE:HD12	1.99	0.44
3:A:978:LEU:HD21	3:A:1045:ARG:HG2	2.00	0.44
3:A:1529:THR:OG1	3:A:1536:GLU:OE2	2.36	0.44
3:B:36:LEU:HD23	3:B:52:PRO:HA	1.99	0.44
3:B:169:ASP:OD1	3:B:202:ASN:ND2	2.51	0.44
3:B:1473:VAL:HG22	3:B:1474:THR:N	2.33	0.44
3:B:2830:GLY:N	3:B:2934:ASN:OD1	2.51	0.44
3:B:4909:LEU:HA	3:B:4912:VAL:HG22	1.99	0.44
3:C:2239:TYR:O	3:C:2243:ILE:HG12	2.18	0.44
3:C:2645:LEU:HD13	3:C:2679:LEU:HD11	1.98	0.44
3:C:2746:VAL:HG22	3:C:2747:ILE:N	2.32	0.44
3:C:3270:VAL:HG12	3:C:3275:LEU:HD23	1.99	0.44
3:C:3394:LEU:HD23	3:C:3398:GLU:OE1	2.17	0.44
3:C:3407:TYR:O	3:C:3411:PRO:CD	2.66	0.44
3:C:3789:CYS:SG	3:C:3834:SER:OG	2.75	0.44
2:N:12:LEU:O	2:N:15:VAL:HG12	2.18	0.44
2:M:21:GLY:HA2	2:M:26:LYS:HA	2.00	0.44
2:O:50:LYS:NZ	2:O:51:ASP:OD2	2.50	0.44
2:J:12:LEU:O	2:J:15:VAL:HG12	2.18	0.44
3:D:3406:LEU:HD11	3:D:3410:TYR:OH	2.18	0.44
3:D:3407:TYR:O	3:D:3411:PRO:CD	2.66	0.44
3:A:581:GLU:HG3	3:A:621:LEU:HD22	1.99	0.44
3:A:619:GLN:OE1	3:A:1679:ASN:ND2	2.49	0.44
3:A:3104:ILE:O	3:A:3107:MET:HB3	2.17	0.44
3:A:3380:LEU:HD21	3:A:3392:GLU:HA	2.00	0.44
3:A:3451:ASN:O	3:A:3454:ARG:HG2	2.18	0.44
3:B:875:LEU:HD11	3:B:1047:LEU:CD2	2.29	0.44
3:B:3380:LEU:HD21	3:B:3392:GLU:HA	2.00	0.44
3:C:1426:GLU:HG2	3:C:1427:ILE:N	2.33	0.44
3:C:2830:GLY:N	3:C:2934:ASN:OD1	2.51	0.44
3:C:3577:TYR:CZ	3:C:3583:ARG:HD3	2.53	0.44
2:I:50:LYS:NZ	2:I:51:ASP:OD2	2.50	0.43
3:D:2239:TYR:O	3:D:2243:ILE:HG12	2.18	0.43
3:D:2528:LEU:HA	3:D:2531:MET:HE2	1.99	0.43
3:D:2952:ILE:H	3:D:2952:ILE:HD12	1.82	0.43
3:A:3406:LEU:HD11	3:A:3410:TYR:OH	2.18	0.43
3:A:3511:ILE:HG23	3:A:3512:VAL:N	2.33	0.43
3:A:4766:ILE:HA	3:A:4769:ILE:HD12	1.99	0.43
3:A:4800:GLY:HA2	3:A:4806:PHE:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:73:SER:O	3:B:100:ARG:NH1	2.51	0.43
3:B:1120:ASP:OD1	3:B:1120:ASP:N	2.50	0.43
3:B:2758:LYS:O	3:B:2761:GLU:HG3	2.18	0.43
3:B:3407:TYR:O	3:B:3411:PRO:CD	2.66	0.43
3:B:3789:CYS:SG	3:B:3834:SER:OG	2.75	0.43
3:C:575:VAL:O	3:C:579:ILE:HG12	2.18	0.43
3:C:690:SER:N	3:C:777:LEU:O	2.52	0.43
3:C:3451:ASN:O	3:C:3454:ARG:HG2	2.18	0.43
2:L:12:LEU:O	2:L:15:VAL:HG12	2.18	0.43
2:P:20:SER:HB3	2:P:27:TYR:HA	1.99	0.43
3:D:73:SER:O	3:D:100:ARG:NH1	2.51	0.43
3:D:2758:LYS:O	3:D:2761:GLU:HG3	2.18	0.43
3:D:4173:ILE:HD12	3:D:4173:ILE:H	1.83	0.43
3:D:4800:GLY:HA2	3:D:4806:PHE:HB2	1.99	0.43
3:A:2239:TYR:O	3:A:2243:ILE:HG12	2.18	0.43
3:A:2268:MET:O	3:A:2269:GLN:HB3	2.18	0.43
3:A:4691:GLU:O	3:A:4692:ASP:CG	2.57	0.43
3:B:1090:TYR:N	3:B:1225:GLU:O	2.50	0.43
3:B:2930:PHE:HA	3:B:2933:MET:HG3	1.99	0.43
3:B:3869:ILE:O	3:B:3869:ILE:HG22	2.17	0.43
3:B:4691:GLU:O	3:B:4692:ASP:CG	2.57	0.43
3:C:1014:ILE:H	3:C:1014:ILE:HD12	1.84	0.43
3:C:2764:HIS:NE2	3:C:2791:MET:SD	2.92	0.43
2:K:74:GLU:O	2:K:78:LEU:HD13	2.19	0.43
2:L:48:VAL:HG23	2:L:49:GLN:N	2.34	0.43
2:P:48:VAL:HG23	2:P:49:GLN:N	2.33	0.43
3:D:2908:PRO:O	3:D:2911:THR:OG1	2.30	0.43
3:A:730:PRO:O	3:A:1477:MET:HE1	2.18	0.43
3:A:1120:ASP:N	3:A:1120:ASP:OD1	2.50	0.43
3:A:1426:GLU:HG2	3:A:1427:ILE:N	2.33	0.43
3:A:1473:VAL:HG22	3:A:1474:THR:N	2.33	0.43
3:A:2624:LEU:O	3:A:2628:VAL:HG23	2.18	0.43
3:A:4155:GLU:OE2	3:A:4183:ARG:NH1	2.50	0.43
3:A:4227:GLU:N	3:A:4227:GLU:OE2	2.51	0.43
3:B:1492:ASN:OD1	3:B:1493:CYS:N	2.51	0.43
3:B:4227:GLU:N	3:B:4227:GLU:OE2	2.51	0.43
3:C:245:LEU:HD23	3:C:301:VAL:HG12	1.99	0.43
3:C:1473:VAL:HG22	3:C:1474:THR:N	2.33	0.43
3:C:2268:MET:O	3:C:2269:GLN:HB3	2.18	0.43
3:C:3380:LEU:HD21	3:C:3392:GLU:HA	2.00	0.43
3:C:3406:LEU:HD11	3:C:3410:TYR:OH	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:74:GLU:O	2:M:78:LEU:HD13	2.19	0.43
2:O:21:GLY:HA2	2:O:26:LYS:HA	2.00	0.43
2:J:20:SER:HB3	2:J:27:TYR:HA	1.99	0.43
3:D:978:LEU:HD21	3:D:1045:ARG:HG2	2.00	0.43
3:D:3337:LYS:HD2	3:D:3465:ILE:HD11	2.01	0.43
3:D:4846:VAL:HG11	3:D:4885:MET:HG2	2.01	0.43
3:A:351:HIS:O	3:A:355:GLY:N	2.44	0.43
3:A:784:PHE:CG	3:A:788:ILE:HD11	2.53	0.43
3:A:2199:MET:SD	3:A:2204:MET:HE1	2.59	0.43
3:A:2764:HIS:NE2	3:A:2791:MET:SD	2.92	0.43
3:A:3324:ILE:HG23	3:A:3336:MET:SD	2.59	0.43
3:A:3526:CYS:SG	3:A:3527:ALA:N	2.92	0.43
3:A:4846:VAL:HG11	3:A:4885:MET:HG2	2.01	0.43
3:B:784:PHE:CG	3:B:788:ILE:HD11	2.54	0.43
3:B:1462:ASP:OD2	3:B:1469:LYS:NZ	2.47	0.43
3:B:1529:THR:OG1	3:B:1536:GLU:OE2	2.35	0.43
3:B:3320:ILE:O	3:B:3324:ILE:CD1	2.65	0.43
3:B:3337:LYS:HD2	3:B:3465:ILE:HD11	2.01	0.43
3:C:2758:LYS:O	3:C:2761:GLU:HG3	2.18	0.43
3:C:2952:ILE:HD12	3:C:2952:ILE:H	1.82	0.43
3:C:3324:ILE:HG23	3:C:3336:MET:SD	2.59	0.43
3:C:3933:ILE:HG22	3:C:3998:VAL:HG11	1.99	0.43
2:P:14:ASN:O	2:P:17:HIS:ND1	2.52	0.43
2:P:51:ASP:HB3	2:P:54:ALA:HB3	2.01	0.43
3:D:575:VAL:O	3:D:579:ILE:HG12	2.18	0.43
3:D:690:SER:N	3:D:777:LEU:O	2.52	0.43
3:D:951:LEU:CB	3:D:971:LEU:HD23	2.45	0.43
3:D:1195:LEU:N	3:D:1195:LEU:HD12	2.34	0.43
3:D:1492:ASN:OD1	3:D:1493:CYS:N	2.51	0.43
3:D:2764:HIS:NE2	3:D:2791:MET:SD	2.92	0.43
3:D:3607:LEU:O	3:D:3607:LEU:HD23	2.19	0.43
3:A:73:SER:O	3:A:100:ARG:NH1	2.51	0.43
3:A:1195:LEU:HD12	3:A:1195:LEU:N	2.34	0.43
3:B:1014:ILE:H	3:B:1014:ILE:HD12	1.84	0.43
3:B:2239:TYR:CE2	3:B:2243:ILE:HD11	2.54	0.43
3:B:3086:PRO:O	3:B:3089:VAL:HG22	2.19	0.43
3:B:3511:ILE:HG23	3:B:3512:VAL:N	2.33	0.43
3:B:4173:ILE:H	3:B:4173:ILE:HD12	1.83	0.43
3:B:4638:GLU:HB3	3:B:4639:PRO:HD3	2.01	0.43
3:B:4846:VAL:HG11	3:B:4885:MET:HG2	2.01	0.43
3:C:1222:GLU:OE1	3:C:1222:GLU:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1492:ASN:OD1	3:C:1493:CYS:N	2.51	0.43
3:C:2239:TYR:CE2	3:C:2243:ILE:HD11	2.54	0.43
3:C:3320:ILE:O	3:C:3324:ILE:CD1	2.65	0.43
3:C:3337:LYS:HD2	3:C:3465:ILE:HD11	2.01	0.43
3:C:3526:CYS:SG	3:C:3527:ALA:N	2.92	0.43
3:C:4909:LEU:HA	3:C:4912:VAL:HG22	1.99	0.43
2:P:12:LEU:O	2:P:15:VAL:HG12	2.18	0.43
2:J:48:VAL:HG23	2:J:49:GLN:N	2.33	0.43
3:D:169:ASP:OD1	3:D:202:ASN:ND2	2.51	0.43
3:D:576:LEU:HD22	3:D:610:CYS:HB2	1.99	0.43
3:D:581:GLU:HG3	3:D:621:LEU:HD22	1.99	0.43
3:D:784:PHE:CG	3:D:788:ILE:HD11	2.54	0.43
3:D:1014:ILE:H	3:D:1014:ILE:HD12	1.84	0.43
3:D:3320:ILE:O	3:D:3324:ILE:CD1	2.65	0.43
3:D:3722:LEU:HD11	3:D:3726:TYR:HE2	1.84	0.43
3:D:4691:GLU:O	3:D:4692:ASP:CG	2.57	0.43
3:A:576:LEU:HD22	3:A:610:CYS:HB2	1.99	0.43
3:A:1014:ILE:H	3:A:1014:ILE:HD12	1.84	0.43
3:A:1080:LYS:HA	3:A:1190:LEU:HD21	2.01	0.43
3:A:1496:VAL:HG12	3:A:1539:THR:HG21	2.00	0.43
3:A:3407:TYR:O	3:A:3411:PRO:CD	2.66	0.43
3:A:4173:ILE:H	3:A:4173:ILE:HD12	1.83	0.43
3:B:1195:LEU:N	3:B:1195:LEU:HD12	2.34	0.43
3:B:2268:MET:O	3:B:2269:GLN:HB3	2.18	0.43
3:B:2755:PHE:CZ	3:B:2931:LEU:HD23	2.54	0.43
3:B:3526:CYS:SG	3:B:3527:ALA:N	2.92	0.43
3:C:73:SER:O	3:C:100:ARG:NH1	2.51	0.43
3:C:3157:VAL:HG13	3:C:3158:ILE:N	2.34	0.43
3:C:3607:LEU:O	3:C:3607:LEU:HD23	2.19	0.43
3:C:4638:GLU:HB3	3:C:4639:PRO:HD3	2.01	0.43
3:C:4691:GLU:O	3:C:4692:ASP:CG	2.57	0.43
2:I:5:LEU:HD21	2:J:15:VAL:HG11	2.01	0.43
2:I:74:GLU:O	2:I:78:LEU:HD13	2.19	0.43
2:J:51:ASP:HB3	2:J:54:ALA:HB3	2.01	0.43
1:G:83:TYR:OH	3:C:1784:PHE:O	2.27	0.43
3:D:575:VAL:HA	3:D:578:ILE:HG22	2.01	0.43
3:D:2384:ALA:HB1	3:D:2423:ILE:CG2	2.49	0.43
3:D:2695:GLU:OE2	2:O:27:TYR:OH	2.37	0.43
3:D:2930:PHE:HA	3:D:2933:MET:HG3	1.99	0.43
3:D:3107:MET:O	3:D:3108:VAL:C	2.57	0.43
3:D:3324:ILE:HG23	3:D:3336:MET:SD	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4935:ILE:HG12	3:A:4932:GLY:HA2	2.00	0.43
3:A:2830:GLY:N	3:A:2934:ASN:OD1	2.51	0.43
3:B:215:VAL:CG1	3:B:275:LEU:HD12	2.47	0.43
3:B:1080:LYS:HA	3:B:1190:LEU:HD21	2.00	0.43
3:B:3157:VAL:HG13	3:B:3158:ILE:N	2.34	0.43
3:C:784:PHE:CG	3:C:788:ILE:HD11	2.54	0.43
3:C:914:LEU:HD23	3:C:919:ARG:HA	2.01	0.43
3:C:2755:PHE:CZ	3:C:2931:LEU:HD23	2.54	0.43
3:C:2883:TYR:HB2	3:C:2920:ASP:OD2	2.19	0.43
3:C:3373:VAL:HG22	3:C:3399:PHE:CE1	2.53	0.43
3:C:4846:VAL:HG11	3:C:4885:MET:HG2	2.01	0.43
2:L:46:LEU:HD23	2:L:47:ASP:N	2.34	0.43
2:P:62:LEU:HD12	2:P:70:VAL:HG11	2.01	0.43
3:A:2473:LEU:O	3:A:2500:LYS:NZ	2.45	0.43
3:A:2758:LYS:O	3:A:2761:GLU:HG3	2.18	0.43
3:A:3157:VAL:HG13	3:A:3158:ILE:N	2.34	0.43
3:A:3337:LYS:HD2	3:A:3465:ILE:HD11	2.01	0.43
3:B:2764:HIS:NE2	3:B:2791:MET:SD	2.92	0.43
3:B:3933:ILE:HG22	3:B:3998:VAL:HG11	1.99	0.43
3:C:575:VAL:HA	3:C:578:ILE:HG22	2.01	0.43
3:C:3086:PRO:O	3:C:3089:VAL:HG22	2.19	0.43
2:N:48:VAL:HG23	2:N:49:GLN:N	2.34	0.43
2:O:5:LEU:HD21	2:P:15:VAL:HG11	2.01	0.43
2:J:46:LEU:HD23	2:J:47:ASP:N	2.34	0.43
3:D:484:MET:HE2	3:D:484:MET:HA	2.00	0.43
3:D:2247:ASN:O	3:D:2250:SER:OG	2.28	0.43
3:D:3451:ASN:O	3:D:3454:ARG:HG2	2.18	0.43
3:D:3526:CYS:SG	3:D:3527:ALA:N	2.92	0.43
3:D:4671:ARG:NH1	3:D:4780:VAL:HG22	2.34	0.43
3:A:2755:PHE:CZ	3:A:2931:LEU:HD23	2.54	0.43
3:A:2930:PHE:HA	3:A:2933:MET:HG3	1.99	0.43
3:B:234:ILE:O	3:B:258:ARG:NH2	2.47	0.43
3:B:961:MET:SD	3:B:962:MET:O	2.77	0.43
3:B:3324:ILE:HG23	3:B:3336:MET:SD	2.59	0.43
3:B:3722:LEU:HD11	3:B:3726:TYR:HE2	1.84	0.43
3:B:3847:LEU:CD1	3:C:77:ARG:HE	2.32	0.43
3:C:880:HIS:CE1	3:C:909:VAL:O	2.72	0.43
3:C:2384:ALA:HB1	3:C:2423:ILE:CG2	2.49	0.43
2:N:46:LEU:HD23	2:N:47:ASP:N	2.34	0.43
3:D:961:MET:SD	3:D:962:MET:O	2.77	0.43
3:D:1106:ALA:HB2	3:D:1192:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:880:HIS:CE1	3:A:909:VAL:O	2.72	0.43
3:A:4638:GLU:HB3	3:A:4639:PRO:HD3	2.01	0.43
3:B:238:ASP:OD1	3:B:238:ASP:O	2.37	0.43
3:B:245:LEU:HD23	3:B:301:VAL:HG12	1.99	0.43
3:B:385:MET:HE1	3:C:169:ASP:OD2	2.18	0.43
3:B:575:VAL:HA	3:B:578:ILE:HG22	2.01	0.43
3:B:3373:VAL:HG22	3:B:3399:PHE:CE1	2.53	0.43
3:C:1106:ALA:HB2	3:C:1192:VAL:HG11	2.01	0.43
3:C:1437:SER:OG	3:C:1566:GLU:HB2	2.19	0.43
3:C:4964:ASP:OD1	3:C:4965:TYR:N	2.47	0.43
2:N:14:ASN:O	2:N:17:HIS:ND1	2.52	0.43
2:O:29:LEU:HB2	2:O:70:VAL:HB	2.01	0.43
3:D:77:ARG:HE	3:C:3847:LEU:CD1	2.32	0.42
3:D:238:ASP:OD1	3:D:238:ASP:O	2.37	0.42
3:D:2239:TYR:CE2	3:D:2243:ILE:HD11	2.54	0.42
3:A:690:SER:N	3:A:777:LEU:O	2.52	0.42
3:A:2384:ALA:HB1	3:A:2423:ILE:CG2	2.49	0.42
3:A:3320:ILE:O	3:A:3324:ILE:CD1	2.65	0.42
3:B:880:HIS:CE1	3:B:909:VAL:O	2.72	0.42
3:B:1426:GLU:HG2	3:B:1427:ILE:N	2.33	0.42
3:B:2883:TYR:HB2	3:B:2920:ASP:OD2	2.19	0.42
3:C:1435:TYR:OH	3:C:1569:LYS:C	2.58	0.42
3:C:4671:ARG:NH1	3:C:4780:VAL:HG22	2.34	0.42
3:C:4766:ILE:HA	3:C:4769:ILE:HD12	1.99	0.42
2:K:29:LEU:HB2	2:K:70:VAL:HB	2.01	0.42
2:N:15:VAL:HG11	2:M:5:LEU:HD21	2.01	0.42
2:P:16:PHE:HE2	2:P:27:TYR:CE2	2.37	0.42
2:P:46:LEU:HD23	2:P:47:ASP:N	2.34	0.42
2:J:14:ASN:O	2:J:17:HIS:ND1	2.52	0.42
3:D:880:HIS:CE1	3:D:909:VAL:O	2.72	0.42
3:D:1496:VAL:HG12	3:D:1539:THR:HG21	2.00	0.42
8:D:8007:PCW:H232	8:D:8007:PCW:H20	1.76	0.42
3:A:575:VAL:HA	3:A:578:ILE:HG22	2.00	0.42
3:A:961:MET:SD	3:A:962:MET:O	2.77	0.42
3:A:1462:ASP:OD2	3:A:1469:LYS:NZ	2.47	0.42
3:A:2239:TYR:CE2	3:A:2243:ILE:HD11	2.54	0.42
3:A:2883:TYR:HB2	3:A:2920:ASP:OD2	2.19	0.42
3:A:3356:ARG:HA	3:A:3360:ILE:HD12	2.01	0.42
3:B:1106:ALA:HB2	3:B:1192:VAL:HG11	2.01	0.42
3:B:2384:ALA:HB1	3:B:2423:ILE:CG2	2.49	0.42
3:B:3405:ASP:O	3:B:3409:LEU:HD23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:961:MET:SD	3:C:962:MET:O	2.77	0.42
3:C:2695:GLU:OE2	2:M:27:TYR:OH	2.37	0.42
3:C:3440:GLY:O	3:C:3444:ILE:HG12	2.19	0.42
3:C:3722:LEU:HD11	3:C:3726:TYR:HE2	1.84	0.42
2:N:16:PHE:HE2	2:N:27:TYR:CE2	2.37	0.42
2:O:62:LEU:HD21	2:O:70:VAL:HG11	2.01	0.42
2:O:74:GLU:O	2:O:78:LEU:HD13	2.18	0.42
2:J:16:PHE:HE2	2:J:27:TYR:CE2	2.37	0.42
3:D:234:ILE:O	3:D:258:ARG:NH2	2.47	0.42
3:D:1090:TYR:HD1	3:D:1153:MET:HG2	1.84	0.42
3:D:3176:LEU:HD23	3:D:3176:LEU:C	2.40	0.42
3:D:3356:ARG:HA	3:D:3360:ILE:HD12	2.01	0.42
3:D:3440:GLY:O	3:D:3444:ILE:HG12	2.19	0.42
3:A:684:ARG:NH1	3:A:708:VAL:O	2.43	0.42
3:A:1521:VAL:HG23	3:A:1521:VAL:O	2.19	0.42
3:A:2197:ASN:OD1	3:A:2200:ARG:NH2	2.46	0.42
3:A:4671:ARG:NH1	3:A:4780:VAL:HG22	2.34	0.42
3:B:575:VAL:O	3:B:579:ILE:HG12	2.18	0.42
3:B:914:LEU:HD23	3:B:919:ARG:HA	2.01	0.42
3:B:3607:LEU:HD23	3:B:3607:LEU:O	2.19	0.42
3:B:4671:ARG:NH1	3:B:4780:VAL:HG22	2.34	0.42
3:B:4766:ILE:HA	3:B:4769:ILE:HD12	1.99	0.42
3:C:914:LEU:O	3:C:919:ARG:NH2	2.53	0.42
3:C:978:LEU:HD21	3:C:1045:ARG:HG2	2.00	0.42
3:C:2438:ALA:HB2	3:C:2510:VAL:HG22	2.01	0.42
3:C:2930:PHE:HA	3:C:2933:MET:HG3	1.99	0.42
2:K:5:LEU:HD21	2:L:15:VAL:HG11	2.01	0.42
2:K:21:GLY:HA2	2:K:26:LYS:HA	2.00	0.42
2:I:27:TYR:OH	3:A:2695:GLU:OE2	2.37	0.42
3:D:2199:MET:HE1	3:D:2202:LEU:HD12	2.01	0.42
3:D:2755:PHE:CZ	3:D:2931:LEU:HD23	2.54	0.42
3:A:352:VAL:HG23	3:A:353:ALA:N	2.35	0.42
3:A:1106:ALA:HB2	3:A:1192:VAL:HG11	2.01	0.42
3:A:2179:MET:HE1	3:A:2183:ILE:CG1	2.50	0.42
3:A:3176:LEU:HD23	3:A:3176:LEU:C	2.40	0.42
3:A:4649:THR:HG1	3:A:4801:HIS:CD2	2.35	0.42
3:B:978:LEU:HD21	3:B:1045:ARG:HG2	2.00	0.42
3:B:4220:PHE:CZ	3:B:4237:PHE:HA	2.55	0.42
3:C:1195:LEU:HD12	3:C:1195:LEU:N	2.34	0.42
2:I:29:LEU:HB2	2:I:70:VAL:HB	2.01	0.42
3:D:102:LEU:HD12	3:D:151:MET:SD	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:351:HIS:O	3:D:355:GLY:N	2.44	0.42
3:D:1120:ASP:N	3:D:1120:ASP:OD1	2.50	0.42
3:D:2438:ALA:HB2	3:D:2510:VAL:HG22	2.01	0.42
3:D:2624:LEU:O	3:D:2628:VAL:HG23	2.18	0.42
3:D:2694:GLN:NE2	2:O:10:GLU:CD	2.63	0.42
3:D:3157:VAL:HG13	3:D:3158:ILE:N	2.34	0.42
3:D:4638:GLU:HB3	3:D:4639:PRO:HD3	2.01	0.42
3:A:234:ILE:O	3:A:258:ARG:NH2	2.46	0.42
3:A:238:ASP:OD1	3:A:238:ASP:O	2.37	0.42
3:A:310:THR:HG23	3:A:311:LYS:N	2.34	0.42
3:A:575:VAL:O	3:A:579:ILE:HG12	2.18	0.42
3:A:1437:SER:OG	3:A:1566:GLU:HB2	2.19	0.42
3:A:3086:PRO:O	3:A:3089:VAL:HG22	2.19	0.42
3:A:3107:MET:O	3:A:3108:VAL:C	2.57	0.42
3:A:3789:CYS:SG	3:A:3834:SER:OG	2.75	0.42
3:B:690:SER:N	3:B:777:LEU:O	2.51	0.42
3:B:2199:MET:HE1	3:B:2202:LEU:HD12	2.02	0.42
3:B:3135:VAL:HG13	3:B:3136:ALA:N	2.35	0.42
3:C:1080:LYS:HA	3:C:1190:LEU:HD21	2.00	0.42
3:C:3771:SER:OG	3:C:3775:ASN:OD1	2.33	0.42
2:L:16:PHE:HE2	2:L:27:TYR:CE2	2.37	0.42
2:I:21:GLY:HA2	2:I:26:LYS:HA	2.00	0.42
2:I:84:VAL:CG1	2:J:72:PHE:HE2	2.23	0.42
3:D:352:VAL:HG23	3:D:353:ALA:N	2.35	0.42
3:D:1080:LYS:HA	3:D:1190:LEU:HD21	2.00	0.42
3:D:1435:TYR:OH	3:D:1569:LYS:C	2.58	0.42
3:D:2160:LEU:HD13	3:D:2204:MET:HG2	2.02	0.42
3:D:3937:TYR:HD1	3:D:4002:MET:CE	2.33	0.42
3:A:102:LEU:HD12	3:A:151:MET:SD	2.60	0.42
3:A:1090:TYR:HD1	3:A:1153:MET:HG2	1.84	0.42
3:A:3937:TYR:HD1	3:A:4002:MET:CE	2.33	0.42
3:B:1437:SER:OG	3:B:1566:GLU:HB2	2.19	0.42
3:B:3107:MET:O	3:B:3108:VAL:C	2.57	0.42
3:B:3638:ARG:CZ	2:K:61:GLU:O	2.67	0.42
3:C:238:ASP:O	3:C:238:ASP:OD1	2.37	0.42
3:C:3135:VAL:HG13	3:C:3136:ALA:N	2.35	0.42
3:C:3176:LEU:HD23	3:C:3176:LEU:C	2.40	0.42
3:C:3356:ARG:HA	3:C:3360:ILE:HD12	2.01	0.42
2:N:51:ASP:HB3	2:N:54:ALA:HB3	2.01	0.42
2:M:29:LEU:HB2	2:M:70:VAL:HB	2.01	0.42
2:I:62:LEU:HD21	2:I:70:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:62:LEU:HD12	2:J:70:VAL:HG11	2.00	0.42
3:D:2199:MET:SD	3:D:2204:MET:HE1	2.60	0.42
3:D:2883:TYR:HB2	3:D:2920:ASP:OD2	2.19	0.42
3:D:3086:PRO:O	3:D:3089:VAL:HG22	2.19	0.42
3:D:3135:VAL:HG13	3:D:3136:ALA:N	2.35	0.42
3:A:2868:LEU:HD22	3:A:2872:LEU:HB3	2.02	0.42
3:A:3722:LEU:HD11	3:A:3726:TYR:HE2	1.84	0.42
3:B:351:HIS:O	3:B:355:GLY:N	2.44	0.42
3:B:352:VAL:HG23	3:B:353:ALA:N	2.34	0.42
3:B:1496:VAL:HG12	3:B:1539:THR:HG21	2.00	0.42
3:C:102:LEU:HD12	3:C:151:MET:SD	2.60	0.42
3:C:1496:VAL:HG12	3:C:1539:THR:HG21	2.00	0.42
3:C:2160:LEU:HD13	3:C:2204:MET:HG2	2.02	0.42
3:C:2528:LEU:HA	3:C:2531:MET:HE2	2.01	0.42
3:C:3402:LEU:HD23	3:C:3402:LEU:C	2.40	0.42
2:L:14:ASN:O	2:L:17:HIS:ND1	2.52	0.42
2:L:62:LEU:HD12	2:L:70:VAL:HG11	2.01	0.42
2:N:62:LEU:HD12	2:N:70:VAL:HG11	2.01	0.42
2:P:16:PHE:CG	2:P:75:TYR:OH	2.60	0.42
3:D:988:ARG:NH1	3:D:1059:GLN:OE1	2.53	0.42
3:D:3405:ASP:O	3:D:3409:LEU:HD23	2.19	0.42
3:D:3994:GLY:O	3:D:3998:VAL:HG23	2.20	0.42
3:A:914:LEU:O	3:A:919:ARG:NH2	2.53	0.42
3:A:3405:ASP:O	3:A:3409:LEU:HD23	2.19	0.42
3:A:3440:GLY:O	3:A:3444:ILE:HG12	2.19	0.42
3:A:3847:LEU:CD1	3:B:77:ARG:HE	2.33	0.42
3:A:4220:PHE:CZ	3:A:4237:PHE:HA	2.55	0.42
3:B:484:MET:HE2	3:B:484:MET:HA	2.01	0.42
3:B:914:LEU:O	3:B:919:ARG:NH2	2.53	0.42
3:B:1090:TYR:HD1	3:B:1153:MET:HG2	1.84	0.42
3:B:2695:GLU:OE2	2:K:27:TYR:OH	2.37	0.42
3:C:2698:ARG:NH2	2:M:17:HIS:CG	2.88	0.42
3:C:3405:ASP:O	3:C:3409:LEU:HD23	2.19	0.42
3:C:4220:PHE:CZ	3:C:4237:PHE:HA	2.55	0.42
2:L:51:ASP:HB3	2:L:54:ALA:HB3	2.01	0.42
3:D:914:LEU:O	3:D:919:ARG:NH2	2.53	0.42
3:D:1521:VAL:O	3:D:1521:VAL:HG23	2.19	0.42
3:D:2204:MET:O	3:D:2207:THR:N	2.53	0.42
3:D:2698:ARG:NH2	2:O:17:HIS:CG	2.88	0.42
3:A:15:LEU:HD12	3:A:166:VAL:HG22	2.02	0.42
3:A:649:ILE:HG23	3:A:815:ALA:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2281:VAL:O	3:A:2281:VAL:HG22	2.20	0.42
3:A:3135:VAL:HG13	3:A:3136:ALA:N	2.35	0.42
3:A:3946:ILE:HD11	3:A:4005:LYS:HE3	2.02	0.42
3:B:1435:TYR:OH	3:B:1569:LYS:C	2.58	0.42
3:B:2654:LYS:HD2	3:B:2658:LEU:HD11	2.02	0.42
3:B:3587:ALA:HA	3:B:3593:ILE:HD11	2.02	0.42
3:B:3946:ILE:HD11	3:B:4005:LYS:HE3	2.02	0.42
3:B:4678:LYS:HD3	3:B:4684:LEU:HD22	2.02	0.42
3:B:4862:ASN:HB2	3:B:4872:MET:HE1	2.01	0.42
2:O:84:VAL:CG1	2:P:72:PHE:HE2	2.23	0.42
3:D:243:ARG:NH1	3:D:482:GLU:OE2	2.48	0.42
3:D:914:LEU:HD23	3:D:919:ARG:HA	2.01	0.42
3:D:1437:SER:OG	3:D:1566:GLU:HB2	2.19	0.42
3:D:3638:ARG:CZ	2:O:61:GLU:O	2.67	0.42
3:D:4862:ASN:HB2	3:D:4872:MET:HE1	2.02	0.42
3:A:2438:ALA:HB2	3:A:2510:VAL:HG22	2.01	0.42
3:A:2939:THR:HG22	3:A:2941:GLY:H	1.85	0.42
3:A:3607:LEU:O	3:A:3607:LEU:HD23	2.19	0.42
3:A:3936:PHE:CD2	3:A:3954:PHE:HE1	2.38	0.42
3:B:2939:THR:HG22	3:B:2941:GLY:H	1.85	0.42
3:B:3176:LEU:C	3:B:3176:LEU:HD23	2.40	0.42
3:B:3937:TYR:HD1	3:B:4002:MET:CE	2.33	0.42
3:B:4993:LEU:HA	3:B:4993:LEU:HD23	1.83	0.42
3:C:352:VAL:HG23	3:C:353:ALA:N	2.35	0.42
3:C:940:VAL:HG12	3:C:1054:ILE:HG22	2.02	0.42
3:C:2968:MET:HE1	3:C:3047:LEU:HD13	2.02	0.42
3:C:3551:ARG:HD3	3:C:3598:GLN:HG3	2.02	0.42
3:C:3587:ALA:HA	3:C:3593:ILE:HD11	2.02	0.42
2:L:29:LEU:CD1	2:L:33:GLU:HB3	2.50	0.42
3:D:1462:ASP:OD2	3:D:1469:LYS:NZ	2.47	0.41
3:D:2420:GLY:O	3:D:2423:ILE:HG22	2.20	0.41
3:D:2939:THR:HG22	3:D:2941:GLY:H	1.85	0.41
3:D:3343:ALA:O	3:D:3346:ILE:HG12	2.20	0.41
3:D:4678:LYS:HD3	3:D:4684:LEU:HD22	2.02	0.41
3:A:4692:ASP:OD1	3:A:4692:ASP:C	2.59	0.41
3:B:1521:VAL:HG23	3:B:1521:VAL:O	2.19	0.41
3:B:2978:LEU:HA	3:B:2981:VAL:HG22	2.02	0.41
3:B:3440:GLY:O	3:B:3444:ILE:HG12	2.19	0.41
3:C:310:THR:HG23	3:C:311:LYS:N	2.35	0.41
3:C:649:ILE:HG23	3:C:815:ALA:HB3	2.02	0.41
3:C:1772:SER:OG	3:C:1957:GLU:OE2	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3937:TYR:HD1	3:C:4002:MET:CE	2.33	0.41
3:D:905:HIS:NE2	3:D:907:CYS:HB2	2.35	0.41
3:D:2417:VAL:HG23	3:D:2417:VAL:O	2.21	0.41
3:D:3355:LEU:HD11	3:D:3431:ASN:ND2	2.35	0.41
3:D:4220:PHE:CZ	3:D:4237:PHE:HA	2.55	0.41
3:D:4692:ASP:OD1	3:D:4692:ASP:C	2.59	0.41
3:A:988:ARG:NH1	3:A:1059:GLN:OE1	2.53	0.41
3:A:3587:ALA:HA	3:A:3593:ILE:HD11	2.02	0.41
3:A:3974:GLY:N	3:A:3975:PRO:HA	2.35	0.41
3:A:4942:ARG:NE	3:B:4936:ASP:OD1	2.52	0.41
3:B:243:ARG:NH1	3:B:482:GLU:OE2	2.48	0.41
3:B:310:THR:HG23	3:B:311:LYS:N	2.35	0.41
3:B:2438:ALA:HB2	3:B:2510:VAL:HG22	2.01	0.41
3:B:3513:ALA:O	3:B:3517:LYS:HG2	2.20	0.41
3:C:1090:TYR:HD1	3:C:1153:MET:HG2	1.84	0.41
3:C:3107:MET:O	3:C:3108:VAL:C	2.57	0.41
3:D:221:LEU:HD21	3:D:263:LEU:HD11	2.02	0.41
3:D:310:THR:HG23	3:D:311:LYS:N	2.35	0.41
3:D:2978:LEU:HA	3:D:2981:VAL:HG22	2.02	0.41
3:D:3131:THR:O	3:D:3135:VAL:HG12	2.21	0.41
3:A:1304:CYS:O	3:A:1305:THR:OG1	2.36	0.41
3:A:2654:LYS:HD2	3:A:2658:LEU:HD11	2.02	0.41
3:A:2768:ALA:HB3	3:A:2858:PRO:HB3	2.03	0.41
3:A:3355:LEU:HD11	3:A:3431:ASN:ND2	2.35	0.41
3:A:3994:GLY:O	3:A:3998:VAL:HG23	2.20	0.41
3:B:760:ILE:HG23	3:B:760:ILE:O	2.20	0.41
3:B:986:VAL:CG2	3:B:1044:VAL:HG11	2.50	0.41
3:B:2698:ARG:NH2	2:K:17:HIS:CG	2.88	0.41
3:B:3895:CYS:HG	3:B:3902:PHE:HD2	1.66	0.41
3:C:986:VAL:CG2	3:C:1044:VAL:HG11	2.50	0.41
3:C:1521:VAL:HG23	3:C:1521:VAL:O	2.19	0.41
3:C:2281:VAL:O	3:C:2281:VAL:HG22	2.20	0.41
3:C:2791:MET:SD	3:C:2791:MET:O	2.79	0.41
3:C:2978:LEU:HA	3:C:2981:VAL:HG22	2.02	0.41
3:C:3343:ALA:O	3:C:3346:ILE:HG12	2.20	0.41
3:C:3638:ARG:CZ	2:M:61:GLU:O	2.67	0.41
2:M:62:LEU:HD21	2:M:70:VAL:HG11	2.01	0.41
2:M:73:LYS:O	2:M:76:VAL:HG22	2.21	0.41
3:D:2925:GLN:OE1	3:D:2929:LYS:CE	2.68	0.41
3:D:3683:GLU:OE1	3:D:3683:GLU:O	2.39	0.41
3:D:4090:LEU:HD13	3:D:4127:ASN:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:760:ILE:HG23	3:A:760:ILE:O	2.20	0.41
3:A:2420:GLY:O	3:A:2423:ILE:HG22	2.20	0.41
3:A:3847:LEU:HD11	3:A:3935:ASP:HB3	2.03	0.41
3:B:15:LEU:HD12	3:B:166:VAL:HG22	2.02	0.41
3:B:221:LEU:HD21	3:B:263:LEU:HD11	2.02	0.41
3:B:940:VAL:HG12	3:B:1054:ILE:HG22	2.02	0.41
3:B:988:ARG:NH1	3:B:1059:GLN:OE1	2.53	0.41
3:B:2281:VAL:HG22	3:B:2281:VAL:O	2.20	0.41
3:B:2698:ARG:HH21	2:K:17:HIS:CE1	2.38	0.41
3:B:2968:MET:HE1	3:B:3047:LEU:HD13	2.03	0.41
3:B:3637:PHE:HE2	2:K:82:LEU:HD22	1.86	0.41
3:B:4552:TYR:O	3:B:4556:ASN:ND2	2.52	0.41
3:C:2420:GLY:O	3:C:2423:ILE:HG22	2.20	0.41
3:C:2654:LYS:HD2	3:C:2658:LEU:HD11	2.02	0.41
3:C:2939:THR:HG22	3:C:2941:GLY:H	1.85	0.41
2:K:62:LEU:HD21	2:K:70:VAL:HG11	2.01	0.41
2:I:61:GLU:O	3:A:3638:ARG:CZ	2.67	0.41
3:D:2940:ARG:NH1	3:D:2942:LEU:HD11	2.36	0.41
3:D:3946:ILE:HD11	3:D:4005:LYS:HE3	2.02	0.41
3:A:905:HIS:NE2	3:A:907:CYS:HB2	2.36	0.41
3:A:914:LEU:HD23	3:A:919:ARG:HA	2.01	0.41
3:A:2204:MET:O	3:A:2207:THR:N	2.53	0.41
3:A:2925:GLN:OE1	3:A:2929:LYS:NZ	2.51	0.41
3:A:2978:LEU:HA	3:A:2981:VAL:HG22	2.02	0.41
3:A:3551:ARG:HD3	3:A:3598:GLN:HG3	2.02	0.41
3:A:3683:GLU:OE1	3:A:3683:GLU:O	2.39	0.41
3:A:4090:LEU:HD13	3:A:4127:ASN:HA	2.02	0.41
3:A:4678:LYS:HD3	3:A:4684:LEU:HD22	2.02	0.41
8:A:8006:PCW:H41	8:A:8006:PCW:H63	1.83	0.41
3:B:649:ILE:HG23	3:B:815:ALA:HB3	2.02	0.41
3:B:1435:TYR:HD1	3:B:1573:ILE:HG21	1.86	0.41
3:B:2204:MET:O	3:B:2207:THR:N	2.53	0.41
3:B:2322:ILE:O	3:B:2322:ILE:HG22	2.21	0.41
3:B:2768:ALA:HB3	3:B:2858:PRO:HB3	2.03	0.41
3:B:3936:PHE:CD2	3:B:3954:PHE:HE1	2.38	0.41
3:B:4090:LEU:HD13	3:B:4127:ASN:HA	2.02	0.41
3:C:1464:SER:O	3:C:1469:LYS:NZ	2.46	0.41
3:C:2698:ARG:HH21	2:M:17:HIS:CE1	2.38	0.41
2:I:17:HIS:CG	3:A:2698:ARG:NH2	2.88	0.41
1:H:26:HIS:HB3	1:H:41:ARG:NE	2.36	0.41
3:D:15:LEU:HD12	3:D:166:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1435:TYR:HD1	3:D:1573:ILE:HG21	1.86	0.41
3:D:2875:MET:HE1	3:D:2938:VAL:HG11	2.02	0.41
3:D:3637:PHE:HE2	2:O:82:LEU:HD22	1.86	0.41
3:A:940:VAL:HG12	3:A:1054:ILE:HG22	2.02	0.41
3:A:1090:TYR:OH	3:A:1092:GLU:OE2	2.35	0.41
3:A:1236:THR:OG1	3:A:1703:ARG:NH1	2.54	0.41
3:A:2247:ASN:O	3:A:2250:SER:OG	2.28	0.41
3:A:2703:CYS:O	3:A:2707:ILE:CD1	2.68	0.41
3:A:3343:ALA:O	3:A:3346:ILE:HG12	2.20	0.41
3:A:4154:SER:HB2	3:A:4167:LEU:HD11	2.02	0.41
3:A:4552:TYR:O	3:A:4556:ASN:ND2	2.52	0.41
3:B:1236:THR:OG1	3:B:1703:ARG:NH1	2.54	0.41
3:B:1930:MET:HG2	3:B:1930:MET:O	2.21	0.41
3:B:2925:GLN:OE1	3:B:2929:LYS:CE	2.68	0.41
3:B:3131:THR:O	3:B:3135:VAL:HG12	2.21	0.41
3:C:1236:THR:OG1	3:C:1703:ARG:NH1	2.54	0.41
3:C:1930:MET:HG2	3:C:1930:MET:O	2.21	0.41
3:C:2322:ILE:O	3:C:2322:ILE:HG22	2.21	0.41
3:C:3231:LEU:HB2	3:C:3233:LEU:HD23	2.03	0.41
3:C:3946:ILE:HD11	3:C:4005:LYS:HE3	2.02	0.41
2:K:12:LEU:O	2:K:15:VAL:HG12	2.21	0.41
1:E:59:GLY:CA	1:E:77:ILE:HD12	2.51	0.41
3:D:1293:SER:C	3:D:1294:LEU:HD22	2.41	0.41
3:D:2281:VAL:O	3:D:2281:VAL:HG22	2.20	0.41
3:D:3551:ARG:HD3	3:D:3598:GLN:HG3	2.02	0.41
3:A:221:LEU:HD21	3:A:263:LEU:HD11	2.03	0.41
3:A:3254:ILE:HD11	3:A:3275:LEU:HD11	2.03	0.41
3:A:3267:MET:HG3	3:A:3271:ILE:CD1	2.51	0.41
3:A:3402:LEU:HD23	3:A:3402:LEU:C	2.40	0.41
3:A:3631:ARG:HA	3:A:3634:VAL:HG12	2.03	0.41
3:B:634:LEU:HB3	3:B:1640:LEU:HD11	2.03	0.41
3:B:1293:SER:C	3:B:1294:LEU:HD22	2.41	0.41
3:B:3267:MET:HG3	3:B:3271:ILE:CD1	2.51	0.41
3:B:3355:LEU:HD11	3:B:3431:ASN:ND2	2.35	0.41
3:C:784:PHE:HB3	3:C:788:ILE:HD13	2.03	0.41
3:C:1293:SER:C	3:C:1294:LEU:HD22	2.41	0.41
3:C:1695:LEU:O	3:C:1699:LEU:HG	2.21	0.41
3:C:2940:ARG:NH1	3:C:2942:LEU:HD11	2.36	0.41
3:C:3254:ILE:HD11	3:C:3275:LEU:HD11	2.03	0.41
3:C:3355:LEU:HD11	3:C:3431:ASN:ND2	2.35	0.41
3:C:3994:GLY:O	3:C:3998:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:4678:LYS:HD3	3:C:4684:LEU:HD22	2.02	0.41
2:I:12:LEU:O	2:I:15:VAL:HG12	2.21	0.41
2:J:29:LEU:CD1	2:J:33:GLU:HB3	2.50	0.41
3:D:215:VAL:HG12	3:D:275:LEU:HD12	2.03	0.41
3:D:1244:PRO:O	3:D:1459:HIS:ND1	2.54	0.41
3:D:3185:GLU:HA	3:D:3188:ARG:HG3	2.03	0.41
3:D:3254:ILE:HD11	3:D:3275:LEU:HD11	2.03	0.41
3:D:3847:LEU:HD11	3:D:3935:ASP:HB3	2.03	0.41
3:D:3974:GLY:N	3:D:3975:PRO:HA	2.35	0.41
3:A:215:VAL:HG12	3:A:275:LEU:HD12	2.03	0.41
3:A:2940:ARG:NH1	3:A:2942:LEU:HD11	2.36	0.41
3:A:3513:ALA:O	3:A:3517:LYS:HG2	2.20	0.41
3:B:2249:ARG:HD3	3:B:2287:LEU:HD21	2.03	0.41
3:B:2420:GLY:O	3:B:2423:ILE:HG22	2.20	0.41
3:B:3356:ARG:HA	3:B:3360:ILE:HD12	2.01	0.41
3:B:4154:SER:HB2	3:B:4167:LEU:HD11	2.02	0.41
3:C:988:ARG:NH1	3:C:1059:GLN:OE1	2.53	0.41
3:C:2417:VAL:HG23	3:C:2417:VAL:O	2.21	0.41
3:C:3637:PHE:HE2	2:M:82:LEU:HD22	1.86	0.41
2:I:82:LEU:HD22	3:A:3637:PHE:HE2	1.86	0.41
1:G:26:HIS:HB3	1:G:41:ARG:NE	2.36	0.41
3:D:610:CYS:O	3:D:613:VAL:HG22	2.21	0.41
3:D:940:VAL:HG12	3:D:1054:ILE:HG22	2.02	0.41
3:D:986:VAL:CG2	3:D:1044:VAL:HG11	2.50	0.41
3:D:1021:ARG:HE	7:D:8005:ATP:N6	2.16	0.41
3:D:1695:LEU:O	3:D:1699:LEU:HG	2.21	0.41
3:D:2171:MET:SD	3:D:2229:MET:CE	3.09	0.41
3:D:2791:MET:SD	3:D:2791:MET:O	2.79	0.41
3:D:2868:LEU:HD22	3:D:2872:LEU:HB3	2.02	0.41
3:D:2925:GLN:OE1	3:D:2929:LYS:NZ	2.51	0.41
3:D:3587:ALA:HA	3:D:3593:ILE:HD11	2.02	0.41
3:A:610:CYS:O	3:A:613:VAL:HG22	2.21	0.41
3:A:986:VAL:CG2	3:A:1044:VAL:HG11	2.50	0.41
3:A:1435:TYR:OH	3:A:1569:LYS:C	2.58	0.41
3:A:1435:TYR:HB3	3:A:1520:LEU:HG	2.03	0.41
3:A:1435:TYR:HD1	3:A:1573:ILE:HG21	1.86	0.41
3:A:1752:GLY:H	3:A:1756:GLU:HA	1.86	0.41
3:A:2160:LEU:HD13	3:A:2204:MET:HG2	2.02	0.41
3:A:2940:ARG:HG2	3:A:2942:LEU:HD22	2.03	0.41
3:A:3862:VAL:HG13	3:A:3863:ASN:N	2.36	0.41
3:B:215:VAL:HG12	3:B:275:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2160:LEU:HD13	3:B:2204:MET:HG2	2.02	0.41
3:B:2207:THR:O	3:B:2211:VAL:HG23	2.21	0.41
3:B:2417:VAL:O	3:B:2417:VAL:HG23	2.21	0.41
3:B:2578:ILE:HG23	3:B:2579:MET:N	2.36	0.41
3:B:2791:MET:SD	3:B:2791:MET:O	2.79	0.41
3:B:2868:LEU:HD22	3:B:2872:LEU:HB3	2.02	0.41
3:B:3231:LEU:HB2	3:B:3233:LEU:HD23	2.03	0.41
3:B:3263:ARG:NH2	3:B:3330:ILE:HD12	2.36	0.41
3:B:3343:ALA:O	3:B:3346:ILE:HG12	2.20	0.41
3:B:3402:LEU:HD23	3:B:3402:LEU:C	2.40	0.41
3:B:3631:ARG:HA	3:B:3634:VAL:HG12	2.03	0.41
3:B:3683:GLU:OE1	3:B:3683:GLU:O	2.39	0.41
3:B:3994:GLY:O	3:B:3998:VAL:HG23	2.20	0.41
3:C:215:VAL:HG12	3:C:275:LEU:HD12	2.03	0.41
3:C:1435:TYR:HD1	3:C:1573:ILE:HG21	1.86	0.41
3:C:2171:MET:SD	3:C:2229:MET:CE	3.09	0.41
3:C:2578:ILE:HG23	3:C:2579:MET:N	2.36	0.41
3:C:2768:ALA:HB3	3:C:2858:PRO:HB3	2.03	0.41
3:C:2925:GLN:OE1	3:C:2929:LYS:NZ	2.51	0.41
3:C:2940:ARG:HG2	3:C:2942:LEU:HD22	2.03	0.41
3:C:3219:VAL:HG13	3:C:3220:TYR:N	2.36	0.41
3:C:3457:GLN:HA	3:C:3460:VAL:HG12	2.03	0.41
3:C:3513:ALA:O	3:C:3517:LYS:HG2	2.20	0.41
3:C:3862:VAL:HG13	3:C:3863:ASN:N	2.36	0.41
3:C:3974:GLY:N	3:C:3975:PRO:HA	2.35	0.41
3:C:4692:ASP:OD1	3:C:4692:ASP:C	2.59	0.41
2:O:73:LYS:O	2:O:76:VAL:HG22	2.21	0.41
2:P:29:LEU:CD1	2:P:33:GLU:HB3	2.50	0.41
3:D:649:ILE:HG23	3:D:815:ALA:HB3	2.02	0.41
3:D:1930:MET:HG2	3:D:1930:MET:O	2.21	0.41
3:D:2226:PHE:N	3:D:2227:PRO:HD3	2.36	0.41
3:D:2564:THR:HG22	3:D:2607:CYS:CA	2.45	0.41
3:D:3513:ALA:O	3:D:3517:LYS:HG2	2.20	0.41
3:D:4154:SER:HB2	3:D:4167:LEU:HD11	2.02	0.41
3:D:4763:LEU:HD12	3:D:4764:THR:N	2.36	0.41
3:A:1217:ILE:HD12	3:A:1217:ILE:H	1.86	0.41
3:A:1244:PRO:O	3:A:1459:HIS:ND1	2.54	0.41
3:A:1293:SER:C	3:A:1294:LEU:HD22	2.41	0.41
3:A:2207:THR:O	3:A:2211:VAL:HG23	2.21	0.41
3:A:2771:LYS:O	3:A:2776:TRP:N	2.53	0.41
3:A:2968:MET:HE1	3:A:3047:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1244:PRO:O	3:B:1459:HIS:ND1	2.54	0.41
3:B:1464:SER:O	3:B:1469:LYS:NZ	2.46	0.41
3:B:2314:LEU:HD12	3:B:2319:TYR:CD2	2.56	0.41
3:B:2940:ARG:NH1	3:B:2942:LEU:HD11	2.36	0.41
3:B:3457:GLN:HA	3:B:3460:VAL:HG12	2.03	0.41
3:C:221:LEU:HD21	3:C:263:LEU:HD11	2.02	0.41
3:C:610:CYS:O	3:C:613:VAL:HG22	2.21	0.41
3:C:634:LEU:HB3	3:C:1640:LEU:HD11	2.03	0.41
3:C:905:HIS:NE2	3:C:907:CYS:HB2	2.35	0.41
3:C:1244:PRO:O	3:C:1459:HIS:ND1	2.54	0.41
3:C:2226:PHE:N	3:C:2227:PRO:HD3	2.36	0.41
3:C:3847:LEU:HD11	3:C:3935:ASP:HB3	2.03	0.41
3:C:4090:LEU:HD13	3:C:4127:ASN:HA	2.02	0.41
3:C:4862:ASN:HB2	3:C:4872:MET:HE1	2.03	0.41
1:F:59:GLY:CA	1:F:77:ILE:HD12	2.51	0.40
3:D:284:ARG:NH1	3:D:291:TYR:OH	2.54	0.40
3:D:1217:ILE:H	3:D:1217:ILE:HD12	1.86	0.40
3:D:1236:THR:OG1	3:D:1703:ARG:NH1	2.54	0.40
3:D:1435:TYR:HB3	3:D:1520:LEU:HG	2.03	0.40
3:D:2505:LEU:HD23	3:D:2505:LEU:C	2.42	0.40
3:D:2654:LYS:HD2	3:D:2658:LEU:HD11	2.02	0.40
3:D:2768:ALA:HB3	3:D:2858:PRO:HB3	2.03	0.40
3:D:3219:VAL:HG13	3:D:3220:TYR:N	2.36	0.40
3:D:3862:VAL:HG13	3:D:3863:ASN:N	2.36	0.40
3:D:4942:ARG:NE	3:A:4936:ASP:OD1	2.51	0.40
3:A:263:LEU:HB3	3:A:281:LEU:HD12	2.04	0.40
3:A:2171:MET:SD	3:A:2229:MET:CE	3.09	0.40
3:A:2322:ILE:HG22	3:A:2322:ILE:O	2.21	0.40
3:A:3263:ARG:NH2	3:A:3330:ILE:HD12	2.36	0.40
3:B:102:LEU:HD12	3:B:151:MET:SD	2.60	0.40
3:B:263:LEU:HB3	3:B:281:LEU:HD12	2.04	0.40
3:B:784:PHE:HB3	3:B:788:ILE:HD13	2.03	0.40
3:B:1821:VAL:HG22	3:B:1927:LEU:HD21	2.04	0.40
3:B:2432:ASP:O	3:B:2436:ARG:HG2	2.21	0.40
3:B:2625:ARG:HA	3:B:2675:LEU:HD23	2.03	0.40
3:B:2701:MET:HE1	3:B:2702:PRO:HG3	2.03	0.40
3:B:4763:LEU:HD12	3:B:4764:THR:N	2.36	0.40
8:B:8007:PCW:H20	8:B:8007:PCW:H232	1.76	0.40
3:C:15:LEU:HD12	3:C:166:VAL:HG22	2.02	0.40
3:C:1041:CYS:O	3:C:1044:VAL:HG12	2.22	0.40
3:C:1567:LEU:HD12	3:C:1567:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2204:MET:O	3:C:2207:THR:N	2.53	0.40
3:C:2249:ARG:HD3	3:C:2287:LEU:HD21	2.03	0.40
3:C:3683:GLU:OE1	3:C:3683:GLU:O	2.39	0.40
2:N:29:LEU:CD1	2:N:33:GLU:HB3	2.50	0.40
2:M:59:MET:SD	2:M:63:ASP:OD2	2.79	0.40
2:I:59:MET:SD	2:I:63:ASP:OD2	2.79	0.40
3:D:2207:THR:O	3:D:2211:VAL:HG23	2.21	0.40
3:D:2260:GLU:OE2	3:D:2298:LYS:NZ	2.22	0.40
3:D:3402:LEU:HD23	3:D:3402:LEU:C	2.40	0.40
3:D:3631:ARG:HA	3:D:3634:VAL:HG12	2.03	0.40
3:D:4883:PHE:CE2	3:D:4895:ILE:HD11	2.57	0.40
3:A:77:ARG:O	3:A:81:GLU:HG2	2.22	0.40
3:A:1930:MET:HG2	3:A:1930:MET:O	2.21	0.40
3:A:1932:LEU:HG	3:A:1936:VAL:HG11	2.03	0.40
3:A:3131:THR:O	3:A:3135:VAL:HG12	2.21	0.40
3:A:4653:PHE:N	3:A:4794:MET:HE1	2.35	0.40
3:A:4883:PHE:CE2	3:A:4895:ILE:HD11	2.57	0.40
3:B:180:TYR:HB2	3:B:197:MET:O	2.22	0.40
3:B:905:HIS:NE2	3:B:907:CYS:HB2	2.35	0.40
3:B:2940:ARG:HG2	3:B:2942:LEU:HD22	2.03	0.40
3:B:3219:VAL:HG13	3:B:3220:TYR:N	2.36	0.40
3:B:3861:MET:HG2	3:B:3863:ASN:O	2.21	0.40
3:B:4692:ASP:OD1	3:B:4692:ASP:C	2.59	0.40
3:C:1932:LEU:HG	3:C:1936:VAL:HG11	2.03	0.40
3:C:2868:LEU:HD22	3:C:2872:LEU:HB3	2.02	0.40
3:C:2925:GLN:OE1	3:C:2929:LYS:CE	2.68	0.40
3:C:4154:SER:HB2	3:C:4167:LEU:HD11	2.02	0.40
3:C:4552:TYR:O	3:C:4556:ASN:ND2	2.52	0.40
2:M:12:LEU:O	2:M:15:VAL:HG12	2.21	0.40
3:D:77:ARG:O	3:D:81:GLU:HG2	2.22	0.40
3:D:2701:MET:HB3	3:D:2701:MET:HE3	2.02	0.40
3:D:3322:ARG:O	3:D:3325:VAL:HG12	2.21	0.40
3:D:3454:ARG:O	3:D:3458:ASN:OD1	2.40	0.40
3:D:3936:PHE:CD2	3:D:3954:PHE:HE1	2.38	0.40
3:A:1116:LEU:HD12	3:A:1194:SER:CB	2.51	0.40
3:B:619:GLN:OE1	3:B:1679:ASN:ND2	2.49	0.40
3:B:1752:GLY:H	3:B:1756:GLU:HA	1.86	0.40
3:C:180:TYR:HB2	3:C:197:MET:O	2.22	0.40
3:C:1021:ARG:HE	7:C:5106:ATP:N6	2.16	0.40
3:C:1821:VAL:HG22	3:C:1927:LEU:HD21	2.04	0.40
3:C:2224:ILE:HD12	3:C:2268:MET:CE	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2314:LEU:HD12	3:C:2319:TYR:CD2	2.56	0.40
3:C:3263:ARG:NH2	3:C:3330:ILE:HD12	2.36	0.40
3:C:3861:MET:HG2	3:C:3863:ASN:O	2.21	0.40
2:K:59:MET:SD	2:K:63:ASP:OD2	2.79	0.40
2:O:59:MET:SD	2:O:63:ASP:OD2	2.79	0.40
3:D:992:ASN:C	3:D:992:ASN:HD22	2.25	0.40
3:D:1567:LEU:HD12	3:D:1567:LEU:N	2.36	0.40
3:D:1821:VAL:HG22	3:D:1927:LEU:HD21	2.04	0.40
3:D:3263:ARG:NH2	3:D:3330:ILE:HD12	2.36	0.40
3:D:3267:MET:HG3	3:D:3271:ILE:CD1	2.51	0.40
3:D:4818:VAL:HG11	3:A:4837:MET:CE	2.52	0.40
3:A:284:ARG:NH1	3:A:291:TYR:OH	2.54	0.40
3:A:1695:LEU:O	3:A:1699:LEU:HG	2.21	0.40
3:A:2314:LEU:HD12	3:A:2319:TYR:CD2	2.56	0.40
3:A:3317:LEU:O	3:A:3321:LEU:HD23	2.22	0.40
3:A:3322:ARG:O	3:A:3325:VAL:HG12	2.21	0.40
3:A:4862:ASN:HB2	3:A:4872:MET:HE1	2.02	0.40
3:B:992:ASN:C	3:B:992:ASN:HD22	2.25	0.40
3:B:1695:LEU:O	3:B:1699:LEU:HG	2.21	0.40
3:B:1964:GLU:HA	3:B:3651:CYS:SG	2.62	0.40
3:B:2171:MET:SD	3:B:2229:MET:CE	3.09	0.40
3:B:2224:ILE:HD12	3:B:2268:MET:CE	2.52	0.40
3:B:3181:ASN:HB2	3:B:3184:VAL:CG2	2.52	0.40
3:B:3454:ARG:O	3:B:3458:ASN:OD1	2.40	0.40
3:B:3974:GLY:N	3:B:3975:PRO:HA	2.35	0.40
3:C:284:ARG:NH1	3:C:291:TYR:OH	2.54	0.40
3:C:1964:GLU:HA	3:C:3651:CYS:SG	2.62	0.40
3:C:2505:LEU:HD23	3:C:2505:LEU:C	2.42	0.40
3:C:3185:GLU:HA	3:C:3188:ARG:HG3	2.03	0.40
3:C:3267:MET:HG3	3:C:3271:ILE:CD1	2.51	0.40
3:C:3936:PHE:CD2	3:C:3954:PHE:CE1	3.10	0.40
2:P:6:GLU:HA	2:P:9:MET:CE	2.52	0.40
2:I:17:HIS:CE1	3:A:2698:ARG:HH21	2.39	0.40
2:I:73:LYS:O	2:I:76:VAL:HG22	2.21	0.40
3:D:760:ILE:O	3:D:760:ILE:HG23	2.20	0.40
3:D:3317:LEU:O	3:D:3321:LEU:HD23	2.22	0.40
3:D:3936:PHE:CD2	3:D:3954:PHE:CE1	3.10	0.40
3:A:1041:CYS:O	3:A:1044:VAL:HG12	2.22	0.40
3:A:1449:VAL:HG22	3:A:1555:VAL:HG23	2.04	0.40
3:A:1481:GLN:O	3:A:1481:GLN:HG2	2.21	0.40
3:A:2417:VAL:HG23	3:A:2417:VAL:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2578:ILE:HG23	3:A:2579:MET:N	2.36	0.40
3:A:2625:ARG:HA	3:A:2675:LEU:HD23	2.03	0.40
3:A:2748:ILE:O	3:A:2748:ILE:HG23	2.21	0.40
3:A:2791:MET:SD	3:A:2791:MET:O	2.79	0.40
3:A:3181:ASN:HB2	3:A:3184:VAL:CG2	2.52	0.40
3:A:3219:VAL:HG13	3:A:3220:TYR:N	2.36	0.40
3:B:1041:CYS:O	3:B:1044:VAL:HG12	2.22	0.40
3:B:1116:LEU:HD12	3:B:1194:SER:CB	2.51	0.40
3:B:1567:LEU:N	3:B:1567:LEU:HD12	2.36	0.40
3:B:3551:ARG:HD3	3:B:3598:GLN:HG3	2.02	0.40
3:B:3847:LEU:HD11	3:B:3935:ASP:HB3	2.03	0.40
3:B:3862:VAL:HG13	3:B:3863:ASN:N	2.36	0.40
3:C:921:TYR:CE2	3:C:925:MET:HE3	2.57	0.40
3:C:1435:TYR:HB3	3:C:1520:LEU:HG	2.03	0.40
3:C:2898:LYS:HZ1	3:C:2900:GLY:C	2.24	0.40
3:C:3131:THR:O	3:C:3135:VAL:HG12	2.21	0.40
2:K:73:LYS:O	2:K:76:VAL:HG22	2.21	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	E	105/108 (97%)	98 (93%)	7 (7%)	0	100	100
1	F	105/108 (97%)	99 (94%)	6 (6%)	0	100	100
1	G	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
1	H	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	I	91/94 (97%)	86 (94%)	5 (6%)	0	100	100
2	J	91/94 (97%)	83 (91%)	8 (9%)	0	100	100
2	K	91/94 (97%)	86 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	91/94 (97%)	83 (91%)	8 (9%)	0	100	100
2	M	91/94 (97%)	86 (94%)	5 (6%)	0	100	100
2	N	91/94 (97%)	83 (91%)	8 (9%)	0	100	100
2	O	91/94 (97%)	86 (94%)	5 (6%)	0	100	100
2	P	91/94 (97%)	83 (91%)	8 (9%)	0	100	100
3	A	4351/5035 (86%)	4238 (97%)	113 (3%)	0	100	100
3	B	4351/5035 (86%)	4240 (97%)	111 (3%)	0	100	100
3	C	4351/5035 (86%)	4241 (98%)	110 (2%)	0	100	100
3	D	4351/5035 (86%)	4240 (97%)	111 (3%)	0	100	100
All	All	18552/21324 (87%)	18032 (97%)	520 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	E	89/90 (99%)	89 (100%)	0	100	100
1	F	89/90 (99%)	89 (100%)	0	100	100
1	G	89/90 (99%)	89 (100%)	0	100	100
1	H	89/90 (99%)	89 (100%)	0	100	100
2	I	80/81 (99%)	78 (98%)	2 (2%)	47	75
2	J	80/81 (99%)	80 (100%)	0	100	100
2	K	80/81 (99%)	78 (98%)	2 (2%)	47	75
2	L	80/81 (99%)	80 (100%)	0	100	100
2	M	80/81 (99%)	78 (98%)	2 (2%)	47	75
2	N	80/81 (99%)	80 (100%)	0	100	100
2	O	80/81 (99%)	78 (98%)	2 (2%)	47	75
2	P	80/81 (99%)	80 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	3811/4296 (89%)	3798 (100%)	13 (0%)	92	97
3	B	3811/4296 (89%)	3798 (100%)	13 (0%)	92	97
3	C	3811/4296 (89%)	3798 (100%)	13 (0%)	92	97
3	D	3811/4296 (89%)	3798 (100%)	13 (0%)	92	97
All	All	16240/18192 (89%)	16180 (100%)	60 (0%)	91	97

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	22	LYS
2	I	57	LYS
3	D	330	ARG
3	D	952	LYS
3	D	953	LYS
3	D	988	ARG
3	D	992	ASN
3	D	1753	ARG
3	D	1997	ARG
3	D	2739	ARG
3	D	2986	ARG
3	D	3551	ARG
3	D	3694	LYS
3	D	3757	GLU
3	D	5011	MET
3	A	330	ARG
3	A	952	LYS
3	A	953	LYS
3	A	988	ARG
3	A	992	ASN
3	A	1753	ARG
3	A	1997	ARG
3	A	2739	ARG
3	A	2986	ARG
3	A	3551	ARG
3	A	3694	LYS
3	A	3757	GLU
3	A	5011	MET
3	B	330	ARG
3	B	952	LYS
3	B	953	LYS
3	B	988	ARG

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Mol	Chain	Res	Type
3	B	992	ASN
3	B	1753	ARG
3	B	1997	ARG
3	B	2739	ARG
3	B	2986	ARG
3	B	3551	ARG
3	B	3694	LYS
3	B	3757	GLU
3	B	5011	MET
3	C	330	ARG
3	C	952	LYS
3	C	953	LYS
3	C	988	ARG
3	C	992	ASN
3	C	1753	ARG
3	C	1997	ARG
3	C	2739	ARG
3	C	2986	ARG
3	C	3551	ARG
3	C	3694	LYS
3	C	3757	GLU
3	C	5011	MET
2	K	22	LYS
2	K	57	LYS
2	M	22	LYS
2	M	57	LYS
2	O	22	LYS
2	O	57	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
2	J	87	ASN
3	D	106	HIS
3	D	726	HIS
3	D	1485	HIS
3	D	2694	GLN
3	A	106	HIS
3	A	726	HIS
3	A	1485	HIS
3	A	2128	GLN
3	A	2694	GLN

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Mol	Chain	Res	Type
3	A	3181	ASN
3	B	106	HIS
3	B	726	HIS
3	B	1485	HIS
3	B	2128	GLN
3	B	2694	GLN
3	B	3181	ASN
3	C	106	HIS
3	C	726	HIS
3	C	1485	HIS
3	C	2694	GLN
2	L	87	ASN
2	N	87	ASN
2	P	87	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 44 ligands modelled in this entry, 24 are monoatomic - leaving 20 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	$\#\|Z\|>2$
6	CFF	B	8002	-	8,15,15	0.91	0	8,23,23	2.82	2 (25%)
8	PCW	B	8006	-	53,53,53	1.14	3 (5%)	59,61,61	2.36	9 (15%)
7	ATP	D	8005	-	26,33,33	0.61	0	31,52,52	1.07	2 (6%)
7	ATP	C	5106	-	26,33,33	0.61	0	31,52,52	1.07	2 (6%)
8	PCW	A	8006	-	53,53,53	1.13	3 (5%)	59,61,61	2.36	9 (15%)
8	PCW	C	5101	-	53,53,53	1.14	4 (7%)	59,61,61	2.30	9 (15%)
8	PCW	A	8007	-	53,53,53	1.14	4 (7%)	59,61,61	2.30	9 (15%)
6	CFF	D	8002	-	8,15,15	0.92	0	8,23,23	2.83	2 (25%)
8	PCW	B	8007	-	53,53,53	1.14	4 (7%)	59,61,61	2.30	9 (15%)
7	ATP	B	8003	-	26,33,33	0.68	0	31,52,52	0.72	1 (3%)
7	ATP	A	8005	-	26,33,33	0.60	0	31,52,52	1.07	2 (6%)
7	ATP	B	8005	-	26,33,33	0.61	0	31,52,52	1.07	2 (6%)
6	CFF	A	8002	-	8,15,15	0.90	0	8,23,23	2.79	2 (25%)
7	ATP	C	5104	-	26,33,33	0.68	0	31,52,52	0.72	1 (3%)
8	PCW	C	5107	-	53,53,53	1.14	3 (5%)	59,61,61	2.36	9 (15%)
8	PCW	D	8006	-	53,53,53	1.14	3 (5%)	59,61,61	2.36	9 (15%)
8	PCW	D	8007	-	53,53,53	1.14	4 (7%)	59,61,61	2.30	9 (15%)
7	ATP	A	8003	-	26,33,33	0.68	0	31,52,52	0.71	1 (3%)
6	CFF	C	5103	-	8,15,15	0.91	0	8,23,23	2.80	2 (25%)
7	ATP	D	8003	-	26,33,33	0.68	0	31,52,52	0.71	1 (3%)

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
6	CFF	B	8002	-	-	-	0/2/2/2
8	PCW	B	8006	-	-	21/57/57/57	-
7	ATP	D	8005	-	-	5/18/38/38	0/3/3/3
7	ATP	C	5106	-	-	5/18/38/38	0/3/3/3
8	PCW	A	8006	-	-	21/57/57/57	-
8	PCW	C	5101	-	-	20/57/57/57	-
8	PCW	A	8007	-	-	20/57/57/57	-
6	CFF	D	8002	-	-	-	0/2/2/2
8	PCW	B	8007	-	-	20/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ATP	B	8003	-	-	7/18/38/38	0/3/3/3
7	ATP	A	8005	-	-	5/18/38/38	0/3/3/3
7	ATP	B	8005	-	-	5/18/38/38	0/3/3/3
6	CFF	A	8002	-	-	-	0/2/2/2
7	ATP	C	5104	-	-	7/18/38/38	0/3/3/3
8	PCW	C	5107	-	-	21/57/57/57	-
8	PCW	D	8006	-	-	21/57/57/57	-
8	PCW	D	8007	-	-	20/57/57/57	-
7	ATP	A	8003	-	-	7/18/38/38	0/3/3/3
6	CFF	C	5103	-	-	-	0/2/2/2
7	ATP	D	8003	-	-	7/18/38/38	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	8006	PCW	O3-C11	3.07	1.42	1.33
8	A	8006	PCW	O3-C11	3.07	1.42	1.33
8	B	8006	PCW	O3-C11	3.07	1.42	1.33
8	C	5107	PCW	O3-C11	3.07	1.42	1.33
8	A	8007	PCW	O3-C11	3.03	1.42	1.33
8	B	8007	PCW	O3-C11	3.03	1.42	1.33
8	C	5101	PCW	O3-C11	3.03	1.42	1.33
8	D	8007	PCW	O3-C11	3.01	1.42	1.33
8	D	8006	PCW	O2-C31	2.87	1.42	1.34
8	C	5107	PCW	O2-C31	2.87	1.42	1.34
8	A	8006	PCW	O2-C31	2.85	1.42	1.34
8	B	8006	PCW	O2-C31	2.85	1.42	1.34
8	A	8007	PCW	O2-C31	2.75	1.42	1.34
8	B	8007	PCW	O2-C31	2.75	1.42	1.34
8	C	5101	PCW	O2-C31	2.75	1.42	1.34
8	D	8007	PCW	O2-C31	2.74	1.42	1.34
8	D	8007	PCW	O2-C2	-2.69	1.39	1.46
8	A	8007	PCW	O2-C2	-2.67	1.39	1.46
8	B	8007	PCW	O2-C2	-2.67	1.39	1.46
8	C	5101	PCW	O2-C2	-2.67	1.39	1.46
8	D	8006	PCW	O2-C2	-2.52	1.40	1.46
8	B	8006	PCW	O2-C2	-2.52	1.40	1.46
8	C	5107	PCW	O2-C2	-2.52	1.40	1.46
8	A	8006	PCW	O2-C2	-2.51	1.40	1.46
8	D	8007	PCW	P-O4P	2.05	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	8007	PCW	P-O4P	2.04	1.67	1.59
8	B	8007	PCW	P-O4P	2.04	1.67	1.59
8	C	5101	PCW	P-O4P	2.04	1.67	1.59

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	8006	PCW	C8-N-C6	11.85	139.44	108.97
8	C	5107	PCW	C8-N-C6	11.85	139.44	108.97
8	D	8006	PCW	C8-N-C6	11.84	139.42	108.97
8	B	8006	PCW	C8-N-C6	11.84	139.42	108.97
8	B	8007	PCW	C8-N-C6	11.22	137.81	108.97
8	A	8007	PCW	C8-N-C6	11.20	137.78	108.97
8	C	5101	PCW	C8-N-C6	11.20	137.78	108.97
8	D	8007	PCW	C8-N-C6	11.20	137.78	108.97
8	D	8007	PCW	C7-N-C5	7.49	140.54	109.92
8	A	8007	PCW	C7-N-C5	7.48	140.51	109.92
8	C	5101	PCW	C7-N-C5	7.48	140.51	109.92
8	B	8007	PCW	C7-N-C5	7.47	140.47	109.92
8	D	8006	PCW	C7-N-C5	7.11	139.00	109.92
8	B	8006	PCW	C7-N-C5	7.11	139.00	109.92
8	C	5107	PCW	C7-N-C5	7.11	139.00	109.92
8	A	8006	PCW	C7-N-C5	7.10	138.96	109.92
6	B	8002	CFF	C5-C6-N1	-5.99	111.82	118.20
6	D	8002	CFF	C5-C6-N1	-5.98	111.82	118.20
6	C	5103	CFF	C5-C6-N1	-5.94	111.87	118.20
6	A	8002	CFF	C5-C6-N1	-5.91	111.89	118.20
8	A	8006	PCW	C8-N-C7	-5.79	94.08	108.97
8	D	8006	PCW	C8-N-C7	-5.79	94.09	108.97
8	B	8006	PCW	C8-N-C7	-5.79	94.09	108.97
8	C	5107	PCW	C8-N-C7	-5.79	94.09	108.97
8	B	8007	PCW	C7-N-C6	-5.27	95.43	108.97
8	A	8007	PCW	C7-N-C6	-5.26	95.44	108.97
8	C	5101	PCW	C7-N-C6	-5.26	95.44	108.97
8	D	8007	PCW	C7-N-C6	-5.26	95.45	108.97
8	D	8007	PCW	C8-N-C7	-5.12	95.82	108.97
8	A	8007	PCW	C8-N-C7	-5.11	95.83	108.97
8	B	8007	PCW	C8-N-C7	-5.11	95.83	108.97
8	C	5101	PCW	C8-N-C7	-5.11	95.83	108.97
8	A	8006	PCW	C7-N-C6	-5.09	95.88	108.97
8	D	8006	PCW	C7-N-C6	-5.09	95.89	108.97
8	B	8006	PCW	C7-N-C6	-5.09	95.89	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	5107	PCW	C7-N-C6	-5.08	95.91	108.97
6	D	8002	CFF	C4-C5-C6	4.76	123.01	119.96
6	B	8002	CFF	C4-C5-C6	4.71	122.99	119.96
6	C	5103	CFF	C4-C5-C6	4.65	122.95	119.96
6	A	8002	CFF	C4-C5-C6	4.63	122.94	119.96
8	D	8006	PCW	C21-C20-C19	3.90	154.63	124.73
8	B	8006	PCW	C21-C20-C19	3.90	154.63	124.73
8	C	5107	PCW	C21-C20-C19	3.90	154.63	124.73
8	A	8006	PCW	C21-C20-C19	3.90	154.63	124.73
8	A	8007	PCW	C21-C20-C19	3.80	153.88	124.73
8	B	8007	PCW	C21-C20-C19	3.80	153.88	124.73
8	C	5101	PCW	C21-C20-C19	3.80	153.88	124.73
8	D	8007	PCW	C21-C20-C19	3.79	153.83	124.73
8	A	8006	PCW	O2-C31-C32	3.57	119.20	111.50
8	D	8006	PCW	O2-C31-C32	3.56	119.18	111.50
8	C	5107	PCW	O2-C31-C32	3.56	119.18	111.50
8	B	8006	PCW	O2-C31-C32	3.56	119.17	111.50
8	D	8007	PCW	O2-C31-C32	3.49	119.02	111.50
8	A	8007	PCW	O2-C31-C32	3.47	118.98	111.50
8	B	8007	PCW	O2-C31-C32	3.47	118.98	111.50
8	C	5101	PCW	O2-C31-C32	3.47	118.98	111.50
8	B	8007	PCW	C8-N-C5	-3.28	96.51	109.92
8	D	8007	PCW	C8-N-C5	-3.28	96.51	109.92
8	A	8007	PCW	C8-N-C5	-3.27	96.52	109.92
8	C	5101	PCW	C8-N-C5	-3.27	96.52	109.92
8	D	8006	PCW	C8-N-C5	-2.95	97.84	109.92
8	B	8006	PCW	C8-N-C5	-2.95	97.84	109.92
8	C	5107	PCW	C8-N-C5	-2.95	97.84	109.92
8	A	8006	PCW	C8-N-C5	-2.95	97.85	109.92
8	C	5107	PCW	C6-N-C5	-2.45	99.89	109.92
8	D	8006	PCW	C6-N-C5	-2.44	99.93	109.92
8	B	8006	PCW	C6-N-C5	-2.44	99.93	109.92
8	A	8006	PCW	C6-N-C5	-2.44	99.93	109.92
8	D	8007	PCW	C6-N-C5	-2.41	100.07	109.92
8	A	8007	PCW	C6-N-C5	-2.40	100.08	109.92
8	C	5101	PCW	C6-N-C5	-2.40	100.08	109.92
8	B	8007	PCW	C6-N-C5	-2.40	100.11	109.92
8	A	8006	PCW	O3-C11-C12	2.33	119.23	111.91
8	D	8006	PCW	O3-C11-C12	2.33	119.22	111.91
8	B	8006	PCW	O3-C11-C12	2.33	119.22	111.91
8	C	5107	PCW	O3-C11-C12	2.33	119.22	111.91
8	D	8007	PCW	O3-C11-C12	2.32	119.19	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	8007	PCW	O3-C11-C12	2.32	119.19	111.91
8	C	5101	PCW	O3-C11-C12	2.32	119.19	111.91
8	B	8007	PCW	O3-C11-C12	2.32	119.18	111.91
7	A	8005	ATP	C5-C6-N6	2.29	123.83	120.35
7	D	8005	ATP	C5-C6-N6	2.28	123.82	120.35
7	B	8005	ATP	C5-C6-N6	2.28	123.82	120.35
7	C	5106	ATP	C5-C6-N6	2.28	123.82	120.35
7	B	8003	ATP	C5-C6-N6	2.22	123.72	120.35
7	C	5104	ATP	C5-C6-N6	2.19	123.68	120.35
7	A	8003	ATP	C5-C6-N6	2.18	123.66	120.35
7	D	8003	ATP	C5-C6-N6	2.18	123.66	120.35
7	A	8005	ATP	PB-O3B-PG	2.09	140.00	132.83
7	D	8005	ATP	PB-O3B-PG	2.08	139.97	132.83
7	B	8005	ATP	PB-O3B-PG	2.08	139.97	132.83
7	C	5106	ATP	PB-O3B-PG	2.07	139.94	132.83

There are no chirality outliers.

All (212) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	8003	ATP	C5'-O5'-PA-O1A
7	D	8005	ATP	C5'-O5'-PA-O1A
7	A	8003	ATP	C5'-O5'-PA-O1A
7	A	8005	ATP	C5'-O5'-PA-O1A
7	B	8003	ATP	C5'-O5'-PA-O1A
7	B	8005	ATP	C5'-O5'-PA-O1A
7	C	5104	ATP	C5'-O5'-PA-O1A
7	C	5106	ATP	C5'-O5'-PA-O1A
8	D	8006	PCW	C1-O3P-P-O2P
8	D	8007	PCW	O4P-C4-C5-N
8	A	8006	PCW	C1-O3P-P-O2P
8	A	8007	PCW	O4P-C4-C5-N
8	B	8006	PCW	C1-O3P-P-O2P
8	B	8007	PCW	O4P-C4-C5-N
8	C	5101	PCW	O4P-C4-C5-N
8	C	5107	PCW	C1-O3P-P-O2P
7	D	8005	ATP	O4'-C4'-C5'-O5'
7	A	8005	ATP	O4'-C4'-C5'-O5'
7	B	8005	ATP	O4'-C4'-C5'-O5'
7	C	5106	ATP	O4'-C4'-C5'-O5'
8	D	8007	PCW	C23-C24-C25-C26
8	B	8007	PCW	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
8	C	5101	PCW	C23-C24-C25-C26
7	D	8005	ATP	C3'-C4'-C5'-O5'
7	A	8005	ATP	C3'-C4'-C5'-O5'
7	B	8005	ATP	C3'-C4'-C5'-O5'
7	C	5106	ATP	C3'-C4'-C5'-O5'
8	A	8007	PCW	C23-C24-C25-C26
8	D	8006	PCW	C1-O3P-P-O4P
8	A	8006	PCW	C1-O3P-P-O4P
8	B	8006	PCW	C1-O3P-P-O4P
8	C	5107	PCW	C1-O3P-P-O4P
8	A	8006	PCW	C43-C44-C45-C46
8	D	8006	PCW	C43-C44-C45-C46
8	B	8006	PCW	C43-C44-C45-C46
8	C	5107	PCW	C43-C44-C45-C46
8	D	8006	PCW	C15-C16-C17-C18
8	D	8007	PCW	C21-C22-C23-C24
8	A	8006	PCW	C15-C16-C17-C18
8	A	8007	PCW	C21-C22-C23-C24
8	B	8006	PCW	C15-C16-C17-C18
8	B	8007	PCW	C21-C22-C23-C24
8	C	5101	PCW	C21-C22-C23-C24
8	C	5107	PCW	C15-C16-C17-C18
8	D	8007	PCW	C13-C14-C15-C16
8	A	8007	PCW	C13-C14-C15-C16
8	B	8007	PCW	C13-C14-C15-C16
8	C	5101	PCW	C13-C14-C15-C16
8	D	8007	PCW	C11-C12-C13-C14
8	A	8007	PCW	C11-C12-C13-C14
8	B	8007	PCW	C11-C12-C13-C14
8	C	5101	PCW	C11-C12-C13-C14
8	D	8007	PCW	C14-C15-C16-C17
8	A	8007	PCW	C14-C15-C16-C17
8	B	8007	PCW	C14-C15-C16-C17
8	C	5101	PCW	C14-C15-C16-C17
8	D	8006	PCW	C17-C18-C19-C20
8	A	8006	PCW	C17-C18-C19-C20
8	B	8006	PCW	C17-C18-C19-C20
8	C	5107	PCW	C17-C18-C19-C20
8	A	8007	PCW	C25-C26-C27-C28
8	D	8007	PCW	C25-C26-C27-C28
8	B	8007	PCW	C25-C26-C27-C28
8	C	5101	PCW	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
8	D	8006	PCW	C32-C31-O2-C2
8	A	8006	PCW	C32-C31-O2-C2
8	B	8006	PCW	C32-C31-O2-C2
8	C	5107	PCW	C32-C31-O2-C2
8	D	8007	PCW	C15-C16-C17-C18
8	A	8007	PCW	C15-C16-C17-C18
8	B	8007	PCW	C15-C16-C17-C18
8	C	5101	PCW	C15-C16-C17-C18
8	D	8006	PCW	O31-C31-O2-C2
8	A	8006	PCW	O31-C31-O2-C2
8	B	8006	PCW	O31-C31-O2-C2
8	C	5107	PCW	O31-C31-O2-C2
8	D	8007	PCW	C40-C41-C42-C43
8	A	8007	PCW	C40-C41-C42-C43
8	B	8007	PCW	C40-C41-C42-C43
8	C	5101	PCW	C40-C41-C42-C43
8	D	8007	PCW	C44-C45-C46-C47
8	A	8007	PCW	C44-C45-C46-C47
8	B	8007	PCW	C44-C45-C46-C47
8	C	5101	PCW	C44-C45-C46-C47
8	D	8006	PCW	C40-C41-C42-C43
8	A	8006	PCW	C40-C41-C42-C43
8	B	8006	PCW	C40-C41-C42-C43
8	C	5107	PCW	C40-C41-C42-C43
8	B	8006	PCW	C23-C24-C25-C26
8	D	8006	PCW	C23-C24-C25-C26
8	A	8006	PCW	C23-C24-C25-C26
8	C	5107	PCW	C23-C24-C25-C26
8	D	8006	PCW	C14-C15-C16-C17
8	A	8006	PCW	C14-C15-C16-C17
8	B	8006	PCW	C14-C15-C16-C17
8	C	5107	PCW	C14-C15-C16-C17
8	D	8007	PCW	C45-C46-C47-C48
8	A	8007	PCW	C45-C46-C47-C48
8	B	8007	PCW	C45-C46-C47-C48
8	C	5101	PCW	C45-C46-C47-C48
8	D	8006	PCW	C19-C20-C21-C22
8	A	8006	PCW	C19-C20-C21-C22
8	B	8006	PCW	C19-C20-C21-C22
8	C	5107	PCW	C19-C20-C21-C22
8	D	8006	PCW	C21-C22-C23-C24
8	A	8006	PCW	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
8	B	8006	PCW	C21-C22-C23-C24
8	C	5107	PCW	C21-C22-C23-C24
7	D	8005	ATP	C4'-C5'-O5'-PA
7	A	8005	ATP	C4'-C5'-O5'-PA
7	B	8005	ATP	C4'-C5'-O5'-PA
7	C	5106	ATP	C4'-C5'-O5'-PA
8	D	8006	PCW	C1-C2-C3-O3
8	A	8006	PCW	C1-C2-C3-O3
8	B	8006	PCW	C1-C2-C3-O3
8	C	5107	PCW	C1-C2-C3-O3
8	D	8006	PCW	C33-C34-C35-C36
8	A	8006	PCW	C33-C34-C35-C36
8	B	8006	PCW	C33-C34-C35-C36
8	C	5107	PCW	C33-C34-C35-C36
8	D	8006	PCW	C25-C26-C27-C28
8	A	8006	PCW	C25-C26-C27-C28
8	C	5107	PCW	C25-C26-C27-C28
8	B	8006	PCW	C25-C26-C27-C28
8	D	8006	PCW	O2-C2-C3-O3
8	A	8006	PCW	O2-C2-C3-O3
8	B	8006	PCW	O2-C2-C3-O3
8	C	5107	PCW	O2-C2-C3-O3
8	D	8007	PCW	C2-C1-O3P-P
8	A	8007	PCW	C2-C1-O3P-P
8	B	8007	PCW	C2-C1-O3P-P
8	C	5101	PCW	C2-C1-O3P-P
8	D	8007	PCW	O3P-C1-C2-C3
8	A	8007	PCW	O3P-C1-C2-C3
8	B	8007	PCW	O3P-C1-C2-C3
8	C	5101	PCW	O3P-C1-C2-C3
8	D	8007	PCW	C32-C31-O2-C2
8	A	8007	PCW	C32-C31-O2-C2
8	B	8007	PCW	C32-C31-O2-C2
8	C	5101	PCW	C32-C31-O2-C2
7	D	8003	ATP	C5'-O5'-PA-O3A
7	A	8003	ATP	C5'-O5'-PA-O3A
7	B	8003	ATP	C5'-O5'-PA-O3A
7	C	5104	ATP	C5'-O5'-PA-O3A
8	D	8007	PCW	C36-C37-C38-C39
8	A	8007	PCW	C36-C37-C38-C39
8	B	8007	PCW	C36-C37-C38-C39
8	C	5101	PCW	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
8	D	8007	PCW	O31-C31-O2-C2
8	A	8007	PCW	O31-C31-O2-C2
8	B	8007	PCW	O31-C31-O2-C2
8	C	5101	PCW	O31-C31-O2-C2
7	D	8003	ATP	PG-O3B-PB-O2B
7	A	8003	ATP	PG-O3B-PB-O2B
7	B	8003	ATP	PG-O3B-PB-O2B
7	C	5104	ATP	PG-O3B-PB-O2B
7	D	8003	ATP	C5'-O5'-PA-O2A
7	A	8003	ATP	C5'-O5'-PA-O2A
7	B	8003	ATP	C5'-O5'-PA-O2A
7	C	5104	ATP	C5'-O5'-PA-O2A
8	D	8007	PCW	C4-C5-N-C8
8	A	8007	PCW	C4-C5-N-C8
8	B	8007	PCW	C4-C5-N-C8
8	C	5101	PCW	C4-C5-N-C8
8	D	8006	PCW	C44-C45-C46-C47
8	C	5107	PCW	C44-C45-C46-C47
8	B	8006	PCW	C44-C45-C46-C47
8	A	8006	PCW	C44-C45-C46-C47
8	D	8007	PCW	O3P-C1-C2-O2
8	A	8007	PCW	O3P-C1-C2-O2
8	B	8007	PCW	O3P-C1-C2-O2
8	C	5101	PCW	O3P-C1-C2-O2
8	D	8006	PCW	O4P-C4-C5-N
8	A	8006	PCW	O4P-C4-C5-N
8	B	8006	PCW	O4P-C4-C5-N
8	C	5107	PCW	O4P-C4-C5-N
8	D	8007	PCW	C1-C2-O2-C31
8	A	8007	PCW	C1-C2-O2-C31
8	B	8007	PCW	C1-C2-O2-C31
8	C	5101	PCW	C1-C2-O2-C31
7	D	8003	ATP	PG-O3B-PB-O1B
7	D	8005	ATP	PG-O3B-PB-O2B
7	A	8003	ATP	PG-O3B-PB-O1B
7	A	8005	ATP	PG-O3B-PB-O2B
7	B	8003	ATP	PG-O3B-PB-O1B
7	B	8005	ATP	PG-O3B-PB-O2B
7	C	5104	ATP	PG-O3B-PB-O1B
7	C	5106	ATP	PG-O3B-PB-O2B
7	D	8003	ATP	C4'-C5'-O5'-PA
7	A	8003	ATP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
7	B	8003	ATP	C4'-C5'-O5'-PA
7	C	5104	ATP	C4'-C5'-O5'-PA
8	A	8006	PCW	C42-C43-C44-C45
8	D	8006	PCW	C42-C43-C44-C45
8	B	8006	PCW	C42-C43-C44-C45
8	C	5107	PCW	C42-C43-C44-C45
8	D	8006	PCW	C2-C1-O3P-P
8	A	8006	PCW	C2-C1-O3P-P
8	B	8006	PCW	C2-C1-O3P-P
8	C	5107	PCW	C2-C1-O3P-P
7	D	8003	ATP	O4'-C4'-C5'-O5'
7	A	8003	ATP	O4'-C4'-C5'-O5'
7	B	8003	ATP	O4'-C4'-C5'-O5'
7	C	5104	ATP	O4'-C4'-C5'-O5'
8	D	8006	PCW	C13-C14-C15-C16
8	B	8006	PCW	C13-C14-C15-C16
8	C	5107	PCW	C13-C14-C15-C16
8	A	8006	PCW	C13-C14-C15-C16
8	D	8007	PCW	C19-C20-C21-C22
8	A	8007	PCW	C19-C20-C21-C22
8	B	8007	PCW	C19-C20-C21-C22
8	C	5101	PCW	C19-C20-C21-C22

There are no ring outliers.

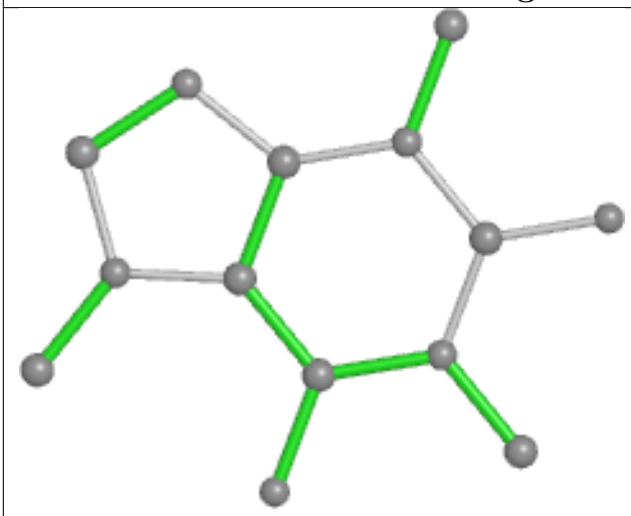
12 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	8006	PCW	1	0
7	D	8005	ATP	3	0
7	C	5106	ATP	3	0
8	A	8006	PCW	2	0
8	C	5101	PCW	3	0
8	A	8007	PCW	4	0
8	B	8007	PCW	5	0
7	A	8005	ATP	2	0
7	B	8005	ATP	2	0
8	C	5107	PCW	1	0
8	D	8006	PCW	1	0
8	D	8007	PCW	4	0

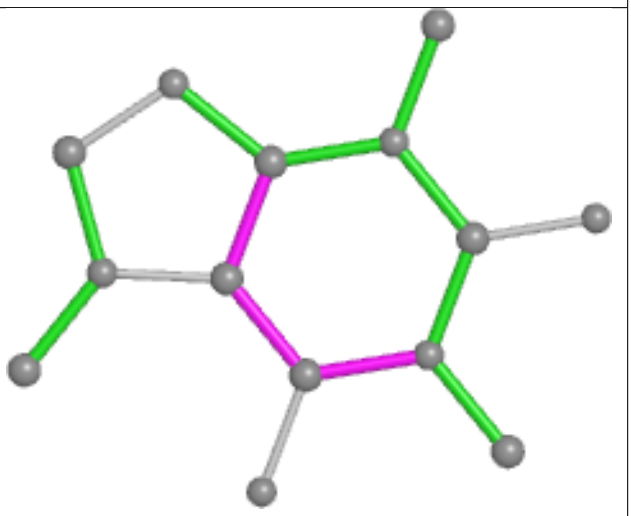
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

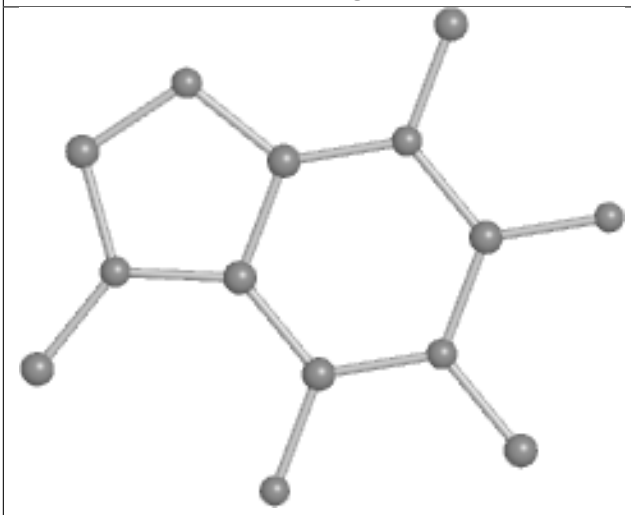
Ligand CFF B 8002



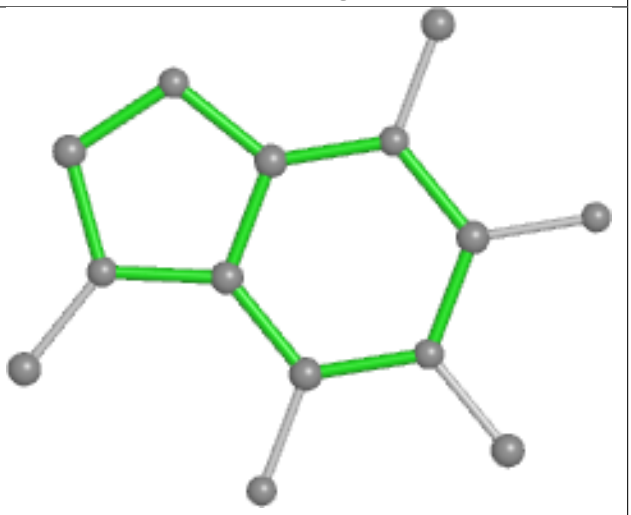
Bond lengths



Bond angles

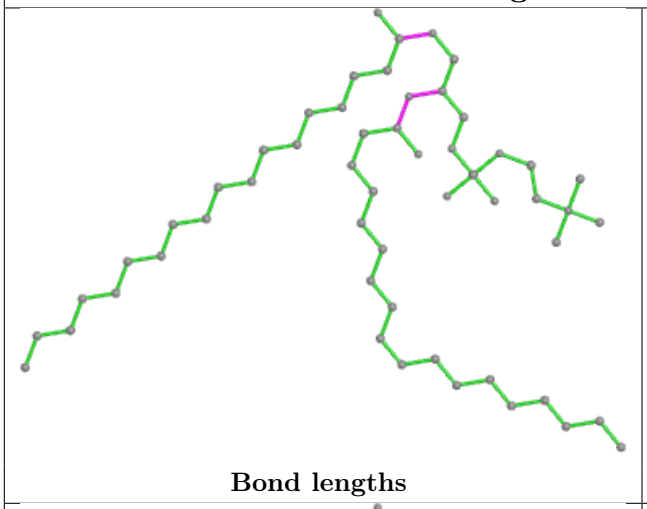


Torsions

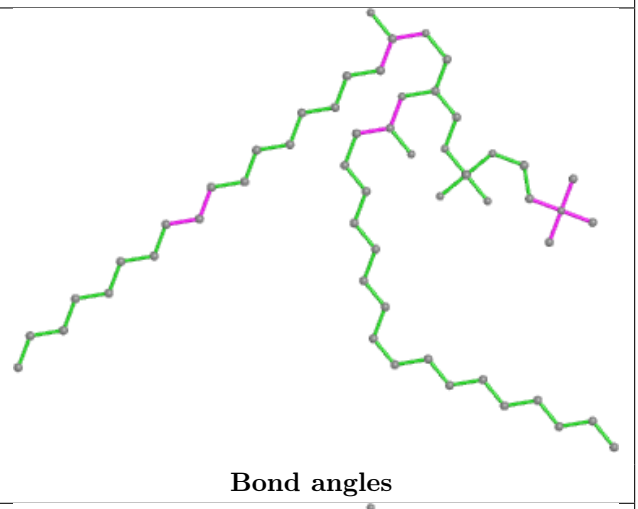


Rings

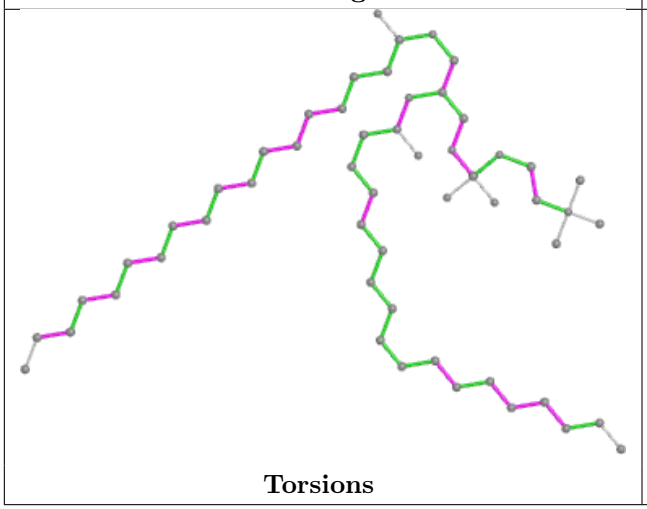
Ligand PCW B 8006



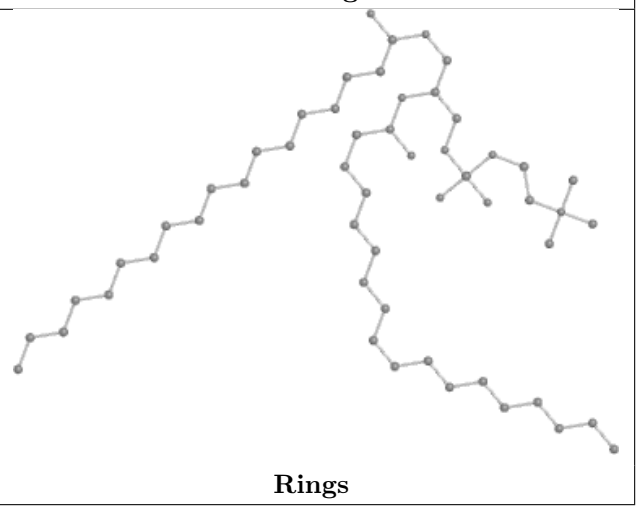
Bond lengths



Bond angles

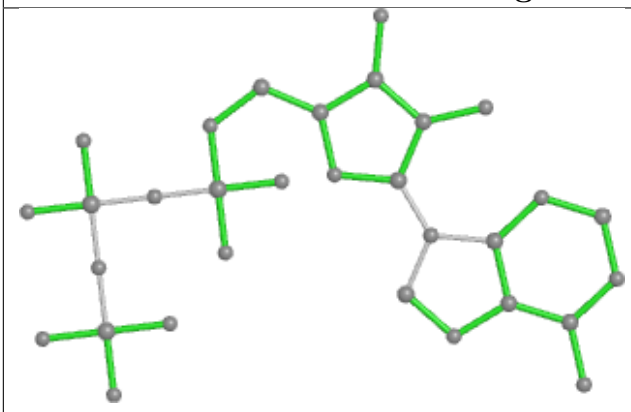


Torsions

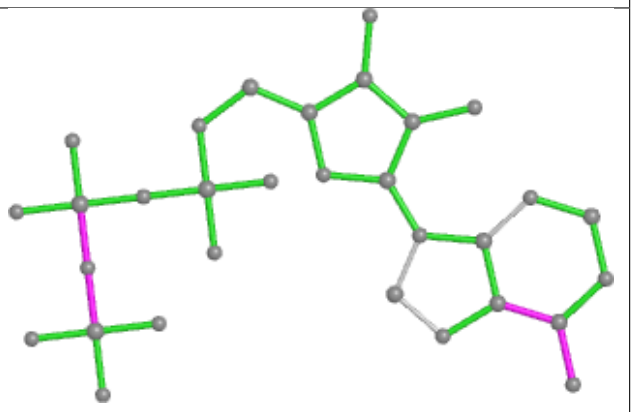


Rings

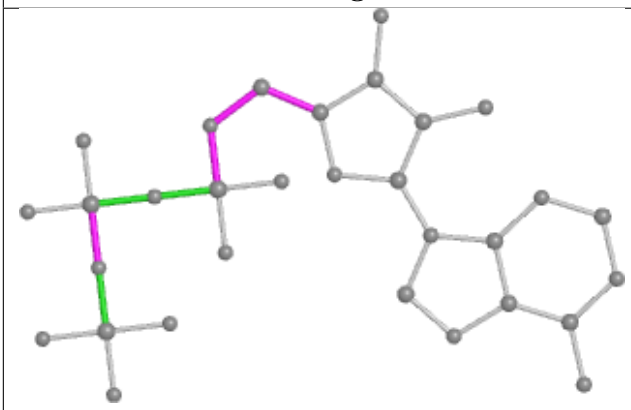
Ligand ATP D 8005



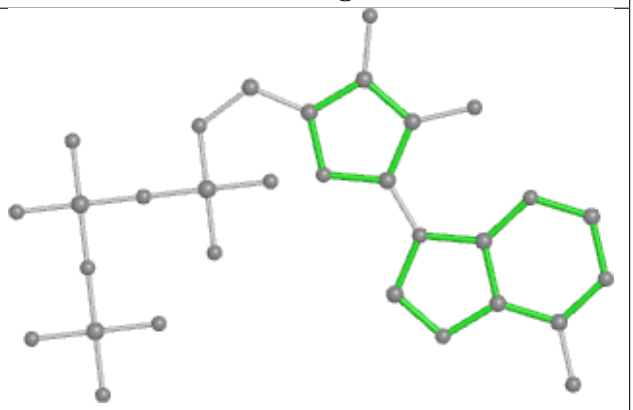
Bond lengths



Bond angles

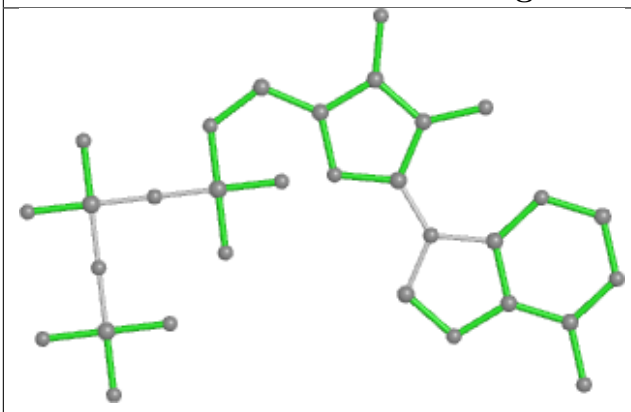


Torsions

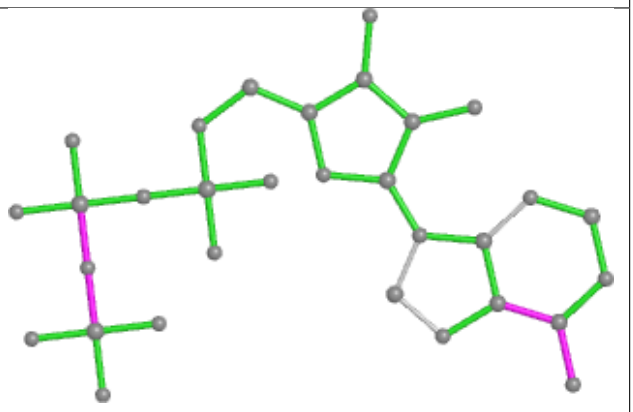


Rings

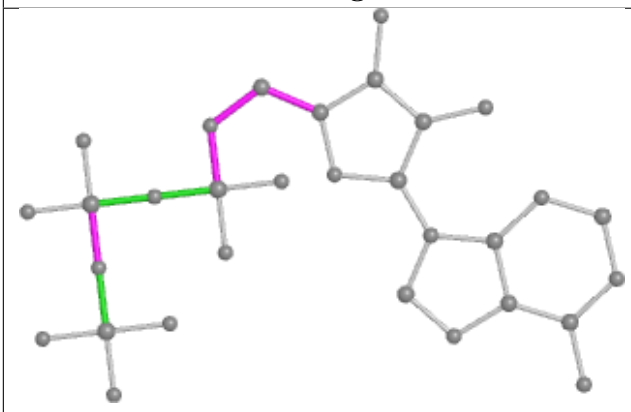
Ligand ATP C 5106



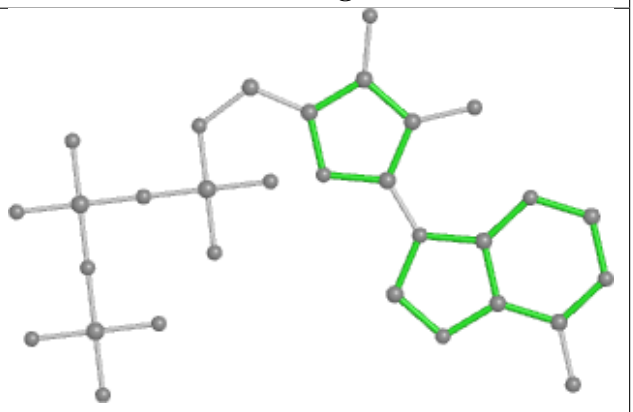
Bond lengths



Bond angles

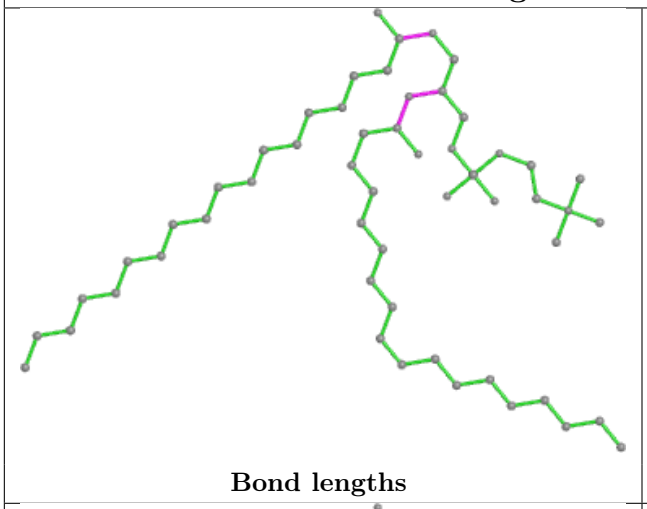


Torsions

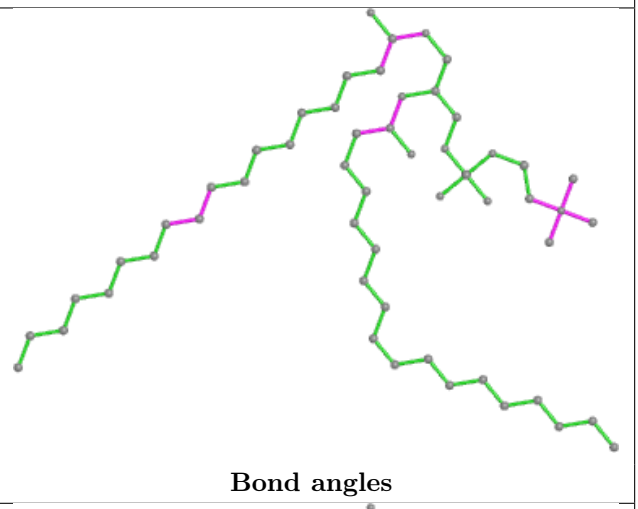


Rings

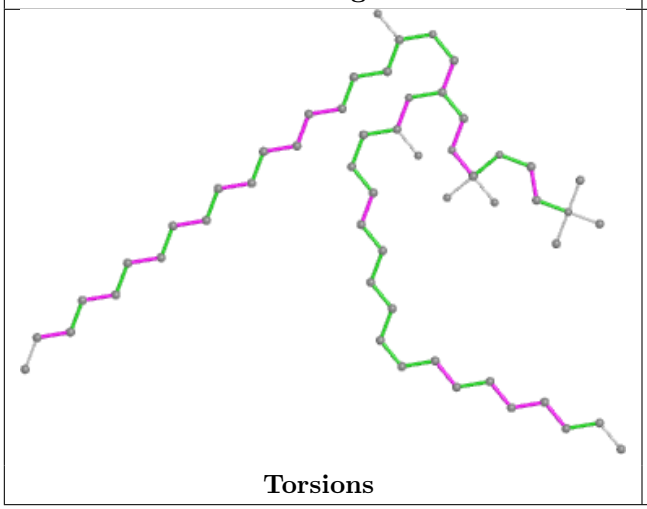
Ligand PCW A 8006



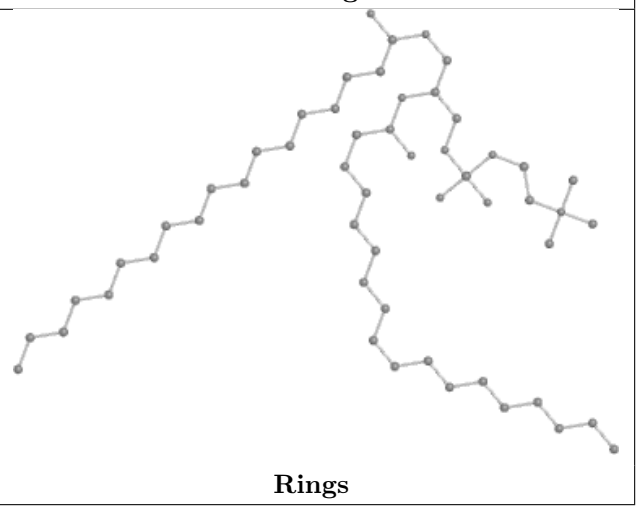
Bond lengths



Bond angles

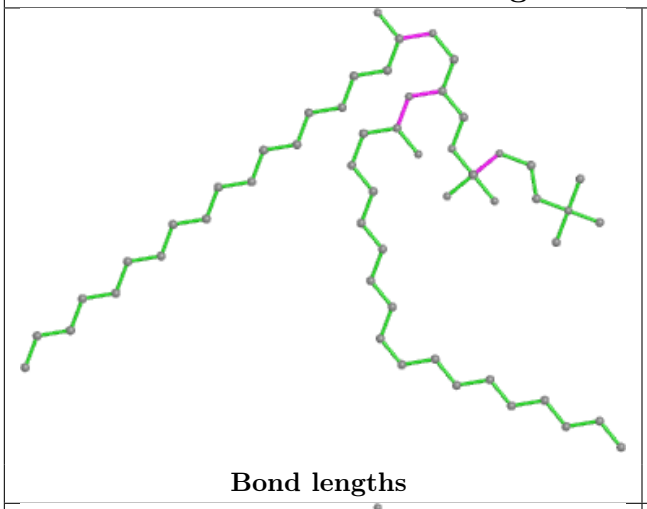


Torsions



Rings

Ligand PCW C 5101



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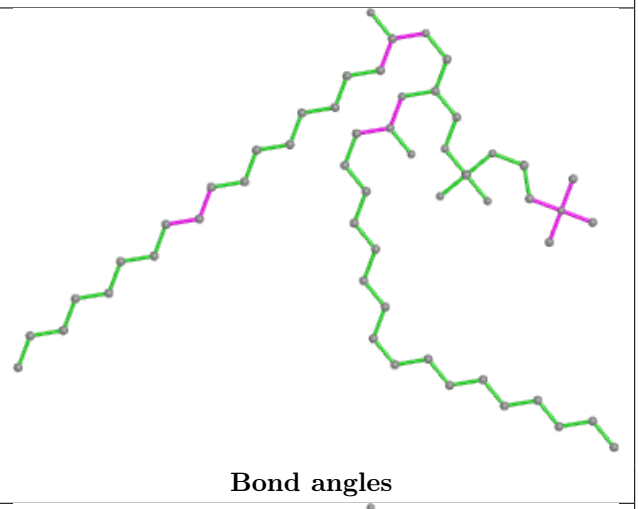
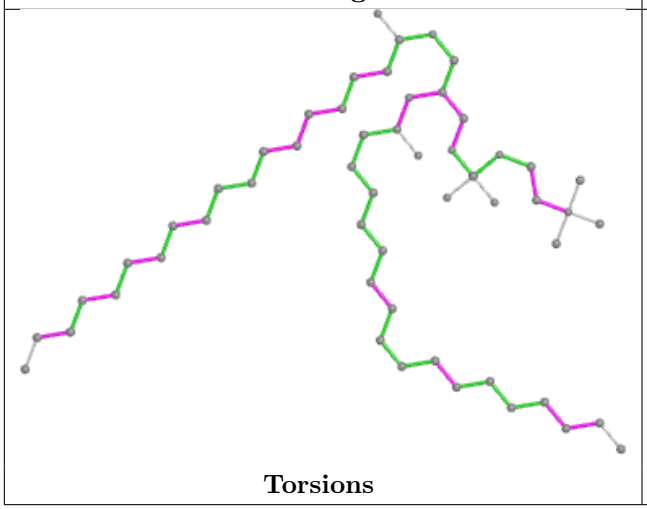


Bond angles



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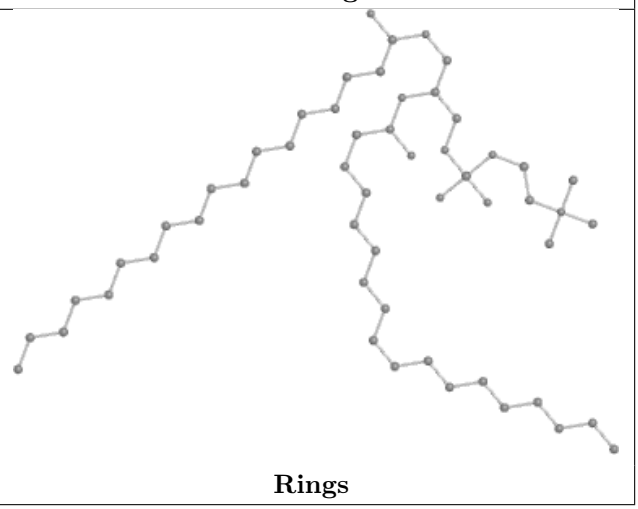
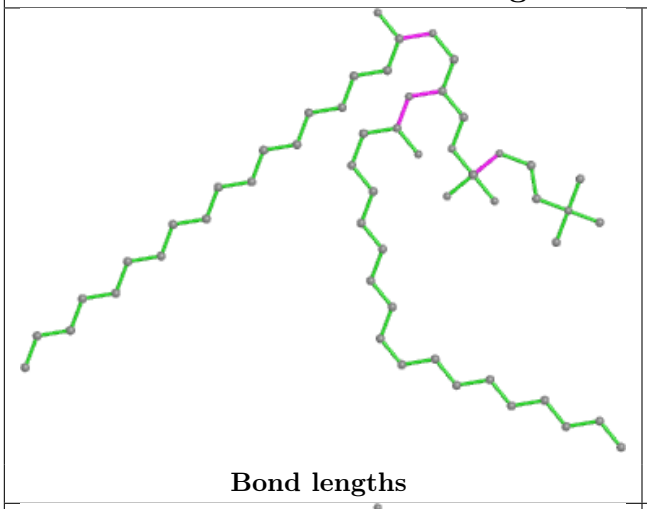
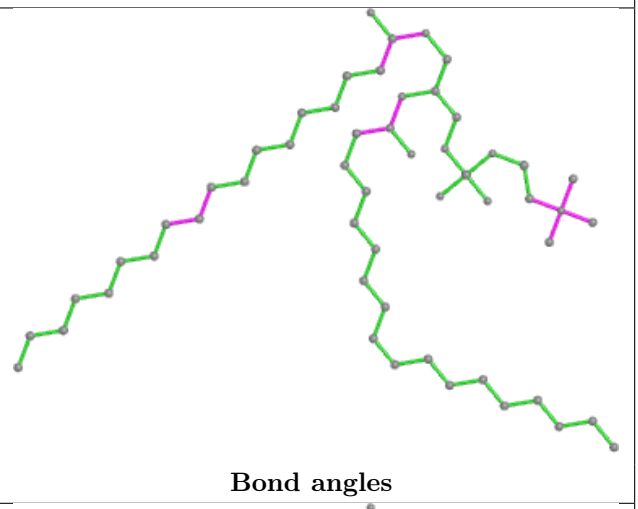


Rings

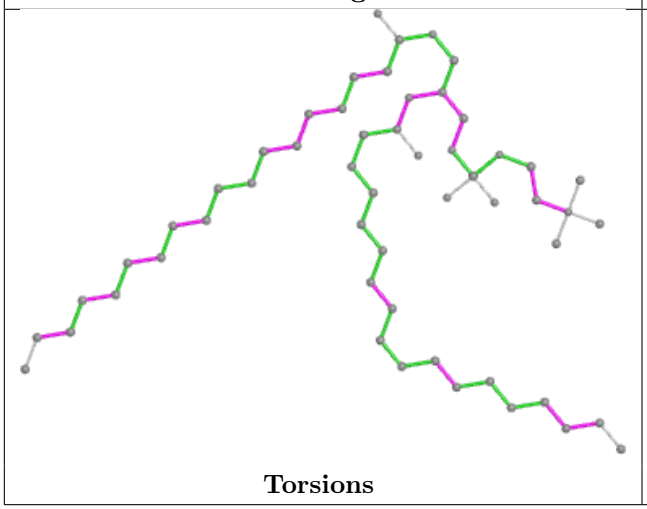
Ligand PCW A 8007



Bond lengths



Bond angles



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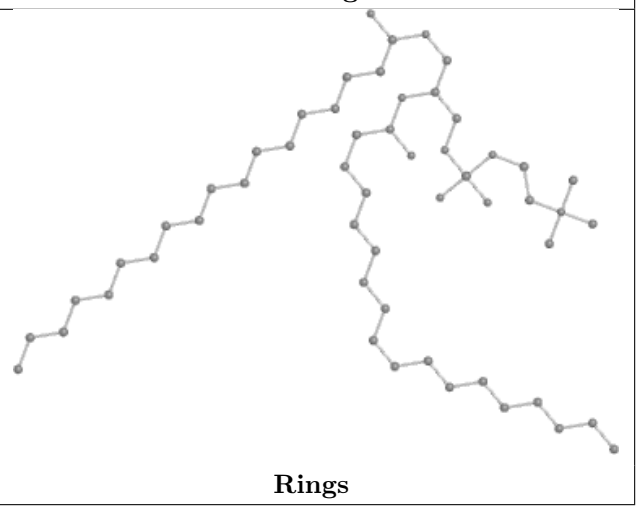
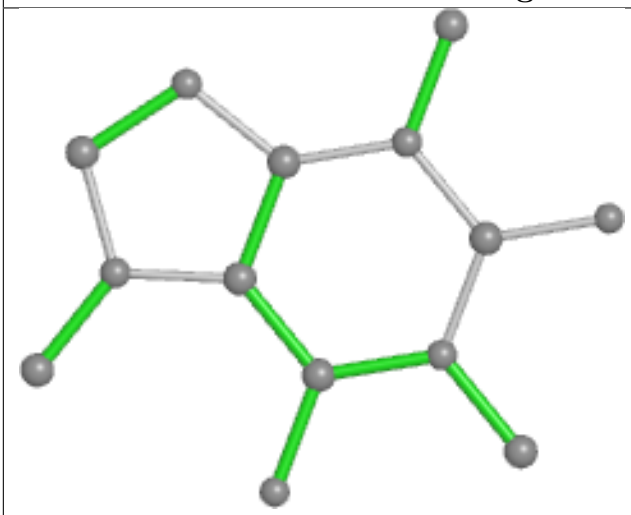


Rings

Ligand CFF D 8002



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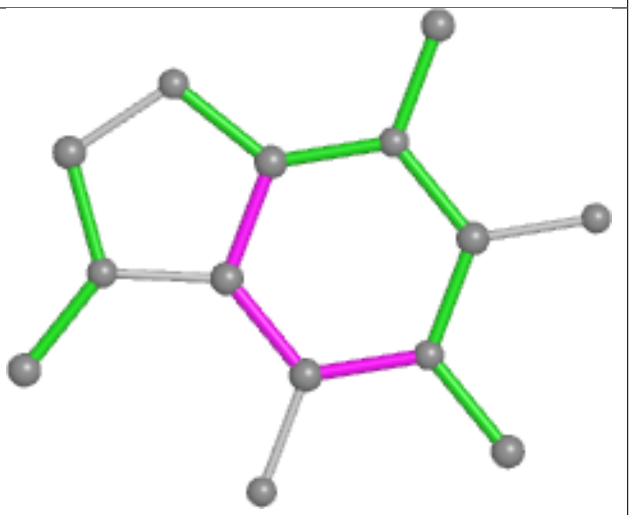
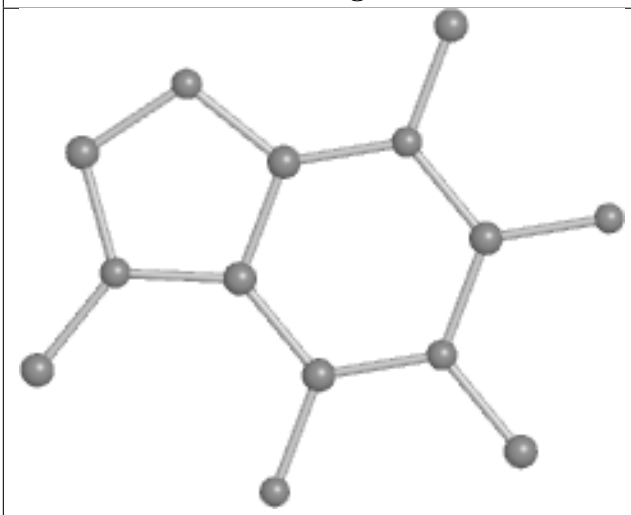
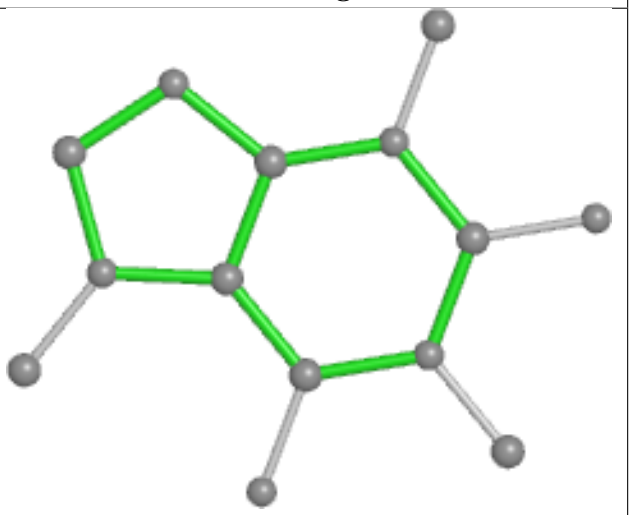


Bond angles

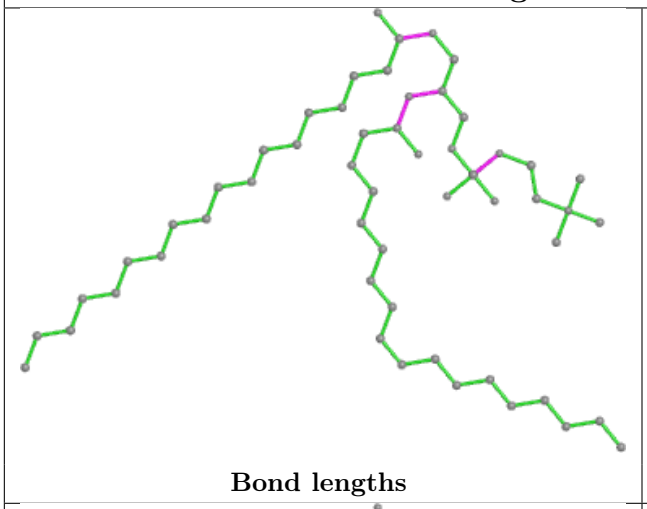


Torsions

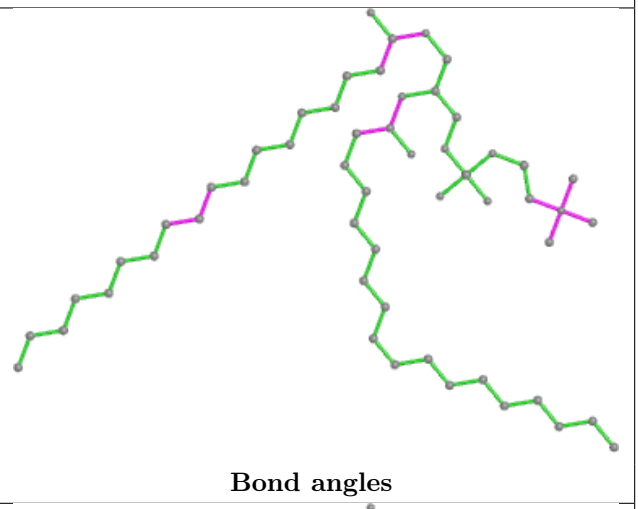


Rings

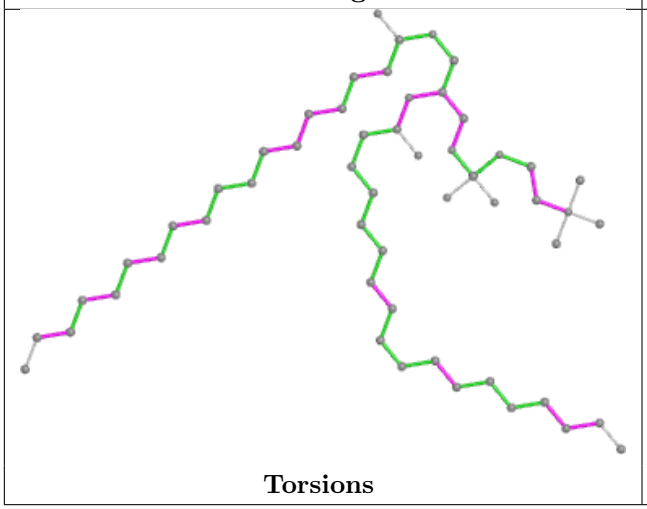
Ligand PCW B 8007



Bond lengths



Bond angles



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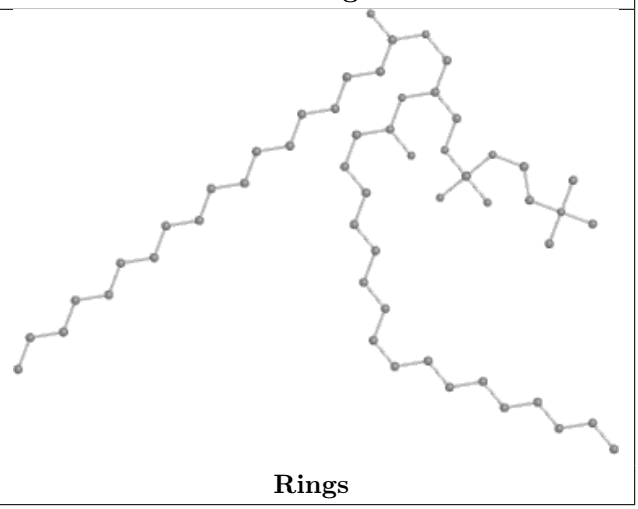
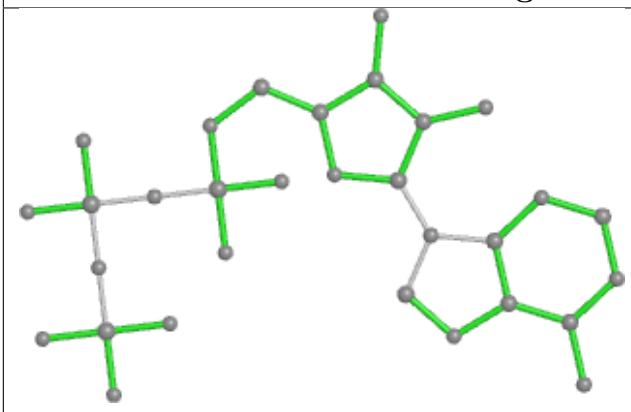
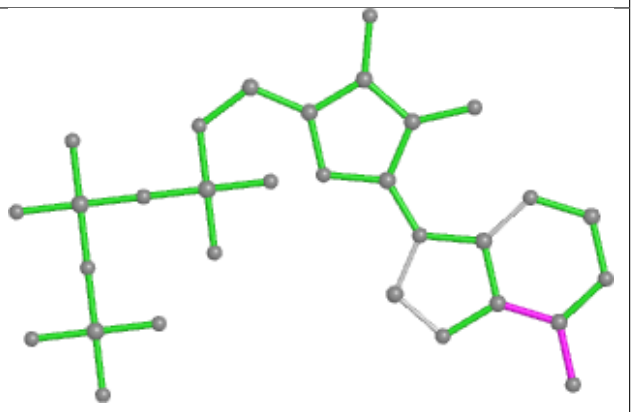


Rings

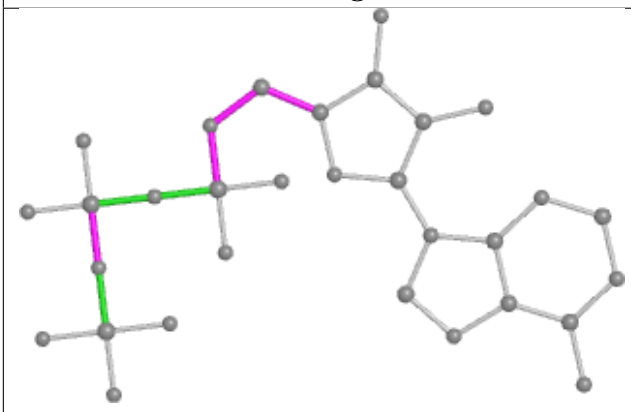
Ligand ATP B 8003



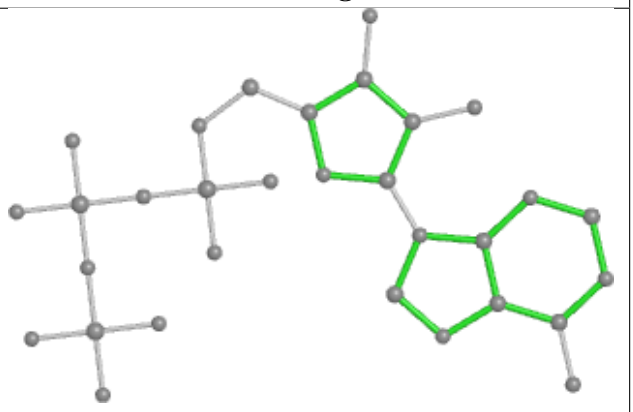
Bond lengths



Bond angles

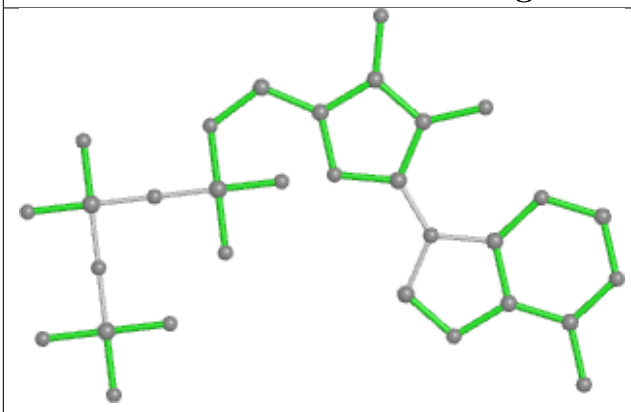


Torsions



Rings

Ligand ATP A 8005



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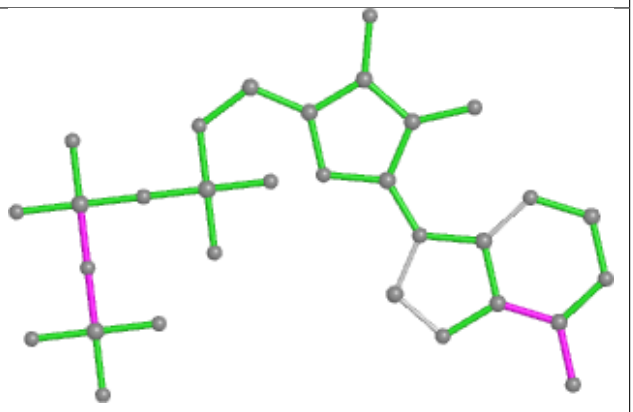
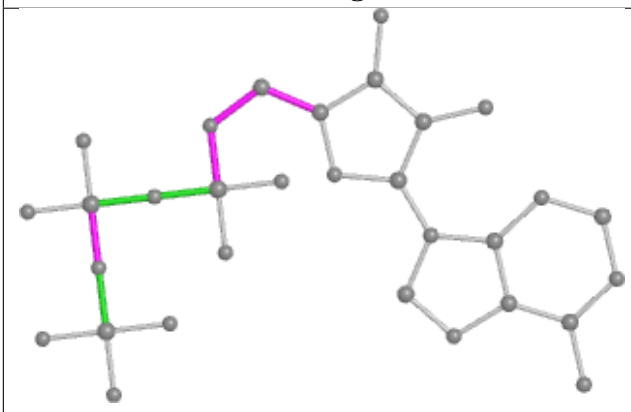
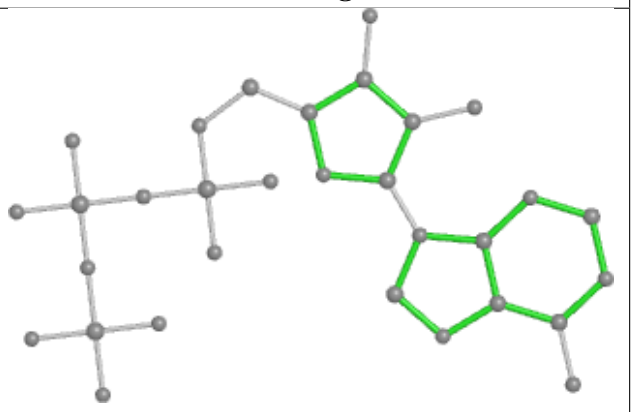


Bond angles

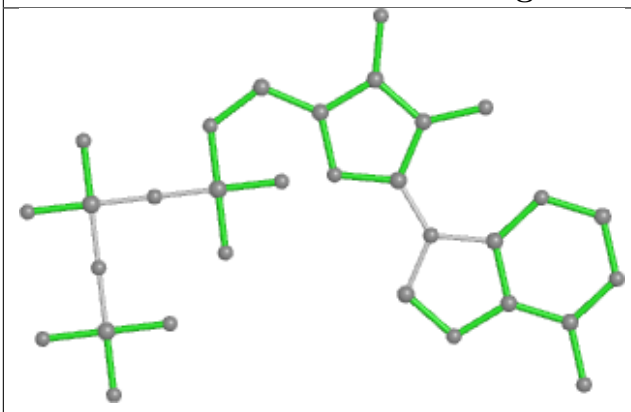


Torsions

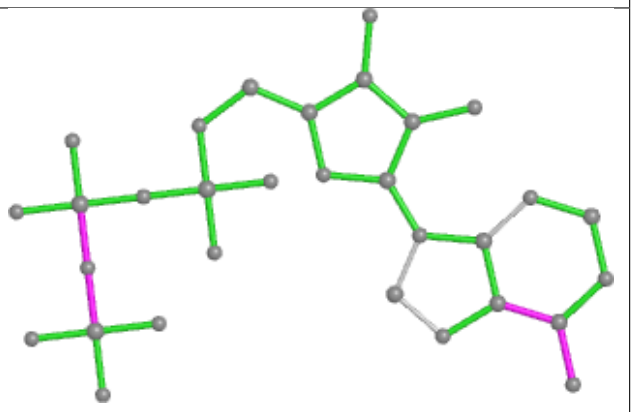


Rings

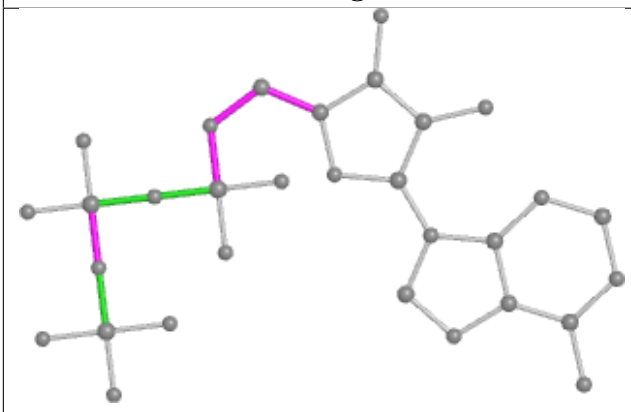
Ligand ATP B 8005



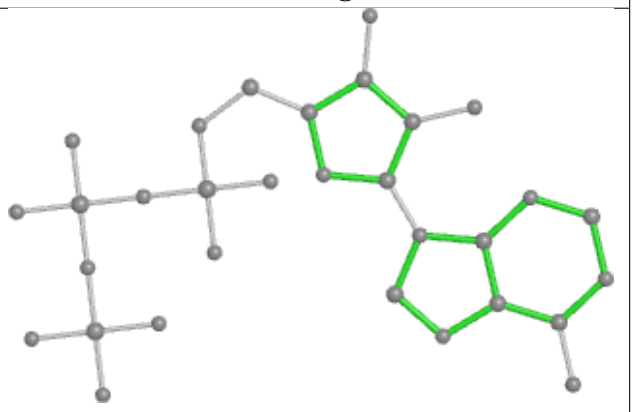
Bond lengths



Bond angles

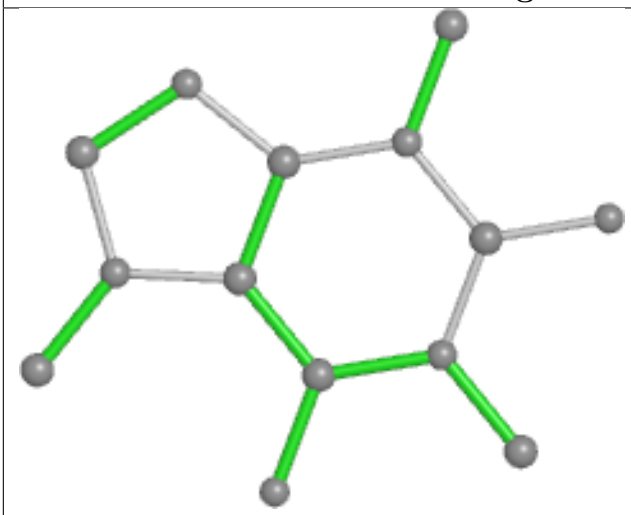


Torsions

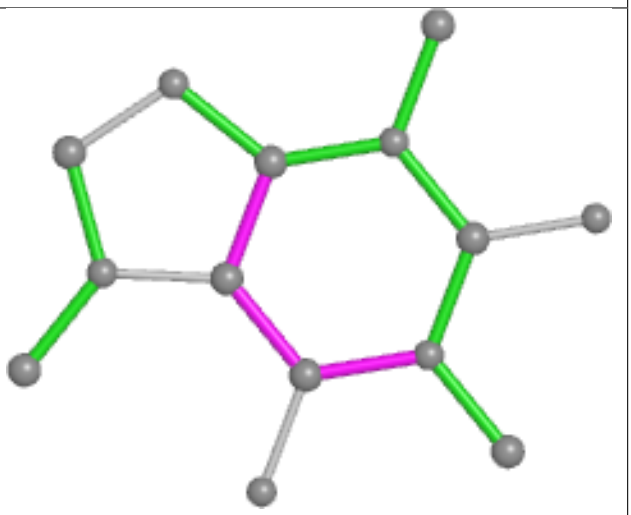


Rings

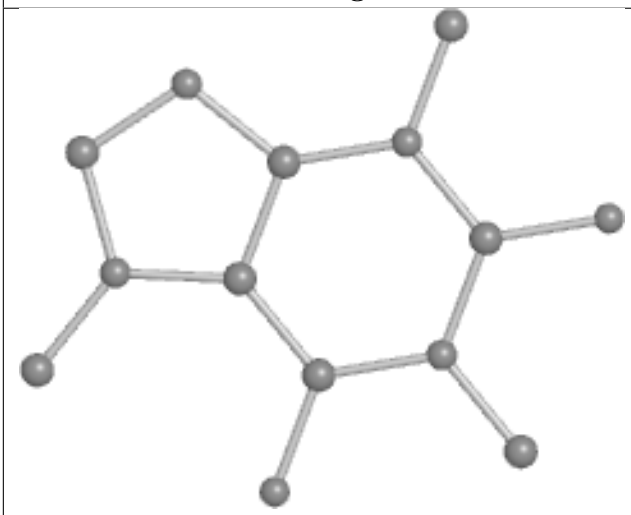
Ligand CFF A 8002



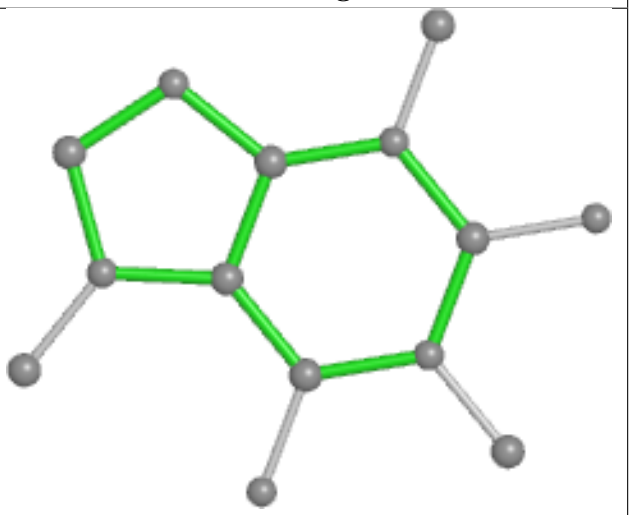
Bond lengths



Bond angles

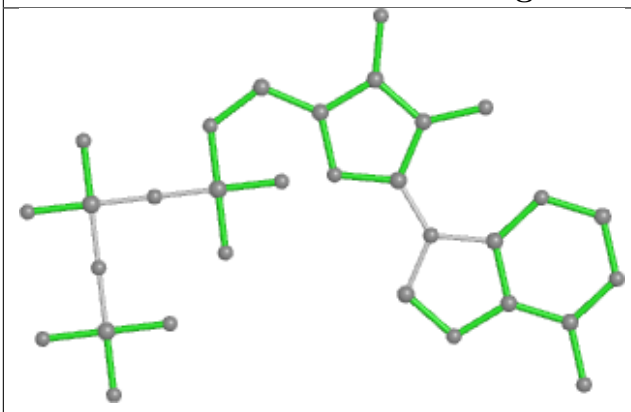


Torsions



Rings

Ligand ATP C 5104



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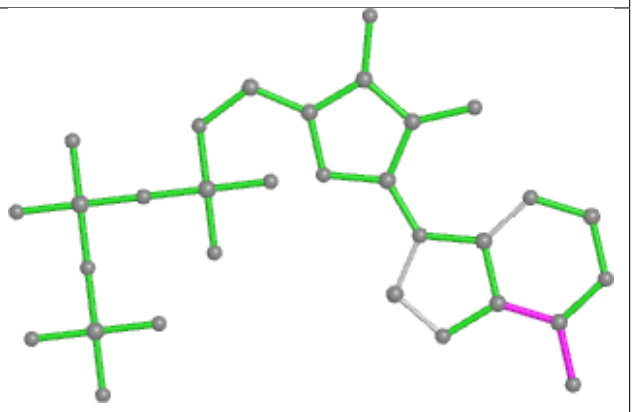
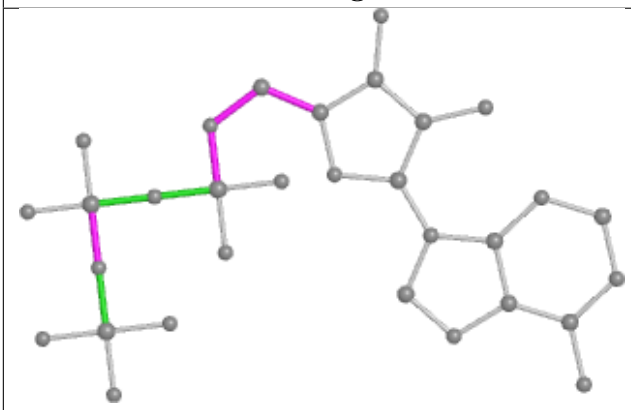
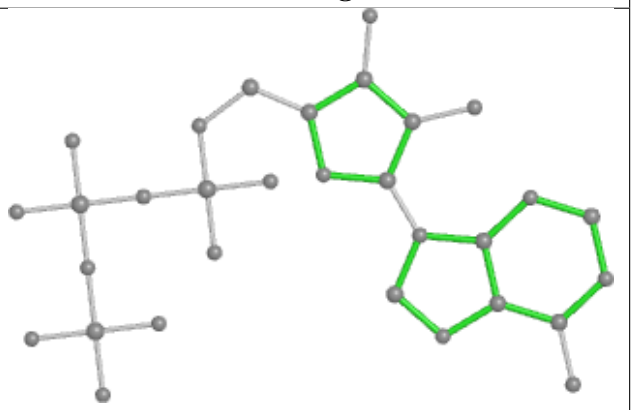


Bond angles

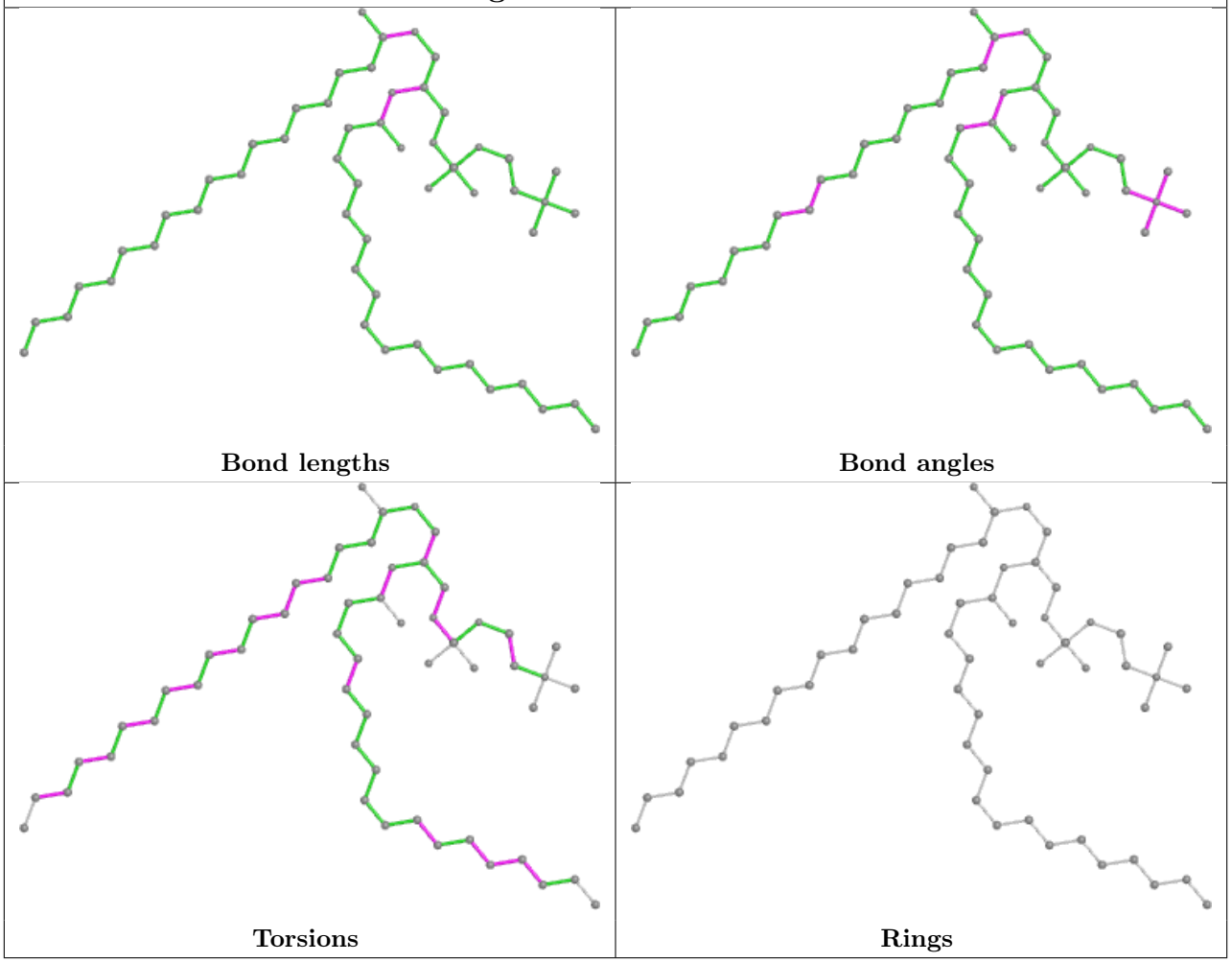


Torsions

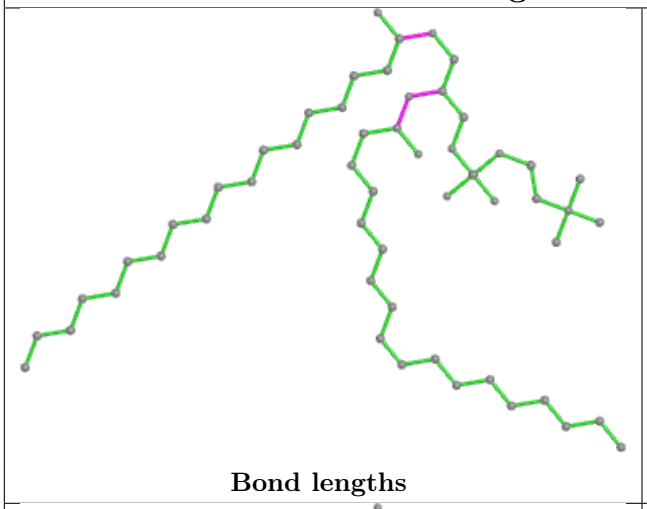


Rings

Ligand PCW C 5107



Ligand PCW D 8006



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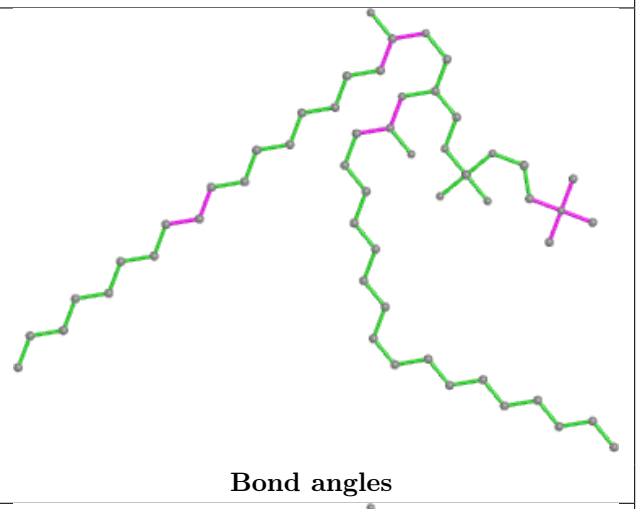
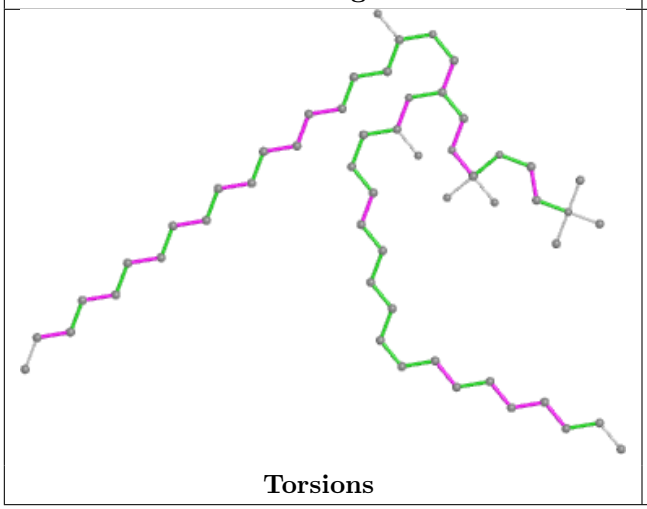
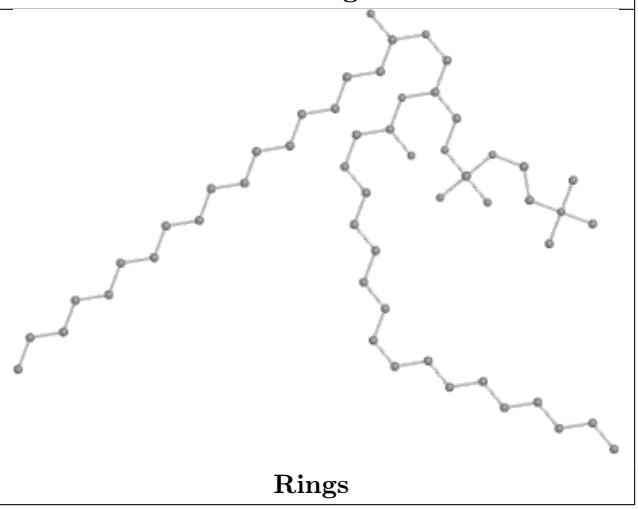


Bond angles

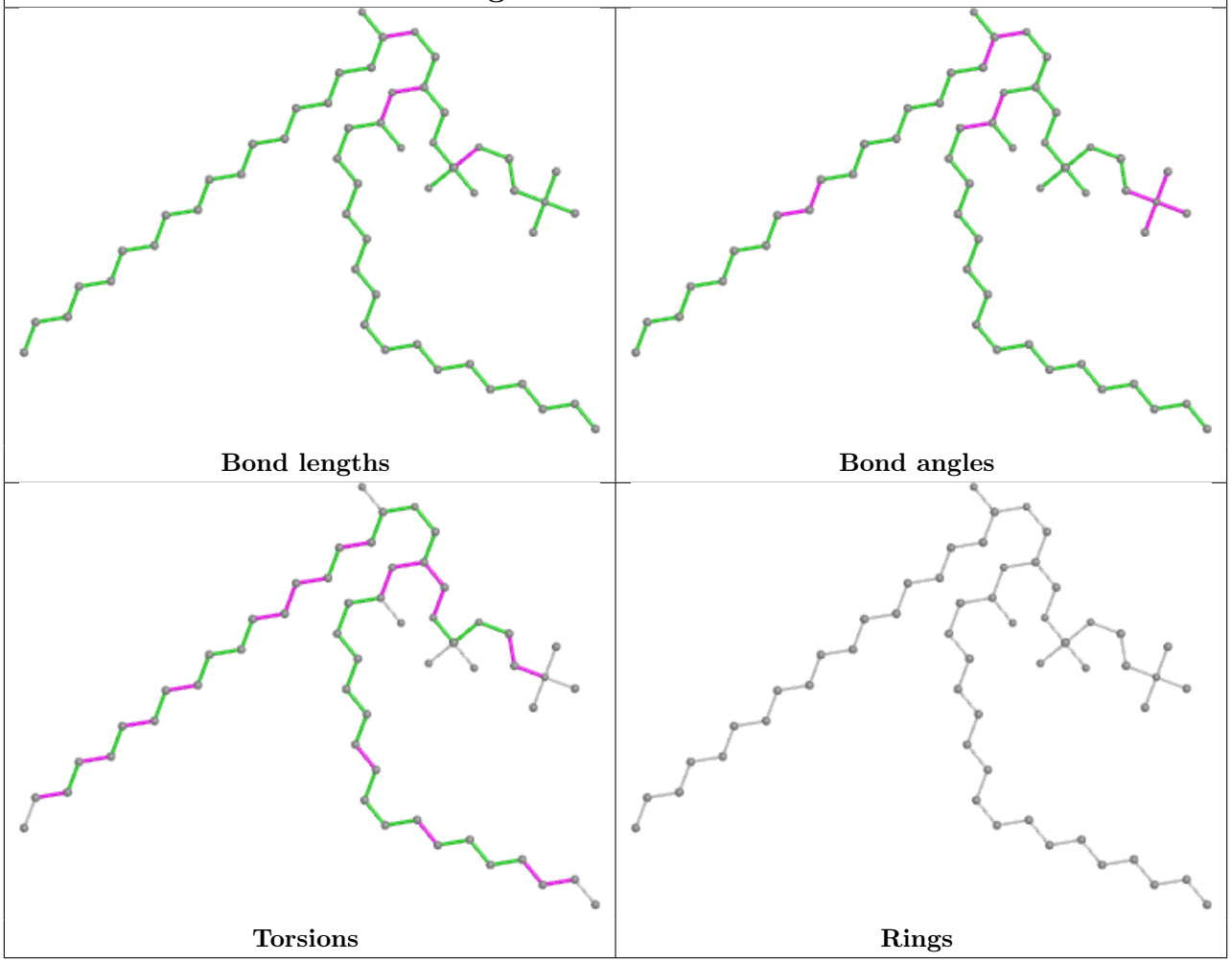


Torsions

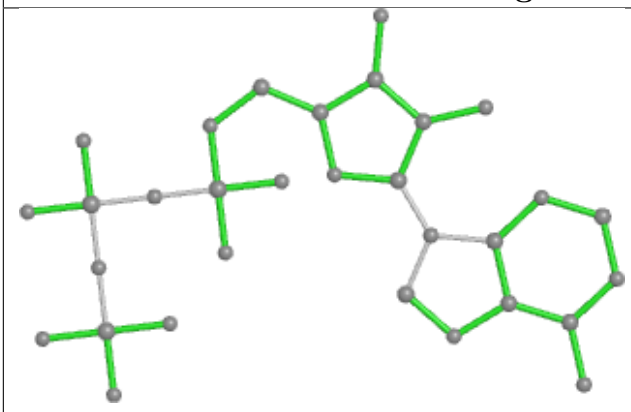


Rings

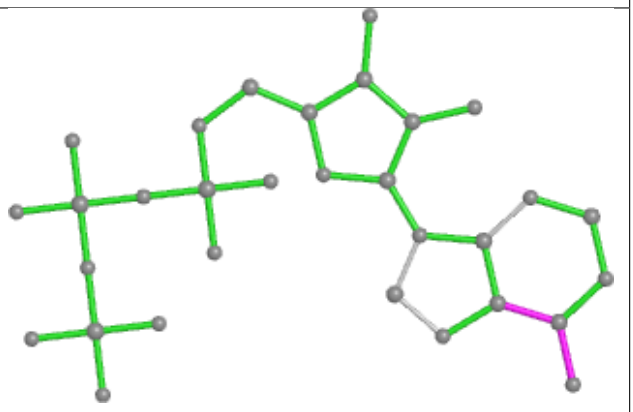
Ligand PCW D 8007



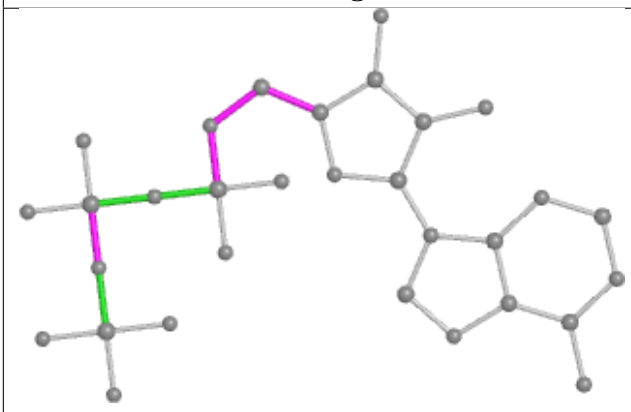
Ligand ATP A 8003



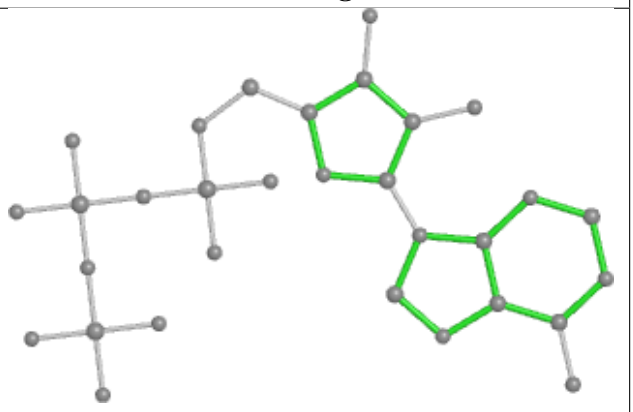
Bond lengths



Bond angles

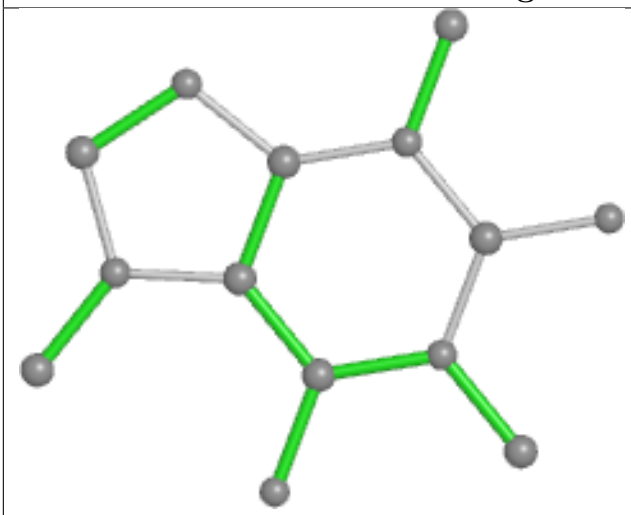


Torsions

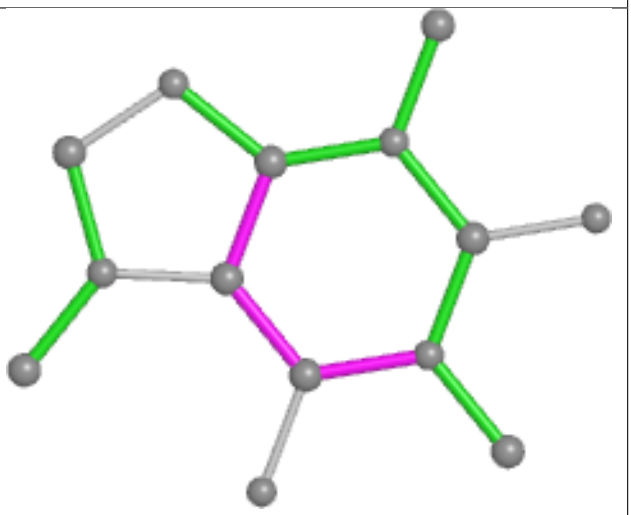


Rings

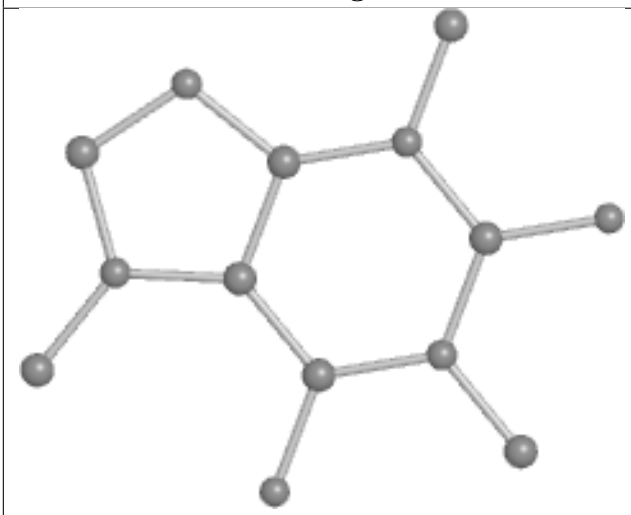
Ligand CFF C 5103



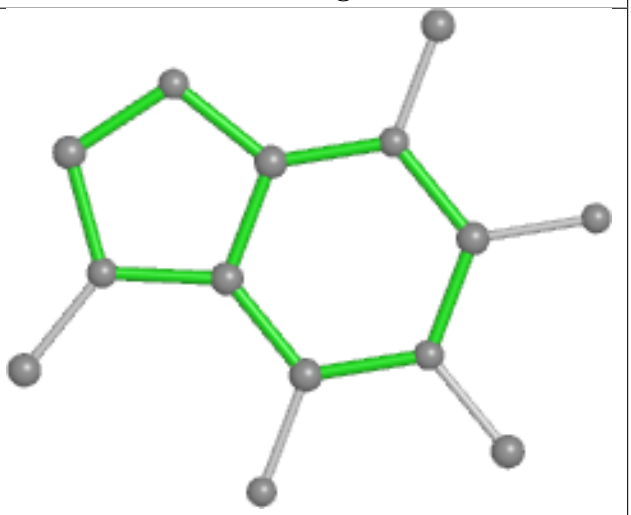
Bond lengths



Bond angles

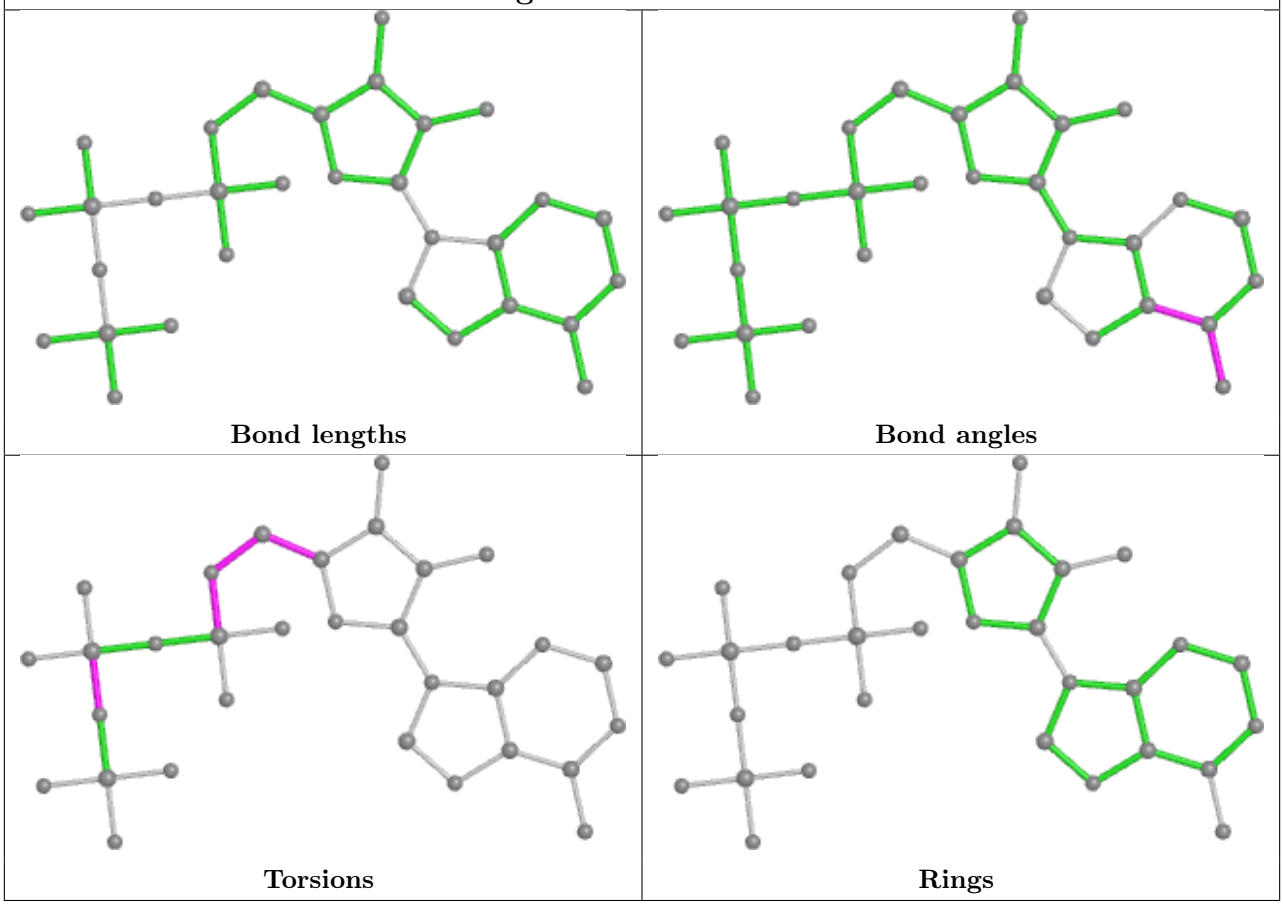


Torsions



Rings

Ligand ATP D 8003



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

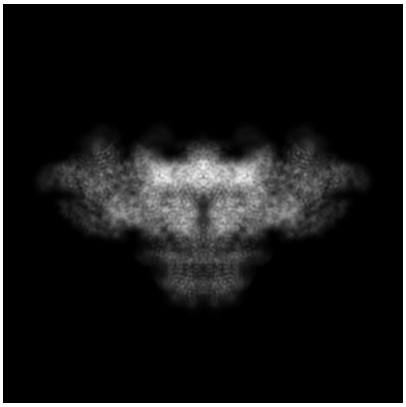
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-43304. These allow visual inspection of the internal detail of the map and identification of artifacts.

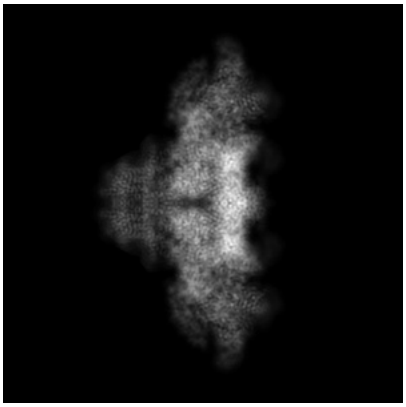
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

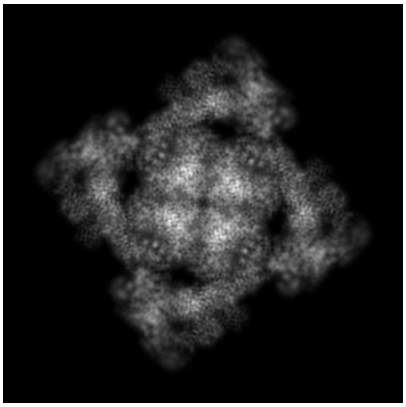
6.1.1 Primary map



X



Y

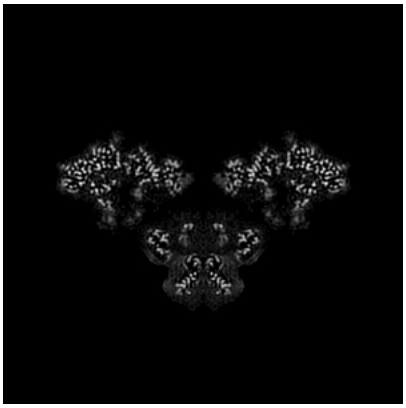


Z

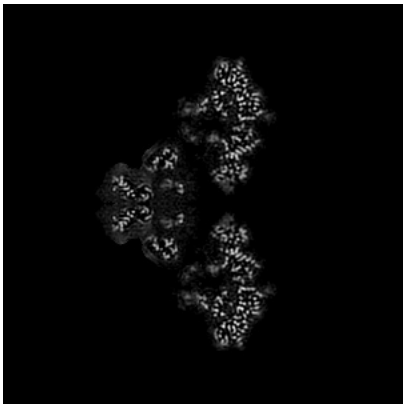
The images above show the map projected in three orthogonal directions.

6.2 Central slices

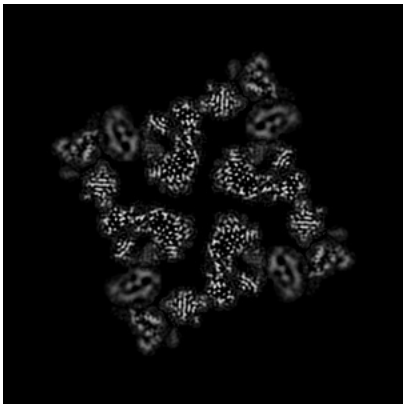
6.2.1 Primary map



X Index: 256



Y Index: 256

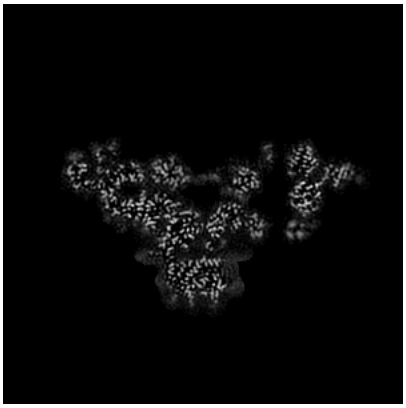


Z Index: 256

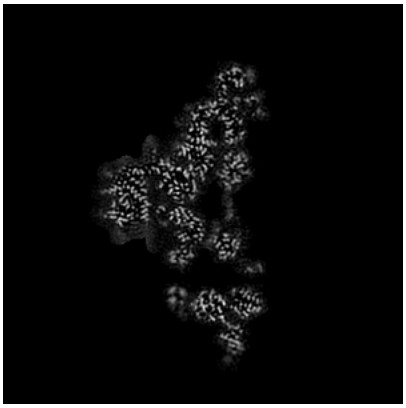
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

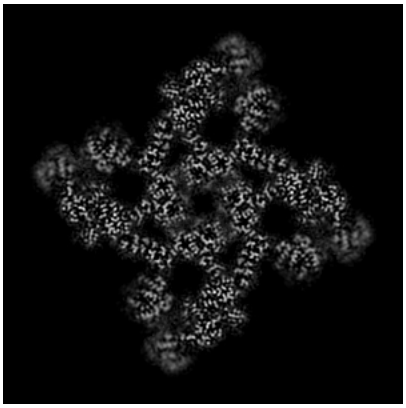
6.3.1 Primary map



X Index: 274



Y Index: 274

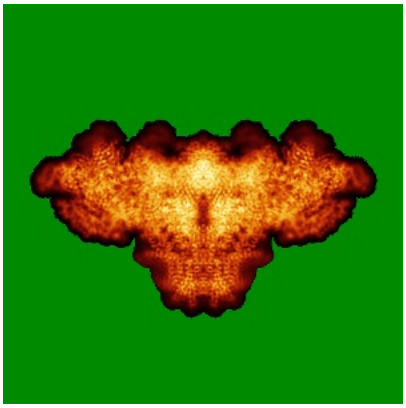


Z Index: 285

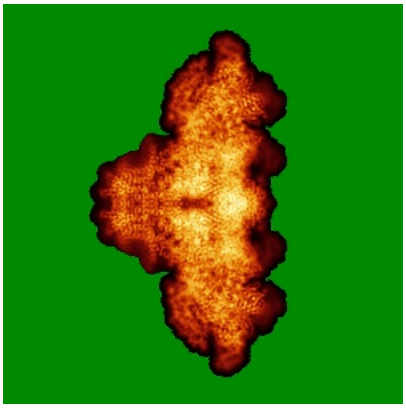
The images above show the largest variance slices of the map in three orthogonal directions.

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

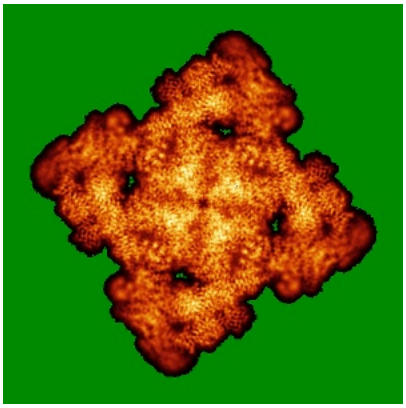
6.4.1 Primary map



X



Y

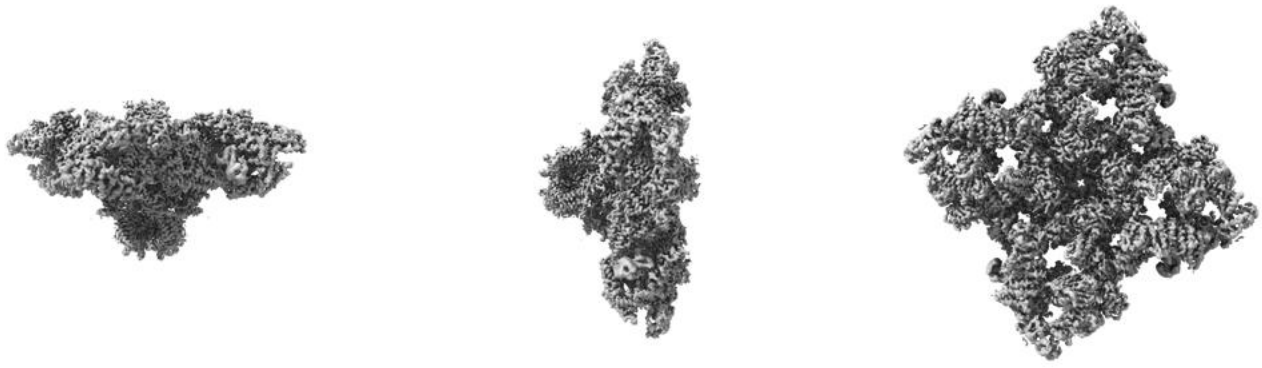


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

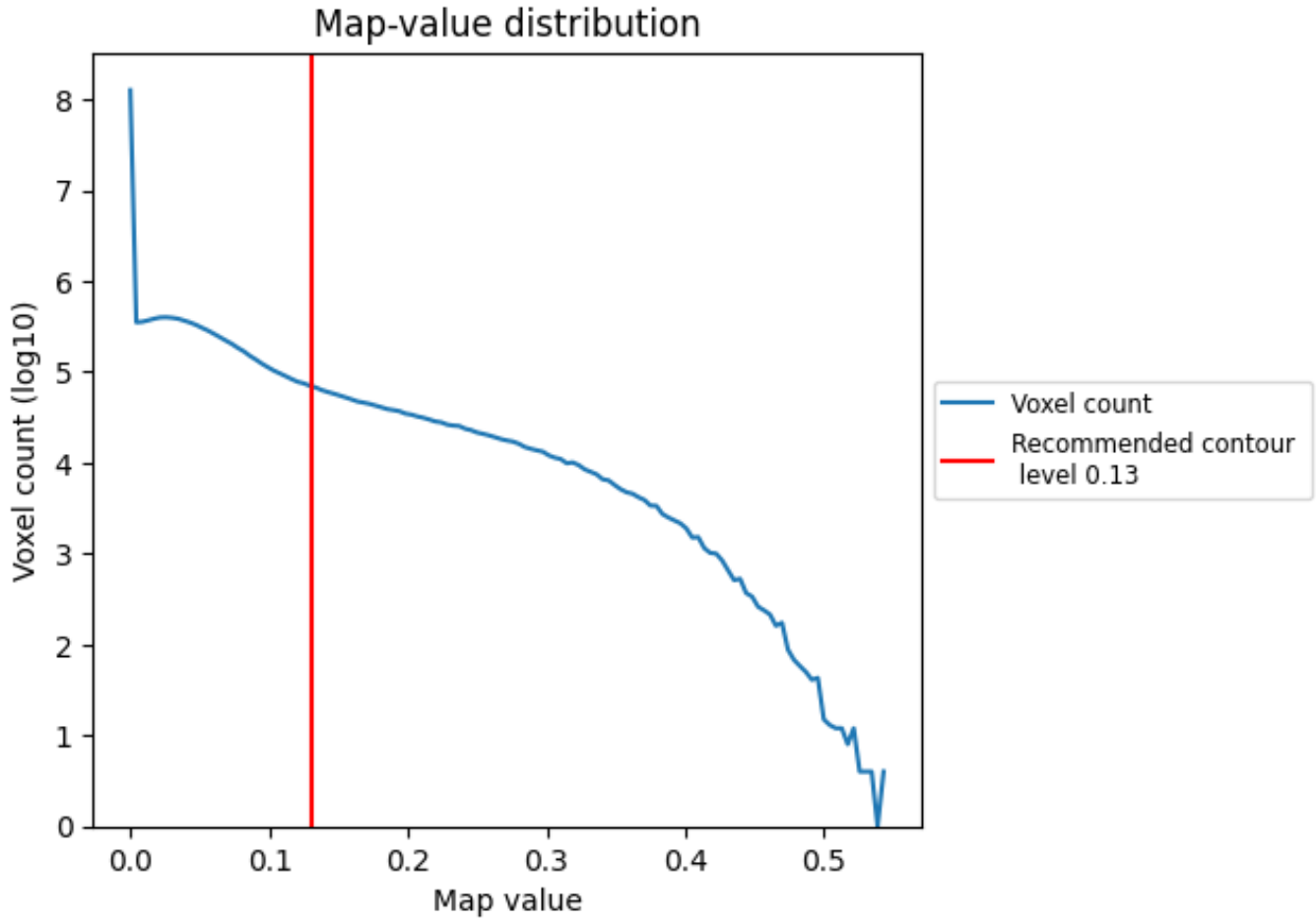
6.6 Mask visualisation (i)

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

7 Map analysis

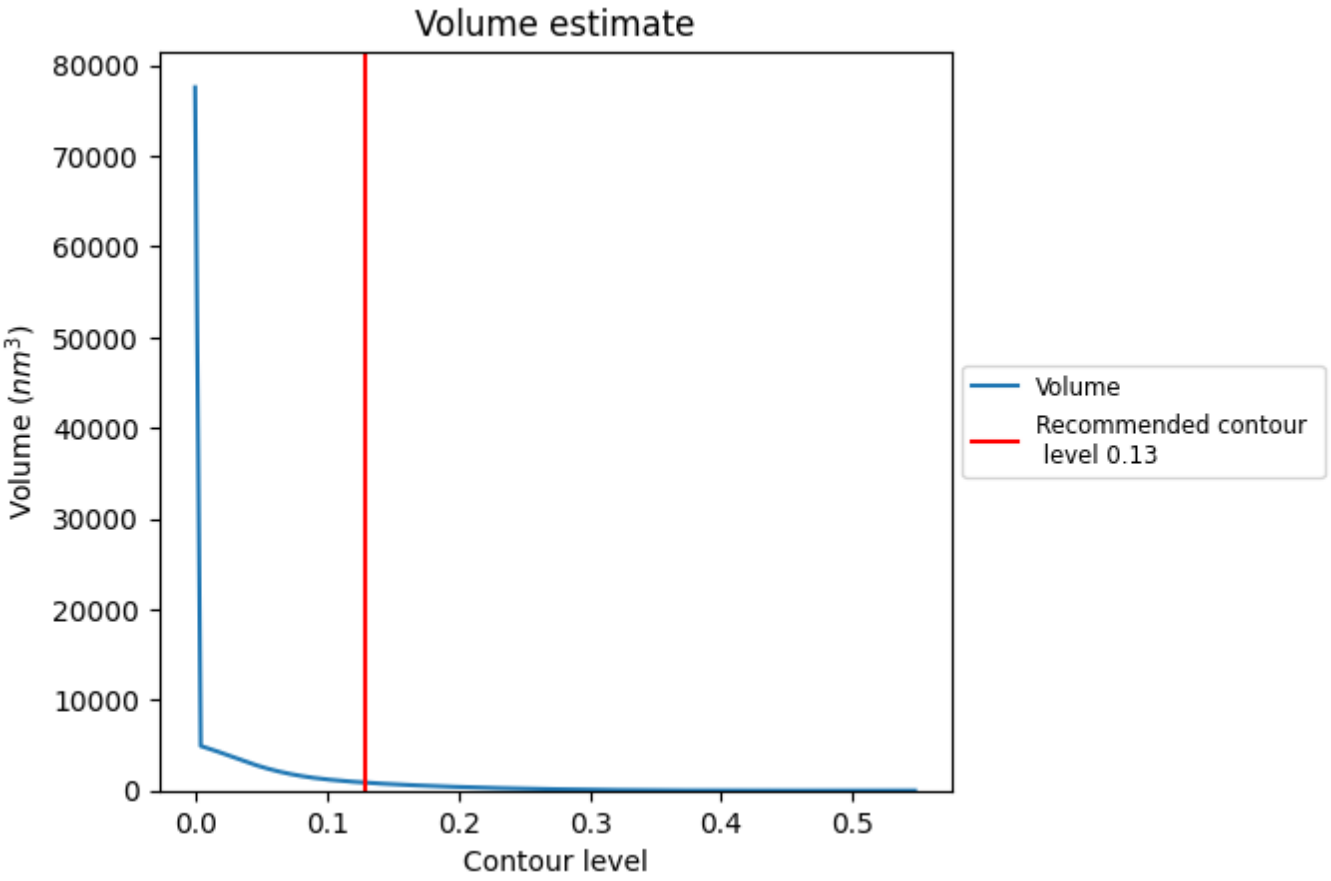
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

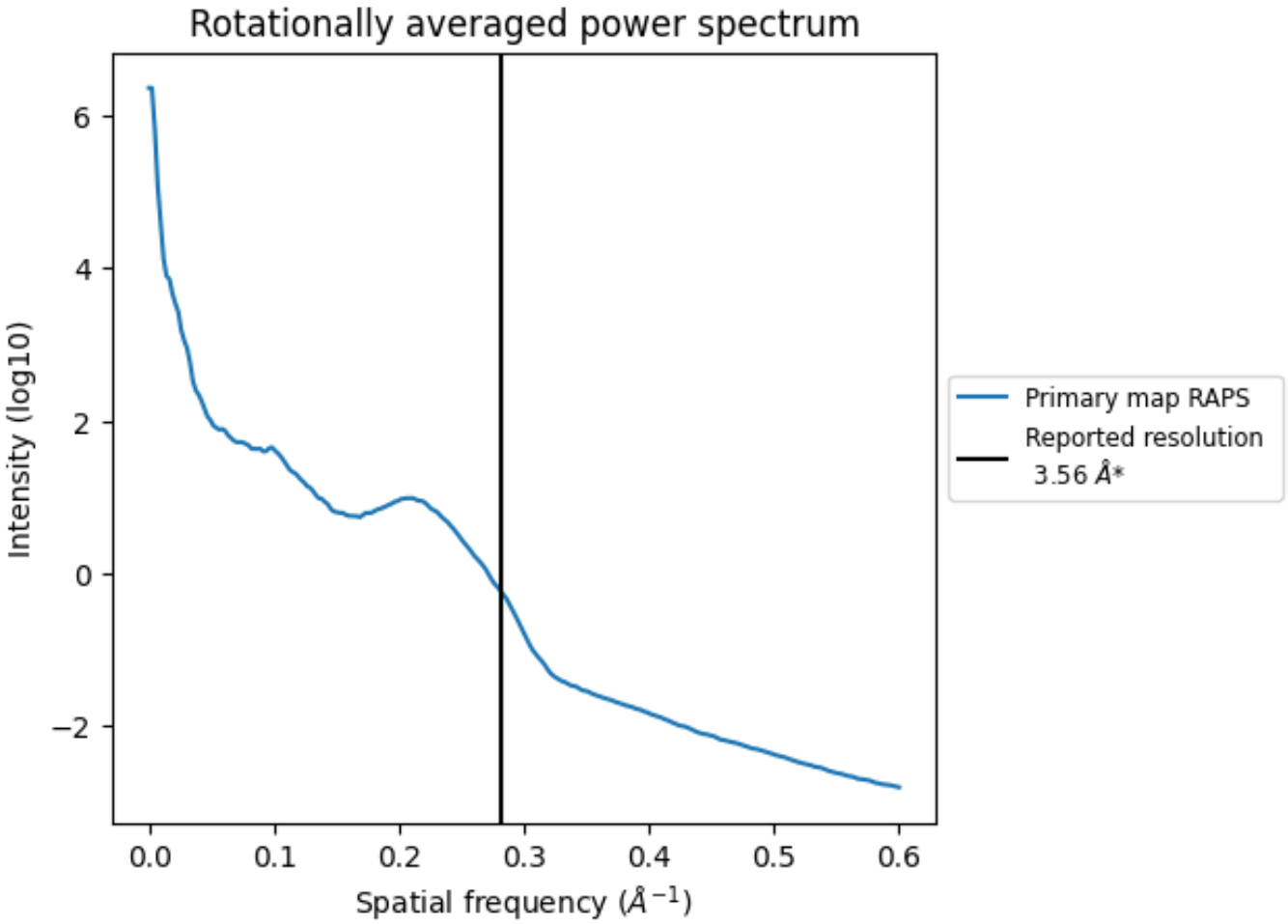
7.2 Volume estimate



The volume at the recommended contour level is 870 nm^3; this corresponds to an approximate mass of 786 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 0.281 Å^{-1}

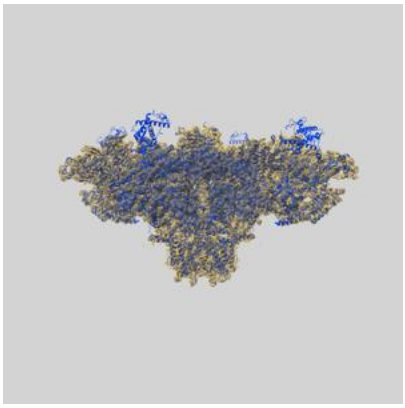
8 Fourier-Shell correlation

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

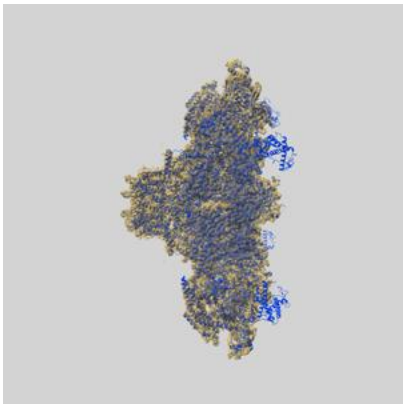
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-43304 and PDB model 8VK4. Per-residue inclusion information can be found in section 3 on page 9.

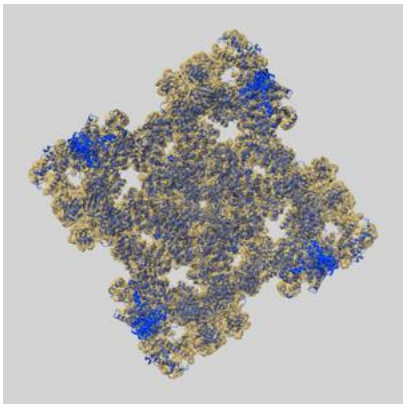
9.1 Map-model overlay



X



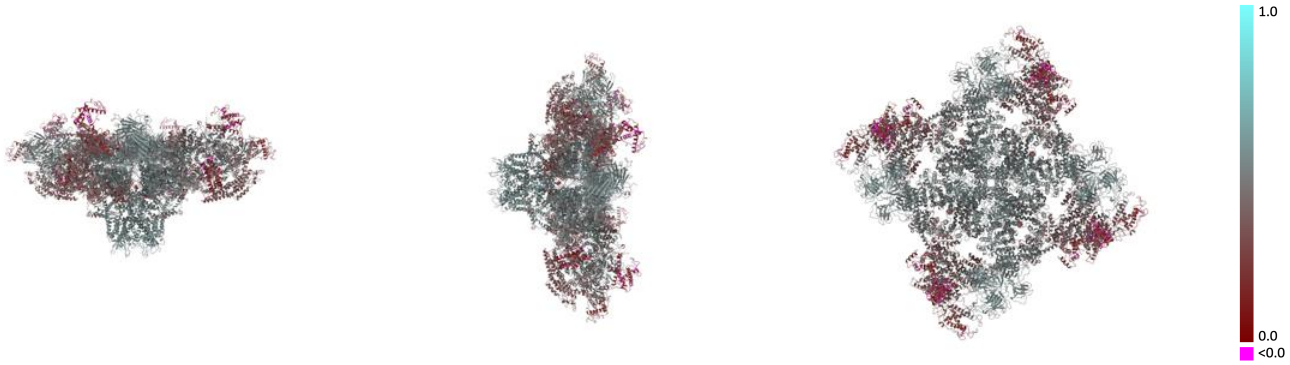
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.13 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.

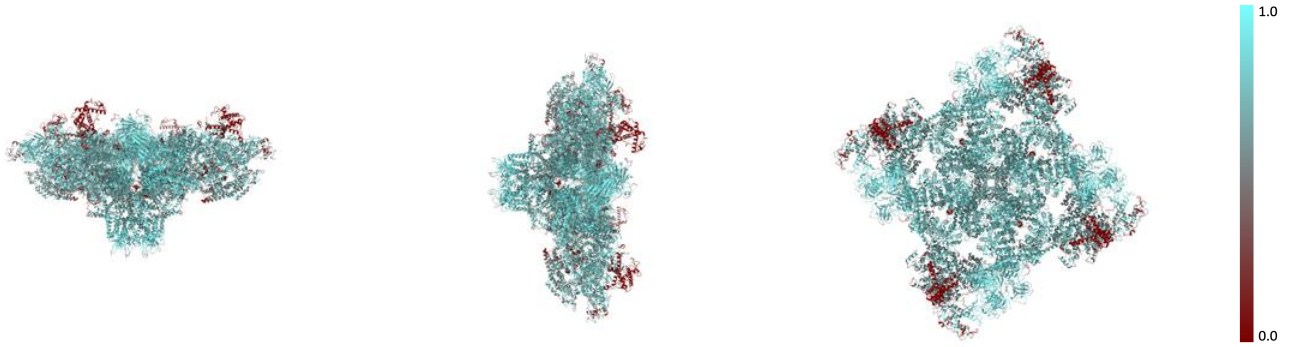
9.2 Q-score mapped to coordinate model (i)



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.

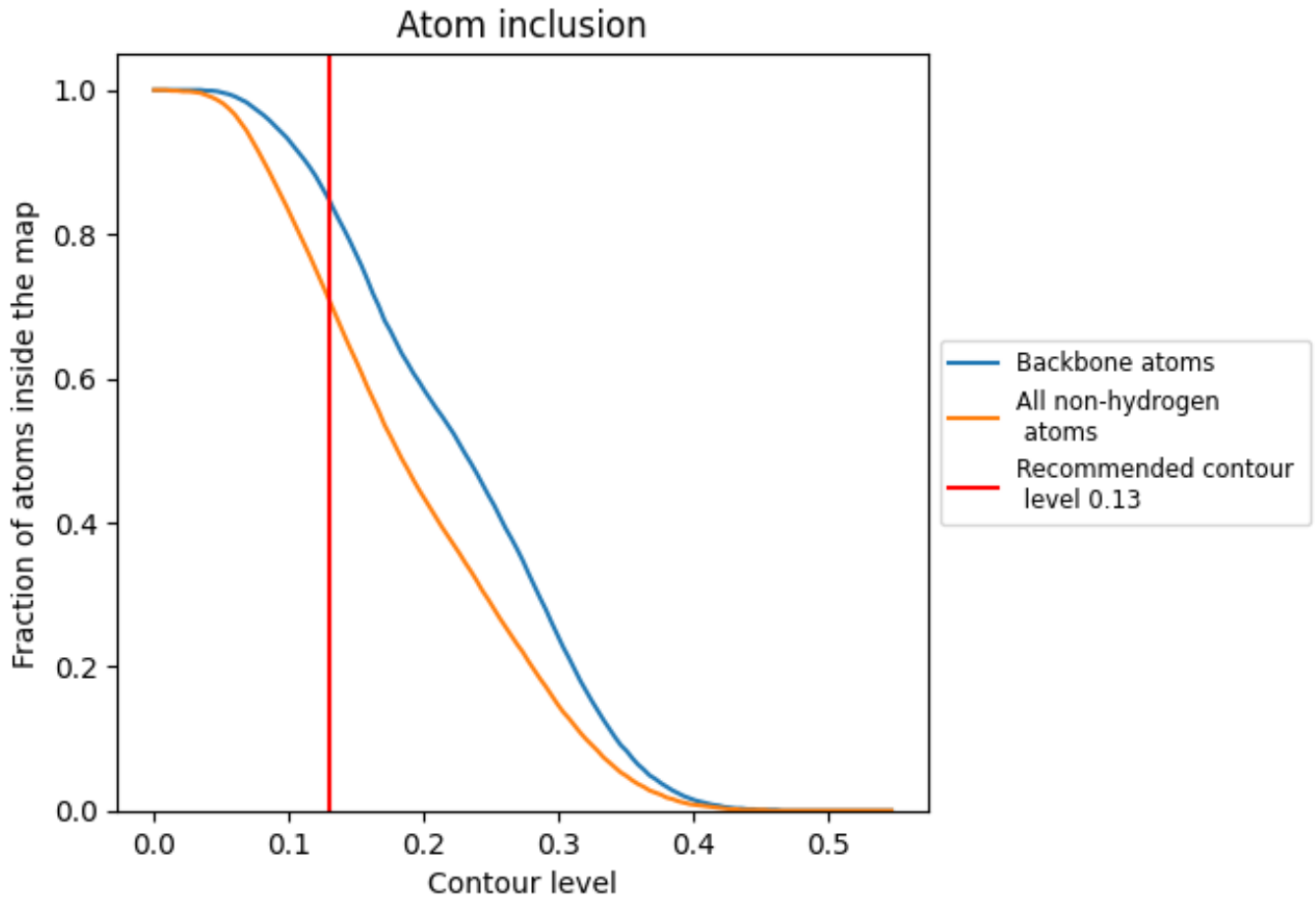
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.13).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 71% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7080	0.4400
A	0.7140	0.4500
B	0.7140	0.4490
C	0.7140	0.4500
D	0.7140	0.4500
E	0.7630	0.5070
F	0.7700	0.5060
G	0.7670	0.5050
H	0.7690	0.5070
I	0.4960	0.1660
J	0.5800	0.1760
K	0.4990	0.1680
L	0.5820	0.1770
M	0.5000	0.1690
N	0.5820	0.1790
O	0.4970	0.1650
P	0.5810	0.1770